The Quantum Nature in the Interaction of Molecular Hydrogen with Porous Materials: Implications for Practical Hydrogen Storage

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Supporting Information

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Computational Details

To estimate the interactions between H$_2$ and the different linkers (with and without TM), we use density functional theory (DFT), as implemented in the Amsterdam Density Functional (ADF) version 2017-r51252.$^{1,2}$ All calculations are completed using the B3LYP-D3 functional.$^{3,4}$ B3LYP is a hybrid functional method, and D3 accounts for Grimme’s dispersion corrections.$^{5–12}$ As the system is weakly bound, it is necessary to incorporate the long-range dispersion correction in the density functional theory (DFT-D)$^{6,8–12}$ to describe the systems properly. Relativistic triple zeta with polarization (ZORA:TZP) basis sets are used for all metals, and triple zeta with polarization (TZP) basis sets are used for the light elements (C, H, O, N, Cl, Tm = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Pd and Pt).$^{13}$ Every basis set is all-electron, and the high numerical quality is used for integration and other convergence criteria. This level of theory will be referred to as B3LYP-D3 for the remainder of this work. The threshold used for evaluating the convergence of the energy, forces, and electron density was $10^{-6}$ a.u. for each parameter. The tolerance (absolute deviation in the Cartesian coordinates) for atomic positions being symmetry equivalent was set at 0.001 Angstrom (Å) and the maximum is 0.1 a.u. by default criteria in ADF.$^{1,2}$ The unrestricted open shell procedure for the self-consistent field (SCF) calculations was used for all spin states. All geometries were optimized using the analytic Hessian to determine that the local minima have no negative curvatures (imaginary frequencies). The vibrational frequencies from the analytic Hessian were used to calculate the zero-point energy correction at 0 K.

For our calculations we used the following nomenclature,

$$\Delta H^\circ_{\text{bind}} = \Delta H^\circ_{\text{host}+H_2} - \Delta H^\circ_{\text{host}} - \Delta H^\circ_{H_2}$$  \hspace{1cm} (1)

Where $\Delta H^\circ_{\text{bind}}$ is the binding enthalpy of H$_2$ to the host, and it represents our estimation of $\Delta H^\circ_{\text{ads}}$. $\Delta H^\circ_{\text{host}}$ is the enthalpy of the host or linker and $\Delta H^\circ_{H_2}$ is the enthalpy of the free H$_2$. From here on, we use the term binding energy instead of binding enthalpy.
The dispersion energy interaction is defined by:\textsuperscript{7}

\[ \Delta E_{\text{Disp}} = E_{\text{Disp}}[\text{Complex+H}_2] - E_{\text{Disp}}[\text{Complex}] - E_{\text{Disp}}[\text{H}_2], \]

where \( E_{\text{Disp}}[\text{Complex+H}_2] \) is the total dispersion energy of the linker-TmCl\textsubscript{x} complex with H\textsubscript{2}, \( E_{\text{Disp}}[\text{Complex}] \) is the total dispersion energy of the linker-TmCl\textsubscript{x} complex alone, and \( E_{\text{Disp}}[\text{H}_2] \) is the dispersion energy of free H\textsubscript{2} molecule. Other relative energies are also defined similarly.

We first find the ground state for a given spin (s) according to the oxidation for the Tm atoms. For our cases we studied the most common oxidation state of the Tm. We also explore the most favorable geometry given the electronic spin state; Tetrahedral (Tet) versus Square Planar (Sqr) when applicable or Trigonal bipyramidal (Tbi) versus Square pyramidal (Spy). The other geometries studied depending on the number ligands are Octahedral (Oct) and Pentagonal bipyramidal (Pbi). Therefore we used the first row transition metals from Sc to Cu because we consider they should be light and abundant. We also include Pd(II) and Pd(0) for comparison.

For the nucleophilic transition metals, we explore:

* Sc(III), geometry = Spy, Tbi with s = 0;
* Ti(IV), geometry = Oct with s = 0;
* V(V), geometry = Pbi with s = 0;
* Cr(III), geometry = Spy, Tbi with s = 1/2, 3/2;

While for the electrophilic transition metals, we studied:

* Mn(II), geometry = Tet, Sqr with s = 1/2, 3/2, 5/2;
* Fe(II), geometry = Tet with s = 0, 2/2;
* Co(II), geometry = Tet, Sqr and s = 1/2, 3/2;
* Ni(II), geometry = Tet, Sqr with s = 0,2/2;
* Cu(II), geometry = Sqr with s = 1/2;
* Pd(II) and Pd(0), geometry = Sqr with s = 0;

All the geometries and their energies are contained in below as supplementary information. Pd is studied to get a comparison to precious metals. The geometry that we show is
the ground state along with the spin state and all the $\Delta H^\circ_{\mathrm{bind}}$ are calculated based on these structures. When the Square and Tetrahedral structure converge to the same coordinates (or Trigonal bipyramidal and Square pyramidal), only one of them is presented. For the V(V) case, we found that the metal does not bind to the linker but interacts mostly by columbic interactions.

**Structure descriptions**

In this Supplementary Information, the details of each Tm-linker complexes and H$_2$ molecules interactions are explained. In each of the chelating ligand (Figure S1), various oxidation states, spins, geometries: square planar (Sqr), tetrahedral (Tet), trigonal bipyramidal (Tbi), square pyramidal (Spy), octahedral (Oct), and pentagonal bipyramidal (Pbi) of chelated Tm are explored to get the optimum binding energy with H$_2$ molecules to be used in porous materials designs. The Tm are chelated by the ligands (the linkers in COFs): (E)-N’-benzylidene-benzohydrazide (BBH), (E)-2-((phenylimino) methyl) phenol (PIP), (E)-N-(pyridin-2-ylmethylene) aniline (PIA), 2,2'-bipyridine (BPY), and phenanthroline (PHEN), shown in FIG S1. The results are tabulated in Table S1, S2, S3, S3, S4, and S5. In this Supporting Informations (SI) we tabulate the type of linkers, geometries, spins, binding enthalpies, and the distances between H atoms in H$_2$. The spins are in unit of 1/2 and the distance between H atoms in 10$^{-12}$ m (pm)

**BBH**

The first linker is BBH. In Table S1, the binding energies of H$_2$ are calculated using first row transition metals (Sc to Cu) as well as Pd and Pt. While Pd and Pt are heavy precious metals, the predominant square geometry given the close shell electronic nature of these metals is explored for a comparison. The ligand BBH alone does not interact strongly with the H$_2$ molecules ($-\Delta H^\circ_{\mathrm{bind}}$=6.03, 6.22, 6.18, 5.68 kJ/mol for the 1$^{\text{st}}$ to the 4$^{\text{th}}$, respectively).
Figure S1: The ligands used as linkers in COFs design: (E)-N′-benzylidene-benzohydrazide (BBH), (E)-2-((phenylimino) methyl) phenol (PIP), (E)-N-(pyridin-2-ylmethylene) aniline (PIA), 2,2′-bipyridine (BPY), and phenanthroline (PHEN) with the plausible transition metal binding sites.

However, the binding energy increases if a Tm bonds to this ligand and reached the ideal range binding energy for H\textsubscript{2} delivery amount at 298K.

Strong interaction between the first 4 H\textsubscript{2} molecules to Pt(II) is observed but there is no evidence for the formation of hydride with its square geometry environment. It can be observed from the short H-H bond distance (maximum 74.7 pm) which is still comparable to isolated H-H bond length (74.4 pm).

The first H\textsubscript{2} occupy the open sites near the Tm. It located at the same plane of the ligand with Mn(II)—H\textsubscript{2} distance was 2.82 Å to both H atoms in H\textsubscript{2} molecule with binding energy -10.7 kJ/mol. A similar pattern is also found in BBH-ScCl\textsubscript{3} and BBH-CrCl\textsubscript{3} with the H\textsubscript{2} occupied the nearest possible site to the Tm. The distance of Sc(II)—H\textsubscript{2} is 3.20 Å.

There is only one coordination from the BBH binding sites in the case of BBH-VCl\textsubscript{5} where the V(V) only make coordination with oxygen atom. The Vanadium atom does not have a coordination with the other binding site (N atom) in BBH. It forms an octahedral...
Table S1: Binding energies ($\Delta H^o_{\text{bind}}$) obtained from Quantum Mechanics (QM) calculations for the ground state of linker BBH and different number of physisorbed $H_2$. We also showed $\Delta H^o_{\text{bind}}$ for the linker + TM(n)Cl$_n$ + $H_2$. The H-H bond of isolated $H_2$ is 0.744 Å

| Linker ligand | Tm Go S  | $-\Delta H^o_{\text{bind}}$ (kJ/mol) | H-H bond (pm) |
|---------------|---------|---------------------------------|----------------|
| BBH Tm n/2    | 6.03, 6.22, 6.18, 5.68 | 75.0, 75.0, 74.6, 74.4 |
| Sc(III) Tbi 0 | 9.06, 8.79, 8.05, 7.40 | 75.0, 74.6, 74.6, 74.4 |
| Ti(IV) Oct 0  | 8.40, 8.74, 8.22, 7.93 | 75.0, 75.0, 75.0, 74.6 |
| V(V) Oct 0    | 11.5, 9.61, 8.57, 7.42 | 75.0, 75.0, 74.4, 74.4 |
| Cr(III) Spi 3 | 10.8, 10.0, 9.03, 7.92 | 75.0, 75.0, 75.0, 74.6 |
| Mn(II) Tet 5  | 10.7, 9.01, 9.29, 9.37 | 75.0, 74.7, 74.7, 74.7 |
| Fe(II) Tet 2  | 9.43, 9.51, 11.2, 10.9 | 74.8, 74.7, 74.7, 74.6 |
| Co(II) Tet 3  | 10.4, 9.87, 9.75, 8.58 | 74.6, 74.6, 74.6, 74.6 |
| Ni(II) Tet 2  | 10.4, 10.1, 9.57, 8.11 | 74.7, 74.6, 74.6, 74.6 |
| Cu(II) Tet 1  | 10.1, 7.99, 7.36, 7.43 | 75.0, 75.0, 74.7, 74.6 |
| Pd(II) Sqr 0  | 7.64, 7.86, 7.44, 7.32 | 75.0, 75.0, 74.7, 74.6 |
| Pt(II) Sqr 0  | 17.2, 17.1, 15.6, 15.2 | 74.7, 74.6, 74.6, 74.6 |

geometry and the difference of the binding energy between the first and the next $H_2$ molecules to the complex is more pronounced compared to other Tm. The interaction is dominated by the interaction of $H_2$ with Cl$^-$, instead of V(V) with $H_2$. The nearest distance between $H_2$–Cl$^-$ is at 3.28 Å much closer than $H_2$–V(V) (4.24 Å). Ti(IV) forms distorted octahedral geometry but it has 2 coordinations with BBH (with O and N atoms) contrast to V(V) which only bond to O in BBH.

The rest of Tm (Fe(II), Co(II), Ni(II), Pd(II), Cu(II)) form tetrahedral or square planar geometries. Generally, non zero total spin Tm with tetrahedral geometry has stronger binding energy than spin 0 such as Pd(II) which forms true Sqr geometry. Cu(II) in BBH forms distorted tetrahedral which the bond to N in BBH is elongated and twisted (2.16 Å) compared to O (1.99 Å). The first $H_2$ binding energy with BBH-CuCl$_2$ is 2.01 kJ/mol higher than the next $H_2$ molecules because the optimum distance of the first $H_2$ is 3.15 Å, almost 1 Å closer than the next $H_2$ (> 4.00 Å) molecules.
The second ligand studied is (E)-N-(pyridin-2-ylmethylene) aniline (PIA) (Table S2). This ligand does not interact strongly with H₂ (−ΔH°ₘₐₓ = 7.05, 5.89, 5.97, 5.74 kJ/mol) but similar property is observed with the addition of Tm. The strongest interaction of H₂ is with Pt(II) but no chemical bond is observed. Cu(II) creates distorted square planar geometry instead of tetrahedral and the first 3 H₂ has similar distances to Cu(II) at 2.80-3.00 Å and relatively similar ΔH°ₘₐₓ to the first three H₂ (-9.91 to -10.3 kJ/mol). With the total spin zero, Pd and Pt formed square planar geometry and the first 4 H₂ local minima energies are near the binding sites (N atoms) and Tm.

Table S2: Binding energies (ΔH°ₘₐₓ) obtained from QM calculations for the ground state of linker PIA and different number of physisorbed H₂. We also show ΔH°ₘₐₓ for the linker + TM(n)Clₙ + H₂. The H-H bond of isolated H₂ is 0.744 Å

| Linker | Geom | S | ΔH°ₘₐₓ (kJ/mol) | H-H bond (pm) |
|--------|------|---|-----------------|---------------|
| linker | N/A  | 3 | 7.05, 5.89, 5.97, 5.74 | 75.0, 75.0, 74.6, 74.4 |
| Sc(III) | Tbi  | 0 | 10.0, 8.63, 7.12, 7.15 | 74.6, 74.4, 75.0, 75.0 |
| Ti(IV) | Oct  | 0 | 7.50, 7.27, 6.91, 6.59 | 75.0, 75.0, 74.6, 74.6 |
| V(V)   | Pbi  | 0 | 9.08, 8.14, 7.49, 7.70 | 75.0, 75.0, 75.0, 74.6 |
| Cr(III) | Spi  | 3 | 8.15, 8.16, 7.49, 9.17 | 75.0, 75.0, 74.6, 74.6 |
| Mn(II) | Tet  | 5 | 8.53, 8.93, 9.04, 9.17 | 74.7, 74.7, 74.6, 74.6 |
| Fe(II) | Tet  | 2 | 11.7, 10.96, 10.5, 9.90 | 75.0, 75.0, 74.6, 74.6 |
| Co(II) | Tet  | 3 | 8.71, 9.01, 8.64, 8.17 | 74.7, 74.7, 74.6, 74.6 |
| Ni(II) | Tet  | 2 | 9.81, 9.64, 9.08, 8.88 | 74.7, 74.7, 74.6, 74.6 |
| Cu(II) | Sqr  | 1 | 9.92, 10.3, 9.91, 8.97 | 74.7, 74.6, 74.6, 75.0 |
| Pd(II) | Sqr  | 0 | 6.26, 6.89, 7.02, 7.20 | 75.0, 74.6, 74.6, 74.4 |
| Pt(II) | Sqr  | 0 | 15.1, 12.7, 14.3, 14.2 | 75.0, 74.6, 74.6, 74.6 |

With the two N binding sites in PIA, V(V) created slightly distorted pentagonal bipyramidal and Ti(IV) formed octahedral geometry. As in BBH, the ΔH°ₘₐₓ are dominated by the H₂–Cl⁻ electrostatics and van der Waals interactions. The typical distance of Tm to the nearest H₂ was more than 4.43 Å. The first H₂ occupies the nearest possible sites to Sc(III) and Cr(III). Sc(III) formed trigonal bypyramidal and Cr(III) formed square pyramidal
geometry with the ligand binding sites (N atoms).

The first two H₂ occupy the open sites near Mn(II) in its tetrahedral geometry. The distance between Mn(II) to H atoms in the first H₂ molecule were at 2.93 and 2.94 and to the second H₂ at 2.96 and 2.99 Å. The rest of the Tm (Fe(II), Co(II), Ni(II), Pd(II)) form tetrahedral and square planar geometries. The favorable H₂ molecules locations were also near the binding sites (N atoms) and Tm.

**PIP**

The third ligand studied (E)-2-((phenylimino) methyl) phenol (PIP) alone had weak interaction with H₂ ($-\Delta H_{\text{bind}}^{\circ}=7.33, 7.09, 6.92, 6.48$ kJ/mol). Generally, H₂ local minima are located close to the binding sites (N atom and OH) and Tm. The fully surrounded V(V) in PIP-V(V)Cl₅ complex has weaker interaction with H₂ than ligand alone. In contrast to BBH-VCl₅ complex which has stronger interaction with the first two H₂ (<-9.00 kJ/mol) molecules, PIP has hydroxy group (-OH) binding site and the H₂ molecules cannot occupy position near both binding sites (N and OH) and ion Cl⁻ at the same time such as in BBH-VCl₅ because of the H atom repulsion from hydroxy group.

Besides with Pt(II), the first H₂ also has a strong interaction (< -14 kJ/mol) with Sc(III) in PIP-Sc(III)Cl₃ complex. It does not form chemical bond but this ligand complex deform slightly with the presence of the first H₂ and give higher calculated $\Delta H_{\text{bind}}^{\circ}$.

As in BBH, the Cu (II) in PIP complex also forms tetrahedral instead of square planar geometry with N and OH binding sites. As in previous ligands, Mn(II), Fe(II), Co(II), and Ni(II) also forms tetrahedral geometry with similar $\Delta H_{\text{bind}}^{\circ}$. Only Pd(II) and Pt(II) with spin zero forms square planar geometry.

**BPY and PHEN**

The fourth (2,2'-bipyridine (BPY)) and the fifth (phenanthroline (PHEN)) ligands alone also does not interact strongly with H₂ ($-\Delta H_{\text{bind}}^{\circ}=6.87, 5.39, 5.47, 5.34$ kJ/mol with BPY
Table S3: Binding energies ($\Delta H_{\text{bind}}$) obtain from QM calculations for the ground state of linker PIP and different number of physisorbed H$_2$. We also showed $\Delta H_{\text{bind}}$ for the linker + TM(n)Cl$_n$ + H$_2$. The H-H bond of isolated H$_2$ is 74.4 pm

| Linker | Geom | S | $-\Delta H_{\text{bind}}$ (kJ/mol) | H-H bond (pm) |
|--------|------|---|-----------------|--------------|
| PIP    | Tm   | $\frac{1}{2}$ |                  |              |
| linker | N/A  | 0  | 7.33, 7.09, 6.92, 6.48 | 75.0, 75.0, 75.0, 74.4 |
| Sc(III)| Tbi  | 0  | 10.1, 9.19, 5.96, 5.82 | 75.0, 75.0, 74.7, 74.4 |
| Ti(IV) | Oct  | 0  | 7.89, 7.53, 7.57, 6.70 | 75.0, 75.0, 74.4, 74.4 |
| V(V)   | Pbi  | 0  | 6.71, 6.21, 6.01, 5.66 | 75.0, 75.0, 74.4, 74.4 |
| Cr(III)| Spi  | 3  | 7.09, 6.79, 6.43, 6.61 | 74.8, 75.0, 74.6, 74.6 |
| Mn(II) | Tet  | 5  | 12.2, 10.2, 9.59, 9.84 | 74.7, 74.7, 75.0, 74.6 |
| Fe(II) | Tet  | 2  | 10.3, 10.5, 8.87, 8.89 | 75.0, 74.6, 74.6, 74.6 |
| Co(II) | Tet  | 3  | 9.11, 8.75, 9.94, 9.22 | 75.0, 74.6, 74.6, 74.4 |
| Ni(II) | Tet  | 2  | 8.30, 8.35, 8.47, 7.15 | 75.0, 75.0, 74.6, 74.3 |
| Cu(II) | Tet  | 1  | 12.7, 11.3, 10.4, 9.82 | 74.6, 74.6, 74.7, 74.9 |
| Pd(II) | Sqr  | 0  | 8.50, 8.10, 7.53, 7.94 | 75.0, 75.0, 74.6, 74.6 |
| Pt(II) | Sqr  | 0  | 16.5, 13.9, 14.1, 12.9 | 74.6, 74.6, 74.6, 74.4 |

and $-\Delta H_{\text{bind}}$=6.42, 5.72, 5.61, 5.56 kJ.mol with PHEN). These ligands-Tm complexes properties are very similar (Table S4 and Table S5).

Table S4: Binding energies ($\Delta H_{\text{bind}}$) obtained from QM calculations for the ground state of linker BPY and different number of physisorbed H$_2$. We also shows $\Delta H_{\text{bind}}$ for the linker + TM(n)Cl$_n$ + H$_2$. The H-H bond of isolated H$_2$ is 74.4 pm

| Linker | Geom | S | $-\Delta H_{\text{bind}}$ (kJ/mol) | H-H bond (pm) |
|--------|------|---|-----------------|--------------|
| BPY    | Tm   | $\frac{1}{2}$ |                  |              |
| linker | N/A  | 0  | 6.42, 5.72, 5.61, 5.56 | 74.6, 74.6, 74.4, 74.4 |
| Sc(III)| Tbi  | 0  | 9.91, 9.34, 9.09, 7.99 | 74.6, 75.0, 75.0, 74.4 |
| Ti(IV) | Oct  | 0  | 7.93, 7.85, 7.81, 7.83 | 75.0, 75.0, 75.0, 75.0 |
| V(V)   | Pbi  | 0  | 8.97, 8.78, 7.99, 7.53 | 75.0, 75.0, 75.0, 75.0 |
| Cr(III)| Spi  | 3  | 7.39, 6.98, 7.55, 7.26 | 74.6, 74.6, 74.6, 74.4 |
| Mn(II) | Tet  | 5  | 10.4, 10.3, 10.1, 8.62 | 74.7, 74.7, 74.7, 74.7 |
| Fe(II) | Tet  | 2  | 8.58, 8.72, 8.74, 8.59 | 74.6, 74.6, 74.6, 74.6 |
| Co(II) | Tet  | 3  | 9.10, 9.36, 9.19, 8.63 | 74.6, 74.6, 74.6, 74.6 |
| Ni(II) | Tet  | 0  | 10.1, 9.74, 9.02, 8.98 | 74.9, 74.9, 74.9, 74.9 |
| Cu(II) | Sqr  | 1  | 10.7, 10.7, 9.75, 7.44 | 74.6, 74.6, 74.6, 74.4 |
| Pd(II) | Sqr  | 0  | 7.83, 7.92, 7.70, 6.99 | 74.6, 74.6, 74.6, 74.4 |
| Pt(II) | Sqr  | 0  | 14.3, 15.5, 13.9, 13.7 | 74.6, 74.6, 74.6, 74.6 |
Table S5: Binding energies ($\Delta H_{\text{bind}}^{\circ}$) obtained from QM calculations for the ground state of linker PHEN and different number of physisorbed H$_2$. We also show $\Delta H_{\text{bind}}^{\circ}$ for the linker + TM(n)Cl$_n$ + H$_2$. The H-H bond of isolated H$_2$ is 0.744 Å

| Linker | Geom | S | $-\Delta H_{\text{bind}}^{\circ}$ (kJ/mol) | H-H bond (pm) |
|--------|------|---|------------------------------------------|----------------|
| linker | N/A  | 0 | 6.87, 5.39, 5.47, 5.34                  | 74.6, 74.6, 74.4, 74.4 |
| Sc(III) | Tbi  | 0 | 10.9, 9.20, 8.76, 7.74                  | 74.6, 75.0, 75.0, 74.4 |
| Ti(IV) | Oct  | 0 | 8.79, 7.82, 7.34, 7.83                  | 75.0, 75.0, 75.0, 75.0 |
| V(V)   | Pbi  | 0 | 9.13, 8.08, 8.03, 7.86                  | 75.0, 75.0, 75.0, 75.0 |
| Cr(III) | Spi  | 3 | 9.52, 8.52, 7.99, 7.22                  | 74.6, 74.6, 74.6, 74.4 |
| Mn(II) | Tet  | 5 | 10.62, 9.76, 9.91, 9.92                  | 74.7, 74.7, 74.7, 74.7 |
| Fe(II) | Tet  | 2 | 9.88, 9.54, 9.52, 9.22                  | 74.7, 74.7, 74.6, 74.6 |
| Co(II) | Tet  | 3 | 8.72, 8.78, 9.16, 7.52                  | 74.7, 74.7, 74.6, 74.6 |
| Ni(II) | Tet  | 2 | 8.88, 9.24, 9.55, 8.87                  | 74.7, 74.7, 74.6, 74.6 |
| Cu(II) | Sqr  | 1 | 10.8, 10.7, 9.44, 9.04                  | 74.6, 74.6, 74.6, 74.4 |
| Pd(II) | Sqr  | 0 | 7.27, 7.47, 7.46, 7.15                  | 75.0, 75.0, 74.6, 74.6 |
| Pt(II) | Sqr  | 0 | 14.1, 12.6, 14.9, 15.0                  | 74.7, 74.7, 74.6, 74.6 |

Pt(II) still has the strongest interaction with H$_2$. The square geometry in Cu(II) and tetrahedral geometry in Mn(II), Co(II), Fe(II), and Ni(II) had similar $\Delta H_{\text{bind}}^{\circ}$ (-10.5 to -7.44 kJ/mol.) with the H$_2$. As in PIA and PIP, the first two H$_2$ occupy the open sites in BPY-Mn(II)Cl$_2$ and PHEN-Mn(II)Cl$_2$ complexes. The H$_2$ molecules in Co(II), Fe (II), and Ni(II) complexes located near the binding sites (N atoms) and Tm, they did not form octahedral environment like in Mn(II).

V(V) formed pentagonal bipyramidal with $-\Delta H_{\text{bind}}^{\circ} = 8.97, 8.78, 7.99, 7.53$ in BPY and $-\Delta H_{\text{bind}}^{\circ} = 9.13, 8.08, 8.03, 7.86$ in PHEN. Octahedral geometry is also observed in these ligands with Ti(IV). As previously observed, the H$_2$ molecules interact more with Cl$^-$ than with Ti(IV) and V(V).

The H$_2$ Sc(III) and Cr(III) form square pyramidal geometry with the ligands and the first H$_2$ occupies the nearest possible sites to the Tm, similar to other ligands. Within B3LYP-D3 functional, Sc(III) always has stronger $\Delta H_{\text{bind}}^{\circ}$ than Cr(III). Weight percentage (%wt) of H$_2$ molecules physisorbed in the linkers and linker-metal complexes has been estimated and it has a range of value between 1.62 to 4.92.
Table S6: Weight percentage (%wt) of H\textsubscript{2} molecules physisorbed in the linkers and linker-metal complexes. Here the equilibrium of 4 H\textsubscript{2} per linker was used.

| Systems Linkers/metal complexes | %wt of H\textsubscript{2} | %wt of H\textsubscript{2} | %wt of H\textsubscript{2} | %wt of H\textsubscript{2} | %wt of H\textsubscript{2} |
|--------------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|
| Pristine BBH                  | 3.48                      | 3.94                      | 4.25                      | 4.92                      | 4.86                      |
| Linker-ScCl\textsubscript{3}  | 2.11                      | 2.26                      | 2.36                      | 2.56                      | 2.54                      |
| Linker-TiCl\textsubscript{4}  | 1.78                      | 1.87                      | 1.94                      | 2.07                      | 2.05                      |
| Linker-VCl\textsubscript{5}   | 1.75                      | 1.86                      | 1.93                      | 2.08                      | 2.05                      |
| Linker-CrCl\textsubscript{3}  | 2.07                      | 2.22                      | 2.32                      | 2.50                      | 2.49                      |
| Linker-MnCl\textsubscript{2}  | 2.26                      | 2.44                      | 2.56                      | 2.79                      | 2.77                      |
| Linker-FeCl\textsubscript{2}  | 2.25                      | 2.43                      | 2.55                      | 2.78                      | 2.76                      |
| Linker-CoCl\textsubscript{2}  | 2.23                      | 2.41                      | 2.52                      | 2.75                      | 2.73                      |
| Linker-NiCl\textsubscript{2}  | 2.22                      | 2.41                      | 2.53                      | 2.74                      | 2.72                      |
| Linker-PdCl\textsubscript{2}  | 1.97                      | 2.11                      | 2.20                      | 2.37                      | 2.35                      |
| Linker-PtCl\textsubscript{2}  | 1.62                      | 1.71                      | 1.77                      | 1.88                      | 1.87                      |

Optimized Geometries

The optimized geometries in xyz files for each of the chelated metals by the ligands and different number of H\textsubscript{2} molecules are listed below. The unit is in Å, and each of structures are calculated within B3LYP-D3 functional in electrically neutral system.

ScCl\textsubscript{3}— H\textsubscript{2}

BBH

C 1.860847 2.920396 0.464176
C 1.202554 2.232080 1.496952
C -0.178827 2.296392 1.616994
C -0.918265 3.038114 0.697863
C -0.273518 3.709207 -0.341518
C 1.105915 3.654801 -0.462887
C 3.308665 2.830277 0.414230
H 1.778435 1.655227 2.212672
H -0.677497 1.769695 2.421371
H -1.997072 3.087997 0.786927
H -0.848616 4.277104 -1.062207
N 4.073310 3.554146 -0.321886
C 6.315265 4.089904 -0.786958
N 5.415864 3.275485 -0.214937
H 3.755560 2.085984 1.082642
H 5.727347 2.522646 0.388479
O 5.955133 5.128008 -1.388725
C 10.473146 3.240210 -0.413222
C 10.026381 4.542351 -0.626219
|   |   |   |
|---|---|---|
| C | 8.668813 | 4.799587 | -0.762482 |
| C | 7.748039 | 3.750392 | -0.665878 |
| C | 8.200985 | 2.440497 | -0.465175 |
| C | 9.560908 | 2.188908 | -0.339083 |
| H | 11.533345 | 3.041932 | -0.309486 |
| H | 10.736224 | 5.357495 | -0.690177 |
| H | 8.304941 | 5.803583 | -0.936532 |
| H | 7.506741 | 1.608323 | -0.447738 |
| H | 9.910172 | 1.174079 | -0.195690 |
| H | 1.595746 | 4.155872 | -1.283605 |
| Sc | 4.077932 | 6.010230 | -1.745867 |
| Cl | 4.925353 | 7.953418 | -2.695121 |
| Cl | 2.958285 | 6.621676 | 0.227477 |
| Cl | 2.991828 | 4.769112 | -3.426946 |
| H2 | 6.047639 | 5.483500 | 1.841639 |
| H2 | 5.391312 | 5.743820 | 1.600880 |
| H2 | 5.818360 | 2.405033 | -3.218507 |
| H2 | 5.216443 | 2.838813 | -3.292954 |
| H2 | 8.521033 | 3.932677 | 2.823002 |
| H2 | 8.728273 | 3.806528 | 2.119681 |
| H2 | 1.365036 | 7.650509 | -2.177173 |
| H2 | 1.391206 | 7.356165 | -2.861052 |
| C | 1.860227 | 2.912428 | 0.455102 |
| C | 1.200007 | 2.213446 | 1.479502 |
| C | -0.181754 | 2.275654 | 1.596624 |
| C | -0.919430 | 3.026293 | 0.683433 |
| C | -0.272547 | 3.708151 | -0.347705 |
| C | 1.107131 | 3.655337 | -0.466499 |
| C | 3.308287 | 2.823842 | 0.408147 |
| H | 1.774441 | 1.629548 | 2.190627 |
| H | -0.681903 | 1.740867 | 2.394758 |
| H | -1.998373 | 3.075226 | 0.770756 |
| H | -0.846250 | 4.283571 | -1.063530 |
| N | 4.074321 | 3.553939 | -0.320303 |
| C | 6.317946 | 4.091379 | -0.778811 |
| N | 5.416738 | 3.275920 | -0.210604 |
| H | 3.753979 | 2.075223 | 1.072441 |
| H | 5.725392 | 2.515943 | 0.384956 |
| O | 5.956751 | 5.129005 | -1.379975 |
| C | 10.481855 | 3.247602 | -0.436977 |
| C | 10.032107 | 4.543070 | -0.683403 |
| C | 8.672414 | 4.798424 | -0.802316 |
| C | 7.751442 | 3.754077 | -0.658840 |
| C | 8.207609 | 2.450305 | -0.424270 |
| C | 9.569397 | 2.200817 | -0.314645 |
| H | 11.543584 | 3.050405 | -0.350060 |
| H | 10.741448 | 5.354719 | -0.787372 |
| H | 8.306817 | 5.796811 | -1.003179 |
| H | 7.514745 | 1.618336 | -0.371639 |
| H | 9.919925 | 1.190011 | -0.146831 |
| H | 1.599089 | 4.164712 | -1.280736 |
| Sc | 4.082276 | 6.015642 | -1.737092 |
| Cl | 4.937728 | 7.959407 | -2.677713 |
Structure descriptions

Cl  2.960338  6.621986  0.236725
Cl  2.992491  4.784087  -3.423124
H2  6.065222  5.498807  1.835653
H2  5.401229  5.750891  1.607921
H2  5.821199  2.422721  -3.219689
H2  5.216041  2.852444  -3.291819
H2  1.383589  7.672875  -2.172028
H2  1.410627  7.382244  -2.857489
C   1.786799  2.925773  0.320932
C   1.095710  2.137567  1.257255
C  -0.282490  2.240921  1.383886
C  -0.986366  3.124511  0.588062
C  -0.309408  3.898736  -0.374803
C   1.067245  3.804760  -0.502855
C   3.228569  2.773037  0.258594
H   1.644272  1.450169  1.892313
H  -0.806127  1.635392  2.113501
H  -2.062789  3.206295  0.662576
H  -0.857342  4.579022  -1.014788
N   4.032028  3.538964  -0.401447
C   6.303051  3.975683  -0.831578
N   5.357164  3.174178  -0.319570
H   3.637384  1.943898  0.846146
H   5.621389  2.353138  0.212980
O   5.999193  5.074125  -1.353415
C  10.413094  2.872658  -0.577768
C  10.038165  4.204300  -0.742993
C   8.695099  4.544774  -0.834371
C   7.715037  3.549251  -0.745138
C   8.096370  2.209469  -0.592342
C   9.441630  1.875290  -0.508945
H  11.461962  2.609375  -0.512345
H  10.792995  4.978284  -0.804834
H   8.387943  5.573168  -0.971992
H   7.357566  1.416350  -0.581740
H   9.733144  0.837588  -0.403902
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Cl  5.153422  8.080376  -2.376438
Cl  3.019918  6.635215  0.357534
Cl  2.920408  5.179265  -3.353978
H2  5.967717  5.151487  1.963874
H2  5.323196  5.454723  1.717715
H2  5.451381  2.503353  -3.357787
H2  4.893085  2.997581  -3.368287
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C  -0.264218  2.478499  1.541146
C  -0.968336  3.243289  0.613047
C  -0.295409  3.858509  -0.443004
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C   3.237507  2.805495  0.309582
| Atoms | X   | Y   | Z   |
|-------|-----|-----|-----|
| H     | 1.659577 | 1.742479 | 2.136440 |
| H     | -0.785083 | 1.995005 | 2.358448 |
| H     | -2.042024 | 3.354332 | 0.707893 |
| H     | -0.844189 | 4.443583 | -1.170396 |
| N     | 4.036844 | 3.505918 | -0.413438 |
| C     | 6.307726 | 3.952271 | -0.834874 |
| N     | 5.362828 | 3.146905 | -0.323203 |
| H     | 3.647473 | 2.025663 | 0.960679 |
| H     | 5.629141 | 2.356310 | 0.252974 |
| O     | 5.996976 | 5.035911 | -1.382070 |
| C     | 10.428515 | 2.915874 | -0.484465 |
| C     | 10.037530 | 4.236591 | -0.694507 |
| C     | 8.691550 | 4.554624 | -0.817416 |
| C     | 7.724516 | 3.547398 | -0.716429 |
| C     | 8.122031 | 2.218354 | -0.517917 |
| C     | 9.470349 | 1.906668 | -0.402635 |
| H     | 11.479682 | 2.670101 | -0.393741 |
| H     | 10.782120 | 5.019578 | -0.765883 |
| H     | 8.372016 | 5.574107 | -0.988732 |
| H     | 7.394331 | 1.415342 | -0.495390 |
| H     | 9.774994 | 0.877026 | -0.261931 |
| H     | 1.588071 | 4.187160 | -1.405858 |
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| Cl    | 5.138743 | 8.029280 | -2.413986 |
| Cl    | 2.979613 | 6.588879 | 0.294285 |
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| H2    | 5.749195 | 4.930840 | 2.032170 |
| H2    | 5.135718 | 5.265728 | 1.771510 |
| C     | 1.788628 | 2.956385 | 0.335675 |
| C     | 1.092974 | 2.281898 | 1.353120 |
| C     | -0.283931 | 2.411129 | 1.468588 |
| C     | -0.981606 | 3.203316 | 0.558737 |
| C     | -0.299852 | 3.859244 | -0.466612 |
| C     | 1.076137 | 3.741683 | -0.583183 |
| C     | 3.229651 | 2.796323 | 0.292468 |
| H     | 1.637200 | 1.665949 | 2.061040 |
| H     | -0.811523 | 1.896370 | 2.262175 |
| H     | -2.057184 | 3.304181 | 0.643837 |
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| N     | 4.036797 | 3.519687 | -0.401267 |
| C     | 6.311267 | 3.957006 | -0.825891 |
| N     | 5.363015 | 3.161563 | -0.302664 |
| H     | 3.633996 | 2.002509 | 0.927928 |
| H     | 5.624143 | 2.348348 | 0.244105 |
| O     | 6.006169 | 5.046387 | -1.365313 |
| C     | 10.423730 | 2.862356 | -0.556915 |
| C     | 10.047212 | 4.188493 | -0.759019 |
| C     | 8.703645 | 4.525612 | -0.854045 |
| C     | 7.724437 | 3.532509 | -0.732304 |
| C     | 8.107458 | 2.197889 | -0.542702 |
| C     | 9.453168 | 1.866923 | -0.455168 |
| H     | 11.472989 | 2.601560 | -0.488184 |
| H     | 10.801224 | 4.960798 | -0.846411 |
| Atom | X      | Y      | Z      |
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| H    | 8.395318 | 5.549540 | -1.020056 |
| H    | 7.369752 | 1.404491 | -0.504930 |
| H    | 9.745771 | 0.832959 | -0.320783 |
| H    | 1.592241 | 4.232542 | -1.395249 |
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| Cl   | 2.941745 | 5.166534 | -3.383270 |
| C    | 1.860582 | 2.911134 | 0.466518  |
| C    | 1.201017 | 2.216845 | 1.494691  |
| C    | -0.181014 | 2.275693 | 1.609623  |
| C    | -0.919572 | 3.017699 | 0.690061  |
| C    | -0.273319 | 3.694662 | -0.34708  |
| C    | 1.106668  | 3.645641 | -0.461415 |
| C    | 3.308726  | 2.827861 | 0.423514  |
| H    | 1.776549  | 1.640213 | 2.210880  |
| H    | -0.680761 | 1.745079 | 2.410781  |
| H    | -1.998810 | 3.063882 | 0.775460  |
| H    | -0.847814 | 4.263001 | -1.065528 |
| N    | 4.074114  | 3.564315 | -0.309396 |
| C    | 6.320360  | 4.090745 | -0.773979 |
| N    | 5.418336  | 3.281855 | -0.192865 |
| H    | 3.755594  | 2.086286 | 1.095374  |
| H    | 5.727411  | 2.523800 | 0.405340  |
| O    | 5.957403  | 5.121118 | -1.387528 |
| C    | 10.487631 | 3.256116 | -0.428421 |
| C    | 10.036402 | 4.542159 | -0.717582 |
| C    | 8.676013  | 4.793492 | -0.837021 |
| C    | 7.755282  | 3.755068 | -0.652543 |
| C    | 8.213553  | 2.460093 | -0.375858 |
| C    | 9.575870  | 2.214401 | -0.264942 |
| H    | 11.549818 | 3.061832 | -0.340539 |
| H    | 10.745026 | 5.345999 | -0.853855 |
| H    | 8.309673  | 5.784637 | -1.070145 |
| H    | 7.522460  | 1.629516 | -0.282623 |
| H    | 9.927204  | 1.210037 | -0.063653 |
| H    | 1.598171  | 4.150615 | -1.278900 |
| Sc   | 4.077596  | 6.015768 | -1.746503 |
| Cl   | 4.950304  | 7.950876 | -2.691977 |
| Cl   | 2.952446  | 6.625979 | 0.220577  |
| Cl   | 2.964285  | 4.791280 | -3.414624 |
| H2   | 1.394992  | 7.730567 | -2.194510 |
| H2   | 1.414057  | 7.437104 | -2.878902 |
| PIP  | C    | 1.718503 | 2.279997 | -0.703578 |
| C    | 1.222879 | 3.519072 | -1.148286 |
| C    | -0.037972 | 3.964664 | -0.789316 |
| C    | -0.840743 | 3.166903 | 0.025958  |
| C    | -0.387659 | 1.929524 | 0.466809  |
| C    | 0.879166  | 1.493597 | 0.101229  |
| C    | 3.067792  | 1.911625 | -1.094486 |
| Atom | X       | Y       | Z       |
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| H    | 1.854597| 4.135175| -1.77561|
| H    | -0.396184| 4.924733|-1.137253|
| H    | -1.828140| 3.504694| 0.315946|
| N    | 3.755418 | 0.889260|-0.722755|
| C    | 7.713181 | 0.709478|-2.181237|
| C    | 7.292925 | 1.814376|-1.444923|
| C    | 5.988958 | 1.880356|-0.967901|
| C    | 5.102652 | 0.833908|-1.228974|
| C    | 5.521228 | -0.281697|-1.951454|
| C    | 6.825471 | -0.333826|-2.431738|
| H    | 8.731341 | 0.656378|-2.547222|
| H    | 7.983592 | 2.620284|-1.227885|
| H    | 5.666909 | 2.715356|-0.357717|
| H    | 4.832245 | -1.096060|-2.126589|
| H    | 7.147637 | -1.198799|-2.998496|
| H    | 3.537091 | 2.615962|-1.784152|
| O    | 1.335265 | 0.268773| 0.503834|
| Sc   | 3.318092 | -0.790749| 0.871071|
| Cl   | 5.373173 | -0.420563| 1.895846|
| Cl   | 1.896968 | -1.373356| 2.739038|
| H    | 0.854711 | -0.104360| 1.279441|
| Cl   | 3.213701 | -2.613028|-0.573420|
| H2   | 1.024958 | -0.272156|-2.486436|
| H2   | 1.413114 | -0.807171|-2.142590|
| H2   | 2.900660 | 2.234920| 2.077753|
| H2   | 3.526242 | 1.904098| 2.313069|
| C    | 1.733141 | 2.227462|-0.533927|
| C    | 1.251577 | 3.546136|-0.502816|
| C    | -0.048482| 3.828840|-0.116982|
| C    | -0.904428| 2.782314| 0.224174|
| C    | -0.464756| 1.465167| 0.171818|
| C    | 0.841613 | 1.191309|-0.206772|
| C    | 3.111072 | 1.999680|-0.941269|
| H    | 1.923915 | 4.352182|-0.773270|
| H    | -0.396153| 4.852968|-0.082478|
| H    | -1.921542| 2.989862| 0.532334|
| H    | -1.128552| 0.650282| 0.436182|
| H    | 3.811269 | 0.948305|-0.700852|
| C    | 7.735706 | 0.707316|-2.212139|
| C    | 7.332849 | 1.855201|-1.533467|
| C    | 6.039398 | 1.954954|-1.033243|
| C    | 5.146990 | 0.897299|-1.215975|
| C    | 5.552174 | -0.264207|-1.873941|
| C    | 6.843923 | -0.349955|-2.379077|
| H    | 8.746194 | 0.630423|-2.594717|
| H    | 8.031018 | 2.668569|-1.376989|
| H    | 5.737380 | 2.823849|-0.461456|
| H    | 4.858561 | -1.089749|-1.981124|
| H    | 7.155664 | -1.250283|-2.893946|
| H    | 3.567037 | 2.814135|-1.508443|
| O    | 1.303482 | -0.100042|-0.315712|
| Sc   | 3.319813 | -0.747105| 0.829533|
### Structure descriptions

| Element | X  | Y  | Z  | X  | Y  | Z  |
|---------|----|----|----|----|----|----|
| Cl      | 5.439822 | -0.622776 | 1.787251 |
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| H       | 0.632882 | -0.725999 | 0.002497 |
| Cl      | 3.066264 | -2.758936 | -0.330543 |
| H2      | 4.351664 | 2.087523  | 2.075705  |
| H2      | 3.777091 | 2.561884  | 2.061779  |
| H2      | 1.123037 | 3.036530  | 2.586376  |
| H2      | 1.291594 | 2.326696  | 2.737231  |

| X  | Y  | Z  |
|----|----|----|
| C  | 1.728418 | 2.225297 | -0.541829 |
| C  | 1.248751 | 3.545067 | -0.534879 |
| C  | -0.051908 | 3.836682 | -0.158619 |
| C  | -0.911394 | 2.797734 | 0.196153 |
| C  | -0.473644 | 1.479362 | 0.168023 |
| C  | 0.834202  | 1.197570 | -0.198690 |
| C  | 3.107092  | 1.991681 | -0.942539 |
| H  | 1.923134  | 4.345307 | -0.817595 |
| H  | -0.397847 | 4.861933 | -0.143310 |
| H  | -1.929963 | 3.012222 | 0.494888 |
| H  | -1.140696 | 0.669790 | 0.440628 |
| N  | 3.808046  | 0.943533 | -0.691980 |
| C  | 7.730536  | 0.709586 | -2.209720 |
| C  | 7.328426  | 1.853811 | -1.524756 |
| C  | 6.035795  | 1.950338 | -1.022096 |
| C  | 5.143700  | 0.893708 | -1.209860 |
| C  | 5.547122  | -0.263648 | -1.875426 |
| C  | 6.838362  | -0.346205 | -2.382223 |
| H  | 8.740966  | 0.634457 | -2.593078 |
| H  | 8.026950  | 2.666162 | -1.363964 |
| H  | 5.733708  | 2.816449 | -0.445892 |
| H  | 4.852683  | -1.087338 | -1.988551 |
| H  | 7.149326  | -1.243343 | -2.903294 |
| H  | 3.563554  | 2.800322 | -1.517320 |
| O  | 1.292277  | -0.097150 | -0.281486 |
| Sc | 3.329945  | -0.743498 | 0.838389 |
| Cl | 5.452718  | -0.637327 | 1.790650 |
| Cl | 1.843378  | -0.585992 | 2.667321 |
| H  | 0.631025  | -0.709954 | 0.079922 |
| Cl | 3.071372  | -2.736839 | -0.347682 |
| H2 | 2.009194  | -0.103107 | -3.471741 |
| H2 | 1.982720  | -0.393188 | -2.786833 |
| H2 | 1.111309  | 3.015452  | 2.554661 |
| H2 | 1.276968  | 2.307810  | 2.718640 |
| H2 | 3.744452  | 2.510099  | 2.074139 |
| H2 | 4.350622  | 2.077238  | 2.098391 |

| X  | Y  | Z  |
|----|----|----|
| C  | 1.636963 | 2.119009 | -0.622575 |
| C  | 1.074366 | 3.406074 | -0.627751 |
| C  | -0.279024 | 3.600635 | -0.407381 |
| C  | -1.106089 | 2.496542 | -0.202548 |
| C  | -0.583054 | 1.208692 | -0.219820 |
| C  | 0.776140  | 1.025766 | -0.423803 |
| C  | 3.058202  | 1.982561 | -0.891426 |
| H  | 1.722854  | 4.257730 | -0.798313 |
Structure descriptions

SP-JLMC

H  -0.691603  4.601015  -0.398776
H  -2.166295  2.636198  -0.030760
H  -1.223427  0.348629  -0.062082
N   3.795780  0.950461  -0.666206
C   7.809198  1.054702  -1.945280
C   7.321865  2.078611  -1.137520
C   5.997893  2.064431  -0.710733
C   5.162826  1.016408  -1.095527
C   5.651449  -0.022158  -1.887082
C   6.971126  0.005838  -2.318646
H   8.842429  1.065201  -2.270178
H   7.975968  2.831414  -0.823991
H   5.625342  2.839111  -0.046658
H   4.997388  -0.841962  -2.159186
H   7.348078  -0.799508  -2.936874
H   3.520139  2.854790  -1.368870
O    1.336853  -0.225255  -0.477001
Sc   3.276915  -0.804509   0.784137
Cl   5.471869  -1.189052  1.439651
Cl   2.199729  0.245347   2.570627
H   0.688166  -0.938505  -0.354668
Cl   2.409856  -2.917353   0.158417
H2   2.143903  0.055829  -3.661720
H2   2.103156  -0.210923  -2.968359
C    1.615456  2.178915  -0.726386
C    1.066769  3.466901  -0.611759
C   -0.296736  3.657257  -0.459902
C   -1.146094  2.551260  -0.446575
C   -0.635415  1.265600  -0.585286
C    0.732737  1.085204  -0.720016
C    3.052202  2.052390  -0.902141
H    1.733534  4.321282  -0.631521
H   -0.699375  4.656363  -0.365371
H   -2.214131  2.687861  -0.329140
H   -1.292878  0.404026  -0.575572
N    3.764527  0.986992  -0.766260
C    7.879518  1.272026  -1.633556
C    7.311673  2.142758  -0.707923
C    5.953835  2.065074  -0.414234
C    5.166089  1.107215  -1.051306
C    5.734485  0.217986  -1.962037
C    7.087853  0.310438  -2.259118
H    8.938101  1.330815  -1.855236
H    7.927330  2.875270  -0.200106
H    5.514181  2.711811   0.335394
H    5.115977  -0.539066  -2.428829
H    7.527033  -0.378339  -2.970144
H    3.556724  2.974272  -1.200048
O    1.283877  -0.160301  -0.882266
Sc   3.108061  -0.935008   0.410721
Cl   2.068502  -2.938912  -0.330922
Cl   2.081810   0.043983   2.261463
H    0.627155  -0.878247  -0.870026

S21
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| Cl   | 5.261128 | -1.565137 | 1.011696 |
| C    | 1.705109 | 2.225945  | -0.550985 |
| C    | 1.222702 | 3.544815  | -0.543812 |
| C    | -0.978126 | 3.833754  | -0.166346 |
| C    | -0.935136 | 2.793306  | 0.190115  |
| C    | -0.494949 | 1.475751  | 0.161304  |
| C    | 0.812719  | 1.196641  | -0.207720 |
| C    | 3.084061  | 1.994999  | -0.952161 |
| H    | 1.895006  | 4.346384  | -0.826959 |
| H    | -0.426095 | 4.858153  | -0.150731 |
| H    | -1.953531 | 3.005855  | 0.490241  |
| H    | -1.159945 | 0.669564  | 0.434629  |
| N    | 3.787958  | 0.948296  | -0.702613 |
| C    | 7.713133  | 0.723646  | -2.214998 |
| C    | 7.304599  | 1.871220  | -1.539321 |
| C    | 6.011019  | 1.965205  | -1.038887 |
| C    | 5.124105  | 0.902740  | -1.219923 |
| C    | 5.534468  | -0.257468 | -1.875931 |
| C    | 6.827112  | -0.338438 | -2.378621 |
| H    | 8.724719  | 0.649876  | -2.595109 |
| H    | 7.998972  | 2.687937  | -1.383615 |
| H    | 5.704687  | 2.833854  | -0.469169 |
| H    | 4.846382  | -1.087318 | -1.981513 |
| H    | 7.144395  | -1.240397 | -2.886507 |
| H    | 3.538272  | 2.804680  | -1.526552 |
| O    | 1.273647  | -0.096845 | -0.293185 |
| Sc   | 3.311446  | -0.748600 | 0.818697 |
| Cl   | 5.451765  | -0.690087 | 1.741151 |
| Cl   | 1.855085  | -0.566148 | 2.664326 |
| H    | 0.609333  | -0.715315 | 0.052066 |
| Cl   | 3.009396  | -2.740053 | -0.357054 |
| H2   | 2.021505  | -0.152282 | -3.480878 |
| H2   | 1.987280  | -0.435709 | -2.793486 |
| H2   | 1.141144  | 3.041183  | 2.527489 |
| H2   | 1.293185  | 2.330960  | 2.693674 |
| H2   | 3.779990  | 2.461975  | 2.085417 |
| H2   | 4.392328  | 2.037261  | 2.089497 |
| H2   | 6.548861  | -2.783597 | -0.060285 |
| H2   | 6.755081  | -3.340193 | -0.510187 |
| C    | 1.728712  | 2.291326  | -0.686053 |
| C    | 1.253899  | 3.557677  | -1.072579 |
| C    | 0.001608  | 4.008105  | -0.689862 |
| C    | -0.814404 | 3.186358  | 0.087469 |
| C    | -0.383092 | 1.921133  | 0.467363 |
| C    | 0.875873  | 1.480826  | 0.080079 |
| C    | 3.073531  | 1.919513  | -1.091707 |
| H    | 1.896208  | 4.192209  | -1.672145 |
| H    | -0.339686 | 4.990047  | -0.990522 |
| H    | -1.795101 | 3.527459  | 0.395685 |
| H    | -1.016439 | 1.271758  | 1.060038 |
| N    | 3.749887  | 0.879887  | -0.746960 |
| C    | 7.699923  | 0.681916  | -2.221638 |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | 7.294669 | 1.779031 | -1.465270 |
| C    | 5.993687 | 1.850961 | -0.981421 |
| C    | 5.095149 | 0.818447 | -1.256365 |
| C    | 5.498991 | -0.290094 | -1.997725 |
| C    | 6.800619 | -0.348174 | -2.484776 |
| H    | 8.716168 | 0.623844 | -2.592230 |
| H    | 7.995263 | 2.573119 | -1.236943 |
| H    | 5.683434 | 2.678145 | -0.354778 |
| H    | 4.801426 | -1.095406 | -2.180666 |
| H    | 7.111690 | -1.207875 | -3.065553 |
| H    | 3.549704 | 2.636827 | -1.763376 |
| O    | 1.311230 | 0.229038 | 0.423572 |
| Sc   | 3.311596 | -0.792741 | 0.859497 |
| Cl   | 5.324935 | -0.334744 | 1.932228 |
| Cl   | 1.842421 | -1.374134 | 2.695462 |
| H    | 0.833021 | -0.158871 | 1.195362 |
| Cl   | 3.323639 | -2.661473 | -0.519608 |
| H2   | 2.800760 | 2.223356 | 2.090864 |
| H2   | 3.434887 | 1.903697 | 2.319194 |

C    | 1.728712 | 2.291326 | -0.686053 |
C    | 1.253899 | 3.557677 | -1.072579 |
C    | 0.001608 | 4.008105 | -0.689862 |
C    | -0.814404 | 3.186358 | 0.087469 |
C    | -0.383092 | 1.921133 | 0.467363 |
C    | 0.875873 | 1.480825 | 0.080079 |
C    | 3.073531 | 1.919513 | -1.091707 |
H    | 1.896208 | 4.192209 | -1.672145 |
H    | -0.339686 | 4.990047 | -0.990522 |
H    | -1.795101 | 3.527459 | 0.395685 |
H    | -1.016439 | 1.271758 | 1.060038 |
N    | 3.749887 | 0.879887 | -0.746960 |
C    | 7.699923 | 0.681916 | -2.221638 |
C    | 7.294669 | 1.779031 | -1.465270 |
C    | 5.993687 | 1.850961 | -0.981421 |
C    | 5.095149 | 0.818447 | -1.256365 |
C    | 5.498991 | -0.290094 | -1.997725 |
C    | 6.800619 | -0.348174 | -2.484776 |
H    | 8.716168 | 0.623844 | -2.592230 |
H    | 7.995263 | 2.573119 | -1.236943 |
H    | 5.683434 | 2.678145 | -0.354778 |
H    | 4.801426 | -1.095406 | -2.180666 |
H    | 7.111690 | -1.207875 | -3.065553 |
H    | 3.549704 | 2.636827 | -1.763376 |
O    | 1.311230 | 0.229038 | 0.423572 |
Sc   | 3.311596 | -0.792741 | 0.859497 |
Cl   | 5.324935 | -0.334744 | 1.932228 |
Cl   | 1.842421 | -1.374134 | 2.695462 |
H    | 0.833021 | -0.158871 | 1.195362 |
Cl   | 3.323639 | -2.661473 | -0.519608 |
H2   | 2.800760 | 2.223356 | 2.090864 |
H2   | 3.434887 | 1.903697 | 2.319194 |

PIA
|   |   |   |
|---|---|---|
| C | 1.105579 | 1.458623 | -0.122111 |
| C | -0.055312 | 2.224124 | -0.165483 |
| C | -1.270140 | 1.619288 | 0.143420 |
| C | -1.278928 | 0.275571 | 0.485513 |
| C | -0.074294 | -0.426602 | 0.498259 |
| N | 1.093888 | 0.146050 | 0.198164 |
| C | 2.412061 | 2.052287 | -0.403891 |
| H | -0.001739 | 3.272401 | -0.431116 |
| H | -2.189549 | 2.191826 | 0.118705 |
| H | -2.197556 | -0.238313 | 0.736053 |
| H | -0.029104 | -1.480176 | 0.741811 |
| N | 3.476065 | 1.361552 | -0.307403 |
| C | 7.210139 | 3.102713 | -1.123465 |
| C | 6.137281 | 3.346800 | -1.977616 |
| C | 4.896489 | 2.775496 | -1.719912 |
| C | 4.731499 | 1.950689 | -0.602916 |
| C | 5.813301 | 1.677176 | 0.236903 |
| C | 7.042647 | 2.269350 | -0.018811 |
| H | 8.177351 | 3.545809 | -1.327941 |
| H | 6.268814 | 3.968893 | -2.854781 |
| H | 4.073462 | 2.927169 | -2.408130 |
| H | 5.673516 | 1.019799 | 1.084660 |
| H | 7.877433 | 2.066395 | 0.640763 |
| H | 2.440975 | 3.111156 | -0.663835 |
| Sc | 3.192446 | -0.980981 | 0.287265 |
| Cl | 4.954290 | -1.419206 | -1.197406 |
| Cl | 3.842055 | -0.544791 | 2.489272 |
| Cl | 1.980009 | -3.008107 | 0.268512 |
| H2 | 1.781904 | -0.501809 | -2.523002 |
| H2 | 2.507721 | -0.606389 | -2.659410 |
| C | 1.601102 | 1.971021 | 0.359558 |
| C | 1.057740 | 3.021986 | 1.091466 |
| C | -0.321881 | 3.077403 | 1.265701 |
| C | -1.105965 | 2.082337 | 0.702247 |
| C | -0.489069 | 1.065206 | -0.024330 |
| N | 0.834790 | 1.005389 | -0.196606 |
| C | 3.046311 | 1.854638 | 0.168478 |
| H | 1.708458 | 3.775772 | 1.517088 |
| H | -0.771080 | 3.883759 | 1.833315 |
| H | -2.182599 | 2.080587 | 0.811403 |
| H | -1.056720 | 0.271021 | -0.492555 |
| N | 3.538292 | 0.846354 | -0.442584 |
| C | 7.687782 | 0.598691 | -1.078183 |
| C | 7.030647 | 1.807960 | -1.292785 |
| C | 5.660205 | 1.903997 | -1.083288 |
| C | 4.941541 | 0.780628 | -0.660383 |
| C | 5.592202 | -0.441614 | -0.477331 |
| C | 6.964992 | -0.521160 | -0.671486 |
| H | 8.755848 | 0.524906 | -1.245414 |
| H | 7.581618 | 2.673949 | -1.640303 |
| H | 5.140307 | 2.830307 | -1.297637 |
| H | 5.019257 | -1.306686 | -0.170859 |
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| H       | 7.469506 | -1.467150 | -0.515912 |
| H       | 3.676823  | 2.642498  | 0.583969  |
| Sc      | 1.948363  | -0.758491 | -1.321867 |
| Cl      | 3.213522  | -0.614304 | -3.285356 |
| Cl      | 2.561856  | -2.302988 | 0.329651  |
| Cl      | -0.164122 | -1.462486 | -2.116549 |
| C       | 1.132662  | 1.478063  | -0.276511 |
| C       | -0.011191 | 2.263629  | -0.370908 |
| C       | -1.239181 | 1.704439  | -0.030655 |
| C       | -1.277480 | 0.383377  | 0.389015  |
| C       | -0.088633 | -0.342476 | 0.445697  |
| N       | 1.091927  | 0.188896  | 0.117863  |
| C       | 2.453765  | 2.031558  | -0.568774 |
| H       | 0.066389  | 3.293659  | -0.695225 |
| H       | -2.145889 | 2.294201  | -0.089983 |
| H       | -2.207019 | -0.094213 | 0.668719  |
| H       | -0.066786 | -1.380135 | 0.752306  |
| N       | 3.503811  | 1.324644  | -0.395296 |
| C       | 7.286826  | 2.955188  | -1.231919 |
| C       | 6.245410  | 3.138893  | -2.138271 |
| C       | 4.988151  | 2.608078  | -1.873253 |
| C       | 4.775864  | 1.883362  | -0.696648 |
| C       | 5.826058  | 1.669367  | 0.198725  |
| C       | 7.071794  | 2.221668  | -0.066140 |
| H       | 8.266701  | 3.366748  | -1.441541 |
| H       | 6.413951  | 3.682525  | -3.060001 |
| H       | 4.188336  | 2.711656  | -2.596825 |
| H       | 5.649560  | 1.087288  | 1.093402  |
| H       | 7.882264  | 2.065551  | 0.635089  |
| H       | 2.506930  | 3.069556  | -0.899351 |
| Sc      | 3.166051  | -0.949660 | 0.363058  |
| Cl      | 5.006391  | -1.520322 | -0.973479 |
| Cl      | 3.693760  | -0.328981 | 2.557840  |
| Cl      | 1.936104  | -2.963973 | 0.438240  |
| H2      | 1.336480  | 1.423128  | 2.834559  |
| H2      | 0.739209  | 1.868085  | 2.798645  |
| H2      | 1.910046  | -0.693563 | -2.513921 |
| H2      | 2.640501  | -0.807445 | -2.614988 |
| C       | 1.134963  | 1.462679  | -0.128054 |
| C       | -0.020578 | 2.236437  | -0.148305 |
| C       | -1.232632 | 1.642245  | 0.189553  |
| C       | -1.243625 | 0.299416  | 0.534636  |
| C       | -0.045144 | -0.412279 | 0.519584  |
| N       | 1.120056  | 0.150293  | 0.191589  |
| C       | 2.440863  | 2.050727  | -0.420974 |
| H       | 0.036198  | 3.284338  | -0.414331 |
| H       | -2.147850 | 2.221772  | 0.185746  |
| H       | -2.159724 | -0.206331 | 0.809425  |
| H       | -0.003202 | -1.465362 | 0.764670  |
| N       | 3.502699  | 1.347604  | -0.320305 |
| C       | 7.250011  | 3.065631  | -1.142293 |
| C       | 6.179409  | 3.315332  | -1.997743 |
Structure descriptions

C  4.934021  2.755272  -1.738211
C  4.761426  1.936797  -0.617836
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H  8.221054  3.499404  -1.348667
H  6.316466  3.933122  -2.877006
H  4.112324  2.910812  -2.427055
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H  7.908563  2.030882   0.626130
H  2.472564  3.107807  -0.687007
Sc  3.204946  -0.977511   0.286770
Cl  4.919351  -1.410751  -1.259602
Cl  3.796335  -0.464529   2.500004
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H2  1.436179   1.227883   2.954872
H2  0.821733   1.648826   2.991381
H2  1.734972  -0.492290  -2.537479
H2  2.453330  -0.629239  -2.684857
H2  5.200550  -3.165633   1.840594
H2  5.404003  -3.344712   1.147455
C  1.120507   1.446381  -0.109073
C  -0.032982   2.223520  -0.100694
C  -1.247876   1.618823   0.206870
C  -1.263757   0.262623   0.494415
C  -0.066246  -0.449839   0.459716
N  1.101664   0.123101   0.161391
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H  0.027589   3.281229   0.224381
H  -2.161608   2.200447   0.743173
H  -2.182458  -0.251796   0.668131
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C  7.218755   3.096488  -1.119840
C  6.140244   3.368807  -1.958905
C  4.900554   2.790157  -1.703777
C  4.741777   1.932949  -0.615171
C  5.829462   1.635209   0.208750
C  7.058227   2.231597  -0.038758
H  8.185147   3.544224  -1.318306
H  6.266441   4.014554  -2.818044
H  4.072037   2.964158  -2.384592
H  5.696283   0.957683   1.041184
H  7.896940   2.009541   0.609423
H  2.459543   3.105726  -0.615744
Sc  3.197539  -0.992132   0.276105
Cl  4.963682  -1.434841  -1.204847
Cl  3.733506  -0.445080   2.499761
Cl  1.996466  -3.022687   0.263711
H2  3.478569   2.505424   2.443145
H2  3.429960   3.247767   2.401537
H2  1.794443  -0.537446  -2.537179
H2  2.517518  -0.654886  -2.677289
H2  1.157224   0.968926   3.014315
| Atom | X  | Y  | Z  |
|------|----|----|----|
| H2   | 0.510066 | 1.338179 | 3.027457 |
| H2   | 5.153633  | -3.153691 | 1.929817  |
| H2   | 5.321046  | -3.383788 | 1.242165  |
| BPY  | C  | 0.644238 | 2.539033 | 1.583759 |
|      | 1.473897 | 3.638083 | 1.363822  |
|      | 2.850610 | 3.462636 | 1.350814  |
|      | 3.369401 | 2.192817 | 1.557767  |
|      | 2.485376 | 1.142136 | 1.760934  |
|      | H  | 3.505271 | 4.309897 | 1.185335 |
|      | 4.435032 | 2.006979 | 1.562769  |
|      | 2.831893 | 0.129168 | 1.915052  |
|      | N  | 1.155686 | 1.304088 | 1.770757 |
|      | Sc | -0.286909 | -0.484431 | 2.351850 |
|      | N  | -1.499058 | 1.497691 | 1.877164 |
|      | C  | -0.833647 | 2.646838 | 1.644579 |
|      | C  | -2.833663 | 1.526720 | 1.980038 |
|      | C  | -1.511313 | 3.855769 | 1.489230 |
|      | C  | -3.516111 | 2.694869 | 1.848218 |
|      | H  | -3.308307 | 0.572622 | 2.164706 |
|      | C  | -2.895379 | 3.788211 | 1.592135 |
|      | H  | -4.648659 | 2.663960 | 1.944046 |
|      | H  | -3.433648 | 4.812120 | 1.478178 |
|      | H  | 1.058339  | 4.623058 | 1.211026 |
|      | H  | -0.973431 | 4.772534 | 1.298449 |
| Cl   | -2.201263 | -1.712138 | 1.704051 |
| Cl   | 1.436897  | -1.990764 | 1.768357 |
| Cl   | -0.252906 | -0.064932 | 4.652887 |
| H2   | -0.713036 | -0.237091 | -0.598429 |
| H2   | -0.048340 | 0.099879  | -0.638146 |
| Cl   | 1.906082  | 2.889501  | 4.448266 |
| H2   | 1.504371  | 2.274956  | 4.577095 |
| H2   | -1.869844 | 3.183912  | 4.541065 |
| H2   | -1.540829 | 2.527288  | 4.667801 |
| C    | 0.640067  | 2.532738  | 1.587064 |
| C    | 1.467330  | 3.632905  | 1.362872 |
| C    | 2.844090  | 3.459550  | 1.342846 |
| C    | 3.365252  | 2.190514  | 1.547914 |
| C    | 2.483767  | 1.138923  | 1.756679 |
| H    | 3.496804  | 4.307492  | 1.173496 |
| H    | 4.431020  | 2.005358  | 1.547589 |
| C    | 2.832527  | 0.126788  | 1.910359 |
| H    | 2.640067  | 1.690764  | 1.768357 |
| Sc   | -0.284709 | -0.492203 | 2.359534 |
| N    | -1.500445 | 1.491048  | 1.896018 |
| C    | -0.837696 | 2.639296  | 1.653363 |
| C    | -2.834631 | 1.518519  | 2.002664 |
| C    | -1.517594 | 3.846189  | 1.491516 |
| C    | -3.574835 | 2.684773  | 1.865603 |
| H    | -3.308143 | 0.565067  | 2.193431 |
| C    | -2.901042 | 3.867993  | 1.599348 |
Structure descriptions

| Atom | X    | Y    | Z    |
|------|------|------|------|
| H    | -4.651579 | 2.652830 | 1.964477 |
| H    | -3.440861 | 4.799749 | 1.480493 |
| H    | 1.048554  | 4.616781 | 1.212198 |
| H    | -0.980812 | 4.761421 | 1.290854 |
| Cl   | -2.191546 | -1.702285 | 1.645386 |
| Cl   | 1.446621  | -1.987100 | 1.767125 |
| Cl   | -0.244403 | -0.033270 | 4.656503 |
| H2   | -0.708434 | 0.150816  | -0.641626 |
| H2   | 1.961558  | 2.883632  | 4.448239 |
| H2   | 1.544519  | 2.279068  | 4.575726 |
| H2   | -1.875433 | 3.207001  | 4.553722 |
| H2   | -1.545001 | 2.549958  | 4.674496 |
| H2   | -0.869570 | -3.437103 | 3.859273 |
| H2   | -0.560206 | -3.148595 | 4.471315 |

| C     | 0.639922  | 2.536712  | 1.581289 |
| C     | 1.466741  | 3.632826  | 1.335375 |
| C     | 2.841532  | 3.450973  | 1.273336 |
| C     | 3.360823  | 2.177841  | 1.456240 |
| C     | 2.480186  | 1.130634  | 1.691106 |
| H     | 3.493920  | 4.295067  | 1.085068 |
| H     | 4.424734  | 1.986134  | 1.419251 |
| H     | 2.827054  | 0.115959  | 1.832445 |
| N     | 1.151473  | 1.298405  | 1.751834 |
| Sc    | -0.284384 | -0.485035 | 2.382999 |
| N     | -1.499760 | 1.497957  | 1.896166 |
| C     | -0.836080 | 2.650353  | 1.677699 |
| C     | -2.833512 | 1.523707  | 2.010112 |
| C     | -1.513673 | 3.864345  | 1.561020 |
| C     | -3.571952 | 2.695112  | 1.911002 |
| H     | -3.306688 | 0.565426  | 2.176724 |
| C     | -2.896602 | 3.885256  | 1.680431 |
| H     | -4.648317 | 2.662428  | 2.013131 |
| H     | -3.435259 | 4.821292  | 1.595653 |
| H     | 1.049345  | 4.618640  | 1.194790 |
| H     | -0.976465 | 4.784361  | 1.385380 |
| Cl    | -2.153092 | -1.691184 | 1.591422 |
| Cl    | 1.461344  | -1.992413 | 1.861354 |
| Cl    | -0.347876 | -0.056281 | 4.672092 |

| C     | 0.641945  | 2.543671  | 1.597731 |
| C     | 1.470485  | 3.643538  | 1.374224 |
| C     | 2.847092  | 3.467018  | 1.347393 |
| C     | 3.366903  | 2.195733  | 1.543293 |
| C     | 2.484261  | 1.144879  | 1.753588 |
| H     | 3.500939  | 4.313825  | 1.176805 |
| H     | 4.432372  | 2.008828  | 1.534383 |
| H     | 2.830821  | 0.130850  | 1.901075 |
| N     | 1.154633  | 1.308166  | 1.778568 |
| Sc    | -0.289641 | -0.486988 | 2.358369 |
| N     | -1.501458 | 1.500425  | 1.889136 |
| C     | -0.836315 | 2.651071  | 1.662591 |
| C     | -2.836657 | 1.526435  | 1.983527 |
C  -1.515044  3.860607  1.512329
C  -3.575953  2.694351  1.853017
H  -3.310733  0.570376  2.160457
C  -2.899750  3.881156  1.608900
H  -4.653684  2.660911  1.940392
H  -3.438851  4.814114  1.496998
H   1.053404  4.628567  1.226159
H  -0.976886  4.778380  1.327250
Cl  -2.199494  -1.710950  1.683138
Cl   1.444366  -1.990254  1.787864
Cl  -0.273509  -0.058787  4.649219
H2  -0.712714  -0.254755  -0.547226
H2   0.042846   0.069914  -0.600658
C   0.641821   2.538816  1.588517
C   1.470043   3.637554  1.360984
C   2.846683   3.462875  1.342137
C   3.366680   2.193883  1.550577
C   2.484129   1.143044  1.759384
H    3.500373   4.309419  1.169945
H    4.432326   2.008209  1.551014
H    2.831802   0.130684  1.914566
N    1.154320   1.304302  1.774515
Sc  -0.288557  -0.488589  2.349769
N  -1.502058   1.495620  1.875612
C  -0.835985   2.647206  1.666740
C  -2.837165   1.522159  1.974132
C  -1.513474   3.859159  1.521171
C  -3.575058   2.692180  1.856314
H  -3.311535   0.565275  2.145573
C  -2.897712   3.880682  1.623290
H  -4.652587   2.659411  1.946176
H  -3.435854   4.815490  1.522290
H   1.052355   4.621031  1.204595
H  -0.974541   4.778099  1.344710
Cl  -2.199163  -1.717711  1.686603
Cl  -0.289083  -0.050615  4.644672
H2  -0.692334  -0.200974  -0.567412
H2   0.026786  -0.006078  -0.605338
H2   1.901606   2.883312  4.453367
H2   1.476413   2.282895  4.574844
PHEN

C   0.614754   2.505736  1.580649
C   1.387047   3.668589  1.361352
C   2.787972   3.518506  1.328599
C   3.339078   2.271516  1.507159
C   2.492666   1.171325  1.715108
H   3.415842   4.387164  1.164969
H   4.410186   2.119727  1.490491
H   2.885897   0.172011  1.851929
N   1.170314   1.279850  1.750620
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| Sc   | -0.288845 | -0.503919 | 2.349524 |
| N    | -1.523771 | 1.468348 | 1.848144 |
| C    | -0.818412 | 2.606005 | 1.633000 |
| C    | -2.846815 | 1.543274 | 1.911579 |
| C    | -1.436006 | 3.865847 | 1.465754 |
| C    | -3.546044 | 2.751127 | 1.762359 |
| H    | -3.363850 | 0.606978 | 2.078885 |
| C    | -2.842754 | 3.911162 | 1.537481 |
| H    | -4.626117 | 2.748929 | 1.825557 |
| H    | -3.354918 | 4.859053 | 1.416007 |
| C    | 0.729423  | 4.929393 | 1.189657 |
| C    | -0.624059 | 5.024524 | 1.240027 |
| Cl   | -2.221122 | -1.726517 | 1.744970 |
| Cl   | 1.451799  | -1.988693 | 1.750811 |
| Cl   | -0.239159 | -0.028270 | 4.632825 |
| H2   | -0.718282 | -0.168633 | -0.600091 |
| H2   | 0.021123  | -0.069892 | -0.600539 |
| H    | -1.114041 | 5.982771 | 1.113211 |
| H    | 1.337035  | 5.811414 | 1.022129 |
| C    | 0.614198  | 2.504189 | 1.583104 |
| C    | 1.387595  | 3.668200 | 1.375628 |
| C    | 2.789023  | 3.518990 | 1.359021 |
| C    | 3.338398  | 2.271452 | 1.539166 |
| C    | 2.490266  | 1.169963 | 1.733391 |
| H    | 3.418496  | 4.388344 | 1.205867 |
| H    | 4.409705  | 2.120153 | 1.534079 |
| H    | 2.882838  | 0.170366 | 1.869425 |
| N    | 1.167721  | 1.278075 | 1.755512 |
| Sc   | -0.291444 | -0.501083 | 2.369504 |
| N    | -1.524771 | 1.462078 | 1.824710 |
| C    | -0.819398 | 2.602194 | 1.619436 |
| C    | -2.849134 | 1.534775 | 1.870004 |
| C    | -1.436975 | 3.860970 | 1.446096 |
| C    | -3.548392 | 2.741642 | 1.713045 |
| H    | -3.366508 | 0.597534 | 2.030287 |
| C    | -2.844756 | 3.903490 | 1.499397 |
| H    | -4.629225 | 2.736992 | 1.761771 |
| H    | -0.357724 | 4.350459 | 1.372673 |
| H    | 1.338428  | 5.811565 | 1.039793 |
| H    | -1.114041 | 5.978797 | 1.100021 |
| Cl   | -2.224017 | -1.727741 | 1.782214 |
| Cl   | 1.423427  | -1.977926 | 1.689869 |
| Cl   | -0.200678 | -0.029692 | 4.650352 |
| C    | 0.730221  | 4.928917 | 1.198714 |
| C    | -0.624050 | 5.021302 | 1.232112 |
| C    | 0.612444  | 2.507774 | 1.572068 |
| C    | 1.383692  | 3.669225 | 1.343614 |
| C    | 2.784489  | 3.520758 | 1.316582 |
| C    | 3.335286  | 2.277088 | 1.513817 |
| C    | 2.490922  | 1.178097 | 1.729398 |
| H    | 3.412289  | 4.388273 | 1.147172 |
| H    | 4.407757  | 2.127294 | 1.506538 |
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| H       | 2.885198 | 0.181288 | 1.879335 |
| N       | 1.168373 | 1.284319 | 1.754322 |
| Sc      | -0.288883 | -0.498808 | 2.348591 |
| N       | -1.524451 | 1.472107 | 1.853296 |
| C       | -2.846975 | 1.547145 | 1.923581 |
| C       | -1.438178 | 3.867040 | 1.456424 |
| C       | -3.546661 | 2.754172 | 1.771323 |
| H       | -3.362874 | 0.611775 | 2.098378 |
| C       | -2.844628 | 3.912761 | 1.535733 |
| H       | -4.626358 | 2.752784 | 1.840770 |
| H       | -3.357482 | 4.859987 | 1.411841 |
| C       | 0.725515 | 4.929107 | 1.164947 |
| C       | -0.627657 | 5.024544 | 1.220456 |
| Cl      | -2.218634 | -1.722125 | 1.736615 |
| Cl      | 1.454206 | -1.983010 | 1.758680 |
| Cl      | -0.248632 | -0.042861 | 4.639413 |
| H2      | -0.698927 | -0.167567 | -0.590640 |
| H2      | 0.037868 | -0.052927 | -0.570007 |
| H2      | 1.813825 | 3.048712 | 4.403083 |
| H2      | 1.413452 | 2.432845 | 4.529360 |
| H       | -1.118138 | 5.982043 | 1.090287 |
| H       | 1.332484 | 5.809567 | 0.990084 |
| C       | 0.610293 | 2.508980 | 1.575853 |
| C       | 1.382649 | 3.671352 | 1.358536 |
| C       | 2.783917 | 3.524288 | 1.347174 |
| C       | 3.334549 | 2.280421 | 1.546127 |
| C       | 2.48793 | 1.180075 | 1.749726 |
| H       | 3.412914 | 4.392489 | 1.185964 |
| H       | 4.406136 | 2.131043 | 1.549130 |
| H       | 2.881949 | 0.183464 | 1.900988 |
| N       | 1.165314 | 1.285763 | 1.761797 |
| Sc      | -0.292486 | -0.495406 | 2.346693 |
| N       | -1.527175 | 1.470254 | 1.838060 |
| C       | -0.822681 | 2.607138 | 1.616261 |
| C       | -2.850235 | 1.545222 | 1.900401 |
| C       | -1.440680 | 3.864470 | 1.437297 |
| C       | -3.549582 | 2.750874 | 1.738592 |
| H       | -3.367144 | 0.610621 | 2.075515 |
| C       | -2.847350 | 3.909167 | 1.503502 |
| H       | -4.629699 | 2.748087 | 1.801546 |
| H       | -3.360285 | 4.855456 | 1.373747 |
| H       | 1.332584 | 5.812526 | 1.009204 |
| H       | -1.119146 | 5.980249 | 1.077081 |
| Cl      | -2.229149 | -1.724796 | 1.773718 |
| Cl      | 1.441058 | -1.977884 | 1.727728 |
| Cl      | -0.213271 | -0.039035 | 4.637193 |
| H2      | -0.701524 | -0.146135 | -0.578692 |
| H2      | 0.042520 | -0.097878 | -0.598755 |
| H2      | 1.846342 | 3.009245 | 4.414082 |
| H2      | 1.453853 | 2.383965 | 4.518209 |
| H2      | -1.827047 | 3.256739 | 4.508838 |
| H2      | -1.531208 | 2.579928 | 4.608257 |
| Atom | x    | y    | z    |
|------|------|------|------|
| C    | -0.629000 | 5.023180 | 1.211630 |
| C    | 0.724964  | 4.930477 | 1.173604 |
| C    | 0.610060  | 2.503280 | 1.579107 |
| C    | 1.381460  | 3.665413 | 1.342923 |
| C    | 2.782800  | 3.519073 | 1.545757 |
| C    | 2.488598  | 1.176420 | 1.754840 |
| H    | 3.410636  | 3.87522  | 1.178403 |
| C    | 4.406145  | 2.127621 | 1.547807 |
| H    | 2.883550  | 0.180425 | 1.907602 |
| N    | 1.166059  | 1.281153 | 1.767998 |
| Sc   | -0.291607 | -0.503320 | 2.355868 |
| N    | -1.526819 | 1.465110 | 1.847403 |
| C    | -0.822833 | 2.601228 | 1.621558 |
| C    | -2.849547 | 1.540160 | 1.913298 |
| C    | -1.441387 | 3.857979 | 1.439877 |
| C    | -3.549514 | 2.745346 | 1.750505 |
| H    | -3.366136 | 0.606125 | 2.092286 |
| C    | -2.847933 | 3.902746 | 1.509242 |
| H    | -4.629421 | 2.742950 | 1.816605 |
| H    | -3.361003 | 4.387522 | 1.397760 |
| H2   | -0.524746 | -3.545271 | 3.958494 |
| H2   | -0.436128 | -3.126047 | 4.666671 |
| C1   | -2.226189 | -1.719669 | 1.748557 |
| C1   | 1.442627  | -1.974529 | 1.712549 |
| C1   | -0.217162 | -0.012758 | 4.643917 |
| H2   | -0.703289 | -0.114476 | -0.587288 |
| H2   | 0.042506  | -0.124475 | -0.605124 |
| H2   | 1.868061  | 3.003600  | 4.402342 |
| H2   | 1.466715  | 2.392196  | 4.545668 |
| H2   | -1.836043 | 3.268825  | 4.503755 |
| H2   | -1.502758 | 2.612947  | 4.622882 |
| C    | -0.630681 | 5.016274  | 1.209069 |
| C    | 0.723216  | 4.923906  | 1.169254 |
| H    | -1.121822 | 5.972387  | 1.071476 |
| H    | 1.330578  | 5.805137  | 0.999659 |

**TiCl₄—H₂**

| Atom | x    | y    | z    |
|------|------|------|------|
| H2   | -0.373152 | -2.152465 | -0.860289 |
| H2   | -1.098204 | -2.315715 | -0.917000 |
| H2   | 6.720303  | 1.309682 | 1.302183 |
| H2   | 6.115192  | 0.922339 | 1.498251 |
| C    | 5.726071  | 1.048737 | -1.723979 |
| C    | 6.829280  | 1.910840 | -1.827829 |
| C    | 8.095647  | 1.400946 | -2.074728 |
| C    | 8.267878  | 0.027427 | -2.243863 |
| C    | 7.171184  | -0.829906 | -2.173885 |
| C    | 5.903484  | -0.327803 | -1.917342 |
| C    | 4.424639  | 1.635299 | -1.453741 |
| H    | 6.692965  | 2.978391 | -1.693546 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 8.945673  | 2.069304  | -2.137856 |
| H    | 9.255509  | -0.372649 | -2.440673 |
| H    | 7.302888  | -1.895183 | -2.317245 |
| N    | 3.425963  | 1.012271  | -0.940017 |
| C    | 1.138581  | 1.175744  | -0.385060 |
| N    | 2.254609  | 1.730554  | -0.889708 |
| H    | 4.311926  | 2.690475  | -1.721168 |
| H    | 2.211745  | 2.636921  | -1.338647 |
| O    | 1.156016  | 0.021993  | 0.089256  |
| C    | -2.531353 | 3.340241  | -0.494823 |
| C    | -2.524246 | 1.947040  | -0.462987 |
| C    | -1.320840 | 1.255631  | -0.418844 |
| C    | -0.112794 | 1.961090  | -0.423192 |
| C    | -0.121885 | 3.361126  | -0.442667 |
| C    | -1.330181 | 4.046307  | -0.476743 |
| H    | -3.472277 | 3.876679  | -0.522518 |
| H    | -3.458126 | 1.396806  | -0.468690 |
| H    | -1.297205 | 0.174496  | -0.388438 |
| H    | -3.334842 | 5.129295  | -0.475910 |
| H    | -5.050811 | -0.989750 | -1.880124 |
| Ti   | 2.869317  | -1.096287 | 0.607789  |
| Cl   | 3.177589  | 0.626564  | 2.131477  |
| Cl   | 2.576895  | -2.042120 | -1.481978 |
| Cl   | 4.976808  | -1.828600 | 0.849153  |
| Cl   | 1.726408  | -2.525360 | 1.842239  |
| H2   | 0.908126  | -0.182404 | -2.980307 |
| H2   | 0.476646  | 0.352687  | -3.268806 |
| H2   | 3.737337  | 3.989294  | 0.786821  |
| H2   | 3.640591  | 3.298100  | 1.050728  |
| H2   | 6.614042  | 1.398652  | 1.283384  |
| H2   | 5.991483  | 1.082308  | 1.542552  |
| C    | 5.720318  | 1.032411  | -1.730899 |
| C    | 6.826131  | 1.891180  | -1.836719 |
| C    | 8.088426  | 1.378703  | -2.098480 |
| C    | 8.253932  | 0.006057  | -2.281447 |
| C    | 7.154646  | -0.847669 | -2.209101 |
| C    | 5.890998  | -0.343171 | -1.937218 |
| C    | 4.422938  | 1.622769  | -1.449673 |
| H    | 6.695031  | 2.957981  | -1.692106 |
| H    | 8.940468  | 2.044327  | -2.162836 |
| H    | 9.238219  | -0.395936 | -2.490539 |
| H    | 7.280874  | -1.912005 | -2.363827 |
| N    | 3.422661  | 1.002494  | -0.935371 |
| C    | 1.135051  | 1.169094  | -0.384410 |
| N    | 2.253884  | 1.725141  | -0.882031 |
| H    | 4.313528  | 2.679461  | -1.711968 |
| H    | 2.215732  | 2.635594  | -1.322915 |
| O    | 1.148597  | 0.012230  | 0.081202  |
| C    | -2.529928 | 3.344174  | -0.492740 |
| C    | -2.526513 | 1.950727  | -0.469882 |
| C    | -1.324766 | 1.256669  | -0.426128 |
| C    | -0.114658 | 1.958155  | -0.421697 |
| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | -0.120381 | 3.358238 | -0.431519 |
| C    | -1.326879  | 4.046657  | -0.492177  |
| H    | -3.469250  | 3.883310  | -0.520230  |
| H    | -3.461687  | 1.404670  | -0.482177  |
| H    | -1.304008  | 0.175286  | -0.400563  |
| H    | 0.804698   | 3.918744  | -0.361510  |
| H    | -1.328793  | 5.129584  | -0.457442  |
| H    | 5.036178   | -1.002203 | -1.898701  |
| Ti   | 2.869570   | -1.094957 | 0.609531   |
| Cl   | 3.142794   | 0.631333  | 2.141544   |
| Cl   | 2.585787   | -2.058176 | -1.471959  |
| Cl   | 4.988746   | -1.786124 | 0.854796   |
| Cl   | 1.748954   | -2.536040 | 1.850819   |
| H2   | 0.868426   | -0.228639 | -2.926599  |
| H2   | 0.438088   | 0.304140  | -3.222556  |
| H2   | 3.753567   | 3.979189  | 0.783898   |
| H2   | 3.650276   | 3.289824  | 1.050111   |
| C    | 2.073512   | 2.660923  | 0.083294   |
| C    | 1.377056   | 2.181112  | 1.204225   |
| C    | -0.007611  | 2.255261  | 1.252871   |
| C    | -0.711124  | 2.784583  | 0.171412   |
| C    | -0.027107  | 3.234532  | -0.956384  |
| C    | 1.358324   | 3.175279  | -1.007054  |
| C    | 3.523091   | 2.547528  | 0.077976   |
| H    | 1.925790   | 1.766395  | 2.042732   |
| H    | -0.538253  | 1.898272  | 2.127036   |
| H    | -1.792896  | 2.836980  | 0.204780   |
| H    | -0.573899  | 3.634946  | -1.800924  |
| N    | 4.321037   | 3.279573  | -0.612803  |
| C    | 6.564756   | 3.590421  | -1.268582  |
| N    | 5.643142   | 2.900898  | -0.572129  |
| H    | 3.942325   | 1.762550  | 0.714420   |
| H    | 5.894653   | 2.034763  | -0.112817  |
| O    | 6.246333   | 4.608062  | -1.914468  |
| C    | 10.60365   | 2.220055  | -1.354785  |
| C    | 10.082115  | 2.981819  | -2.400617  |
| C    | 8.768139   | 3.427872  | -2.354165  |
| C    | 7.958589   | 3.097756  | -1.262476  |
| C    | 8.484445   | 2.343432  | -0.206721  |
| C    | 9.803236   | 1.908254  | -0.255412  |
| H    | 11.628017  | 1.878932  | -1.390497  |
| H    | 10.704018  | 3.231429  | -3.251376  |
| H    | 8.352083   | 4.026461  | -3.153655  |
| H    | 7.891702   | 2.134768  | 0.676409   |
| H    | 10.212382  | 1.338378  | 0.569634   |
| H    | 1.888501   | 3.509252  | -1.887062  |
| Ti   | 4.425310   | 5.669407  | -1.704939  |
| Cl   | 5.230878   | 6.040260  | 0.443017   |
| Cl   | 3.789150   | 4.436983  | -3.555562  |
| Cl   | 2.338242   | 6.272724  | -1.146057  |
| Cl   | 5.192067   | 7.480087  | -2.712167  |
| H2   | 5.579061   | 2.163687  | -3.615524  |
| H2   | 6.063033   | 1.598746  | -3.563536  |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H2   | 5.614276| 3.119812| 2.598683|
| H2   | 5.519179| 3.713374| 2.156258|
| C    | 2.057585| 2.643735| 0.039661|
| C    | 1.337143| 2.132001| 1.130889|
| C    | -0.048336| 2.205226| 1.151821|
| C    | -0.728417| 2.766413| 0.071530|
| C    | -0.020331| 3.249077| -1.027540|
| C    | 1.365740| 3.189710| -1.050519|
| C    | 3.507346| 2.530565| 0.060308|
| H    | 1.867384| 1.691508| 1.968310|
| H    | -0.597753| 1.822744| 2.003364|
| H    | -1.810739| 2.818105| 0.082990|
| H    | -0.548806| 3.674550| -1.871544|
| N    | 4.316105| 3.277711| -0.600316|
| C    | 6.566299| 3.595590| -1.232214|
| N    | 5.638413| 2.898127| -0.548977|
| H    | 3.914593| 1.728897| 0.685278|
| H    | 5.876044| 1.998278| -0.150438|
| O    | 6.259976| 4.634821| -1.846866|
| C    | 10.585518| 2.180134| -1.393841|
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| H    | 1.119413| 4.813809| 0.735429|
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Ti  3.004767  -1.016352  0.265694
Cl  2.803351  -1.715460  -1.918279
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H  0.235190  -0.695051  0.269159
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Cl  5.019230  -1.842596  0.648632
H2  1.122139  0.299216  -3.124762
H2  0.745413  0.889466  -3.379629
H2  3.176463  3.228837  1.873361
H2  3.373882  3.936075  1.746350
H2  0.137030  -0.402067  2.710536
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C  -0.789220  1.604945  0.310261
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C  2.707366  1.886751  -1.126312
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H  -2.205612  3.199234  0.483314
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C  6.513896  0.193323  -2.844565
H  8.465005  1.033893  -2.499105
H  7.735132  2.376664  -0.545230
H  5.370258  2.269342  0.215244
H  4.471462  -0.497615  -2.921667
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Ti  3.039660  -0.892767  0.524967
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| Cl | 1.782495 | -2.303822| 1.789689 |
| Cl | 5.093937 | -1.603959| 0.927083 |
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| H2 | 0.724591 | 0.402975 | -3.270162|
| H2 | 3.466520 | 3.581849 | 1.319992 |
| H2 | 3.691163 | 4.246273 | 1.068054 |
| H2 | -1.003004| -2.098898| 0.895001 |
| H2 | -1.519669| -1.783476| 0.457626 |
| H2 | 8.614170 | -1.311784| 0.318186 |
| H2 | 8.015035 | -0.965339| 0.044659 |
| C  | 1.356392 | 2.199857 | -0.747385|
| C  | 0.889834 | 3.513744 | -0.920015|
| C  | -0.390060| 3.884828 | -0.541271|
| C  | -1.240596| 2.930274 | 0.013680 |
| C  | -0.815205| 1.617089 | 0.175397 |
| C  | 0.469250 | 1.255137 | -0.207415|
| C  | 2.733725 | 1.927574 | -1.121032|
| H  | 1.560639 | 4.250215 | -1.347182|
| H  | -0.723952| 4.905597 | -0.673723|
| H  | -2.243198| 3.204750 | 0.318119 |
| H  | -1.478574| 0.869745 | 0.595895 |
| N  | 3.445059 | 0.897434 | -0.844342|
| C  | 7.515615 | 1.062656 | -1.930347|
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| C  | 4.830921 | 0.959690 | -1.239741|
| C  | 5.269414 | 0.294361 | -2.381474|
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| H  | 8.564486 | 1.098515 | -2.199210|
| H  | 7.762694 | 2.263725 | -0.160991|
| H  | 5.357837 | 2.141871 | 0.468226 |
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| Cl | 2.982318 | 0.748986 | 2.075731 |
| H  | 0.260494 | -0.599232| 0.372468 |
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| H2 | 1.155823 | -0.043071| -3.009400|
| H2 | 0.791215 | 0.500567 | -3.369560|
| C  | 1.373446 | 2.238961 | -0.691312|
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| C  | -0.360425| 3.935371 | -0.461340|
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| C  | -0.806624| 1.659731 | 0.215687 |
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Structure descriptions

SP-JLMC

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C  5.723117  1.686907 -0.346251
C  4.847275  0.992970 -1.180316
C  5.307524  0.348489 -2.325718
C  6.660139  0.416198 -2.643045
H  8.598221  1.149466 -2.067643
H  7.758558  2.275182 -0.022388
H  5.342760  2.141230  0.559818
H  4.613786 -0.207741 -2.939980
H  7.023116 -0.081189 -3.534228
H  3.252461  2.792252 -1.569479
O  0.884746 -0.009006 -0.093761
Ti  3.016185 -0.928303  0.399095
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Cl  3.012413  0.647602  2.096734
H  0.255152 -0.568784  0.390685
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PIA

C  1.062941  1.324641 -0.305979
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S40
| Atom | x      | y      | z      | Coordinates |
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| Cl   | 2.014830 | -2.740327 | 1.482321 |
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| H2   | 1.158464 | 1.130686 | -3.788138 |
| H2   | -0.333827 | -2.631184 | -1.036954 |
| H2   | -1.058937 | -2.779846 | -0.949597 |
| C    | 1.064351 | 1.326733 | -0.295812 |
| C    | -0.053557 | 2.145640 | -0.408273 |
| C    | -1.245956 | 1.736523 | 0.178700 |
| C    | -1.273202 | 0.526435 | 0.856513 |
| C    | -0.111602 | -0.239777 | 0.923185 |
| N    | 1.031042 | 0.147537 | 0.359279 |
| C    | 2.349662 | 1.708285 | -0.864940 |
| H    | 0.018032 | 3.083183 | -0.944529 |
| H    | -2.134029 | 2.352404 | 0.107094 |
| H    | -2.176408 | 0.164895 | 1.329847 |
| H    | -0.085813 | -1.191309 | 1.435101 |
| N    | 3.367596 | 0.954866 | -0.707501 |
| C    | 7.030042 | 2.099107 | -2.416736 |
| C    | 5.898535 | 1.989251 | -3.220321 |
| C    | 4.680127 | 1.613589 | -2.662873 |
| C    | 4.606879 | 1.340237 | -1.296150 |
| C    | 5.741353 | 1.423558 | -0.488649 |
| C    | 6.947030 | 1.816781 | -1.053435 |
| H    | 7.978126 | 2.389351 | -2.853240 |
| H    | 5.963233 | 2.184257 | -4.283931 |
| H    | 3.800196 | 1.488952 | -3.281456 |
| H    | 5.663115 | 1.187805 | 0.563226 |
| H    | 7.827396 | 1.892810 | -0.427170 |
| H    | 2.421752 | 2.652058 | -1.402244 |
| Ti   | 3.012211 | -1.047279 | 0.378747 |
| Cl   | 2.290530 | -1.645691 | -1.748928 |
| Cl   | 3.428049 | 0.269818 | 2.244951 |
| Cl   | 5.100360 | -1.796606 | 0.126423 |
| Cl   | 2.020124 | -2.744320 | 1.472447 |
| H2   | 3.102747 | 3.087078 | 1.598283 |
| H2   | 3.044517 | 3.804343 | 1.402676 |
| H2   | 1.358604 | 0.511954 | -3.415649 |
| H2   | 1.141951 | 1.111246 | -3.803342 |
| H2   | -0.367335 | -2.626774 | -1.037474 |
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| H2   | 7.056588 | 0.031079 | 2.622376 |
| H2   | 6.494465 | -0.336798 | 2.300414 |

| C    | 1.657256 | 2.149070 | -0.576091 |
| C    | 0.894872 | 3.196621 | -1.081749 |
| C    | -0.466913 | 3.229180 | -0.804263 |
| C    | -1.012984 | 2.215217 | -0.030058 |
| C    | -0.183762 | 1.198800 | 0.438864 |
| N    | 1.120671 | 1.162513 | 0.171074 |
| C    | 3.092377 | 2.067960 | -0.812253 |
Structure descriptions SP-JLMC

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N  3.771615 1.113409 -0.306558
C  7.900521 0.941114 -1.058779
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C  5.637452 1.056961 -1.885365
C  5.169839 1.049134 -0.570245
C  6.057977 0.966395  0.502893
C  7.422720 0.927199  0.251466
H  8.966467 0.894554 -1.247206
H  7.372274 0.986067 -3.14519
H  4.929284 1.066166 -2.704581
H  5.668529 0.941391  1.511482
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H  3.566757 2.848302 -1.405085
Ti  2.583579  0.495600  0.853051
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H2  3.632100  3.630201  1.604090
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C  1.664934  1.978942  0.406647
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C  -0.252113  2.971988  1.442567
C  -1.044457  2.136658  0.668621
C  -0.433134  1.249731 -0.215471
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H  1.788919  3.519731  1.896427
H  -0.698061  3.673201  2.137598
H  -2.124265  2.161219  0.736677
H  -1.010678  0.582293 -0.840495
N  3.568038  0.964765 -0.579525
C  7.728872  0.655128 -1.063265
C  7.101937  1.836748 -1.251487
C  5.724193  1.995414 -1.092946
C  4.977729  0.866158 -0.751501
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C  6.973320 -0.469397 -0.731546
H  8.801954  0.569520 -1.188081
H  7.680951  2.754937 -1.533702
H  5.218471  2.936215 -1.274362
H  4.991475 -1.238324 -0.345800
H  7.458232 -1.428047 -0.592044
H  3.765858  2.465458  0.825224
Ti  2.017120 -0.226612 -1.813758
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Cl  2.101808 -1.594711  0.061199
### Structure descriptions

#### Cl

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| Cl | 3.523459 | -1.345868 | -3.023072 |
| Cl | 0.064307 | -1.006266 | -2.620179 |

#### C

|   |   |   |   |
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| C | 1.668776 | 2.173010 | -0.549963 |
| C | 0.914609 | 3.236623 | -1.034810 |
| C | -0.448130 | 3.271758 | -0.761206 |
| C | -1.002863 | 2.245129 | -0.010593 |
| C | -0.181416 | 1.213150 | 0.438451 |
| N | 1.123262 | 1.174031 | 0.173999 |
| C | 3.105428 | 2.090685 | -0.777730 |
| H | 1.393682 | 4.018405 | -1.610182 |
| H | -1.061162 | 4.087084 | -1.125268 |
| H | -2.057298 | 2.229545 | 0.231454 |
| H | -0.570508 | 0.391736 | 1.023841 |
| N | 3.777696 | 1.123045 | -0.287358 |
| C | 7.912775 | 0.955228 | -1.009136 |
| C | 7.028011 | 1.035150 | -2.080992 |
| C | 5.656977 | 0.901681 | -1.851357 |
| C | 5.17786 | 1.059656 | -0.540710 |
| C | 6.057162 | 0.952899 | 0.537577 |
| C | 7.423822 | 0.915716 | 0.296459 |
| H | 8.980012 | 0.909664 | -1.189647 |
| H | 7.401302 | 1.041960 | -3.097851 |
| H | 4.956028 | 1.115718 | -2.676661 |
| H | 5.659241 | 0.908650 | 1.541952 |
| H | 8.109753 | 0.846123 | 1.131768 |
| H | 3.587519 | 2.883274 | -1.347750 |
| Ti | 2.578815 | -0.510793 | 0.823411 |
| Cl | 2.207844 | -1.208051 | -1.351882 |
| Cl | 2.943260 | 0.935565 | 2.611567 |
| Cl | 4.334085 | -1.835099 | 1.202134 |
| Cl | 0.887315 | -1.654999 | 1.769884 |
| H2 | 3.518711 | 3.621869 | 1.698189 |
| H2 | 3.719364 | 4.275327 | 1.400187 |

#### BPY

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| C | 0.558389 | 2.470579 | 1.788442 |
| C | 1.391882 | 3.588555 | 1.777160 |
| C | 2.767245 | 3.416866 | 1.800950 |
| C | 3.281820 | 2.129255 | 1.837320 |
| C | 2.396745 | 1.061562 | 1.851114 |
| H | 3.424601 | 4.277723 | 1.792810 |
| H | 4.347072 | 1.942524 | 1.856199 |
| H | 2.745418 | 0.039624 | 1.881974 |
| N | 1.070127 | 1.224922 | 1.828130 |
| Ti | -0.382947 | -0.544212 | 1.872799 |
| N | -1.586930 | 1.398057 | 1.813066 |
| C | -0.916351 | 2.565787 | 1.759035 |
| C | -2.923589 | 1.407661 | 1.795006 |
| C | -1.596918 | 3.780069 | 1.673727 |
| C | -3.662103 | 2.578906 | 1.713148 |
| H | -3.403292 | 0.440997 | 1.844172 |
| C | -2.983360 | 3.787265 | 1.647931 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -4.742640 | 2.531227  | 1.699861  |
| H    | -3.522466 | 4.724347  | 1.579769  |
| H    | 0.976011  | 4.584795  | 1.753238  |
| H    | -1.054768 | 4.712533  | 1.623494  |
| Cl   | -2.218579 | -1.848568 | 1.917556  |
| Cl   | 1.269467  | -2.074485 | 1.910994  |
| Cl   | -0.354203 | -0.098316 | 4.150859  |
| Cl   | -0.371976 | -0.219572 | -0.422253 |
| H2   | 1.945570  | 2.439004  | -1.160964 |
| H2   | 1.489086  | 1.852956  | -1.101549 |
| H2   | 1.473036  | 2.023449  | 4.753942  |
| H2   | 1.987450  | 2.220451  | 4.675791  |
| H2   | -2.347613 | 2.864638  | 4.573404  |
| C    | 0.556744  | 2.470326  | 1.781053  |
| C    | 1.391044  | 3.587507  | 1.753453  |
| C    | 2.766262  | 3.415258  | 1.770846  |
| C    | 3.280332  | 2.127636  | 1.815848  |
| C    | 2.394992  | 1.060556  | 1.842291  |
| H    | 3.424159  | 4.275445  | 1.749263  |
| H    | 4.345492  | 1.940043  | 1.630865  |
| H    | 2.743353  | 0.038715  | 1.877939  |
| N    | 1.068132  | 1.224465  | 1.825508  |
| Ti   | -0.381523 | -0.544756 | 1.871698  |
| N    | -1.587982 | 1.397762  | 1.795385  |
| C    | -0.918209 | 2.566588  | 1.764214  |
| C    | -2.924867 | 1.407729  | 1.781352  |
| C    | -1.599302 | 3.782699  | 1.718804  |
| C    | -3.663215 | 2.580816  | 1.736946  |
| H    | -3.403895 | 0.439901  | 1.808200  |
| C    | -2.985273 | 3.790681  | 1.705256  |
| H    | -4.743770 | 2.533082  | 1.727907  |
| H    | -3.524999 | 4.729119  | 1.670168  |
| H    | 0.974872  | 4.583217  | 1.718643  |
| H    | -1.056503 | 4.715728  | 1.694178  |
| C1   | -2.218985 | -1.849076 | 1.898476  |
| C1   | 1.269826  | -2.076576 | 1.938887  |
| C1   | -0.378240 | -0.090543 | 4.145896  |
| C1   | -0.336592 | -0.244643 | -0.427699 |
| H2   | 1.964905  | 2.445385  | -1.190958 |
| H2   | 1.504390  | 1.863680  | -1.123045 |
| H2   | 1.459448  | 2.052353  | 4.731590  |
| H2   | 1.922813  | 2.634494  | 4.769437  |
| H2   | -1.942987 | 2.270247  | 4.689361  |
| H2   | -2.333992 | 2.903814  | 4.716521  |
| H2   | -2.268903 | 2.706622  | -1.238196 |
| H2   | -1.881051 | 2.075629  | -1.157658 |
| C    | 0.563428  | 2.477673  | 1.786406  |
| C    | 1.398203  | 3.594963  | 1.754566  |
| C    | 2.773876  | 3.421458  | 1.782190  |
| C    | 3.287451  | 2.133462  | 1.840557  |
| C    | 2.401151  | 1.066797  | 1.867280  |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| H    | 3.423776 | 4.270721 | 1.663376 |
| H    | 4.344613  | 1.939931 | 1.843064 |
| H    | 2.740591  | 0.041903 | 1.956371 |
| N    | 1.066562  | 1.225643 | 1.851708 |
| Ti   | -0.382264 | -0.545863 | 1.878788 |
| N    | -1.590509 | 1.398747 | 1.825005 |
| C    | -0.920227 | 2.565544 | 1.753787 |
| C    | -2.927226 | 1.408938 | 1.825731 |
| C    | -1.600902 | 3.779950 | 1.670638 |
| C    | -3.666164 | 2.580199 | 1.744214 |
| H    | -3.406204 | 0.442655 | 1.889403 |
| C    | -2.987617 | 3.787731 | 1.661662 |
| H    | -4.746864 | 2.535351 | 1.746212 |
| H    | -3.527411 | 4.724565 | 1.594857 |
| H    | 0.974910  | 4.579292 | 1.630599 |
| H    | -1.058709 | 4.712083 | 1.612737 |
| Cl   | -2.219747 | -1.850947 | 1.886176 |
| Cl   | 1.268563  | -2.080228 | 1.920886 |
| Cl   | -0.374695 | -0.116647 | 4.160828 |
| Cl   | -0.335798 | -0.189779 | -0.408618 |
| H2   | -2.014235 | 2.221341 | 4.722184 |
| H2   | -2.381988 | 2.865598 | 4.654593 |
| H2   | 1.476906  | 2.033819 | 4.705844 |
| H2   | 1.945054  | 2.612652 | 4.682999 |
| C    | 0.563106  | 2.477592 | 1.786944 |
| C    | 1.398155  | 3.594866 | 1.756850 |
| C    | 2.774036  | 3.421275 | 1.783463 |
| C    | 3.287388  | 2.133115 | 1.840303 |
| C    | 2.400536  | 1.066789 | 1.866472 |
| H    | 3.432763  | 4.280894 | 1.759954 |
| H    | 4.352513  | 1.945469 | 1.863801 |
| H    | 2.746826  | 0.044268 | 1.909313 |
| N    | 1.074161  | 1.232132 | 1.839923 |
| Ti   | -0.378089 | -0.536528 | 1.874458 |
| N    | -1.583925 | 1.406807 | 1.786787 |
| C    | -0.912753 | 2.574815 | 1.763092 |
| C    | -2.920547 | 1.416666 | 1.765837 |
| C    | -1.592845 | 3.792175 | 1.720363 |
| C    | -3.658884 | 2.590287 | 1.722037 |
| H    | -3.399151 | 0.448182 | 1.786320 |
| C    | -2.979752 | 3.800438 | 1.700219 |
| H    | -4.739540 | 2.543345 | 1.707239 |
| H    | -3.518789 | 4.739490 | 1.668221 |
| H    | 0.983306  | 4.590892 | 1.711614 |
| H    | -1.050059 | 4.725613 | 1.704725 |
| Cl   | -2.214996 | -1.840756 | 1.887528 |
| Cl   | 1.270649  | -2.069332 | 1.955423 |
| Cl   | -0.391990 | -0.052246 | 4.140526 |
| Cl   | -0.311259 | -0.208690 | -0.418702 |

PHEN

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | 0.519718  | 2.422866 | 1.769377 |
|         |  x     |  y     |  z     |
|---------|--------|--------|--------|
|        C | 1.293599 | 3.602775 | 1.728187 |
|        C | 2.694368 | 3.460287 | 1.722615 |
|        C | 3.244248 | 2.200116 | 1.757286 |
|        H | 2.398318 | 1.082309 | 1.796643 |
|        H | 3.242065 | 4.341899 | 1.691515 |
|        H | 4.315966 | 2.051622 | 1.754341 |
|        H | 2.794602 | 0.076659 | 1.824956 |
|        N | 1.078054 | 1.189804 | 1.803239 |
|        Ti | -0.383340 | -0.574596 | 1.872753 |
|        N | -1.615999 | 1.356022 | 1.818421 |
|        C | -0.910724 | 2.511251 | 1.777679 |
|        C | -2.939560 | 1.412388 | 1.826518 |
|        C | -1.533901 | 3.777344 | 1.743816 |
|        H | -3.641633 | 2.625799 | 1.795342 |
|        H | -3.456555 | 0.463309 | 1.859411 |
|        C | -2.941415 | 3.807772 | 1.754058 |
|        H | -4.723439 | 2.610187 | 1.804197 |
|        H | -3.457652 | 4.761496 | 1.729418 |
|        C | 0.632903 | 4.872316 | 1.694642 |
|        C | -0.722386 | 4.966065 | 1.702497 |
|        H2 | -2.224337 | -1.868201 | 1.931450 |
|        Cl | 1.283334 | -2.086923 | 1.910395 |
|        Cl | -0.337654 | -0.083030 | 4.140120 |
|        Cl | -0.374234 | -0.241478 | -0.421675 |
|        N | 1.078054 | 1.189804 | 1.803239 |
|        Ti | -0.383340 | -0.574596 | 1.872753 |
|        N | -1.615999 | 1.356022 | 1.818421 |
|        C | -0.910724 | 2.511251 | 1.777679 |
|        C | -2.939560 | 1.412388 | 1.826518 |
|        C | -1.533901 | 3.777344 | 1.743816 |
|        H | -3.641633 | 2.625799 | 1.795342 |
|        H | -3.456555 | 0.463309 | 1.859411 |
|        C | -2.941415 | 3.807772 | 1.754058 |
|        H | -4.723439 | 2.610187 | 1.804197 |
|        H | -3.457652 | 4.761496 | 1.729418 |
|        C | 0.632903 | 4.872316 | 1.694642 |
|        C | -0.722386 | 4.966065 | 1.702497 |
|        Cl | -2.224337 | -1.868201 | 1.931450 |
|        Cl | 1.283334 | -2.086923 | 1.910395 |
|        Cl | -0.337654 | -0.083030 | 4.140120 |
|        Cl | -0.374234 | -0.241478 | -0.421675 |
|        N | 1.078054 | 1.189804 | 1.803239 |
|        Ti | -0.383340 | -0.574596 | 1.872753 |
|        N | -1.615999 | 1.356022 | 1.818421 |
|        C | -0.910724 | 2.511251 | 1.777679 |
|        C | -2.939560 | 1.412388 | 1.826518 |
|        C | -1.533901 | 3.777344 | 1.743816 |
|        H | -3.641633 | 2.625799 | 1.795342 |
|        H | -3.456555 | 0.463309 | 1.859411 |
|        C | -2.941415 | 3.807772 | 1.754058 |
|        H | -4.723439 | 2.610187 | 1.804197 |
|        H | -3.457652 | 4.761496 | 1.729418 |
|        C | 0.632903 | 4.872316 | 1.694642 |
|        C | -0.722386 | 4.966065 | 1.702497 |
|        Cl | -2.224337 | -1.868201 | 1.931450 |
|        Cl | 1.283334 | -2.086923 | 1.910395 |
|        Cl | -0.337654 | -0.083030 | 4.140120 |
|        Cl | -0.374234 | -0.241478 | -0.421675 |
| Atoms | X-Coordinates | Y-Coordinates | Z-Coordinates |
|-------|---------------|---------------|---------------|
| Cl    | -0.350422     | -0.060055     | 4.124290      |
| Cl    | -0.354278     | -0.280347     | -0.438250     |
| H2    | 1.872482      | 2.464128      | -1.262012     |
| H2    | 1.427105      | 1.879901      | -1.136930     |
| H2    | -0.120825     | 2.840969      | 4.661773      |
| H2    | -0.063077     | 3.583730      | 4.641226      |
| H     | 1.262110      | 5.772118      | 1.756457      |
| H     | -1.191889     | 5.929818      | 1.756094      |
| H2    | -2.079882     | 2.820212      | -1.162206     |
| H2    | -1.757139     | 2.150969      | -1.107186     |
| C     | 0.506121      | 2.424193      | 1.773220      |
| C     | 1.275933      | 3.607773      | 1.755495      |
| C     | 2.337311      | 3.470369      | 1.781641      |
| C     | 3.231057      | 2.212346      | 1.825256      |
| C     | 2.385842      | 1.091074      | 1.843374      |
| H     | 3.303797      | 4.354855      | 1.770212      |
| H     | 4.303068      | 2.067599      | 1.847797      |
| H     | 2.788072      | 0.086914      | 1.879910      |
| N     | 1.668296      | 1.193106      | 1.818383      |
| Ti    | -0.387883     | -0.577224     | 1.863153      |
| N     | -1.627163     | 1.350008      | 1.785748      |
| C     | -0.925086     | 2.507557      | 1.756325      |
| C     | -2.950595     | 1.402269      | 1.780279      |
| C     | -1.551800     | 3.772334      | 1.723124      |
| C     | -3.656494     | 2.613708      | 1.745758      |
| H     | -3.464821     | 0.451327      | 1.805514      |
| C     | -2.959808     | 3.798997      | 1.717631      |
| H     | -4.738271     | 2.594186      | 1.743669      |
| H     | -3.478443     | 4.750509      | 1.693751      |
| C     | 0.611441      | 4.876022      | 1.722120      |
| C     | -0.743927     | 4.954962      | 1.706404      |
| Cl    | -2.225025     | -1.878748     | 1.897656      |
| Cl    | 1.284545      | -2.082729     | 1.942100      |
| Cl    | -0.387545     | -0.080315     | 4.133235      |
| Cl    | -0.340434     | -0.249863     | -0.427417     |
| H2    | -0.247942     | 2.821307      | 4.679646      |
| H2    | -0.196242     | 3.564726      | 4.699808      |
| H     | 1.215122      | 5.775756      | 1.710716      |
| H     | -1.238892     | 5.918620      | 1.683144      |
| C     | 0.519218      | 2.435537      | 1.780432      |
| C     | 1.292499      | 3.616470      | 1.748281      |
| C     | 2.693064      | 3.474978      | 1.762181      |
| C     | 3.243308      | 2.215964      | 1.805728      |
| C     | 2.398010      | 1.097413      | 1.835838      |
| H     | 3.322152      | 4.357403      | 1.738901      |
| H     | 4.314858      | 2.067979      | 1.817464      |
| H     | 2.796586      | 0.092653      | 1.870250      |
| N     | 1.077697      | 1.202594      | 1.824042      |
| Ti    | -0.383104     | -0.565784     | 1.872675      |
| N     | -1.615962     | 1.366949      | 1.799364      |
| C     | -0.911144     | 2.522963      | 1.767585      |
| C     | -2.939292     | 1.423498      | 1.788969      |
Structure descriptions

\begin{align*}
\text{C} & \ -1.534378 \ 3.788979 \ 1.723154 \\
\text{C} & \ -3.641487 \ 2.636521 \ 1.746180 \\
\text{H} & \ -3.456833 \ 0.474669 \ 1.815649 \\
\text{C} & \ -2.941753 \ 3.819253 \ 1.713028 \\
\text{H} & \ -4.723115 \ 2.619733 \ 1.739855 \\
\text{H} & \ -3.457913 \ 4.771864 \ 1.679580 \\
\text{C} & \ 0.631720 \ 4.886322 \ 1.703711 \\
\text{C} & \ -0.723400 \ 4.969087 \ 1.691752 \\
\text{Cl} & \ -2.224460 \ -1.859814 \ 1.898263 \\
\text{Cl} & \ 1.286706 \ -2.073178 \ 1.939645 \\
\text{Cl} & \ -0.379403 \ -0.098211 \ 4.145607 \\
\text{Cl} & \ -0.339500 \ -0.252306 \ -0.426436 \\
\text{H} & \ 1.831221 \ 2.533443 \ -1.187453 \\
\text{H} & \ 1.395938 \ 1.933674 \ -1.110135 \\
\text{H} & \ 1.374400 \ 2.109356 \ 4.698250 \\
\text{H} & \ 1.793188 \ 2.722324 \ 4.761549 \\
\text{H} & \ -1.823575 \ 2.324238 \ 4.677200 \\
\text{H} & \ -2.169278 \ 2.982648 \ 4.723865 \\
\text{H} & \ -2.150054 \ 2.764272 \ -1.225720 \\
\text{H} & \ -1.804704 \ 2.111703 \ -1.125294 \\
\text{H} & \ -1.215977 \ 5.933716 \ 1.657720 \\
\text{H} & \ 1.238394 \ 5.783869 \ 1.679671 \\
\text{C} & \ 0.522005 \ 2.424422 \ 1.776937 \\
\text{C} & \ 1.295782 \ 3.605511 \ 1.742706 \\
\text{C} & \ 2.696875 \ 3.462713 \ 1.750844 \\
\text{C} & \ 3.246381 \ 2.202676 \ 1.791020 \\
\text{C} & \ 2.400387 \ 1.084427 \ 1.823082 \\
\text{H} & \ 3.326828 \ 4.344422 \ 1.725475 \\
\text{H} & \ 4.317974 \ 2.053969 \ 1.797995 \\
\text{H} & \ 2.796195 \ 0.078563 \ 1.854806 \\
\text{N} & \ 1.080174 \ 1.191457 \ 1.816693 \\
\text{Ti} & \ -0.382327 \ -0.574611 \ 1.872499 \\
\text{N} & \ -1.615839 \ 1.358248 \ 1.804854 \\
\text{C} & \ -0.909691 \ 2.513148 \ 1.770919 \\
\text{C} & \ -2.939140 \ 1.415193 \ 1.799913 \\
\text{C} & \ -1.531627 \ 3.780417 \ 1.730462 \\
\text{C} & \ -3.640431 \ 2.629212 \ 1.761014 \\
\text{H} & \ -3.456471 \ 0.465947 \ 1.828059 \\
\text{C} & \ -2.939687 \ 3.811856 \ 1.725968 \\
\text{H} & \ -4.722188 \ 2.613058 \ 1.759224 \\
\text{H} & \ -3.454948 \ 4.765017 \ 1.695524 \\
\text{C} & \ 0.635556 \ 4.876237 \ 1.702392 \\
\text{C} & \ -0.719438 \ 4.960129 \ 1.696318 \\
\text{Cl} & \ -2.222804 \ -1.868798 \ 1.911640 \\
\text{Cl} & \ 1.283834 \ -2.086007 \ 1.929066 \\
\text{Cl} & \ -0.382571 \ -0.084432 \ 4.137323 \\
\text{Cl} & \ -0.350880 \ -0.239502 \ -0.420287 \\
\text{H} & \ 1.242568 \ 5.773495 \ 1.676627 \\
\text{H} & \ -1.211066 \ 5.925317 \ 1.664717 \\
\end{align*}

\[ \text{VCl}_5 - \text{H}_2 \]
Structure descriptions

SP-JLMC

BBH

C1  3.371639  7.723136  -2.430966
C  1.770946  1.500203  -0.034423
C  1.056209  0.516817  0.662295
C -0.318439  0.391724  0.492663
C -0.991205  1.252118  -0.370746
C -0.285510  2.238814  -1.063028
C  1.084841  2.367490  -0.899513
C  3.211695  1.606135  0.169328
H  1.579436 -0.152815  1.336689
H -0.862109 -0.373365  1.033737
H -2.062821  1.158472  -0.503298
H -0.810095  2.912076  -1.730282
N  3.933723  2.422946  -0.498462
C  6.129007  3.295722  -0.784067
N  5.262607  2.438908  -0.196487
H  3.650043  0.952759  0.935145
H  5.623068  1.797474  0.503713
O  5.784256  4.214040  -1.542367
C  10.300638  2.798248  0.019653
C  9.784395  4.037565  -0.352504
C  8.428161  4.179346  -0.617004
C  7.572293  3.079859  -0.490736
C  8.097975  1.831421  -0.132235
C  9.457099  1.693568  0.122079
H 11.360273  2.688870  0.217848
H 10.439748  4.895212  -0.442298
H  8.015634  5.133115  -0.916504
H  7.465368  0.952196  -0.092007
H  9.859809  0.723331  0.386078
H  1.638002  3.132506  -1.427778
V  4.550080  5.953815  -1.972634
Cl  6.110300  7.051907  -0.720561
Cl  3.260437  4.521257  -3.126629
Cl  3.465098  5.466828  -0.059934
Cl  5.936646  6.118215  -3.734866
H2  5.183209  2.217740  -3.318882
H2  5.547365  1.578796  -3.437106

Cl  3.311086  7.702961  -2.450050
C  1.757183  1.480224  -0.083872
C  1.044083  0.465357  0.567963
C -0.333212  0.357724  0.409223
C -1.010440  1.267322  -0.398360
C -0.306457  2.285215  -1.045896
C  1.066746  2.396938  -0.893622
C  3.200572  1.565905  0.110103
H  1.571049 -0.242175  1.199415
H -0.875568 -0.431615  0.915677
H -2.084058  1.187652  -0.521813
H -0.834947  2.996235  -1.669472
N  3.921492  2.410624  -0.522691
C  6.111418  3.303052  -0.766497
Structure descriptions

N  5.252147  2.407266  -0.231137
H  3.541774  0.872666  0.838089
H  5.614188  1.744050  0.838089
O  5.763304  4.253527  -1.482111
C  9.739592  4.090260  -0.214406
C  8.387159  2.199162  -0.502350
C  7.553639  3.097269  -0.462094
C  8.096925  1.841032  -0.164526
H  9.452994  1.715810  0.113058
H 11.331105  2.742578  0.313367
H 10.378197  4.964754  -0.237299
H  7.959527  5.181533  -0.751883
H  7.481408  0.949152  -0.189823
H  9.870443  0.740026  0.329478
H  1.618339  3.185069  -1.389635
V  4.511652  5.958418  -1.955371
Cl  6.012095  7.091236  -0.663544
Cl  3.282581  4.499716  -3.141352
Cl  3.373696  5.455477  -0.074115
Cl  5.940150  6.148459  -3.680910
H2  5.257722  2.262942  -3.337922
H2  5.666648  1.647493  -3.431684
H2  5.672902  5.031673  1.730452
H2  6.169980  4.681737  2.169046
Cl  3.173264  7.449266  -2.865261
C  1.798278  1.510621  0.138474
C  1.107696  0.498871  0.819160
C -0.266402  0.355194  0.661748
C -0.963148  1.226133  -0.171775
C -0.282227  2.242620  -0.845208
C  1.087688  2.389339  -0.694821
C  3.239396  1.635112  0.327238
H  1.650301  -0.177987  1.470602
H -0.791235  -0.432236  1.189172
H -2.034491  1.118456  -0.293972
H -0.824124  2.926841  -1.486599
N  3.942645  2.456112  -0.354848
C  6.112265  3.723566  -0.669641
N  5.272311  2.503542  -0.063623
H  3.695127  0.993262  1.092766
H  5.646712  1.907284  0.668672
O  5.747042  4.249067  -1.465939
C  10.276765  3.096004  0.255726
C  9.708665  4.304861  -0.141594
C  8.356177  4.374362  -0.449137
C  7.556176  3.231977  -0.340853
C  8.133114  2.014982  0.043522
C  9.489461  1.949432  0.339867
H 11.333724  3.043597  0.482257
H 10.321259  5.194904  -0.216486
H  7.902422  5.303977  -0.766132
H  7.543126  1.106151  0.071977
Structure descriptions

SP-JLMC

H  9.933683  1.003219  0.623667
H  1.617653  3.180375 -1.207824
V  4.436750  5.828860 -2.154308
Cl  5.879237  7.163497 -0.996144
Cl  3.279485  4.189222 -3.164360
Cl  3.291537  5.517163 -0.235978
Cl  5.876996  5.868709 -3.880863
H2  5.290650  2.017638 -3.104942
H2  5.750416  1.429391 -3.152659
H2  5.610787  5.348151  1.580239
H2  6.117970  5.047721  2.035570
H2  0.755192  5.454018 -2.164135
H2  0.026020  5.512286 -2.026001
Cl  3.181546  7.444189 -2.875974
C  1.795571  1.501372  0.136617
C  1.111302  0.461421  0.780128
C -0.263869  0.322900  0.627197
C -0.967743  1.226730  0.164349
C -0.293077  2.71453  -0.799689
C  1.077889  2.413235  0.653677
C  3.238825  1.618278  0.316918
H  1.659234 -0.241744  1.398395
H -0.784283 -0.486350  1.125156
H -2.039816  1.22248  -0.282774
H -0.840074  2.981248  1.408137
N  3.937461  2.457022 -0.348296
C  6.108334  3.69148  -0.666320
N  5.269725  2.495282 -0.066857
H  3.699826  0.953287  1.058744
H  5.649600  1.882663  0.648874
O  5.741440  4.257448  1.448970
C 10.274781  3.080969  0.245211
C  9.704673  4.295457 -0.130846
C  8.351974  4.368008  0.435939
C  7.553683  3.223393 -0.344796
C  8.131974  2.000883  0.196657
C  9.488888  1.932049  0.312127
H 11.332150  3.026029  0.475270
H 10.314759  5.188284  0.189783
H  7.897221  5.302328 -0.736337
H  7.542700  1.091204  0.035296
H  9.934647  0.981897  0.579944
H  1.603419  3.226279 -1.135413
V  4.442772  5.827108  2.153096
Cl  5.884851  7.175413 -1.005477
Cl  3.283016  4.184759 -3.158946
Cl  3.293752  5.532661 -0.233182
Cl  5.885297  5.853955 -3.876949
H2  5.229360  1.965566  3.057557
H2  5.709435  1.398614 -3.110664
H2  5.572394  5.292858  1.575009
H2  6.126056  5.040467  2.004358
H2  0.761799  5.442676 -2.197981

S52
|    |    |    |    |    |    |
|----|----|----|----|----|----|
| N  | 3.999338 | 1.675991 | -1.496119 |
| C  | 7.966314  | 1.425538  | -2.843624 |
| C  | 7.485821  | 2.651791  | -2.384713 |
| C  | 6.177617  | 2.769935  | -1.933164 |
| C  | 5.330393  | 1.652982  | -1.944667 |
| C  | 5.824794  | 0.417826  | -2.379220 |
| C  | 7.132733  | 0.309465  | -2.834445 |
| H  | 8.989375  | 1.338865  | -3.189368 |
| H  | 8.138620  | 3.516459  | -2.364695 |
| H  | 5.829962  | 3.718263  | -1.542611 |
| H  | 5.171740  | -0.445261 | -2.346622 |
| H  | 7.504127  | -0.650283 | -3.172643 |
| H  | 3.632174  | 3.711655  | -1.746990 |
| O  | 2.160874  | 0.315883  | -0.452141 |
| V  | 2.712082  | -1.383588 | 1.082556  |
| Cl | 3.476638  | -2.291466 | -0.835125 |
| Cl | 1.830358  | 0.017988  | 2.582275  |
| H  | 3.052717  | 0.608984  | -0.904658 |
| Cl | 0.660000  | -2.134495 | 0.571856  |
| Cl | 4.651309  | -0.241134 | 1.229509  |
| H2 | 3.824029  | 2.535884  | 1.792640  |
| H2 | 3.578275  | 3.230880  | 1.891291  |
| Cl | 3.235415  | -2.998818 | 2.415881  |
| C  | 1.933547  | 2.671902  | -0.878455 |
| C  | 1.123233  | 3.815493  | -0.845290 |
| C  | -0.154461 | 3.768546  | -0.311219 |
| C  | -0.642911 | 2.561199  | 0.192290  |
| C  | 0.132748  | 1.408691  | 0.169443  |
| C  | 1.419604  | 1.458493  | -0.356813 |
| C  | 3.270573  | 2.735329  | -1.434397 |
| H  | 1.513774  | 4.744856  | -1.245363 |
| H  | -0.769522 | 4.659073  | -0.287651 |
| H  | -1.642843 | 2.514912  | 0.606691  |
| H  | -0.242262 | 0.472139  | 0.553416  |
| N  | 4.004868  | 1.682243  | -1.487958 |
| C  | 7.967107  | 1.431466  | -2.846636 |
| C  | 7.483412  | 2.660371  | -2.398679 |
| C  | 6.175971  | 2.777774  | -1.944323 |
| C  | 5.333970  | 1.657153  | -1.942032 |
| C  | 5.831270  | 0.419339  | -2.364948 |
| C  | 7.138046  | 0.312102  | -2.823557 |
| H  | 8.989484  | 1.345254  | -3.194363 |
| H  | 8.132971  | 3.527618  | -2.389024 |
| H  | 5.824797  | 3.727838  | -1.561013 |
| H  | 5.181760  | -0.445907 | -2.322083 |
| H  | 7.512242  | -0.649467 | -3.153313 |
| H  | 3.616166  | 3.704022  | -1.804352 |
| O  | 2.191226  | 0.335048  | -0.413276 |
| V  | 2.714301  | -1.380290 | 1.085080  |
| Cl | 3.478282  | -2.278161 | -0.832633 |
| Cl | 1.840173  | 0.003601  | 2.606766  |
| H  | 3.085524  | 0.633831  | -0.873857 |
| Cl | 0.657914  | -2.110975 | 0.558274  |
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| Cl   | 4.665964 | -0.258376 | 1.251919 |
| H2   | 3.746990 | 2.465477 | 1.833911 |
| H2   | 3.484101 | 3.160131 | 1.833911 |
| H2   | 0.782344 | -0.811632 | -3.068753 |
| H2   | 1.128506 | -0.741612 | -2.413447 |
| Cl   | 3.195567 | -3.003318 | 2.413072 |
| C    | 1.929045 | 2.670293 | -0.870357 |
| C    | 1.110198 | 3.808152 | -0.841295 |
| C    | -0.178436 | 3.747557 | -0.335597 |
| C    | -0.669981 | 2.531363 | 0.142445 |
| C    | 0.113962 | 1.384284 | 0.123605 |
| C    | 1.412234 | 1.447831 | -0.372958 |
| C    | 3.273743 | 2.749538 | -1.406215 |
| H    | 1.503315 | 4.744265 | -1.222687 |
| H    | -0.799217 | 4.634078 | -0.315700 |
| H    | -1.678398 | 2.473569 | 0.534148 |
| H    | -0.263633 | 0.441144 | 0.488354 |
| N    | 4.018558 | 1.703929 | -1.461649 |
| C    | 7.979162 | 1.501838 | -2.835022 |
| C    | 7.478045 | 2.727847 | -2.398596 |
| C    | 6.172215 | 2.829757 | -1.937635 |
| C    | 5.348336 | 1.696090 | -1.916353 |
| C    | 5.863914 | 0.461893 | -2.372433 |
| C    | 7.169075 | 0.369888 | -2.793232 |
| H    | 9.000663 | 1.428088 | -3.188385 |
| H    | 8.113436 | 3.605568 | -2.403244 |
| H    | 5.809269 | 3.779168 | -1.564219 |
| H    | 5.228992 | -0.413231 | -2.270031 |
| H    | 7.569687 | -0.589545 | -3.112951 |
| H    | 3.612709 | 3.724523 | -1.765232 |
| O    | 2.193848 | 0.330467 | -0.420696 |
| V    | 2.690878 | -1.382678 | 1.077609 |
| Cl   | 3.531768 | -2.259476 | -0.823761 |
| Cl   | 1.755449 | -0.025280 | 2.586274 |
| H    | 3.090822 | 0.636548 | -0.862323 |
| Cl   | 0.663115 | -2.139610 | 0.484366 |
| Cl   | 4.623012 | -0.234210 | 1.315928 |
| H2   | 3.646171 | 2.463731 | 1.911045 |
| H2   | 3.395725 | 3.164592 | 1.919763 |
| H2   | 7.882130 | 1.192518 | 0.343573 |
| H2   | 7.224883 | 0.875680 | 0.487938 |
| Cl   | 3.168629 | -3.071711 | 2.337982 |
| C    | 1.875585 | 2.645703 | -0.966959 |
| C    | 1.001507 | 3.738395 | -1.052104 |
| C    | -0.263921 | 3.684213 | -0.490614 |
| C    | -0.673106 | 2.519643 | 0.161710 |
| C    | 0.166320 | 1.416509 | 0.260041 |
| C    | 1.440465 | 1.472504 | -0.297364 |
| C    | 3.200715 | 2.720623 | -1.545274 |
| H    | 1.333875 | 4.634597 | -1.564164 |
| H    | -0.929384 | 4.535160 | -0.559658 |
| H    | -1.662148 | 2.467249 | 0.600824 |
|  | x   | y   | z   |
|---|------|------|------|
| H | -0.154156 | 0.516610 | 0.760221 |
| N | 4.004598 | 1.720253 | -1.464623 |
| C | 7.962912 | 1.528981 | -2.843088 |
| C | 7.395527 | 2.777176 | -2.588050 |
| C | 6.086799 | 2.874931 | -2.134582 |
| C | 5.328584 | 1.713381 | -1.936164 |
| C | 5.908472 | 0.461625 | -1.68524 |
| C | 7.216162 | 0.373508 | -2.628094 |
| H | 8.986534 | 1.459548 | -3.190850 |
| H | 7.981125 | 3.677839 | -2.729061 |
| H | 5.673067 | 3.848163 | -1.901747 |
| H | 5.322648 | -0.428926 | -1.980445 |
| H | 7.655209 | -0.600225 | -2.807677 |
| H | 3.479168 | 3.649081 | -0.049170 |
| O | 2.288057 | 0.409270 | -0.246086 |
| V | 2.702471 | -1.364555 | 1.093464 |
| Cl | 3.472472 | -2.217086 | -0.860842 |
| Cl | 1.859703 | -0.067296 | 2.706518 |
| H | 3.177187 | 0.725533 | -0.741080 |
| Cl | 0.639530 | -2.031603 | 0.504065 |
| Cl | 4.703471 | -0.332263 | 1.344660 |
| H2 | 3.713605 | 2.397069 | 1.764667 |
| H2 | 3.370104 | 3.055307 | 1.713842 |
| H2 | 7.730199 | 1.671154 | 0.453077 |
| H2 | 7.117152 | 1.259862 | 0.544600 |
| H2 | 1.427591 | -0.057898 | -3.274623 |
| H2 | 1.685082 | -0.419511 | -2.677087 |
| Cl | 3.193962 | -2.994595 | 2.423572 |
| C | 1.942721 | 2.677976 | -0.833754 |
| C | 1.130645 | 3.820452 | -0.778346 |
| C | -0.164438 | 3.753150 | -0.290924 |
| C | -0.670597 | 2.525893 | 0.142032 |
| C | 0.105962 | 1.374841 | 0.096370 |
| C | 1.410798 | 1.44018 | -0.382719 |
| C | 3.289653 | 2.763023 | -1.364613 |
| H | 1.534641 | 4.765338 | -1.125176 |
| H | -0.779107 | 4.643224 | -0.250253 |
| H | -1.683956 | 2.463037 | 0.519876 |
| H | -0.281332 | 0.423169 | 0.427719 |
| N | 4.025380 | 1.713356 | -1.45953 |
| C | 7.984088 | 1.489591 | -2.833501 |
| C | 7.476017 | 2.728361 | -2.442620 |
| C | 6.171205 | 2.839748 | -1.981966 |
| C | 5.353668 | 1.702997 | -1.914387 |
| C | 5.875231 | 0.458407 | -2.284922 |
| C | 7.180385 | 0.355889 | -2.748994 |
| H | 9.005123 | 1.409022 | 3.186801 |
| H | 8.105379 | 3.609460 | -2.484316 |
| H | 5.805258 | 3.802438 | -1.647878 |
| H | 5.245000 | -0.417504 | -2.196473 |
| H | 7.572415 | -0.612608 | -3.034542 |
| H | 3.633910 | 3.747279 | -1.691879 |
| O | 2.181023 | 0.320063 | -0.456240 |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| V    | 2.690558 | -1.387810 | 1.071159 |
| Cl   | 3.518776  | -2.280053  | 0.826821  |
| Cl   | 1.755879  | -0.008016  | 2.562230  |
| H    | 3.080388  | 0.628432   | -0.885076 |
| Cl   | 0.658610  | -2.146116  | 0.491993  |
| Cl   | 4.617832  | -0.237001  | 1.289731  |
| H2   | 7.180824  | 1.019389   | 0.525265  |
| H2   | 7.817796  | 1.384706   | 0.406820  |
| Cl   | 0.743542  | -2.860553  | 1.250495  |
| C    | 2.874600  | 1.900835   | -3.00528  |
| C    | 2.575589  | 2.582774   | -4.188294 |
| C    | 1.669070  | 2.064429   | -5.098821 |
| C    | 1.052710  | 0.841121   | -4.829007 |
| C    | 1.329932  | 0.136657   | -3.663636 |
| C    | 2.235002  | 0.660023   | -2.744824 |
| C    | 3.812777  | 2.460618   | -2.050530 |
| H    | 3.065125  | 3.530604   | -4.383963 |
| H    | 1.443383  | 2.601192   | -6.011327 |
| H    | 0.345016  | 0.426687   | -5.536951 |
| N    | 0.856050  | -0.810301  | -3.460140 |
| C    | 6.601196  | 3.130440   | 2.139804  |
| C    | 6.055245  | 4.076827   | 1.273058  |
| C    | 5.221812  | 3.681354   | 0.235295  |
| C    | 4.930467  | 2.322852   | 0.053501  |
| C    | 5.459065  | 1.378204   | 0.939718  |
| C    | 6.296934  | 1.782126   | 1.971146  |
| H    | 7.245756  | 3.446369   | 2.951158  |
| H    | 6.268285  | 5.129519   | 1.418079  |
| H    | 4.772535  | 4.430547   | -0.404569 |
| H    | 5.200262  | 0.335479   | 0.807844  |
| H    | 6.703401  | 1.042772   | 2.650345  |
| H    | 4.274495  | 3.418158   | -2.302353 |
| O    | 2.554997  | -0.005092  | -1.601699 |
| V    | 1.600035  | -1.472748  | -0.171098 |
| Cl   | 3.774958  | -2.001094  | 0.188882  |
| Cl   | 0.320988  | -0.564796  | -0.864190 |
| H    | 3.257354  | 0.615350   | -1.094414 |
| Cl   | 1.610383  | -2.875772  | -1.925945 |
| Cl   | 1.852469  | 0.240372   | 1.289800  |
| H2   | 0.864494  | 2.402160   | -0.429523 |
| H2   | 0.738919  | 2.881869   | -0.984469 |
| H2   | 3.392057  | 3.222542   | 2.934796  |
| H2   | 3.165223  | 2.612118   | 2.675223  |
| H2   | 5.031189  | -0.913734  | -3.308187 |
| H2   | 4.766994  | -1.035193  | -2.605448 |
| H2   | 7.966678  | 2.081397   | -1.702822 |
| H2   | 7.507531  | 2.158340   | -1.121981 |

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| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| Cl   | 3.468885  | -1.915319  | -1.411860  |
| C    | 1.847355  | 2.143351  | 0.985612  |
|   |   |   |   |
|---|---|---|---|
| C | 1.305018 | 3.234246 | 1.657624 |
| C | -0.076137 | 3.372948 | 1.704623 |
| C | -0.867477 | 2.417567 | 1.079407 |
| C | -0.257659 | 1.356485 | 0.419778 |
| N | 1.070053 | 1.224639 | 0.371673 |
| C | 3.274351 | 1.910402 | 0.908788 |
| H | 1.961936 | 3.950107 | 2.134494 |
| H | -0.526494 | 4.210199 | 2.223553 |
| H | -1.947155 | 2.481781 | 1.093073 |
| H | -0.828619 | 0.589653 | -0.083485 |
| N | 3.702408 | 0.865888 | 0.308094 |
| C | 7.857415 | 0.370390 | -0.122621 |
| C | 7.242968 | 1.542874 | -0.554269 |
| C | 5.868844 | 1.700394 | -0.417457 |
| C | 5.109714 | 0.678055 | 0.159119 |
| C | 5.715178 | -0.508986 | 0.571610 |
| C | 7.090446 | -0.650037 | 0.376053 |
| H | 8.923057 | 0.246310 | -0.233234 |
| H | 7.828393 | 2.330554 | -1.012765 |
| H | 5.369425 | 2.583656 | -0.792989 |
| H | 5.110237 | -1.290249 | 1.007055 |
| H | 7.563859 | -1.565689 | 0.770200 |
| V | 3.960389 | 2.615040 | 1.370465 |
| V | 2.086221 | -0.441598 | -0.627980 |
| Cl | 0.389946 | -1.905021 | 0.007160 |
| Cl | 2.942196 | 1.216393 | -2.179755 |
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| Cl | 2.578761 | -1.093853 | 1.706294 |

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C  1.869988   2.139182   0.993955
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C  -0.042101  3.401632   1.684560
C  -0.838676   2.459190   1.049012
C  -0.237561   1.384278   0.404897
N  1.087864   1.228632   0.374873
C  3.294030   1.896970   0.917534
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H  -0.485413   4.248212   2.193987
H  -1.917251   2.541545   1.043649
H  -0.815690   0.625612  -0.102096
N  3.719122   0.856729   0.306301
C  7.873342   0.393315  -0.165851
C  7.254356   1.585704  -0.530741
C  5.881127   1.730757  -0.381290
C  5.125648   0.677690   0.143626
C  5.737085  -0.526469   0.491364
C  7.111432  -0.657154   0.342382
H  8.943650   0.277883  -0.281616
H  7.835051   2.397201  -0.951950
H  5.379362   2.630533  -0.712231
H  5.139081  -1.330719   0.892048
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| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| V    | 2.094119 | -0.445123 | -0.621961 |
| Cl   | 0.967475  | 1.194870  | -2.188182 |
| Cl   | 2.967475  | 1.194870  | -2.188182 |
| Cl   | 0.497900  | -0.279177 | -2.328360 |
| Cl   | 2.639284  | -1.130392 | 1.699360 |
| H2   | 1.022704  | 3.285323  | -1.755391 |
| H2   | 0.625608  | 3.849927  | -1.474370 |
| H2   | 0.263838  | 0.796922  | 3.560289 |
| H2   | 0.687072  | 0.294257  | 3.208542 |
| H2   | 3.444040  | 0.577247  | 3.302161 |
| H2   | 4.799936  | 1.065372  | 3.634386 |
| Cl   | 3.473797  | -1.913397 | -1.409534 |
| C    | 1.341831  | 3.247341  | 1.646388 |
| C    | -0.038493 | 3.381856  | 1.716601 |
| C    | -0.836728 | 2.420789  | 1.110092 |
| C    | -0.235034 | 1.358677  | 0.445208 |
| N    | 1.091863  | 1.229609  | 0.376524 |
| C    | 3.301327  | 1.917607  | 0.883092 |
| H    | 2.004646  | 3.968352  | 2.106914 |
| H    | -0.482499 | 4.221644  | 2.236817 |
| H    | -1.916183 | 2.482085  | 1.140013 |
| H    | -0.812732 | 0.590245  | -0.047233 |
| N    | 3.719996  | 0.865651  | 0.288882 |
| C    | 7.871521  | 0.346281  | -0.149910 |
| C    | 7.260217  | 1.514487  | -0.597549 |
| C    | 5.887130  | 1.679493  | -0.459079 |
| C    | 5.126096  | 0.669228  | 0.135575 |
| C    | 5.728209  | -0.513316 | 0.565463 |
| C    | 7.102413  | -0.662235 | 0.428594 |
| H    | 8.941408  | 0.216476  | -0.261307 |
| H    | 7.847080  | 2.292562  | -1.070377 |
| H    | 5.390008  | 2.559026  | -0.846303 |
| H    | 5.121651  | -1.284913 | 1.015717 |
| H    | 7.573661  | -1.573811 | 0.775124 |
| H    | 3.994130  | 2.623105  | 1.333013 |
| V    | 2.092123  | -0.440028 | -0.624506 |
| Cl   | 0.411306  | -1.916915 | 0.012028 |
| Cl   | 2.958832  | 1.200343  | -2.202592 |
| Cl   | 0.470035  | -0.240075 | -2.308705 |
| Cl   | 2.588943  | -1.075828 | 1.714682 |
| H2   | 0.953181  | 3.232674  | -1.771090 |
| H2   | 0.541680  | 3.788423  | -1.492425 |
| Cl   | 3.462710  | -1.924187 | -1.416486 |
| C    | 1.877173  | 2.144147  | 0.985847 |
| C    | 1.343881  | 3.237211  | 1.661247 |
| C    | -0.036053 | 3.387271  | 1.708549 |
| C    | -0.835246 | 2.441663  | 1.078630 |
| C    | -0.234376 | 1.375591  | 0.418889 |
| N    | 1.092090  | 1.231995  | 0.372216 |
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| C       | 3.302092 | 1.903411 | 0.901419 |
| H       | 2.006964 | 3.945783 | 2.140341 |
| H       | -0.479476 | 4.227292 | 2.228959 |
| H       | -1.914265 | 2.516607 | 1.089753 |
| N       | 7.873720 | 0.362175 | -0.154448 |
| C       | 7.258037 | 1.537586 | -0.576117 |
| C       | 5.884405 | 1.693717 | -0.434519 |
| C       | 5.126516 | 0.667274 | 0.136762 |
| H       | 8.944279 | -0.62738 | 0.399344 |
| H       | 7.842316 | 2.329150 | -1.029350 |
| H       | 5.384274 | 2.580063 | -0.801872 |
| H       | 5.131204 | -1.306333 | 0.972485 |
| H       | 7.582843 | -1.580071 | 0.725526 |
| H       | 3.994299 | 2.600083 | 1.364444 |
| V       | 2.094520 | -0.441243 | -0.627600 |
| Cl      | 0.387022 | -1.879964 | 0.043710 |
| Cl      | 2.938230 | 1.218319 | -2.185122 |
| Cl      | 0.491458 | -0.283589 | -2.330235 |
| Cl      | 2.610739 | -1.097590 | 1.708774 |
| H2      | 4.306011 | 0.617008 | 3.313857 |
| H2      | 4.759087 | 1.106976 | 3.646946 |
| Cl      | 3.468815 | -1.905383 | -1.421495 |
| C       | 1.860377 | 2.127726 | 1.010284 |
| C       | 1.322328 | 3.232131 | 1.664005 |
| C       | -0.058346 | 3.408868 | 1.661774 |
| C       | -0.853276 | 2.471514 | 1.013768 |
| C       | -0.250157 | 1.385908 | 0.385591 |
| N       | 1.080603 | 1.220914 | 0.378147 |
| C       | 3.282500 | 1.881469 | 0.943411 |
| H       | 1.981552 | 3.934815 | 2.156976 |
| H       | -0.503000 | 4.260822 | 2.161044 |
| H       | -1.930589 | 2.564631 | 0.989582 |
| H       | -0.826079 | 0.630437 | -0.128743 |
| N       | 3.704120 | 0.857315 | 0.325858 |
| C       | 7.858048 | 0.374960 | -0.174895 |
| C       | 7.235516 | 1.551420 | -0.583605 |
| C       | 5.862319 | 1.705543 | -0.421748 |
| C       | 5.111438 | 0.674837 | 0.156149 |
| C       | 5.726742 | -0.514562 | 0.547993 |
| C       | 7.100819 | -0.651391 | 0.390685 |
| H       | 8.927083 | 0.253732 | -0.303216 |
| H       | 7.812753 | 2.345087 | -1.042369 |
| H       | 5.355637 | 2.591713 | -0.780634 |
| H       | 5.130088 | -1.300984 | 0.985240 |
| H       | 7.581000 | -1.569587 | 0.705991 |
| H       | 3.972020 | 2.575134 | 1.417087 |
| V       | 2.086602 | -0.442783 | -0.619959 |
| Cl      | 0.356177 | -1.855312 | 0.050266 |
| Cl      | 2.917849 | 1.255377 | -2.151504 |
| Element | X   | Y     | Z     |
|---------|-----|-------|-------|
| Cl      | 0.517593 | -0.326900 | -2.350246 |
| Cl      | 2.634452 | -1.132980 | 1.696634 |
| H2      | 0.662423 | 0.322965 | 3.176563 |
| H2      | 0.198184 | 0.798923 | 3.514250 |
| Cl      | 3.458167 | -1.923904 | -1.423356 |
| C       | 1.875064 | 2.138353 | 0.996107 |
| C       | 1.342604 | 3.242797 | 1.653051 |
| C       | -0.035725 | 3.410889 | 1.671781 |
| C       | -0.834500 | 2.466448 | 1.040518 |
| C       | -0.235042 | 1.384203 | 0.406698 |
| N       | 1.090499 | 1.227578 | 0.379727 |
| C       | 3.299385 | 1.891964 | 0.920906 |
| H       | 2.005575 | 3.948877 | 2.135852 |
| H       | -0.478109 | 4.262342 | 2.174059 |
| H       | -1.912597 | 2.553039 | 1.032272 |
| H       | -0.812884 | 0.622730 | -0.096498 |
| N       | 3.719737 | 0.851297 | 0.307444 |
| C       | 7.872748 | 0.373572 | -0.164220 |
| C       | 7.251573 | 1.552654 | -0.567214 |
| C       | 5.877990 | 1.702193 | -0.418245 |
| C       | 5.125328 | 0.668178 | 0.143104 |
| C       | 5.738365 | -0.526646 | 0.526933 |
| C       | 7.112769 | -0.660710 | 0.379622 |
| H       | 8.943159 | 0.255782 | -0.283584 |
| H       | 7.831193 | 2.351839 | -1.012993 |
| H       | 5.373714 | 2.591554 | -0.772421 |
| H       | 5.140872 | -1.318480 | 0.952589 |
| H       | 7.591455 | -1.581088 | 0.690880 |
| H       | 3.991172 | 2.585813 | 1.388713 |
| H       | -0.909952 | -0.443448 | -0.623224 |
| Cl      | 0.376612 | -1.865605 | 0.058551 |
| Cl      | 2.931219 | 1.227176 | -2.170092 |
| Cl      | 0.496901 | -0.294980 | -2.331835 |
| Cl      | 2.633457 | -1.130103 | 1.701795 |
| H2      | 4.316768 | 0.579548 | 3.324415 |
| H2      | 4.767053 | 1.068438 | 3.662676 |
| H2      | 0.264974 | 0.807177 | 3.563058 |
| H2      | 0.686681 | 0.302742 | 3.211890 |
| Cl      | 3.455342 | -1.931647 | -1.411803 |
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| C       | 1.293065 | 3.241550 | 1.634495 |
| C       | -0.086489 | 3.395295 | 1.638637 |
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| N       | 1.074923 | 1.217273 | 0.364562 |
| C       | 3.275076 | 1.905128 | 0.918625 |
| H       | 1.945012 | 3.956262 | 2.118889 |
| H       | -0.542521 | 4.241565 | 2.137711 |
| H       | -1.947558 | 2.517129 | 0.981437 |
| H       | -0.819064 | 0.592512 | -0.126092 |
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| C       | 7.862962 | 0.405580 | -0.173311 |
Structure descriptions

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C1  3.470795  -1.916266  -1.414154
C   1.876483   2.145326   0.985286
C   1.341681   3.239533   1.657425
C  -0.038694   3.386908   1.705741
C  -0.836619   2.437402   1.080206
C  -0.234177   1.371552   0.421299
N   1.092633   1.231037   0.372919
C   3.301958   1.904707   0.902345
H   2.003407   3.951742   2.133091
H  -0.483141   4.227700   2.224042
H  -1.915799   2.509582   1.093066
H  -0.810454   0.608869  -0.082187
N   3.721197   0.858699   0.297972

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Structure descriptions

C  7.871881  0.353111  -0.163050
C  7.256010  1.523935  -0.596748
C  5.883125  1.684493  -0.449996
C  5.127290  0.666969   0.139041
C  5.734220  -0.518190  0.555076
C  7.107969  -0.662514  0.410042
H  8.941522   0.226859  -0.280705
H  7.838982  2.308032  -1.064429
H  5.381777  2.566082  -0.826816
H  5.131332  -1.294808  1.001389
H  7.582988  -1.576414  0.745195
H  3.994250  2.605522  1.360210
V  2.094255  -0.441587  -0.625012
Cl  0.392534  -1.891593   0.034364
Cl  2.938744   1.222077 -2.182927
Cl  0.488367  -0.275767 -2.326123
Cl  2.603520  -1.091626  1.710543

BPY

C  0.454025  2.370552   2.089286
C  1.003324  3.574206   2.525066
C  2.157244  3.559540   3.292164
C  2.740050  2.340377   3.609310
C  2.150245  1.178188   3.141688
H  2.593376   4.488800   3.637548
H  3.639390   2.276936   4.206495
H  2.564512   0.204692   3.354659
N  1.036413   1.193046   2.398065
V  0.133596  -0.641538   1.653798
N  1.149806   1.034151   0.949256
C  0.769944   2.280418   1.284582
C  2.254223   0.845977   0.221123
C  1.515414   3.385574   0.879888
C  3.036164   1.903222  -0.210571
H  2.503682  -0.177112  -0.012516
C  2.660326   3.198319   0.124384
H  3.921985   1.701944  -0.797828
H  3.249064   4.048529  -0.196374
H  0.534049   4.512110   2.268791
H  1.203034   4.382208   1.153402
Cl  0.688809  -1.721599   3.644679
Cl  1.069924  -2.212137   0.732458
Cl  0.815206   0.181204  -0.572431
Cl  2.268488 -0.1500569  1.264806
Cl  1.679927  -0.127879   3.246785
H  0.134025   2.194089   5.292217
H  0.281904   1.635963   5.026365
H  2.815924   2.505050   3.737362
H  3.096415   3.182604   3.870262
H  3.020447   1.830293   0.252794
H  3.425048   2.399254   0.513062
H  0.926788   3.036771  -1.254187
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H2   | 0.920213| 3.764160| -1.415954|
| C    | 0.478798| 2.371866| 2.104470 |
| C    | 1.034516| 3.569821| 2.549719 |
| C    | 2.203010| 3.544740| 3.295142 |
| C    | 2.794096| 3.20777| 3.581903|
| C    | 2.193341| 1.164662| 3.11568 |
| H    | 2.645104| 4.469039| 3.646720|
| H    | 3.705788| 2.250097| 4.159547|
| H    | 2.608900| 0.187115| 3.304546|
| N    | 1.064443| 1.190483| 2.391100|
| V    | 0.136742| -0.638033| 1.654548|
| N    | -1.138543| 1.052119| 0.961144|
| C    | -0.752618| 2.293761| 1.307698|
| C    | -2.245070| 0.876682| 0.233757|
| C    | -1.496187| 3.406458| 0.918189|
| C    | -3.025669| 1.940605| -0.184108|
| H    | -2.498236| -0.143215| -0.010551|
| C    | -2.645600| 3.230903| 0.164615|
| H    | -3.913638| 1.748850| -0.771434|
| H    | -3.233478| 4.086077| -0.144916|
| H    | 0.560784| 4.511819| 2.316412|
| H    | -1.179972| 4.399611| 1.201400|
| Cl   | 0.706294| -1.717291| 3.648980|
| Cl   | -1.094051| -2.192416| 0.744537|
| Cl   | 0.830611| 0.201763| -0.551912|
| Cl   | 2.254038| -1.543130| 1.244599|
| Cl   | -1.640204| -0.090728| 3.270383|
| C    | 0.455681| 2.373720| 2.109660|
| C    | 0.983878| 3.572448| 2.584074|
| C    | 2.150230| 3.555442| 3.331802|
| C    | 2.767033| 3.38951| 3.590108|
| C    | 2.187381| 1.180510| 3.100916|
| H    | 2.571313| 4.480542| 3.705825|
| H    | 3.680200| 2.273815| 4.165794|
| H    | 2.619564| 0.208051| 3.280676|
| N    | 1.057634| 1.197523| 2.381519|
| V    | 0.140179| -0.637097| 1.647092|
| N    | -1.138664| 1.044601| 0.947191|
| C    | -0.761631| 2.288533| 1.293690|
| C    | -2.235792| 0.861406| 0.206423|
| C    | -1.498815| 3.397693| 0.881948|
| C    | -3.011632| 1.921411| -0.228766|
| H    | -2.483038| -0.160421| -0.034984|
| C    | -2.635568| 3.215060| 0.112697|
| H    | -3.891878| 1.724733| -0.825889|
| H    | -3.219284| 4.067015| -0.212823|
| H    | 0.488427| 4.507930| 2.371675|
| H    | -1.187445| 4.392593| 1.163230|
| Cl   | 0.706824| -1.681672| 3.655919|
| Cl   | -1.082530| -2.204939| 0.745967|
| Cl   | 0.822004| 0.181799| -0.574168|
| Cl   | 2.252153| -1.538256| 1.245763|
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| Cl   | -1.680408 | -0.111350 | 3.244919  |
| H2   | 0.230616  | 1.981640  | 5.463862  |
| H2   | -0.149260 | 1.445059  | 5.113139  |
| H2   | -2.442594 | 2.638211  | 3.856261  |
| H2   | -2.636532 | 3.338388  | 4.022172  |
| H2   | 2.830270  | 2.084059  | 0.149714  |
| H2   | 3.240920  | 2.642715  | 0.423502  |
| C    | 0.448051  | 2.369364  | 2.087539  |
| C    | 0.978170  | 3.572142  | 2.549949  |
| C    | 2.114519  | 3.556840  | 3.343260  |
| C    | 2.702601  | 2.338044  | 3.654811  |
| C    | 2.133103  | 1.177174  | 3.158448  |
| H    | 2.534854  | 4.484784  | 3.711236  |
| H    | 3.589953  | 2.274369  | 4.269796  |
| N    | 1.032843  | 1.193004  | 2.394686  |
| V    | 0.134597  | -0.645592 | 1.649207  |
| N    | -1.151977 | 1.032195  | 0.941539  |
| C    | -0.765965 | 2.279151  | 1.266315  |
| C    | -2.255829 | 0.842912  | 0.213373  |
| C    | -1.500189 | 3.385872  | 0.842335  |
| C    | -3.030042 | 1.899894  | -0.233047 |
| H    | -2.509637 | -0.181543 | -0.010254 |
| C    | -2.644204 | 3.196659  | 0.084183  |
| H    | -3.916136 | 1.698477  | -0.819835 |
| H    | -3.224844 | 4.046612  | -0.252165 |
| H    | 0.505517  | 4.509750  | 2.297891  |
| H    | -1.180664 | 4.384235  | 1.102406  |
| Cl   | 0.682214  | -1.764148 | 3.619570  |
| Cl   | -1.085884 | -2.218140 | 0.748227  |
| Cl   | 0.792666  | 0.148989  | -0.583554 |
| Cl   | 2.293185  | -1.469244 | 1.268205  |
| Cl   | -1.639564 | -0.089288 | 3.267290  |
| H2   | 3.276480  | 2.536373  | 0.484142  |
| H2   | 2.890211  | 1.957465  | 0.217075  |
| C    | 0.460766  | 2.378578  | 2.104731  |
| C    | 1.007355  | 3.578112  | 2.555887  |
| C    | 2.171769  | 3.557900  | 3.306599  |
| C    | 2.768119  | 2.337168  | 3.591180  |
| C    | 2.175980  | 1.179043  | 3.115921  |
| H    | 2.606812  | 4.483549  | 3.662786  |
| H    | 3.677068  | 2.268909  | 4.171881  |
| H    | 2.596852  | 0.204140  | 3.309337  |
| N    | 1.049772  | 1.199322  | 2.391168  |
| V    | 0.131128  | -0.634474 | 1.651735  |
| N    | -1.141003 | 1.053378  | 0.947622  |
| C    | -0.763760 | 2.295629  | 1.298724  |
| C    | -2.240018 | 0.872059  | 0.209493  |
| C    | -1.509195 | 3.405602  | 0.902736  |
| C    | -3.021125 | 1.932547  | -0.215058 |
| H    | -2.485263 | -0.149146 | -0.037171 |
| C    | -2.650011 | 3.224560  | 0.138307  |
| Atom | X    | Y    | Z    |
|------|------|------|------|
| H    | -3.902427 | 1.737822 | -0.811207 |
| H    | -3.239098  | 4.076914  | -0.176576 |
| H    | 0.528736   | 4.517423  | 2.322319  |
| H    | -1.199878  | 4.399872  | 1.189200  |
| Cl   | 0.694497   | -1.689147 | 3.660075  |
| Cl   | -1.077828  | -2.205843 | 0.733069  |
| Cl   | 0.820213   | 0.184732  | -0.666251 |
| Cl   | 2.253367   | -1.526736 | 1.259474  |
| Cl   | -1.685364  | -0.121395 | 3.230381  |
| H2   | 0.093985   | 2.192519  | 5.352737  |
| H2   | -0.271654  | 1.626782  | 5.033752  |
| H2   | 3.290228   | 2.603340  | 0.431812  |
| H2   | 2.877307   | 2.031363  | 0.174698  |
| PHEN  |
| C    | 0.411799   | 2.330869  | 2.073479  |
| C    | 0.890451   | 3.592036  | 2.481194  |
| C    | 2.088331   | 3.617989  | 3.218381  |
| C    | 2.729681   | 2.434480  | 3.509086  |
| C    | 2.178088   | 1.223495  | 3.073970  |
| H    | 2.495768   | 4.566371  | 3.549114  |
| H    | 3.653147   | 2.416463  | 4.072029  |
| H    | 2.647522   | 0.274271  | 3.288666  |
| N    | 1.050227   | 1.175922  | 2.376321  |
| V    | 0.134218   | -0.666644 | 1.653495  |
| N    | -1.171277  | 0.999189  | 0.917476  |
| C    | -0.778251  | 2.235892  | 1.298009  |
| C    | -2.259846  | 0.865696  | 0.178250  |
| C    | -1.487612  | 3.400656  | 0.944035  |
| C    | -3.024046  | 1.970116  | -0.219592 |
| H    | -2.532580  | -0.140693 | -0.102783 |
| C    | -2.645860  | 3.237848  | 0.161370  |
| H    | -3.905482  | 1.803539  | -0.824385 |
| H    | -3.223348  | 4.105355  | -0.135686 |
| C    | 0.148319   | 4.763078  | 2.118769  |
| C    | -0.990811  | 4.670750  | 1.384618  |
| Cl   | 0.718010   | -1.665316 | 3.686283  |
| Cl   | -1.080160  | -2.214674 | 0.713681  |
| Cl   | 0.873709   | 0.194648  | -0.542318 |
| Cl   | 2.227507   | -1.606006 | 1.260033  |
| Cl   | -1.688250  | -0.154430 | 3.225670  |
| H2   | 0.050473   | 2.244857  | 5.280270  |
| H2   | -0.305715  | 1.665709  | 4.974601  |
| H2   | 1.300078   | 3.072958  | -0.747591 |
| H    | 1.311030   | 3.816395  | -0.693504 |
| H    | -1.542883  | 5.562453  | 1.112002  |
| H    | 0.518557   | 5.729150  | 2.440889  |
| C    | 0.422507   | 2.328422  | 2.074774  |
| C    | 0.899845   | 3.587921  | 2.489143  |
| C    | 2.076390   | 3.608606  | 3.260006  |
| C    | 2.700796   | 2.422147  | 3.572430  |
| C    | 2.156978   | 1.213994  | 3.120753  |
### Structure descriptions

|   |   |   |   |
|---|---|---|---|
| H | 2.479824 | 4.555253 | 3.600165 |
| H | 3.606907 | 2.399533 | 4.162679 |
| H | 2.617552 | 0.263031 | 3.346312 |
| N | 1.048363 | 1.170585 | 2.392602 |
| V | 0.140375 | 0.667758 | 1.652948 |
| N | -1.166086 | 1.000857 | 0.921219 |
| C | -0.761288 | 2.237258 | 1.289025 |
| C | -2.258961 | 0.868428 | 0.188041 |
| C | -1.460599 | 3.404858 | 0.923377 |
| C | -3.014106 | 1.975375 | -0.219724 |
| H | -2.541218 | -0.138773 | -0.080654 |
| C | -2.621690 | 3.243923 | 0.144268 |
| H | -3.900090 | 1.810427 | -0.818319 |
| H | -3.192388 | 4.113163 | -0.160550 |
| C | 0.172672 | 4.762882 | 2.107422 |
| C | 0.957029 | 4.674939 | 1.358278 |
| C1 | 0.698917 | -1.718395 | 3.658570 |
| C1 | -1.080953 | -2.216879 | 0.725466 |
| C1 | 0.848187 | 0.172510 | -0.559082 |
| C1 | 2.262659 | -1.551506 | 1.269518 |
| C1 | -1.671851 | -0.131656 | 3.242852 |
| H2 | -0.019979 | 2.277741 | 5.296575 |
| H2 | -0.370979 | 1.707231 | 4.968941 |
| H | 0.544943 | 5.727912 | 2.429967 |
| H | -1.499494 | 5.568942 | 1.074574 |
| H2 | 2.793436 | 2.104825 | 0.145215 |
| H2 | 3.189298 | 2.685659 | 0.394143 |
| C | 0.415461 | 2.331836 | 2.070883 |
| C | 0.885352 | 3.591447 | 2.492754 |
| C | 2.059062 | 3.614046 | 3.268288 |
| C | 2.691821 | 2.429768 | 3.571630 |
| C | 2.155217 | 1.221177 | 3.112986 |
| H | 2.455584 | 4.560917 | 3.615994 |
| H | 3.597642 | 2.408916 | 4.162407 |
| H | 2.619899 | 0.271598 | 3.335486 |
| N | 1.045861 | 1.175275 | 2.386270 |
| V | 0.141838 | -0.663562 | 1.649530 |
| N | -1.165343 | 1.001315 | 0.911392 |
| C | -0.762372 | 2.239097 | 1.276979 |
| C | -2.255417 | 0.866664 | 0.174535 |
| C | -1.459522 | 3.405267 | 0.903807 |
| C | -3.008244 | 1.972421 | -0.240409 |
| H | -2.536940 | -0.141312 | -0.091675 |
| C | -2.616546 | 3.242237 | 0.119855 |
| H | -3.892132 | 1.805456 | -0.841558 |
| H | -3.186520 | 4.110368 | -0.189356 |
| C | 0.157744 | 4.764484 | 2.107553 |
| C | -0.962625 | 4.674966 | 1.344713 |
| C1 | 0.694165 | -1.704452 | 3.660475 |
| C1 | -1.085989 | -2.214297 | 0.733804 |
| C1 | 0.852409 | 0.164997 | -0.559572 |
| C1 | 2.260895 | -1.556134 | 1.272998 |
| C1 | -1.679666 | -0.118558 | 3.241016 |

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| Atom | X    | Y    | Z    |
|------|------|------|------|
| H2   | 0.278977 | 1.723488 | 5.634452 |
| H2   | -0.067467 | 1.196644 | 5.237224 |
| H2   | -2.087057 | 2.676276 | 3.936204 |
| H2   | -2.135089 | 3.416403 | 4.009270 |
| H2   | 2.771313 | 2.138809 | 0.143727 |
| H2   | 3.152554 | 2.729642 | 0.391546 |
| H    | -1.504450 | 5.568443 | 1.057539 |
| H    | 0.523111 | 5.730052 | 2.436701 |
| C    | 0.409886 | 2.335357 | 2.065645 |
| C    | 0.883660 | 3.596554 | 2.477437 |
| C    | 2.059566 | 3.621335 | 3.250372 |
| C    | 2.686345 | 2.437359 | 3.566375 |
| C    | 2.146272 | 1.226976 | 3.16759 |
| H    | 2.460277 | 4.569964 | 3.588469 |
| H    | 3.591818 | 2.418492 | 4.157725 |
| H    | 2.609102 | 0.277960 | 3.345020 |
| N    | 1.039226 | 1.179382 | 2.386911 |
| V    | 0.137013 | -0.660250 | 1.650764 |
| N    | -1.174468 | 1.001217 | 0.916374 |
| C    | -0.773161 | 2.239848 | 1.280209 |
| C    | -2.267494 | 0.863767 | 0.184163 |
| C    | -1.475594 | 3.403970 | 0.911455 |
| C    | -3.025467 | 1.967543 | -0.226331 |
| H    | -2.547588 | -0.144691 | -0.081652 |
| C    | -2.636005 | 3.238145 | 0.133754 |
| H    | -3.911278 | 1.798637 | -0.824015 |
| H    | -3.208926 | 4.105065 | -0.173322 |
| C    | 0.153820 | 4.767947 | 2.092044 |
| C    | -0.975306 | 4.674885 | 1.342704 |
| Cl   | 0.697673 | -1.711535 | 3.656335 |
| Cl   | -1.082259 | -2.213938 | 0.728212 |
| Cl   | 0.840389 | 0.170908 | -0.566652 |
| Cl   | 2.263770 | -1.537283 | 1.269513 |
| Cl   | -1.675986 | -0.127727 | 3.244252 |
| H2   | 0.273697 | 1.802034 | 5.589820 |
| H2   | -0.108017 | 1.288936 | 5.207322 |
| H2   | -2.126724 | 2.696527 | 3.930962 |
| H2   | -2.173028 | 3.436432 | 4.005166 |
| H2   | 3.154988 | 1.687537 | 0.252085 |
| H2   | 3.615921 | 2.220128 | 0.495286 |
| H2   | 1.070526 | 3.062202 | -0.948207 |
| H2   | 1.051841 | 3.826904 | -0.933780 |
| H    | 0.523304 | 5.734812 | 2.412612 |
| H    | -1.520043 | 5.566900 | 1.056609 |
| C    | 0.414127 | 2.328465 | 2.075957 |
| C    | 0.890491 | 3.588551 | 2.491144 |
| C    | 2.066802 | 3.609587 | 3.264016 |
| C    | 2.691774 | 2.422898 | 3.577457 |
| C    | 2.148871 | 1.213908 | 3.124659 |
| H    | 2.469689 | 4.556379 | 3.604603 |
| H    | 3.597447 | 2.401424 | 4.168833 |
| H    | 2.609190 | 0.262522 | 3.349555 |
Structure descriptions

N  1.041817  1.171237  2.394481
V  0.138181 -0.667116  1.650851
N -1.174431  1.000454  0.921506
C  -0.769945  2.237262  1.289830
C  -2.267830  0.869033  0.189582
C  -1.469791  3.404651  0.925219
C  -3.023833  1.975913 -0.217110
H  -2.550063 -0.137840 -0.080175
C  -2.631829  3.244355  0.146845
H  -3.910232  1.810828 -0.815232
H  -3.202888  4.113662 -0.157082
C  0.162893  4.763635  2.109465
C  -0.966711  4.675095  1.360319
Cl  0.697644 -1.740231  3.648281
Cl  -1.087123 -2.210483  0.721086
Cl  0.859180  0.190372 -0.540488
Cl  2.267752 -1.551554  1.268489
Cl  -1.647407 -0.114821  3.257166
H  -1.509611  5.569355  1.076900
H  0.534550  5.728729  2.432566

C  0.420136  2.328786  2.068559
C  0.893080  3.588979  2.486244
C  2.052291  3.609269  3.283718
C  2.666473  2.422247  3.615152
C  2.133233  1.213852  3.150470
H  2.450663  4.556135  3.629408
H  3.558431  2.400009  4.226725
H  2.588988  0.262378  3.384211
N  1.040912  1.171516  2.398350
V  0.140494 -0.667328  1.652130
N -1.170998  0.997610  0.921894
C  -0.759262  2.236025  1.276075
C  -2.267571  0.864036  0.194804
C  -1.452242  3.403470  0.898749
C  -3.017299  1.970903 -0.223726
H  -2.556477 -0.144260 -0.062431
C  -2.615401  3.241070  0.122858
H  -3.906387  1.804206 -0.817222
H  -3.181158  4.110294 -0.191170
C  0.176635  4.764398  2.085745
C  -0.944856  4.675189  1.324544
Cl  0.680404 -1.779939  3.620377
Cl  -1.095729 -2.213230  0.734381
Cl  0.825421  0.151481 -0.568146
Cl  2.294906 -1.498923  1.279347
Cl  -1.631939 -0.091310  3.275466
H2  3.203346  2.641971  0.426979
H2  2.812498  2.054116  0.186978
H  -1.480215  5.569283  1.027876
H  0.549185  5.730357  2.405200
CrCl$_3$— H$_2$

BBH

C 2.150484 3.167697 0.509951
C 1.365614 2.139835 1.058475
C -0.015479 2.262774 1.111801
C -0.626346 3.422589 0.638869
C 0.148278 4.461253 0.123044
C 1.527622 4.341070 0.057626
C 3.583364 2.951326 0.445322
H 1.840345 1.236348 1.425035
H -0.614163 1.458936 1.522076
H -1.704215 3.522780 0.683548
H -0.323854 5.371875 -0.223758
N 4.393765 3.566312 0.339145
C 6.591479 3.741606 -1.124587
N 5.728156 3.235063 -0.225282
H 3.982383 2.178211 1.106675
H 6.052779 2.726856 0.587122
O 6.173800 4.490345 -2.040422
C 10.758707 2.918181 -1.124587
C 10.298762 4.047801 -1.514031
C 8.936310 4.298134 -1.607567
C 8.025136 3.418518 -1.011451
C 8.489608 2.277343 -0.34433
C 9.853518 2.030753 -0.260671
H 11.822318 2.723644 -0.773006
H 11.002364 4.733909 -1.968654
H 8.562932 5.169341 -2.129257
H 7.798311 1.555069 0.074212
H 10.210014 1.141843 0.244679
H 2.123961 5.174268 -0.288054
Cr 4.281237 5.011735 -2.04897
Cl 4.375898 6.617274 -0.431404
Cl 3.230112 3.288461 -3.129419
Cl 4.309927 6.405973 -3.801721

C 2.150484 3.167696 0.509952
C 1.365614 2.139834 1.058475
C -0.015479 2.262773 1.111801
C -0.626346 3.422589 0.638870
C 0.148278 4.461253 0.123045
C 1.527622 4.341070 0.057628
C 3.583364 2.951326 0.445323
H 1.840345 1.236347 1.425034
H -0.614163 1.458935 1.522075
H -1.704215 3.522781 0.683549
H -0.323853 5.371876 -0.223756
N 4.393765 3.566312 -0.339145
C 6.591479 3.741606 -1.124587
N 5.728156 3.235063 -0.225282
H 3.982383 2.178210 1.106675
H 6.052779 2.726855 0.587121
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| O       | 6.173800  | 4.490345  | -2.040422 |
| C       | 10.758707 | 2.918183  | -0.840304 |
| C       | 10.298761 | 4.047802  | -1.514031 |
| C       | 8.936310  | 2.981394  | -1.607567 |
| C       | 8.025136  | 3.418518  | -1.011451 |
| C       | 8.489609  | 2.77344   | -0.344332 |
| C       | 9.853518  | 2.030755  | -0.260670 |
| H       | 11.82318  | 2.723646  | -0.773006 |
| H       | 11.002363 | 4.733910  | -1.968655 |
| H       | 8.562931  | 5.169340  | -2.129258 |
| H       | 7.798312  | 1.555070  | 0.074214  |
| H       | 10.210015 | 1.141845  | 0.244681  |
| H       | 2.123961  | 5.174268  | -0.280052 |
| Cr      | 4.281237  | 5.011735  | -2.074597 |
| Cl      | 4.375898  | 6.617274  | -0.431405 |
| Cl      | 3.230112  | 3.288461  | -3.129419 |
| Cl      | 4.309927  | 6.405972  | -3.801722 |
| C       | 2.067188  | 3.038468  | 0.259262  |
| C       | 1.553524  | 4.338799  | 0.381221  |
| C       | 0.214501  | 4.521992  | 0.691227  |
| C       | -0.625803 | 3.425355  | 0.875700  |
| C       | -0.121349 | 2.129365  | 0.771686  |
| C       | 1.220708  | 1.937249  | 0.481609  |
| C       | 3.458271  | 2.753255  | -0.027869 |
| H       | 2.203000  | 5.192212  | 0.258200  |
| H       | -0.175125 | 5.527836  | 0.785111  |
| H       | -1.672203 | 3.579706  | 1.111340  |
| H       | -0.770579 | 1.275931  | 0.923680  |
| N       | 4.313342  | 3.520955  | -0.613729 |
| C       | 6.585672  | 3.778821  | -1.183602 |
| N       | 5.612498  | 3.038826  | -0.610430 |
| H       | 3.806189  | 1.773252  | 0.312622  |
| H       | 5.843756  | 2.63065   | -0.003391 |
| O       | 6.301792  | 4.841200  | -1.770444 |
| C       | 10.655277 | 2.529628  | -0.938435 |
| C       | 10.328360 | 3.860241  | -1.191471 |
| C       | 8.997753  | 4.248087  | -1.277387 |
| C       | 7.982730  | 3.301880  | -1.095362 |
| C       | 8.314686  | 1.962670  | -0.852940 |
| C       | 9.647837  | 1.580413  | -0.775627 |
| H       | 11.69404  | 2.229265  | -0.877149 |
| H       | 11.111277 | 4.596325  | -1.325399 |
| H       | 8.726129  | 5.275567  | -1.480610 |
| H       | 7.545985  | 1.203517  | -0.764583 |
| H       | 9.901040  | 0.542183  | -0.600230 |
| H       | 1.616552  | 0.929891  | 0.409255  |
| Cr      | 4.336498  | 5.428869  | -1.955512 |
| Cl      | 4.297693  | 6.695885  | -0.110846 |
| Cl      | 2.277618  | 4.949524  | -2.712009 |
| Cl      | 4.913984  | 6.829697  | -3.580811 |
| H2      | 4.280742  | 2.689820  | -3.543051 |
| H2      | 4.985961  | 2.451179  | -3.575706 |
|   |   |   |
|---|---|---|
| C | 2.061380 | 3.031704 | 0.238827 |
| C | 1.546856 | 4.331785 | 0.360332 |
| C | 0.208581 | 4.514441 | 0.673590 |
| C | -0.630453 | 3.417462 | 0.862040 |
| C | -0.125258 | 2.121746 | 0.758826 |
| C | 3.451224 | 2.745766 | -0.053108 |
| H | 2.194967 | 5.185633 | 0.234256 |
| H | -1.676352 | 3.571292 | 1.100275 |
| H | -0.773334 | 1.268045 | 0.914182 |
| N | 4.307299 | 3.514205 | -0.636806 |
| C | 6.581273 | 3.781017 | -1.183930 |
| N | 5.605094 | 3.026264 | -0.640856 |
| H | 3.797451 | 1.762988 | 0.280872 |
| H | 5.836893 | 2.258325 | -0.024066 |
| O | 6.299291 | 4.850908 | -1.762398 |
| C | 10.651348 | 2.549173 | -0.895536 |
| C | 10.321486 | 3.885306 | -1.114415 |
| C | 8.990804 | 4.267959 | -1.217856 |
| C | 7.978607 | 3.310433 | -1.08067 |
| C | 8.313077 | 1.966431 | -0.879318 |
| C | 9.646770 | 1.589731 | -0.783638 |
| H | 11.690847 | 2.253255 | -0.820136 |
| H | 11.102431 | 4.629738 | -1.207446 |
| H | 8.716730 | 5.299444 | -1.392519 |
| H | 7.546349 | 1.201665 | -0.832053 |
| H | 9.902648 | 0.548036 | -0.634571 |
| H | 1.612330 | 0.922983 | 0.393404 |
| Cr | 4.334807 | 5.424534 | -1.974005 |
| Cl | 4.267108 | 6.708372 | -0.138259 |
| Cl | 2.75061 | 4.952016 | -2.732244 |
| Cl | 4.922488 | 6.817838 | -3.601524 |
| H2 | 4.429708 | 2.750161 | -3.641033 |
| H2 | 5.169120 | 2.677362 | -3.699413 |
| H2 | 6.406889 | 5.368550 | 1.264674 |
| H2 | 6.950833 | 4.958132 | 1.569295 |
| C | 2.033496 | 3.043104 | 0.219600 |
| C | 1.506127 | 4.337749 | 0.341822 |
| C | 0.162896 | 4.506631 | 0.642078 |
| C | -0.668078 | 3.401138 | 0.815522 |
| C | -0.150111 | 2.110538 | 0.710914 |
| C | 1.196122 | 1.932673 | 0.431080 |
| C | 3.428878 | 2.769828 | -0.065851 |
| H | 2.148178 | 5.197935 | 0.228029 |
| H | -0.237230 | 5.508237 | 0.737081 |
| H | -1.717784 | 3.544232 | 1.043225 |
| H | -0.792183 | 1.250235 | 0.854484 |
| N | 4.283823 | 3.545472 | -0.634417 |
| C | 6.556690 | 3.811794 | -1.195626 |
| N | 5.582582 | 3.066574 | -0.634570 |
| H | 3.779332 | 1.789376 | 0.276747 |
| H | 5.803323 | 2.242979 | -0.090260 |
Structure descriptions

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| O    | 6.278532 | 4.895971 | -1.745820 |
| C    | 10.610385 | 2.500763 | -1.041164 |
| C    | 10.299935 | 3.845185 | -1.235655 |
| C    | 8.974145  | 4.254244 | -1.292037 |
| C    | 7.948091  | 3.315097 | -1.138376 |
| C    | 8.262837  | 1.962285 | -0.955546 |
| C    | 9.591354  | 1.559357 | -0.907892 |
| H    | 11.645719 | 2.183894 | -1.003272 |
| H    | 11.091817 | 4.575375 | -1.347405 |
| H    | 8.714825  | 5.292651 | -1.461133 |
| H    | 7.484082  | 1.210885 | -0.893642 |
| H    | 9.831828  | 0.511300 | -0.779184 |
| H    | 1.602572  | 0.929620 | 0.357380 |
| Cr   | 4.314028  | 5.473824 | -1.942506 |
| Cl   | 4.237447  | 6.712313 | -0.080022 |
| Cl   | 2.272459  | 4.979150 | -2.742121 |
| Cl   | 4.900023  | 6.906203 | -3.536732 |
| H2   | 4.310356  | 2.774403 | -3.562733 |
| H2   | 5.007122  | 2.514290 | -3.614540 |
| H2   | 5.027546  | -0.114044 | -1.442323 |
| H2   | 4.898534  | 0.476555 | -1.877102 |
| C    | 2.058371  | 3.042683 | 0.245658 |
| C    | 1.538770  | 4.343315 | 0.334350 |
| C    | 0.198048  | 4.528454 | 0.635600 |
| C    | -0.638228 | 3.433135 | 0.844495 |
| C    | -0.127990 | 2.137154 | 0.774106 |
| C    | 1.215584  | 1.943593 | 0.492682 |
| C    | 3.451168  | 2.755148 | -0.30118 |
| H    | 2.184633  | 5.196204 | 0.192117 |
| H    | -0.196085 | 5.534597 | 0.703691 |
| H    | -1.685918 | 3.588897 | 1.073221 |
| H    | -0.774240 | 1.285132 | 0.945292 |
| N    | 4.308254  | 3.509990 | -0.630284 |
| C    | 6.584413  | 3.779060 | -1.165834 |
| N    | 5.608369  | 3.029204 | -0.610357 |
| H    | 3.800133  | 1.784218 | 0.334092 |
| H    | 5.841911  | 2.287266 | 0.036925 |
| O    | 6.296853  | 4.829048 | -1.773281 |
| C    | 10.663956 | 2.609453 | -0.790336 |
| C    | 10.319631 | 3.935240 | -1.046303 |
| C    | 8.985710  | 4.298157 | -1.176025 |
| C    | 7.985071  | 3.329611 | -1.035259 |
| C    | 8.333760  | 1.995889 | -0.786936 |
| C    | 9.670872  | 1.639398 | -0.666203 |
| H    | 11.706143 | 2.329198 | -0.695037 |
| H    | 11.092143 | 4.687230 | -1.148301 |
| H    | 8.699375  | 5.322184 | -1.375836 |
| H    | 7.576323  | 1.222634 | -0.729568 |
| H    | 9.938946  | 0.605469 | -0.487678 |
| H    | 1.616192  | 0.936660 | 0.446338 |
| Cr   | 4.332417  | 5.383846 | -2.008128 |
| Cl   | 4.258520  | 6.715774 | -0.207026 |
| Cl   | 2.275715  | 4.897587 | -2.765330 |
Structure descriptions

| Element | X    | Y    | Z    |
|---------|------|------|------|
| Cl      | 4.929275 | 6.750232 | -3.655430 |
| H2     | 4.493158  | 2.731139  | -3.666427  |
| H2     | 5.233964  | 2.740629  | -3.745265  |
| H2     | 6.333686  | 5.361400  | 1.293319   |
| H2     | 6.869493  | 4.951951  | 1.612900   |
| H2     | 7.880470  | 7.715330  | -0.911167  |
| H2     | 7.218331  | 7.473553  | -1.153219  |
| C      | 2.056040  | 3.041125  | 0.243886   |
| C      | 1.526511  | 4.338460  | 0.318693   |
| C      | 0.183429  | 4.516098  | 0.613807   |
| C      | -0.644064 | 3.415924  | 0.832036   |
| C      | -0.123856 | 2.123196  | 0.776878   |
| C      | 1.221897  | 1.937494  | 0.500050   |
| C      | 3.450599  | 2.758753  | -0.029610  |
| H      | 2.165754  | 5.195628  | 0.172486   |
| H      | -0.218287 | 5.519757  | 0.665045   |
| H      | -1.693973 | 3.565351  | 1.054566   |
| H      | -0.764220 | 1.268015  | 0.954524   |
| N      | 4.305423  | 3.510436  | -0.636409  |
| C      | 6.582889  | 3.777077  | -1.169149  |
| N      | 5.605670  | 3.028778  | -0.616288  |
| H      | 3.801878  | 1.791054  | 0.342670   |
| H      | 5.833801  | 2.274219  | 0.018164   |
| O      | 6.298517  | 4.832799  | -1.769057  |
| C      | 10.658503 | 2.590105  | -0.808718  |
| C      | 10.318486 | 3.918657  | -1.056016  |
| C      | 8.985659  | 4.287239  | -1.180903  |
| C      | 7.981939  | 3.321362  | -1.044349  |
| C      | 8.326101  | 1.984922  | -0.804870  |
| C      | 9.662214  | 1.622857  | -0.688853  |
| H      | 11.699947 | 2.305969  | -0.716354  |
| H      | 11.093425 | 4.668733  | -1.154199  |
| H      | 8.702858  | 5.313598  | -1.374127  |
| H      | 7.566229  | 1.213690  | -0.750371  |
| H      | 9.926467  | 0.586932  | -0.515902  |
| H      | 1.630316  | 0.933098  | 0.464077   |
| Cr     | 4.340507  | 5.395408  | -2.000130  |
| Cl     | 4.274213  | 6.704645  | -0.183800  |
| Cl     | 2.279933  | 4.928800  | -2.767452  |
| Cl     | 4.942095  | 6.782366  | -3.630399  |
| H2     | 4.488224  | 2.746329  | -3.675257  |
| H2     | 5.230067  | 2.731153  | -3.741177  |
| H2     | 6.364423  | 5.370701  | 1.277449   |
| H2     | 6.902126  | 4.955224  | 1.586023   |
| H2     | 0.971999  | 7.127867  | -1.248278  |
| H2     | 0.596572  | 7.611570  | -0.823847  |
| H2     | 7.870827  | 7.688489  | -0.858979  |
| H2     | 7.208584  | 7.434431  | -1.087359  |

PIP

| Element | X    | Y    | Z    |
|---------|------|------|------|
| C      | 1.654205 | 2.030803 | -0.454752 |
| C      | 1.180792 | 3.352450 | -0.501138 |
Structure descriptions

C  -0.104857  3.672678  -0.097060
C   -0.955322  2.661921   0.348108
C   -0.524181  1.340328  0.380544
C    0.767187  1.035668  -0.017508
C    3.029431  1.791495  -0.861732
H     1.850729  4.132646  -0.842586
H    -0.444178  4.699782  -0.125351
H    -1.961795  2.899302  0.669838
H    -1.180453  0.549360  0.721473
N     3.738875  0.732771  -0.681816
C     7.728086   0.938544  -2.030107
C     7.301560  1.758564  -0.990328
C     5.984020  1.697695  -0.545547
C     5.099454  0.806895  -1.147708
C     5.521870  -0.030599  -2.177010
C     6.835335   0.046903  -2.622851
H     8.755085   0.984235  -2.371549
H     7.995351  2.439403  -0.512423
H     5.647949  2.301535   0.287289
H     4.829674  -0.737141  -2.614816
H     7.165270  -0.599164  -3.427211
H     3.503749  2.635185  -1.364657
O     1.209605  -0.268443  -0.043898
Cr    3.150221  -0.915209   0.596792
Cl    1.880752  -2.673443  1.346524
Cl    3.134802   0.440932  2.374685
H     0.653627  -0.891246   0.472846
Cl    5.149897  -1.882095   0.680577
H2     2.691158  -1.790867  -1.762298
H2     3.123963  -2.321316  -1.461484
H2     3.953864   3.891298   1.571586
H2     3.768481   3.192262   1.753894
H2     6.486045   0.258486   2.290806
H2     6.964581   0.727407   2.616699
H2    -0.349734  -0.379730   3.120394
H2     0.392230  -0.386395   3.046675
C     1.638852   2.035667  -0.610872
C     1.160796   3.346635  -0.773495
C    -0.134478   3.689627  -0.420649
C    -0.988631   2.711313   0.086292
C    -0.554326   1.397671   0.223603
C     0.746164   1.064745  -0.128105
C     3.029930   1.769142  -0.951502
H     1.833180   4.101222  -1.165113
H    -0.478759   4.708802  -0.537811
H     2.002056   2.967341   0.369592
H    -1.219050   0.629517   0.600359
N     3.746668   0.768548  -0.576933
C     7.763996   0.756608  -1.863856
C     7.279401   1.822233  -1.109740
C     5.956119   1.830258  -0.683436
C     5.118719   0.764552  -1.013538
C     5.600689  -0.315037  -1.749424
| Atom | X-Coordinate | Y-Coordinate | Z-Coordinate |
|------|--------------|--------------|--------------|
| C    | 6.922630     | -0.307479    | -2.180420    |
| C    | 8.796526     | 0.748673     | -2.191390    |
| H    | 7.933752     | 2.642123     | -0.839566    |
| H    | 5.581767     | 2.633823     | -0.061175    |
| H    | 4.946539     | -1.146648    | -1.969138    |
| H    | 7.296700     | -1.143109    | -2.759257    |
| H    | 3.502627     | 2.528487     | -1.576388    |
| O    | 1.186361     | -0.238525    | -0.057604    |
| Cr   | 3.128130     | -0.649423    | 0.898761     |
| Cl   | 3.293832     | -2.498323    | -0.292417    |
| Cl   | 1.710640     | -1.158790    | 2.613167     |
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| Cl   | 4.959776     | -0.338238    | 2.083742     |
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| C    | 1.094438     | 3.262925     | -0.721990    |
| C    | -0.220665    | 3.546243     | -0.389838    |
| C    | -1.054125    | 2.519363     | 0.049945     |
| C    | -0.578628    | 1.215447     | 0.144262     |
| C    | 0.739835     | 0.948221     | -0.185426    |
| C    | 3.017814     | 1.760095     | -0.922293    |
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| C    | 7.813658     | 1.032931     | -1.731691    |
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| H    | 7.940024     | 2.570301     | -0.232091    |
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| H    | 5.004203     | -0.731551    | -2.471472    |
| H    | 7.385225     | -0.544969    | -3.131513    |
| H    | 3.491952     | 2.597097     | -1.436662    |
| O    | 1.233048     | -0.336740    | -0.153058    |
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| H2   | 3.363353     | -2.350196    | -1.329413    |
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| Atom | X     | Y     | Z     |
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| H2   | 3.399097  | -2.369765 | -1.247873 |
| C    | 1.608899  | 1.961069 | -0.609834 |
| C    | 1.090876  | 3.260717 | -0.729664 |
| C    | -0.224633 | 3.545255 | -0.399016 |
| C    | -1.057650 | 2.519959 | 0.045042 |
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| C    | 3.014937  | 1.757868 | -0.923097 |
| H    | 1.747171  | 4.054097 | -1.068148 |
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| H    | 3.489434  | 2.595388 | -1.437072 |
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| C    | -0.242979 | 3.516715 | -0.510962 |
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| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
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| H    | 5.567160  | 2.312942  | 0.385784  |
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| H2   | 2.820628  | -2.03597 | -1.573087 |
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| Cl   | 1.854093  | -2.655972 | 1.342246  |
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| H    | 0.675230  | -0.924815 | 0.402296  |
| Cl   | 5.147823  | -1.875328 | 0.708036  |
| H2   | 2.719588  | -1.816776 | -1.765090 |
| H2   | 3.156331  | -2.338959 | -1.455753 |
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C  7.296243  1.852643  -0.717632
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| C       | 4.908912  | 1.948548  | -2.102671 |
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| H       | -2.004575 | 2.111230  | 0.451817 |
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| H       | 4.052722  | 1.941529  | -2.804652 |
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|------|---------|---------|---------|
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| H2   | 2.413527| 2.948830 | 2.456495 |
| H2   | 2.695438| 2.259441 | 2.500491 |
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| H    | 6.276909| 2.910426|-3.434353 |
| H    | 4.066453| 2.060062|-2.714061 |
| H    | 5.790909| 0.623831| 0.939423 |
| H    | 8.007788| 1.487673| 0.227826 |
| H    | 2.600384| 2.661360|-0.827833 |
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| Cl   | 4.886092| -1.975202| -0.593243 |
| H2   | 1.890767| -0.828870| -2.599369 |
| H2   | 2.565779| -1.144217| -2.573432 |
| H2   | 2.720039| 3.081398| 2.345781 |
| H2   | 2.926945| 2.372529| 2.453495 |
| C    | 1.279140| 1.274916|-0.047047 |
| C    | 0.203800| 2.154495|-0.098533 |
| C    | -1.027817| 1.731764| 0.391196 |
| C    | -1.138799| 0.451292| 0.914136 |
| C    | -0.016611| -0.377693| 0.923729 |
| N    | 1.163819| 0.023611| 0.449996 |
| C    | 2.614636| 1.658616|-0.486167 |
| H    | 0.338473| 3.148446|-0.505776 |
| H    | -1.884102| 2.394979| 0.368285 |
| H    | -2.072666| 0.083228| 1.313374 |
| H    | -0.048836| -1.387497| 1.310558 |
| N    | 3.583131| 0.828887|-0.372004 |
| C    | 7.438115| 2.012475|-1.554712 |
| C    | 6.359568| 2.236295|-2.406402 |
Structure descriptions

C  5.079896  1.846440  -2.026151
C  4.886186  1.224218  -0.790636
C  5.968001  0.969957   0.054344
C  7.237420  1.381810  -0.327491
H  8.434970  2.315058  -1.852704
H  6.513582  2.701931  -3.372382
H  4.242976  1.981190  -2.701176
H  5.799008  0.465566   0.995588
H  8.076460  1.196181  -0.331782
H  7.769835  2.669003  -0.861595
Cr  3.003891  -1.121369   0.432202
Cl  1.843452  -3.031199   0.743812
Cl  3.554212  -0.451015   2.502819
Cl  4.768152  -2.083592  -0.558233
H2  1.836155  -0.806141  -2.653113
H2  2.521635  -1.095878  -2.623852
H2  0.346750  -1.374213   4.076194
H2  1.002270  -1.369532  -3.721222
H2  2.886750   3.132852   2.281971
H2  3.052155   2.410476   2.368273
C  1.281249  -1.280081  -0.050841
C  0.207732   2.162053  -0.097350
C  -1.025567  1.738865   0.388007
C  -1.138140  0.454435   0.900204
C  -0.019423  -0.376267   0.906686
N  1.163273   0.025363   0.438429
C  2.616659   1.663901   0.488470
H  0.344258   3.158614  -0.497235
H  -1.879866  2.404527   0.368355
H  -2.075236  0.085257   1.295207
H  -0.054178  -1.388131   1.287171
N  3.584695   0.833678  -0.376381
C  7.440289   0.211082  -1.559622
C  6.362598   2.230730  -2.413984
C  5.082493   1.843365  -2.032374
C  4.887234   1.228445  -0.793994
C  5.967689   0.979641   0.053742
C  7.237918   1.387284  -0.329282
H  8.437827   2.309654  -1.859297
H  6.518006   2.690624  -3.382378
H  4.246211   1.974436  -2.706995
H  5.799646   0.481568   0.997852
H  8.075407   1.201111   0.331488
H  2.771968   2.674331  -0.862887
Cr  3.003086  -1.115340   0.429711
Cl  1.840162  -3.027539   0.716642
Cl  3.548161  -0.450707   2.503053
Cl  4.799018  -2.082110  -0.503270
H2  1.984455  -0.782303  -2.732920
H2  2.670447  -1.066626  -2.671136
H2  6.850633  -1.708541   1.569345
H2  7.389580  -1.512473   2.045385
H2  0.318716  -1.256206   4.059787
| Symbol | X    | Y    | Z    |
|--------|------|------|------|
| H2     | 0.983904 | -1.239737 | 3.723532 |
| BPY    |       |      |      |
| C      | 0.628241 | 2.483648 | 1.666634 |
| C      | 1.463441 | 3.579624 | 1.459909 |
| C      | 2.839185 | 3.407427 | 1.666634 |
| C      | 3.349033 | 2.145035 | 1.459909 |
| C      | 2.462723 | 1.093140 | 1.786785 |
| H      | 3.500494 | 4.251432 | 1.364697 |
| H      | 4.413458 | 1.964898 | 1.854233 |
| H      | 2.800706 | 0.083955 | 2.158032 |
| N      | 1.136076 | 1.254870 | 1.893818 |
| Cr     | -0.280963 | -0.335001 | 2.199922 |
| N      | -1.498720 | 1.420690 | 1.932042 |
| C      | -0.846785 | 2.576026 | 1.682487 |
| C      | -2.833524 | 1.424463 | 2.026257 |
| C      | -1.542987 | 3.766990 | 1.488296 |
| C      | -3.585739 | 2.577766 | 1.855173 |
| H      | -3.289718 | 0.465874 | 2.232557 |
| C      | -2.928073 | 3.766433 | 1.570938 |
| H      | -4.662914 | 2.531930 | 1.943332 |
| H      | -3.482620 | 4.685351 | 1.424151 |
| H      | 1.049779  | 4.558553 | 1.266998 |
| H      | -1.015293 | 4.686238 | 1.279023 |
| Cl     | -2.044674 | -1.693765 | 1.787249 |
| Cl     | 1.278357  | -1.890892 | 1.696102 |
| Cl     | -0.224243 | -0.046050 | 4.420296 |
| H2     | -1.192037 | -0.125075 | -0.733798 |
| H2     | -0.773106 | 0.417920  | -1.027603 |
| H2     | 1.818499  | 2.961923  | 4.670644 |
| H2     | 1.397330  | 2.346752  | 4.67419 |
| H2     | -1.855987 | 3.188534  | 4.702861 |
| H2     | -1.534287 | 2.515975  | 4.722641 |
| H2     | 1.813536  | 1.810826  | -1.096298 |
| H2     | 1.760051  | 1.071791  | -1.032186 |
| C      | 0.627041  | 2.484021  | 1.665026 |
| C      | 1.462438  | 3.587575  | 1.499289 |
| C      | 2.838861  | 3.408864  | 1.526103 |
| C      | 3.349525  | 2.132782  | 1.717702 |
| C      | 2.462704  | 1.075618  | 1.866405 |
| H      | 3.499586  | 4.258331  | 1.402809 |
| H      | 4.414611  | 1.946907  | 1.753753 |
| H      | 2.798892  | 0.057670  | 2.010406 |
| N      | 1.135146  | 1.244472  | 1.834694 |
| Cr     | -0.284302 | -0.341511 | 2.194563 |
| N      | -1.503299 | 1.413793  | 1.886879 |
| C      | -0.848132 | 2.578552  | 1.693154 |
| C      | -2.839310 | 1.415605  | 1.969891 |
| C      | -1.541362 | 3.779858  | 1.554346 |
| C      | -3.588910 | 2.577573  | 1.851030 |
| H      | -3.296789 | 0.448747  | 2.130765 |
Structure descriptions

C  -2.927139  3.778101  1.633911
H   -4.666827  2.529245  1.928560
H    -3.478682  4.704925  1.532244
H     1.049652  4.575720  1.359171
H   -1.011459  4.707108  1.393694
Cl   -2.045896 -1.707693  1.823402
Cl    1.273639 -1.920181  1.758201
Cl   -0.214839  0.060316  4.393382

C    0.626554  2.480584  1.659854
C    1.460513  3.575664  1.442137
C    2.836552  3.399033  1.471568
C    3.347831  2.133413  1.721344
C    2.462254  1.082288  1.912231
H    3.497280  4.241856  1.308378
H    4.412994  1.949989  1.763444
H    2.800195  0.070812  2.092838
N    1.134916  1.248045  1.872268
Cr   -0.285049 -0.340652  2.195589
N   -1.502337  1.414791  1.906957
C   -0.848222  2.577491  1.700667
C   -2.837070  1.417527  2.002792
C   -1.541286  3.779286  1.566687
C   -3.586711  2.579545  1.886753
H   -3.294349  0.451663  2.170243
C   -2.926150  3.779194  1.660195
H   -4.663885  2.532460  1.974926
H   -3.478138  4.706217  1.562724
H    1.046123  4.556209  1.259150
H   -1.011539  4.706028  1.402390
Cl   -2.036864 -1.699967  1.751337
Cl    1.273639 -1.920181  1.758201
Cl   -0.214839  0.060316  4.393382
H2   -0.230680  0.595719 -0.927339
H2   -0.364901 -0.133741 -0.857187
H2    1.832014  2.951490  4.572177
H2    1.377352  2.361476  4.611194

C    0.627937  2.486975  1.671934
C    1.463374  3.590363  1.505170
C    2.839546  3.413029  1.543320
C    3.349992  2.138877  1.748840
C    2.462639  1.082242  1.898476
H    3.500392  4.262554  1.419358
H    4.415008  1.954773  1.795082
H    2.799029  0.065666  2.051450
N    1.135796  1.249702  1.853925
Cr   -0.286392 -0.337647  2.194705
N   -1.504256  1.419977  1.900799
C   -0.847761  2.581052  1.690079
C   -2.840445  1.423346  1.979214
C   -1.540735  3.779412  1.525257
C   -3.589603  2.582750  1.836750
H   -3.298593  0.459187  2.154521
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -2.926707 | 3.779166 | 1.599555 |
| H    | -4.667849 | 2.536795 | 1.910881 |
| H    | -3.477879 | 4.703694 | 1.476460 |
| H    | 1.051393  | 4.577517 | 1.355901 |
| H    | -1.010735 | 4.703628 | 1.348134 |
| Cl   | -2.053931 | -1.702596| 1.850876 |
| Cl   | 1.269785  | -1.910948| 1.724830 |
| Cl   | -0.195918 | 0.038333 | 4.397842 |
| H2   | -0.464578 | 0.397842 | -0.871074|
| H2   | 0.136828  | -0.035465| -0.794435|
| C    | 0.628045  | 2.481646 | 1.665539 |
| C    | 1.463343  | 3.581911 | 1.483665 |
| C    | 2.83953   | 3.405327 | 1.524403 |
| C    | 3.348822  | 2.134568 | 1.749013 |
| C    | 2.462370  | 1.079314 | 1.909946 |
| H    | 3.500724  | 4.252420 | 1.389880 |
| H    | 4.413722  | 1.951396 | 1.800624 |
| H    | 2.799234  | 0.064794 | 2.074420 |
| N    | 1.135410  | 1.245994 | 1.861001 |
| Cr   | -0.286064 | -0.340908| 2.188659 |
| N    | -1.501034 | 1.415577 | 1.908048 |
| C    | -0.847048 | 2.575491 | 1.685755 |
| C    | -2.836385 | 1.419329 | 1.995639 |
| C    | -1.541052 | 3.771330 | 1.512500 |
| C    | -3.586238 | 2.577452 | 1.849029 |
| H    | -3.294198 | 0.456834 | 2.179769 |
| C    | -2.926328 | 3.771228 | 1.594126 |
| H    | -4.663737 | 2.531417 | 1.933129 |
| H    | -3.479354 | 4.694005 | 1.467134 |
| H    | 1.050800  | 4.567005 | 1.322732 |
| H    | -1.012665 | 4.694229 | 1.325691 |
| Cl   | -2.048865 | -1.702683| 1.803122 |
| Cl   | 1.271005  | -1.915007| 1.731233 |
| Cl   | -0.220298 | -0.014404| 4.404030 |
| H2   | -0.291866 | 0.557938 | -0.881918|
| H2   | -0.392402 | -0.179592| -0.849131|
| H2   | 1.947245  | 2.899786 | 4.586526 |
| H2   | 1.489880  | 2.315878 | 4.666398 |
| H2   | -1.972709 | 3.157665 | 4.657501 |
| H2   | -1.615006 | 2.503407 | 4.672811 |

**PHEN**

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 0.602776 | 2.439787 | 1.650093 |
| C    | 1.378558 | 3.609470 | 1.505337 |
| C    | 2.779919 | 3.458409 | 1.524907 |
| C    | 3.322803 | 2.204424 | 1.684383 |
| C    | 2.473311 | 1.094507 | 1.819357 |
| H    | 3.414285 | 4.331359 | 1.420802 |
| H    | 4.393926 | 2.054660 | 1.712292 |
| H    | 2.856260 | 0.089599 | 1.947693 |
| N    | 1.152760 | 1.208821 | 1.796555 |
| Cr   | -0.291543| -0.377534| 2.136931 |
|   |   |   |   |
|---|---|---|---|
| N | -1.526890 | 1.379357 | 1.820099 |
| C | -0.827240 | 2.531329 | 1.663721 |
| C | -2.851092 | 1.433842 | 1.868209 |
| C | -1.450689 | 3.790417 | 1.533335 |
| C | -3.554159 | 2.643350 | 1.750069 |
| H | -3.355509 | 0.484921 | 2.003164 |
| C | -2.859223 | 3.818532 | 1.579976 |
| H | -4.634915 | 2.631490 | 1.797884 |
| C | -3.379849 | 4.764977 | 1.487352 |
| H | 0.718295  | 4.873182 | 1.360943 |
| C | -0.637838  | 4.960023 | 1.374558 |
| Cl | -2.081147 | -1.744404 | 1.899226 |
| Cl | 1.305053  | -1.961585 | 1.826556 |
| Cl | -0.227579 | 0.050269  | 4.334405 |
| H2 | -0.571283 | -0.077131 | -0.345750 |
| H2 | 0.047880  | -0.494915 | -0.297536 |
| H | -1.128795 | 5.920433  | 1.270785 |
| H | 1.325291  | 5.763418  | 1.246153 |
| C | 0.611703  | 2.424534  | 1.646181 |
| C | 1.390632  | 3.587732  | 1.474184 |
| C | 2.790956  | 3.431885  | 1.486566 |
| C | 3.329425  | 2.178798  | 1.666544 |
| C | 2.477224  | 1.075937  | 1.829514 |
| H | 3.429042  | 4.299158  | 1.361021 |
| H | 4.400184  | 2.024858  | 1.688176 |
| H | 2.859100  | 0.073056  | 1.971093 |
| N | 1.156773  | 1.194444  | 1.814904 |
| Cr | -0.286014 | -0.376535 | 2.185867 |
| N | -1.516680 | 1.375246  | 1.860979 |
| C | -0.816818 | 2.521376  | 1.670762 |
| C | -2.839969 | 1.435773  | 1.923309 |
| C | -1.437659 | 3.779444  | 1.524333 |
| C | -3.540849 | 2.644088  | 1.789326 |
| H | -3.347943 | 0.492915  | 2.080506 |
| C | -2.844759 | 3.813726  | 1.587420 |
| H | -4.620710 | 2.635990  | 1.850272 |
| H | -3.363937 | 4.759633  | 1.483261 |
| C | 0.733404  | 4.851007  | 1.316736 |
| C | -0.621976 | 4.942995  | 1.340744 |
| Cl | -2.064199 | -1.727857 | 1.858147 |
| Cl | 1.279922  | -1.952452 | 1.766291 |
| Cl | -0.204984 | 0.047200  | 4.385188 |
| H2 | -0.222608 | 0.311024  | -0.961375 |
| H2 | 0.185695  | -0.289728 | -0.792916 |
| H2 | -0.016690 | 3.712186  | 4.511902 |
| H2 | -0.052457 | 2.968928  | 4.565810 |
| H | -1.109868 | 5.903811  | 1.227975 |
| H | 1.342289  | 5.737408  | 1.184588 |
| C | 0.603558  | 2.435983  | 1.655284 |
| C | 1.379458  | 3.597005  | 1.457521 |
| C | 2.779913  | 3.446224  | 1.481171 |
| C | 3.321365  | 2.200736  | 1.700178 |
|   |   |   |   |
|---|---|---|---|
| C | 2.471847 | 1.099181 | 1.883540 |
| H | 3.415771  | 4.312175  | 1.335591  |
| H | 4.392229  | 2.050533  | 1.734790  |
| H | 2.856842  | 0.101447  | 2.049416  |
| N | 1.151154  | 1.211850  | 1.853260  |
| Cr| -0.290917 | -0.366597 | 2.198365  |
| N | -1.522189 | 1.383564  | 1.879975  |
| C | -0.825596 | 2.528070  | 1.669646  |
| C | -2.846055 | 1.441327  | 1.934942  |
| C | -1.450180 | 3.779357  | 1.486015  |
| C | -3.550056 | 2.643088  | 1.767200  |
| H | -3.352195 | 0.500868  | 2.109983  |
| C | -2.857675 | 3.809419  | 1.537773  |
| H | -4.630450 | 2.630978  | 1.822627  |
| H | -3.379610 | 4.750173  | 1.403864  |
| C | 0.718198  | 4.853120  | 1.260891  |
| C | -0.637333 | 4.940628  | 1.274578  |
| Cl| -2.063759 | -1.717804 | 1.845979  |
| Cl| 1.281860  | -1.928655 | 1.754720  |
| Cl| -0.224553 | 0.004635  | 4.407096  |
| H2| -0.337832 | 0.330092  | -0.920027 |
| H2| 0.205822  | -0.154479 | -0.763995 |
| H2| 1.758232  | 3.041101  | 4.497148  |
| H2| 1.379023  | 2.403634  | 4.573007  |
| H2| -1.908054 | 3.214510  | 4.605694  |
| H2| -1.594835 | 2.538074  | 4.625191  |
| H | 1.324589  | 5.737954  | 1.107328  |
| H | -1.128341 | 5.896123  | 1.132514  |
| C | 0.597010  | 2.436385  | 1.652101  |
| C | 1.371504  | 3.603867  | 1.486253  |
| C | 2.772650  | 3.453075  | 1.497213  |
| C | 3.315636  | 2.200560  | 1.667262  |
| C | 2.467694  | 1.093005  | 1.821348  |
| H | 3.407593  | 4.323340  | 1.376484  |
| H | 4.386915  | 2.050047  | 1.687207  |
| H | 2.853333  | 0.090325  | 1.954054  |
| N | 1.146641  | 1.206493  | 1.809350  |
| Cr| -0.290404 | -0.371328 | 2.189276  |
| N | -1.527610 | 1.375427  | 1.850048  |
| C | -0.832428 | 2.526771  | 1.673607  |
| C | -2.851738 | 1.429381  | 1.899419  |
| C | -1.458199 | 3.782685  | 1.527116  |
| C | -3.557246 | 2.635100  | 1.766693  |
| H | -3.356679 | 0.483170  | 2.045897  |
| C | -2.866195 | 3.809640  | 1.578269  |
| H | -4.637994 | 2.620160  | 1.816094  |
| H | -3.389647 | 4.752909  | 1.471545  |
| C | 0.708925  | 4.864547  | 1.327453  |
| C | -0.646883 | 4.950193  | 1.346595  |
| Cl| -2.061856 | -1.729979 | 1.854808  |
| Cl| 1.279874  | -1.938104 | 1.769099  |
| Cl| -0.221388 | 0.076610  | 4.380424  |
| H | -1.138759 | 5.908619  | 1.229971  |
Structure descriptions

Table

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| H    | 1.313942 | 5.753915 | 1.196886 |
| C    | 0.597344  | 2.443739 | 1.658259  |
| C    | 1.371251  | 3.608705 | 1.480857  |
| C    | 2.771881  | 3.459302 | 1.502323  |
| C    | 3.315141  | 2.210034 | 1.690782  |
| C    | 2.467331  | 1.104096 | 1.852724  |
| H    | 3.406424  | 4.328724 | 1.373339  |
| H    | 4.386179  | 2.060252 | 1.717630  |
| H    | 2.853312  | 0.103236 | 1.996082  |
| N    | 1.146733  | 1.216842 | 1.832615  |
| Cr   | -0.292306 | -0.363664 | 2.187611 |
| N    | -1.527279 | 1.384898 | 1.868169  |
| C    | -0.831963 | 2.530606 | 1.671642  |
| C    | -2.851539 | 1.439542 | 1.916221  |
| C    | -1.458078 | 3.785023 | 1.498588  |
| C    | -3.557340 | 2.641412 | 1.753388  |
| H    | -3.356353 | 0.496436 | 2.080845  |
| C    | -2.866154 | 3.811374 | 1.541864  |
| H    | -4.638022 | 2.627004 | 1.803919  |
| H    | -3.389454 | 4.752401 | 1.415018  |
| C    | 0.708758  | 4.866270 | 1.299610  |
| C    | -0.646938 | 4.950531 | 1.305832  |
| Cl   | -2.067996 | -1.723492 | 1.879078  |
| Cl   | 1.277295  | -1.927446 | 1.740987  |
| Cl   | -0.209823 | 0.015196  | 4.395161  |
| H2   | -0.445256 | 0.197298  | -0.921758 |
| H2   | -0.137817 | -0.466897 | -0.781150 |
| H2   | 1.818424  | 3.009472  | 4.552689  |
| H2   | 1.423480  | 2.378725  | 4.598859  |
| H2   | -1.908801 | 3.214747  | 4.574952  |
| H2   | -1.585457 | 2.544235  | 4.618568  |
| H2   | 1.806526  | 2.293994  | -1.077764 |
| H2   | 1.689025  | 1.731830  | -1.549489 |
| H    | 1.314153  | 5.754316  | 1.161239  |
| H    | -1.139204 | 5.906577  | 1.172074  |
| C    | 0.602671  | 2.438739  | 1.649094  |
| C    | 1.378337  | 3.608338  | 1.507636  |
| C    | 2.779291  | 3.457479  | 1.527449  |
| C    | 3.321401  | 2.203339  | 1.684089  |
| C    | 2.472390  | 1.093641  | 1.816036  |
| H    | 3.414196  | 4.329819  | 1.423944  |
| H    | 4.392417  | 2.052918  | 1.710181  |
| H    | 2.855560  | 0.088881  | 1.941639  |
| N    | 1.152484  | 1.207942  | 1.793761  |
| Cr   | -0.291461 | -0.377507 | 2.136204  |
| N    | -1.526579 | 1.378588  | 1.817980  |
| C    | -0.827054 | 2.530109  | 1.662392  |
| C    | -2.850170 | 1.432840  | 1.865596  |
| C    | -1.450591 | 3.788899  | 1.534764  |
| C    | -3.553097 | 2.641700  | 1.749224  |
| H    | -3.354752 | 0.484321  | 1.999659  |
| C    | -2.858729 | 3.816981  | 1.581277  |

S91
Structure descriptions

H  -4.633829  2.629060  1.796626
H  -3.379707  4.763034  1.489765
C   0.717827  4.871635  1.365105
C  -0.637739  4.958228  1.378210
Cl -2.081883  -1.743191  1.900563
Cl  1.305529  -1.960953  1.827500
Cl  -0.227115  0.054860  4.330356
H2  -0.571672  -0.081397  -0.347872
H2   0.047751  -0.498113  -0.299204
H  -1.128288  5.918894  1.277056
H   1.324394  5.762302  1.253122
C   0.612469  2.426349  1.657433
C   1.391236  3.589013  1.477461
C   2.791765  3.432446  1.484222
C   3.329952  2.179222  1.663439
C   2.477774  1.076786  1.831361
H   3.429828  4.298830  1.352499
H   4.400644  2.024019  1.679422
H   2.859773  0.073529  1.969997
N   1.157463  1.195970  1.824167
Cr  -0.286327  -0.376800  2.190200
N  -1.516671  1.376554  1.869646
C  -0.816638  2.523025  1.681243
C  -2.840372  1.436273  1.921087
C  -1.437600  3.780319  1.524328
C  -3.541082  2.643730  1.778236
H  -3.348828  0.493180  2.075396
C  -2.845422  3.813539  1.577741
H  -4.621800  2.638554  1.829663
H  -3.365073  4.758142  1.464364
C   0.733520  4.851102  1.309824
C  -0.621822  4.942818  1.331982
Cl  -2.065322  -1.727157  1.860587
Cl   1.279229  -1.949895  1.756285
Cl  -0.204949  0.040037  4.387538
H2  -0.226946  0.324638  -0.954858
H2   0.184205  -0.274735  -0.789014
H  -1.109883  5.902506  1.209752
H   1.341968  5.736700  1.169842
C   0.611511  2.423181  1.638994
C   1.390853  3.587311  1.476128
C   2.790910  3.431408  1.492011
C   3.328960  2.176958  1.665029
C   2.476831  1.073042  1.819046
H   3.429492  4.299376  1.374189
H   4.399569  2.022449  1.689134
H   2.858283  0.069065  1.953557
N   1.155701  1.191329  1.800694
Cr  -0.284873  -0.378828  2.187295
N  -1.515338  1.372398  1.854374
C  -0.817029  2.519882  1.666561
C  -2.838809  1.433465  1.921764
Structure descriptions

C  -1.437917  3.778622  1.527920
C  -3.539527  2.642148  1.793968
H  -3.346873  0.490283  2.076137
C  -2.844554  3.812930  1.595552
H  -4.619570  2.632970  1.857874
H  -3.364369  4.759083  1.497294
C   0.733337  4.851390  1.325169
C  -0.621993  4.943020  1.349624
Cl  -2.062270 -1.728829  1.854116
Cl   1.278974 -1.953564  1.772362
Cl  -0.208571  0.059548  4.383247
H  -1.109711  5.904459  1.241475
H   1.341739  5.738774  1.197489
H2  -0.006814  3.722460  4.499474
H2  -0.045311  2.979669  4.558024

\textbf{MnCl}_2—\textbf{H}_2

BBH

C   2.186652  2.727725  0.117646
C   1.501736  2.144179  1.195596
C   0.129504  2.307073  1.328079
C  -0.575432  3.042317  0.377400
C   0.094326  3.604068  -0.709639
C   1.465290  3.448726  -0.846525
C   3.627921  2.548895  0.057280
H   2.050295  1.575131  1.938393
H  -0.388695  1.863041  2.169233
H  -1.646846  3.169658  0.477673
H  -0.452767  4.162327  -1.459136
N   4.421722  3.264505  -0.654594
C   6.672533  3.693127  -1.251452
N   5.752776  2.921549  -0.614732
H   4.040746  1.755788  0.688595
H   6.026767  2.047431  -0.183866
O   6.337719  4.716206  -1.867871
C  10.766030  2.469577  -1.198177
C  10.272064  3.277663  -2.220473
C   8.940478  3.672190  -2.16287
C   8.087590  3.245630  -1.93148
C   8.590423  2.443550  -0.161335
C   9.925979  2.059154  -0.165394
H  11.806516  2.167646  -1.200463
H  10.926430  3.603394  -3.019671
H   8.543798  4.307072  -2.997532
H   7.963825  2.150675  0.673375
H  10.313175  1.450246  0.642316
H   1.961303  3.860283  -1.716586
Mn   4.297460  5.435939  -1.727368
Cl   4.073913  6.654156  0.186090
Cl   3.180506  5.157226  -3.704445
H2   5.531568  7.482402  -3.229465
H2   5.699997  7.739494  -2.548893

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Structure descriptions

C  2.178957  2.702809  0.110186
C  1.487167  2.111020  1.179308
C  0.115188  2.278546  1.307837
C -0.582657  3.026915  0.361983
C  0.093802  3.596782 -0.716386
C  1.464384  3.435654 -0.849760
C  3.620479  2.522083  0.054284
H  2.030937  1.532765  1.918456
H -0.408538  1.828406  2.142268
H -1.653795  3.158430  0.459536
H -0.447522  4.167626 -1.460285
N  4.418195  3.250138 -0.639869
C  6.670215  3.685759 -1.227873
N  5.748604  2.906485 -0.601709
H  4.029226  1.716473  0.672344
H  6.020212  2.022320 -0.190352
O  6.337930  4.717721 -1.829181
C  10.761070  2.456040 -1.191820
C  10.266487  3.271065 -2.207163
C  8.935675  3.677750 -2.197309
C  8.083956  3.234659 -1.175841
C  8.587241  2.423920 -0.151116
C  9.922266  2.037652 -0.160639
H  11.801143  2.151365 -1.198058
H  10.919709  3.601698 -3.005253
H  8.537931  4.308955 -2.972828
H  7.961511  2.126062  0.682441
H  10.310213  1.422455  0.641896
H  1.966655  3.850628 -1.714399
Mn 4.291942  5.427205 -1.698704
Cl 4.119241  6.28914  0.234680
Cl 3.283652  5.066785 -3.724611
H2 1.463838  6.801186 -1.255115
H2 1.345914  6.16704 -1.967392
H2 5.463940  7.507227 -3.054262
H2 5.629433  7.767765 -2.525338

C  2.177785  2.705769  0.086122
C  1.499144  2.151196  1.182891
C  0.131413  2.337905  1.330627
C -0.575162  3.069117  0.377969
C  0.088287  3.602808 -0.726769
C  1.454472  3.421950 -0.879903
C  3.616568  2.510142  0.011486
H  2.048372  1.588095  1.928812
H -0.381889  1.916670  2.186386
H -1.642738  3.216007  0.491339
H -0.459548  4.160645 -1.475890
N  4.406350  3.212476 -0.717119
C  6.656881  3.654990 -1.304214
N  5.736070  2.871226 -0.683941
H  4.029799  1.722820  0.648706
H  6.019981  2.030997 -0.196536

S94
| Element | X    | Y    | Z    |
|---------|------|------|------|
| Mn      | 4.284387 | 5.418425 | -1.655046 |
| Cl      | 4.113015 | 6.572206 | 0.312993  |
| Cl      | 3.300612 | 5.112705 | -3.706961 |
| H2      | 5.524423 | 3.898888 | 2.346458  |
| H2      | 5.211194 | 4.441708 | 1.939931  |
| H2      | 1.564277 | 6.922103 | -1.267398 |
| H2      | 1.451438 | 6.735595 | -1.980086 |
| H2      | 5.470799 | 7.540303 | -3.104870 |
| H2      | 5.632248 | 7.789352 | -2.419609 |
| C       | 2.163629 | 2.801255 | 0.089475  |
| C       | 1.460832 | 2.222865 | 1.158908  |
| C       | 0.092012 | 2.414507 | 1.286722  |
| C       | -0.592253 | 3.172944 | 0.339114  |
| C       | 0.094425  | 3.729168 | -0.740157 |
| C       | 1.462380 | 3.545045 | -0.872517 |
| C       | 3.600752  | 2.589769 | 0.033661  |
| H       | 1.994064 | 1.635144 | 1.898262  |
| H       | -0.439633 | 1.975573 | 2.122049  |
| H       | -1.661104 | 3.322419 | 0.435466  |
| N       | 4.417726 | 3.296812 | -0.661348 |
| C       | 6.682499 | 3.665693 | -1.252709 |
| N       | 5.738797 | 2.916487 | -0.621993 |
| H       | 3.990934 | 1.775155 | 0.651756  |
| H       | 5.984918 | 2.026203 | -0.207997 |
| O       | 6.377995 | 4.702955 | -1.860626 |
| C       | 10.734782 | 2.313764 | -1.204636 |
| C       | 10.266843 | 3.140814 | -2.239555 |
| C       | 8.948538 | 3.577446 | -2.218110 |
| C       | 8.082476 | 3.174508 | -1.196249 |
| C       | 8.559813 | 2.353425 | -0.167079 |
| C       | 9.882311 | 1.926584 | -0.172973 |
| H       | 11.765141 | 1.979057 | -1.208016 |
| H       | 10.931082 | 3.448195 | -3.022156 |
| H       | 8.571729 | 4.226923 | -2.997122 |
| H       | 7.924563 | 2.078199 | 0.667039  |
| H       | 10.250347 | 1.303267 | 0.632612  |
| Mn      | 4.346025 | 5.458400 | -1.720687 |
| Cl      | 4.173620 | 6.746346 | 0.145924  |
| Cl      | 3.257906 | 5.220920 | -3.715403 |

**PIP**

| Element | X    | Y    | Z    |
|---------|------|------|------|
| H2      | 2.711114 | 0.269673 | 0.592271  |
| H2      | 2.489248 | 0.629838 | -0.023700 |
| C       | 6.421972 | 3.062684 | 2.232289  |
| C       | 6.946693 | 3.438518 | 3.480854  |
| C       | 6.155718 | 3.509944 | 4.615553  |
| C       | 4.796254 | 3.221132 | 4.517675  |
| C       | 4.240631 | 2.874386 | 3.292313  |
| C       | 5.040648 | 2.798903 | 2.159999  |
| C       | 7.358704 | 2.980841 | 1.118405  |
Structure descriptions

H  8.005526  3.659615  3.550625
H  6.590613  3.787008  5.566829
H  4.162786  3.269289  5.394777
H  3.181095  2.657433  3.212270
N  7.173792  2.392853 -0.007749
C 10.239945  2.267590 -2.890541
C 10.546133  2.015855 -1.554910
C  9.549913  2.064503 -0.586114
C  8.236974  2.370137 -0.956917
C  7.921350  2.594228 -2.29756
C  8.926593  2.553022 -3.258543
H 11.017776  2.222656 -3.643164
H 11.559579  2.176178 -1.267099
H  9.778194  1.819760  0.44079
H  6.892261  2.784854 -2.579067
H  8.678278  2.736944 -4.297197
H  8.316992  3.473630  1.301866
O  4.493123  2.504304  0.933240
Mn 5.520061  0.968814 -0.473361
Cl  4.376706  1.430893 -2.391179
Cl  5.749239 -0.706231  1.068274
H  3.547580  2.309747  1.020924
H2  7.439192 -0.838693 -1.532552
H2  7.550935 -0.379716 -2.110789
H2  5.380947  5.337733 -0.417072
H2  5.180842  4.627188 -0.514946
H2  5.394876  0.640565  3.560450
H2  5.225842  1.099151  4.123977
C  5.821651  3.304611  1.849927
C  5.902997  3.970897  3.084660
C  4.789244  4.172285  3.882600
C  3.546312  3.719329  3.446108
C  3.427439  3.075369  2.220719
C  4.549538  2.870832  1.429770
C  7.064541  3.132279  1.107251
H  6.872547  4.321517  3.418926
H  4.885500  4.676988  4.834984
H  2.665052  3.865998  4.058057
H  2.461156  2.721876  1.877994
N  7.269941  2.350680  0.109578
C 11.083503  2.102065 -1.659883
C 10.975967  2.131480 -0.270926
C  9.727537  2.182368  0.334253
C  8.576392  2.281703 -0.468101
C  8.679616  2.219505 -1.851287
C  9.933645  2.141304 -2.445486
H 12.058238  2.029271 -2.126850
H 11.864991  2.067433  0.344931
H  9.640478  2.190632  1.413463
H  7.777544  2.231898 -2.452180
H  7.100927  2.103006 -3.525243
H  7.891369  3.746904  1.471603
O  4.441941  2.267607  0.197948
|   |   |   |   |
|---|---|---|---|
| Mn | 5.947120 | 0.696133 | -0.577057 |
| Cl | 5.289026 | 0.795724 | -2.755226 |
| Cl | 6.011930 | -0.813442 | 1.125740 |
| H  | 3.516134 | 2.098664 | -0.030582 |
| H2 | 5.526454 | 4.394874 | -1.902169 |
| H2 | 5.408902 | 3.679073 | -2.074260 |
| C  | 5.827849 | 3.314249 | 1.835227 |
| C  | 5.916620 | 4.018544 | 3.048589 |
| C  | 4.816215 | 4.210041 | 3.866766 |
| C  | 3.578266 | 3.707378 | 3.471841 |
| C  | 3.450698 | 3.029716 | 2.266384 |
| C  | 4.559877 | 2.835220 | 1.453556 |
| C  | 7.062531 | 3.145719 | 1.079667 |
| H  | 6.883178 | 4.404820 | 3.350729 |
| H  | 4.918709 | 4.744411 | 4.802065 |
| H  | 2.706630 | 3.845046 | 4.099569 |
| H  | 2.486819 | 2.644110 | 1.952950 |
| N  | 7.273924 | 2.342854 | 0.100518 |
| C  | 11.082325 | 2.141032 | -1.684331 |
| C  | 10.974666 | 2.148885 | -0.295829 |
| C  | 9.726060 | 2.193773 | 0.311721 |
| C  | 8.578012 | 2.300623 | -0.477952 |
| C  | 8.679694 | 2.299481 | -1.871570 |
| C  | 9.933138 | 2.230694 | -2.467673 |
| H  | 12.056075 | 2.073602 | -2.154174 |
| H  | 11.862408 | 2.016040 | 0.317253 |
| H  | 9.634703 | 2.126483 | 1.389016 |
| H  | 7.777727 | 2.341483 | -2.469528 |
| H  | 10.009336 | 2.237339 | -3.548068 |
| H  | 7.882799 | 3.785369 | 1.415061 |
| O  | 4.433872 | 2.202502 | 0.241251 |
| Mn | 5.966068 | 0.672875 | -0.564368 |
| Cl | 5.383306 | 0.804021 | -2.771055 |
| Cl | 5.860908 | -0.828148 | 1.158435 |
| H  | 3.526635 | 1.886946 | 0.110160 |
| H2 | 8.219739 | -1.007531 | -0.820268 |
| H2 | 8.434855 | -0.600647 | -1.408922 |
| H2 | 2.990988 | -0.230952 | -0.255652 |
| H2 | 2.942405 | 0.031328 | -0.953789 |
| H2 | 5.371441 | 1.160014 | 4.172495 |
| H2 | 5.485546 | 0.686700 | 3.607425 |
| H2 | 8.491329 | -0.628355 | -1.243052 |
| H2 | 8.233086 | -1.005789 | -0.652519 |
| C  | 5.845649 | 3.258592 | 1.847916 |
| C  | 5.925220 | 3.861273 | 3.115104 |
| C  | 4.808081 | 4.026491 | 3.917003 |
| C  | 3.565050 | 3.603261 | 3.451092 |
| C  | 3.448178 | 3.027035 | 2.191847 |
| C  | 4.573188 | 2.858553 | 1.396452 |
| C  | 7.088836 | 3.115750 | 1.099026 |
| H  | 6.894959 | 4.189708 | 3.471048 |
| H  | 4.901687 | 4.480694 | 4.894786 |
Structure descriptions

SP-JLMC

H2  5.449908  3.803564  -1.793236
C  5.854765  3.236999  1.918279
C  5.958967  3.906322  3.150667
C  4.861721  4.107255  3.971559
C  3.610969  3.649764  3.562610
C  3.469240  2.999432  2.342717
C  4.575444  2.794733  1.528701
C  7.080798  3.087622  1.142695
H  6.933245  4.265048  3.461630
H  4.976565  4.617238  4.919034
H  2.741465  3.798674  4.190683
H  2.497153  2.642342  2.020874
N  7.269389  2.332617  0.122326
C  11.038157  2.197619  -1.751998
C  10.966105  2.173047  -0.360632
C  9.732635  2.221489  0.278767
C  8.560964  2.299491  -0.481095
C  8.628648  2.291440  -1.877534
C  9.867890  2.251953  -2.505958
H 12.001313  2.155008  -2.245766
H 11.871367  2.098475  0.229689
H  9.673723  2.153021  1.358032
H  7.712093  2.318925  -2.454779
H  9.915615  2.256372  -3.587878
H  7.909870  3.703264  1.499139
O  4.441238  2.179994  0.306086
Mn  5.941449  0.693188  -0.594649
Cl  5.188995  0.957243  -2.732156
Cl  6.104011  -0.908208  1.002621
H  3.510064  2.025813  0.089649
H2  5.521831  4.602301  -1.608061
H2  5.405074  3.898938  -1.826256
C  5.854499  3.199068  1.943245
C  5.961636  3.16610  3.201596
C  4.860283  4.017156  4.016948
C  3.603111  3.608726  3.577189
C  3.458968  3.009143  2.331851
C  4.568882  2.806858  1.522152
C  7.087673  3.035220  1.182771
H  6.942025  4.132962  3.538283
H  4.977273  4.486704  4.984829
H  2.730280  3.756188  4.201180
H  2.481415  2.690802  1.986311
N  7.263401  2.322927  0.130438
C 11.065952  2.066496  -1.656853
C 10.952856  1.95821  -0.272340
C  9.707131  2.047701  0.338708
C  8.566591  2.250531  -0.444448
C  8.672381  2.326002  -1.836593
C  9.924146  2.245742  -2.435141
H 12.038167  1.991337  -2.128704
H 11.834310  1.786504  0.333569
H  9.608301  1.912489  1.408479

S100
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| H    | 7.774987 | 2.445916 | -2.432008 |
| H    | 10.004333 | 2.314172 | -3.513079 |
| H    | 7.937189  | 3.591488 | 1.586000 |
| O    | 4.431530  | 2.244358 | 0.279482 |
| Mn   | 5.911080  | 0.770657 | -0.682382 |
| Cl   | 5.202925  | 1.126013 | -2.821045 |
| Cl   | 6.034123  | -0.900147 | 0.859196 |
| H    | 3.499162  | 2.113050 | 0.048932 |
| H2   | 7.645452  | 0.484740 | 2.792700 |
| H2   | 8.028333  | 0.865293 | 3.308557 |
| H2   | 5.388799  | 0.664243 | 3.642855 |
| H2   | 5.255896  | 1.120016 | 4.218081 |
| C    | 5.836149  | 3.289741 | 1.849484 |
| C    | 5.917694  | 3.951663 | 3.086574 |
| C    | 4.805542  | 4.143795 | 3.888612 |
| C    | 3.563956  | 3.685384 | 3.453453 |
| C    | 3.444591  | 3.049003 | 2.224577 |
| C    | 4.564837  | 2.854477 | 1.427747 |
| C    | 7.076711  | 3.128942 | 1.101136 |
| H    | 6.886681  | 4.304872 | 3.419812 |
| H    | 4.901853  | 4.644537 | 4.843036 |
| H    | 2.683552  | 3.824226 | 4.068500 |
| H    | 2.478602  | 2.694245 | 1.882185 |
| N    | 7.286001  | 2.347756 | 0.103617 |
| C    | 11.086292 | 2.149427 | -1.698070 |
| C    | 10.987357 | 2.139781 | -0.308506 |
| C    | 9.742464  | 2.216268 | 0.306380 |
| C    | 8.587959  | 2.306039 | -0.476666 |
| C    | 8.681589  | 2.286390 | -1.870972 |
| C    | 9.931433  | 2.219453 | -2.479444 |
| H    | 12.057594 | 2.083212 | -2.173064 |
| H    | 11.879701 | 2.054799 | 0.299954 |
| H    | 9.661209  | 2.159307 | 1.385023 |
| H    | 7.775248  | 2.311035 | -2.464673 |
| H    | 10.000062 | 2.210773 | -3.555790 |
| H    | 7.898811  | 3.754912 | 1.457397 |
| O    | 4.455040  | 2.262828 | 0.189926 |
| Mn   | 5.969694  | 0.681741 | -0.569743 |
| Cl   | 5.350656  | 0.762103 | -2.760861 |
| Cl   | 5.846824  | -0.785926 | 1.176056 |
| H    | 3.531204  | 2.062955 | -0.017476 |
| H2   | 8.243698  | -1.012505 | -0.748582 |
| H2   | 8.497834  | -0.609686 | -1.323807 |
| H2   | 5.540805  | 4.485544 | -1.830464 |
| H2   | 5.414562  | 3.770404 | -1.998376 |
| C    | 5.811703  | 3.320855 | 1.842235 |
| C    | 5.892249  | 4.019390 | 3.059217 |
| C    | 4.779959  | 4.235556 | 3.853499 |
| C    | 3.538095  | 3.765331 | 3.434175 |
| C    | 3.419791  | 3.088686 | 2.226612 |
| C    | 4.541115  | 2.867070 | 1.439059 |
| C    | 7.055056  | 3.137224 | 1.103309 |
Structure descriptions

H  6.860687  4.384533  3.380932
H  4.876197  4.765915  4.793669
H  2.657445  3.924413  4.043918
N  7.263712  2.341326  0.118262
C 11.081103  2.084006 -1.641292
C 10.969938  2.117538 -0.252784
C  9.719869  2.208053  0.348623
C  8.571336  2.270107 -0.447218
C  8.677964  2.205803 -1.840006
C  9.933615  2.12926  -2.430263
H 12.056959  2.008836 -2.105548
H 11.857138  2.054068  0.365740
H  9.628715  2.183426  1.427560
H  7.778229  2.222743 -2.443784
H 10.012450  2.084454 -3.509754
H  7.880774  3.758485  1.458534
O  4.432317  2.220118  0.230860
Mn 5.953099  0.689454  -0.517265
Cl 5.252455  0.848213  -2.739089
Cl 6.075790 -0.869681  1.079814
H  3.506476  2.049112  0.004342
H2 5.263258  1.100982  4.041472
H2 5.436332  0.629427  3.489882
H2 5.490636  4.355229 -1.959377
H2 5.338734  3.627245 -2.007602
C  5.869539  3.344006  1.829166
C  5.996422  4.041656  3.042654
C  4.916967  4.246028  3.885743
C  3.662834  3.764090  3.516915
C  3.498553  3.089006  2.313524
C  4.587078  2.881188  1.476913
C  7.079068  3.173858  1.033436
H  6.974816  4.413974  3.323021
H  5.048209  4.775202  4.820451
H  2.807397  3.913659  4.163986
H  2.523243  2.714362  2.022945
N  7.255183  2.359317  0.057716
C 10.978641  2.128872 -1.891621
C 10.936750  2.163000 -0.499688
C  9.717369  2.254005  0.162926
C  8.531580  2.308294 -0.575354
C  8.567820  2.241857 -1.970835
C  9.792624  2.164005 -2.622714
H 11.930214  2.054699 -2.403859
H 11.853935  2.108635  0.073955
H  9.676530  2.229769  1.244644
H  7.637808  2.243445 -2.526295
H  9.818025  2.120754 -3.704585
H  7.907207  3.821076  1.331361
O  4.433140  2.246130  0.266925
Mn 5.929199  0.655572 -0.482122
Cl  5.188043  0.680784 -2.638785
Structure descriptions

| Atom | x     | y     | z     |
|------|-------|-------|-------|
| Cl   | 5.926710 | -0.709498 | 1.349140 |
| H    | 5.502532 | 2.039794 | 0.096006 |
| H2   | 7.805429 | 0.850849 | 2.901317 |
| H2   | 8.274147 | 1.261141 | 3.312685 |
| H2   | 8.218080 | -1.019852 | -0.708429 |
| H2   | 8.444165 | -0.621895 | -1.299095 |
| H2   | 5.581167 | 4.456871 | -1.891297 |
| H2   | 5.439556 | 3.740259 | -2.039263 |
| C    | 5.829872 | 3.299929 | 1.840884 |
| C    | 5.911352 | 3.986451 | 3.064663 |
| C    | 4.800701 | 4.188109 | 3.866517 |
| C    | 3.560167 | 3.715068 | 3.442220 |
| C    | 3.440601 | 3.053381 | 2.228764 |
| C    | 4.559759 | 2.848136 | 1.433374 |
| C    | 7.070405 | 3.130999 | 1.994339 |
| H    | 6.879264 | 4.352119 | 3.387370 |
| H    | 4.897124 | 4.708328 | 4.810447 |
| H    | 2.680881 | 3.861695 | 4.059046 |
| H    | 2.475849 | 2.686091 | 1.896405 |
| N    | 7.283683 | 2.336231 | 0.109074 |
| C    | 11.086009 | 2.147796 | -1.689618 |
| C    | 10.985171 | 2.131406 | -0.300309 |
| C    | 9.739247 | 2.205496 | 0.313047 |
| C    | 8.586359 | 2.298014 | -0.471532 |
| C    | 8.681567 | 2.286428 | -1.865677 |
| C    | 9.932418 | 2.222875 | -2.467869 |
| H    | 12.057973 | 2.084272 | -2.163642 |
| H    | 11.876591 | 2.043438 | 0.309078 |
| H    | 9.655103 | 2.144208 | 1.391246 |
| H    | 7.776450 | 2.318339 | -2.460097 |
| H    | 10.002952 | 2.221914 | -3.548644 |
| H    | 7.890067 | 3.765866 | 1.439959 |
| O    | 4.449241 | 2.229076 | 0.211650 |
| Mn   | 5.977473 | 0.670805 | -0.562763 |
| Cl   | 5.330243 | 0.807920 | -2.747365 |
| Cl   | 5.870759 | -0.828422 | 1.155114 |
| H    | 3.525767 | 2.021491 | 0.007904 |
| H2   | 8.245050 | -1.023074 | -0.783191 |
| H2   | 8.499466 | -0.608350 | -1.349896 |
| H2   | 5.290553 | 1.141835 | 4.162210 |
| H2   | 5.420428 | 0.672289 | 3.597384 |
| H2   | 5.581167 | 4.456871 | -1.891297 |
| H2   | 5.439556 | 3.740259 | -2.039263 |
| C    | 5.829872 | 3.299929 | 1.840884 |
| C    | 5.911352 | 3.986451 | 3.064663 |
| C    | 4.800701 | 4.188109 | 3.866517 |
| C    | 3.560167 | 3.715068 | 3.442220 |
| C    | 3.440601 | 3.053381 | 2.228764 |
| C    | 4.559759 | 2.848136 | 1.433374 |
| C    | 7.070405 | 3.130999 | 1.094439 |
| H    | 6.879264 | 4.352119 | 3.387370 |
| H    | 4.897124 | 4.708328 | 4.810447 |
Structure descriptions

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| H    | 2.680881 | 3.861695 | 4.059046 |
| H    | 2.475849 | 2.686091 | 1.896405 |
| N    | 11.086009 | 2.147796 | -1.689618 |
| C    | 10.985171 | 2.131406 | -0.300309 |
| C    | 9.7939247 | 2.205496 | 0.313047 |
| C    | 8.586359 | 2.298014 | -0.471532 |
| C    | 8.681567 | 2.286428 | -1.865677 |
| C    | 9.932418 | 2.222875 | -2.467869 |
| H    | 12.057973 | 2.084272 | -2.163642 |
| H    | 11.876591 | 2.043438 | 0.309078 |
| H    | 9.655103 | 2.144208 | 1.391246 |
| H    | 7.776450 | 2.318339 | -2.460097 |
| H    | 10.002952 | 2.221914 | -3.548644 |
| H    | 7.890067 | 3.765866 | 1.439959 |
| O    | 4.449241 | 2.229076 | 0.211650 |
| Mn   | 5.977473 | 0.670805 | -0.562763 |
| Cl   | 5.330243 | 0.807920 | -2.747365 |
| Cl   | 5.870759 | -0.828422 | 1.155114 |
| H    | 3.525767 | 2.021491 | 0.007094 |
| H2   | 8.245050 | -1.023074 | -0.783191 |
| H2   | 8.499466 | -0.608350 | -1.349896 |
| H2   | 5.290553 | 1.141835 | 4.162210 |
| H2   | 5.420428 | 0.672289 | 3.597384 |
| H2   | 5.540360 | 4.461790 | -1.810079 |
| H2   | 5.423830 | 3.743218 | -1.969554 |
| C    | 5.823672 | 3.314845 | 1.832096 |
| C    | 5.912435 | 4.024693 | 3.041960 |
| C    | 4.811824 | 4.220201 | 3.859189 |
| C    | 3.573784 | 3.716614 | 3.466039 |
| C    | 3.446173 | 3.033378 | 2.263630 |
| C    | 4.555669 | 2.839522 | 1.452613 |
| C    | 7.058536 | 3.143785 | 1.076809 |
| H    | 6.879011 | 4.411844 | 3.542937 |
| C    | 4.914245 | 4.758393 | 4.792297 |
| H    | 2.702059 | 3.857901 | 4.092889 |
| H    | 2.482157 | 2.646263 | 1.952386 |
| N    | 7.270142 | 2.340201 | 0.098457 |
| C    | 11.080767 | 2.107912 | -0.293033 |
| C    | 9.721241 | 2.187604 | 0.312556 |
| C    | 8.574556 | 2.296623 | -0.478805 |
| C    | 8.678512 | 2.297389 | -1.872129 |
| C    | 9.932980 | 2.228175 | -2.466268 |
| H    | 12.055182 | 2.067523 | -2.149755 |
| H    | 11.857271 | 2.007380 | 0.321557 |
| H    | 9.629250 | 2.118945 | 1.389697 |
| H    | 7.777923 | 2.340443 | -2.472061 |
| H    | 10.010539 | 2.235915 | -3.546570 |
| H    | 7.878620 | 3.783809 | 1.412454 |
| O    | 4.431017 | 2.192219 | 0.245175 |
| Mn   | 5.962643 | 0.673305 | -0.563554 |
| Cl   | 5.382370 | 0.817702 | -2.769302 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Cl      | 5.869340| -0.834813| 1.154299|
| H       | 3.520475| 1.889882| 0.107208|
| H2      | 8.230192| -1.026121| -0.826498|
| H2      | 8.483252| -0.600630| -1.385337|
| H2      | 3.041761| -0.279203| -0.236235|
| H2      | 2.979109| -0.021702| -0.934800|
| H2      | 5.362721| 1.161630| 4.158478|
| H2      | 5.482186| 0.686889| 3.595672|
| C       | 5.781976| 3.256385| 1.881683|
| C       | 5.829676| 3.890671| 3.135335|
| C       | 4.713048| 3.988956| 3.949020|
| C       | 3.500603| 3.461254| 3.510662|
| C       | 3.413842| 2.846737| 2.267061|
| C       | 4.538701| 2.747014| 1.459652|
| C       | 7.023521| 3.199409| 1.118225|
| H       | 6.775038| 4.301157| 3.470528|
| H       | 4.783671| 4.472281| 4.914621|
| H       | 2.617600| 3.528387| 4.133941|
| H       | 2.470841| 2.437405| 1.921818|
| N       | 7.271276| 2.457669| 0.100229|
| C       | 11.058479| 2.548173| -1.738541|
| C       | 10.975047| 2.539701| -0.347580|
| C       | 9.735190| 2.514603| 0.280585|
| C       | 8.567914| 2.503205| -0.490432|
| C       | 8.649550| 2.476885| -1.885989|
| C       | 9.894435| 2.512051| -2.503258|
| H       | 12.027045| 2.562314| -2.223370|
| H       | 11.877732| 2.534314| 0.251354|
| H       | 9.671069| 2.458599| 1.360272|
| H       | 7.738254| 2.426918| -2.470413|
| H       | 9.705351| 2.501026| -3.584631|
| H       | 7.805907| 3.868094| 1.584936|
| O       | 4.459433| 2.177103| 0.209052|
| Mn      | 6.054202| 0.712690| -0.583342|
| Cl      | 5.387012| 0.783940| -2.760485|
| Cl      | 6.216686| -0.760017| 1.137391|
| H       | 3.545079| 1.946290| -0.011570|
| PIA     |        |        |         |
| C       | 5.959493| 2.837359| 1.729740|
| C       | 5.692218| 3.647993| 2.831247|
| C       | 4.406503| 3.658587| 3.361131|
| C       | 3.431756| 2.861134| 2.776274|
| C       | 3.780052| 2.076886| 1.678248|
| N       | 5.009178| 2.062687| 1.167001|
| C       | 7.299962| 2.789674| 1.134371|
| H       | 6.479102| 4.256501| 3.259312|
| H       | 4.171970| 4.281088| 4.216057|
| H       | 2.418183| 2.839507| 3.154401|
| H       | 3.053175| 1.441276| 1.187718|
| N       | 7.534868| 2.049086| 0.120371|
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 11.296820 | 1.789421 | -1.724924 |
| C    | 10.868189  | 3.019068 | -1.225618 |
| C    | 9.629842   | 3.130676 | -0.606586 |
| C    | 8.810190   | 2.001518 | -0.487262 |
| C    | 9.223498   | 0.774378 | -1.016274 |
| C    | 10.470442  | 0.671674 | -1.619560 |
| H    | 12.260803  | 1.708548 | -2.210466 |
| H    | 11.493503  | 3.897069 | -1.334217 |
| H    | 9.280851   | 4.096491 | -0.261775 |
| H    | 8.569407   | -0.085805 | -0.927121 |
| H    | 10.792815  | -0.283130 | -2.016255 |
| Mn   | 5.708895   | 0.929022 | -0.670033 |
| Cl   | 6.107113   | -1.273851 | -0.187236 |
| Cl   | 4.897656   | 2.164849 | -2.409339 |
| H2   | 3.074710   | -0.373296 | -0.531578 |
| H2   | 2.885374   | 0.212527 | -0.954490 |
| C    | 5.962982   | 2.834638 | 1.703900 |
| C    | 5.685597   | 3.661842 | 2.789846 |
| C    | 4.399853   | 3.663149 | 3.320464 |
| C    | 3.437236   | 2.839863 | 2.752041 |
| C    | 3.796146   | 2.040948 | 1.667813 |
| N    | 5.024943   | 2.035371 | 1.157093 |
| C    | 7.303492   | 2.791491 | 1.107435 |
| H    | 6.463664   | 4.290402 | 3.204804 |
| H    | 4.156522   | 4.297710 | 4.163986 |
| H    | 2.424427   | 2.810070 | 3.131680 |
| H    | 3.078910   | 1.385484 | 1.189431 |
| N    | 7.544276   | 2.039246 | 0.104006 |
| C    | 11.330871  | 1.771239 | -1.684358 |
| C    | 10.858751  | 3.018288 | -1.278042 |
| C    | 9.610499   | 3.132383 | -0.678120 |
| C    | 8.827742   | 1.987881 | -0.488750 |
| C    | 9.285372   | 0.739909 | -0.923108 |
| C    | 10.541950  | 0.636337 | -1.505181 |
| H    | 12.303180  | 1.687786 | -2.154564 |
| H    | 11.457048  | 3.906368 | -1.442355 |
| H    | 9.223863   | 4.105994 | -0.402147 |
| H    | 8.653470   | -0.129228 | -0.780965 |
| H    | 10.900785  | -0.332811 | -1.829379 |
| H    | 8.079369   | 3.403258 | 1.571265 |
| Mn   | 5.720863   | 0.925484 | -0.698698 |
| Cl   | 6.117888   | -1.277327 | -0.194688 |
| Cl   | 4.793732   | 2.242743 | -2.328478 |
| H2   | 3.108024   | -0.418878 | -0.559623 |
| H2   | 2.904638   | 0.174879 | -0.964791 |
| H2   | 7.195470   | -0.266684 | -3.018217 |
| H2   | 6.954343   | 0.366463 | -3.329787 |
| C    | 5.956994   | 2.848856 | 1.697225 |
| C    | 5.687637   | 3.656055 | 2.799665 |
| C    | 4.409365   | 3.637571 | 3.347903 |
| C    | 3.445258   | 2.817712 | 2.777195 |
|  |  |  |  |
|---|---|---|---|
| C  | 3.794844 | 2.042365 | 1.673009 |
| N  | 5.016745 | 2.052221 | 1.146679 |
| C  | 7.295409 | 2.808703 | 1.097116 |
| H  | 6.467181 | 4.280746 | 3.217602 |
| H  | 4.172728 | 4.254202 | 4.206466 |
| H  | 2.438517 | 2.771706 | 3.171258 |
| H  | 3.075583 | 1.391408 | 1.191554 |
| N  | 7.537004 | 2.052491 | 0.096649 |
| C  | 11.33428 | 1.761211 | -1.668472 |
| C  | 10.866412 | 3.011766 | -1.266586 |
| C  | 9.614715 | 3.134095 | -0.675725 |
| C  | 8.823548 | 1.994944 | -0.489948 |
| C  | 9.276679 | 0.743834 | -0.919685 |
| C  | 10.536297 | 0.631556 | -1.493641 |
| H  | 12.308399 | 1.671270 | -2.132162 |
| H  | 11.471689 | 3.895761 | -1.427248 |
| H  | 9.232950 | 4.110746 | -0.403464 |
| H  | 8.640225 | -0.122367 | -0.780336 |
| H  | 10.890824 | -0.340143 | -1.814866 |
| H  | 8.071991 | 3.418785 | 1.561332 |
| Mn | 5.717193 | 0.938694 | -0.698251 |
| Cl | 6.091432 | -1.266011 | -0.165647 |
| Cl | 4.803914 | 2.235984 | -2.350452 |
| H2 | 2.890989 | 0.203506 | -0.975602 |
| H2 | 3.090981 | -0.390224 | -3.285892 |
| H2 | 6.762388 | -0.155640 | 2.416476 |
| H2 | 6.916495 | 0.196836 | 3.056240 |
| H2 | 7.177661 | -0.303078 | -3.003965 |
| H2 | 6.942965 | 0.328490 | -3.323472 |
| C  | 5.967469 | 2.850181 | 1.725755 |
| C  | 5.699254 | 3.635187 | 2.844657 |
| C  | 4.415306 | 3.624012 | 3.379516 |
| C  | 3.443640 | 2.833060 | 2.780612 |
| C  | 3.792588 | 2.077800 | 1.662618 |
| N  | 5.019946 | 2.083984 | 1.149027 |
| C  | 7.308251 | 2.806825 | 1.132526 |
| H  | 6.483724 | 4.237975 | 3.284966 |
| H  | 4.179796 | 4.223724 | 4.250287 |
| H  | 2.432307 | 2.795017 | 3.163520 |
| H  | 3.067929 | 1.448306 | 1.160188 |
| N  | 7.543666 | 2.072821 | 0.113489 |
| C  | 11.320051 | 1.775236 | -1.694099 |
| C  | 10.900936 | 3.008977 | -1.197724 |
| C  | 9.657237 | 3.133977 | -0.592042 |
| C  | 8.823898 | 2.014249 | -0.482859 |
| C  | 9.230460 | 0.782687 | -1.006688 |
| C  | 10.481710 | 0.666234 | -1.598375 |
| H  | 12.288925 | 1.684426 | -2.170161 |
| H  | 11.537323 | 3.879908 | -1.298491 |
| H  | 9.316342 | 4.103183 | -0.248577 |
| H  | 8.568051 | -0.072021 | -0.924080 |
| H  | 10.797722 | -0.291875 | -1.992028 |
| H  | 8.087642 | 3.398711 | 1.614668 |
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Mn      | 5.724714 | 0.958265 | -0.680101 |
| Cl      | 6.053299 | -1.245697 | -0.165382 |
| Cl      | 4.826933 | 2.121813 | -2.414901 |
| H2      | 6.889613 | 0.188728 | 3.066445 |
| H2      | 6.733478 | -0.159159 | 2.424607 |
| C       | 5.969565 | 2.845430 | 1.699105 |
| C       | 5.684004 | 3.668967 | 2.786012 |
| C       | 4.396726 | 3.659233 | 3.313089 |
| C       | 3.440814 | 2.829967 | 2.741274 |
| C       | 3.808992 | 2.034462 | 1.667577 |
| N       | 5.038378 | 2.040269 | 1.150243 |
| C       | 7.311260 | 2.806588 | 1.104361 |
| H       | 6.455819 | 4.303184 | 3.204148 |
| H       | 4.146529 | 2.991109 | 4.156620 |
| H       | 2.427182 | 2.792987 | 3.118108 |
| H       | 3.095844 | 1.376982 | 1.174119 |
| N       | 7.554455 | 2.059499 | 0.099449 |
| C       | 11.352936 | 1.766325 | -1.661965 |
| C       | 10.890993 | 3.014886 | -1.248235 |
| C       | 9.638808 | 3.137591 | -0.658304 |
| C       | 8.841973 | 2.000137 | -0.485576 |
| C       | 9.290082 | 0.751059 | -0.926710 |
| C       | 10.550128 | 0.638771 | -1.499819 |
| H       | 12.328121 | 1.676446 | -2.124867 |
| H       | 11.500837 | 3.897543 | -1.398769 |
| H       | 9.261464 | 4.113278 | -0.376670 |
| H       | 8.648931 | -0.113332 | -0.795783 |
| H       | 10.900766 | -0.331240 | -1.830331 |
| H       | 8.086507 | 3.416061 | 1.572234 |
| Mn      | 5.740227 | 0.937561 | -0.701946 |
| Cl      | 6.061859 | -1.268515 | -0.182757 |
| Cl      | 4.735947 | 2.219159 | -2.306855 |
| H2      | 6.958167 | 0.360299 | -3.338650 |
| H2      | 7.197094 | -0.272781 | -3.025146 |
| C       | 5.960233 | 2.794787 | 1.744610 |
| C       | 5.646581 | 3.583423 | 2.848887 |
| C       | 4.336003 | 3.599596 | 3.314406 |
| C       | 3.384934 | 2.816987 | 2.665883 |
| C       | 3.781522 | 2.050322 | 1.572096 |
| N       | 5.034476 | 2.036393 | 1.124006 |
| C       | 7.319504 | 2.764166 | 1.193096 |
| H       | 6.414816 | 4.179679 | 3.325257 |
| H       | 4.063236 | 4.201867 | 4.168468 |
| H       | 2.353387 | 2.798761 | 2.992233 |
| H       | 3.074592 | 1.431068 | 1.032894 |
| N       | 7.582286 | 2.064718 | 0.156496 |
| C       | 11.389798 | 1.879558 | -1.593737 |
| C       | 10.943853 | 3.090630 | -1.072137 |
| C       | 9.689000 | 3.176879 | -0.480416 |
| C       | 8.874360 | 2.040634 | -0.418317 |
| C       | 9.307136 | 0.831979 | -0.974127 |
| C       | 10.569004 | 0.754481 | -1.549457 |
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| H    | 12.366833 | 1.81832 | -2.063554 |
| H    | 11.567300 | 3.972491| -1.137159 |
| H    | 9.325400  | 4.128904| -0.113949 |
| H    | 8.656189  | -0.034255| -0.926311 |
| H    | 10.907072 | -0.185749| -1.967357 |
| H    | 8.084753  | 3.345229| 1.710208  |
| Mn   | 5.792032  | 0.952101| -0.702080 |
| Cl   | 6.158604  | -1.260432| -0.267869 |
| Cl   | 4.879361  | 2.147500| -2.418718 |
| H2   | 5.393034  | 5.026440| -0.308307 |
| H2   | 5.285525  | 4.473349| -0.798707 |
| C    | 5.965170  | 2.788425| 1.745715  |
| C    | 5.662144  | 3.544020| 2.875217  |
| C    | 4.354783  | 3.545020| 3.350115  |
| C    | 3.396127  | 2.792654| 2.684264  |
| C    | 3.781500  | 2.061587| 1.562410  |
| N    | 5.031256  | 2.056832| 1.106031  |
| C    | 7.325011  | 2.751245| 1.197556  |
| H    | 6.436825  | 4.119227| 3.366613  |
| H    | 4.090826  | 4.125106| 4.225964  |
| H    | 2.367325  | 2.762655| 3.018470  |
| H    | 3.068278  | 1.462615| 1.008727  |
| N    | 7.583858  | 2.060922| 0.154095  |
| C    | 11.405393 | 1.828271| -1.565733 |
| C    | 10.973623 | 3.042084| -1.033151 |
| C    | 9.715028  | 3.144056| -0.453895 |
| C    | 8.880344  | 2.021018| -0.409657 |
| C    | 9.299546  | 0.809995| -0.970691 |
| C    | 10.565905 | 0.716356| -1.533420 |
| H    | 12.386079 | 1.755067| -2.020093 |
| H    | 11.612061 | 3.915826| -1.084201 |
| H    | 9.362165  | 4.095851| -0.082770 |
| H    | 8.634652  | -0.046050| -0.936019 |
| H    | 10.893262 | -0.225832| -1.955308 |
| H    | 8.095845  | 3.312386| 1.727589  |
| Mn   | 5.785674  | 0.984670| -0.723650 |
| Cl   | 6.107604  | -1.238004| -0.283799 |
| Cl   | 4.911774  | 2.176042| -2.460449 |
| H2   | 5.505324  | 5.027424| -0.345166 |
| H2   | 5.386118  | 4.475371| -0.834058 |
| H2   | 6.706186  | -0.253654| 2.354257 |
| H2   | 6.844420  | 0.071144| 3.012170  |
| C    | 5.981763  | 2.836465| 1.712718  |
| C    | 5.705287  | 3.640654| 2.814947  |
| C    | 4.413128  | 3.648956| 3.329941  |
| C    | 3.443669  | 2.856811| 2.728969  |
| C    | 3.803040  | 2.079614| 1.629549  |
| N    | 5.038419  | 2.066437| 1.136882  |
| C    | 7.324582  | 2.784460| 1.124626  |
| H    | 6.487630  | 4.246582| 3.254682  |
| H    | 4.169087  | 4.265603| 4.186376  |
| H    | 2.425891  | 2.834970| 3.095833  |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 5.959816   | 2.837704   | 1.709733   |
| C       | 5.689674   | 3.647026   | 2.809955   |
| C       | 4.405816   | 3.644610   | 3.345035   |
| C       | 3.437304   | 2.837091   | 2.764113   |
| C       | 3.788460   | 2.057553   | 1.663563   |
| N       | 5.015833   | 2.055428   | 1.149697   |
| C       | 7.299436   | 2.791589   | 1.113806   |
| H       | 6.472298   | 4.263329   | 3.234370   |
| H       | 4.167907   | 4.264192   | 4.201060   |
| H       | 2.425856   | 2.804628   | 3.147201   |
| H       | 3.066104   | 1.415366   | 1.175080   |
| N       | 7.539454   | 2.033813   | 0.114872   |
| C       | 11.315782  | 1.781307   | -1.694719  |
| C       | 10.831856  | 3.028810   | -1.304317  |
| C       | 9.586627   | 3.137282   | -0.696923  |
| C       | 8.820013   | 1.986345   | -0.484046  |
| C       | 9.288682   | 0.737366   | -0.902848  |
| C       | 10.541991  | 0.639631   | -1.492837  |
| H       | 12.28574   | 1.702190   | -2.170991  |
| H       | 11.418130  | 3.921208   | -1.487263  |
| H       | 9.187536   | 4.109524   | -0.434602  |
| H       | 8.667240   | -0.136599  | -0.745406  |
| H       | 10.909870  | -0.329687  | -1.806013  |
| H       | 8.075819   | 3.405834   | 1.572403   |
| Mn      | 5.721714   | 0.933443   | -0.689330  |
| Cl      | 6.080619   | -1.274697  | -0.169423  |
| Cl      | 4.838403   | 2.246217   | -2.351117  |
| H       | 6.090480   | 5.132857   | -0.577548  |
| H       | 5.842492   | 4.564021   | -0.993379  |
| H       | 6.698067   | -0.185670  | 2.435489   |
| H       | 6.838826   | 0.161891   | 3.080964   |
| H       | 7.195637   | -0.311714  | -2.982387  |
| H       | 6.970536   | 0.322051   | -3.304842  |
| H       | 2.891728   | 0.222028   | -0.994463  |
| H       | 3.085651   | -0.375602  | -0.590650  |
| C       | 2.634570   | 1.885802   | 0.480673   |
| C       | 1.907043   | 2.646633   | 1.393523   |
| C       | 2.591889   | 3.505807   | 2.246504   |
| C       | 3.976076   | 3.578298   | 2.160610   |
| C       | 4.629292   | 2.785015   | 1.219012   |
| N       | 3.978484   | 1.962789   | 0.399878   |
| C       | 1.966745   | 0.964521   | -0.445391  |
| H       | 0.828199   | 2.562086   | 1.431725   |
| H       | 2.050916   | 4.107353   | 2.966823   |
| H       | 4.548203   | 4.231676   | 2.805937   |
| H       | 5.707937   | 2.803700   | 1.118708   |
| N       | 2.647742   | 0.261753   | -1.266583  |
| C       | 0.922979   | -2.411094  | -4.004996  |
| C       | 0.360215   | -2.283304  | -2.735775  |
### Structure descriptions

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 0.909603  | -1.403429 | -1.811887 |
| C    | 2.033908  | -0.645104 | -2.160864 |
| C    | 2.618922  | -0.795068 | -3.422983 |
| C    | 2.051325  | -1.666696 | -4.343454 |
| H    | 0.492910  | -3.101247 | -4.720610 |
| H    | -0.498807 | -2.882614 | -2.459261 |
| H    | 0.498830  | -1.339518 | -0.811608 |
| H    | 3.495443  | -0.206859 | -3.671732 |
| H    | 2.498025  | -1.770178 | -5.324531 |
| H    | 0.875539  | 0.928252  | -0.415614 |
| Mn   | 4.903138  | 0.542150  | -1.095303 |
| Cl   | 5.546623  | 1.650998  | -2.989095 |
| Cl   | 5.780074  | -1.085188 | 0.237094  |
| C    | 5.956732  | 2.797152  | 1.742845  |
| C    | 5.643460  | 3.579385  | 2.851373  |
| C    | 4.335224  | 3.580340  | 3.323091  |
| C    | 3.385482  | 2.801622  | 2.675377  |
| C    | 3.780848  | 2.043333  | 1.575569  |
| N    | 5.031710  | 2.038143  | 1.122148  |
| C    | 7.315407  | 2.769182  | 1.189792  |
| H    | 6.410700  | 4.176624  | 3.327627  |
| H    | 4.063439  | 4.182053  | 4.181587  |
| H    | 2.355900  | 2.775652  | 3.006771  |
| H    | 3.074776  | 1.423329  | 1.036267  |
| N    | 7.579256  | 2.064767  | 0.157106  |
| C    | 11.385612 | 1.878700  | -1.598656 |
| C    | 10.931272 | 3.094455  | -1.090401 |
| C    | 9.677487  | 3.180799  | -0.498934 |
| C    | 8.870684  | 2.040010  | -0.418390 |
| C    | 9.311257  | 0.826165  | -0.956022 |
| C    | 10.573202 | 0.748755  | -1.530474 |
| H    | 12.362540 | 1.817594  | -2.062603 |
| H    | 11.548053 | 3.981351  | -1.169960 |
| H    | 9.305659  | 4.135167  | -0.146797 |
| H    | 8.665726  | -0.043134 | -0.895780 |
| H    | 10.917671 | -0.195100 | -1.934326 |
| H    | 8.079638  | 3.354748  | 1.702794  |
| Mn   | 5.792243  | 0.954715  | -0.704725 |
| Cl   | 6.157590  | -1.256752 | -0.264039 |
| Cl   | 4.882072  | 2.153049  | -2.420687 |
| H2   | 5.653720  | 5.034952  | -0.400561 |
| H2   | 5.495036  | 4.478729  | -0.872946 |

### BPY

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H2   | -2.445783 | -2.420985 | 2.512219  |
| H2   | -2.372428 | -2.555339 | 1.781476  |
| Cl   | 0.196096  | -1.943123 | 0.102466  |
| Cl   | -0.213266 | -1.153250 | 4.307725  |
| H    | -1.185212 | 4.259421  | 1.019202  |
| H    | 0.870847  | 4.340126  | 1.160083  |
| C    | 0.639655  | 2.228115  | 1.550679  |
| C    | 1.367487  | 3.407841  | 1.385357  |
Structure descriptions

C  2.749616  3.377323  1.512960
C  3.379907  2.173871  1.801456
C  2.590843  1.041346  1.951068
H  4.454124  2.105854  1.909071
H  3.025771  0.075447  2.176217
N  1.262551  1.067931  1.829635
Mn  -0.027639  -0.762547  2.055612
N  -1.405279  0.955179  1.606982
C  -0.844325  2.166437  1.432707
C  -2.729645  0.819457  1.516180
C  -1.631880  3.285898  1.158085
C  -3.575630  1.886080  1.244875
H  -3.113498  -0.181598  1.667777
C  -3.009363  3.141308  1.063741
H  -4.644147  1.730396  1.180145
H  -3.631390  4.002308  0.851476
H2  2.374467  -2.227740  2.948446
H2  2.446408  -2.365335  2.217818

C  0.764282  2.413967  1.542677
C  1.427384  3.641401  1.491987
C  2.812710  3.668466  1.584586
C  3.508925  2.479666  1.731929
C  2.780541  1.294166  1.784112
H  3.340299  4.614013  1.548071
H  4.587699  2.453329  1.811518
H  3.267686  0.334957  1.912800
N  1.449860  1.264550  1.688666
Mn  0.250398  -0.617634  1.917878
N  -1.219725  1.060888  1.691803
C  -0.716067  2.285699  1.451578
C  -2.535982  0.859010  1.608899
C  -1.552865  3.351293  1.116857
C  -3.430578  1.870593  1.287744
H  -2.873331  -0.152808  1.799220
C  -2.922549  3.139148  1.036335
H  -4.490560  1.662092  1.229848
H  -3.583628  3.955584  0.771754
H  0.876566  4.565733  1.394205
H -1.146922  4.329692  0.904007
Cl  0.569645  -1.240830  4.087442
Cl  0.071440  -1.714090  -0.081840
H2  -1.267470  1.360166  -1.453469
H2  -0.984501  0.701936  -1.242794

H2  0.276085  1.624985  4.631553
H2  0.317695  2.370564  4.635456
Cl  -0.208884  -1.970002  0.143142
Cl  0.175585  -1.239537  4.281915
H2  -1.019415  0.456663  -1.235516
H2  -1.236008  1.123900  -1.491055
C  0.644431  2.237225  1.576011
C  1.360096  3.434644  1.548216
Structure descriptions

SP-JLMC

C  2.732463  3.409241  1.757421
C  3.362690  2.193692  1.995094
C  2.583766  1.044914  2.014595
H  4.428651  2.132114  2.169541
H  3.017129  0.071494  2.211262
N  1.265801  1.065868  1.806799
Mn -0.034429 -0.739974  2.062225
N -1.406580  0.984438  1.660489
C  -0.829498  2.168537  1.384977
C  -2.723081  0.836996  1.500685
C  -1.588668  3.247630  0.931302
C  -3.544229  1.866860  1.063028
H  -3.120689 -0.145805  1.724044
C  -2.959216  3.093180  0.772017
H  -4.607389  1.703850  0.946591
H  -3.560988  3.920569  0.415702
H  0.857765  4.377305  1.385324
H  -1.121383  4.190785  0.687187
H2  -0.237019  1.532604  4.556926
H2  -0.272153  2.277972  4.543752
H2  1.951159  1.120454 -1.177328
H2  1.600909  0.489309 -0.988935
H2  -1.274662  0.400063 -1.197515
H2  -1.616209  1.013699 -1.449181
C  0.652013  2.222313  1.529268
C  1.393693  3.375243  1.271860
C  2.774998  3.338858  1.406762
C  3.389748  2.156562  1.798439
C  2.586799  1.049848  2.035278
H  3.362881  4.226719  1.208618
H  4.462688  2.085581  1.916376
H  3.010142  0.099832  2.339072
N  1.260200  1.065868  1.806799
Mn -0.026679 -0.727490  2.109985
N  -1.403528  0.981998  1.693639
C  -0.831236  2.166651  1.411948
C  -2.727920  0.849038  1.613842
C  -1.607776  3.261961  1.033928
C  -3.564400  1.893443  1.246154
H  -3.121063 -0.132414  1.850901
C  -2.986377  3.120947  0.949578
H  -4.634075  1.741325  1.193044
H  -3.600821  3.963099  0.655640
H  0.908806  4.291570  0.968766
H  -1.151741  4.213885  0.804699
Cl  0.140170 -1.820037  0.102106
Cl -0.146757 -1.347272  4.302907
H2  1.063287  1.485420  4.745799
H2  1.380191  2.159325  4.787167
H2  1.909969  1.046122 -1.256692
H2  1.577082  0.416579 -1.035137
| Element | x   | y   | z     |
|---------|-----|-----|-------|
| H2      | -1.724274 | 1.391377 | 4.512027 |
| H2      | -2.088631  | 2.041813  | 4.491281  |
| C       | 0.640079   | 2.221993  | 1.553421  |
| C       | 1.374483   | 3.397504  | 1.396235  |
| C       | 2.756268   | 3.357656  | 1.525324  |
| C       | 3.379359   | 2.149784  | 1.811454  |
| C       | 2.583411   | 1.022167  | 1.952527  |
| H       | 3.338196   | 4.263596  | 1.407372  |
| H       | 4.452793   | 2.076356  | 1.922494  |
| H       | 3.013191   | 0.052864  | 2.175080  |
| N       | 1.256786   | 1.058467  | 1.827860  |
| Mn      | -0.034926  | -0.739289 | 2.050378  |
| N       | -1.406084  | 0.956658  | 1.608368  |
| C       | -0.842848  | 2.165382  | 1.431971  |
| C       | -2.728835  | 0.819575  | 1.516462  |
| C       | -1.628888  | 3.283411  | 1.152369  |
| C       | -3.574279  | 1.884822  | 1.242107  |
| H       | -3.114480  | -0.181108 | 1.670398  |
| C       | -3.006406  | 3.138864  | 1.057444  |
| H       | -4.642688  | 1.729480  | 1.176108  |
| H       | -3.628198  | 3.998953  | 0.840868  |
| H       | 0.883619   | 4.334151  | 1.175903  |
| H       | -1.181031  | 4.256069  | 1.010362  |
| Cl      | 0.178669   | -1.942538 | 0.115138  |
| Cl      | -0.209544  | -1.152937 | 4.294965  |
| H2      | -1.556421  | 0.874121  | -1.549026 |
| H2      | -1.209553  | 0.279423  | -1.262077 |
| C       | 0.764219   | 2.411916  | 1.535296  |
| C       | 1.430300   | 3.637742  | 1.486300  |
| C       | 2.816047   | 3.660540  | 1.572477  |
| C       | 3.510466   | 2.465225  | 1.710676  |
| C       | 2.779407   | 1.285767  | 1.759887  |
| H       | 3.345846   | 4.604680  | 1.537488  |
| H       | 4.589353   | 2.441071  | 1.784865  |
| H       | 3.265476   | 0.324691  | 1.879741  |
| N       | 1.448476   | 1.260759  | 1.671432  |
| Mn      | 0.251923   | -0.625004 | 1.897774  |
| N       | -1.219060  | 1.053117  | 1.648658  |
| C       | -0.717573  | 2.286956  | 1.453783  |
| C       | -2.536794  | 0.854510  | 1.585162  |
| C       | -1.560284  | 3.366593  | 1.183415  |
| C       | -3.436815  | 1.880306  | 1.329109  |
| H       | -2.871694  | -0.164388 | 1.739915  |
| C       | -2.931813  | 3.158136  | 1.123361  |
| H       | -4.498150  | 1.675696  | 1.287204  |
| H       | -3.597068  | 3.986518  | 0.912378  |
| H       | 0.882458   | 4.564014  | 1.392133  |
| H       | -1.159186  | 4.354761  | 1.011251  |
| Cl      | 0.515966   | -1.191058 | 4.094124  |
| Cl      | 0.120722   | -1.761332 | -0.079624 |
Structure descriptions SP-JLMC

H2  4.259306 -0.025435  3.170809
H2  4.162595  0.485757  3.706788
H2  -0.206524 -1.548690  4.749871
H2  -0.195874 -1.024836  5.282253
H2  0.112047  0.137573 -0.648837
H2  0.436189 -0.267645 -0.111629
C   0.641196  2.615758  1.130502
C   0.717214  3.600505  0.119398
C   2.001880  3.996750 -0.303097
C   3.113774  3.422427  0.269424
C   2.938630  2.450854  1.266515
H   2.102182  4.748784 -0.774111
H   4.113500  3.703477 -0.034770
H   3.790643  1.974959  1.737934
N   1.744891  2.061001  1.683318
Mn  1.322622  0.464931  3.224866
N  -0.697734  1.214829  2.548979
C  -0.652468  2.168083  1.589380
C  -1.874872  0.785819  2.974702
C  -1.821646  2.723120  1.021148
C  -3.088712  1.278914  2.472739
H  -1.857748  0.021293  3.742720
C  -3.064087  2.247540  1.495376
H  -4.023554  0.892076  2.856686
H  -3.901999  2.647958  1.084295
C  -0.489586  4.142921 -0.431500
C  -1.705891  3.722687  0.005343
Cl  1.744841  1.319768  5.294620
Cl  1.653808 -1.534906  2.164808
H  -0.411680  4.897455 -1.205424
H  -2.613221  4.136919 -0.423228
H2  1.701468  0.585347 -1.013452
H2  1.699000  0.128727 -0.422899
C   0.637088  2.612551  1.143252
C   0.712832  3.521421  0.063581
C   1.997472  3.915029 -0.361572
C   3.109036  3.412629  0.274936
C   2.933981  2.512207  1.336555
H   2.097453  4.609139 -1.183038
H   4.108448  3.694219 -0.029539
H   3.786262  2.090530  1.856458
N   1.740859  2.125749  1.756804
Mn  1.314765  0.511387  3.269798
N  -0.700967  1.294052  2.639414
C  -0.655989  2.172237  1.610668
C  -1.876839  0.875576  3.077329
C  -1.824648  2.657968  0.981479
C  -3.090352  1.303277  2.518066
H  -1.859644  0.169781  3.899579
C  -3.062466  2.193260  1.468998
H  -4.024609  0.927193  2.913751
H  -3.981720  2.540046  1.010828

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Structure descriptions

C  -0.493330  3.993289  -0.549373
C   -1.709168  3.579603  -0.109626
Cl   1.828380  1.179178   5.383159
Cl   1.527069 -1.403580   2.018988
H2  -1.461727 -0.488398   0.141378
H2  -0.856843 -0.738534   0.500102
H    -0.415163  4.688328  -1.377126
H   -2.616281  3.939185  -0.580989
H2   1.834299  1.604904  -1.238412
H2   1.527163  0.938331  -1.102651
H2  -0.226184  1.147050   4.571273
H2  -0.256099  1.899896   4.639084
C    0.645977  2.235466   1.616618
C    1.299019  3.478326   1.456265
C    2.705769  3.485306   1.539167
C    3.380127  2.308228   1.770246
C    2.644751  1.122572   1.915844
H    3.243831  4.416989   1.418821
H    4.459659  2.260945   1.838266
H    3.142208  0.176074   2.092732
N    1.324620  1.086497   1.841379
Mn   0.033533  -0.756916   1.846001
N   -1.394984  0.972642   1.689749
C   -0.793984  2.175247   1.537738
C   -2.713807  0.898194   1.624209
C   -1.527112  3.360353   1.303859
C   -3.525792  2.019946   1.399049
H   -3.146489  -0.087398   1.750252
C   -2.930523  3.249858   1.236389
H   -4.600525  1.903168   1.353256
H   -3.528281  4.136220   1.056797
C    0.523278  4.659366   1.217140
C   -0.831156  4.602924   1.144599
C    0.197732  -1.522041  -0.310146
C1   -0.071513  -1.677868   3.930092
H2  -1.700411  1.443600  -1.383870
H2  -1.328725  0.816105  -1.226061
H   -1.410276   5.500583   0.962796
H   1.042236   5.602646   1.093794
H2  -3.206554   0.160789   0.952296
H2  -3.131673   0.652576   1.508138
H2   2.427055  -1.991811   1.634002
H2   2.113443  -2.361030   1.066675
H2  -2.716702   1.114142  -1.581276
H2  -2.519143   1.832032  -1.626408
C    0.104554   0.186055   0.885140
C    0.480616   0.962081   2.004281
C    0.202811   0.433644   3.280922
C   -0.411524  -0.792715   3.391293
C   -0.745863  -1.490814   2.221867
H    0.476185   0.999053   4.164721
H   -0.638373  -1.225540   4.356702
Structure descriptions

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H  -1.228536 -2.459824  2.269506
N  -0.496488 -1.019226  1.012047
Mn -0.947357 -2.031410 -0.936510
N  -0.007537 -0.076289 -1.498901
C   0.365565  0.684056 -0.444451
C   0.224913  0.362141 -2.724432
C   0.996672  1.937949 -0.605413
C   0.846782  1.592024 -2.983841
H  -0.092838 -0.284209 -3.534031
C   1.232010  2.379291 -1.922923
H   1.013645  1.902494 -4.006840
C   1.118344  2.229775  1.803000
C   1.365937  2.696993  0.552952
Cl  -3.197445 -1.814459 -1.286248
Cl   0.685676 -3.609003 -1.219978
H2  3.039805  -0.725250 -1.453012
H2  2.628949  -1.347584 -1.436303
H   1.849223  3.656524  0.410341
H   1.400960  2.810783  2.673151
C   0.810566  0.160820  0.241270
C   1.466736  1.400188  0.061054
C   2.875559  1.398304  0.107302
C   3.548778  0.216903  0.321115
C   2.810140 -0.964675  0.489996
H   3.415795  2.328565  0.027334
H   4.629505  0.184014  0.361075
H   3.306124 -1.913385  0.660065
N   1.487805  -0.992234  0.451752
Mn  0.180735  -2.820893  0.697124
N  -1.236220 -1.089630  0.373558
C  -0.632155  0.109290  0.200964
C  -2.557366 -1.156140  0.341351
C  -1.364080  1.299527 -0.015428
C  -3.368062 -0.029266  0.132883
H  -2.992980 -2.138031  0.486516
C  -2.769672  1.197454 -0.045124
H  -4.444379  0.138758  0.116291
H  -3.366358  2.087910 -0.207557
C   0.691813  2.585910 -0.157311
C  -0.664720  2.537805 -0.193105
Cl  0.102948  -3.331211  2.921310
Cl  0.304603  -3.988409 -1.260891
H  -1.243383  3.439248 -0.357283
H   1.213312  3.526214 -0.292840

FeCl$_2$—H$_2$

BBH

H$_2$  4.456276  1.590747 -2.650035
H$_2$  4.649934  0.905382 -2.425340
C   2.209105  3.130680  0.227698
Structure descriptions

SP-JLMC

C 1.580703  2.556005  1.347308
C 0.215195  2.700068  1.543873
C -0.547784  3.403619  0.613980
C 0.060886  3.951274 -0.514598
H 2.172387  2.008443  2.072871
H -0.253612  2.263788  2.417416
H  1.615341  3.515308  0.762233
H -0.532909  4.481217 -1.248942
N 4.473382  3.627713 -0.598483
C 6.750947  3.912429 -1.190591
N 5.794186  3.180186  0.554217
H 4.061654  2.152277  0.739686
H 5.943902  2.198219 -0.370669
O 6.459805  4.987663 -1.730288
C 10.727066  2.369531 -1.348949
C 10.271348  3.273268 -2.306937
C  8.976906  3.771574 -2.235273
C  8.125271  3.356136  0.206902
C  8.589110  2.456504 -0.239539
C  9.887536  1.966685 -0.312412
H 11.738496  1.984918 -1.404807
H 10.925824  3.590163 -3.109521
H  8.606656  4.477052 -2.967395
H  7.961074  2.167678  0.595140
H 10.247604  1.280407  0.444202
H  1.873458  4.211124 -1.615573
Fe 4.324326  5.209246 -1.680652
Cl 3.742142  6.880778  0.141796
Cl  3.727033  4.261270 -3.615597

H2  3.987952  1.538543 -2.625175
H2  4.060617  0.845669  2.357723
C  2.214174  3.130548  0.227049
C  1.592669  2.545611  1.345367
C  0.228813  2.689417  1.553289
C -0.539570  3.403894  0.636346
C  0.062111  3.962925 -0.490467
C  1.426082  3.830474 -1.070676
C  3.646565  2.940924  0.107994
H  2.188380  1.988643  2.060396
H  -0.234492  2.244091  2.425203
H  -1.605869  3.515624  0.793271
H  -0.535969  4.502133 -1.214493
N  4.475072  3.615432 -0.620202
N  6.753513  3.896881 -1.211516
N  5.794306  3.163656 -0.582519
H  4.065032  2.143819  0.722264
H  5.949071  2.189141 -0.366432
O  6.458555  4.965240  1.764845
C 10.747804  2.397274 -1.297433
C 10.299642  3.296629 -2.263402
C  8.999314  3.781313 -2.214838
| Atom | X  | Y  | Z  |
|------|----|----|----|
| C    | 2.213391 | 3.127864 | 0.225926 |
| C    | 1.593220 | 2.574286 | 1.360334 |
| C    | 0.232278 | 2.738128 | 1.572775 |
| C    | -0.534084 | 3.439391 | 0.643865 |
| C    | 0.066213  | 3.965329 | -0.499426 |
| C    | 1.427662 | 3.814063 | -0.713860 |
| C    | 3.643701  | 2.924694 | 0.099970 |
| H    | 2.187952 | 2.028736 | 2.084899 |
| H    | -0.230509 | 2.319009 | 2.457872 |
| H    | -1.598126 | 3.566190 | 0.804571 |
| H    | -0.530707 | 4.493570 | -1.232449 |
| N    | 4.470743 | 3.602943 | -0.626418 |
| C    | 6.747560  | 3.896541 | -1.206925 |
| N    | 5.785222 | 3.141820 | -0.611592 |
| H    | 4.061249 | 2.120710 | 0.705579 |
| H    | 5.937110 | 2.161260 | -0.424248 |
| O    | 6.458351 | 4.985993 | -1.720572 |
| C    | 10.738846 | 2.391332 | -1.317319 |
| H    | 10.290429 | 3.299032 | -2.275277 |
| C    | 8.990754  | 3.785349 | -2.220474 |
| C    | 8.126218 | 3.352807 | -1.210159 |
| C    | 8.582197 | 2.449228 | -0.242804 |
| C    | 9.886364 | 1.972075 | -0.298158 |
| H    | 11.754688 | 2.016829 | -1.359495 |
| H    | 10.955164 | 3.628682 | -3.064187 |
| H    | 8.626259 | 4.494356 | -2.952125 |
| H    | 7.942557 | 2.148018 | 0.578493 |
| H    | 10.240435 | 1.283103 | 0.458851 |
| H    | 1.868749 | 4.189904 | -1.626063 |
| Fe   | 4.325591 | 5.200148 | -1.685776 |
| Cl   | 3.724132 | 6.661362 | -0.136422 |
| Cl   | 3.718972 | 4.278133 | -3.629242 |
| H2   | 4.590839 | 0.894291 | -2.481812 |
| H2   | 4.396521 | 1.583771 | -2.692844 |
| H2   | 6.312647 | 4.953230 | 1.795909 |
| H2   | 5.771722 | 5.340177 | 1.457447 |
| C    | 2.213044 | 3.126448 | 0.226799 |
| C    | 1.594482 | 2.575450 | 1.363244 |
| C    | 0.233638 | 2.738722 | 1.576610 |
| C    | -0.534059 | 3.437154 | 0.646863 |
| C    | 0.064691 | 3.960981 | -0.498176 |
| C    | 1.425953 | 3.810002 | -0.713705 |
| C    | 3.643315 | 2.923870 | 0.099763 |
| H    | 2.190479 | 2.032132 | 2.088432 |
| H    | -0.228070 | 2.321346 | 2.463061 |
| H    | -1.598027 | 3.563622 | 0.808314 |
| H    | -0.533626 | 4.486865 | -1.231719 |
| N    | 4.468765 | 3.599925 | -0.630569 |
| C    | 6.744682 | 3.895742 | -1.212672 |
| N    | 5.783528 | 3.141230 | -0.615444 |
| H    | 4.062336 | 2.122342 | 0.707708 |
| H    | 5.938790 | 2.162805 | -0.419334 |
| O    | 6.453836 | 4.983014 | -1.729861 |
Structure descriptions

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| C | 10.738168 | 2.396852 | -1.310866 |
| C | 10.287193 | 3.292593 | -2.278800 |
| C | 8.986814 | 3.777318 | -2.228261 |
| C | 8.124250 | 3.354659 | -1.212214 |
| C | 8.582686 | 2.463224 | -0.234910 |
| C | 9.887547 | 1.987635 | -0.286255 |
| H | 11.754661 | 2.023816 | -1.349753 |
| H | 10.950642 | 3.614237 | -3.072089 |
| H | 8.620351 | 4.477464 | -2.967448 |
| H | 7.943520 | 2.170838 | 0.589926 |
| H | 10.243814 | 1.308265 | 0.478367 |
| H | 1.865605 | 4.183785 | -1.627504 |
| Fe | 4.322023 | 5.200110 | -1.687735 |
| Cl | 3.739212 | 6.658755 | -0.129263 |
| Cl | 3.716782 | 4.281012 | -3.632313 |
| H2 | 4.627071 | 0.911435 | -2.537541 |
| H2 | 4.429817 | 1.596888 | -2.759223 |
| H2 | 6.295888 | 4.871267 | 1.791641 |
| H2 | 5.768759 | 5.277363 | 1.453546 |
| C | 2.217610 | 3.119756 | 0.213044 |
| C | 1.601031 | 2.552774 | 1.343208 |
| C | 0.240385 | 2.711591 | 1.561317 |
| C | -0.529464 | 3.422995 | 0.643132 |
| C | 0.066985 | 3.963103 | -0.495576 |
| C | 1.427843 | 3.816058 | -0.716071 |
| C | 3.647477 | 2.917533 | 0.082178 |
| H | 2.198261 | 1.999846 | 2.060070 |
| H | -0.219169 | 2.281078 | 2.442594 |
| H | -1.593180 | 3.546633 | 0.808351 |
| H | -0.532798 | 4.498717 | -1.220855 |
| N | 4.474609 | 3.594167 | -0.646127 |
| C | 6.752190 | 3.893608 | -1.218870 |
| N | 5.792464 | 3.147638 | -0.614089 |
| H | 4.066914 | 2.119996 | 0.695564 |
| H | 5.965374 | 2.190999 | -0.341590 |
| O | 6.455073 | 4.962506 | -1.770968 |
| C | 10.751931 | 2.411825 | -1.275499 |
| C | 10.292307 | 3.268480 | -2.274395 |
| C | 8.990155 | 3.749510 | -2.235849 |
| C | 8.134643 | 3.362544 | -1.200082 |
| C | 8.601372 | 2.510791 | -0.192063 |
| C | 9.907957 | 2.038496 | -0.231711 |
| H | 11.769355 | 2.040548 | -1.306007 |
| H | 10.949635 | 3.560820 | -3.083943 |
| H | 8.615077 | 4.414549 | -3.002448 |
| H | 7.968003 | 2.246347 | 0.646816 |
| H | 10.270510 | 1.389712 | 0.556087 |
| H | 1.864376 | 4.201616 | -1.626157 |
| Fe | 4.334189 | 5.199394 | -1.697177 |
| Cl | 3.773426 | 6.643173 | -0.115259 |
| Cl | 3.659997 | 4.338138 | -3.644912 |
| H2 | 6.235275 | 2.221067 | -3.611174 |
| H2 | 5.751134 | 2.789313 | -3.669884 |
Structure descriptions

H2  6.226419  4.865185  1.824680
H2  5.706643  5.269874  1.473790
C   2.218636  3.126188  0.223846
C   1.604616  2.561406  1.356196
C   0.245612  2.726341  1.579802
C  -0.524881  3.440643  0.664340
C   0.069286  3.978827 -0.476372
C   1.428819  3.826270 -0.701987
C   3.646870  2.918157  0.086035
H   2.202520  2.005781  2.070429
H  -0.212215  2.298140  2.463144
H  -1.587479  3.568316 -0.835765
H  -0.530807  4.517535 -1.199134
N   4.472102  3.591716 -0.646210
C   6.748877  3.882865  0.664340
N   5.784539  3.170404 -0.639489
H   4.064527  2.110450  0.686756
H   5.944761  2.157190 -0.408667
O   6.456314  4.966121 -1.753271
C  10.755507  2.417945 -1.270176
C  10.312089  3.316922 -2.238841
C   9.007025  3.789938 -2.205756
C   8.132213  3.356666 -1.206019
C   8.583045  2.459780 -0.227633
C   9.892412  1.994824 -0.261745
H  11.775463  2.053261 -1.295882
H  10.984882  3.649391  3.019715
H   8.649336  4.486666 -2.948119
H   7.934734  2.155939  0.585959
H  10.241998  1.312614  0.503444
H  1.864631  4.212821 -1.612041
Fe  4.334912  5.194735 -1.701125
Cl  3.752365  6.647784 -0.135890
Cl  3.668898  4.305646 -3.645423
H2  6.090687  2.808123  3.875910
H2  6.709691  2.392571 -3.850546
H2  4.012223  0.839781 -2.399099
H2  3.947742  1.535363 -2.662391
C   2.170438  2.887788  0.073560
C   1.480332  2.321235  1.158236
C   0.108773  2.488783  1.284630
C  -0.592332  3.209509  0.319861
C   0.081523  3.752601 -0.773857
C   1.453013  3.595045 -0.903832
C   3.609010  2.700257  0.029081
H   2.026658  1.764816  1.911875
H  -0.412438  2.059430  2.131455
H  -1.663987  3.339255  0.414230
H  -0.464002  4.297434 -1.534272
N   4.433189  3.402824 -0.664923
C   6.702661  3.785919 -1.219063
N   5.759904  3.035242 -0.588612
Structure descriptions

H  4.006817  1.906845  0.666621
H  5.997224  2.135269 -0.193711
O  6.391432  4.818517 -1.831675
C 10.755970  2.455534 -1.131775
C 10.281016  3.233891 -2.185828
C  8.961017  3.665474 -2.195172
C  8.102171  3.304947 -1.152221
C  8.584549  2.532792 -0.088737
C  9.908995  2.111902 -0.080177
H 11.787886  2.125331 -1.128333
H 10.941417  3.507418 -2.999471
H  8.57703  4.277252 -3.001163
H  7.950606  2.297656  0.758424
H 10.282918  1.527879  0.751806
H  1.953446  3.988354 -1.779423
Fe 4.348086  5.292153 -1.709193
Cl 4.124040  6.671589  0.026658
Cl 3.438740  4.960228 -3.720082
H2 5.234139  2.683234 -3.610164
H2 5.691993  2.101151 -3.516719
H2 4.194757  4.709810  2.182493
H2 4.255892  4.204843  2.728763
H2 6.650574  5.650534  1.071221
H2 7.297873  5.339031  1.272724
H2 6.961726  5.124785  1.497252
H2 6.354636  5.481208  1.251040
C  2.196696  3.049087  0.138570
C  1.570373  2.398571  1.216589
C  0.212582  2.560840  1.448530
C -0.544287  3.360212  0.594327
C  0.061712  3.985825 -0.494444
C  1.420421  3.835378 -0.727099
C  3.624309  2.840346 -0.002918
H  2.158814  1.779721  1.884874
H -0.254591  2.065606  2.290914
H -1.605857  3.487437  0.770082
H -0.528640  4.591893 -1.170270
N  4.463403  3.558535 -0.673786
C  6.747342  3.864060 -1.227397
N  5.775462  3.094255 -0.671879
H  4.028829  1.989577  0.545040
H  5.938062  2.123927 -0.442277
O  6.463764  4.962108 -1.727026
C 10.749565  2.389867 -1.269097
C 10.312364  3.299207 -2.230913
C  9.008074  3.774455 -2.199244
C  8.127845  3.329323 -1.208135
C  8.572082  2.424781 -0.236584
C  9.981044  1.983888 -0.268873
H 11.769047  2.023900 -1.293547
H 10.989670  3.638658 -3.004847
H  8.651031  4.483018 -2.934726
H  7.919264  2.115195  0.571242
| Symbol | X       | Y       | Z       |
|--------|---------|---------|---------|
| H      | 10.225857 | 1.268357 | 0.491412 |
| H      | 1.864086  | 4.292659 | -1.599684 |
| Fe     | 4.350511  | 5.234490 | -1.615113 |
| Cl     | 3.871674  | 6.565275 | 0.092413  |
| Cl     | 3.631103  | 4.539355 | -3.614650 |
| H2     | 6.035950  | 2.977699 | -3.947611 |
| H2     | 6.614741  | 2.506953 | -3.940779 |
| H2     | 3.909761  | 4.250966 | 2.960695  |
| H2     | 3.883123  | 4.726309 | 2.386461  |
| H2     | 3.818269  | 0.978158 | -2.639890 |
| H2     | 3.790372  | 1.692059 | -2.854824 |
| C      | 2.173809  | 2.952902 | 0.043325  |
| C      | 1.498853  | 2.384643 | 1.136953  |
| C      | 0.133417  | 2.572320 | 1.296140  |
| C      | -0.577492 | 3.315163 | 0.355530  |
| C      | 0.080156  | 3.858995 | -0.747368 |
| C      | 1.445724  | 3.681215 | -0.910208 |
| C      | 3.608088  | 2.743120 | -0.02869 |
| H      | 2.052877  | 1.811977 | 1.872537  |
| H      | -0.375122 | 2.142674 | 2.150479  |
| H      | -1.644244 | 3.462014 | 0.476237  |
| H      | -0.473785 | 4.420112 | -1.489665 |
| N      | 4.444500  | 3.448342 | -0.707275 |
| C      | 6.727005  | 3.806278 | -1.236332 |
| N      | 5.766578  | 3.049516 | -0.642194 |
| H      | 3.999215  | 1.926542 | 0.582354  |
| H      | 5.979571  | 2.131505 | -0.277872 |
| O      | 6.436178  | 4.861483 | -1.817945 |
| C      | 10.763168 | 2.424833 | -1.139128 |
| C      | 10.312574 | 3.247771 | -2.169776 |
| C      | 8.997333  | 3.693325 | -2.182463 |
| C      | 8.119032  | 3.303662 | -1.166490 |
| C      | 8.576840  | 2.486156 | -0.126398 |
| C      | 9.896588  | 2.050527 | -0.114294 |
| H      | 11.791410 | 2.083658 | -1.128313 |
| H      | 10.987977 | 3.544013 | -2.962909 |
| H      | 8.631935  | 4.338431 | -2.970540 |
| H      | 7.928111  | 2.226047 | 0.701840  |
| H      | 10.251735 | 1.431362 | 0.700336  |
| H      | 1.933410  | 4.072878 | -1.793101 |
| Fe     | 4.358703  | 5.280387 | -1.704120 |
| Cl     | 4.006086  | 6.570916 | 0.089641  |
| Cl     | 3.512425  | 4.810848 | -3.726265 |
| H2     | 5.463226  | 2.677155 | -3.707415 |
| H2     | 5.972791  | 2.137147 | -3.628745 |
| H2     | 4.207096  | 4.608110 | 2.213464  |
| H2     | 4.301482  | 4.100773 | 2.753166  |
| H2     | 6.573187  | 5.629263 | 1.094175  |
| H2     | 7.220951  | 5.324528 | 1.305660  |
| H2     | 5.267837  | 7.698642 | -2.498430 |
| H2     | 5.209149  | 7.411355 | -3.186348 |
| C      | 2.163207  | 3.047155 | 0.025884  |
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| C       | 1.503588 | 2.380203 | 1.074228 |
| C       | 0.135325 | 2.521503 | 1.253093 |
| C       | -0.599045| 3.316127 | 0.375104 |
| C       | 0.040819 | 3.957926 | -0.684437|
| C       | 1.409470 | 3.828482 | -0.864691|
| H       | 2.072829 | 1.761600 | 1.759565 |
| H       | -0.357746| 2.012407 | 2.072213 |
| H       | -1.668623| 3.426256 | 0.509438 |
| H       | -0.530759| 4.560193 | -1.379575|
| N       | 4.453490 | 3.584069 | -0.705809|
| C       | 6.754228 | 3.893536 | -1.201642|
| N       | 5.768667 | 3.126122 | -0.659627|
| H       | 3.992083 | 2.006095 | 0.493769 |
| H       | 5.922987 | 2.149162 | -0.454981|
| O       | 6.488159 | 5.000210 | -1.687530|
| C       | 10.731275| 2.343633 | -1.274110|
| C       | 10.313969| 3.288970 | -2.209238|
| C       | 9.019414 | 3.790193 | -2.164390|
| C       | 8.128485 | 3.334947 | -1.187527|
| C       | 8.553719 | 2.393650 | -0.242317|
| C       | 9.852854 | 1.901815 | -0.286967|
| H       | 11.742961| 1.957331 | -1.308539|
| H       | 10.998821| 3.636433 | -2.972875|
| H       | 8.679222 | 4.528232 | -2.878811|
| H       | 7.894441 | 2.072125 | 0.555647 |
| H       | 10.182614| 1.183437 | 0.453463 |
| H       | 1.881174 | 4.297166 | -1.716447|
| Fe      | 4.351289 | 5.263800 | -1.639041|
| Cl      | 3.819048 | 6.584017 | 0.049840 |
| Cl      | 3.741465 | 4.561865 | -3.663742|

**PIP**

| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| C       | 1.360169 | 2.076840 | -0.611214|
| C       | 0.770198 | 3.220485 | -1.183307|
| C       | -0.581970| 3.491132 | -1.064094|
| C       | -1.392415| 2.611291 | -0.349669|
| C       | -0.842728| 1.479480 | 0.238498 |
| C       | 0.514805 | 1.211431 | 0.112226 |
| C       | 2.790817 | 1.913803 | -0.825592|
| H       | 1.404531 | 3.901779 | -1.738351|
| H       | -1.002508| 4.376903 | -1.521932|
| H       | -2.452984| 2.804131 | -0.245775|
| H       | -1.469664| 0.795642 | 0.800612 |
| N       | 3.538097 | 0.906406 | -0.535809|
| C       | 7.673299 | 1.168256 | -1.283257|
| C       | 7.043890 | 2.156838 | -0.531294|
| C       | 5.676824 | 2.084167 | -0.284848|
| C       | 4.941523 | 1.014255 | -0.797134|
| C       | 5.568927 | 0.007926 | -1.533812|
| C       | 6.933285 | 0.996831 | -1.781068|
| H       | 8.739032 | 1.224653 | -1.469205|
| H       | 7.618458 | 2.978811 | -0.121575|
Structure descriptions

H  5.185835  2.823842  0.335419
H  4.979881  -0.820900  -1.907827
H  7.420182  -0.677954  -2.360580
H  3.266792  2.763463  -1.315859
Fe  3.001659  -0.834398   0.250711
Cl  2.458201  -2.104730  -1.496501
Cl  3.973820  -0.962188   2.238372
O2  1.056917   0.104262  0.715886
H2  0.372151  -0.427223   1.146136
H2  2.648253   2.409861  2.302564
H2  2.955074   1.731641  2.358130

C  1.405652   2.180196  -0.581281
C  0.871365   3.382049  -1.084074
C  -0.455295  3.731861  -0.900848
C  -1.293939  2.874951  -0.190411
C  -0.801337  1.681531   0.321401
C   0.530013  1.332491   0.127263
C   2.825568  1.957384  -0.812132
H   1.529874   4.049087  -1.628235
H   0.372151   4.662382  -1.302881
H   2.648253   2.409861   2.302564
H   2.955074   1.731641   2.358130
C   1.405652   2.180196  -0.581281
C   0.871365   3.382049  -1.084074
C   -0.455295  3.731861  -0.900848
C   -1.293939  2.874951  -0.190411
C   -0.801337  1.681531   0.321401
C    0.530013  1.332491   0.127263
C    2.825568  1.957384  -0.812132
H    1.529874   4.049087  -1.628235
H    0.372151   4.662382  -1.302881
H    2.648253   2.409861   2.302564
H    2.955074   1.731641   2.358130

Fe   3.001659  -0.834398   0.250711
Cl   2.458201  -2.104730  -1.496501
Cl   3.973820  -0.962188   2.238372
O2   1.056917   0.104262  0.715886
H2   0.372151  -0.427223   1.146136
H2   2.648253   2.409861  2.302564
H2   2.955074   1.731641  2.358130
C   1.405652   2.180196  -0.581281
C   0.871365   3.382049  -1.084074
C  -0.455295  3.731861  -0.900848
C  -1.293939  2.874951  -0.190411
C  -0.801337  1.681531   0.321401
C   0.530013  1.332491   0.127263
C   2.825568  1.957384  -0.812132
H   1.529874   4.049087  -1.628235
H   0.372151   4.662382  -1.302881
H   2.648253   2.409861   2.302564
H   2.955074   1.731641   2.358130

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### Structure descriptions

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| H    | -0.890755 | 4.607943 | -1.116531 |
| H    | -2.426548  | 2.914039  | -0.124825  |
| H    | -1.541267  | 0.727832  | 0.603832   |
| N    | 3.514148   | 0.868546  | -0.569545  |
| C    | 7.647642   | 1.119368  | -1.341386  |
| C    | 7.040886   | 2.060611  | -0.513205  |
| C    | 5.676405   | 1.988841  | -0.255215  |
| C    | 4.919963   | 0.969594  | -0.835806  |
| C    | 5.523715   | 0.008978  | -1.648127  |
| C    | 6.887146   | 0.096078  | -1.904151  |
| H    | 8.711955   | 1.174475  | -1.535521  |
| H    | 7.632128   | 2.842441  | -0.051939  |
| H    | 5.203225   | 2.687183  | 0.423798   |
| H    | 4.920504   | -0.787993 | -2.064805  |
| H    | 7.356647   | -0.643744 | -2.540905  |
| H    | 3.286637   | 2.787253  | -1.191740  |
| Fe   | 2.995408   | -0.838244 | 0.223568   |
| Cl   | 2.692180   | -2.280052 | -1.447283  |
| Cl   | 3.849550   | -0.711708 | 2.266295   |
| O2   | 0.953930   | -0.047251 | 0.438585   |
| H2   | 0.233683   | -0.638958 | 0.698328   |
| H2   | 2.341003   | 2.541947  | 2.325087   |
| H2   | 2.597201   | 1.892426  | 2.417118   |
| H2   | 0.992296   | -0.339202 | -2.689631  |
| H2   | 0.563738   | 0.237614  | -2.890563  |
| C    | 1.362372   | 2.126209  | -0.597829  |
| C    | 0.852577   | 3.395277  | -0.935733  |
| C    | -0.457791  | 3.756045  | -0.676171  |
| C    | -1.308105  | 2.839536  | -0.097957  |
| C    | -0.843864  | 1.574589  | 0.275198   |
| C    | 0.472681   | 1.217590  | 0.008030   |
| C    | 2.774054   | 1.910317  | -0.872001  |
| H    | 1.520254   | 4.108556  | -1.404858  |
| H    | -0.814981  | 4.741470  | -0.945430  |
| H    | -2.335986  | 3.104695  | 0.154920   |
| H    | -1.505719  | 0.851345  | 0.738474   |
| N    | 3.499469   | 0.870500  | -0.637502  |
| C    | 7.639730   | 1.132546  | -1.374418  |
| C    | 7.016939   | 2.085140  | -0.571443  |
| C    | 5.650195   | 2.007550  | -0.326999  |
| C    | 4.907351   | 0.970314  | -0.894767  |
| C    | 5.527796   | -0.002052 | -1.679885  |
| C    | 6.893270   | 0.091695  | -1.923518  |
| H    | 8.705503   | 1.192456  | -1.569133  |
| H    | 7.596617   | 2.881452  | -0.120364  |
| H    | 5.164193   | 2.715946  | 0.332210   |
| H    | 4.937733   | -0.815084 | -2.082888  |
| H    | 7.374892   | -0.657107 | -2.540496  |
| H    | 3.272589   | 2.767404  | -1.323847  |
| Fe   | 2.595984   | -0.807549 | 0.214960   |
| Cl   | 2.869392   | -2.391780 | -1.346154  |
| Cl   | 3.574721   | -0.520156 | 2.340522   |
| O2   | 0.913228   | -0.044894 | 0.314529   |
### Structure descriptions

|          |          |          |          |          |          |          |
|----------|----------|----------|----------|----------|----------|----------|
| H2       | 0.337955 | -0.477816| 0.964878 |          |          |          |
| H2       | 2.811359 | 2.989338 | 2.134005 |          |          |          |
| H2       | 3.038660 | 2.285861 | 2.237458 |          |          |          |
| H2       | 1.242240 | -0.407674| -2.656822|          |          |          |
| H2       | 0.850511 | 0.182250 | -2.891299|          |          |          |
| H2       | 0.203103 | -1.787492| 2.488113 |          |          |          |
| H2       | 0.880230 | -1.496337| 2.627942 |          |          |          |
| C        | 1.413868 | 2.195515 | -0.416718|          |          |          |
| C        | 0.948252 | 3.515945 | -0.570967|          |          |          |
| C        | -0.385495| 3.849053 | -0.412970|          |          |          |
| C        | -1.305113| 2.850715 | -0.095221|          |          |          |
| C        | -0.880910| 1.539033 | 0.070377 |          |          |          |
| C        | 0.460951 | 1.212875 | -0.083484|          |          |          |
| C        | 2.831484 | 1.980334 | -0.659431|          |          |          |
| H        | 1.665089 | 4.287241 | -0.082789|          |          |          |
| H        | -0.709617| 4.873937 | -0.538485|          |          |          |
| H        | -2.353362| 3.092052 | 0.030769 |          |          |          |
| H        | -1.587930| 0.761019 | 0.334687 |          |          |          |
| N        | 3.514916 | 0.892646 | -0.555809|          |          |          |
| C        | 7.658295 | 1.021120 | -1.303065|          |          |          |
| C        | 7.087008 | 1.937973 | -0.423780|          |          |          |
| C        | 5.719948 | 1.908096 | -0.171570|          |          |          |
| C        | 4.924350 | 0.954341 | -0.809484|          |          |          |
| C        | 5.492881 | 0.155599 | -1.671555|          |          |          |
| C        | 6.859507 | 0.061582 | -1.921909|          |          |          |
| H        | 8.724643 | 1.044271 | -1.492790|          |          |          |
| H        | 7.707709 | 2.667907 | 0.081837 |          |          |          |
| H        | 5.275411 | 2.584204 | 0.547551 |          |          |          |
| H        | 4.862111 | -0.735532| -2.130306|          |          |          |
| H        | 7.300166 | -0.660990| -2.597912|          |          |          |
| H        | 3.366202 | 2.872151 | -0.985338|          |          |          |
| Fe       | 2.912464 | -0.837084| 0.144584 |          |          |          |
| Cl       | 2.691988 | -2.339192| -1.507741|          |          |          |
| Cl       | 3.635596 | -0.689548| 2.240269 |          |          |          |
| O2       | 0.876145 | -0.080566| 0.095771 |          |          |          |
| H2       | 0.151706 | -0.719877| 0.000756 |          |          |          |
| H2       | 3.314029 | 2.928666 | 2.363180 |          |          |          |
| H2       | 3.436655 | 2.192762 | 2.380092 |          |          |          |
| H2       | 1.422458 | -0.091452| -2.829494|          |          |          |
| H2       | 1.073256 | 0.533006 | -3.040537|          |          |          |
| H2       | 0.454682 | 0.957770 | 2.970521 |          |          |          |
| H2       | 1.069622 | 0.541130 | 2.903630 |          |          |          |
| H2       | -0.072475| -2.505485| -0.704478|          |          |          |
| H2       | -0.751408| -2.422805| -0.397479|          |          |          |
| C        | 1.703541 | 2.433297 | -0.311207|          |          |          |
| C        | 0.985179 | 3.583752 | 0.032784 |          |          |          |
| C        | -0.396972| 3.546037 | -0.008808|          |          |          |
| C        | -1.034787| 2.361276 | -0.398046|          |          |          |
| C        | -0.273556| 1.256330 | -0.730457|          |          |          |
| N        | 1.071917 | 1.281028 | -0.687658|          |          |          |
| C        | 3.126164 | 2.318858 | -0.326832|          |          |          |
| H        | 1.518566 | 4.478069 | 0.328967 |          |          |          |
Structure descriptions

PIA

H  -0.976670  4.421565  0.253901
H  -2.113509  2.298584 -0.450437
H  -0.709749  0.323534 -1.060109
N   3.616431  1.139035 -0.613092
C   7.754837  0.776992 -1.316685
C   7.046938  1.846843 -1.860585
C   5.682193  1.969385 -1.630668
C   5.016516  1.016992 -0.846777
C   5.720541 -0.068904 -0.320793
C   7.086829 -0.176319 -0.551113
H   8.818014  0.679791 -1.501302
H   7.553434  2.578560 -2.478468
H   5.123192  2.776876 -2.087683
H   5.187974 -0.808127  0.260444
H   7.629753 -1.014905 -0.13218
H   3.765884  3.171484 -0.465460

Fe   2.249845 -0.268635 -0.915736
Cl   1.044191 -1.274973 -2.472124
Cl   2.925963 -1.867797  0.465460

C   1.404717  2.095871 -0.539176
C   0.931415  3.419946 -0.598276
C  -0.382727  3.745285 -0.307623
C  -1.273299  2.733393  0.043982
C  -0.844604  1.412716  0.095468
C   0.475937  1.093558 -0.193969
C   2.814271  1.898241 -0.850557
H   1.628398  4.203520 -0.871779
H  -0.711808  4.775160 -0.353842
H  -2.304555  2.968037  0.276926
H  -1.536815  0.622033  0.363874
N   3.530356  0.838495 -0.701255
C   7.638401  1.052896 -1.614092
C   7.064824  2.015584 -0.786883
C   5.709919  1.956291 -0.479529
C   4.926770  0.927765 -1.009192
C   5.501925 -0.057708 -1.813036
C   6.855086  0.177514 -2.121337
H   8.695148  1.090060 -1.048009
H   7.674875  2.805032 -0.364642
H   5.267163  2.673214  0.200785
H   4.887172 -0.871624 -2.175300
H   7.299031 -0.742086 -2.752825
H   3.307597  2.785530 -1.248948
Fe   2.989303 -0.835276  0.258454
Cl   3.087563 -2.636026 -1.044630
Cl   3.223028 -0.179226  2.365128
O2   0.896900 -0.212528 -0.180352
H2   0.176315 -0.813578  0.056599

PIA

H2   2.097027  0.596407 -2.579253
H2   2.300117 -0.001804 -2.975576
C 1.426894 1.778904 -0.397083
C 0.480345 2.784652 -0.622220
C -0.861773 2.478542 -0.497043
C -1.234519 1.172714 -0.152290
C -0.255203 0.219313 0.055768
N 1.054144 0.509072 -0.058481
C 2.840946 1.934535 -0.505886
H 0.811689 3.780533 -0.887649
H -1.615414 3.237680 -0.663000
H -2.275680 0.895025 -0.056047
H -0.484368 -0.809196 0.297900
N 3.572192 0.893372 -0.199243
C 7.687767 0.971354 -1.094528
C 6.764402 1.453401 -2.019988
C 5.406503 1.428751 -1.728044
C 4.963784 0.928751 -1.728044
C 5.886825 0.414064 0.413777
C 7.243123 0.451144 0.119165
H 8.746291 0.987257 -1.324996
H 7.099515 1.835016 -2.976982
H 4.685292 1.762626 -2.463850
H 5.527840 0.00758 1.351163
H 7.955279 0.064851 0.838216
H 3.283165 2.867455 -0.840165
Fe 2.535020 -0.692287 0.389854
Cl 1.573934 -2.544999 -0.353672
Cl 3.544390 -1.237505 2.285031
H2 2.049444 -0.645508 -2.521164
H2 2.265327 -0.088680 -2.968077
H2 2.461533 1.401161 2.640035
H2 2.078009 2.039095 2.592379
C 1.478799 1.819025 -0.376165
C 0.547427 2.840566 -0.584630
C -0.795050 2.569072 -0.393267
C -1.179576 1.280552 -0.003439
C -0.212887 0.308424 0.179912
N 1.095633 0.565404 0.001972
C 2.893248 1.945943 -0.534789
H 0.889166 3.822939 -0.884982
H -1.538404 3.341864 -0.544981
H -2.220980 1.029044 0.147384
H -0.453382 -0.709419 0.453998
N 3.615459 0.905069 -0.217823
C 7.703259 0.930403 -1.234653
C 6.748659 1.320689 -2.172336
C 5.399806 1.311778 -1.838348
C 5.000495 0.913266 -0.555960
C 5.953805 0.503779 0.378441
C 7.300355 0.528839 0.036053
H 8.754300 0.936689 -1.497170
H 7.051330 1.615366 -3.169968
H 4.651823 1.572437 -2.576861
H 5.626602 0.170949 1.352796
|     | X     | Y     | Z     |
|-----|-------|-------|-------|
| H   | 8.037787 | 0.216711 | 0.766371 |
| H   | 3.341126  | 2.859644   | -0.912244 |
| Fe  | 2.568701  | -0.657624  | 0.429473 |
| Cl  | 1.521681  | -2.499730  | -0.226883 |
| Cl  | 3.713449  | -1.255788  | 2.231463 |
| H2  | 2.404510  | 3.976158   | -3.110760 |
| H2  | 2.239897  | 3.456682   | -2.601029 |
| H2  | 6.235882  | 5.599181   | 1.368019 |
| H2  | 5.557236  | 5.787943   | 1.122246 |
| C   | 6.804331  | 3.667940   | -0.925818 |
| C   | 8.156708  | 3.363241   | -0.753554 |
| C   | 9.104960  | 4.183758   | -1.339048 |
| C   | 8.679214  | 5.286139   | -2.086624 |
| C   | 7.323978  | 5.531071   | -2.228458 |
| N   | 6.396154  | 4.741131   | -1.660470 |
| C   | 5.716532  | 2.915650   | -0.378160 |
| H   | 8.440448  | 2.501467   | -0.162989 |
| H   | 10.160913 | 3.975094   | -1.219574 |
| H   | 9.390649  | 5.946675   | -2.564276 |
| H   | 6.937427  | 6.353016   | -2.814762 |
| N   | 4.517377  | 3.391909   | -0.561968 |
| C   | 1.236604  | 0.955602   | 0.456464 |
| C   | 2.280176  | 0.436497   | -0.304677 |
| C   | 3.365417  | 1.239071   | -0.636990 |
| C   | 3.406613  | 2.570231   | -0.205485 |
| C   | 2.352007  | 3.099246   | 0.539940 |
| C   | 1.277158  | 2.284451   | 0.874447 |
| H   | 0.387221  | 0.331609   | 0.710749 |
| H   | 2.245360  | -0.588570  | -0.653410 |
| H   | 4.160836  | 0.852934   | -1.262403 |
| H   | 2.384561  | 4.137958   | 0.834727 |
| H   | 0.463190  | 2.695472   | 1.459131 |
| H   | 5.887180  | 1.986367   | 0.156434 |
| Fe  | 4.456720  | 5.099090   | -1.595552 |
| Cl  | 4.380793  | 6.120502   | -3.574450 |
| Cl  | 3.053187  | 6.285719   | -0.346997 |
| H2  | 5.142213  | 3.167283   | -3.754649 |
| H2  | 5.290401  | 2.449098   | -3.620100 |
| H2  | 6.109274  | 6.466632   | 0.701131 |
| H2  | 6.840493  | 6.371062   | 0.810665 |
| C   | 6.798324  | 3.716364   | -0.932416 |
| C   | 8.158609  | 3.453815   | -0.742088 |
| C   | 9.086732  | 4.275137   | -1.362869 |
| C   | 8.635979  | 5.329697   | -2.164568 |
| C   | 7.276141  | 5.534259   | -2.317903 |
| N   | 6.367994  | 4.748299   | -1.714178 |
| C   | 5.727234  | 2.958459   | -0.364239 |
| H   | 8.464010  | 2.633340   | -0.111016 |
| H   | 10.147182 | 4.100312   | -1.229667 |
| H   | 9.331793  | 5.985034   | -2.671397 |
| H   | 6.869844  | 6.322542   | -2.936498 |
| N   | 4.517112  | 3.393605   | -0.586845 |

S133
| Atoms | X      | Y      | Z      |
|-------|--------|--------|--------|
| C     | 1.218390 | 0.962898 | 0.390029 |
| C     | 2.374746  | 0.388014  | -0.134144 |
| C     | 3.465396  | 1.184806  | -0.456639 |
| C     | 3.407249  | 2.341965  | 0.575082  |
| H     | 0.366143  | 0.340708  | 0.635716  |
| H     | 2.421445  | -0.679966 | -0.310256 |
| H     | 4.344038  | 0.742607  | -0.909812 |
| H     | 2.199696  | 4.221469  | 0.387931  |
| H     | 0.255793  | 2.796513  | 0.972278  |
| Fe    | 5.920380  | 2.059801  | 0.212593  |
| Cl    | 4.442476  | 5.101351  | -1.607498 |
| Cl    | 4.231212  | 6.014814  | -3.614015 |
| H2    | 6.199260  | 7.943220  | -0.716968 |
| C     | 6.808033  | 3.667362  | -0.926998 |
| C     | 8.159037  | 3.356586  | -0.758209 |
| C     | 9.109400  | 4.171184  | -1.349265 |
| H     | 8.440498  | 2.494571  | -0.166970 |
| H     | 10.164736 | 3.957697  | -1.233170 |
| N     | 4.521043  | 3.397122  | -0.557830 |
| C     | 1.241303  | 0.969578  | 0.464617  |
| C     | 2.277243  | 0.445993  | -0.311641 |
| C     | 3.361523  | 1.249414  | -0.645044 |
| C     | 4.410050  | 2.575650  | -0.200187 |
| C     | 5.264316  | 3.099284  | 0.561059  |
| H     | 1.290540  | 2.283625  | 0.896915  |
| H     | 0.393591  | 0.335208  | 0.720049  |
| H     | 2.236600  | -0.575137 | -0.670999 |
| H     | 4.150259  | 0.868130  | -1.281998 |
| H     | 2.401692  | 4.134529  | 0.866545  |
| H     | 0.483387  | 2.690231  | 1.493918  |
| Fe    | 5.887955  | 1.986248  | 0.153339  |
| Cl    | 4.464662  | 5.105568  | -1.593506 |
| Cl    | 3.390633  | 6.132449  | -3.567960 |
| H2    | 5.148647  | 3.155834  | -3.742525 |
| H2    | 5.278645  | 4.346673  | -3.597570 |
| H2    | 6.084010  | 5.461539  | 1.501568  |
|       |        |        |        |
|-------|--------|--------|--------|
| H2    | 5.426513 | 5.658494 | 1.209591 |

BPy

|       |        |        |        |
|-------|--------|--------|--------|
| C1    | -0.046854 | -1.813522 | 0.140917 |
| C1    | -0.397092 | -0.962843 | 4.182562 |
| H2    | 0.337553  | 1.430946  | -1.427506 |
| H2    | 0.247200  | 0.740056  | -1.159511 |
| H     | 0.891615  | 4.296866  | 1.280858  |
| H     | -1.234529 | 4.096867  | 1.092262  |
| C     | 0.714364  | 2.169471  | 1.600847  |
| C     | 1.413438  | 3.369904  | 1.471951  |
| C     | 2.795844  | 3.391756  | 1.590311  |
| C     | 3.452293  | 2.156053  | 1.835300  |
| C     | 2.690666  | 1.003180  | 1.954694  |
| H     | 3.356392  | 4.280910  | 1.492125  |
| H     | 4.528826  | 2.109513  | 1.932357  |
| H     | 3.143677  | 0.038321  | 2.147201  |
| N     | 1.360316  | 1.009589  | 1.840989  |
| Fe    | 0.029675  | -0.624592 | 2.024099  |
| N     | -1.216969 | 0.775060  | 1.634289  |
| C     | -0.748196 | 2.037649  | 1.480095  |
| C     | -2.532620 | 0.536811  | 1.526381  |
| C     | -1.617244 | 3.093494  | 1.214400  |
| C     | -3.443331 | 1.545147  | 1.261553  |
| H     | -2.834847 | -0.492968 | 1.668536  |
| C     | -2.977974 | 2.847631  | 1.103609  |
| H     | -4.495707 | 1.307951  | 1.181507  |
| H     | -3.664685 | 3.658858  | 0.896124  |

C1    | 0.052155  | -1.664983 | 0.096495  |
| C1    | -0.490554 | -1.084355 | 4.189189  |
| H2    | 1.918004  | 1.225779  | -1.170453 |
| H2    | 1.558198  | 0.597463  | -0.990966 |
| H2    | -1.680558 | 1.180052  | -1.416107 |
| H2    | -1.333884 | 0.557015  | -1.196949 |
| C     | 0.704612  | 2.157829  | 1.557129  |
| C     | 1.413413  | 3.31924  | 1.301933  |
| C     | 2.797158  | 3.317157  | 1.401110  |
| C     | 3.444970  | 2.136337  | 1.752254  |
| C     | 2.673614  | 1.008649  | 1.990317  |
| H     | 3.365111  | 4.218143  | 1.203380  |
| H     | 4.522302  | 2.085984  | 1.837513  |
| H     | 3.121264  | 0.059849  | 2.259699  |
| N     | 1.342260  | 1.019012  | 1.895899  |
| Fe    | 0.015452  | -0.618188 | 2.073330  |
| N     | -1.240046 | 0.787970  | 1.708258  |
| C     | -0.762525 | 2.033828  | 1.472552  |
| C     | -2.560327 | 0.561521  | 1.658921  |
| C     | -1.627667 | 3.083999  | 1.174123  |
| C     | -3.468263 | 1.563989  | 1.363922  |
| H     | -2.869789 | -0.454377 | 1.862976  |
| C     | -2.993382 | 2.843289  | 1.115693  |
| H     | -4.525067 | 1.335603  | 1.331113  |
| Atom | X    | Y    | Z    |
|------|------|------|------|
| H    | -3.677089 | 3.654834 | 0.881571 |
| H    | 0.897988  | 4.240203 | 1.023453 |
| H    | -1.237892 | 4.074804 | 0.988249 |
| H2   | -0.214169 | 1.690376 | 4.518717 |
| H2   | -0.121676 | 2.431021 | 4.523451 |
| H2   | 1.978185  | 1.190703 | -1.198049 |
| H2   | 1.597303  | 0.580350 | -1.000397 |
| H2   | -1.724608 | 1.141336 | -1.406805 |
| H2   | -1.365411 | 0.528592 | -1.178393 |
| C    | 0.719505  | 2.160888 | 1.523563 |
| C    | 1.431132  | 3.326026 | 1.240474 |
| C    | 2.815135  | 3.309923 | 1.338102 |
| C    | 3.460319  | 2.135208 | 1.712989 |
| C    | 2.687019  | 1.014068 | 1.973927 |
| H    | 3.385397  | 2.046464 | 1.120011 |
| H    | 4.537635  | 2.083332 | 1.797138 |
| H    | 3.132678  | 0.069097 | 2.259252 |
| C    | 0.978525  | 1.590951 | 4.691956 |
| C    | 1.310993  | 2.257352 | 4.733958 |
| H    | 1.857420  | 1.119398 | -1.259589 |
| H    | 1.489187  | 0.509962 | -1.037267 |
| H2   | -1.807602 | 1.612120 | 4.408569 |
| H2   | -2.172160 | 2.241935 | 4.246115 |
| C    | 0.701411  | 2.159819 | 1.570487 |
| C    | 1.404763  | 3.352273 | 1.404163 |
| C    | 2.786859  | 3.341015 | 1.527657 |
| C    | 3.437935  | 2.144842 | 1.813946 |
| C    | 2.671555  | 0.999182 | 1.966149 |
| H    | 3.350817  | 4.257210 | 1.401376 |
| H    | 4.513718  | 2.096293 | 1.917673 |
| H    | 3.120959  | 0.039380 | 2.189503 |
| N    | 1.342936  | 1.007223 | 1.847525 |
| Fe   | 0.017949  | -0.620818 | 2.036853 |
| N    | -1.237116 | 0.778513 | 1.658243 |
| C    | -0.762835 | 2.032296 | 1.463596 |
| C    | -2.554025 | 0.545617 | 1.580943 |
| C    | -1.629860 | 3.085232 | 1.184891 |
C  -3.464043  1.551612  1.306246
H  -2.860294 -0.478203  1.746295
C  -2.993661  2.845230  1.104753
H  -4.518795  1.318098  0.887925
H  -3.678822  3.655239  1.252290
H   0.886868  4.274489  1.181868
H  -1.243619  4.082987  1.031166
Cl  -0.041510 -1.738991  0.105332
Cl  -0.388455 -0.976029  4.204673
H2  -1.658178  1.170613 -1.483383
H2  -1.328105  0.542872  1.031166
C    0.670016  2.095771  1.707183
C    1.507135  3.210256  1.710130
C    2.882081  3.032814  1.663101
C    3.394839  1.739541  1.614418
C    2.514312  0.671183  1.664937
H    4.460211  1.553326  1.577058
H    2.853336 -0.355042  1.581220
N    1.184826  0.842396  1.660860
Fe  -0.021107  -0.650042  1.658921
N   -1.412730  0.954755  1.746882
C   -0.802180  2.157476  1.752122
C   -2.745491  0.888030  1.782783
C   -1.542069  3.340399  1.794684
C   -3.546706  2.019735  1.826528
H   -3.168408 -0.109246  1.774741
C   -2.927081  3.266399  1.832495
H   -4.624018  1.923777  1.854426
H   -3.517856  4.173955  1.865386
H    1.089329  4.206396  1.748665
H   -1.049828  4.302761  1.797548
Cl    0.333590 -1.465208  3.700790
Cl    0.150808 -1.323318 -0.457432

PHEN

H   -0.269682  4.806339  1.086822
H   -2.523336  4.151754 -0.368607
C    0.600363  2.472252  1.253043
C    0.767717  3.452520  0.255681
C    2.085969  3.774348 -0.120828
C    3.137400  3.124551  0.491234
C    2.884731  2.158589  1.472288
H    2.263108  4.522043 -0.884759
H    4.162753  3.345434  0.225855
H    3.683400  1.627179  1.971399
N    1.648269  1.837688  1.844163
Fe   1.219602  0.522831  3.157661
N   -0.789137  1.132231  2.629295
C   -0.710465  2.089534  1.675422
C   -1.986352  0.742147  3.038073
C   -1.843644  2.693371  1.090819
Structure descriptions

C  -3.173061  1.284471  2.520534
H  -2.006734 -0.026399  3.801482
C  -3.102786  2.259110  1.547370
H  -4.126324  0.929858  2.890193
H  -4.005248  2.691223  1.130284
C  -0.402041  4.052894  -0.319277
C  -1.650592  3.690476   0.078408
Cl  1.850582  1.583293  5.003339
Cl  1.694548 -1.338978  2.032995
H2  -0.127165  0.176760  -0.724841
H2   0.249503 -0.204421  -0.205165
H2   1.730550  0.695961  -1.073759
H2   1.725986  0.219321  -0.499562
C   0.608578  2.487857  1.265304
C   0.778114  3.449797  0.246315
C   2.098043  3.805854  -0.092706
C   3.147736  3.208748  0.577338
C   2.892522  2.258093  1.572753
H   2.277144  4.531393  -0.872432
H   4.173780  3.460450   0.344175
H   3.689632  1.768210  2.114778
N   1.655456  1.900212  1.903612
Fe   1.220181  0.553333  3.185347
N  -0.783242  1.164826  2.666143
C  -0.702948  2.083352  1.664763
C  -1.980427  0.753484  3.041977
C  -1.834067  2.631422  1.024416
C  -3.165643  1.237185  2.466193
H  -2.003705  0.012857  3.832319
C  -3.093634  2.175375  1.458380
H  -4.119001  0.866080  2.818827
H  -3.994596  2.562936  0.996723
C  -0.389844  3.989240  -0.384866
C  -1.638804  3.590053  -0.015591
Cl  2.000581  1.516762  5.025963
Cl  1.547766 -1.283714  1.953976
H2  -1.451473 -0.478520   0.022893
H2  -0.850054 -0.714596   0.396120
H   0.255500  4.721995  -1.171802
H   2.510658  4.016621  -0.505279
H2   1.772245  1.728172  -1.259065
H2   1.442445  1.066835  -1.158879
H2  -0.945461  1.456733  4.551487
H2  -1.088410  2.187323  4.602309
C   0.739136  2.165750  1.604118
C   1.335711  3.436871  1.473183
C   2.741727  3.488424  1.531189
C   3.457156  2.323403  1.711918
C   2.769645  1.106168  1.836555
H   3.249845  4.440905  1.432333
H   4.538200  2.331805  1.758230
H   3.302893  0.173522  1.976558
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| N       | 1.449442 | 1.027577 | 1.786115 |
| Fe      | 0.076946  | -0.637144 | 1.809837  |
| N       | -1.190917 | 0.779904  | 1.663381  |
| C       | -0.682798 | 2.035294  | 1.545672  |
| C       | -2.510086 | 0.616335  | 1.645208  |
| C       | -1.494971 | 3.172722  | 1.380413  |
| C       | -3.388655 | 1.695683  | 1.494919  |
| H       | -2.864386 | -0.399726 | 1.752090  |
| C       | -2.889002 | 2.973305  | 1.355965  |
| H       | -4.453905 | 1.507125  | 1.485740  |
| H       | -3.553553 | 3.820169  | 1.231708  |
| C       | 0.490882  | 4.581257  | 1.291713  |
| C       | -0.862197 | 4.454067  | 1.250616  |
| Cl      | 0.059690  | -1.406277 | -0.286733 |
| Cl      | -0.378503 | -1.350131 | 3.865804  |
| H2      | -1.762023 | 1.605831  | -1.341018 |
| H2      | -1.392388 | 0.962738  | -1.263748 |
| H       | -1.490063 | 5.327168  | 1.117207  |
| H       | 0.953267  | 5.555942  | 1.189558  |

H2 -2.997575  | 0.371246   | 1.173537  |
H2 -2.845995  | 0.853465   | 1.721704  |
H2 2.446963   | -1.699315  | 1.804847  |
H2 2.179619   | -2.123497  | 1.252878  |
H2 -2.586879  | 1.241171   | -1.435705 |
H2 -2.380191  | 1.953732   | -1.511706 |
C 0.063687    | 0.097048   | 0.747709  |
C 0.393538    | 0.819667   | 1.910800  |
C 0.086710    | 0.225122   | 3.149813  |
C -0.512691   | -1.015735  | 3.172075  |
C -0.806295   | -1.665809  | 1.967698  |
H 0.323074    | 0.745485   | 4.070594  |
H -0.762379   | -1.501148  | 4.106090  |
H -1.276252   | -2.639686  | 1.945974  |
N -0.526384   | -1.125026  | 0.788126  |
Fe -0.893690  | -1.946904  | -0.930234 |
N 0.002784    | -0.108558  | -1.615591 |
C 0.347416    | 0.641983   | -0.544171 |
C 0.249674    | 0.362713   | -2.826794 |
C 0.960292    | 1.907466   | -0.654249 |
C 0.855601    | 1.609879   | -3.041022 |
H -0.041031   | -0.268475  | -3.657832 |
C 1.210587    | 2.382685   | -1.955912 |
H 1.035931    | 1.947839   | -4.053017 |
H 1.680318    | 3.349993   | -2.093924 |
C 1.016262    | 2.104422   | 1.766829  |
C 1.287631    | 2.625307   | 0.543152  |
Cl -3.103317  | -1.652458  | -1.015779 |
Cl 0.718790   | -3.488120  | -0.955853 |
H2 3.102061   | -0.677104  | -1.435995 |
H2 2.671394   | -1.282760  | -1.373974 |
H 1.758289    | 3.597232   | 0.452269  |
H 1.268378    | 2.656520   | 2.666716  |

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Structure descriptions

\begin{verbatim}
Cl  -3.090738  -1.718005  -1.016654
Cl  0.632031  -3.564444  -0.927513
C   1.003634   2.111412   1.767373
C   1.273768   2.642365   0.545314
H   1.736660   3.618764   0.463118
H   1.249684   2.661115   2.668313
C   0.069688   0.103839   0.732760
C   0.391022   0.820714   1.902074
C  -0.503690  -1.031358   3.144977
C  -0.791679  -1.677008   1.937102
H   0.314954   0.729027   4.062487
H  -0.751575  -1.526192   4.074796
H  -1.253334  -2.654348   1.905639
N  -0.878526  -1.933176  -0.927351
N   0.015955  -0.094276  -1.628081
C   0.353051   0.657683  -0.553843
C   0.261612   0.384279  -2.837621
C   0.956009   1.929396  -0.657587
C   0.857497   1.637878  -3.045016
H  -0.023024  -0.247382  -3.670584
C   1.204877   2.410644  -1.956931
H   1.036806   1.981285  -4.055501
H   1.666469   3.381995  -2.092602
\end{verbatim}

\[ \text{CoCl}_2 \rightarrow \text{H}_2 \]

\begin{verbatim}
BBH
H2   5.043994   4.218945   2.153045
H2   4.564838   4.662767   1.791817
C   0.783031   1.985080   0.766220
C  -0.060844   0.890277   1.021625
C  -1.430434   1.071616   1.150741
C  -1.971078   2.351220   1.041797
C  -1.137855   3.446068   0.811025
C   0.230584   3.272985   0.675185
C   2.200228   1.710933   0.620501
H   0.359750  -0.106042   1.105317
H  -2.073632   0.220319   1.337067
H  -3.039838   2.497276   1.145129
H  -1.554890   4.442866   0.740209
N   3.072655   2.519408   0.130628
C   5.336132   2.831545  -0.486556
N   4.378449   2.078759   0.117142
H   2.529310   0.721295   0.950086
H   4.596814   1.161150   0.483276
O   5.044451   3.883251  -1.080825
C   9.378911   1.469573  -0.393549
C   8.926350   2.297265  -1.419441
C   7.609153   2.736671  -1.431477
C   6.730577   2.335759  -0.419460
C   7.191241   1.513704   0.616328
C   8.512719   1.084036   0.627449
\end{verbatim}

S140
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 10.4086 | 1.1328  | -0.3836 |
| H    | 9.6017  | 2.6026  | -2.2090 |
| H    | 7.2435  | 3.3863  | -2.2157 |
| H    | 6.5423  | 1.2425  | 1.4413  |
| H    | 8.8693  | 0.4601  | 1.4378  |
| H    | 0.8634  | 4.1389  | 0.5311  |
| Co   | 3.0285  | 4.3397  | -1.0633 |
| Cl   | 2.5987  | 6.1167  | 0.1951  |
| Cl   | 2.0216  | 3.7505  | -2.9390 |
| H2   | 4.8157  | 3.6586  | 2.5603  |
| H2   | 4.3281  | 4.1470  | 2.2741  |
| H2   | 4.2039  | 1.4570  | -2.9155 |
| H2   | 3.7594  | 2.0568  | -2.9292 |
| C    | 0.7702  | 1.9340  | 0.6006  |
| C    | 0.0340  | 1.1669  | 1.5207  |
| C    | -1.3379 | 1.3347  | 1.6399  |
| C    | -1.9934 | 2.2606  | 0.8306  |
| C    | -1.2742 | 3.0083  | -0.1019 |
| C    | 0.0974  | 2.8509  | -0.2235 |
| C    | 2.2039  | 1.7184  | 0.5599  |
| H    | 0.5447  | 0.4474  | 2.1515  |
| H    | -1.8946 | 0.7465  | 2.3592  |
| H    | -3.0653 | 2.3929  | 0.9192  |
| H    | -1.7845 | 3.7173  | -0.7419 |
| N    | 3.0660  | 2.4873  | -0.0067 |
| C    | 5.3533  | 2.8763  | -0.4551 |
| N    | 4.3792  | 2.0736  | 0.0463  |
| H    | 2.5629  | 0.8249  | 1.0784  |
| H    | 4.5843  | 1.1190  | 0.3104  |
| O    | 5.0813  | 3.9895  | -0.9369 |
| C    | 9.3757  | 1.4556  | -0.4458 |
| C    | 8.9471  | 2.3834  | -1.3933 |
| C    | 7.6370  | 2.8435  | -1.3762 |
| C    | 6.7414  | 2.3619  | -0.4160 |
| C    | 7.1776  | 1.4388  | 0.5423  |
| C    | 8.4925  | 0.9897  | 0.5259  |
| H    | 10.4000 | 1.1028  | -0.4578 |
| H    | 9.6358  | 2.7505  | -2.1442 |
| H    | 7.2890  | 3.5695  | -2.0992 |
| H    | 6.5143  | 1.1020  | 1.3306  |
| H    | 8.8310  | 0.2868  | 1.2772  |
| H    | 0.6308  | 3.4122  | -0.9788 |
| Co   | 3.0814  | 4.4820  | -0.8681 |
| Cl   | 2.5724  | 5.8599  | 0.7849  |
| Cl   | 2.1678  | 4.4637  | -2.8937 |
| H2   | 4.8698  | 4.1434  | 2.3051  |
| H2   | 4.4248  | 4.6217  | 1.9446  |
| C    | 0.8192  | 1.9446  | 0.5976  |
| C    | -0.0274 | 0.8272  | 0.6926  |
| C    | -1.4024 | 0.9918  | 0.7788  |
| C    | -1.9460 | 2.2749  | 0.7867  |
| C    | -1.1106 | 3.3897  | 0.7157  |
| Atom | X  | Y  | Z  |
|------|----|----|----|
| C    | 0.263740 | 3.233842 | 0.623492 |
| C    | 2.243125  | 1.692883 | 0.480785 |
| H    | 0.395527  | -0.171230 | 0.681670 |
| H    | -2.048313 | 0.124513  | 0.839513 |
| H    | -3.019311 | 2.406833  | 0.856518 |
| H    | -1.530235 | 4.387781  | 0.735369 |
| N    | 3.120962  | 2.549466  | 0.094475 |
| C    | 5.388700  | 2.927603  | -0.466407 |
| N    | 4.431868  | 2.124524  | 0.079712 |
| H    | 2.570598  | 0.679641  | 0.728040 |
| H    | 4.642874  | 1.165492  | 0.324224 |
| O    | 5.096154  | 4.027073  | -0.956580 |
| C    | 9.421783  | 1.543791  | -0.503581 |
| C    | 8.963765  | 2.445093  | -1.463038 |
| C    | 7.650012  | 2.893166  | -1.427765 |
| C    | 6.781135  | 2.427326  | -0.435519 |
| C    | 7.246370  | 1.530258  | 0.533641 |
| C    | 8.564756  | 1.092367  | 0.498026 |
| H    | 10.448783 | 1.199764  | -0.530361 |
| H    | 9.631934  | 2.800035  | -2.237882 |
| H    | 7.277386  | 3.595297  | -2.161701 |
| H    | 6.602494  | 1.205346  | 1.342836 |
| H    | 8.926472  | 0.409686  | 1.257017 |
| H    | 0.897255  | 4.111098  | 0.599870 |
| Co   | 3.075760  | 4.433231  | -0.983407 |
| Cl   | 2.544508  | 6.157488  | 0.307068 |
| Cl   | 2.183403  | 3.878890  | -2.935120 |
| H2   | 2.016500  | 0.282712  | -2.340012 |
| H2   | 2.014551  | 1.016760  | -2.476600 |
| H2   | 5.081112  | 1.666647  | -3.150392 |
| H2   | 4.512427  | 2.150183  | -3.161407 |
| H2   | 5.425892  | 4.381154  | 2.157000 |
| H2   | 4.926695  | 4.794818  | 1.788210 |
| C    | 0.810625  | 1.921801  | 0.563704 |
| C    | -0.015149 | 0.793177  | 0.702925 |
| C    | -1.393690 | 0.933236  | 0.772334 |
| C    | -1.962384 | 2.204137  | 0.717493 |
| C    | -1.148667 | 3.351212  | 0.601635 |
| C    | 0.228868  | 3.198978  | 0.526701 |
| C    | 2.238346  | 1.688306  | 0.466908 |
| H    | 0.427561  | -0.196194 | 0.740839 |
| H    | -2.022603 | 0.056751  | 0.868528 |
| H    | -3.038542 | 2.317588  | 0.772754 |
| H    | -1.588530 | 4.320236  | 0.573691 |
| N    | 3.114928  | 2.543601  | 0.075078 |
| C    | 5.384679  | 2.916451  | -0.473270 |
| N    | 4.428747  | 2.125612  | 0.081376 |
| H    | 2.573014  | 0.683150  | 0.738963 |
| H    | 4.642631  | 1.174182  | 0.351678 |
| O    | 5.091929  | 4.005628  | -0.995591 |
| C    | 9.419238  | 1.536066  | -0.490031 |
| C    | 8.960236  | 2.415226  | -1.469335 |
| C    | 7.645731  | 2.861954  | -1.444635 |
Structure descriptions

C 6.777035 2.416847 -0.442770
C 7.243260 1.542162 0.546240
C 8.562273 1.105485 0.520750
H 10.446813 1.193229 -0.508680
H 9.628310 2.754291 -2.251358
H 7.273234 3.548652 -2.193134
H 6.600166 1.234865 1.362872
H 8.924552 0.440623 1.295132
H 0.844551 4.086614 0.474129
Co 3.081282 4.442115 -0.959711
Cl 2.615125 6.097320 0.447058
Cl 2.125261 4.021356 -2.912591
H2 1.697471 0.440289 -2.409185
H2 1.757447 1.174170 -2.531371
H2 2.254013 3.646606 3.189321
H2 2.406499 4.180065 2.691272
H2 4.884408 1.610288 -3.116674
H2 4.348312 2.129633 -3.117361

C 2.121277 2.956705 0.090548
C 1.406182 2.298310 1.106188
C 0.034984 2.470973 1.227983
C -0.640457 3.291423 0.326479
C 0.057904 3.929194 -0.698778
C 1.428720 3.766664 -0.824243
C 3.555925 2.745367 0.048087
H 1.932285 1.660545 1.808394
H -0.505564 1.967652 2.020171
H -1.711960 3.425985 0.416193
H -0.468020 4.564408 -1.409419
N 4.401374 3.456158 -0.611763
C 6.682283 3.805589 -1.146134
N 5.719967 3.053081 -0.546742
H 3.930288 1.912633 0.650435
H 5.936707 2.134584 -0.182357
O 6.395442 4.864966 -1.728307
C 10.717287 2.413072 -1.090524
C 10.272440 3.280837 -2.086043
C 8.958628 3.730689 -2.083302
C 8.075094 3.300519 -1.087637
C 8.528505 2.437389 -0.082290
C 9.846508 1.997426 -0.085353
H 11.744255 2.067996 -1.091705
H 10.951074 3.609606 -2.863351
H 8.599017 4.410991 -2.843973
H 7.877895 2.138786 0.731750
H 10.196964 1.341284 0.701803
H 1.946275 4.239884 -1.648153
Co 4.384086 5.360815 -1.667338
Cl 3.908830 6.876555 -0.134944
Cl 3.440084 5.130823 -3.662787

PIP
| atom | x     | y     | z     |
|------|-------|-------|-------|
| H2   | 8.491512 | -0.625023 | -1.237575 |
| H2   | 8.238185 | -1.000680 | -0.643789 |
| C    | 5.845375 | 3.260013  | 1.847030  |
| C    | 5.925707 | 3.864444  | 3.113253  |
| C    | 4.809720 | 4.028349  | 3.917006  |
| C    | 3.449091 | 3.024484  | 2.195068  |
| C    | 4.572958 | 2.857091  | 1.397417  |
| C    | 7.087965 | 3.117604  | 1.097462  |
| H    | 6.895429 | 4.194675  | 3.467555  |
| H    | 4.903940 | 4.483590  | 4.894208  |
| H    | 2.683884 | 3.720340  | 4.069332  |
| H    | 2.482157 | 2.695260  | 1.830555  |
| N    | 7.297881 | 2.348006  | 0.091371  |
| C    | 11.093377 | 2.165899 | -1.721694 |
| C    | 10.999580 | 2.164723 | -0.331701 |
| C    | 9.756455  | 2.236036  | 0.287210  |
| C    | 8.598065  | 2.311774  | -0.491929 |
| C    | 8.687133  | 2.282737  | -1.886400 |
| C    | 9.935167  | 2.221621  | -2.494689 |
| H    | 12.063500 | 2.104435  | -2.199789 |
| H    | 11.894784 | 2.090275  | 0.273958  |
| H    | 9.680270  | 2.185027  | 1.366489  |
| H    | 7.778340  | 2.295921  | -2.476574 |
| H    | 9.999917  | 2.206464  | -3.575708 |
| H    | 7.908288  | 3.740306  | 1.463424  |
| O    | 4.469312  | 2.328266  | 0.131903  |
| Mn   | 5.961340  | 0.685258  | -0.564349 |
| Cl   | 5.375381  | 0.724710  | -2.766115 |
| Cl   | 5.783584  | -0.688356 | 1.251011  |
| H    | 3.545840  | 2.139803  | -0.090976 |
| C    | 1.390485  | 2.079566  | -0.628603 |
| C    | 0.858944  | 3.379086  | -0.717137 |
| C    | -0.459063 | 3.657429  | -0.397561 |
| C    | -1.295184 | 2.621696  | 0.011997  |
| C    | -0.809830 | 1.322418  | 0.089726  |
| C    | 0.513726  | 1.052114  | -0.228880 |
| C    | 2.803090  | 1.930776  | -0.960401 |
| H    | 1.513403  | 4.182455  | -1.034183 |
| H    | -0.833076 | 4.670425  | -0.465406 |
| H    | -2.328050 | 2.820472  | 0.268941  |
| H    | -1.459276 | 0.511959  | 0.401653  |
| N    | 3.564477  | 0.918132  | -0.742074 |
| C    | 7.656039  | 1.112843  | -1.717567 |
| C    | 7.047177  | 2.202380  | -1.099322 |
| C    | 5.696909  | 2.157277  | -0.772804 |
| C    | 4.950281  | 1.013742  | -1.071810 |
| C    | 5.564970  | -0.093436 | -1.661085 |
| C    | 6.913002  | -0.033083 | -1.991879 |
| H    | 8.710022  | 1.149075  | -1.964600 |
| H    | 7.627904  | 3.082551  | -0.851652 |
| H    | 5.236238  | 2.983102  | -0.245055 |
| H    | 4.983373  | -0.988399 | -1.844873 |
Structure descriptions

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| Atom | X-coordinate | Y-coordinate | Z-coordinate |
|------|--------------|--------------|--------------|
| H2   | 3.344520     | 1.320542     | 2.976075     |
| H2   | 3.530574     | -0.835941    | -2.375437    |
| H2   | 3.920564     | -0.231727    | -2.575982    |
| C    | 3.877412     | 1.465055     | -0.094292    |
| C    | 4.465443     | 2.711700     | -0.383690    |
| C    | 5.829435     | 2.925008     | -0.287940    |
| C    | 6.656824     | 1.876061     | 0.107205     |
| C    | 6.113107     | 0.632055     | 0.398560     |
| C    | 4.742883     | 0.425468     | 0.299590     |
| C    | 2.429385     | 1.392313     | -0.230252    |
| N    | 3.818187     | 3.525451     | -0.689068    |
| C    | 6.246156     | 3.897085     | -0.517019    |
| H    | 7.726724     | 2.022413     | 0.189248     |
| H    | 6.754152     | -0.187503    | 0.705060     |
| N    | 1.651048     | 0.395179     | -0.000286    |
| C    | -2.481434    | 0.797491     | -0.702958    |
| C    | -1.575867    | 1.240686     | -1.663839    |
| C    | -0.207849    | 1.119010     | -1.445217    |
| C    | 0.253372     | 0.551555     | -0.254631    |
| C    | -0.650556    | 0.078812     | 0.699408     |
| C    | -2.015072    | 0.215085     | 0.474037     |
| H    | -3.546424    | 0.888548     | -0.878914    |
| H    | -1.933075    | 1.665435     | -2.594231    |
| H    | 0.498013     | 1.416960     | -2.210909    |
| H    | -0.275983    | -0.383512    | 1.605098     |
| H    | -2.714805    | -0.143481    | 1.218897     |
| H    | 1.973594     | 2.328280     | -0.568155    |
| O    | 4.221001     | -0.810450    | 0.588603     |
| Co   | 2.205289     | -1.495422    | 0.582961     |
| Cl   | 1.782829     | -1.921663    | 2.721200     |
| Cl   | 2.069254     | -2.928529    | -1.092300    |
| H    | 4.908529     | -1.429606    | 0.873547     |
| H2   | 3.460708     | 1.277634     | 2.954849     |
| H2   | 3.092459     | 0.630904     | 3.011617     |
| H2   | 3.472544     | -0.798677    | -2.427957    |
| H2   | 3.861879     | -0.198524    | -2.641308    |
| C    | 3.841724     | 1.489052     | -0.096370    |
| C    | 4.428368     | 2.735681     | -0.390927    |
| C    | 5.782969     | 2.969632     | -0.232288    |
| C    | 6.602147     | 1.942691     | 0.232877     |
| C    | 6.061874     | 0.697020     | 0.522986     |
| C    | 4.700608     | 0.467421     | 0.359629     |
| C    | 2.397682     | 1.400950     | -0.275913    |
| H    | 3.786544     | 3.534339     | -0.744209    |
| H    | 6.198550     | 3.941281     | -0.464896    |
| H    | 7.664457     | 2.106504     | 0.365303     |
| H    | 6.696759     | -0.110425    | 0.869745     |
| N    | 1.622055     | 0.402749     | -0.041525    |
| C    | -2.503508    | 0.725018     | -0.815260    |
| C    | -1.591269    | 1.177197     | -1.765674    |
| C    | -0.224894    | 1.083310     | -1.525033    |
| C    | 0.228026     | 0.535067     | -0.322532    |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -0.682124 | 0.053332  | 0.621427  |
| C    | -2.045062 | 0.161386  | 0.373973  |
| H    | -3.567140 | 0.794171  | -1.008850 |
| H    | -1.941790 | 1.586933  | -2.705299 |
| H    | 0.486632  | 1.387634  | -2.282877 |
| H    | -0.312830 | -0.392438 | 1.538001  |
| H    | -2.749646 | -0.204351 | 1.110711  |
| H    | 1.943442  | 2.326192  | -0.635384 |
| O    | 4.188804  | -0.777299 | 0.629890  |
| Co   | 2.187446  | -1.470408 | 0.577804  |
| Cl   | 1.869589  | -1.845233 | 2.752943  |
| Cl   | 1.934607  | -2.934293 | -1.050679 |
| H    | 4.773492  | -1.298276 | 1.206387  |
| H2   | 4.644985  | -2.458193 | 2.711387  |
| H2   | 5.368181  | -2.562772 | 2.542089  |
| H2   | 3.476473  | -0.886444 | -2.358300 |
| H2   | 3.880388  | -0.291088 | -2.557896 |
| C    | 3.861401  | 1.460254  | -0.070160 |
| C    | 4.445650  | 2.714853  | -0.330911 |
| C    | 5.808655  | 2.930950  | -0.226748 |
| C    | 6.638585  | 1.876276  | 0.147210  |
| C    | 6.098456  | 0.624488  | 0.410873  |
| C    | 4.729187  | 0.415508  | 0.304765  |
| C    | 2.414491  | 1.384352  | -0.215599 |
| H    | 3.796075  | 3.532475  | -0.620628 |
| H    | 6.222679  | 3.909075  | -0.433957 |
| H    | 7.707840  | 2.024341  | 0.234654  |
| H    | 6.741521  | -0.198979 | 0.702327  |
| N    | 1.639793  | 0.380410  | -0.003397 |
| C    | -2.485914 | 0.809011  | -0.722375 |
| C    | -1.573744 | 1.236693  | -1.683701 |
| C    | -0.207756 | 1.101351  | -1.461244 |
| C    | 0.244233  | 0.536202  | -0.266596 |
| C    | -0.666363 | 0.075869  | 0.686851  |
| C    | -2.028540 | 0.226133  | 0.457863  |
| H    | -3.549286 | 0.913682  | -0.899701 |
| H    | -1.924253 | 1.663590  | -2.615471 |
| H    | 0.503910  | 1.393034  | -2.223731 |
| H    | -0.297931 | -0.383692 | 1.596384  |
| H    | -2.733709 | -0.119363 | 1.203583  |
| H    | 1.955730  | 2.322089  | -0.533500 |
| O    | 4.210478  | -0.827538 | 0.567837  |
| Co   | 2.192431  | -1.511154 | 0.574544  |
| Cl   | 1.755171  | -1.931250 | 2.710921  |
| Cl   | 2.061890  | -2.945227 | -1.100119 |
| H    | 4.902089  | -1.455090 | 0.822870  |
| H2   | 3.096976  | 0.604010  | 3.024498  |
| H2   | 3.471025  | 1.247626  | 2.971099  |
| H2   | 3.421744  | -0.791994 | 2.423462  |
| H2   | 3.801145  | -0.182588 | -2.628701 |
| H2   | -0.707931 | 3.069148  | 0.657654  |
| H2   | -0.597600 | 3.735142  | 0.971470  |
Structure descriptions

C  3.844970  1.457941  -0.013656
C  4.411674  2.742075   0.084748
C  5.768237  2.933665   0.282760
C  6.608921  1.825887   0.368822
C  6.086009  0.543731   0.263087
C  4.722258  0.360419   0.080864
C  2.399890  1.397967  -0.194276
H  3.754619  3.600893   0.013335
H  6.170037  3.935038   0.366166
H  7.673008  1.956671   0.521799
H  6.735460  -0.321647  0.336889
N  1.632203  0.373848  -0.080758
C  -2.495439  0.766209  -0.802419
C  -1.586242  1.314236  -1.703567
C  -0.218827  1.197859  -1.476144
C   0.237726  0.530032  -0.337352
C  -0.670235  -0.041683  0.557107
C  -2.033409  0.088940  0.324886
H  -3.559536  0.852245  -0.985916
H  -1.939353  1.817877  -2.595383
H   0.492034  1.580354  -2.198445
H  -0.300706  -0.562990  1.432612
H  -2.736200  -0.346934  1.024231
H   1.999552  2.361904  -0.418056
O   4.206449  -0.910360  -0.024761
Co  2.230104  -1.497176  0.531729
Cl  2.115322  -1.546990  2.749360
Cl  1.873942  -3.137792  -0.902310
H   4.902017  -1.583552  0.004314
H2  1.433038  1.324021  2.798196
H2  1.214052  2.036282  2.812179
H2  2.741696  -0.905315  -2.622575
H2  3.000516  -0.311235  -2.992772
H2  4.132604   0.589025   3.121496
H2  4.625794   1.144165   3.051683

C  3.846974  1.497910  -0.106782
C  4.423170  2.745396  -0.414980
C  5.783600  2.976964  -0.308863
C  6.618534  1.946268  0.116817
C  6.086432  0.701803  0.427824
C  4.720031  0.476782  0.318025
C  2.401428  1.405349  -0.255618
H  3.769703  3.545043  -0.743504
H  6.191216  3.949125  -0.553450
H  7.685715  2.107008  0.207187
H  6.733868  -0.103415  0.757750
N  1.633819  0.401894  -0.016967
C  -2.494704  0.783293  -0.747157
C  -1.585477  1.923727  -1.719422
C  -0.218570  1.071858  -1.493897
C  0.237156  0.540770  -0.285218
C  -0.670135  0.098579  0.679792
C  -2.033355  0.233778  0.447378
Structure descriptions

SP-JLMC

H  -3.558758   0.876301  -0.926837
H  -1.938935   1.348871  -2.263635
H   0.491149   1.348871  -2.263635
H  -0.298612  -0.335394  1.600559
H  -2.736109  -0.097315  1.201872
H   1.936408   2.330046  -0.601464
O    4.209128  -0.758896   0.626586
Co   2.199638  -1.472364   0.604225
Cl   1.754556  -1.466015   2.745874
Cl   2.105956  -2.934020  -1.047605
H    4.899582  -1.362613   0.937153
H2   3.013431   0.710185   2.998545
H2   3.372392   1.361490   2.935119
H2   3.505792  -0.828710  -2.381823
H2   3.882205  -0.220101  -2.594919
H2  -0.803883   3.117270   0.524225
H2  -0.663222   3.765076   0.862917
C    3.833538   1.427227  -0.127142
C    4.465940   2.564578  -0.663385
C    5.839666   2.730618  -0.627730
C    6.629878   1.747784  -0.035963
C    6.040124   0.617310   0.513528
C    4.661363   0.455801   0.470142
C    2.381301   1.381404  -0.246404
H    3.847423   3.327328  -1.121489
H    6.292351   3.615382  -1.055284
H    7.706095   1.859344  -0.002796
H    6.651161  -0.148248   0.979024
N    1.888229   0.411873   0.040707
C   -2.539100   0.819434  -0.685625
C   -1.628516   1.222291  -1.659839
C   -0.261912   1.097529  -1.435674
C    0.193254   0.568202  -0.224760
C   -0.715962   0.132440   0.741975
C   -2.079101   0.271927   0.510334
H   -3.603151   0.913513  -0.866157
H   -1.981339   1.617235  -2.604907
H    0.447067   1.359365  -2.211103
H   -0.346158  -0.311309   1.658309
H   -2.782597  -0.058097   1.264828
H    1.944071   2.301443  -0.637617
O    4.084228  -0.653767   1.037949
Co    2.165442  -1.476807   0.612470
Cl   1.527485  -2.118049   2.640656
Cl   2.400584  -2.700663  -1.212977
H    4.743785  -1.229813   1.451200
H2    2.448579   0.627892   3.077681
H2    2.688948   1.333870   3.067993
H2    2.737161  -0.319283   2.809145
H2    2.889676   0.311267  -3.178720
H2    5.080349   3.084929   2.191421
H2    4.860373   3.079530   2.901882
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 3.844776| 1.486190| -0.116239|
| C    | 4.431502| 2.728783| -0.425856|
| C    | 5.784142| 2.968031| -0.258005|
| C    | 6.599733| 1.950739| 0.233951 |
| C    | 6.058285| 0.709373| 0.540187 |
| C    | 4.699807| 0.474971| 0.365653 |
| H    | 3.791790| 3.519950| -0.799208|
| H    | 6.200711| 3.936228| -0.503215|
| H    | 7.660342| 2.118817| 0.374718 |
| H    | 6.690704| -0.090310| 0.908582 |
| N    | 1.625938| 0.401893| -0.044705|
| C    | -2.503618| 0.737085| -0.792555|
| C    | -1.595931| 1.176294| -1.753317|
| C    | -0.228291| 1.077247| -1.521549|
| C    | 0.230401| 0.537236| -0.317577|
| C    | -0.675501| 0.068330| 0.636737 |
| C    | -2.039676| 0.181272| 0.398159 |
| H    | -3.568160| 0.810046| -0.979186|
| H    | -1.951131| 1.579657| -2.693930|
| H    | 0.479710| 1.371239| -2.286759|
| H    | -0.302266| -0.372747| 1.553777 |
| H    | -2.740930| -0.174692| 1.142808|
| H    | 1.947320| 2.317891| -0.660935|
| O    | 4.186597| -0.764316| 0.654222|
| Co   | 2.190843| -1.470678| 0.575663 |
| Cl   | 1.834015| -1.873797| 2.743633 |
| Cl   | 1.958458| -2.933606| -1.055473|
| H    | 4.766692| -1.272689| 1.246355 |
| H2   | 4.622657| -2.416533| 2.756204 |
| H2   | 5.351670| -2.501228| 2.598872 |
| H2   | 3.523268| -0.900962| -2.359824|
| H2   | 3.932536| -0.309521| -2.559639|
| H2   | 2.993034| 0.750245| 3.011694 |
| H2   | 3.366737| 1.393738| 2.955115 |
| C    | 1.389857| 2.080756| -0.633608|
| C    | 0.857506| 3.379028| -0.739073|
| C    | -0.461652| 3.660546| -0.426308|
| C    | -1.298341| 2.629202| -0.006134|
| C    | -0.812375| 1.330971| 0.088571 |
| C    | 0.512241| 1.057433| -0.223990|
| C    | 2.803373| 1.928070| -0.961141|
| H    | 1.512349| 4.178992| -1.064418|
| H    | -0.836174| 4.672540| -0.507853|
| H    | -2.332170| 2.830443| 0.245554 |
| N    | -1.462320| 0.523721| 0.408213 |
| C    | 3.565293| 0.919201| -0.734506|
| C    | 7.653965| 1.121313| -1.723561|
| C    | 7.043832| 2.211864| -1.107776|
| C    | 5.694932| 2.163255| -0.775103|
| C    | 4.950973| 1.015505| -1.065905|
| C    | 5.567293| -0.092994| -1.651538|
| C    | 6.913825| -0.028846| -1.989031|
| Atom | X  | Y  | Z  |
|------|----|----|----|
| H    | 8.706632 | 1.160578 | -1.976282 |
| H    | 7.622416 | 3.095553 | -0.867014 |
| H    | 5.233167 | 2.990288 | -0.249861 |
| H    | 4.987787 | -0.990670 | -1.829366 |
| H    | -7.386835 | -0.886840 | -2.450706 |
| H    | -3.240509 | 2.807431 | -1.440867 |
| O    | 0.982898 | -0.234810 | -0.177452 |
| Co   | 2.996044 | -0.740106 | 0.367346 |
| Cl   | 3.212241 | -2.718453 | -0.606008 |
| Cl   | 3.161494 | -0.188899 | 2.499516 |
| H    | 0.301309 | -0.850384 | 0.130713 |

PIA

| Atom | X  | Y  | Z  |
|------|----|----|----|
| C    | 1.031164 | 1.361555 | -0.155910 |
| C    | -0.120802 | 2.141355 | -0.208227 |
| C    | -1.309887 | 1.611814 | 0.285864 |
| C    | -1.310409 | 0.327734 | 0.814887 |
| C    | -0.114830 | -0.389210 | 0.833983 |
| N    | 1.021547 | 0.115254 | 0.362199 |
| C    | 2.323253 | 1.850084 | -0.653365 |
| H    | -0.082988 | 3.138732 | -0.628064 |
| H    | -2.221483 | 2.196080 | 0.256574 |
| H    | -2.213414 | -0.120371 | 1.207794 |
| H    | -0.059276 | -1.394525 | 1.233995 |
| N    | 3.356402 | 1.096927 | -0.593514 |
| C    | 7.175063 | 2.229968 | -1.911624 |
| C    | 6.054625 | 2.710941 | -2.588851 |
| C    | 4.778956 | 2.352706 | -2.172899 |
| C    | 4.623141 | 1.503507 | -1.070007 |
| C    | 5.746129 | 0.993699 | -0.409909 |
| C    | 7.016539 | 1.372038 | -0.825064 |
| H    | 8.168001 | 2.509262 | -2.242861 |
| H    | 6.175853 | 3.352538 | -3.453285 |
| H    | 3.913644 | 2.691443 | -2.729576 |
| H    | 5.602975 | 0.326614 | 0.432870 |
| H    | 7.884101 | 0.986348 | -0.304161 |
| H    | 2.363232 | 2.867132 | -1.044316 |
| Co   | 2.914063 | -0.809595 | 0.249207 |
| Cl   | 2.807172 | -2.358752 | -1.328105 |
| Cl   | 3.862611 | -0.981473 | 2.250789 |

| Atom | X  | Y  | Z  |
|------|----|----|----|
| C    | 5.391520 | 2.781610 | -0.506794 |
| C    | 6.697124 | 2.302918 | -0.468614 |
| C    | 7.706442 | 3.066967 | -1.047900 |
| C    | 7.379811 | 4.277119 | -1.645277 |
| C    | 6.047245 | 4.686613 | -1.644188 |
| N    | 5.083036 | 3.958324 | -1.090230 |
| C    | 4.277010 | 2.046387 | 0.104265 |
| H    | 6.914679 | 1.355435 | 0.008228 |
| H    | 8.733248 | 2.719853 | -1.030764 |
| H    | 8.134915 | 4.900652 | -2.105407 |
| H    | 5.737031 | 5.620602 | -2.096143 |
| N    | 3.094316 | 2.533493 | 0.065023 |
| Atom | X  | Y  | Z  |
|------|----|----|----|
| C    | -0.263679 | 0.683527 | 1.768435 |
| C    | 0.739536  | -0.111665 | 1.215091 |
| C    | 1.862292  | 0.474856  | 0.645970 |
| C    | 1.980929  | 1.869916  | 0.628960 |
| C    | 0.961290  | 2.670130  | 1.154351 |
| C    | -0.149666 | 2.071761  | 1.734550 |
| H    | -1.139520 | 0.221195  | 2.207583 |
| H    | 0.638572  | -1.190259 | 1.212080 |
| H    | 2.617386  | -0.143890 | 0.176480 |
| H    | 1.067064  | 3.748457  | 1.118155 |
| H    | -0.932348 | 2.693159  | 2.151855 |
| H    | 4.504036  | 1.106376  | 0.607017 |
| Co   | 3.028189  | 4.395274  | -0.959532 |
| Cl   | 2.139991  | 4.192602  | -2.972704 |
| Cl   | 2.651470  | 6.028906  | 0.501639 |
| H2   | 5.471469  | 4.408128  | 2.126155 |
| H2   | 4.891462  | 4.792162  | 1.854770 |
| C    | 5.391678  | 2.786262  | -0.484391 |
| C    | 6.690366  | 2.287159  | -0.482616 |
| C    | 7.693011  | 3.030301  | -1.099165 |
| C    | 7.368050  | 4.242192  | -1.694174 |
| C    | 6.044001  | 4.676315  | -1.649543 |
| N    | 5.086149  | 3.967534  | -1.060045 |
| C    | 4.276943  | 2.054619  | 0.131609 |
| H    | 6.906114  | 1.336183  | -0.011837 |
| H    | 8.712429  | 2.664436  | -1.114687 |
| H    | 8.117686  | 4.847832  | -2.186039 |
| H    | 5.735133  | 5.612731  | -2.097242 |
| N    | 3.098336  | 2.544519  | 0.082963 |
| C    | -0.282227 | 0.668879  | 1.723448 |
| C    | 0.722346  | -0.116383 | 1.158806 |
| C    | 1.852845  | 0.479639  | 0.615073 |
| C    | 1.976790  | 1.874020  | 0.635886 |
| C    | 0.955889  | 2.665709  | 1.171599 |
| C    | -0.162385 | 2.057215  | 1.726580 |
| H    | -1.164104 | 0.199231  | 2.142338 |
| H    | 0.616235  | -1.194005 | 1.125835 |
| H    | 2.608954  | -0.128640 | 0.133803 |
| H    | 1.065602  | 3.744331  | 1.159942 |
| H    | -0.946644 | 2.670967  | 2.152165 |
| H    | 4.499699  | 1.107597  | 0.623106 |
| Co   | 3.030265  | 4.407146  | -0.927385 |
| Cl   | 2.169155  | 4.163858  | -2.953964 |
| Cl   | 2.606662  | 6.041861  | 0.508183 |
| H2   | 4.221511  | 1.200916  | -2.938189 |
| H2   | 3.752479  | 1.780967  | -2.979761 |
| C    | 5.394588  | 2.785161  | -0.496530 |
| C    | 6.697759  | 2.300178  | -0.470099 |
| C    | 7.704268  | 3.054893  | -1.066269 |
| C    | 7.377288  | 4.263313  | -1.666823 |
| C    | 6.047403  | 4.681080  | -1.650527 |
| N    | 5.086139  | 3.961234  | -1.080866 |
| Atoms | X  | Y  | Z  |
|-------|----|----|----|
| C     | 4.280937 | 2.053137 | 0.118837 |
| C     | 6.915540 | 1.353307 | 0.007793 |
| H     | 8.728144 | 2.701511 | -1.059904 |
| H     | 8.129799 | 4.879362 | -2.141071 |
| C     | -0.268866 | 0.677327 | 1.744424 |
| C     | 6.915540 | -1.11398 | 1.177638 |
| C     | 1.858569 | 0.481010 | 0.622365 |
| C     | 0.966025 | 2.670226 | 1.171772 |
| C     | -0.148778 | 2.065531 | 1.737973 |
| H     | -1.147690 | 0.210279 | 2.172420 |
| H     | 0.625827 | -1.189222 | 1.152579 |
| H     | 2.611690 | -0.130545 | 0.140577 |
| H     | 1.075898 | 3.748643 | 1.153844 |
| H     | -0.929681 | 2.682404 | 2.165238 |
| Co    | 3.031896 | 4.398180 | -0.948505 |
| Cl    | 2.141807 | 4.172566 | -2.961935 |
| Cl    | 2.639078 | 6.041670 | 0.495811 |
| H2    | 5.540918 | 4.546997 | 2.097626 |
| H2    | 4.943023 | 4.906426 | 1.831331 |
| H2    | 3.735872 | 1.780808 | -2.997120 |
| H2    | 4.200540 | 1.198229 | -2.945888 |
| C     | 5.392760 | 2.773728 | -0.522140 |
| C     | 6.687535 | 2.265548 | -0.542713 |
| C     | 7.698124 | 3.036693 | -1.112064 |
| C     | 7.383929 | 4.282369 | -1.637596 |
| C     | 6.060972 | 4.717944 | -1.581921 |
| N     | 5.096008 | 3.983086 | -1.041047 |
| C     | 4.277167 | 2.032833 | 0.078874 |
| H     | 6.896051 | 1.291481 | -0.120765 |
| H     | 8.715679 | 2.666630 | -1.141660 |
| H     | 8.140290 | 4.911946 | -2.087125 |
| H     | 5.760346 | 5.678041 | -1.982452 |
| N     | 3.102860 | 2.541363 | 0.080697 |
| C     | -0.272463 | 0.688501 | 1.743233 |
| C     | 0.718431 | -0.104012 | 1.164376 |
| C     | 1.846857 | 0.482918 | 0.607549 |
| C     | 1.984226 | 1.876133 | 0.630121 |
| C     | 0.976610 | 2.674873 | 1.180738 |
| C     | -0.140984 | 2.075612 | 1.747092 |
| H     | -1.153017 | 0.225478 | 2.172109 |
| H     | 0.602461 | -1.180561 | 1.130500 |
| H     | 2.590335 | -0.131139 | 0.115062 |
| H     | 1.095281 | 3.752602 | 1.171155 |
| H     | -0.914502 | 2.695337 | 2.183494 |
| H     | 4.495489 | 1.067678 | 0.535260 |
| Co    | 3.044122 | 4.406847 | -0.926803 |
| Cl    | 2.216858 | 4.134048 | -2.967711 |
| Cl    | 2.605056 | 6.064417 | 0.483346 |
| H2    | 5.457865 | 2.539687 | -3.846519 |
Structure descriptions

H2  4.785319  2.847042  -3.747565
H2  2.710951  1.289641  -2.662070
H2  2.898745  0.571717  -2.583161
H2  5.640267  4.673313   2.013316
H2  5.020188  5.000671   1.757326
C   5.395154  2.799523  -0.486859
C   6.701729  2.324725  -0.448462
C   7.076534  3.082077  -1.046138
C   7.373206  4.282855  -1.658886
C   6.040926  4.691195  -1.652097
N   5.083207  3.968744  -1.081850
C   4.282475  2.062019   0.124047
H   6.923976  1.383711   0.038648
H   8.732058  2.736644  -1.032070
H   8.123951  4.899710  -2.134651
H   5.726503  5.618942  -2.113460
N   3.094281  2.533382   0.062570
C  -0.272680  0.667112  1.729261
C   0.763254  -0.123304  1.231791
C   1.889241  0.468685  0.675873
C   1.979794  1.864594  0.615319
C   0.928458  2.657928  1.085272
C  -0.187037  2.055457  1.651876
H  -1.150954  0.200134  2.158465
H   0.685142  -1.203376  1.261711
H   2.668925  -0.148562  0.247177
H   1.013557  3.736503  1.022981
H  -0.993768  2.673233  2.026447
H   4.514549  1.131092  0.640313
Co  3.038280  4.392168  -0.952139
Cl  2.171923  4.203729  -2.983693
Cl  2.695381  6.002068   0.544403
H2  3.407050  4.063796  2.634661
H2  3.552954  3.520278  3.123766
H2  2.348220  1.332332  -2.633934
H2  2.439893  0.602110  -2.512005
H2  6.188057  5.094761  1.581469
H2  5.499429  5.319211  1.404059
H2  5.271318  2.196694  -3.643308
H2  4.648972  2.597712  -3.553007

BPY

Cl  -0.177747  -1.358817   4.154293
Cl  0.155739   -1.796722   0.224840
H2  1.935688   1.038648  -1.161884
H2  1.592830   0.414793  -0.937192
H2  -1.262503  0.328884  -1.169737
H2  -1.611936   0.927408  -1.446515
C   0.644377   2.194429   1.536778
C   1.391104   3.342430   1.278246
C   2.773130   3.294757   1.410060
C   3.382043   2.108089   1.798080
|   |        |        |        |
|---|--------|--------|--------|
| C | 2.575289 | 1.004184 | 2.037344 |
| H | 3.366840 | 4.178029 | 1.208823 |
| H | 4.455112 | 2.031571 | 1.909965 |
| H | 2.986698 | 0.048121 | 2.335428 |
| N | 1.249465 | 1.049837 | 1.908653 |
| Co | -0.038006 | -0.589989 | 2.086898 |
| N | -1.402356 | 0.942862 | 1.698320 |
| C | -0.840440 | 2.135440 | 1.421970 |
| C | -2.724350 | 0.790805 | 1.622031 |
| C | -1.627907 | 3.223379 | 1.049674 |
| C | -3.570295 | 1.830048 | 1.259938 |
| H | -3.098468 | -0.197866 | 1.855804 |
| C | -3.005490 | 3.064858 | 0.967310 |
| H | -4.638345 | 1.668077 | 1.206275 |
| H | -3.629879 | 3.900732 | 0.676347 |
| H | 0.910117 | 4.261017 | 0.975448 |
| H | -1.181305 | 4.180507 | 0.823205 |
| H2 | -0.226062 | 1.527625 | 4.534912 |
| H2 | -0.240223 | 2.274066 | 4.543981 |
| H2 | 1.925670 | 1.040445 | -1.208052 |
| H2 | 1.594188 | 0.412767 | -0.978149 |
| H2 | -1.271774 | 0.330715 | -1.176641 |
| H2 | -1.605165 | 0.938013 | -1.453356 |
| C | 0.652434 | 2.192504 | 1.534674 |
| C | 1.397086 | 3.346388 | 1.298781 |
| C | 2.779008 | 3.299335 | 1.431882 |
| C | 3.389803 | 2.106606 | 1.797674 |
| C | 2.585208 | 0.996647 | 2.014161 |
| H | 3.371284 | 4.187841 | 1.250443 |
| H | 4.462728 | 2.030828 | 1.911475 |
| H | 2.998110 | 0.036380 | 2.296216 |
| N | 1.259521 | 1.042375 | 1.884599 |
| Co | -0.026300 | -0.591917 | 2.069419 |
| N | -1.393157 | 0.939643 | 1.690150 |
| C | -0.831938 | 2.134566 | 1.424515 |
| C | -2.715838 | 0.789946 | 1.622701 |
| C | -1.620868 | 3.227654 | 1.071700 |
| C | -3.563227 | 1.834505 | 1.280770 |
| H | -3.089728 | -0.200783 | 1.848140 |
| C | -2.999355 | 3.072403 | 0.999205 |
| H | -4.632016 | 1.674967 | 1.235122 |
| H | -3.625213 | 3.912623 | 0.724465 |
| H | 0.914842 | 4.270295 | 1.014973 |
| H | -1.175469 | 4.187323 | 0.853965 |
| Cl | 0.147960 | -1.837076 | 0.234378 |
| Cl | -0.148478 | -1.319998 | 4.158678 |
| H2 | 1.024668 | 1.462909 | 4.744654 |
| H2 | 1.323643 | 2.142672 | 4.814260 |
| H2 | 1.915411 | 0.958970 | -1.280005 |
| H2 | 1.576756 | 0.345459 | -1.024640 |
| H2 | -1.760550 | 1.302864 | 4.492896 |
| H2 | -2.117581 | 1.957429 | 4.507415 |
Structure descriptions

PHEN

C 0.814604  0.058732  0.223146
C 1.468107  1.293059  0.024385
Structure descriptions

S158
| Atom | x      | y      | z      |
|------|--------|--------|--------|
| H    | -2.598574 | 3.972147 | -0.513130 |
| H2   | 1.834609  | 1.501866 | -1.253083 |
| H2   | 1.522187  | 0.843047 | -1.094190 |
| H2   | -0.205122 | 1.165720 | 4.555085  |
| H2   | -0.237888 | 1.905460 | 4.649854  |
| C    | 0.646029  | 2.201174 | 1.617421  |
| C    | 1.301198  | 3.442831 | 1.482987  |
| C    | 2.708158  | 3.439900 | 1.569845  |
| C    | 3.375629  | 2.254563 | 1.779482  |
| C    | 2.637629  | 1.067053 | 1.899012  |
| H    | 3.252566  | 4.371734 | 1.469971  |
| H    | 4.454646  | 2.221563 | 1.849935  |
| H    | 3.124057  | 0.112621 | 2.057702  |
| N    | 1.318367  | 1.043879 | 1.819491  |
| Co   | 0.027789  | -0.617131 | 1.825294 |
| N    | -1.384714 | 0.931660 | 1.668806  |
| C    | -0.792154 | 2.141524 | 1.537276  |
| C    | -2.702054 | 0.845255 | 1.601230  |
| C    | -1.528789 | 3.325339 | 1.325179  |
| C    | -3.517854 | 1.968223 | 1.395415  |
| H    | -3.122424 | -0.146915 | 1.708928 |
| C    | -2.931632 | 3.205679 | 1.255747  |
| H    | -4.591577 | 1.845779 | 1.345920  |
| H    | -3.536794 | 4.089786 | 1.091974  |
| C    | 0.523069  | 4.626852 | 1.266487  |
| C    | -0.831951 | 4.570622 | 1.190898  |
| Cl   | 0.174222  | -1.566858 | -0.182933 |
| Cl   | -0.386607 | -1.625709 | 3.795935  |
| H2   | -1.643822 | 1.343673 | -1.442039 |
| H2   | -1.293493 | 0.715816 | -1.242308 |
| H    | -1.410211 | 5.471879 | 1.026248  |
| H    | 1.039605  | 5.573527 | 1.162791  |
| H2   | -3.141421 | 0.156056 | 0.949316  |
| H2   | -3.071714 | 0.662898 | 1.491935  |
| H2   | 2.442820  | -2.026771 | 1.582418 |
| H2   | 2.099290  | -2.399841 | 1.035663 |
| H2   | -2.691064 | 1.082592 | -1.641133 |
| H2   | -2.513294 | 1.805344 | -1.690634 |
| C    | 0.094012  | 0.159367 | 0.872759  |
| C    | 0.450460  | 0.933532 | 1.993059  |
| C    | 0.170413  | 0.399001 | 3.265636  |
| C    | -0.425981 | -0.836429 | 3.366559 |
| C    | -0.743877 | -1.538447 | 2.194229 |
| H    | 0.427661  | 0.965408 | 4.150405  |
| H    | -0.652800 | -1.274690 | 4.329292 |
| H    | -1.213275 | -2.513719 | 2.229076 |
| N    | -0.491504 | -1.055030 | 0.990611 |
| Co   | -0.880632 | -1.918148 | -0.882534 |
| N    | -0.001304 | -0.117890 | -1.504970 |
| C    | 0.354887  | 0.657040 | -0.454867 |
| C    | 0.225333  | 0.311602 | -2.733927 |
| C    | 0.964416  | 1.918990 | -0.619349 |
Structure descriptions

C   0.826588  1.551726 -2.996378
H  -0.079650 -0.349423 -3.535590
C   1.195281  2.353918 -1.940451
H   0.991132  1.858790 -4.020589
H   1.661555  3.317361 -2.112535
C   1.068235  2.216033  1.790978
C   1.314195  2.685397  0.540527
Cl  -3.064188 -1.843118 -1.282008
Cl   0.546214 -3.585228 -1.230566
H2   3.061925 -0.843906 -1.572804
H2   2.602015 -1.430179 -1.541255
H   1.781932  3.652585  0.399039
H   1.336848  2.803768  2.660826
C   0.820445  0.056319  0.215622
C   1.475099  1.294697  0.043657
C   2.884781  1.284669  0.062039
C   3.555361  0.096074  0.242428
C   2.817961 -1.087104  0.405479
H   3.428248  2.213570 -0.066446
H   4.636383  0.057702  0.260800
H   3.306261 -2.042835  0.550313
N   1.495760 -1.104141  0.392110
Co  0.199891 -2.755636  0.614332
N  -1.213367 -1.201945  0.373828
C  -0.621098  0.004260  0.206072
C  -2.533822 -1.280148  0.369212
C  -1.360886  1.192399  0.024496
C  -3.351885  0.153132  0.195456
H  -2.953580 -2.286849  0.507644
C  -2.766251  1.080783  0.023584
H  -4.427502 -0.269033  0.199707
H  -3.373583  1.968187 -0.112072
C   0.693218  2.482092 -0.138074
C  -0.664193  2.433121 -0.147255
Cl   0.217618 -3.444297  2.719293
Cl   0.256523 -4.004296 -1.214552
H  -1.244743  3.337428 -0.285685
H   1.209019  3.425920 -0.268954
C   0.815092  0.059179  0.226284
C   1.468503  1.293337  0.023317
C   2.878425  1.282054  0.021718
C   3.550071  0.095436  0.212114
C   2.813533 -1.083942  0.404936
H   3.421102  2.207776 -0.131906
H   4.631371  0.055225  0.213794
H   3.303120 -2.042835  0.550313
N   1.491082 -1.099401  0.411988
Co  0.194397 -2.749110  0.634131
N  -1.216795 -1.197838  0.408750
C  -0.626238  0.006708  0.225010
C  -2.536857 -1.278860  0.398779
C  -1.367285  1.190279  0.021394
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -3.356877 | -0.155957 | 0.205804  |
| H    | -2.955777 | -2.266004 | 0.547594  |
| C    | -2.772597 | 1.076456  | 0.017967  |
| H    | -4.432461 | -0.274236 | 0.205751  |
| H    | -3.381107 | 1.960377  | -0.135282 |
| C    | 0.685464  | 2.477775  | -0.176121 |
| C    | -0.672094 | 2.428419  | -0.176758 |
| Cl   | 0.221960  | -3.495368 | 2.717039  |
| Cl   | 0.237644  | -3.962757 | -1.225233 |
| H2   | 0.099273  | -0.663725 | -2.713145 |
| H2   | 0.125204  | -1.375637 | -2.488463 |
| H    | -1.253875 | 3.329537  | -0.330749 |
| H    | 1.200646  | 3.418649  | -0.329769 |
| H2   | 1.705713  | 0.501399  | -0.961733 |
| H2   | 1.722062  | 0.070325  | -0.352481 |
| C    | 0.649050  | 2.593446  | 1.167418  |
| C    | 0.731289  | 3.520840  | 0.107224  |
| C    | 2.021424  | 3.912135  | -0.305619 |
| C    | 3.126939  | 3.387900  | 0.325335  |
| C    | 2.945847  | 2.466298  | 1.366611  |
| H    | 2.131292  | 4.621058  | -1.118350 |
| H    | 4.129166  | 3.667793  | 0.028874  |
| H    | 3.789198  | 2.023887  | 1.884654  |
| N    | 1.747077  | 2.083716  | 1.774175  |
| Co   | 1.247852  | 0.593562  | 3.177038  |
| N    | -0.680736 | 1.251864  | 2.640827  |
| C    | -0.643497 | 2.149696  | 1.628038  |
| C    | -1.850836 | 0.818425  | 3.078283  |
| C    | -1.812280 | 2.645980  | 1.012436  |
| C    | -3.066423 | 1.257723  | 2.530737  |
| H    | -1.822064 | 0.096526  | 3.885196  |
| C    | -3.046558 | 2.168294  | 1.498359  |
| H    | -3.998352 | 0.871934  | 2.922435  |
| H    | -3.969716 | 2.520670  | 1.052512  |
| C    | -0.475640 | 4.006997  | -0.494475 |
| C    | -1.693252 | 3.587977  | -0.061538 |
| C1   | 1.824692  | 1.133022  | 5.242160  |
| C1   | 1.534595  | -1.365237 | 2.150722  |
| H2   | -1.389459 | -0.537594 | 0.148106  |
| H2   | -0.798068 | -0.778467 | 0.534730  |
| H    | -0.397411 | 4.717815  | -1.308662 |
| H    | -2.598861 | 3.960087  | -0.525922 |
| H2   | 1.820171  | 1.505169  | -1.256799 |
| H2   | 1.509404  | 0.845704  | -1.096266 |
| H2   | -0.212573 | 1.171339  | 4.531372  |
| H2   | -0.246079 | 1.911638  | 4.622516  |
| C    | 0.647104  | 2.201421  | 1.617776  |
| C    | 1.301894  | 3.443786  | 1.483988  |
| C    | 2.708866  | 3.441411  | 1.572248  |
| C    | 3.376516  | 2.255957  | 1.781892  |
| C    | 2.638912  | 1.067829  | 1.899266  |
| H    | 3.253144  | 4.373661  | 1.473403  |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | 4.455611  | 2.223599  | 1.854152  |
| H       | 3.125898  | 0.113576  | 2.058049  |
| N       | 1.319615  | 1.043892  | 1.818542  |
| Co      | 0.028490  | -0.617452 | 1.825072  |
| N       | -1.383810 | 0.931482  | 1.671752  |
| C       | -0.791551 | 2.141264  | 1.537668  |
| C       | -2.701163 | 0.844646  | 1.604315  |
| C       | -1.528431 | 3.324885  | 1.323638  |
| C       | -3.517453 | 1.967087  | 1.395496  |
| H       | -3.121473 | -0.147300 | 1.715492  |
| C       | -2.931418 | 3.204487  | 1.253159  |
| H       | -4.591381 | 1.844361  | 1.346755  |
| H       | -3.536986 | 4.088370  | 1.088653  |
| C       | 0.523101  | 4.627715  | 1.266343  |
| C       | -0.831791 | 4.570704  | 1.189280  |
| Cl      | 0.171691  | -1.566829 | -0.183882 |
| Cl      | -0.039334 | -1.626396 | 3.796288  |
| H2      | -1.643317 | 1.344274  | -1.439885 |
| H2      | -1.300012 | 0.712703  | -1.238861 |
| H       | -1.410321 | 5.471701  | 1.023093  |
| H       | 1.039363  | 5.574765  | 1.162350  |
| H2      | -3.142899 | 0.163784  | 0.930027  |
| H2      | -3.929595 | 0.681461  | 1.464664  |
| H2      | 2.433169  | -2.011361 | 1.627571  |
| H2      | 2.089386  | -2.372740 | 1.072919  |
| H2      | -2.726021 | 1.068327  | -1.656984 |
| H2      | -2.545613 | 1.789809  | -1.716550 |
| C       | 0.093038  | 0.158158  | 0.870974  |
| C       | 0.462733  | 0.930803  | 1.991729  |
| C       | 0.182193  | 0.392597  | 3.264436  |
| C       | -0.427316 | -0.837493 | 3.365362  |
| C       | -0.757127 | -1.536363 | 2.192696  |
| H       | 0.450021  | 0.953159  | 4.153006  |
| H       | -0.654627 | -1.275514 | 4.328220  |
| H       | -1.236065 | -2.504420 | 2.227235  |
| N       | -0.504532 | -1.050555 | 0.988819  |
| Co      | -0.890117 | -1.917060 | -0.883362 |
| N       | -0.017415 | -0.111068 | -1.507389 |
| C       | 0.352664  | 0.657413  | -0.456735 |
| C       | 0.207978  | 0.319591  | -2.736206 |
| C       | 0.975599  | 1.912482  | -0.620480 |
| C       | 0.822650  | 1.553520  | -2.998151 |
| H       | -0.108598 | -0.335594 | -3.538326 |
| C       | 1.205523  | 2.348448  | -1.941573 |
| H       | 0.986066  | 1.861501  | -4.022390 |
| H       | 1.682585  | 3.306858  | -2.110345 |
| C       | 1.094146  | 2.202117  | 1.790281  |
| C       | 1.339719  | 2.671951  | 0.539791  |
| Cl      | -3.072069 | -1.862938 | -1.289626 |
| Cl      | 0.563789  | -3.561229 | -1.219419 |
| H2      | 3.047227  | -0.770671 | -1.466541 |
| H2      | 2.602416  | -1.369204 | -1.449085 |
| H       | 1.817909  | 3.634147  | 0.398332  |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| H       | 1.373428| 2.784320| 2.660641|
| C       | 0.820274| 0.056390| 0.215596|
| C       | 1.475023| 1.294926| 0.043220|
| C       | 2.884901| 1.284597| 0.061407|
| C       | 3.555243| 0.095812| 0.243045|
| C       | 2.817562|-1.087257| 0.406590|
| H       | 3.428547| 2.213490|-0.067591|
| H       | 4.636352| 0.057125| 0.261903|
| H       | 3.305753|-2.043193| 0.551772|
| N       | 1.495191|-1.104386| 0.392685|
| Co      | 0.199470|-2.755829| 0.614590|
| N       | -1.213816|-1.201768| 0.374119|
| C       | -0.621272| 0.004413| 0.205900|
| C       | -2.534038|-1.279615| 0.368834|
| C       | -1.360846| 1.192977| 0.024311|
| C       | -3.352514|-0.152398| 0.195552|
| H       | -2.954408|-2.68305| 0.506802|
| C       | -2.766366| 1.081517| 0.023755|
| H       | -4.428271|-0.268203| 0.198692|
| H       | -3.373611| 1.969019|-0.112762|
| C       | 0.693407| 2.482744|-0.139105|
| C       | -0.664243| 2.433912|-0.148038|
| Cl      | 0.218860|-3.445601| 2.718779|
| Cl      | 0.257142|-4.004079|-1.214158|
| H       | -1.244858| 3.338325|-0.286454|
| H       | 1.209541| 3.426524|-0.270416|

\( \text{NiCl}_2 \rightarrow \text{H}_2 \)

BBH

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | 2.048422| 2.919725| 0.075910|
| C       | 1.338611| 2.236433| 1.077361|
| C       | -0.027699| 2.427688| 1.226445|
| C       | -0.703529| 3.289430| 0.364746|
| C       | -0.010677| 3.949335|-0.649713|
| C       | 1.355885| 3.769558|-0.800997|
| C       | 3.480439| 2.692089| 0.001133|
| H       | 1.864639| 1.566555| 1.748907|
| H       | -0.564362| 1.906312| 2.009571|
| H       | -1.771098| 3.437939| 0.476145|
| H       | -0.538014| 4.603265|-1.333025|
| N       | 4.326407| 3.456035|-0.591656|
| C       | 6.589785| 3.867522|-1.131574|
| N       | 5.643087| 3.047787|-0.592116|
| H       | 3.853146| 1.801899| 0.514161|
| H       | 5.862438| 2.089166|-0.355996|
| O       | 6.271053| 4.979337|-1.582352|
| C       | 10.62168| 2.504884|-1.355143|
| C       | 10.135828| 3.453984|-2.252822|
| C       | 8.828301| 3.893942|-2.159903|
| C       | 7.981593| 3.372685|-1.171622|
| C       | 8.474869| 2.427589|-0.283575|
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| C       | 9.793103 | 1.997784 | -0.356796 |
| H       | 11.649050 | 2.166830 | -1.426857 |
| H       | 10.783559 | 3.852600 | -3.024621 |
| H       | 8.430281  | 4.639617  | -2.845213  |
| H       | 7.854922  | 2.056809  | 0.544566  |
| H       | 10.176240 | 1.277086  | 0.355105  |
| H       | 1.870063  | 4.251448  | -1.622593 |
| Ni      | 4.284344  | 5.387165  | -1.435024 |
| Cl      | 3.974590  | 6.610459  | 0.374835  |
| Cl      | 3.578359  | 5.059204  | -3.519569 |
| H2      | 5.330198  | 2.938103  | -3.668956 |
| H2      | 5.508000  | 2.365007  | -3.639711 |
| C       | 2.041093  | 2.936766  | 0.060675  |
| C       | 1.329858  | 2.205119  | 1.026998  |
| C       | -0.306816 | 2.868343  | 1.182882  |
| C       | -0.712309 | 3.289822  | 0.364237  |
| C       | -0.018638 | 3.999789  | -0.615281 |
| C       | 1.347957  | 3.827597  | -0.774251 |
| C       | 3.472821  | 2.711141  | -0.020810 |
| H       | 1.855660  | 1.502683  | 1.664571  |
| H       | -0.574204 | 1.826098  | 1.937780  |
| H       | -1.780078 | 3.432202  | 0.481456  |
| H       | -0.545556 | 4.687339  | -1.264998 |
| N       | 4.323681  | 3.483901  | -0.595463 |
| C       | 6.578014  | 3.875312  | -1.162295 |
| N       | 5.638160  | 3.090133  | -0.597724 |
| C       | 3.842571  | 1.807917  | 0.471408  |
| H       | 5.843657  | 2.097164  | -0.407174 |
| U       | 6.268609  | 4.593200  | -1.601056 |
| C       | 10.578254 | 2.437533  | -1.505001 |
| C       | 10.081980 | 3.390091  | -2.393154 |
| C       | 8.780312  | 3.855583  | -2.261141 |
| C       | 7.962136  | 3.357313  | -1.242186 |
| C       | 8.466110  | 2.408634  | -0.344281 |
| C       | 9.772208  | 1.952525  | -0.477136 |
| H       | 11.595640 | 2.079319  | -1.607558 |
| H       | 10.716000 | 3.770934  | -1.188514 |
| H       | 8.378581  | 4.596323  | -2.939848 |
| H       | 7.865158  | 2.054876  | 0.485569  |
| H       | 10.164139 | 1.228836  | 0.226863  |
| H       | 1.861370  | 4.349630  | -1.570915 |
| Ni      | 4.292531  | 5.430489  | -1.394108 |
| Cl      | 4.048806  | 6.618219  | 0.448842  |
| Cl      | 3.530165  | 5.190329  | -3.473073 |
| H2      | 5.303475  | 2.937036  | -3.702733 |
| H2      | 5.779552  | 2.363181  | -3.660364 |
| C       | 2.066112  | 2.960265  | 0.111758  |
| C       | 1.374118  | 2.322009  | 1.154446  |
| C       | 0.010490  | 2.519910  | 1.318183  |
| C       | -0.680974 | 3.342410  | 0.430857  |
| C       | -0.006156 | 3.957686  | -0.623089 |
| C       | 1.357861  | 3.771366  | -0.789187 |

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| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| C       | 3.496967 | 2.732132 | 0.022755 |
| H       | 1.913017 | 1.684109 | 1.846381 |
| H       | -0.512279 | 2.033921 | 2.132704 |
| H       | -1.746507 | 3.495898 | 0.553994 |
| N       | 4.330353  | 3.472757 | -0.615923 |
| C       | 6.578573  | 3.877111 | -1.192698 |
| N       | 5.647407  | 3.074636 | -0.614933 |
| H       | 3.881845  | 1.867390 | 0.568277 |
| H       | 5.878586  | 2.133534 | -0.326840 |
| O       | 6.252414  | 4.970659 | -1.681869 |
| C       | 10.611571 | 2.512242 | -1.423931 |
| C       | 10.103970 | 3.404570 | -2.366544 |
| C       | 8.791244  | 3.847588 | -2.271267 |
| C       | 7.973401  | 3.380555 | -1.235442 |
| C       | 8.488304  | 2.497150 | -0.283405 |
| C       | 9.805609  | 2.064627 | -0.379293 |
| H       | 11.637513 | 2.171889 | -1.497679 |
| H       | 10.732535 | 3.756773 | -3.175023 |
| H       | 8.380848  | 4.543366 | -2.991102 |
| H       | 7.886848  | 2.176522 | 0.559447 |
| H       | 10.206220 | 1.389072 | 0.366396 |
| N       | 4.278509  | 5.397169 | -1.462352 |
| C       | 4.099881  | 6.584008 | 0.397084 |
| C       | 3.472278  | 5.168024 | -3.521785 |
| H2      | 5.429535  | 3.925235 | 2.414131 |
| H2      | 5.151881  | 4.502552 | 2.029052 |
| H2      | 3.080907  | 0.368707 | 1.109501 |
| H2      | 2.570384  | 0.210072 | 0.588045 |
| C       | 6.281758  | 3.783184 | -0.483293 |
| C       | 6.936561  | 4.496502 | -1.500760 |
| C       | 5.310081  | 4.687480 | -1.453053 |
| C       | 9.047446  | 4.152123 | -0.398607 |
| C       | 8.408092  | 3.418898 | 0.600464 |
| C       | 7.034749  | 3.229683 | 0.564148 |
| C       | 4.838452  | 3.658592 | -0.580141 |
| H       | 6.361734  | 4.917249 | -2.318413 |
| H       | 8.804911  | 5.250720 | -2.234679 |
| H       | 10.120586 | 4.297045 | -0.360672 |
| H       | 8.981944  | 2.986420 | 1.410580 |
| N       | 4.049025  | 3.379066 | 0.393933 |
| C       | 1.827920  | 3.068684 | 1.116659 |
| N       | 2.706635  | 3.282462 | 0.103007 |
| H       | 4.403355  | 3.850825 | -1.563402 |
| H       | 2.414376  | 3.215069 | -0.862508 |
| O       | 2.224389  | 2.997478 | 2.290374 |
| C       | -2.301382 | 2.544872 | 0.194304 |
| C       | -1.745212 | 1.968011 | 1.334611 |
| C       | -0.399935 | 2.153580 | 1.625000 |
| C       | 0.400848  | 2.908222 | 0.762155 |
| C       | -0.161711 | 3.495420 | -0.377138 |
| C       | -1.510616 | 3.313390 | -0.657393 |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| H    | -3.352746 | 2.403959 | -0.026235 |
| H    | -2.361569 | 1.375938 | 1.999747 |
| H    | 0.047449  | 1.719181 | 2.509229 |
| H    | 0.429999  | 4.135063 | -1.021704 |
| H    | -1.946979 | 3.781414 | -1.531132 |
| H    | 6.558842  | 2.623762 | 1.324636 |
| Ni   | 4.218551  | 3.312439 | 2.487071 |
| Cl   | 4.448452  | 5.485889 | 2.863097 |
| Cl   | 5.016715  | 1.311608 | 3.028622 |
| H2   | 3.874758  | 6.626964 | -0.523303 |
| H2   | 4.014441  | 6.414309 | 0.178976 |
| H2   | 1.157696  | 5.979058 | 1.463421 |
| H2   | 1.817721  | 5.927717 | 1.808426 |
| H2   | 2.624826  | 0.285936 | 1.516737 |
| H2   | 2.057477  | 0.077285 | 1.078859 |
| C    | 6.280356  | 3.796759 | -0.475296 |
| C    | 6.932522  | 4.500241 | -1.501116 |
| C    | 8.302758  | 4.712130 | -1.446714 |
| C    | 9.039449  | 4.207031 | -0.377119 |
| C    | 8.403359  | 3.482644 | 0.630408 |
| C    | 7.033559  | 3.273086 | 0.586977 |
| C    | 4.840386  | 3.648103 | -0.580329 |
| H    | 6.358102  | 4.897279 | -2.330758 |
| H    | 8.795543  | 5.267887 | -2.234956 |
| H    | 10.110071 | 4.368057 | -0.334114 |
| H    | 8.977499  | 3.072503 | 1.451782 |
| N    | 4.048925  | 3.381177 | 0.394879 |
| C    | 1.826833  | 3.073615 | 1.115803 |
| N    | 2.711097  | 3.240430 | 0.098116 |
| H    | 4.410900  | 3.803308 | -1.572673 |
| H    | 2.428724  | 3.116260 | -0.864656 |
| O    | 2.216897  | 3.062294 | 2.294048 |
| C    | -2.298021 | 2.501344 | 0.201612 |
| C    | -1.748923 | 1.991257 | 1.376682 |
| C    | -0.404935 | 2.190926 | 1.662956 |
| C    | 0.401720  | 2.894417 | 0.762816 |
| C    | -0.154015 | 3.415211 | -0.411559 |
| C    | -1.501404 | 3.218068 | -0.688877 |
| H    | -3.348231 | 2.348545 | -0.016507 |
| H    | -2.369751 | 1.439247 | 2.071494 |
| H    | 0.037561  | 1.805368 | 2.571767 |
| H    | 0.442305  | 4.014625 | -1.089691 |
| H    | -1.931991 | 3.634182 | -1.591344 |
| H    | 6.561336  | 2.670351 | 1.351976 |
| Ni   | 4.218707  | 3.328811 | 2.481192 |
| C1   | 4.543114  | 5.479194 | 2.894613 |
| C1   | 4.937564  | 1.273913 | 2.954972 |
| H2   | 4.256078  | 6.754055 | -0.501474 |
| H2   | 4.335374  | 6.503578 | 0.197360 |
| H2   | 1.347225  | 6.035242 | 1.251898 |
| H2   | 1.985279  | 5.974318 | 1.634298 |
| H2   | 5.057610  | 0.534809 | 0.145025 |
| H2   | 5.130506  | 0.393674 | -0.583900 |
Structure descriptions

**PIP**

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| C       | 1.659643 | 4.045507 | 0.385407 |
| C       | 0.755483  | 4.777158  | -0.401605 |
| C       | -0.470512 | 5.193251  | 0.091702 |
| C       | -0.827968 | 4.867962  | 1.397645 |
| C       | 0.035908  | 4.127823  | 2.196553 |
| C       | 1.261547  | 3.718578  | 1.694328 |
| C       | 2.932732  | 3.680410  | -0.223473 |
| H       | 1.039540  | 5.029758  | -1.416458 |
| H       | -1.142037 | 5.766846  | -0.533562 |
| H       | -1.780730 | 5.188857  | 1.799843 |
| H       | -0.239943 | 3.870575  | 3.213128 |
| N       | 3.982316  | 3.244915  | 0.373282 |
| C       | 7.506332  | 2.520632  | -1.810156 |
| C       | 6.790705  | 3.695143  | -2.032332 |
| C       | 5.623302  | 3.948604  | -1.321310 |
| C       | 5.169258  | 3.015131  | -0.385173 |
| C       | 5.900734  | 1.852081  | -0.134522 |
| C       | 7.060694  | 1.605233  | -0.858917 |
| H       | 8.418748  | 2.329535  | -2.361970 |
| H       | 7.150763  | 4.425474  | -2.746828 |
| H       | 5.092377  | 4.883223  | -1.453301 |
| H       | 5.555919  | 1.162773  | 0.626217 |
| H       | 7.622217  | 0.698589  | -0.669919 |
| H       | 2.972200  | 3.815784  | -1.305586 |
| O       | 2.104932  | 2.933318  | 2.448607 |
| Ni      | 4.201576  | 3.164793  | 2.396069 |
| Cl      | 4.653080  | 1.164639  | 3.230987 |
| Cl      | 4.456807  | 5.332166  | 2.792977 |
| H       | 1.728088  | 2.721637  | 3.315319 |
| H2      | 1.460343  | 7.022951  | 1.64673 |
| H2      | 2.101140  | 6.752067  | 1.914093 |

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| C       | 1.620356 | 3.704174 | 0.425931 |
| C       | 0.626587 | 4.199134 | -0.434330 |
| C       | -0.618589 | 4.586628 | 0.033130 |
| C       | -0.904471 | 4.471050 | 1.391217 |
| C       | 0.050252 | 3.967420 | 2.266783 |
| C       | 1.295127 | 3.586893 | 1.789452 |
| C       | 2.902818 | 3.354275 | -0.171744 |
| H       | 0.854786 | 4.289240 | -1.489888 |
| H       | -1.359971 | 4.975648 | -0.652269 |
| H       | -1.871621 | 4.771439 | 1.774397 |
| H       | -0.169212 | 3.873764 | 3.324512 |
| N       | 4.006037 | 3.115040 | 0.437800 |
| C       | 7.501075 | 2.336959 | -1.773844 |
| C       | 6.685131 | 3.407700 | -2.132433 |
| C       | 5.526517 | 3.676385 | -1.412627 |
| C       | 5.182553 | 2.862423 | -0.329715 |
| C       | 6.013519 | 1.807486 | 0.054034 |
| C       | 7.164179 | 1.543347 | -0.679158 |
| H       | 8.405599 | 2.133497 | -2.334159 |
| Atom | x     | y     | z     |
|------|-------|-------|-------|
| H    | 6.959862 | 4.046894 | -2.963085 |
| H    | 4.915791  | 4.536949  | -1.655987  |
| H    | 5.750677  | 1.214666  | 0.920932   |
| H    | 7.802852  | 0.718958  | -0.386662  |
| H    | 2.895466  | 3.307621  | -1.261747  |
| O    | 2.232120  | 3.038285  | 2.635643   |
| Ni   | 4.298694  | 3.386571  | 2.430704   |
| Cl   | 4.907819  | 1.548629  | 3.512365   |
| Cl   | 4.419771  | 5.596852  | 2.478313   |
| H    | 1.902155  | 2.960393  | 3.542771   |
| H2   | 2.870863  | 0.597547  | 1.594464   |
| H2   | 2.387592  | 0.333518  | 1.091686   |
| H2   | 1.247294  | 6.793361  | 1.168707   |
| H2   | 1.918464  | 6.652138  | 1.462244   |
| H2   | -0.138288 | 1.152254  | 0.664818   |
| H2   | -0.755272 | 1.453040  | 0.378686   |
| C    | 1.608411  | 3.757119  | 0.473286   |
| C    | 0.620951  | 4.271431  | -0.382387  |
| C    | -0.618227 | 4.671641  | 0.089466   |
| C    | -0.903408 | 4.553390  | 1.447502   |
| C    | 0.045365  | 4.032131  | 2.318527   |
| C    | 1.282322  | 3.635502  | 1.835413   |
| C    | 2.882969  | 3.389690  | -0.129946  |
| H    | 0.848055  | 4.364042  | -1.437867  |
| H    | -1.355860 | 5.074720  | -0.592213  |
| H    | -1.866183 | 4.864528  | 1.833443   |
| H    | -0.173983 | 3.933211  | 3.375641   |
| N    | 3.982428  | 3.120020  | 0.474112   |
| C    | 7.460957  | 2.309922  | -1.752595  |
| C    | 6.661759  | 3.397510  | -2.098054  |
| C    | 5.508657  | 3.677282  | -1.373478  |
| C    | 5.153257  | 2.857050  | -0.299176  |
| C    | 5.967472  | 1.784481  | 0.071562   |
| C    | 7.112840  | 1.509800  | -0.666227  |
| H    | 8.361501  | 2.098650  | -2.316457  |
| H    | 6.944745  | 4.041477  | -2.921992  |
| H    | 4.912221  | 4.550536  | -1.606841  |
| H    | 5.695820  | 1.185621  | 0.931631   |
| H    | 7.738333  | 0.672000  | -0.383383  |
| H    | 2.873096  | 3.357973  | -1.220434  |
| O    | 2.209874  | 3.060759  | 2.675944   |
| Ni   | 4.283071  | 3.350925  | 2.467040   |
| Cl   | 4.842142  | 1.482397  | 3.526321   |
| Cl   | 4.468526  | 5.558423  | 2.556400   |
| H    | 1.881347  | 2.981493  | 3.583370   |
| H2   | 2.819930  | 0.498579  | 1.629329   |
| H2   | 2.365497  | 0.262447  | 1.087145   |
| H2   | 1.323786  | 6.855782  | 1.240139   |
| H2   | 1.992593  | 6.685590  | 1.523437   |
| H2   | -0.140976 | 1.249913  | 0.594958   |
| H2   | -0.773060 | 1.509961  | 0.302802   |
| H2   | 3.714890  | 6.314850  | -0.226366  |
| Atom | X    | Y    | Z    |
|------|------|------|------|
| H2   | 3.486930 | 6.487032 | -0.915792 |
| C    | 1.626405 | 3.784993 | 0.466987 |
| C    | 0.642795 | 4.325378 | 0.466987 |
| C    | -0.597958 | 3.784993 | 0.466987 |
| C    | -0.597958 | 4.325378 | 0.466987 |
| C    | -0.597958 | 4.710494 | 1.823950 |
| C    | -0.597958 | 4.547522 | 1.454804 |
| C    | 0.055833 | 4.002967 | 2.313615 |
| C    | 1.296302 | 3.627344 | 1.823950 |
| C    | 2.897792 | 3.417249 | -0.142178 |
| H    | 0.874626 | 4.449478 | -1.427052 |
| H    | -1.332638 | 5.134566 | -0.568595 |
| H    | -1.855471 | 4.844240 | 1.845197 |
| H    | -0.166104 | 3.873288 | 3.366701 |
| N    | 3.993643 | 3.130147 | 0.459922 |
| C    | 7.473570 | 2.273630 | -1.745315 |
| C    | 6.678133 | 3.356661 | -2.112111 |
| C    | 5.523509 | 3.652190 | -1.396877 |
| C    | 5.162881 | 2.852301 | -0.309010 |
| C    | 5.973176 | 1.783982 | 0.082147 |
| C    | 7.120213 | 1.493754 | -0.646308 |
| H    | 8.375299 | 2.050350 | -2.302316 |
| H    | 6.965878 | 3.986000 | -2.945452 |
| H    | 4.931548 | 4.523393 | -1.644920 |
| H    | 5.698607 | 1.201557 | 0.952313 |
| H    | 7.742767 | 0.659628 | -0.347157 |
| H    | 2.887813 | 3.397269 | -1.232469 |
| O    | 2.227620 | 3.040587 | 2.652345 |
| Ni   | 4.290676 | 3.386227 | 2.451696 |
| Cl   | 4.877062 | 1.559549 | 3.561154 |
| Cl   | 4.419076 | 5.604002 | 2.481005 |
| H    | 1.896801 | 2.923661 | 3.554769 |
| H2   | 2.793650 | 0.557044 | 1.679337 |
| H2   | 2.344170 | 0.282710 | 1.151832 |
| H2   | 1.154658 | 6.879787 | 1.496831 |
| H2   | 1.830489 | 6.696119 | 1.751809 |
| C    | 1.477158 | 2.093472 | -0.572328 |
| C    | 0.970850 | 3.402713 | -0.540505 |
| C    | -0.347787 | 3.665792 | -0.204732 |
| C    | -1.202425 | 2.606957 | 0.091699 |
| C    | -0.738004 | 1.297067 | 0.044420 |
| C    | 0.584398 | 1.045490 | -0.286114 |
| C    | 2.887946 | 1.926395 | -0.901953 |
| H    | 1.640748 | 4.223068 | -0.770786 |
| H    | -0.708060 | 4.685787 | -0.173841 |
| H    | -2.235229 | 2.795763 | 0.356969 |
| H    | -1.402011 | 0.469633 | 0.268610 |
| N    | 3.608034 | 0.883716 | -0.699035 |
| C    | 7.709861 | 0.939226 | -1.639532 |
| C    | 7.146536 | 2.018996 | -0.963255 |
| C    | 5.793272 | 2.016274 | -0.644765 |
| C    | 4.999662 | 0.926202 | -1.013193 |
| C    | 5.566487 | -0.173893 | -1.660585 |
| C    | 6.918312 | -0.155211 | -1.981698 |
| H    | 8.765922 | 0.942329 | -1.880937 |
Structure descriptions

H  7.764385  2.857356  -0.664805
H  5.362000  2.829869  -0.074744
H  4.944108 -1.028112  -1.895919
H  7.354819 -1.004910  -2.492239
O  1.052281  -0.247156  -0.395495
Ni  2.966687  -0.736148  0.365969
Cl  3.125354  -2.682975  -0.674198
Cl  2.879775   0.197269   2.374718
H  0.363496  -0.897804  -0.193757

H2  1.848404  6.730680   1.770699
H2  1.172984  6.924341   1.521897
H2  3.735421  6.347306  -0.221447
H2  3.509566  6.528235  -0.909373
C  1.623349  3.777114   0.465345
C  0.640668  4.318312  -0.379240
C  -0.598704  4.709829  0.099613
C  -0.890919  4.550710   1.451684
C  0.053953  4.004861   2.312008
C  1.294324  3.624622   1.823979
C  2.895385  3.407297  -0.142083
H  0.873150  4.439736  -1.430459
H  -1.332008  5.134714  -0.572930
H  -1.854803  4.851993   1.842001
H  -0.167869  3.880819   3.365924
N  3.993014  3.128485   0.460878
C  7.472877  2.278492  -1.747046
C  6.673866  3.358720  -2.114352
C  5.519539  3.652010  -1.397768
C  5.162645  2.852643  -0.308258
C  5.976656  1.974748   0.083474
C  7.123080  3.889586  -0.646683
H  8.374596  2.056992  -2.304828
H  6.958482  3.987476  -2.949196
H  4.924765  4.521293  -1.640676
H  5.704886  1.204755   0.964377
H  7.748541  0.667166  -0.347125
H  2.885100  3.380694  -1.232314
O  2.226066  3.042562   2.653458
Ni  4.290015  3.386025   2.453203
Cl  4.875651  1.558796   3.562323
Cl  4.426474  5.602788   2.480526
H  1.894522  2.925346   3.555631
H2  2.796806  0.557718   1.673747
H2  2.323128  0.282010   1.168588

C  0.947513  3.040270   1.209153
C  -0.379967  2.713043   0.953435
C  -1.180919  2.300462   2.013143
C  -0.633372  2.229265   3.287837
C  0.703743  2.574461   3.463535
N  1.467897  2.966733   2.450422
C  1.869259  3.493971   0.169149
Structure descriptions

SP-JLMC

H  -0.771150  2.782421  -0.053669
H  -2.218259  2.038569   1.844288
H  -1.223242  1.913322   4.137935
H   1.181179  2.537900   4.434528
N   3.071575  3.785227   0.496332
C   5.991105  5.108555  -2.206260
C   5.049560  4.170930  -2.628538
C   4.072009  3.717932  -1.752386
C   4.997766  5.127885  -0.007439
C   5.962810  5.582541  -0.896289
H   6.754421  5.455098  -2.892641
H   5.088054  3.777860  -3.637350
H   3.373720  2.951798  -2.064510
H   4.955655  5.489705   1.013180
H   6.698080  6.303852  -0.561566
H   1.501008  3.595095  -0.850259
Ni   3.435152  3.485981   2.499672
Cl   4.463660  1.521684   2.581383
Cl   3.452572  5.520469   3.405545
H2   3.511844  0.818645  -0.057190
H2   3.214591  0.637616  -0.717353
H2   1.900172  6.831306   0.366954
H2   2.185673  6.588462   1.011766
H2   1.945155  0.119141   2.057375
H2   1.269764  0.148690   1.887618
H2  -0.201053  5.605185   2.857097
H2   0.529725  5.632979   3.004269

PIA

C   0.952636  3.063805   1.189984
C  -0.383587  2.770216   0.938109
C  -1.174211  2.312004   1.986432
C  -0.607631  2.161947   3.246355
C   0.736708  2.480376   3.420030
N   1.490763  2.918873   2.417515
C   1.869156  3.545941   0.158784
H  -0.788428  2.898893  -0.057527
H  -2.218184  2.075869   1.821136
H  -1.189782  1.807787   4.086597
H   1.228105  2.386763   4.379903
N   3.078421  3.807740   0.484822
C   6.001491  5.136387  -2.211107
C   5.047237  4.215345  -2.641657
C   4.067728  3.763162  -1.767311
C   4.044098  4.237608  -0.450859
C   5.016649  5.139221  -0.008158
C   5.983408  5.593881  -0.894986
H   6.766691  5.482110  -2.895511
H   5.077489  3.834702  -3.655314
H   3.358054  3.010346  -2.087452
H   4.981870  5.488932   1.016729
H   6.728495  6.301857  -0.554163
### Structure descriptions

**SP-JLMC**

| Element | X    | Y    | Z    |
|---------|------|------|------|
| N       | 3.074747 | 3.761951 | 0.470442 |
| C       | 5.978571  | 5.018557  | −2.278164 |
| C       | 5.099666  | 3.997210  | −2.636447 |
| C       | 4.126502  | 3.567707  | −1.743447 |
| C       | 4.036053  | 4.166495  | −0.481847 |
| C       | 4.935421  | 5.169185  | −0.106883 |
| C       | 5.894044  | 5.600174  | −1.014404 |
| H       | 6.739093  | 5.346721  | −2.976466 |
| H       | 5.184328  | 3.521958  | −3.606149 |
| H       | 3.476270  | 2.740302  | −1.999552 |
| H       | 4.852532  | 5.604736  | 0.882206  |
| H       | 6.583332  | 6.385267  | −0.729337 |
| H       | 1.523025  | 3.468755  | −0.878779 |
| Ni      | 3.453735  | 3.535604  | 2.483622  |
| Cl      | 4.517701  | 1.590751  | 2.614356  |
| Cl      | 3.464506  | 5.584196  | 3.334378  |
| H2      | 2.927334  | 0.569192  | 0.496006  |
| H2      | 2.453929  | 0.353816  | −0.040720 |
| C       | 1.080319  | 1.351343  | −0.069649 |
| C       | −0.074732 | 2.128272  | −0.056853 |
| C       | −1.251711 | 1.563935  | 0.423660  |
| C       | −1.237534 | 0.249837  | 0.875420  |
| C       | −0.041361 | −0.462746 | 0.831998  |
| N       | 1.082572  | 0.076855  | 0.371403  |
| C       | 2.368602  | 1.849913  | −0.549057 |
| H       | −0.045837 | 3.149144  | −0.416583 |
| H       | −2.166625 | 2.143503  | 0.444953  |
| H       | −2.132402 | −0.224185 | 1.256491  |
| H       | 0.026889  | −1.489063 | 1.170309  |
| N       | 3.381604  | 1.068217  | −0.518406 |
| C       | 7.219130  | 2.155588  | −1.811302 |
| C       | 6.107687  | 2.640052  | −2.499944 |
| C       | 4.826637  | 2.294403  | −2.090191 |
| C       | 4.658555  | 1.456607  | −0.981507 |
| C       | 5.771362  | 0.944007  | −0.307616 |
| C       | 7.047035  | 1.308087  | −0.718694 |
| H       | 8.216709  | 2.424502  | −2.137831 |
| H       | 6.239702  | 3.273635  | −3.368791 |
| H       | 3.965402  | 2.631010  | −2.654446 |
| H       | 5.614842  | 0.288237  | 0.541346  |
| H       | 7.908549  | 0.921356  | −0.188360 |
| H       | 2.435961  | 2.879926  | −0.897386 |
| Ni      | 2.912223  | −0.816657 | 0.180829  |
| Cl      | 2.646307  | −2.021035 | −1.661341 |
| Cl      | 3.749756  | −0.937117 | 2.233355  |

**BPY**

| C       | −0.344950 | 1.747535 | 0.413836 |
| C       | −1.095924 | 2.866552 | 0.058965 |
| C       | −2.400835 | 2.691118 | −0.382484 |
| C       | −2.929263 | 1.407640 | −0.458752 |
| C       | −2.123803 | 0.340100 | −0.087360 |
| Atom | X-coordinate | Y-coordinate | Z-coordinate |
|------|--------------|--------------|--------------|
| N    | -0.872091    | 0.511352     | 0.335626     |
| H    | -0.672244    | 3.858930     | 0.117447     |
| H    | -2.997279    | 3.549542     | -0.666573    |
| H    | -3.940161    | 1.231115     | -0.800860    |
| H    | -2.471876    | -0.684127    | -0.127248    |
| C    | 3.668066     | 1.665240     | 1.746113     |
| C    | 2.888505     | 0.532814     | 1.553500     |
| N    | 1.626041     | 0.605873     | 1.133096     |
| C    | 1.062426     | 1.802101     | 0.878955     |
| C    | 1.785434     | 2.981574     | 1.050981     |
| C    | 3.101692     | 2.908318     | 1.488345     |
| H    | 4.689854     | 1.568384     | 2.080101     |
| H    | 3.267776     | -0.464336    | 1.736914     |
| H    | 1.333800     | 3.942283     | 0.848840     |
| H    | 3.677860     | 3.815183     | 1.626226     |
| Ni   | 0.404423     | -0.994528    | 0.831773     |
| Cl   | -0.182635    | -1.640367    | 2.868447     |
| Cl   | 1.028221     | -1.817377    | -1.138785    |
| H2   | 0.149110     | 0.610337     | -2.415587    |
| H2   | -0.113976    | 1.264544     | -2.661747    |
| C    | -0.624076    | 1.447698     | 0.477804     |
| C    | -1.639204    | 2.369691     | 0.223637     |
| C    | -2.759559    | 1.964235     | -0.495491    |
| C    | -2.852897    | 0.651186     | -0.952564    |
| C    | -1.812225    | -0.220504    | -0.664856    |
| N    | -0.747481    | 0.176508     | 0.024485     |
| H    | -1.561906    | 3.387527     | 0.578149     |
| H    | -3.554208    | 2.671669     | -0.699219    |
| H    | -3.709851    | 0.306816     | -1.515978    |
| H    | -1.816369    | -1.256155    | -0.981143    |
| C    | 3.024170     | 2.153999     | 2.591238     |
| C    | 2.674020     | 0.923301     | 2.053538     |
| N    | 1.529539     | 0.751256     | 1.398094     |
| C    | 0.651402     | 1.772274     | 1.227139     |
| C    | 0.949193     | 3.032174     | 1.742756     |
| C    | 2.143422     | 3.220925     | 2.431376     |
| H    | 3.961311     | 2.265777     | 3.120080     |
| H    | 3.302821     | 0.048410     | 2.152176     |
| H    | 0.259667     | 3.854620     | 1.616554     |
| H    | 2.383688     | 4.195289     | 2.838806     |
| Ni   | 0.848829     | -0.944253    | 0.554374     |
| Cl   | -0.065863    | -2.168945    | 2.166083     |
| Cl   | 2.049921     | -1.121412    | -1.316746    |
| H2   | 3.696067     | -2.269387    | 2.491509     |
| H2   | 2.981096     | -2.386206    | 2.306077     |
| H2   | 2.111242     | 1.768161     | -1.577256    |
| H2   | 1.965793     | 2.500098     | -1.570348    |
| H2   | -0.016146    | -0.027189    | 3.744014     |
| H2   | 0.009502     | 0.616911     | 4.121970     |

| Atom | X-coordinate | Y-coordinate | Z-coordinate |
|------|--------------|--------------|--------------|
| C    | -0.346911    | 1.756960     | 0.428066     |
| C    | -1.112345    | 2.882620     | 0.126692     |
| C    | -2.424904    | 2.713070     | -0.294792    |
Structure descriptions

C  -2.945574  1.429185  -0.408232
C  -2.125250  0.354710  -0.091776
N  -0.866785  0.520066   0.313554
H   -0.695761  3.875617   0.217551
H   -3.033421  3.576938  -0.533270
H   -3.962621  1.257092  -0.734175
H   -2.468259  -0.669869  -0.159249
C   3.671595   1.659688   1.743899
C   2.892978   0.529211   1.535580
N   1.629349   0.607332   1.120022
C   1.063171   1.806128   0.886787
C   1.784765   2.984008   1.075917
C   3.102164   2.905841   1.508991
H   4.694432   1.559020   2.081501
H   3.274664  -0.470203   1.701203
H   1.331129   3.947035   1.660464
Ni  0.407190  -0.991800   0.800342
Cl  -0.212924  -1.620860   2.837475
Cl  1.046024  -1.825354  -1.156637
H   0.905191   4.237157   1.227029
H  -1.221909   4.151092   1.063314
H2  0.097533   1.451152  -1.446788
H2  0.117995   0.750766  -1.187965
Cl  -0.191391  -0.958413   4.222364
Cl  0.163144  -1.767236   0.133023
C   0.635513   2.126750   1.583077
C   1.386061   3.291463   1.432577
C   2.768458   3.222514   1.546392
C   3.372164   1.997986   1.808281
C   2.561492   0.880087   1.950049
H   3.367466   4.117592   1.430272
H   4.445920   1.904710   1.901604
H   2.967632  -0.102186   2.155492
N   1.235250   0.949046   1.839780
Ni  -0.032322  -0.632940   2.033667
N  -1.376417   0.842028   1.630357
C  -0.841294   2.066383   1.465925
C  -2.693407   0.665331   1.529126
C  -1.650871   3.167899   1.193977
C  -3.559437   1.715132   1.255887
H  -3.045854  -0.348273   1.672003
C  -3.023664   2.986844   1.088059
H  -4.623200   1.534225   1.178253
H  -3.667498   3.831599   0.875145
Cl  -0.204215  -1.044308   4.229479
Cl  0.176293  -1.666406   0.101525
H2  1.959853   1.279657  -1.188856
H2  1.620136   0.638849  -1.014224
H2  -1.324237   0.496730  -1.220631
H2  -1.687272   1.100944  -1.464774
C   0.639168   2.118771   1.555534
Structure descriptions

C 1.394914 3.270768 1.347493
C 2.775334 3.205396 1.480623
C 3.372168 1.997325 1.820724
C 2.557147 0.890831 2.013348
H 3.378187 4.090590 1.319462
H 4.444035 1.907316 1.933772
H 2.958699 -0.079371 2.275922
N 1.233233 0.956357 1.882464
Ni -0.033828 -0.628877 2.063472
N -1.380028 0.849995 1.670081
C -0.837955 2.058775 1.438712
C -2.696133 0.676807 1.594739
C -3.560424 1.716845 1.276546
C -3.056568 -0.325074 1.793702
H -3.017320 2.972317 1.031517
H -4.626127 1.540447 1.222425
H -3.657222 3.808676 0.778528
H 0.919084 4.203770 1.082096
H -1.208413 4.120406 0.926510
H2 -0.408264 1.853521 4.534744
H2 -0.473685 2.596998 4.512838
H2 0.136198 1.442757 -1.470310
H2 0.147415 0.744064 -1.207106
Cl -0.188001 -0.969029 4.221531
Cl 0.160515 -1.765460 0.131718
C 0.636018 2.125504 1.568378
C 1.387669 3.289135 1.415578
C 2.767222 3.223944 1.548091
C 3.392326 2.003041 1.829304
C 2.559095 0.885059 1.968802
H 3.366115 4.118952 1.432713
H 4.441376 1.912752 1.940024
H 2.964274 -0.094311 2.188380
N 1.234331 0.951002 1.840660
Ni -0.032674 -0.631556 2.031222
N -1.376509 0.844343 1.632188
C -0.839872 2.065053 1.450285
C -2.695034 0.670297 1.549285
C -1.648813 3.164824 1.173001
C -3.560919 1.719852 1.276612
H -3.049091 -0.340148 1.707993
C -3.022961 2.987203 1.085971
H -4.626148 1.542142 1.216571
H -3.666585 3.831399 0.871309
H 0.906976 4.232087 1.196769
H -1.218526 4.14982 1.026736
H2 -0.374108 1.769153 4.513209
H2 -0.423184 2.514241 4.489729
H2 2.019483 1.212917 -1.183290
H2 1.654928 0.590991 -0.990533
H2 -1.274648 0.499222 -1.234660
| Atoms | x      | y      | z       |
|-------|--------|--------|---------|
| H2    | -1.642858 | 1.096915 | -1.487711 |
| C     | 0.638940  | 2.117447 | 1.543665  |
| C     | 1.395729  | 3.266485 | 1.326780  |
| C     | 2.774905  | 3.204464 | 1.474638  |
| C     | 3.368926  | 2.001731 | 1.837002  |
| C     | 2.552893  | 0.897031 | 2.035399  |
| H     | 3.378757  | 4.088076 | 1.308682  |
| H     | 4.439702  | 1.914067 | 1.962098  |
| H     | 2.952911  | -0.069480 | 2.313829 |
| N     | 1.230396  | 0.959299 | 1.890298  |
| Ni    | -0.035721 | -0.621431 | 2.070296  |
| N     | -1.380814 | 0.852836 | 1.678946  |
| C     | -0.837147 | 2.057196 | 1.424114  |
| C     | -2.700034 | 0.682817 | 1.610016  |
| C     | -1.639742 | 3.142801 | 1.081607  |
| C     | -3.560349 | 1.719408 | 1.276935  |
| H     | -3.060105 | -0.314680 | 1.826886 |
| C     | -3.015123 | 2.968581 | 1.006699  |
| H     | -4.627191 | 1.544716 | 1.229640  |
| H     | -3.653955 | 3.801564 | 0.740287  |
| H     | 0.921784  | 4.196044 | 1.046329  |
| H     | -1.203569 | 4.109329 | 0.874352  |
| Cl    | 0.157011  | -1.643699 | 0.098417  |
| Cl    | -0.183375 | -1.065514 | 4.236755  |
| H2    | 1.088929 | 1.664978 | 4.700159  |
| H2    | 1.404640 | 2.340763 | 4.689788  |
| H2    | 1.961634 | 1.199436 | -1.229714 |
| H2    | 1.620634 | 0.560848 | -1.049733 |
| H2    | -1.781945 | 1.529945 | 4.439684  |
| H2    | -2.157448 | 2.171700 | 4.380693  |
| C     | 0.636973 | 2.115959 | 1.571585  |
| C     | 1.388171 | 3.278714 | 1.417731  |
| C     | 2.768511 | 3.213475 | 1.552604  |
| C     | 3.369248 | 1.993758 | 1.839044  |
| C     | 2.558525 | 0.876574 | 1.977631  |
| H     | 3.368239 | 4.107717 | 1.435833  |
| H     | 4.441013 | 1.903591 | 1.952847  |
| H     | 2.963435 | -0.102076 | 2.200745 |
| N     | 1.235069 | 0.942599 | 1.846904  |
| Ni    | -0.031965 | -0.631186 | 2.032024 |
| N     | -1.376441 | 0.835152 | 1.634658  |
| C     | -0.839596 | 2.055173 | 1.451751  |
| C     | -2.693653 | 0.660203 | 1.549662  |
| C     | -1.648608 | 3.153762 | 1.171726  |
| C     | -3.559779 | 1.708031 | 1.273412  |
| H     | -3.047802 | -0.349986 | 1.709702  |
| C     | -3.022603 | 2.975104 | 1.082360  |
| H     | -4.624807 | 1.529734 | 1.212691  |
| H     | -3.666845 | 3.818585 | 0.866818  |
| H     | 0.908583 | 4.221009 | 1.195214  |
| H     | -1.218236 | 4.133974 | 1.025341  |
| Cl    | 0.159288 | -1.728185 | 0.108396  |
| Cl    | -0.187485 | -0.954628 | 4.225243  |
### Structure descriptions

| Atom | X  | Y  | Z  |
|------|----|----|----|
| H2   | -1.605805 | 1.116004 | -1.485068 |
| H2   | -1.260389 | 0.503003 | -1.237825 |
| Cl   | -0.189245 | -0.962992 | 4.221281 |
| Cl   | 0.162149  | -1.737016 | 0.115031 |
| H    | 0.908847  | 4.228400  | 1.196485 |
| H    | -1.218751 | 4.140522  | 1.021632 |
| H    | -3.666426 | 3.826380  | 0.864140 |
| H    | -4.626887 | 1.537196  | 1.214432 |
| C    | 0.637107  | 2.121373  | 1.570086 |
| C    | 1.388408  | 3.285552  | 1.416727 |
| C    | 2.768923  | 3.220362  | 1.552069 |
| C    | 3.370530  | 2.000271  | 1.836614 |
| C    | 2.559909  | 0.882036  | 1.975436 |
| H    | 3.367306  | 4.115757  | 1.436794 |
| H    | 4.442405  | 1.909718  | 1.949802 |
| H    | 2.964479  | -0.097118 | 2.197114 |
| N    | 1.235461  | 0.947007  | 1.845099 |
| Ni   | -0.031844 | -0.637429 | 2.032393 |
| N    | -1.377415 | 0.840063  | 1.635273 |
| C    | -0.840143 | 2.060784  | 1.450793 |
| C    | -2.695819 | 0.666511  | 1.551195 |
| C    | -1.649241 | 3.160652  | 1.169875 |
| C    | -3.561816 | 1.715672  | 1.275212 |
| H    | -3.049631 | -0.343762 | 1.711566 |
| C    | -3.023595 | 2.982333  | 1.081922 |

### PHEN

| Atom | X  | Y  | Z  |
|------|----|----|----|
| H2   | -2.976590 | 0.363936 | 1.170242 |
| H2   | -2.871203 | 0.837494 | 1.737226 |
| H2   | 2.580199  | -1.733042 | 1.577939 |
| H2   | 2.455833  | -2.085769 | 1.011887 |
| H2   | -2.582850 | 1.393887  | -1.382641 |
| H2   | -2.378512 | 2.109690  | -1.434474 |
| C    | 0.124273  | 0.186865  | 0.857614 |
| C    | 0.516400  | 0.933926  | 1.986000 |
| C    | 0.282468  | 0.354452  | 3.248891 |
| C    | -0.306181 | -0.888212 | 3.328195 |
| C    | -0.662217 | -1.556416 | 2.147010 |
| H    | 0.567004  | 0.890733  | 4.147041 |
| H    | -0.498598 | -1.358573 | 4.283347 |
| H    | -1.126628 | -2.534267 | 2.166668 |
| N    | -0.451989 | -1.031695 | 0.953069 |
| Ni   | -0.878816 | -1.818665 | -0.888707 |
| N    | -0.061379 | -0.045986 | -1.504099 |
| C    | 0.333567  | 0.715456  | -0.460037 |
| C    | 0.113314  | 0.402086  | -2.734439 |
| C    | 0.931278  | 1.980949  | -0.623565 |
| C    | 0.699480  | 1.649371  | -2.997213 |
| H    | -0.220328 | -0.247338 | -3.533858 |
| C    | 1.107667  | 2.438339  | -1.944609 |
| H    | 0.822176  | 1.973362  | -4.022184 |
| H    | 1.563413  | 3.405892  | -2.121722 |
Structure descriptions

| Atom | x   | y   | z   |
|------|-----|-----|-----|
| C    | 1.122366 | 2.219076 | 1.790383 |
| C    | 1.320624  | 2.719721  | 0.542536 |
| Cl   | -3.066870 | -1.494369 | -1.104404 |
| Cl   | 0.756628  | -3.287601  | -1.220792 |
| H2   | 3.057845  | -0.444257  | 0.542536 |
| H2   | 0.756628  | -3.287601  | -1.220792 |
| H    | 1.779697  | 3.692273  | 0.409091 |
| H    | 1.421549  | 2.788062  | 2.662835 |
| C    | 0.658876  | 2.075800  | 1.508875 |
| C    | 1.329979  | 3.293750  | 1.273853 |
| C    | 2.738478  | 3.263815  | 1.304746 |
| C    | 3.387166  | 2.074880  | 1.557103 |
| H    | 3.299203  | 4.174623  | 1.129548 |
| H    | 4.467362  | 2.020298  | 1.586921 |
| H    | 3.10444   | -0.040732 | 1.981610 |
| N    | 1.310771  | 0.916820  | 1.755144 |
| Ni   | 0.013210  | -0.648146 | 2.055948 |
| N    | -1.365059 | 0.838988  | 1.725650 |
| C    | -0.776311 | 2.033911  | 1.492785 |
| C    | -2.684463 | 0.750766  | 1.719412 |
| C    | -1.511817 | 3.210770  | 1.241314 |
| C    | -3.500466 | 1.873452  | 1.478199 |
| C    | -3.104193 | -0.222415 | 1.90825 |
| C    | -2.916508 | 3.098333  | 1.239850 |
| H    | -4.576090 | 1.756418  | 1.483206 |
| H    | -3.525895 | 3.974616  | 1.051451 |
| C    | 0.556141  | 4.474417  | 1.021038 |
| C    | -0.802587 | 4.434670  | 1.005324 |
| Cl   | 0.008775  | -0.905332 | 4.261106 |
| Cl   | 0.053590  | -1.790985 | 0.156468 |
| H    | 1.078196  | 5.406823  | 0.841333 |
| H    | -1.373755 | 5.335217  | 0.812969 |
| H    | 1.447220  | 2.776572  | 2.678196 |
| H    | 1.817699  | 3.678158  | 0.425232 |
| H2   | 2.976648  | -0.807944 | 0.149432 |
| H2   | 2.577865  | -1.373154 | -0.132462 |
| Cl   | 0.733351  | -3.300716 | -1.19983 |
| Cl   | -3.076062 | -1.533598 | -1.135916 |
| C    | 0.113344  | 0.194912  | 0.870171 |
| C    | 0.517420  | 0.935299  | 1.999664 |
| C    | 0.285350  | 0.353409  | 3.261907 |
| C    | -0.310822 | -0.886216 | 3.339365 |
| C    | -0.676384 | -1.549232 | 2.157217 |
| H    | 0.679211  | 0.883783  | 4.160423 |
| H    | -0.500290 | -1.359010 | 4.294041 |
| H    | -1.143951 | -2.525782 | 2.175592 |
| N    | -0.469302 | -1.021522 | 0.962962 |
| Ni   | -0.892865 | -1.817354 | -0.882483 |
| N    | -0.063463 | -0.040023 | -1.492321 |
| C    | 0.330532  | 0.721808  | -0.447372 |
| C    | 0.128794  | 0.402532  | -2.723129 |

S179
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 0.947163| 1.979224| -0.609356|
| C    | 0.731785| 1.643076| -2.983991|
| H    | -0.203522| -0.246390| -3.523735|
| C    | 1.140547| 2.430768| -1.930118|
| H    | 0.868580| 1.962249| -4.008814|
| H    | 1.610987| 3.391281| -2.106382|
| C    | 1.139409| 2.213036| 1.805311|
| C    | 1.344584| 2.712310| 0.557666|
| H    | 1.563357| 2.730160| 2.649514|
| H    | 1.937609| 3.625216| 0.394524|
| H2   | 2.492915| -1.697190| 1.680628|
| H2   | 2.198314| -2.064175| 1.101210|
| H2   | -2.742780| 1.009727| -0.107871|
| H2   | -2.550916| 1.672133| 0.178537|
| C    | 0.122582| 0.200558| 0.851041|
| C    | 0.560873| 0.925096| 1.977397|
| C    | 0.309516| 0.354956| 3.241163|
| C    | -0.341139| -0.856503| 3.323298|
| C    | -0.738986| -1.504767| 2.143850|
| H    | 0.629406| 0.873342| 4.137790|
| H    | -0.548762| -1.318386| 4.279441|
| H    | -1.248771| -2.459790| 2.165642|
| N    | -0.511312| -0.989282| 0.948329|
| Ni   | -0.912525| -1.795828| -0.893539|
| N    | -0.103527| -0.014022| -1.508521|
| C    | 0.341654| 0.723533| -0.467178|
| C    | 0.071497| 0.433604| -2.739651|
| C    | 0.994376| 1.961413| -0.633350|
| C    | 0.709625| 1.655114| -3.004889|
| H    | -0.301777| -0.196388| -3.537229|
| C    | 1.172346| 2.417193| -1.954715|
| H    | 0.831244| 1.979504| -4.029874|
| H    | 1.670982| 3.362694| -2.134463|
| C    | 1.226283| 2.180007| 1.778944|
| C    | 1.433558| 2.675644| 0.530188|
| C1   | -3.101573| -1.632876| -1.187318|
| C1   | 0.796483| -3.201818| -1.173260|
| H2   | 3.043518| -0.378216| -1.630537|
| H2   | 2.639041| -1.002140| -1.564421|
| H    | 1.581756| 2.715178| 2.659879|
| H    | 1.934202| 3.622447| 0.406625|
| H2   | 2.508690| -1.689941| 1.643340|
| H2   | 2.197951| -2.065680| 1.077885|
| H2   | 2.606461| -1.020827| -1.558364|
| H2   | 3.016000| -0.400225| -1.628025|
| C    | 0.116107| 0.198779| 0.862234|
| C    | 0.569172| 0.915650| 1.988183|
| C    | 0.338669| 0.334379| 3.250950|
| C    | -0.305150| -0.880685| 3.323674|
| C    | -0.718057| -1.521162| 2.154027|
| H    | 0.671387| 0.845770| 4.146867|
| H    | -0.494826| -1.352321| 4.287823|
|  | x    | y    | z    |
|---|------|------|------|
| H | -1.220156 | -2.480290 | 2.175474 |
| N | -0.510754 | -0.995314 | 0.959245 |
| Ni | -0.916477 | -1.798939 | -0.885359 |
| N | -0.123155 | -0.007694 | -1.497773 |
| C | 0.323768 | 0.728529 | -0.455683 |
| C | 0.051314 | 0.441428 | -2.728493 |
| C | 0.979345 | 1.965417 | -0.621386 |
| C | 0.689426 | 1.663254 | -2.992785 |
| H | -0.323125 | -0.187624 | -3.526310 |
| C | 1.155352 | 2.423081 | -1.942438 |
| C | 1.233536 | 2.170986 | 1.789911 |
| C | 1.429255 | 2.673230 | 0.541818 |
| Cl | -3.103821 | -1.633189 | -1.172305 |
| Cl | 0.800425 | -3.195004 | -1.171787 |

|  | x    | y    | z    |
|---|------|------|------|
| H | 1.413572 | 2.804712 | 2.654761 |
| H | 1.782809 | 3.702538 | 0.400004 |
| H2 | 2.979147 | -0.835325 | 0.113429 |
| H2 | 2.574930 | -1.397009 | -0.168377 |
| H2 | -2.698480 | 1.111290 | -0.023736 |
| H2 | -2.502039 | 1.767369 | 0.274229 |
| C | 0.125186 | 0.198319 | 0.850466 |
| C | 0.511702 | 0.948605 | 1.978868 |
| C | 0.270423 | 0.373485 | 3.242257 |
| C | -0.320477 | -0.868628 | 3.321932 |
| C | -0.670930 | -1.540660 | 2.140612 |
| H | 0.550077 | 0.912181 | 4.140347 |
| H | -0.518871 | -1.335485 | 4.277697 |
| H | -1.136447 | -2.518147 | 2.160421 |
| N | -0.453268 | -1.019582 | 0.945149 |
| Ni | -0.877646 | -1.817175 | -0.897103 |
| N | -0.048751 | -0.042894 | -1.510703 |
| C | 0.341518 | 0.722832 | -0.467611 |
| C | 0.132014 | 0.402200 | -2.742492 |
| C | 0.939992 | 1.988052 | -0.631950 |
| C | 0.719282 | 1.649482 | -3.005747 |
| H | -0.198816 | -0.249291 | -3.541607 |
| C | 1.122846 | 2.441827 | -1.953257 |
| H | 0.846486 | 1.971084 | -4.031025 |
| H | 1.578850 | 3.408948 | -2.131341 |
| C | 1.118713 | 2.233358 | 1.782565 |
| C | 1.323315 | 2.730430 | 0.534051 |
| Cl | -3.063910 | -1.510797 | -1.144034 |
| Cl | 0.721491 | -3.323530 | -1.222722 |

|  | x    | y    | z    |
|---|------|------|------|
| H | 1.389735 | 2.819703 | 2.655884 |
| H | 1.760380 | 3.716331 | 0.400974 |
| Cl | -3.053226 | -1.498405 | -1.134898 |
| Cl | 0.719348 | -3.331118 | -1.228680 |
| H2 | -2.680916 | 1.124348 | -0.016508 |
| H2 | -2.489458 | 1.782398 | 0.280461 |
| C | 0.136021 | 0.195705 | 0.851365 |
Structure descriptions

PdCl₂ — H₂

BBH

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| Element | x   | y   | z   |
|---------|-----|-----|-----|
| Pd      | 4.405078 | 5.487899 | -1.467473 |
| Cl      | 2.434131 | 6.328476 | -0.604270 |
| Cl      | 4.807364 | 7.453315 | -2.580380 |
| H2      | 4.796928 | 2.181385 | -3.544677 |
| H2      | 4.866954 | 2.914906 | -3.437411 |
| C       | 2.140498 | 2.798102 | 0.055342 |
| C       | 1.428403 | 2.223648 | 1.121955 |
| C       | 0.041646 | 2.237053 | 1.127822 |
| C       | -0.648348 | 2.79879 | 0.054027 |
| C       | 0.050598 | 3.343990 | -1.021356 |
| C       | 1.436894 | 3.349336 | -1.025073 |
| C       | 3.588321 | 2.726735 | 0.095424 |
| H       | 1.967486 | 1.781765 | 1.952976 |
| H       | -0.500888 | 1.808196 | 1.961278 |
| H       | -1.731824 | 2.804695 | 0.052789 |
| H       | -0.485887 | 3.777071 | -1.855937 |
| N       | 4.410198 | 3.478790 | -0.551614 |
| C       | 6.670821 | 3.702794 | -1.266120 |
| N       | 5.741694 | 3.086201 | -0.487964 |
| H       | 4.003884 | 1.929057 | 0.718269 |
| H       | 5.952406 | 2.196366 | -0.055656 |
| C       | 6.373287 | 4.680257 | -1.971129 |
| C       | 10.670421 | 2.203344 | -1.320975 |
| C       | 10.181367 | 2.982861 | -2.368231 |
| C       | 8.880013 | 3.465766 | -2.330593 |
| C       | 8.051380 | 3.159257 | -1.245625 |
| C       | 8.550046 | 2.386989 | -0.189005 |
| C       | 9.855748 | 1.912890 | -0.228977 |
| H       | 11.688060 | 1.83915 | -1.349808 |
| H       | 10.816985 | 3.218811 | -3.212749 |
| H       | 8.489436 | 4.083062 | -3.128835 |
| H       | 7.947702 | 2.187323 | 0.689705 |
| H       | 10.240862 | 1.327409 | 0.596782 |
| H       | 1.973743 | 3.774681 | -1.859361 |
| Pd      | 4.423637 | 5.485939 | -1.504688 |
| Cl      | 2.449046 | 6.339718 | -0.662211 |
| Cl      | 4.877868 | 7.472237 | -2.555203 |
| H2      | 6.460538 | 5.508523 | 1.569415 |
| H2      | 5.966340 | 5.763016 | 1.073215 |

| C       | 2.149627 | 2.785348 | 0.084098 |
| C       | 1.430868 | 2.203103 | 1.141692 |
| C       | 0.044108 | 2.203018 | 1.131076 |
| C       | -0.639016 | 2.758085 | 0.049376 |
| C       | 0.067269 | 3.310805 | -1.017287 |
| C       | 1.453342 | 3.330113 | -1.004376 |
| C       | 3.597934 | 2.725588 | 0.135471 |
| H       | 1.964472 | 1.765400 | 1.978424 |
| H       | -0.504149 | 1.768352 | 1.957753 |
| H       | -1.722441 | 2.752698 | 0.035162 |
| H       | -0.463359 | 3.738323 | -1.858505 |
| N       | 4.416090 | 3.491756 | -0.498515 |
| C       | 6.654073 | 3.697846 | -1.274727 |
| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| Cl   | 2.445401 | 6.328108 | -0.601506|
| Cl   | 4.795119 | 7.408084 | -2.631339|
| H2   | 7.325306 | 6.136019 | 0.667940 |
| H2   | 6.927102 | 6.356276 | 0.077987 |
| H2   | 4.725973 | 2.874236 | -3.371315|
| H2   | 4.628717 | 2.142942 | -3.472288|
| H2   | 1.689764 | 5.048073 | -4.053093|
| H2   | 1.947705 | 5.519068 | -3.535198|
| C    | 2.160444 | 2.766990 | 0.090387 |
| C    | 1.433296 | 2.226476 | 1.163553 |
| C    | 0.046542 | 2.241770 | 1.147416 |
| C    | -0.626489| 2.770256 | 0.046067 |
| C    | 0.088705 | 3.281030 | -1.035508|
| C    | 1.474611 | 3.284311 | -1.017368|
| C    | 3.607956 | 2.705038 | 0.148331 |
| H    | 1.959545 | 1.814002 | 2.017445 |
| H    | -0.509476| 1.841171 | 1.986007 |
| H    | -1.709893| 2.777850 | 0.029062 |
| H    | -0.432915| 3.689015 | -1.891882|
| N    | 4.422211 | 3.463278 | -0.498460|
| C    | 6.656503 | 3.686272 | -1.272730|
| N    | 5.761535 | 3.095721 | -0.435507|
| H    | 4.027386 | 1.916261 | 0.779291 |
| H    | 5.986229 | 2.205810 | -0.009249|
| O    | 6.324516 | 4.635004 | -2.002422|
| C    | 10.657415| 2.208189 | -1.423640|
| C    | 10.116375| 2.921418 | -2.491711|
| C    | 8.814695 | 3.399897 | -2.422986|
| C    | 8.039159 | 3.152930 | -1.285196|
| C    | 8.589519 | 2.446558 | -0.208351|
| C    | 9.896659 | 1.977446 | -0.280133|
| H    | 11.675412| 1.841336 | -1.477247|
| H    | 10.711405| 3.109056 | -3.376906|
| H    | 8.383600 | 3.966906 | -3.237440|
| H    | 8.027011 | 2.298436 | 0.706153 |
| H    | 10.322836| 1.444326 | 0.560257 |
| H    | 2.023282 | 3.680381 | -1.858281|
| Pd   | 4.391618 | 5.440332 | -1.477142|
| Cl   | 2.441656 | 6.293997 | -0.573187|
| Cl   | 4.784008 | 7.407712 | -2.589410|
| H2   | 7.263185 | 5.944816 | 0.846249 |
| H2   | 6.844204 | 6.212152 | 0.291437 |
| H2   | 4.798366 | 2.858600 | -3.422488|
| H2   | 4.722680 | 2.129575 | -3.553228|
| H2   | 1.550428 | 5.133073 | -3.994048|
| H2   | 1.808354 | 5.560733 | -3.439739|
| H2   | 3.821130 | 4.936015 | 2.508940 |
| H2   | 3.529978 | 5.243204 | 1.893887 |
| C    | 2.187470 | 2.796496 | 0.161394 |
| C    | 1.495584 | 2.235786 | 1.248695 |
| C    | 0.109180 | 2.210600 | 1.261273 |
| C    | -0.600948| 2.720061 | 0.174563 |
### Structure descriptions

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 0.078335 | 3.250813 | -0.920432 |
| C    | 1.464080 | 3.294169 | -0.931926 |
| C    | 3.636510 | 2.764243 | 0.197330  |
| H    | 2.049870 | 1.834045 | 2.090073  |
| H    | -0.417196 | 1.792400 | 2.110368  |
| H    | -1.684237 | 2.696179 | 0.178304  |
| H    | -0.473053 | 3.642862 | -1.765593 |
| N    | 4.439582 | 3.509797 | -0.480206 |
| C    | 6.683363 | 3.717880 | -1.250496 |
| N    | 5.782188 | 3.149794 | -0.401639 |
| H    | 4.073069 | 2.001892 | 0.849525  |
| H    | 6.004662 | 2.269270 | 0.044811  |
| O    | 6.359341 | 4.649409 | -2.002997 |
| C    | 10.682087 | 2.218295 | -1.349250 |
| C    | 10.158331 | 2.936596 | -2.422406 |
| C    | 8.858320 | 3.421857 | -2.369673 |
| C    | 8.066046 | 3.178363 | -1.242388 |
| C    | 8.600045 | 2.467176 | -0.160256 |
| C    | 9.904123 | 1.990256 | -0.216255 |
| H    | 11.698521 | 1.845662 | -1.390428 |
| H    | 10.765384 | 3.122898 | -3.299684 |
| H    | 8.441273 | 3.992317 | -3.189063 |
| H    | 8.026823 | 2.317855 | 0.747404  |
| H    | 10.316742 | 1.452484 | 0.628450  |
| H    | 1.984212 | 3.703833 | -1.782570 |
| Pd   | 4.404200 | 5.454516 | -1.545389 |
| Cl   | 2.427847 | 6.317606 | -0.715834 |
| Cl   | 4.795482 | 7.375224 | -2.737723 |

### PIP

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| H2   | 4.298965 | -3.497581 | -1.517185 |
| H2   | 4.356965 | -3.128708 | -0.871296 |
| Cl   | 4.761646 | -1.203114 | 1.352420 |
| H    | 0.381924 | -0.724854 | -0.175583 |
| C    | 1.506257 | 2.232957 | -0.741576 |
| C    | 1.063910 | 3.564300 | -0.665581 |
| C    | -0.236904 | 3.880174 | -0.305144 |
| C    | -1.140995 | 2.855059 | -0.036229 |
| C    | -0.747388 | 1.526335 | -0.148157 |
| C    | 0.559019 | 1.219676 | -0.501750 |
| C    | 2.919214 | 2.022161 | -1.063852 |
| H    | 1.772069 | 4.358933 | -0.870645 |
| H    | -0.544560 | 4.915155 | -0.232470 |
| H    | -2.159878 | 3.085812 | 0.249137 |
| H    | -1.451440 | 0.722548 | 0.031766 |
| N    | 3.652233 | 1.005699 | -0.776870 |
| C    | 7.710476 | 1.068796 | -1.897000 |
| C    | 7.165374 | 2.157994 | -1.223400 |
| C    | 5.826908 | 2.146760 | -0.844350 |
| C    | 5.034029 | 1.037873 | -1.142858 |
| C    | 5.584870 | -0.069930 | -1.785967 |
| C    | 6.917069 | -0.043286 | -2.174555 |
| H    | 8.754344 | 1.076659 | -2.186250 |
### Structure descriptions

| Element | X  | Y  | Z     |
|---------|----|----|-------|
| H       | 7.784081 | 3.012182 | -0.976342 |
| H       | 5.410088 | 2.973329 | -0.281976 |
| H       | 4.972467 | -0.942910 | -1.966451 |
| H       | 7.341253 | -0.902302 | -2.679487 |
| H       | 3.391649 | 2.855693 | -1.585153 |
| O       | 0.937548 | -0.095476 | -0.690230 |
| Pd      | 2.811316 | -0.640263 | 0.270310 |
| Cl      | 1.456332 | -2.237425 | 1.301749 |
| Cl      | 4.761910 | -1.190256 | 1.351152 |
| H       | 0.380180 | -0.724506 | -0.177706 |
| H₂      | 1.453878 | 1.862846 | 2.420744 |
| H₂      | 1.790222 | 1.201060 | 2.484769 |
| C       | 1.503814 | 2.230695 | -0.750150 |
| C       | 1.065176 | 3.562223 | -0.662592 |
| C       | -0.232196 | 3.878457 | -0.292226 |
| C       | -1.136230 | 2.853230 | -0.021616 |
| C       | -0.745555 | 1.524683 | -0.143552 |
| C       | 0.557388 | 1.218060 | -0.507931 |
| C       | 2.916354 | 2.019864 | -1.072835 |
| H       | 1.773310 | 4.356662 | -0.868461 |
| H       | -0.537341 | 4.913522 | -0.208916 |
| H       | -2.152210 | 3.084053 | 0.273857 |
| H       | -1.448604 | 0.721159 | 0.041075 |
| N       | 3.648774 | 1.002849 | -0.786211 |
| C       | 7.712853 | 1.064392 | -1.885590 |
| C       | 7.164594 | 2.153663 | -1.214763 |
| C       | 5.824011 | 2.143316 | -0.843140 |
| C       | 5.031927 | 1.035368 | -1.146624 |
| C       | 5.586176 | -0.072978 | -1.785845 |
| C       | 6.920568 | -0.047487 | -2.166888 |
| H       | 8.758404 | 1.071402 | -2.168536 |
| H       | 7.782560 | 3.007178 | -0.963624 |
| H       | 5.404480 | 2.969653 | -0.282511 |
| H       | 4.973064 | -0.945108 | -1.969799 |
| H       | 7.347159 | -0.906619 | -2.669625 |
| H       | 3.389257 | 2.853879 | -1.593044 |
| O       | 0.935479 | -0.096953 | -0.694712 |
| Pd      | 2.810069 | -0.640429 | 0.265862 |
| Cl      | 1.457805 | -2.235186 | 1.305469 |
| H₂      | 1.481494 | 1.923817 | 2.416855 |
| H₂      | 1.834861 | 1.269992 | 2.467698 |
| C       | 1.505600 | 2.240792 | -0.714341 |
| C       | 1.064022 | 3.569831 | -0.603239 |
| C       | -0.235055 | 3.876549 | -0.229279 |
| C       | -1.138375 | 2.844845 | 0.018266 |
| C       | -0.745156 | 1.519594 | -0.130453 |
| C       | 0.559764 | 1.222433 | -0.495577 |
| C       | 2.920119 | 2.040205 | -1.033125 |
| H       | 1.771748 | 4.369210 | -0.790245 |
| H       | -0.542195 | 4.909321 | -0.128805 |
| H       | -2.155849 | 3.068248 | 0.312165 |
| H       | -1.447332 | 0.711294 | 0.035501 |
Structure descriptions

SP-JLMC
| Atom | x    | y    | z    |
|------|------|------|------|
| H2   | 4.538244 | -3.263310 | -0.572655 |
| H2   | 1.617973  | 2.057779  | 2.379791  |
| H2   | 1.985466  | 1.419500  | 2.492061  |
| C    | 1.508062  | 2.197204  | -0.764401 |
| C    | 1.093733  | 3.539063  | -0.741430 |
| C    | -0.178440 | 3.901223  | -0.326342 |
| C    | -1.082489 | 2.911442  | 0.052684  |
| C    | -0.718085 | 1.571058  | -0.003337 |
| C    | 0.560294  | 1.219021  | -0.410864 |
| C    | 2.898279  | 1.939573  | -1.144202 |
| H    | 1.802169  | 4.306106  | -1.032282 |
| H    | -0.463898 | 4.944568  | -0.296432 |
| H    | -2.078908 | 3.178494  | 0.382218  |
| N    | 3.627841  | 0.928654  | -0.831256 |
| C    | 7.623833  | 0.819426  | -2.150890 |
| C    | 7.141265  | 1.957440  | -1.511018 |
| C    | 5.822985  | 2.005039  | -1.069082 |
| C    | 4.988251  | 0.905254  | -1.270038 |
| C    | 5.476466  | -0.249533 | -1.880402 |
| C    | 6.788281  | -0.281711 | -2.332406 |
| H    | 8.652372  | 0.781880  | -2.488624 |
| H    | 7.793840  | 2.804897  | -1.339380 |
| H    | 5.455555  | 2.870844  | -0.531915 |
| H    | 4.831489  | -1.111223 | -1.986913 |
| H    | 7.164196  | -1.177257 | -2.811399 |
| H    | 3.356832  | 2.728733  | -1.741603 |
| O    | 0.909988  | -0.110902 | -0.532297 |
| Pd   | 2.823510  | -0.630799 | 0.361519  |
| Cl   | 1.512432  | -2.152205 | 1.553156  |
| Cl   | 4.819641  | -1.133195 | 1.390920  |
| H    | 0.367489  | -0.697095 | 0.042410  |
| H2   | 2.133461  | -2.097708 | -2.756273 |
| H2   | 2.324192  | -2.423419 | -2.114648 |
| H2   | 4.574762  | -3.723756 | -1.104423 |
| H2   | 4.616463  | -3.248771 | -0.530688 |
| H2   | 1.167740  | 1.543953  | 2.618178  |
| H2   | 1.386829  | 0.832616  | 2.653684  |
| C    | 1.516284  | 2.202833  | -0.768058 |
| C    | 1.105676  | 3.545942  | -0.743653 |
| C    | -0.169500 | 3.910333  | -0.340029 |
| C    | -1.080847 | 2.921845  | 0.024447  |
| C    | -0.719260 | 1.580817  | -0.031741 |
| C    | 0.562747  | 1.226667  | -0.425306 |
| C    | 2.905564  | 1.941322  | -1.149754 |
| H    | 1.818605  | 4.312004  | -1.028212 |
| H    | -0.452293 | 4.954456  | -0.309030 |
| H    | -2.080261 | 3.190719  | 0.343372  |
| H    | -1.428449 | 0.804342  | 0.229184  |
| N    | 3.628459  | 0.924482  | -0.843654 |
| C    | 7.622824  | 0.779350  | -2.161800 |
| C    | 7.150487  | 1.921520  | -1.521876 |
| C    | 5.832336  | 1.981823  | -1.080667 |
Structure descriptions

|   | C     | H     | O    |
|---|-------|-------|------|
|   | 4.987956 | 0.890125 | -1.283909 |
|   | 5.465011 | -0.268893 | -1.894815 |
|   | 6.777159 | -0.313851 | -2.344944 |
|   | 8.651391 | 0.732358  | -2.498517 |
|   | 7.811107 | 2.762363  | -1.348149 |
|   | 5.473643 | 2.848099  | -0.539205 |
|   | 4.811976 | -1.124392 | -2.003309 |
|   | 7.144595 | -1.212564 | -2.824731 |
|   | 3.366959 | 2.730461  | -1.745042 |
|   | 0.909248 | -0.106021 | -0.544198 |
|   | 0.360975 | -0.685798 | 0.030156  |
|   | 0.1518131 | -2.132489 | 1.571294 |
|   | 0.4815864 | -1.091868 | 1.411322 |
|   | 0.360975 | -0.685798 | 0.030156  |
|   | 2.166070 | -2.193377 | -2.710057 |
|   | 2.369400 | -2.453843 | -2.042893 |
|   | 4.253100 | 2.529285  | 2.034615 |
|   | 4.408842 | 1.808267  | 1.923940 |

C 1.504396  2.244185  -0.698157
C 1.058521  3.573187  -0.599090
C -0.248315  3.879658  -0.253202
C -1.15055   2.847833  -0.021433
C -0.757471  1.522389  -0.155568
C 0.554904   1.225009  -0.494973
C 2.922630   2.045319  -1.003365
H 1.768260   4.373223  -0.776086
H -0.558868  4.912540  -0.163664
H -2.178975  3.071192  0.251744
H -1.463100  0.719060  -0.004816
N 3.655110   1.021242  -0.742519
C 7.729934   1.154307  -1.796439
C 7.167134   2.212136  -1.088440
C 5.823026   2.177229  -0.731046
C 5.042685   1.075982  -1.085115
C 5.611271  -0.001793  -1.762627
C 6.948614   0.49263   -2.130605
H 8.777735   1.180863  -2.070092
H 7.775828   3.060086  -0.798492
H 5.391729   2.978252  -0.143097
H 5.006591  -0.870755  -1.985609
H 7.386970  -0.786166  -2.662400
H 3.400777   2.898415  -1.486617
O 0.937842  -0.084448  -0.705562
Pd 2.810710  -0.670004  0.232497
Cl 1.448520  -2.308309  1.192301
Cl 4.760111  -1.284120  1.287851
H 0.378177  -0.728367  -0.213855

PIA

H2 3.444692  1.132324  -4.760641
H2 3.375955  0.486996  -4.392587
C 1.431951  2.336593  -0.611937
|  |   |   |   |
|---|---|---|---|
| H | 4.715055 | -1.119397 | -0.587328 |
| H | 7.164329 | -1.443397 | -0.802524 |
| H2 | 3.453261 | 1.147809 | -4.742356 |
| H2 | 3.416838 | 0.487231 | -4.397808 |
| C | 1.422427 | 2.327067 | -0.607832 |
| C | 0.861885 | 3.506409 | -0.125434 |
| C | -0.517086 | 3.576697 | 0.039173 |
| C | -1.287692 | 2.465842 | -0.278872 |
| C | -0.661937 | 1.316344 | -0.756466 |
| N | 0.659544 | 1.250433 | -0.916478 |
| C | 2.856216 | 2.177665 | -0.810771 |
| H | 1.500191 | 4.348703 | 0.109502 |
| H | -0.979792 | 4.483214 | 0.409401 |
| H | -2.363641 | 2.477085 | -0.165014 |
| H | -1.207967 | 0.421366 | -1.031387 |
| N | 3.337719 | 1.079219 | -1.274724 |
| C | 7.481464 | 0.738915 | -1.865080 |
| C | 6.814440 | 1.877153 | -2.313628 |
| C | 5.442736 | 1.997850 | -2.129228 |
| C | 4.735927 | 0.970205 | -1.495578 |
| C | 5.394527 | -0.187459 | -1.077840 |
| C | 6.769149 | -0.288282 | -1.249461 |
| H | 8.550522 | 0.646628 | -2.013538 |
| H | 7.358496 | 2.664292 | -2.821448 |
| H | 4.912380 | 2.859587 | -2.515730 |
| H | 4.825213 | -0.994141 | -0.634941 |
| H | 7.281747 | -1.182313 | -0.916734 |
| H | 3.507711 | 3.007245 | -0.540493 |
| Pd | 1.783033 | -0.363804 | -1.743931 |
| Cl | 3.164803 | -1.952158 | -2.710365 |
| Cl | -0.114429 | -1.648178 | -2.137888 |
| H2 | 0.639938 | 2.872736 | -3.696555 |
| H2 | 0.727313 | 2.138311 | -3.111328 |
| H2 | 2.018560 | 0.271552 | 1.996861 |
| H2 | 1.892847 | -0.097317 | 1.362456 |
| H2 | 1.892834 | 2.821007 | -3.913170 |
| H2 | 1.879747 | 2.083981 | -3.807010 |
| Cl | -0.213742 | -1.490911 | -2.236360 |
| Cl | 3.055696 | -1.990881 | -2.696799 |
| C | 1.508824 | 2.369433 | -0.605215 |
| C | 1.007812 | 3.556248 | -0.078608 |
| C | -0.367840 | 3.697349 | 0.070166 |
| C | -1.194685 | 2.648755 | -0.311430 |
| C | -0.626858 | 1.488125 | -0.833040 |
| N | 0.691349 | 1.353919 | -0.974821 |
| C | 2.935260 | 2.138670 | -0.779718 |
| H | 1.688254 | 4.348659 | 0.206103 |
| H | -0.784449 | 4.610393 | 0.476872 |
| H | -2.270120 | 2.715167 | -0.211800 |
| H | -1.217197 | 0.637081 | -1.152460 |
| N | 3.359228 | 1.023780 | -1.259468 |
| C | 7.488872 | 0.459431 | -1.772724 |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | 6.891 | 1.629 | -2.237|
| C    | 5.524 | 1.822 | -2.077|
| C    | 4.754 | 0.837 | -1.453|
| C    | 5.342 | -0.352| -1.018|
| H    | 6.712 | -0.525| -1.165|
| H    | 8.653 | 0.308 | -1.901|
| H    | 7.485 | 2.384 | -2.737|
| H    | 5.046 | 2.711 | -2.471|
| H    | 4.724 | -1.122| -0.581|
| H    | 7.171 | -1.443| -0.818|
| H    | 3.629 | 2.919 | -0.474|
| Pd   | 1.741 | -0.316| -1.788|
| H2   | 1.962 | -0.156| 1.327 |
| H2   | 2.106 | 0.185 | 1.972 |
| H2   | 1.714 | 2.841 | -3.873|
| H2   | 1.678 | 2.109 | -3.740|
| Cl   | -0.217| -1.491| -0.972|
| Cl   | 3.052 | -1.992| -2.692|
| C    | 1.504 | 2.369 | -0.605|
| C    | 1.003 | 3.560 | -0.078|
| C    | -0.373| 3.696 | 0.071 |
| C    | -1.199| 2.647 | -0.308|
| C    | -0.630| 1.486 | -0.829|
| N    | 0.687 | 1.353 | -0.971|
| C    | 2.930 | 2.140 | -0.781|
| H    | 1.683 | 4.349 | 0.206 |
| H    | -0.789| 4.609 | 0.477 |
| H    | -2.274| 2.712 | -0.208|
| H    | -1.220| 0.634 | -1.148|
| N    | 3.356 | 1.026 | -1.260|
| C    | 7.486 | 0.466 | -1.776|
| C    | 6.887 | 1.634 | -2.241|
| C    | 5.519 | 1.827 | -2.080|
| C    | 4.750 | 0.840 | -1.457|
| C    | 5.340 | -0.347| -1.020|
| C    | 6.710 | -0.519| -1.167|
| H    | 8.550 | 0.315 | -1.904|
| H    | 7.479 | 2.390 | -2.741|
| H    | 5.041 | 2.715 | -2.475|
| H    | 4.722 | -1.118| -0.582|
| H    | 7.170 | -1.437| -0.820|
| H    | 3.624 | 2.922 | -0.478|
| Pd   | 1.738 | -0.317| -1.786|
| H2   | 1.921 | -0.119| 1.383 |
| H2   | 2.058 | 0.261 | 2.009 |
| H2   | 1.154 | 2.938 | -3.774|
| H2   | 1.255 | 2.202 | -3.719|
| H2   | 3.646 | 1.010 | -4.745|
| H2   | 3.525 | 0.359 | -4.411|
| C    | 1.507 | 2.369 | -0.604|
| C    | 1.005 | 3.560 | -0.090|
| C    | -0.371| 3.702 | 0.054 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| Cl   | 3.167082  | -1.947218 | -2.738586 |
| Cl   | -0.110445 | -1.642932 | -2.172253 |
| H2   | 2.031308  | -0.058957 | 1.405898  |
| H2   | 2.170995  | 0.363626  | 2.002714  |
| H2   | 2.861357  | -2.616633 | 0.179675  |
| H2   | 3.004997  | -2.617477 | 0.909192  |
| H2   | 0.863238  | 2.927982  | -3.761751 |
| H2   | 0.912758  | 2.190187  | -3.674918 |
| H2   | 3.562790  | 1.080799  | -4.743747 |
| H2   | 3.479895  | 0.428247  | -4.392022 |
| C    | 1.507830  | 2.370104  | -0.610830 |
| C    | 1.004116  | 3.563558  | -0.102870 |
| C    | -0.371467 | 3.701598  | 0.049419  |
| C    | -1.195309 | 2.642648  | -0.309104 |
| C    | -0.624820 | 1.475724  | -0.813045 |
| N    | 0.693022  | 1.345139  | -0.958963 |
| C    | 2.934561  | 2.143809  | -0.789891 |
| H    | 1.682698  | 4.363638  | 0.164555  |
| H    | -0.790478 | 4.619990  | 0.441470  |
| H    | -2.270515 | 2.706762  | -0.205878 |
| H    | -1.213505 | 0.618228  | -1.117545 |
| N    | 3.360930  | 1.026144  | -1.260579 |
| C    | 7.489341  | 0.444214  | -1.757172 |
| C    | 6.898601  | 1.615216  | -2.227499 |
| C    | 5.532352  | 1.815641  | -2.072983 |
| C    | 4.755386  | 0.834937  | -1.448311 |
| C    | 5.336717  | -0.354813 | -1.006777 |
| C    | 6.706624  | -0.534877 | -1.148354 |
| H    | 8.554082  | 0.287432  | -1.881965 |
| H    | 7.497649  | 2.365935  | -2.728537 |
| H    | 5.059373  | 2.703515  | -2.474492 |
| H    | 4.714524  | -1.118833 | -0.564873 |
| H    | 7.160239  | -1.453237 | -0.796757 |
| H    | 3.627744  | 2.928461  | -0.491650 |
| Pd   | 1.742656  | -0.315204 | -1.785622 |
| Cl   | 3.058888  | -1.978026 | -2.725033 |
| Cl   | -0.209744 | -1.494477 | -2.228339 |
| H2   | 1.964888  | -0.050860 | 1.405249  |
| H2   | 2.023284  | 0.412824  | 1.984750  |
| C    | 1.543707  | 2.355888  | -0.091208 |
| C    | 0.980605  | 3.535146  | 0.389280  |
| C    | -0.401045 | 3.612116  | 0.528516  |
| C    | -1.171991 | 2.509323  | 0.184743  |
| C    | -0.544191 | 1.360087  | -0.292055 |
| N    | 0.780166  | 1.286908  | -0.425521 |
| C    | 2.981316  | 2.192008  | -0.251855 |
| H    | 1.618609  | 4.371060  | 0.646580  |
| H    | -0.864636 | 4.517561  | 0.900077  |
| H    | -2.249833 | 2.524804  | 0.278910  |
| H    | -1.089168 | 0.469146  | -0.581784 |
| N    | 3.465296  | 1.083200  | -0.689075 |
| C    | 7.625605  | 0.719201  | -1.144134 |
**Structure descriptions**

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 6.97409| 1.84535| -1.643472 |
| C    | 5.59795| 1.97280| -1.504297 |
| C    | 4.86978| 0.96308| -0.866028 |
| C    | 5.51303| -0.18334| -0.396369 |
| C    | 6.89190| -0.28981| -0.523082 |
| H    | 8.69853| 0.61979| -1.256149 |
| H    | 7.53669| 2.61924| -2.153358 |
| H    | 5.08210| 2.82767| -0.924946 |
| H    | 4.92856| -0.97356| 0.051272 |
| H    | 7.39229| -1.17479| -0.150112 |
| H    | 3.63253| 3.01823| 0.029433 |
| Pd   | 1.91833| -0.35830| -1.175672 |
| Cl   | 3.31698| -2.00275| -2.013585 |
| Cl   | 0.02238| -1.64144| -1.587614 |

**BPY**

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 0.69602| 2.36287| 1.481559 |
| C    | 1.42793| 3.53677| 1.307885 |
| C    | 2.81528| 3.48608| 1.320554 |
| C    | 3.44596| 2.26281| 1.506773 |
| C    | 2.66478| 1.12766| 1.675280 |
| H    | 3.39342| 4.39210| 1.185648 |
| H    | 4.52438| 2.17830| 1.522580 |
| H    | 3.08610| 0.14017| 1.823922 |
| N    | 1.32891| 1.17914| 1.662670 |
| Pd   | 0.04539| -0.49490| 1.889984 |
| N    | -1.34085| 1.09380| 1.649168 |
| C    | -0.78312| 2.31575| 1.475007 |
| C    | -2.67082| 0.95728| 1.648555 |
| C    | -1.58677| 3.44091| 1.296084 |
| C    | -3.52130| 2.04079| 1.473376 |
| H    | -3.03005| -0.05490| 1.792160 |
| C    | -2.96819| 3.30206| 1.294963 |
| H    | -4.59225| 1.88769| 1.478301 |
| H    | -3.60157| 4.16974| 1.155823 |
| H    | 0.92443| 4.48153| 1.162756 |
| H    | -1.14323| 4.41618| 1.157506 |
| Cl   | 1.78141| -2.02848| 2.113218 |
| Cl   | -1.59257| -2.13549| 2.094840 |
| H2   | -0.07378| 1.27049| -1.510112 |
| H2   | -0.05841| 0.65932| -1.085174 |
| H2   | 1.80113| 0.75926| -1.429424 |
| H2   | 1.62266| 0.23703| -0.929832 |
| C    | 0.66314| 2.38157| 1.482406 |
| C    | 1.37225| 3.56668| 1.285121 |
| C    | 2.75870| 3.55289| 1.356812 |
| C    | 3.41116| 2.35703| 1.626021 |
| C    | 2.65213| 1.20943| 1.809337 |
| H    | 3.31885| 4.46718| 1.203084 |
| H    | 4.48958| 2.30131| 1.690439 |
| H    | 3.09280| 0.23965| 2.008879 |
| N    | 1.31769| 1.22379| 1.738109 |

S196
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| Pd   | 0.070172 | -0.480372 | 1.919902 |
| N    | -1.348421 | 1.070549 | 1.639637 |
| C    | -0.813570 | 2.296685 | 1.427875 |
| C    | -2.674204 | 0.903726 | 1.612619 |
| C    | -1.637201 | 3.392935 | 1.174667 |
| C    | -3.544033 | 1.958005 | 1.370099 |
| H    | -3.014904 | -0.110817 | 1.782896 |
| C    | -3.014632 | 3.221675 | 1.144659 |
| H    | -4.610899 | 1.779381 | 1.355929 |
| H    | -3.662948 | 4.066985 | 0.948188 |
| H    | 0.851835  | 4.489208 | 1.076856 |
| H    | -1.211910 | 4.370896 | 1.001755 |
| Cl   | 1.838556  | -1.972982 | 2.163168 |
| Cl   | -1.530302 | -2.165426 | 2.039477 |
| H2   | -1.601382 | 0.585306 | -1.553473 |
| H2   | -1.394130 | 0.080149 | -1.045739 |
| H2   | 0.706683  | 1.450084 | -1.451828 |
| H2   | 0.659261  | 0.845834 | -1.019671 |
| H2   | -0.072127 | 1.219588 | 4.474913 |
| C    | 0.693276  | 2.386867 | 1.631604 |
| C    | 1.418323  | 3.575817 | 1.574652 |
| C    | 2.803769  | 3.537284 | 1.656006 |
| C    | 3.438826  | 2.310034 | 1.793159 |
| C    | 2.664166  | 1.159286 | 1.845663 |
| H    | 3.376966  | 4.455105 | 1.611663 |
| H    | 4.516014  | 2.234156 | 1.859218 |
| H    | 3.089883  | 0.168279 | 1.951557 |
| N    | 0.650385  | 1.909577 | 1.767245 |
| Pd   | 0.058001  | -0.494562 | 1.828854 |
| N    | -1.333406 | 1.092359 | 1.618697 |
| C    | -0.782010 | 2.327365 | 1.546788 |
| C    | -2.660043 | 0.945361 | 1.550859 |
| C    | -1.589357 | 3.454327 | 1.400644 |
| C    | -3.514239 | 2.030058 | 1.406621 |
| H    | -3.015649 | -0.076091 | 1.614336 |
| C    | -2.967860 | 3.304282 | 1.329557 |
| H    | -4.582530 | 1.867315 | 1.355284 |
| H    | -3.603908 | 4.173611 | 1.215548 |
| H    | 0.910818  | 4.523378 | 1.466810 |
| H    | -1.150828 | 4.439856 | 1.341607 |
| Cl   | 1.797725  | -2.023465 | 2.047356 |
| Cl   | -1.566846 | -2.162682 | 1.860755 |
| H2   | -2.052105 | -0.565323 | -1.407081 |
| H2   | -1.904379 | -1.007538 | -0.824474 |
| H2   | 2.060643  | -0.256556 | 4.530990 |
| H2   | 2.160999 | 0.299282 | 5.018491 |
| H2   | 2.188308 | -0.417192 | -1.191950 |
| H2   | 2.069240 | -0.834855 | -0.585417 |
| H2   | -0.324849 | 1.457698 | 4.420105 |
| H2   | -0.543189 | 2.141035 | 4.618864 |
| C    | 0.650385 | 2.404709 | 1.513317 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 1.356199   | 3.599976   | 1.385905   |
| C    | 2.741620   | 3.589352   | 1.478471   |
| C    | 3.396025   | 2.384143   | 1.695557   |
| C    | 2.639848   | 1.226022   | 1.812242   |
| H    | 3.299543   | 4.512754   | 1.381730   |
| H    | 4.473562   | 2.330045   | 1.774172   |
| H    | 3.082653   | 0.251620   | 1.979191   |
| N    | 1.306766   | 1.238973   | 1.723737   |
| Pd   | 0.061201   | -0.468476  | 1.883322   |
| N    | -1.355976  | 1.080611   | 1.592793   |
| C    | -0.824444  | 2.316393   | 1.437570   |
| C    | -2.680555  | 0.909450   | 1.548149   |
| C    | -1.650507  | 3.419481   | 1.227215   |
| C    | -3.552801  | 1.970255   | 1.345372   |
| H    | -3.019098  | -0.111439  | 1.679274   |
| C    | -3.027175  | 3.244893   | 1.181333   |
| H    | -4.618933  | 1.788958   | 1.316862   |
| H    | -3.677790  | 4.095597   | 1.019198   |
| H    | 0.834404   | 4.530744   | 1.217457   |
| H    | -1.227789  | 4.405548   | 1.100714   |
| Cl   | 1.825435   | -1.964575  | 2.167904   |
| Cl   | -1.535277  | -2.157905  | 2.011810   |
| H2   | -1.815345  | -0.659015  | -1.367711  |
| H2   | -1.694994  | -1.048415  | -0.742809  |
| C    | 0.718002   | 2.339480   | 1.725626   |
| C    | 1.484429   | 3.495302   | 1.714322   |
| C    | 2.863372   | 3.393813   | 1.700903   |
| C    | 3.451256   | 2.143640   | 1.699870   |
| C    | 2.634828   | 1.027901   | 1.710549   |
| H    | 3.471042   | 4.289161   | 1.691260   |
| H    | 4.525122   | 2.022560   | 1.690799   |
| H    | 3.018751   | 0.011481   | 1.709777   |
| N    | 1.308944   | 1.128605   | 1.722784   |
| Pd   | -0.023557  | -0.511098  | 1.737009   |
| N    | -1.351242  | 1.132422   | 1.746150   |
| C    | -0.756888  | 2.341603   | 1.740419   |
| C    | -2.677397  | 1.035405   | 1.758231   |
| C    | -1.520050  | 3.499616   | 1.748708   |
| C    | -3.490672  | 2.153471   | 1.766002   |
| H    | -3.063980  | 0.020003   | 1.761578   |
| C    | -2.899279  | 3.401971   | 1.761946   |
| H    | -4.564900  | 2.035633   | 1.775213   |
| H    | -3.504606  | 4.298928   | 1.769164   |
| H    | 1.014312   | 4.468269   | 1.715474   |
| H    | -1.047179  | 4.471244   | 1.745313   |
| Cl   | 1.647106   | -2.106605  | 1.724367   |
| Cl   | -1.698750  | -2.101795  | 1.755543   |
| C    | 0.720769   | 2.346412   | 1.725892   |
| C    | 1.490355   | 3.508973   | 1.717443   |
| C    | 2.875047   | 3.412623   | 1.703904   |
| C    | 3.466573   | 2.155842   | 1.698757   |
| C    | 2.647986   | 1.034316   | 1.708253   |
|   |   |   |
|---|---|---|
| H | 3.482036 | 4.309781 | 1.697104 |
| H | 4.540584 | 2.034769 | 1.687840 |
| H | 3.037176 | 0.022979 | 1.705134 |
| N | 1.314594 | 1.128882 | 1.721517 |
| Pd | -0.023559 | -0.516886 | 1.738208 |
| N | -1.356966 | 1.132721 | 1.748178 |
| C | -0.759670 | 2.348525 | 1.739913 |
| C | -2.690627 | 1.041984 | 1.761079 |
| C | -1.525938 | 3.513297 | 1.744192 |
| C | -3.505009 | 2.165854 | 1.766437 |
| H | -3.082697 | 0.031774 | 1.767273 |
| C | -2.910894 | 3.420934 | 1.757546 |
| H | -4.580363 | 2.047849 | 1.771180 |
| H | -3.515315 | 4.319843 | 1.761022 |
| H | 1.017711 | 4.480467 | 1.721368 |
| H | -1.050515 | 4.483412 | 1.737079 |
| Cl | 1.662649 | -2.119566 | 1.721431 |
| Cl | -1.714255 | -2.114810 | 1.755760 |

**PHEN**

|   |   |   |
|---|---|---|
| C | 0.669895 | 2.316011 | 1.483360 |
| C | 1.332257 | 3.547354 | 1.294201 |
| C | 2.742027 | 3.531158 | 1.305605 |
| C | 3.404866 | 2.340063 | 1.495211 |
| C | 2.669648 | 1.157308 | 1.674249 |
| H | 3.289464 | 4.455856 | 1.163286 |
| H | 4.485807 | 2.294304 | 1.507677 |
| H | 3.141222 | 0.192732 | 1.824085 |
| N | 1.345037 | 1.149570 | 1.668311 |
| Pd | 0.048261 | -0.523315 | 1.895623 |
| N | -1.358319 | 1.055876 | 1.646692 |
| C | -0.762774 | 2.266301 | 1.472179 |
| C | -2.680175 | 0.971513 | 1.629515 |
| C | -1.505626 | 3.448929 | 1.271448 |
| C | -3.492682 | 2.100487 | 1.437231 |
| H | -3.086297 | -0.035252 | 1.771607 |
| C | -2.910830 | 3.334904 | 1.259236 |
| H | -4.567981 | 1.980225 | 1.430888 |
| H | -3.518891 | 4.219422 | 1.107826 |
| C | 0.551850 | 4.733167 | 1.097100 |
| C | -0.806227 | 4.686019 | 1.086384 |
| Cl | 1.800724 | -2.034269 | 2.124342 |
| Cl | -1.599463 | -2.151898 | 2.098084 |
| H2 | -0.112394 | 1.485510 | -1.512964 |
| H2 | -0.072987 | 0.829766 | -1.162291 |
| H | -1.385340 | 5.589247 | 0.934756 |
| H | 1.069477 | 5.674358 | 0.954037 |
| C | 0.669878 | 2.314964 | 1.480945 |
| C | 1.332479 | 3.546343 | 1.291029 |
| C | 2.742149 | 3.530819 | 1.304357 |
| C | 3.405038 | 2.340239 | 1.497095 |
| C | 2.669752 | 1.157554 | 1.676258 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 3.289413  | 4.455584  | 1.162076  |
| H    | 4.485905  | 2.293618  | 1.512393  |
| H    | 3.142287  | 0.193900  | 1.828766  |
| N    | 1.345294  | 1.149024  | 1.668235  |
| Pd   | 0.048261  | -0.523751 | 1.896800  |
| N    | -1.358480 | 1.056045  | 1.650690  |
| C    | -0.763028 | 2.265788  | 1.472019  |
| C    | -2.680263 | 0.972278  | 1.635671  |
| C    | -1.505587 | 3.448363  | 1.270276  |
| C    | -3.492601 | 2.100866  | 1.441405  |
| H    | -3.087340 | -0.021901 | 1.780591  |
| C    | -2.910708 | 3.334706  | 1.259425  |
| H    | -4.567929 | 1.980754  | 1.436560  |
| H    | -3.519252 | 4.218595  | 1.106579  |
| C    | 0.552042  | 4.731934  | 1.093061  |
| C    | -0.806058 | 4.684952  | 1.083075  |
| Cl   | 1.800908  | -2.033687 | 2.126603  |
| Cl   | -1.599473 | -2.152653 | 2.092456  |
| H2   | -0.548341 | 1.351846  | -1.532669 |
| H2   | -0.589856 | 0.718947  | -1.143155 |
| H    | -1.384448 | 5.588468  | 0.930443  |
| H    | 1.069080  | 5.673255  | 0.948711  |
| H2   | 2.415082  | -0.237391 | -1.221414 |
| H2   | 2.229504  | -0.679669 | -0.650010 |
| H    | 1.021861  | 5.745036  | 1.290503  |
| H    | -1.429771 | 5.634153  | 1.179634  |
| C    | 0.648051  | 2.356956  | 1.605849  |
| C    | 1.300413  | 3.604966  | 1.515902  |
| C    | 2.708669  | 3.609771  | 1.584606  |
| C    | 3.379480  | 2.411536  | 1.732235  |
| C    | 2.654059  | 1.211994  | 1.811477  |
| H    | 3.248725  | 4.541535  | 1.519175  |
| H    | 4.459562  | 2.377515  | 1.786121  |
| H    | 3.133429  | 0.246144  | 1.920785  |
| N    | 1.331391  | 1.189356  | 1.750532  |
| Pd   | 0.049763  | -0.505473 | 1.829634  |
| N    | -1.368799 | 1.067723  | 1.631419  |
| C    | -0.782750 | 2.292359  | 1.542223  |
| C    | -2.688271 | 0.971325  | 1.573769  |
| C    | -1.533805 | 3.477047  | 1.388652  |
| C    | -3.508732 | 2.101138  | 1.425452  |
| H    | -3.087089 | -0.033923 | 1.644565  |
| C    | -2.936858 | 3.349283  | 1.331677  |
| H    | -4.581907 | 1.970169  | 1.382676  |
| H    | -3.550929 | 4.234679  | 1.213465  |
| C    | 0.511793  | 4.791532  | 1.360388  |
| C    | -0.844390 | 4.730144  | 1.299016  |
| Cl   | 1.814183  | -2.011960 | 2.012891  |
| Cl   | -1.579026 | -2.166714 | 1.867206  |
| H2   | -2.035293 | -0.479021 | -1.378575 |
| H2   | -1.898001 | -0.920158 | -0.792529 |
| H    | -1.441430 | 5.635855  | 1.217453  |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 1.010825 | 5.747335 | 1.314150 |
| H2   | -0.166339 | 1.285737 | 4.442946 |
| H2   | -0.215207 | 1.963864 | 4.746558 |
| C    | 0.641106  | 2.356115 | 1.595068 |
| C    | 1.292034  | 3.605002 | 1.513846 |
| C    | 2.700626  | 3.604936 | 1.575116 |
| C    | 3.373038  | 2.411572 | 1.707352 |
| C    | 2.648794  | 1.210822 | 1.779874 |
| H    | 3.239486  | 4.543665 | 1.516506 |
| H    | 4.453335  | 2.377712 | 1.756701 |
| H    | 3.128671  | 0.244396 | 1.884184 |
| N    | 1.325566  | 1.187988 | 1.725651 |
| Pd   | 0.045840  | -0.508503 | 1.819875 |
| N    | -1.374021 | 1.066026 | 1.623842 |
| C    | -0.789422 | 2.291299 | 1.540344 |
| C    | -2.694018 | 0.968832 | 1.576610 |
| C    | -1.542305 | 3.476288 | 1.403441 |
| C    | -3.516170 | 2.099224 | 1.441677 |
| H    | -3.091340 | -0.037198 | 1.648837 |
| C    | -2.945648 | 3.345513 | 1.354772 |
| H    | -4.589644 | 1.968113 | 1.408047 |
| H    | -3.560852 | 4.234866 | 1.250133 |
| C    | 0.501784  | 4.792671 | 1.375641 |
| C    | -0.854617 | 4.730943 | 1.322333 |
| Cl   | 1.809769  | -2.008974 | 2.023877 |
| Cl   | -1.584769 | -2.164288 | 1.893982 |
| H2   | -0.053266 | 0.825970 | -1.112709 |
| H2   | -0.027619 | 1.480990 | -1.466141 |
| H2   | 2.419348  | -0.256406 | -1.226083 |
| H2   | 2.232383  | -0.694918 | -0.652266 |
| H2   | -0.195037 | 1.247366 | 4.447070 |
| H2   | -0.243360 | 1.925460 | 4.750917 |
| C    | 0.648247  | 2.356477 | 1.598342 |
| C    | 1.300160  | 3.604997 | 1.516817 |
| C    | 2.708080  | 3.604672 | 1.592326 |
| C    | 3.378906  | 2.412157 | 1.738867 |
| C    | 2.653812  | 1.212058 | 1.810524 |
| H    | 3.247726  | 4.542927 | 1.533558 |
| H    | 4.458681  | 2.378791 | 1.798755 |
| H    | 3.132974  | 0.246393 | 1.922097 |
| N    | 1.331537  | 1.189145 | 1.742911 |
| Pd   | 0.050189  | -0.505481 | 1.824246 |
| N    | -1.368028 | 1.067521 | 1.624223 |
| C    | -0.782156 | 2.291776 | 1.534050 |
| C    | -2.687643 | 0.971110 | 1.573770 |
| C    | -1.533700 | 3.476750 | 1.387951 |
| C    | -3.508573 | 2.100957 | 1.429167 |
| H    | -3.086473 | -0.033774 | 1.649040 |
| C    | -2.936996 | 3.349230 | 1.335856 |
| H    | -4.589201 | 1.970276 | 1.392610 |
| H    | -3.551341 | 4.235199 | 1.223403 |
| C    | 0.511350  | 4.791976 | 1.365755 |
| C    | -0.844740 | 4.730413 | 1.303495 |
| Atom | X  | Y  | Z  |
|------|----|----|----|
| Cl   | 1.813731 | -2.011816 | 2.018655 |
| Cl   | -1.579434 | -2.165300 | 1.876144 |
| H2   | -2.046040 | -0.491259 | -1.375597 |
| H2   | -1.907478 | -0.930238 | -0.788241 |
| H    | -1.430676 | 5.634801  | 1.189769  |
| H    | 1.021229  | 5.746040  | 1.302406  |
| H2   | -3.448839 | -1.597671 | 1.051778  |
| H2   | -3.787871 | -1.035378 | 1.406238  |
| H2   | 1.756689  | -3.689779 | 1.371657  |
| H2   | 1.104335  | -3.812472 | 1.030706  |
| H2   | -2.866835 | -0.057345 | -2.748082 |
| H2   | -3.139643 | 0.636018  | -2.709473 |
| C    | 0.196021  | 0.331500  | 0.917140  |
| C    | 0.568185  | 1.095749  | 2.042794  |
| C    | 0.350026  | 0.523637  | 3.312935  |
| C    | -0.205134 | -0.731943 | 3.404277  |
| C    | -0.547427 | -1.426266 | 2.232792  |
| H    | 0.622230  | 1.077228  | 4.204298  |
| H    | -0.385065 | -1.199159 | 4.363528  |
| H    | -0.987001 | -2.416479 | 2.251040  |
| N    | -0.351587 | -0.908463 | 1.030451  |
| Pd   | -0.792675 | -1.783996 | -0.855878 |
| N    | 0.031961  | 0.079881  | -1.456395 |
| C    | 0.398495  | 0.855640  | -0.401065 |
| C    | 0.212586  | 0.528566  | -2.688798 |
| C    | 0.970696  | 2.134068  | -0.569323 |
| C    | 0.775558  | 1.789541  | -2.943300 |
| H    | -0.103405 | -0.139732 | -3.481369 |
| C    | 1.152874  | 2.591230  | -1.890658 |
| H    | 0.902299  | 2.111081  | -3.968677 |
| H    | 1.589173  | 3.568226  | -2.064499 |
| C    | 1.143686  | 2.392862  | 1.842292  |
| C    | 1.335880  | 2.889947  | 0.592168  |
| C    | -1.653092 | -3.734932 | 0.082780  |
| Cl   | -1.175323 | -2.484944 | -3.040420 |
| H2   | 2.932916  | -1.032152 | -0.254838 |
| H2   | 2.414310  | -1.541828 | -0.414164 |
| H    | 1.772715  | 3.871781  | 0.453043  |
| H    | 1.425004  | 2.973260  | 2.713025  |
| C    | 0.670116  | 2.307676  | 1.465402  |
| C    | 1.331716  | 3.540998  | 1.285231  |
| C    | 2.741372  | 3.527517  | 1.307588  |
| C    | 3.404973  | 2.337422  | 1.501057  |
| C    | 2.670898  | 1.153038  | 1.672785  |
| H    | 3.288234  | 4.453522  | 1.172222  |
| H    | 4.485881  | 2.293665  | 1.523501  |
| H    | 3.143734  | 0.189800  | 1.827320  |
| N    | 1.346186  | 1.141924  | 1.654694  |
| Pd   | 0.049647  | -0.529138 | 1.891141  |
| N    | -1.358291 | 1.046105  | 1.630015  |
| C    | -0.763004 | 2.256878  | 1.452640  |
| C    | -2.680635 | 0.963428  | 1.623971  |
### Structure descriptions

- **C**  -1.506780  3.440626  1.260580
- **C**  -3.493515  2.093272  1.439384
- **H**  -3.086858  -0.031107  1.769405
- **C**  -2.912111  3.327526  1.258456
- **H**  -4.568962  1.973871  1.442217
- **H**  -3.520974  4.212576  1.113934
- **C**   0.550260  4.726566  1.091482
- **C**  -0.807843  4.678499  1.079839
- **Cl**  1.803917  -2.034639  2.148816
- **Cl**  -1.598476  -2.154998  2.119526
- **H**   1.066812  5.669106  0.953469
- **H**  -1.387126  5.582326  0.932494

**PtCl₂ — H₂**

|   |   |   |
|---|---|---|
| **C** | 2.183771 | 2.797332 | 0.113297 |
| **C** | 1.426967 | 2.201989 | 1.135849 |
| **C** | 0.041404 | 2.228872 | 1.084133 |
| **C** | -0.599168 | 2.826167 | -0.001797 |
| **C** | 0.146202 | 3.394135 | -0.032981 |
| **C** | 1.530889 | 3.383846 | -0.980142 |
| **C** | 3.628610 | 2.718630 | 0.187627 |
| **H** | 1.928579 | 1.732954 | 1.975396 |
| **H** | -0.539308 | 1.783301 | 1.882397 |
| **H** | -1.681599 | 2.841045 | -0.046599 |
| **H** | -0.351703 | 3.857850 | -1.875000 |
| **N** | 4.444840 | 3.492674 | -0.437399 |
| **C** | 6.676177 | 3.689459 | -1.259577 |
| **N** | 5.784994 | 3.123826 | -0.398095 |
| **H** | 4.043100 | 1.910200 | 0.795978 |
| **H** | 6.010288 | 2.239629 | 0.034922 |
| **O** | 6.352146 | 4.632979 | -1.999614 |
| **C** | 10.656094 | 2.162210 | -1.475800 |
| **C** | 10.127702 | 2.941769 | -2.502949 |
| **C** | 8.832627 | 3.433331 | -2.409777 |
| **C** | 8.050046 | 3.136165 | -1.288553 |
| **C** | 8.589290 | 2.364155 | -0.251685 |
| **C** | 9.888002 | 1.879748 | -0.348164 |
| **H** | 11.668150 | 1.783058 | -1.548320 |
| **H** | 10.727411 | 3.171253 | -3.374979 |
| **H** | 8.409876 | 4.053229 | -3.189360 |
| **H** | 8.025568 | 2.169430 | 0.653370 |
| **H** | 10.304644 | 1.293118 | 0.461189 |
| **H** | 2.112008 | 3.830614 | -1.773041 |
| **Pt** | 4.393111 | 5.449999 | -1.469549 |
| **Cl** | 2.415926 | 6.379123 | -0.604878 |
| **Cl** | 4.730811 | 7.444704 | -2.600644 |
| **H₂** | 6.865359 | 6.137896 | 0.752701 |
| **H₂** | 6.303304 | 6.277739 | 0.281165 |
| **H₂** | 4.401669 | 3.372760 | -3.212464 |
| **H₂** | 4.338949 | 2.684818 | -3.495063 |
| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | 2.212034 | 2.851093 | 0.180917 |
| C    | 1.476769  | 2.306260  | 1.246827  |
| C    | 0.091117  | 2.279870  | 1.198530  |
| C    | -0.571155 | 2.773233  | -0.998492 |
| C    | 0.153293  | 3.289356  | -0.998492 |
| C    | 1.537832  | 3.331574  | -0.950597 |
| C    | 3.658374  | 2.815917  | 0.256663  |
| H    | 1.995407  | 1.917379  | 2.116512  |
| H    | -0.472466 | 1.874215  | 2.029658  |
| H    | -1.653523 | 2.746519  | 0.031655  |
| H    | -0.361499 | 3.670072  | -1.871318 |
| N    | 4.466360  | 3.562299  | -0.412889 |
| C    | 6.696366  | 3.740607  | -1.229475 |
| N    | 5.809893  | 3.200184  | -0.349551 |
| H    | 4.086561  | 2.051528  | 0.910531  |
| H    | 6.033415  | 2.324417  | 0.103007  |
| O    | 6.374217  | 4.663831  | -1.993855 |
| C    | 10.671971 | 2.194390  | -1.429428 |
| C    | 10.135385 | 2.937726  | -2.479027 |
| C    | 8.843544  | 3.438174  | -2.389859 |
| C    | 8.072506  | 3.184499  | -1.250194 |
| C    | 8.619528  | 2.448789  | -0.191423 |
| C    | 9.915602  | 1.956403  | -0.283731 |
| H    | 11.682004 | 1.808788  | -1.498923 |
| H    | 10.726169 | 3.131215  | -3.365735 |
| H    | 8.413686  | 4.027718  | -3.186777 |
| H    | 8.063624  | 2.290630  | 0.725465  |
| H    | 10.339167 | 1.398016  | 0.541842  |
| H    | 2.100762  | 3.736937  | -1.778110 |
| Pt   | 4.407513  | 5.469810  | -1.521203 |
| Cl   | 2.368319  | 6.351756  | -0.759576 |
| Cl   | 4.748237  | 7.407191  | -2.760003 |
| C    | 2.192729  | 2.815639  | 0.120418  |
| C    | 1.425202  | 2.237817  | 1.144799  |
| C    | 0.040139  | 2.264647  | 1.077928  |
| C    | -0.588417 | 2.846479  | -0.023382 |
| C    | 0.168111  | 3.399048  | -1.055232 |
| C    | 1.551817  | 3.386041  | -0.988519 |
| C    | 3.636564  | 2.737747  | 0.209544  |
| H    | 1.917624  | 1.782555  | 1.997309  |
| H    | -0.549396 | 1.832503  | 1.877077  |
| H    | -1.670412 | 2.864062  | -0.078571 |
| H    | -0.319631 | 3.851363  | -1.909172 |
| N    | 4.455602  | 3.496226  | -0.429659 |
| C    | 6.682830  | 3.689566  | -1.254800 |
| N    | 5.797471  | 3.135188  | -0.379230 |
| H    | 4.046551  | 1.943385  | 0.838279  |
| H    | 6.025876  | 2.255222  | 0.063475  |
| O    | 6.350311  | 4.608018  | -2.021882 |
| C    | 10.677799 | 2.196939  | -1.415525 |
| C    | 10.134039 | 2.912039  | -2.480883 |
| C    | 8.834293  | 3.394200  | -2.405713 |
| C    | 8.062752  | 3.150513  | -1.264397 |
| Atom | x    | y    | z    | Cartesian Coordinates |
|------|------|------|------|-----------------------|
| C    | 8.616665 | 2.443674 | -0.189626 |
| C    | 9.920598 | 1.969706 | -0.268189 |
| H    | 11.693703 | 1.825722 | -1.474136 |
| H    | 10.725214 | 3.098545 | -3.368833 |
| H    | 8.399000 | 3.964945 | -3.215436 |
| H    | 8.060024 | 2.296232 | 0.728476 |
| H    | 10.349479 | 1.434274 | 0.569694 |
| H    | 2.141648 | 3.823293 | -1.780089 |
| Pt   | 4.380288 | 5.424555 | -1.494349 |
| Cl   | 2.444458 | 6.380332 | -0.549948 |
| Cl   | 4.723191 | 7.404409 | -2.667664 |
| H2   | 6.667073 | 5.946283 | 0.892374 |
| H2   | 6.096279 | 6.115797 | 0.441423 |
| H2   | 4.380314 | 3.411742 | -3.266342 |
| H2   | 4.272400 | 2.720704 | -3.526298 |
| H2   | 1.969969 | 5.326161 | -3.924294 |
| H2   | 2.365106 | 5.700970 | -3.412843 |
| C    | 2.179413 | 2.768464 | 0.093409 |
| C    | 1.410279 | 2.143421 | 1.088434 |
| C    | 0.025164 | 2.176924 | 1.022787 |
| C    | -0.601615 | 2.813430 | -0.048814 |
| C    | 0.156664 | 3.414445 | -1.052029 |
| C    | 1.540137 | 3.393254 | -0.986470 |
| C    | 3.623098 | 2.687886 | 0.182412 |
| H    | 1.901420 | 1.646643 | 1.918195 |
| H    | -0.566652 | 1.707825 | 1.799822 |
| H    | -1.683535 | 2.837728 | -0.102333 |
| H    | -0.329559 | 3.911146 | -1.881849 |
| N    | 4.442425 | 3.464228 | -0.432860 |
| H    | 6.662265 | 3.666142 | -1.266824 |
| N    | 5.788415 | 3.122119 | -0.371670 |
| H    | 4.032045 | 1.877465 | 0.790332 |
| H    | 6.026091 | 2.246224 | 0.075128 |
| O    | 6.313312 | 4.563093 | -2.052417 |
| C    | 10.677409 | 2.228847 | -1.406551 |
| C    | 10.123716 | 2.916176 | -2.482777 |
| C    | 8.816850 | 3.383101 | -2.415443 |
| C    | 8.048543 | 3.145795 | -1.270513 |
| C    | 8.612339 | 2.463440 | -0.184952 |
| C    | 9.922760 | 2.006896 | -0.256483 |
| H    | 11.698924 | 1.872193 | -1.459054 |
| H    | 10.712767 | 3.102148 | -3.372970 |
| H    | 8.374230 | 3.935974 | -3.233507 |
| H    | 8.057765 | 2.322291 | 0.735315 |
| H    | 10.359248 | 1.490967 | 0.589678 |
| H    | 2.131387 | 3.869448 | -1.754029 |
| Pt   | 4.372636 | 5.405244 | -1.496552 |
| Cl   | 2.460753 | 6.378105 | -0.483668 |
| Cl   | 4.719601 | 7.388825 | -2.64216 |
| H2   | 7.137070 | 6.563334 | 0.137700 |
| H2   | 6.585787 | 6.628448 | -0.360848 |
| H2   | 4.319391 | 3.406033 | -3.270867 |
| H2   | 4.185668 | 2.717829 | -3.526350 |
### Structure descriptions

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H2   | 1.882137| 5.400608| -3.876006|
| H2   | 2.312690| 5.749407| -3.375264|
| H2   | 4.974590| 5.338824| 2.030102 |
| H2   | 4.569035| 5.560604| 1.444736 |
| C    | 2.182022| 2.797702| 0.110092 |
| C    | 1.427489| 2.193746| 1.129629 |
| C    | 0.041908| 2.209195| 1.075324 |
| C    | -0.601424| 2.805752| -0.009422|
| C    | 0.141684| 3.383302| -1.037011|
| C    | 1.526363| 3.382922| -0.982221|
| C    | 3.626916| 2.724159| 0.185291 |
| H    | 1.931228| 1.724190| 1.967658 |
| H    | -0.536627| 1.755581| 1.870628 |
| H    | -1.683875| 2.812017| -0.056466|
| H    | -0.358076| 3.844502| -1.879170|
| N    | 4.445328| 3.501429| -0.432976|
| C    | 6.675723| 3.690484| -1.257822|
| N    | 5.784563| 3.126514| -0.394254|
| H    | 4.041050| 1.910694| 0.786996 |
| H    | 6.005187| 2.236089| 0.029825 |
| U    | 6.351685| 4.630840| -2.001779|
| C    | 10.649563| 2.147661| -1.476523|
| C    | 10.12172| 2.923301| -2.506741|
| C    | 8.828930| 3.421653| -2.412303|
| C    | 8.048735| 3.134584| -1.286791|
| C    | 8.588071| 2.367045| -0.246687|
| C    | 9.884243| 1.876119| -0.344323|
| H    | 11.659595| 1.763081| -1.550270|
| H    | 10.718624| 3.143426| -3.382796|
| H    | 8.405843| 4.035993| -3.195935|
| H    | 8.025894| 2.180967| 0.661146 |
| H    | 10.300877| 1.292530| 0.467264 |
| H    | 2.105147| 3.834086| -1.773876|
| Pt   | 4.397907| 5.456847| -1.467112|
| C1   | 2.421974| 6.379534| -0.592928|
| C1   | 4.761289| 7.441684| -2.618971|
| H2   | 4.418123| 3.356478| -3.182198|
| H2   | 4.352952| 2.666946| -3.459716|

### PIP

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C1   | 4.767647| -1.181820| 1.379681|
| H    | 0.369991| -0.748809| -0.243766|
| H2   | 3.301057| 2.260913| 2.205096|
| H2   | 3.399713| 1.538086| 2.049594|
| C    | 1.500247| 2.219082| -0.763413|
| C    | 1.061639| 3.549081| -0.657693|
| C    | -0.230739| 3.860142| -0.263075|
| C    | -1.129009| 2.832499| 0.013774|
| C    | -0.739965| 1.505494| -0.131037|
| C    | 0.553755| 1.204520| -0.526656|
| C    | 2.916260| 2.013083| -1.077993|
| H    | 1.768588| 4.345516| -0.859036|
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| H    | -0.534320 | 4.894298 | -0.166138 |
| H    | -2.138950 | 3.059773 | 0.331501 |
| H    | -1.441759 | 0.700856 | 0.054433 |
| N    | 7.705555  | 1.057843 | -1.887588 |
| C    | 7.157555  | 2.180957 | -1.273986 |
| C    | 5.823130  | 2.182233 | -0.879671 |
| C    | 5.042120  | 1.049619 | -1.105107 |
| C    | 5.596359  | -0.092604 | -1.680313 |
| C    | 6.922969  | -0.079367 | -2.085469 |
| H    | 8.746079  | 1.059006 | -2.188615 |
| H    | 7.771638  | 3.053492 | -1.086947 |
| H    | 5.402355  | 3.038081 | -0.366500 |
| H    | 4.984434  | -0.980829 | -1.766241 |
| H    | 7.353047  | -0.965013 | -2.536387 |
| H    | 3.380669  | 2.830250 | -1.628407 |
| O    | 0.915874  | -0.111742 | -0.757936 |
| Pt   | 2.790857  | -0.627631 | 0.260706 |
| Cl   | 1.460425  | -2.304723 | 1.275049 |
| Cl   | 4.768843  | -1.216169 | 1.344919 |
| H    | 0.383666  | -0.753973 | -0.269820 |
| C    | 1.502879  | 2.225645 | -0.728477 |
| C    | 1.061650  | 3.551809 | -0.588831 |
| C    | -0.231374 | 3.850236 | -0.186539 |
| C    | -1.126748 | 2.814082 | 0.066885 |
| C    | -0.734599 | 1.491734 | -0.109352 |
| C    | 0.558983  | 1.203343 | -0.514870 |
| C    | 2.919176  | 2.032388 | -1.053132 |
| H    | 1.766703  | 4.354445 | -0.771551 |
| H    | 0.537363  | 4.881010 | -0.064385 |
| H    | -2.136987 | 3.031332 | 0.390464 |
| H    | -1.434175 | 0.681210 | 0.057498 |
| N    | 3.667492  | 1.034074 | -0.744884 |
| C    | 7.724262  | 1.131467 | -1.842285 |
| C    | 7.158040  | 2.238416 | -1.215795 |
| C    | 5.819766  | 2.218430 | -0.836219 |
| C    | 5.051907  | 1.082094 | -1.088956 |
| C    | 5.625233  | -0.045009 | 1.674966 |
| C    | 6.955822  | -0.010306 | -2.063666 |
| H    | 8.767554  | 1.148484 | -2.132918 |
| H    | 7.760504  | 3.114268 | -1.007660 |
| H    | 5.385908  | 3.062382 | -0.313986 |
| H    | 5.025026  | -0.938492 | -1.783884 |
| H    | 7.400004  | -0.883862 | -2.527063 |
| H    | 3.381826  | 2.869116 | -1.575947 |
| O    | 0.923441  | -0.106183 | -0.778196 |
| Pt   | 2.798713  | -0.638416 | 0.233792 |
| Cl   | 1.465754  | -2.320935 | 1.222312 |
| H2   | 3.834514  | -3.544786 | -1.414751 |
| H2   | 3.612387  | -3.163074 | -0.813359 |
| H2   | 3.041263  | 2.221314 | 2.232052 |
| H2   | 3.125391  | 1.497794 | 2.070714 |
C 1.504221 2.218275 -0.755995
C 1.059550 3.542876 -0.618733
C -0.234001 3.837363 -0.214900
C -1.126593 2.798819 0.038387
C -0.730919 1.477579 -0.137968
C 0.563540 1.193420 -0.542769
C 2.920911 2.022850 -1.076641
H 1.762308 4.347547 -0.801231
H -0.542863 4.867230 -0.092164
H -2.136948 3.013352 0.363356
H -1.428194 0.665237 0.030249
N 3.667597 1.029729 -0.750807
C 7.709512 1.035824 -1.900440
C 7.167514 2.171883 -1.305076
C 5.834195 2.185830 -0.907998
C 5.047743 1.052810 -1.112102
C 5.596226 -0.102161 -1.667209
C 6.922057 -0.101680 -2.075421
H 8.749307 1.027149 -2.203673
H 7.785607 3.045009 -1.134589
H 5.419225 3.053307 -0.409631
H 4.980863 -0.989496 -1.736098
H 7.347425 -0.996914 -2.511626
H 3.380720 2.843159 -1.626678
O 0.934578 -0.115908 -0.802059
Pt 2.796459 -0.621671 0.256523
Cl 1.462484 -2.308657 1.258286
Cl 4.755913 -1.150041 1.418975
H 0.378746 -0.763281 -0.313767
H2 3.834984 -3.710477 -1.016329
H2 3.711576 -3.266179 -0.429898
H2 3.061423 2.282991 2.213496
H2 3.154339 1.555175 2.078000
C 1.501649 2.167536 -0.779419
C 1.093346 3.510792 -0.736890
C -0.165108 3.876309 -0.283990
C -1.061485 2.890539 0.120946
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H 1.799125 4.276749 -1.036585
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H -1.408839 0.773643 0.324164
N 3.643591 0.933280 -0.824223
C 7.636000 0.823058 -2.138887
C 7.111662 2.014233 -1.643830
C 5.796074 2.066283 -1.195580
C 5.005784 0.917689 -1.248101
C 5.540503 -0.288001 -1.699960
C 6.848907 -0.327450 -2.159371
H 8.662647 0.784417 -2.481801
H 7.730939 2.901339 -1.589238
| Atoms | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| H     | 5.400210  | 2.980273  | -0.770018 |
| H     | 4.930728  | -1.179771 | -1.655455 |
| H     | 7.261199  | -1.263296 | -2.515460 |
| H     | 3.331627  | 2.693003  | -1.792672 |
| O     | 0.871933  | -0.143941 | -0.577667 |
| Pt    | 2.809048  | -0.629976 | 0.342725  |
| Cl    | 1.511384  | -2.196597 | 1.564146  |
| Cl    | 4.822108  | -1.114771 | 1.441766  |
| H     | 0.353390  | -0.728849 | 0.020897  |
| H2    | 2.433095  | -1.094971 | -3.232172 |
| H2    | 2.420856  | -0.990186 | -2.495565 |
| H2    | 3.860294  | -3.641651 | -1.033726 |
| H2    | 3.700817  | -3.206684 | -0.448907 |
| H2    | 1.105307  | 1.163946  | 2.650044  |
| H2    | 1.441604  | 0.522848  | 2.469064  |
| C     | 1.515547  | 2.192926  | -0.773114 |
| C     | 1.108182  | 3.536429  | -0.732342 |
| C     | -0.157798 | 3.902241  | -0.302602 |
| C     | -1.062852 | 2.916506  | 0.083294  |
| C     | -0.705290 | 1.575327  | 0.013225  |
| C     | 0.561935  | 1.220405  | -0.421111 |
| C     | 2.900865  | 1.939881  | -1.178908 |
| H     | 1.816893  | 4.302606  | -1.024680 |
| H     | -0.434888 | 4.947326  | -0.260732 |
| H     | -2.053121 | 3.187206  | 0.427790  |
| H     | -1.411127 | 0.799295  | 0.284197  |
| N     | 3.653606  | 0.958882  | -0.830396 |
| C     | 7.625585  | 0.747576  | -2.191717 |
| C     | 7.116181  | 1.969419  | -1.759099 |
| C     | 5.807201  | 2.057218  | -1.297776 |
| C     | 5.008138  | 0.912763  | -1.272497 |
| C     | 5.529898  | -0.320973 | -1.659741 |
| C     | 6.830834  | -0.296106 | -2.135243 |
| H     | 8.647208  | 0.681558  | -2.545863 |
| H     | 7.742275  | 2.853398  | -1.763769 |
| H     | 5.426248  | 2.996900  | -0.917454 |
| H     | 4.914141  | -1.203740 | -1.562045 |
| H     | 7.231643  | -1.353718 | -2.443091 |
| H     | 3.333320  | 2.703986  | -1.823168 |
| O     | 0.886367  | -0.116901 | -0.572136 |
| Pt    | 2.822400  | -0.609096 | 0.356804  |
| Cl    | 1.518007  | -2.210711 | 1.538399  |
| Cl    | 4.822433  | -1.105044 | 1.478130  |
| H     | 0.362866  | -0.699769 | 0.023432  |
| H2    | 2.489513  | -1.151743 | -3.144818 |
| H2    | 2.419771  | -1.132901 | -2.404171 |
| H2    | 3.889102  | 2.406094  | 1.927269  |
| H2    | 3.999330  | 1.669971  | 1.884680  |

PIA

| H2    | 1.383669  | -2.712928 | -0.076083 |
| H2    | 1.501059  | -3.084059 | 0.560181  |
| Element | X  | Y  | Z  |
|---------|----|----|----|
| H2      | 0.244755 | 1.957696 | -4.128856 |
| H2      | 0.535889  | 1.427045  | -3.693237  |
| H2      | 3.382247  | 1.058269  | -4.596362  |
| H2      | 3.196932  | 0.466414  | -4.181777  |
| C       | 1.506273  | 2.393983  | -0.632972  |
| C       | 0.992655  | 3.586918  | -0.134337  |
| C       | -0.379569 | 3.698305  | 0.061246   |
| C       | -1.194598 | 2.614971  | -0.244433  |
| C       | -0.618900 | 1.452295  | -0.748693  |
| N       | 0.696271  | 1.349699  | -0.937779  |
| C       | 2.932105  | 2.180653  | -0.827147  |
| H       | 1.663102  | 4.405209  | 0.093018   |
| H       | -0.804189 | 4.615588  | 0.448698   |
| H       | -2.266035 | 2.658988  | -0.100750  |
| H       | -1.192801 | 0.574068  | -1.020511  |
| N       | 3.369664  | 1.050408  | -1.260580  |
| C       | 7.487142  | 0.439015  | -1.764015  |
| C       | 6.909900  | 1.621776  | -2.223182  |
| C       | 5.545986  | 1.835895  | -2.069354  |
| C       | 4.759854  | 0.856034  | -1.455751  |
| C       | 5.325481  | -0.347653 | -1.032287  |
| C       | 6.693439  | -0.541070 | -1.171261  |
| H       | 8.550522  | 0.273333  | -1.888421  |
| H       | 7.519130  | 2.371120  | -2.713787  |
| H       | 5.084929  | 2.734455  | -2.460818  |
| H       | 4.686504  | -1.112983 | -0.616696  |
| H       | 7.136566  | -1.469948 | -0.834630  |
| H       | 3.619212  | 2.981031  | -0.563916  |
| Pt      | 1.762196  | -0.300069 | -1.773374  |
| Cl      | 3.076559  | -2.022198 | -2.707340  |
| Cl      | -0.214877 | -1.501794 | -2.290853  |
| H2      | 2.072112  | 0.041446  | 1.123808   |
| H2      | 2.168509  | 0.176855  | 1.849982   |
| H2      | 0.660957  | 2.309048  | -3.887129  |
| H2      | 0.834496  | 1.642540  | -3.601679  |
| H2      | 3.477256  | 1.036343  | -4.584539  |
| H2      | 3.319685  | 0.399715  | -4.229157  |
| C       | 1.418715  | 2.328593  | -0.594152  |
| C       | 0.855849  | 3.485142  | -0.063946  |
| C       | -0.519155 | 3.532523  | 0.137822   |
| C       | -1.288811 | 2.422599  | -0.193209  |
| C       | -0.661475 | 1.297419  | -0.723107  |
| N       | 0.655886  | 1.255688  | -0.916662  |
| C       | 2.850278  | 2.192810  | -0.813695  |
| H       | 1.490301  | 4.326614  | 0.181001   |
| H       | -0.981500 | 4.421049  | 0.547793   |
| H       | -2.359214 | 2.415845  | -0.050263  |
| H       | -1.199092 | 0.401836  | -1.011945  |
| N       | 3.337823  | 1.103636  | -1.295112  |
| C       | 7.476502  | 0.718499  | -1.847406  |
| C       | 6.838051  | 1.887152  | -2.259668  |
| C       | 5.466432  | 2.027508  | -2.090296  |
| C       | 4.734257  | 0.988025  | -1.508469  |
Structure descriptions

C 5.362248 -0.198109 -1.127426
C 6.737036 -0.319215 -1.283574
H 8.545730 0.609588 -1.984906
H 7.405220 2.682709 -2.727338
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H 4.767196 -1.007269 -0.730610
H 7.227919 -1.235877 -0.981360
H 3.499380 3.017672 -0.531065
Pt 1.793589 -0.383895 -1.774664
Cl 3.160821 -2.007900 -2.723174
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H2 1.966631 -0.311545 1.006073
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H 1.486981 4.344015 0.145758
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C 7.468772 0.708329 -1.841314
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C 6.732716 -0.303769 -1.277577
H 8.538174 0.596749 -1.974323
H 7.392097 2.629515 -2.810308
H 4.942462 2.868527 -2.538875
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H2 0.821810 2.485482 -3.805663
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C 2.972721 2.209347 -0.265375
H 1.603212 4.379872 0.635656
| Atom | X     | Y     | Z     | R     |
|------|-------|-------|-------|-------|
| H    | -0.879753 | 4.510889 | 0.910617 |
| H    | -2.258424 | 2.508638 | 0.307880 |
| H    | -1.087559 | 0.455541 | -0.560122 |
| N    | 3.462285  | 1.103247 | -0.705552 |
| C    | 7.612471  | 0.682162 | -1.131461 |
| C    | 6.984690  | 1.818205 | -1.638746 |
| C    | 5.609089  | 1.969373 | -1.510807 |
| C    | 4.863279  | 0.970862 | -0.877816 |
| C    | 5.481615  | -0.185489 | -0.400069 |
| C    | 6.859233  | -0.314738 | -0.513596 |
| H    | 8.684771  | 0.566351 | -1.234141 |
| H    | 7.563677  | 2.581492 | -2.144317 |
| H    | 5.109993  | 2.832517 | -1.934671 |
| H    | 4.872023  | -0.962191 | 0.038071 |
| H    | 7.342898  | -1.207055 | -0.136181 |
| H    | 3.620262  | 3.038391  | 0.012885 |
| Pt   | 1.924052  | -0.343341 | -1.176246 |
| Cl   | 3.330735  | -2.022032 | -2.028590 |
| Cl   | 0.025931  | -1.685713 | -1.576839 |

| H2   | 1.658103  | 2.485495 | -3.802000 |
| H2   | 1.604537  | 1.751700 | -3.681455 |
| C    | 1.435697  | 2.344856 | -0.627504 |
| C    | 0.881218  | 3.510993 | -0.108026 |
| C    | -0.496421 | 3.580442 | 0.066949 |
| C    | -1.275160 | 2.482624 | -0.278884 |
| C    | -0.658141 | 1.344756 | -0.791123 |
| N    | 0.662782  | 1.281069 | -0.968717 |
| C    | 2.867968  | 2.188650 | -0.832253 |
| H    | 1.524695  | 4.342445 | 0.147863 |
| H    | -0.952667 | 4.476631 | 0.468026 |
| H    | -2.350261 | 2.494782 | -0.157353 |
| H    | -1.202377 | 0.454605 | -1.084048 |
| N    | 3.344502  | 1.091018 | -1.305235 |
| C    | 7.484268  | 0.674918 | -1.825091 |
| C    | 6.845523  | 1.815495 | -2.307906 |
| C    | 5.472876  | 1.965640 | -2.148663 |
| C    | 4.741558  | 0.960668 | -1.509658 |
| C    | 5.369974  | -0.199381 | -1.855148 |
| C    | 6.744692  | -0.327682 | -1.199725 |
| H    | 8.553944  | 0.560059 | -1.952739 |
| H    | 7.413205  | 2.583140 | -2.819671 |
| H    | 4.963321  | 2.831533 | -2.553922 |
| H    | 4.769607  | -0.979978 | -0.610897 |
| H    | 7.236361  | -1.223263 | -0.840748 |
| H    | 3.525476  | 3.006505 | -0.546503 |
| Pt   | 1.794563  | -0.344251 | -1.762252 |
| Cl   | 3.180294  | -2.010353 | -2.668665 |
| Cl   | -0.111570 | -1.679233 | -2.143152 |

| H2   | 1.614307  | 2.431458 | -3.823061 |
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| H2   | 2.015649  | -0.240690 | 1.028885 |
### Structure descriptions

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H 4.782160 -1.000466 -0.697430
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#### BPY

H2 -3.083740 -0.257835 0.645608
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C -0.307048 2.657346 0.812018
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| H2   | 3.161620  | -1.565364 | 0.165599 |
| H2   | 2.629981  | -1.416336 | -0.335671 |
| H2   | 2.947264  | 1.907348  | 0.232031 |
| H2   | 2.434434  | 1.685908  | -0.261943 |
| H2   | -2.954952 | -1.804453 | -0.510344 |
| H2   | -2.325517 | -1.590780 | -0.848654 |
| H2   | -3.108976 | 1.609047  | -0.526550 |
| H2   | -2.437140 | 1.430766  | -0.796770 |
| Cl   | 0.163541  | 1.735238  | -2.347422 |
| C    | -0.198261 | 0.732519  | 2.129527 |
| C    | -0.319583 | 1.491982  | 3.291432 |
| C    | -0.355690 | 2.877448  | 3.204903 |
| C    | -0.269387 | 3.481902  | 1.957179 |
| C    | -0.148852 | 2.676399  | 0.834822 |
| H    | -0.385891 | 1.010969  | 4.256015 |
| H    | -0.450134 | 3.474581  | 4.103450 |
| H    | -0.294005 | 4.557543  | 1.845200 |
| H    | -0.074914 | 3.067813  | -0.173319 |
| N    | -0.114600 | 1.343545  | 0.923701 |
| Pt   | 0.069947  | 0.010724  | -0.723553 |
| Cl   | 0.264730  | -1.692680 | -2.360883 |
| N    | -0.036777 | -1.345094 | 0.913971 |
| C    | -0.155101 | -0.748709 | 2.124064 |
| C    | 0.005523  | -2.677152 | 0.814864 |
| C    | -0.231019 | -1.522333 | 3.280666 |
| C    | -0.066334 | -3.495962 | 1.931805 |
| H    | 0.100597  | -3.056045 | -0.196230 |
| C    | -0.185825 | -2.906552 | 3.184005 |
| H    | -0.324561 | -1.052492 | 4.248513 |
| H    | -0.028697 | -4.570380 | 1.811806 |
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| H2   | 3.127359  | -1.630204 | 0.034967 |
| H2   | 2.524207  | -1.440323 | -0.360471 |
| H2   | 3.009269  | 1.826139  | 0.049351 |
| H2   | 2.438721  | 1.613999  | -0.381591 |
| Cl   | 0.079033  | 1.699406  | -2.392621 |
| C    | -0.146454 | 0.730748  | 2.118197 |
| C    | -0.240917 | 1.496145  | 3.278931 |
| C    | -0.256059 | 2.881844  | 3.185785 |
| C    | -0.177454 | 3.479730  | 1.934353 |
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| H    | -0.299921 | 1.020210  | 4.246790 |
| H    | -0.328633 | 3.484239  | 4.082354 |
| H    | -0.182596 | 4.554959  | 1.816370 |
| H    | -0.027302 | 3.056572  | -0.197109 |
| N    | -0.076237 | 1.335598  | 0.907147 |
| Pt   | 0.043295  | 0.004300  | -0.750720 |
| Cl   | 0.165371  | -1.677193 | -2.402396 |
| N    | -0.006519 | -1.344049 | 0.899822 |
| C    | 0.105640  | -0.750528 | 2.114291 |
| C    | 0.053029  | 2.674406  | 0.797506 |

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Structure descriptions

C  -0.154543  -1.526097   3.271093
C   0.011985  -3.495979   1.914972
H   0.132664  -3.053080  -0.214724
C  -0.094836  -2.910023   3.169990
H  -0.235441  -1.059328   4.241815
H   0.063560  -4.569302   1.790789
H  -0.131726  -3.520648   4.063180
H2   2.940773   0.090335   1.240267
H2   2.501199   0.077256   0.637763

Cl  0.044643   1.689614  -2.392980
C  -0.118909   0.722991   2.120681
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C  -0.241182   2.871646   3.191624
C  -0.207860   3.471035   1.938977
C  -0.130894   1.093360   4.251871
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H  -0.247855   4.546075   1.822542
H  -0.101014   3.050135  -0.195602
N  -0.087631   1.329029   0.909264
Pt  0.031631  -0.004995  -0.748949
Cl  0.164260  -1.684839  -2.402769
N   0.007426  -1.353199   0.902131
C  -0.065732  -0.757368   2.117135
C   0.061249  -2.684060   0.801540
C  -0.086337  -1.530255   3.276021
C   0.044356  -3.503417   1.921043
H   0.118341  -3.065028  -0.211483
C  -0.030799  -2.914464   3.179151
H  -0.144460  -1.060979   4.246900
H   0.089430  -4.577425   1.799195
H  -0.046120  -3.522893   4.072099
H2   2.942345   0.099269   1.122873
H2   2.515187   0.096021   0.512151
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Cl  0.000000   1.692865  -2.405060
C  0.000000   0.740947   2.113732
C  0.000000   1.512400   3.274379
C  0.000000   2.897879   3.175399
C  0.000000   3.489257   1.913331
C  0.000000   2.671653   0.796991
H  0.000000   1.041699   4.246805
H  0.000000   3.505092   4.071886
H  0.000000   4.569370   1.794850
H  0.000000   3.055225  -0.216593
N  0.000000   1.339641   0.897318
Pt  0.000000   0.000000  -0.756889
Cl  0.000000  -1.692865  -2.405060
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C  0.000000  -0.740947   2.113732
C  0.000000  -2.671653   0.796991

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| C | 0.000000 | -1.512400 | 3.274379 |
| C | 0.000000 | -3.489257 | 1.918331 |
| H | 0.000000 | -3.055225 | -0.216593 |
| C | 0.000000 | -2.897879 | 3.175399 |
| H | 0.000000 | -1.041699 | 4.246805 |
| H | 0.000000 | -4.563970 | 1.794850 |
| H | 0.000000 | -3.505092 | 4.071886 |

**PHEN**

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| C | 0.670646 | 2.321386 | 1.463718 |
| C | 1.331679 | 3.553600 | 1.282937 |
| C | 2.741724 | 3.540961 | 1.304685 |
| C | 3.407017 | 2.351411 | 1.498143 |
| C | 2.675303 | 1.166603 | 1.670756 |
| H | 3.287663 | 4.466894 | 1.169264 |
| H | 4.487969 | 2.308126 | 1.520373 |
| H | 3.144971 | 0.20371 | 1.826288 |
| N | 1.351847 | 1.157431 | 1.652876 |
| Pt | 0.049089 | -0.515901 | 1.891604 |
| N | -1.364282 | 1.061068 | 1.629531 |
| C | -0.764048 | 2.270401 | 1.451722 |
| C | -2.685168 | 0.976239 | 1.624968 |
| C | -1.507710 | 3.452831 | 1.259706 |
| C | -3.496168 | 2.106402 | 1.440448 |
| H | -3.087733 | -0.019013 | 1.773064 |
| C | -2.913464 | 3.340244 | 1.258462 |
| H | -4.571596 | 1.986859 | 1.445068 |
| H | -3.521534 | 4.225308 | 1.114800 |
| C | 0.549487 | 4.739010 | 1.089042 |
| C | -0.808524 | 4.690803 | 1.078271 |
| Cl | 1.805835 | -2.068342 | 2.155010 |
| Cl | -1.599029 | -2.187531 | 2.127238 |
| H | -1.387522 | 5.594501 | 0.931260 |
| H | 1.066378 | 5.681493 | 0.950528 |

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| H2 | 1.785172 | -2.048378 | -2.234971 |
| H2 | 2.508628 | -1.882906 | -2.306078 |
| H2 | 1.988247 | -3.160311 | 1.013594 |
| H2 | 1.328757 | -3.170720 | 0.666240 |
| H | 1.407695 | 2.981367 | 2.723832 |
| H | 1.778030 | 3.868859 | 0.464393 |
| C | 0.187137 | 0.335703 | 0.930051 |
| C | 0.550691 | 1.103909 | 2.054917 |
| C | 0.312434 | 0.542967 | 3.326670 |
| C | -0.254375 | -0.707603 | 3.422046 |
| C | -0.587181 | -1.408777 | 2.253879 |
| H | 0.577738 | 1.101947 | 4.215968 |
| H | -0.447420 | -1.166035 | 4.382968 |
| H | -1.029370 | -2.398173 | 2.267442 |
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| Pt | -0.788343 | -1.785597 | -0.843177 |
| N | 0.037010 | 0.083893 | -1.451557 |
| C | 0.403749 | 0.854430 | -0.390843 |
Structure descriptions

C  0.223428  0.529843 -2.683518
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H  0.921389  2.110403 -3.959165
H  1.605762  3.563224 -2.050743
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H2  1.313978 -3.210133  0.678055
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H  1.788980  3.856504  0.470396
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C  0.560351  1.091985  2.059526
C  0.317434  0.533830  3.31355
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C  1.152509  2.381352  1.857977
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H2  2.483645 -1.894749 -2.382941
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C  0.668746  2.327882  1.474554
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C  3.405963  2.351822  1.470352
C  2.674203  1.166094  1.634802
H  3.286234  4.472593  1.180705
H  4.487091  2.307715  1.474598
H  3.142765  0.198277  1.770611
N  1.350392  1.160448  1.637396
Pt  0.045749 -0.510715  1.882972
Structure descriptions

| Atoms | X     | Y     | Z     |
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| N     | -1.367675 | 1.067053 | 1.621170 |
| C     | -0.766832 | 2.278553 | 1.466607 |
| C     | -2.688515 | 0.981810 | 1.603537 |
| C     | -1.508223 | 3.464062 | 1.290290 |
| C     | -3.498328 | 2.114748 | 1.431825 |
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| C     | -2.914042 | 3.351338 | 1.277478 |
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| H     | -3.520523 | 4.239243 | 1.145153 |
| C     | 0.548938 | 4.751565 | 1.136851 |
| C     | -0.809065 | 4.704851 | 1.129939 |
| Cl    | 1.797665 | -2.062109 | 2.158538 |
| Cl    | -1.601072 | -2.177789 | 2.132045 |
| H2    | -0.032225 | 0.769131 | -1.341745 |
| H2    | -0.004882 | 0.291953 | -0.768625 |
| H     | -1.388800 | 5.610497 | 0.999394 |
| H     | 1.066560 | 5.694868 | 1.011699 |
| H2    | -3.211149 | -1.259066 | 0.694816 |
| H2    | -3.738548 | -0.861927 | 1.041735 |
| H2    | 1.933766 | -3.331315 | 0.962393 |
| H2    | 1.271162 | -3.226615 | 0.636589 |
| H2    | -2.723690 | -0.091790 | -2.218196 |
| H2    | -3.173587 | 0.493597 | -2.323732 |
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| C     | 0.542680 | 1.102754 | 2.052037 |
| C     | 0.305822 | 0.543153 | 3.324535 |
| C     | -0.256202 | -0.709069 | 3.422770 |
| C     | -0.585594 | -1.413372 | 2.255602 |
| H     | 0.568916 | 1.105580 | 4.212701 |
| H     | -0.449957 | -1.164181 | 4.385063 |
| H     | -1.029518 | -2.402787 | 2.269352 |
| N     | -0.370700 | -0.904905 | 1.052202 |
| Pt    | -0.785050 | -1.783060 | -0.841757 |
| N     | 0.042907 | 0.079284 | -1.456004 |
| C     | 0.401409 | 0.850165 | -0.393431 |
| C     | 0.230066 | 0.526135 | -2.688143 |
| C     | 0.974316 | 2.127455 | -0.560208 |
| C     | 0.794212 | 1.785682 | -2.937243 |
| H     | -0.082145 | -0.147140 | -3.478947 |
| C     | 1.165376 | 2.584913 | -1.880350 |
| H     | 0.928417 | 2.109634 | -3.960821 |
| H     | 1.602952 | 3.561911 | -2.048941 |
| C     | 1.122767 | 2.397357 | 1.851110 |
| C     | 1.329198 | 2.887560 | 0.601283 |
| Cl    | -1.658223 | -3.770947 | 0.110437 |
| Cl    | -1.145253 | -2.520205 | -3.066028 |
| H2    | 2.464114 | -2.048201 | -2.417721 |
| H2    | 1.731874 | -2.105449 | -2.288412 |
| H     | 1.768510 | 3.867669 | 0.461019 |
| H     | 1.395013 | 2.980731 | 2.722213 |
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