Magnetic Exchange Interactions in Binuclear and Tetranuclear Iron(III) Complexes Described by Spin-Flip DFT and Heisenberg Effective Hamiltonians: Supplemental Information

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1. MULTIPLE-CENTER MOLECULAR MAGNETS: MAYHALL’S APPROACH

For strongly correlated systems that are well described by the Heisenberg model, Mayhall and Head-Gordon proposed to parameterize the Heisenberg-Dirac-van Vleck (HDvV) Hamiltonian using single spin-flip (1SF) methods in which a single spin-flipping excitation operator from the highest spin state generates a manifold of adjacent spin states\[^1\ 2\]. For systems with two radical centers, the Landé interval rule can be used to obtain the $J$ parameter from a 1SF calculation using energies alone. For systems with multiple radical centers, $J$ parameters can be obtained by fitting of energy levels. However, without considering the wave functions it is difficult to judge whether the fit correctly represents the underlying interactions. Mayhall and Head-Gordon introduced an effective Hamiltonian-based approach to parameterize the HDvV spin Hamiltonian for systems with an arbitrary number of radical centers and unpaired electrons using energies and wave functions from 1SF calculations.

Effective Hamiltonian theory provides an effective tool to parameterize phenomenological models like the HDvV Hamiltonian by mapping states of the \textit{ab initio} electronic Hamiltonian onto the states of the model Hamiltonian. To do so, one computes a set of energies and the corresponding eigenfunctions of the many-body electronic Hamiltonian, which correspond to electronic states whose properties the model is to capture. The effective Hamiltonian is then defined such that the computed electronic states are mapped onto the states of a model Hamiltonian that have the same energies as the full Hamiltonian. Via this connection between the model states and electronic wave functions, matrix elements of the effective Hamiltonian can be interpreted as the interactions between effective local spins.

The HDvV Hamiltonian describes the low-energy part of the spectrum under the assumption that the respective states are dominated by the neutral configurations. For a system with $M$ radical centers, one computes the $M$ lowest energy 1SF excitations starting from the reference state with maximum spin projection $S$ at each site thus an overall spin projection of $S \times M$. By localizing all partially occupied molecular orbitals and transforming the excited-state solution vectors to this local orbital basis, one can verify that the obtained solutions are predominantly neutral and assign each partially occupied orbital to a specific radical site.

If the 1SF states are indeed not ionic, the flipped spin of that state is located at a specific radical site, which can be interpreted as a local $S-1$ spin. Determinants of the partially occupied orbitals at that site $I$ are used to define a local $S-1$ spin function $|\Psi_I^{S-1}\rangle$. If the
$M$ lowest energy SF excitations each result in a local SF at a different radical site, one obtains a local $S - 1$ spin functions at each site. The $|\Psi^{S-1}\rangle$ functions are then used as the basis for representing the effective Hamiltonian. Following the approach of des Cloizeaux$^3$, the local spin functions are orthonormalized to form the orthonormalized spin functions $|\tilde{\Psi}_I^{ON}\rangle$. One then defines the effective Hamiltonian via the spectral representation:

$$\hat{H}^{\text{eff}} = \sum_I |\tilde{\Psi}_I^{ON}\rangle E_I \langle \tilde{\Psi}_I^{ON}|,$$  \hspace{1cm} (1)

where $E_I$ refers to the energy of the single SF excitation that resulted in $(S - 1)$ spin at site $I$. Each of these states thus maps onto one specific vector of model spin states in which all but one site have maximum spin projection $S$ and one site has the projection $(S - 1)$. By this construction, the energy differences between two 1SF excited states result from the coupling between their local spin functions and the off-diagonal matrix elements of the effective Hamiltonian represented in the basis of local spin functions provide the exchange coupling parameters $J_{IJ}$ for the HDvV Hamiltonian.

Fig. S1: Flowchart of the protocol. $H^{HDvV}$ is the Heisenberg-Dirac-van Vleck Hamiltonian and $|\tilde{\Psi}_I^{ON}\rangle$ are the local spin functions.

FIG. S1: Flowchart of the computational protocol we apply to compute $J$ couplings of tetranuclear iron (III) compounds. The first step requires a simple 1SF calculation from the high-spin reference state. The next step is parameterization of the HDvV Hamiltonian, as prescribed by Mayhall and Head-Gordon$^2$; it requires eigenstates and energies, and provides all $J$-values. Mayhall’s approach is implemented as a post-processing Python script (available within the ezMagnet module $^4$). The script reads the raw data from the Q-Chem output (energies and projected eigenvectors) and provides the $J$-values. Therefore, two separate calculations need to be performed: 1) 1SF calculation using Q-Chem and 2) construct the effective Hamiltonian by executing the Python script in which Mayhall’s approach of Ref. $^2$ is implemented. For additional details about Mayhall’s approach, see Refs. $^1$ $^2$ and ezMagnet.
The following example illustrates the assignment of exchange parameters $J_{AB}$ from the effective Hamiltonian for the (Fe)$_4$ YAYPOD complex. The section of the Q-Chem input below contains the keywords used to compute the four lowest energy SF-TDDFT states and request the partially occupied orbitals of the respective eigenvectors to be localized; the molecular geometry is given in Section 5. Any ionic determinants, i.e. those that move charges between radical centers, are projected out and only the neutral determinant coefficients are kept.

$comment
Spin-flip calculation for building effective spin models
$end

$rem
BASIS = 6-31G(d,p)  
CIS_N_ROOTS = 4        [ Sets the number of CI-Singles (CIS) roots ]
EXCHANGE = LRC-wPBEh  
WANG_ZIEGLER_KERNEL = TRUE  [ non-collinear exchange-correlation kernel SF-DFT ]
MEM_TOTAL 230000        [ Sets the total memory in megabyte ]
SCF_MAX_CYCLES = 500    [ the maximum number of SCF iterations permitted ]
MAX_CIS_CYCLES = 150    [ Maximum number of CIS iterative cycles allowed ]
SPIN_FLIP = 1           [ spin flip dft used]  
SCF_CONVERGENCE = 7     [ decreased criterion for convergence ]
SCF_ALGORITHM = diis_gdm
$end

$development
1sf_heis_projection 1   [ Requests eigenvectors projected onto local orbitals ]
$end

The combined weight of the neutral coefficients for each eigenvector is listed, which can be used as an additional check for the assumptions that ionic configurations can be neglected. The weights for our example YAYPOD complex is printed below

\[
\begin{bmatrix}
9.731619E-01 & 9.803481E-01 & 9.845902E-01 & 9.986758E-01 \\
\end{bmatrix}
\]

as well as the energies in Hartrees

\[
\begin{bmatrix}
-4.902195E-03 & -3.549901E-03 & -2.509316E-03 & -1.136423E-03 \\
\end{bmatrix}
\]

and the projected eigenvector coefficients

\[
\begin{bmatrix}
-2.357448E-01 & -1.451038E-01 & 2.445182E-01 & 2.432505E-01 \\
-2.560876E-01 & -1.563791E-01 & 2.499574E-01 & 2.444646E-01 \\
-1.726807E-01 & 2.247644E-01 & -2.558274E-01 & 2.249857E-01 \\
\end{bmatrix}
\]
In addition to the projected vectors, the calculation lists for each of the neutral determinants which radical center the localization procedure has assigned it to. For our example this list reads

```
2 2 3 2 2 0 2 0 1 3 1 3 1 0 0 3 3 1 0 1
```

with labels 0-3 indicating one of the four radical centers. The projected eigenvectors are then sorted according to the radical center and the vectors are orthonormalized to yield the orthonormalized projected eigenvectors $\tilde{b}$. A determinant-wise effective Hamiltonian $\tilde{H}_{\text{det}}^{\text{eff}}$ is constructed
as an intermediate for defining local spin functions. The determinant-wise effective Hamiltonian is defined via the spectral representation

\[ H^{\text{eff}}_{\text{det}} = \sum_i^M \tilde{b}_i E_i \tilde{b}_i^T, \]  

where \( \tilde{b}_i \) are the orthonormalized projected eigenvector and the \( E_i \) are the energies of the excitation localized at radical center \( i \). The resulting effective Hamiltonian matrix then reads

\[
\begin{bmatrix}
-2.001038E-01 & -1.966752E-01 & -1.964967E-01 & -2.021006E-01 & -2.054433E-01 \\
-1.304710E-05 & -7.746025E-04 & -1.062858E-03 & -5.464950E-04 \\
6.060696E-03 & 1.471196E-03 & 2.626110E-03 \\
-4.62224E-03 & -2.15807E-03 & -2.43947E-03 \\
-3.018491E-03 & 1.177874E-03 & -8.698211E-04
\end{bmatrix}
\]
Each of the 5 × 5 sub-block matrices that describe effective interactions within a specific radical site is then diagonalized. Since only one SF excited state is located on each site and the matrix is thus rank deficient each diagonal block only yields one non-zero eigenvalue. The
resulting eigenvectors of this block-diagonalization are a linear combination of local SF excited determinants that can be interpreted a local spin function. Only the local spin functions that correspond to non-zero eigenvalues are kept and all others projected out. The remaining eigenvectors are orthonormalized yet again to restore orthonormality after the projection. The final effective Hamiltonian is then constructed from the spectral representation in the basis of the orthonormalized local spin functions $|\tilde{\Psi}^{ON}_I\rangle$ as defined in equation [1]. The resulting effective Hamiltonian matrix is printed below:

$$
\begin{bmatrix}
-1.001885E+00 & 2.152256E-05 & 6.327713E-04 & 1.040924E-03 \\
2.152256E-05 & -1.002200E+00 & 1.335355E-03 & 6.852854E-04 \\
6.327713E-04 & 1.335355E-03 & -1.001802E+00 & 4.339833E-05 \\
1.040924E-03 & 6.852854E-04 & 4.339833E-05 & -1.001665E+00
\end{bmatrix}
$$

The exchange coupling parameters are then obtained from the off-diagonal matrix element that corresponds to the pair of radical sites via

$$J_{AB} = -\frac{H_{AB}^{\text{off}}}{2\sqrt{S_A S_B}}. \quad (3)$$
2. STRUCTURES OF MONONUCLEAR Fe(III) SYSTEMS

FIG. S2: Model mononuclear Fe (III) systems: [Fe(Cl)$_6$]$^{3-}$ (left), a monomer unit built from ABIZOA complex (center), and [Fe(CN)$_6$]$^{3-}$ (right).
3. NATURAL ORBITALS IN MONONUCLEAR Fe(III) SYSTEMS

FIG. S3: Frontier $\alpha$ and $\beta$ natural orbitals of the lowest hextet (left) and quartet state (right) in [Fe(Cl)$_6$]$^{3-}$ with their occupations.
FIG. S4: Frontier $\alpha$ and $\beta$ natural orbitals of the lowest hextet (left) and quartet state (right) in ABI-m with their occupations.
FIG. S5: Frontier $\alpha$ and $\beta$ natural orbitals of the lowest hextet (left) and quartet state (right) in $\text{[Fe(CN)$_6$]}^{3-}$ with their occupations.
4. NATURAL ORBITALS IN BINUCLEAR Fe(III) SYSTEMS

FIG. S6: Frontier $\alpha$ and $\beta$ natural orbitals of the lowest $S = 4$ state in complex 2 with their occupations.
FIG. S7: Frontier $\alpha$ and $\beta$ natural orbitals of the lowest $S = 4$ state in complex 7 with their occupations.
FIG. S8: Frontier $\alpha$ and $\beta$ natural orbitals of the lowest $S = 4$ state in complex 12 with their occupations.
5. MAGNETO-STRUCTURAL CORRELATIONS

TABLE S1: Structural (from experiments of Refs. [5 20]) and magnetic data of this work (LRC-$\omega$PBEh/6-31G(d,p)) for the 16 complexes under study.

| Complex | $J$ (cm$^{-1}$) | Fe–Fe (Å) | Fe-O-Fe (°) |
|---------|----------------|------------|-------------|
| 1       | -7.1           | 3.34       | 103.8       |
| 2       | -16.6          | 3.17       | 104.4       |
| 3       | -15.7          | 3.09       | 102.7       |
| 4       | -20.4          | 3.20       | 107.3       |
| 5       | -106.8         | 3.45       | 151.6       |
| 6       | -91.9          | 3.45       | 143.7       |
| 7       | -100.7         | 3.62       | 180.0       |
| 8       | -105.4         | 3.20       | 125.5       |
| 9       | -109.8         | 3.11       | 119.8       |
| 10      | -124.7         | 3.15       | 123.6       |
| 11      | -123.1         | 3.11       | 121.4       |
| 12      | -119.4         | 3.15       | 123.9       |
| 13$^a$  | -10.9          | 3.10       | 102.6       |
| 14$^a$  | -11.3          | 3.10       | 102.0       |
| 15$^{a,b}$ | -43.5      | 3.40       | 127.9       |
| 16$^{a,b}$ | -40.6      | 3.40       | 133.2       |

$^a$ Average $J$ values, average Fe–Fe distances, and average Fe-O-Fe bond angles. $^b$ Only dominant wing-body exchange interaction is considered.

FIG. S9: Left: Plot of the Fe–Fe distance vs the exchange interactions ($J$) for the 16 complexes under study. Right: Plot of the (Fe-O-Fe) bond angle vs the exchange interactions ($J$) for the 16 complexes under study.
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properties of dinuclear oxo-bridged iron(III) complexes, Polyhedron 33, 25 (2012).

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structure and magnetism of a tetranuclear Fe(III) complex containing an $[\text{Fe}_4(\mu_3-O)_2]^{8+}$ core, Inorg. Chim. Acta \textbf{212}, 241 (1993).
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Cl  6.3995100 -1.7566430  0.2466030
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Cl  6.3995100 -1.7566430  0.2466030
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$comment
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Nuclear Repulsion Energy = 3757.36986576 hartrees
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Fe  -0.2037531 -1.7030953  0.0357681
N  -0.4369491  -3.2517367  -1.2717061
N  -0.3062356  -2.9013332   1.5839169
N  -2.2279851  -1.7408506   0.0954634
N   1.7456780  -2.0541891   0.1480624
O  -0.0017983  -0.1698386   1.1326195
N  -1.0630873  -3.1299327  -2.3121113
N  -1.6968562  -3.0002627  -3.3456193
N  -3.8683536  -3.1253945   0.8528112
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N  3.3289137  -3.3832510   1.0351028
H  3.7808280  -4.1247413   1.6150442
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$end

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N 3.5207530 2.8228110 2.7748080
Cl 2.6761840 1.4458820 0.0090800
Cl 6.9095920 0.2811050 -4.8668660
Cl -1.0249530 6.3237400 5.5169760
C 4.8318420 3.0258850 -1.9194070
C 4.5208290 3.0514690 -3.2765630
H 3.8907140 3.6607980 -3.5867710
C 5.1273760 2.1921000 -4.1711090
H 4.8946540 2.2112330 -5.0715440
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C 6.4060190 1.2337420 -2.3798090
H 7.0470360 0.6267860 -2.0884990
C 5.7730490 2.0736570 -1.4601090
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Cl   2.1112440  8.9899300   4.8668660
Cl   10.045790   2.9472950  -5.5169760
C    4.1889950  6.2451500   1.9194070
C    4.5003770  6.2195660   3.2765630
H    5.1301220  5.6102370   3.5867710
C    3.8934600  7.0789350   4.1711090
H    4.1261820  7.0598020   5.0715440
Cl   2.9388760  7.9676450   3.7174550
C    2.6148170  8.0372920   2.3798090
H    1.9738000  8.6442490   2.0884990
C    3.2477870  7.1973770   1.4601090
C    2.7684910  7.1992430   0.0858960
H    1.9498680  7.6075140  -0.0809880
C    2.6788070  6.5490450  -2.1856840
H    2.7335740  5.6243230  -2.4713500
H    1.7413910  6.7583330  -2.0480050
C    3.2194450  7.4418180  -3.3090810
C    2.5843180  8.8334350  -3.2408550
H    3.0077040  9.4096130  -3.8812710
H    1.6474390  8.7678240  -3.4395200
H    2.7000420  9.1953220  -2.3584580
C    2.8735110  6.7789270  -4.6434140
H    3.3186310  5.9302680  -4.7034180
H    1.9246190  6.6475550  -4.6985100
H    3.1611690  7.3427560  -5.3648170
C    4.7357140  7.6463870  -3.1691930
H    4.8923540  8.3412110  -2.5106170
H    5.0813600  7.9660770  -4.0174800
C    6.3907560  6.0114550  -3.5947470
H    6.3970290  6.3834810  -4.4469570
C    7.3827040  4.9961270  -3.3154620
C    8.1457150  4.5136710  -4.3956650
H    7.9775260  4.8181810  -5.2580610
C    9.1386130  3.5921720  -4.1735630
C    9.4558610  3.1688970  -2.8862280
H   10.1421090  2.5565980  -2.7498980
C   8.7435880   3.6648650  -1.8169450
Complex 2: BAZCOV structure
Nuclear Repulsion Energy = 6542.17529318 hartrees

$end

$molecule
0
11
Fe  6.1424250  0.2042960  1.4088310
Cl  7.9028810  1.4738330  2.2803370
O  6.0573340  0.9989700 -0.3754410
O  4.7532450  1.2487130  2.2242060
N  6.0651270 -1.0650990  3.0853030
N  7.6354570 -1.3401670  0.8661150
C  4.3942220  1.3563480  3.4960580
C  3.6421430  2.4819480  3.8930820
C  3.2358740  2.6303870  5.2004090
C  3.5561420  1.6799580  6.1445860
C  4.2705110  0.5824980  5.7840150
C  4.7369390  0.4024020  4.4643970
C  5.5184460 -0.7724430  4.1986150
C  6.8702170 -2.2870790  2.9756450
C  8.0638350 -1.9979400  2.1225400
C  8.7591220 -0.8948520  0.0260210
C  9.6408530 -2.0014570 -0.4850990
C  6.8470600  2.0359290  1.4088310
H  7.0095570 -1.9698000  0.4497850
H  3.4174170  3.1305750  3.2674480
H  2.7423770  3.3782070  5.4494640
H  3.2835110  1.7897040  7.0255700
H  4.4570430 -0.0668320  6.4215200
H  5.6351040 -1.3725280  4.8993130
H  6.3424540 -2.9976130  2.5779010
H  7.1558830 -2.5762170  3.8566290
H  8.6764520 -1.4189590  2.6020630
H  8.5277330 -2.8252560  1.9162340
H  9.3037560 -0.2778820  0.5408570
H  8.4039530 -0.4073270 -0.7341540
H 10.3160310 -1.6335270 -1.0594110
H  9.1101610 -2.6310900  0.9776320
H 10.0589540 -2.4460700  0.2564890
H  6.3550360  2.8597270 -0.8698330
H  7.0747850  1.8347280 -1.8102920
H  7.6490240  2.1224600 -0.3810160
Fe  4.7405750  -0.2042960  -1.4088310
Cl  2.9801190  -1.4738330  -2.2803370
O  6.1297550  -1.2487130  -2.2242060
N  4.8178730   1.0650990  -3.0853030
N  3.2475430   1.3401670  -0.8661150
C  6.4887780  -1.3563480  -3.4960580
C  7.2408570  -2.4819480  -3.8938020
C  7.6471260  -2.6303870  -5.2004090
C  7.3268580  -1.6799580  -6.1445860
C  6.6124890  -0.5824980  -5.7840150
C  6.1460610  -0.4024020  -4.4643970
C  5.3645540   0.7724430  -4.1986150
C  4.0127830   2.2870790  -2.9756450
C  2.8191650   1.9979400  -2.1225400
C  2.1238780   0.8948520  -0.0260210
C  1.2421470   2.0014570   0.4850990
C  4.0359400  -2.0359290   0.9014290
H  3.8734430   1.9698000  -0.4497850
H  7.4655830  -3.1305750  -3.2674480
H  8.1406230  -3.3782070  -5.4494640
H  7.5994890  -1.7897040  -7.0255700
H  6.4259570   0.0668320  -6.4215200
H  5.2478960   1.3725280  -4.8993130
H  4.5405460   2.9976130  -2.5779010
H  3.7271170   2.5762170  -3.8566290
H  2.2065480   1.4189590  -2.602630
H  2.3552670   2.8252650  -1.9162340
H  1.5792440   0.2778820  -0.5408570
H  2.4790470   0.4073270   0.7341540
H  0.5669690   1.6335270   1.0594110
H  1.7728390   2.6310900   0.9776320
H  0.8240460   2.4460700  -0.2564890
H  4.5279640  -2.8597270   0.8698330
H  3.8082150  -1.8347280   1.8102920
H  3.2339760  -2.1224600   0.3810160
$end

$comment
Complex 3: QOHVUF structure
Nuclear Repulsion Energy = 17862.42895125  hartrees
$end

$molecule
0 11
 Fe  7.7031670  0.0577830  4.6715320
 Fe  8.6142600  1.6093790  7.1775940
C 10.3078550 0.6459050 0.0785510
C 11.2451340 0.2422140 -0.8591510
H 12.0754760 -0.8279610 -0.5911780
H 12.6973370 -1.1160850 -1.2498600
C 11.0381470 -1.1097530 1.5393120
H 10.9637190 -1.5925990 2.3544830
C 10.3097640 -0.0459100 1.2883180
C 9.1285960 0.2802090 2.2761370
C 6.8279290 2.6501900 2.9612080
C 5.1673900 6.1157000 1.8287650
H 4.7643920 4.1619700 1.3685050
C 5.2383230 4.6907250 3.3056860
H 4.3019040 4.9741000 3.4591060
H 5.8395630 5.3556270 3.7270790
C 7.5734260 6.6933470 6.1531590
C 7.4808860 7.7841030 5.3021900
C 7.0633250 8.5851510 5.5947100
C 7.9976580 7.6986150 4.0318740
C 7.9330560 8.4458380 3.4488780
C 8.6114990 6.5366200 3.5900240
C 8.9716950 6.4891270 2.7124630
C 8.6956970 5.4490300 4.4409930
C 9.1094030 4.6495650 4.1382450
C 8.1808200 5.5044390 5.7407660
C 8.2597890 4.3107810 6.5925530
C 7.3528860 3.2326900 9.6908160
C 6.5272540 4.1192260 12.0035690
H 7.1489000 4.5783250 12.6233850
H 5.6059640 4.3598570 12.2776790
C 6.6851740 2.7577600 12.1569890
H 5.8040770 2.3683180 12.3881410
H 7.2873690 2.6010330 12.9261340
C 10.4011970 -2.2353370 10.2218530
C 10.2515710 -3.4812370 10.8437150
H 11.0143940 -4.0179080 11.0237270
C 8.9947040 -3.9245050 11.1914660
H 8.8968560 -4.7540490 11.6435440
C 7.8781300 -3.1725320 10.8846270
H 7.0142110 -3.4812370 11.1321440
C 8.0170800 -1.9709590 10.2167390
H 7.2436040 -1.4707000 9.9845640
C 9.2860870 -1.4833650 9.8794200
C 9.3959880 -0.2279660 9.1110930
C 11.5768090 2.2020920 8.2010070
Complex 4: ABIZOA structure

Nuclear Repulsion Energy = 10644.04975278 hartrees

$molecule

2 11

Fe  2.4918390  7.2964270  12.0883100
N  2.8937820  7.2085840  10.1280470
N  4.0830990  8.3563220  13.4083070
N  2.0886640  9.3407440  11.9202210
N  3.9585750  5.8688230  12.3692340
O  1.7647120  7.0176230  13.9621340
N  2.3743290  7.7208020  9.1937870
N  1.9033240  8.1601420  8.2711730
N  2.8842820 11.4004730 11.7998800
H  3.4216640 12.0652670 11.8943410
N  5.9196900  5.1544760  13.0731640
H  6.6902360  5.1587560  13.4535970
C  4.3767690  9.6551140  12.7639010
H  4.7025370 10.2884030 13.4212470
H  5.0535240  9.5448370  12.0793810
C  3.1218520 10.1398460 12.1673720
C  1.1167850 10.1484740 11.3353380
C  0.2816710  9.8727340  10.9251430
H  0.5401160  9.0173570  11.0001950
C  0.2816710 11.196180 11.283250
H  0.9132050 12.8606710 10.9067750
C  0.8776340 12.4935190 10.7012830

$end
| Atom | x      | y      | z      |
|------|--------|--------|--------|
| H    | 1.2240100 | 13.3537180 | 10.6275260 |
| C    | 1.6211090  | 11.4513110  | 11.2395830 |
| C    | 5.3056260  | 7.5299400  | 13.6036990 |
| H    | 6.0625440  | 7.9468430  | 13.1624490 |
| H    | 5.5062170  | 7.4528380  | 14.5496050 |
| C    | 5.0619620  | 6.1816980  | 13.0252870 |
| C    | 4.1190680  | 4.5439230  | 11.9564520 |
| C    | 3.2703310  | 3.7003560  | 11.2538170 |
| H    | 2.4351720  | 3.9892880  | 10.9639630 |
| C    | 3.7107820  | 2.4203210  | 11.0027830 |
| H    | 3.1707910  | 1.8372040  | 10.5201250 |
| C    | 4.9486220  | 1.9858150  | 11.4608550 |
| H    | 5.2094660  | 1.1114360  | 11.2822840 |
| C    | 5.7990270  | 2.7981700  | 12.1673720 |
| H    | 6.6279480  | 2.5007480  | 12.4675780 |
| C    | 5.3515770  | 4.0874090  | 12.4067600 |
| C    | 2.5802590  | 7.3784010  | 15.0749640 |
| H    | 3.1784520  | 6.6476880  | 15.3001180 |
| H    | 2.0244110  | 7.5660050  | 15.8474750 |
| C    | 3.3755600  | 8.5961180  | 14.7074710 |
| H    | 2.7853910  | 9.3609940  | 14.6233620 |
| H    | 4.0242210  | 8.7885460  | 15.4036370 |
| Fe   | 0.0744590  | 6.0832360  | 13.7914570 |
| N    | -0.3274840 | 6.1710800  | 15.7517200 |
| N    | -1.5168010 | 5.0233420  | 12.4714600 |
| N    | 0.4776340  | 4.0389200  | 13.9595460 |
| N    | -1.3922770 | 7.5108410  | 13.5105320 |
| O    | 0.8015860  | 6.3620410  | 11.9176330 |
| N    | 0.1919690  | 5.6588620  | 16.6859800 |
| N    | 0.6629740  | 5.2195220  | 17.6085930 |
| N    | -0.3179840 | 1.9791910  | 14.0798870 |
| H    | -0.8553660 | 1.3143960  | 13.9854260 |
| N    | -3.3533920 | 8.2251880  | 12.8066030 |
| H    | -4.1239380 | 8.2209080  | 12.4261700 |
| C    | -1.8104710 | 3.7245500  | 13.1158660 |
| H    | -2.1362390 | 3.0912610  | 12.4585200 |
| H    | -2.4872270 | 3.8348270  | 13.8003860 |
| C    | -0.5555540 | 3.2398180  | 13.7123940 |
| C    | 1.4495130  | 3.2311900  | 14.5444290 |
| C    | 2.7479690  | 3.5069300  | 14.9546230 |
| H    | 3.1064130  | 4.3623070  | 14.8795720 |
| C    | 3.4792900  | 2.4733500  | 15.4748060 |
| H    | 4.3514940  | 2.6330760  | 15.7543080 |
| C    | 2.9544870  | 1.1880460  | 15.5964410 |
| H    | 3.4795030  | 0.5189930  | 15.9729920 |
| C    | 1.6886640  | 0.8861450  | 15.1784830 |
| H    | 1.3422880  | 0.0259460  | 15.2522400 |
| C    | 0.9451890  | 1.9283530  | 14.6401840 |
Complex 5: MHQINF structure
Nuclear Repulsion Energy = 8674.45767240 hartrees

$molecule
0 11
C  3.3668200  2.2302500  3.4757400
C  1.3207300  2.1449700  0.1893700
C  4.5516300  4.8386600  1.0780900
C  2.6550600  1.1545200  1.2364000
C  2.6798900  0.9030200  1.6902800
C  5.6422200  2.3627000  3.4436700
C  9.0069300  1.4905000  1.5600200
C  6.2845500  2.1726600  4.7171400
C 10.0649600  0.6471500  1.5640300
C  6.1412400  0.9957100  5.4094800
C  9.9667900  0.7178000  1.7353600
C  5.4177100  0.0200400  4.8544100
C 10.9563700  1.6350400  1.7513900
C  5.2330800  1.3378200  5.4716000
C 10.6892800  2.9228300  1.9217200
C  4.4322000  2.2970600  4.8453900
C  3.6746300  4.1428300  2.1211100
C  1.7598700  0.0231600  1.1071500
Complex 6: JOJGAS structure

Nuclear Repulsion Energy = 11591.38628089 hartrees

$end

$molecule
0 11
Fe 9.9100950 5.2055760 12.0047640
Fe 6.8617640 3.8723210 12.9327670
O 8.6220970 4.0267640 12.5159890
O 10.8483530 4.3441480 10.5050570
C 10.2228020 3.8447730 9.4354710
C 10.5251970 2.5717800 8.9360310
H 11.1843910 2.0469030 9.3753370
C 9.8866250 2.0565650 7.8193090
H 10.1092870 1.1881370 7.5037360
C 8.9217010 2.8060050 7.1587030
H 8.4749760 2.4529910 6.3981040
C 8.6188380 4.0780430 7.6259100
H 7.9567500 4.5906370 7.1779380
C 9.2656620 4.6186420 8.7389930
C 9.0333520 6.0357690 9.1536910
H 9.8810280 6.5373210 9.0582050
H 8.3737730 6.4423770 8.5383150
N 8.5418960 6.1914820 10.5504600
H 7.7832700 5.6902850 10.6040090
C 8.1235790 7.5964810 10.7989680
H 7.1728680 7.5881220 11.0753750
$end

$comment
Complex 7: FAJQEO structure
Nuclear Repulsion Energy = 9380.72884738 hartrees
$end
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| C    | 6.9797920 | 1.3988840 | 19.4123200 |
| N    | 8.5156900 | 2.4577930 | 16.6347310 |
| C    | 5.6640570 | 2.0924330 | 16.9880450 |
| C    | 9.2138950 | 0.0000000 | 18.1186490 |
| C    | 6.4234240 | -0.9066000 | 17.8305620 |
| N    | 5.8640570 | 2.0924330 | 16.9880450 |
| O    | 8.5156900 | 2.4577930 | 16.6347310 |
| O    | 9.2138950 | 0.0000000 | 18.1186490 |
| O    | 6.4234240 | -0.9066000 | 17.8305620 |
| O    | 7.5372540 | -0.0825010 | 14.4931070 |
| O    | 2.9801260 | 3.2220560 | 16.7108300 |
| H    | 2.9150370 | 3.1731000 | 17.6838010 |
| C    | 7.3502310 | 0.7887420 | 20.5447360 |
| H    | 8.0377070 | 0.1622810 | 20.5193690 |
| C    | 6.7275360 | 1.0734140 | 21.7586850 |
| H    | 6.9906840 | 0.6382460 | 22.5377870 |
| C    | 5.7183260 | 2.0090260 | 21.7876750 |
| H    | 5.2922980 | 2.2193570 | 22.5867070 |
| C    | 5.3498250 | 2.6273270 | 20.6172100 |
| H    | 4.6632670 | 3.2556010 | 20.6172100 |
| C    | 6.0050710 | 2.3118300 | 19.4358740 |
| C    | 5.7413770 | 3.0244180 | 18.1512620 |
| H    | 6.3731240 | 3.7524170 | 18.0497980 |
| H    | 4.8479790 | 3.4015630 | 18.1693810 |
| C    | 6.2848650 | 2.8449110 | 15.7831550 |
| H    | 5.7328570 | 3.6367330 | 15.6835020 |
| H    | 6.1629340 | 2.2918850 | 14.9949940 |
| C    | 7.7287620 | 3.2492540 | 15.8973020 |
| C    | 8.1917390 | 4.3525870 | 15.2504660 |
| H    | 7.6117130 | 4.9047060 | 14.7775700 |
| C    | 9.5590320 | 4.6381660 | 15.3102580 |
| H    | 9.9048110 | 5.3706980 | 14.8536680 |
| C    | 10.3944930 | 3.8231320 | 16.0531230 |
| H    | 11.3057930 | 3.9981060 | 16.1183500 |
| C    | 9.8264260 | 2.7451850 | 16.6963350 |
| H    | 10.3787620 | 2.1885320 | 17.1964090 |
| C    | 4.6036690 | 1.3535540 | 16.7470670 |
| H    | 4.2795040 | 1.0371500 | 17.6040790 |
| H    | 4.8189250 | 0.5702510 | 16.2180020 |
| C    | 3.4472970 | 2.0770210 | 16.0513110 |
| H    | 3.7347960 | 2.3317750 | 15.1598730 |
| H    | 2.7057970 | 1.4560000 | 15.9552820 |
| C    | 16.2522320 | -1.7080340 | 16.8304130 |
| C    | 6.89180000 | -1.2030580 | 15.5240580 |
| Fe   | 10.7741870 | -0.6878370 | 18.7283410 |
| N    | 11.4479980 | -1.3988840 | 16.8249770 |
| N    | 12.5637330 | -2.0924330 | 19.2492520 |
|    |         |         |         |
|----|---------|---------|---------|
| Fe | 4.3705830 | 3.685660 | 13.38260 |
| Fe | 7.0943580 | 3.729200 | 15.063019 |
| O  | 6.1190610 | 3.267287 | 13.643420 |
| C  | 4.5708430 | 5.056081 | 15.997564 |
| O  | 4.0353500 | 4.911880 | 14.811360 |
| O  | 3.9643410 | 5.638352 | 16.891280 |
| N  | 4.1417840 | 2.365589 | 11.634590 |
| N  | 3.7393650 | 1.839902 | 14.250751 |
| N  | 2.2755200 | 4.012009 | 12.788300 |
| N  | 4.7552100 | 4.992196 | 11.766190 |
| C  | 3.9536520 | 0.766626 | 13.480930 |
| C  | 3.6803850 | -0.526860 | 13.946074 |
| C  | 3.2289270 | -0.684487 | 15.219623 |
| C  | 0.1767030 | 5.165599 | 12.861424 |
| C  | 1.4463930 | 4.897280 | 13.357032 |
| C  | 5.0759000 | 4.389847 | 10.594629 |
| C  | 5.4322100 | 5.110840 | 9.479512 |
| C  | 5.4643190 | 6.483466 | 9.589195 |
| C  | 5.1222560 | 7.120495 | 10.734780 |
| C  | 4.7718910 | 6.339267 | 11.795055 |
| C  | 4.5270860 | 1.025819 | 12.115982 |
| C  | 2.7453840 | 2.340035 | 11.104450 |
| C  | 5.1137760 | 2.876673 | 10.651502 |
| N  | 8.5500860 | 4.251124 | 16.690196 |
| N  | 7.9064940 | 5.618273 | 14.435588 |
| N  | 8.9177870 | 2.814613 | 14.366528 |
| N  | 7.0807400 | 2.004179 | 16.361145 |
| C  | 8.5337550 | 6.333791 | 15.424772 |
| C  | 9.1540720 | 7.543965 | 15.105877 |
| C  | 9.0386950 | 8.040447 | 13.850608 |
| C  | 8.3934410 | 7.297549 | 12.873611 |
| C  | 7.8615380 | 6.089201 | 13.200610 |
| C  | 9.9975400 | 2.907703 | 15.174930 |
| C  | 11.1514270 | 2.184884 | 14.921040 |
| C  | 11.2155910 | 1.392704 | 13.818110 |
| C  | 10.1133370 | 1.306915 | 12.983295 |
| C  | 8.9939410 | 2.042511 | 13.294065 |
| C  | 7.6266230 | 2.166631 | 17.557510 |
| C  | 7.7663960 | 1.058674 | 18.445135 |
| C  | 7.2927840 | -0.182530 | 18.057180 |
| C  | 6.7733960 | -0.328554 | 16.777537 |
## Complex 9: DIBXAN10 structure

Nuclear Repulsion Energy = 6561.2383334 hartrees
$molecule$

2 11

Fe 3.2695000 3.4118140 6.0884780
O 3.2695000 2.5090780 7.6450000
O 1.7524520 4.6901140 6.5349460
N 4.6845400 2.1686240 4.9554890
N 3.2695000 4.4631440 4.0793720
C 5.1579630 2.9009550 3.7705140
C 4.4818310 4.0588550 3.3745030
C 3.9783280 0.9327030 4.5686520
C 1.2816440 5.0092900 7.6450000
C 0.0614670 5.8036840 7.6450000
C 5.8484820 1.7944780 5.7582140
C 3.2695000 5.9278080 4.2857870
H 6.0603450 3.1669350 3.9601100
H 5.1527320 2.2892010 3.0320070
H 4.2385800 3.9258650 2.4540450
H 5.0951890 4.7947330 3.4402500
H 6.3127510 2.5995110 6.0043830
H 5.5699200 1.3299000 6.5502360
H 6.4343760 1.2323740 5.2459990
H 3.2695000 6.3338700 3.4066120
Fe 3.2695000 3.4118140 9.2015220
O 4.7865480 4.6901140 8.7550540
C 5.2573560 5.0092900 7.6450000
O 4.7865480 4.6901140 6.5349460
O 1.7524520 4.6901140 8.7550540
N 1.8544600 2.1686240 10.3345110
C 1.3810370 2.9009550 11.5194860
C 2.0571690 4.0588550 11.9154970
N 3.2695000 4.4631440 11.2106280
N 4.6845400 2.1686240 10.3345110
C 5.1579630 2.9009550 11.5194860
C 4.4818310 4.0588550 11.9154970
C 3.2695000 5.9278080 11.0042130
H 3.2695000 6.3338700 11.8833880
H 4.2385800 3.9258650 12.8359550
H 5.0951890 4.7947330 11.8497500
H 6.0603450 3.1669350 11.3298900
H 5.1527320 2.2892010 12.2579930
C 3.9783280 0.9327030 10.7213480
C 2.5606720 0.9327030 10.7213480
C 0.6905180 1.7944780 9.5317860
H 0.2262490 2.5995110 9.2856170
H 0.9690800 1.3299000 8.7397640
H 0.1046240 1.2323740 10.0440010
C 5.8484820 1.7944780 9.5317860
H 6.3127510 2.5995110 9.2856170
Complex 10: CACZIP structure

Nuclear Repulsion Energy = 7218.18459304 hartrees

$end

$molecule
0 11
Fe -2.5939820 0.6370610 5.1644460
$end
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Fe      | -0.1275000| 2.5893980 | 5.1743920 |
| O       | -0.8414720| 0.9498110 | 5.1642390 |
| O       | -3.0623710| 1.9356900 | 6.6664350 |
| O       | -3.0913840| 2.0070570 | 3.7355990 |
| O       | -1.3336790| 3.3550110 | 6.6440570 |
| O       | -1.3421280| 3.3984790 | 3.7492740 |
| N       | -2.5423600| -0.9983650| 6.5638710 |
| N       | -4.7424160| 0.1644670 | 5.1379250 |
| N       | -3.2670220| -2.1447040| 6.344470  |
| N       | -1.3336790| 3.3550110 | 6.6440570 |
| N       | -1.3421280| 3.3984790 | 3.7492740 |
| N       | 1.4071800 | 2.1547230 | 6.6152570 |
| N       | 0.8346180 | 4.5406560 | 5.1735630 |
| N       | 1.3955750 | 2.1829310 | 3.7152930 |
| N       | 2.6959510 | 2.5440810 | 6.4078500 |
| N       | 2.1895490 | 4.6553360 | 5.1920040 |
| N       | 2.6871260 | 2.5724420 | 3.9185560 |
| C       | -1.8734260| -1.1899610| 7.7656280 |
| C       | -2.1537990| -2.4292460| 8.2314120 |
| C       | -3.0338900| -2.9980230| 7.3535080 |
| C       | -5.8375750| 0.9171330 | 5.1136820 |
| C       | -6.9671110| 0.1294780 | 5.0556660 |
| C       | -6.4979490| -1.1529670| 5.0494500 |
| C       | -1.8313520| -1.0774390| 2.5756960 |
| C       | -2.0830130| -2.3043930| 1.9926370 |
| C       | -2.9779730| -2.9163290| 2.8282720 |
| C       | 1.3872780 | 1.4936170 | 7.7656280 |
| C       | 2.6526490 | 1.4473750 | 8.3066260 |
| C       | 3.4412030 | 2.1194250 | 7.4343160 |
| C       | 0.3607410 | 5.7802500 | 5.1779140 |
| C       | 1.3787330 | 6.6927590 | 5.1944900 |
| C       | 2.5193260 | 5.9636770 | 5.1998770 |
| C       | 1.3684300 | 1.5552730 | 2.5352920 |
| C       | 2.6425090 | 1.5290690 | 1.9704670 |
| C       | 3.4298990 | 2.1779980 | 2.8655680 |
| C       | -2.4141190| 2.9194120 | 7.1096350 |
| C       | -3.0013430| 3.6562010 | 8.2796900 |
| C       | -2.4613840| 3.0149780 | 3.3212000 |
| C       | -3.1012440| 3.8396270 | 2.2452130 |
| B       | -4.1376450| -2.2704820| 5.0867460 |
| B       | 3.0555540 | 3.3802900 | 5.1737700 |
| H       | -4.6683010| -3.2353990| 5.0991780 |
| H       | 3.9891250 | 3.5976280 | 5.2234980 |
| H       | -1.2830380| -0.5579870| 8.0828500 |
| H       | -1.8108370| -2.8038070| 9.0318240 |
| H       | -3.4215910| -3.8596660| 7.4426040 |
| H       | -5.8387180| 1.8666350 | 5.1344020 |
Complex 11: YUPSAE structure

Nuclear Repulsion Energy = 6285.40992966 hartrees

$molecule
4 11
Fe  5.5983160  3.5998000  1.1948770
Fe  3.6806600  1.4810050  2.4295720
O   6.4162130  3.3859960  3.0688090
O   4.9179130  1.9761080  3.9847860
O   4.0649750  4.7347320  1.9598720
O   2.5754280  3.2025400  2.6535210
O   4.7559030  2.0315970  1.1129010
N   6.5838610  5.5591480  0.9675050
H   6.5206320  6.0064620  1.7584440
N   7.4936710  3.0281450  0.3765520
H   7.7193830  2.2093900  0.7044590
N   5.2436710  4.0575330 -0.8756190
H   4.3599600  3.9329640 -1.0521840
N   2.1165290  0.6239740  1.2359650
H   1.9792130  1.1630160  0.5152820
N   2.3567710  0.6330340  3.9673090
H   2.2392250  1.2660680  4.6105110
N   4.3019330 -0.5662200  2.4322740

$end
Complex 12: VABMUG structure

Nuclear Repulsion Energy = 6256.81653582 hartrees

$molecule
0 11
Fe 16.8282870 2.8408430 5.0234490
Fe 14.0209430 1.5496990 4.4071950
Cl 18.4682590 1.3552370 5.9216050
Cl 13.6908630 0.3755480 2.3871630
O 15.5803670 4.3869540 4.2178940
C 14.4224950 4.3830990 3.7335780
O 13.6529040 3.3738960 3.6450730
C 13.8876890 5.6813800 3.2246770
O 15.9413320 3.1771340 6.7935380
C 14.7302730 2.9452880 7.1024850
O 13.8554260 2.5203090 6.3256120
C 14.3133690 3.2439130 8.5095420
O 15.8070030 1.5386520 4.3596650
N 18.0276130 3.1007320 3.2631930
C 17.9303470 2.2887280 2.1904860
C 18.7029270 2.4495910 1.0612340
C 19.6017510 3.4966390 1.0186210
C 19.7081910 4.3524630 2.1134540
C 18.9162210 4.1290750 3.2213990
C 18.9562600 4.9632330 4.4645590
C 19.778310 6.0773060 4.5817460
C 19.7095180 6.8166120 5.7626250
C 18.8559780 6.4200790 6.7542030
C 18.0874820 5.2933380 6.5821110
N 18.1187130 4.5755860 5.4495820
Complex 13: AGAQIJ structure

Nuclear Repulsion Energy = 36777.12046167 hartrees

$end

$molecule
0 21
  Fe  -2.8968660  8.3643640  6.1190450
  Fe  -3.4288590 10.0269600  3.5705880
  Fe  -4.4285370  5.7187690  6.6525790
  Fe  -0.8279450  9.5172590  8.1124500

$end
H -4.9748220 13.9974070 4.7255790
C -1.8490440 14.0255800 5.9302930
H -0.9532270 14.0746290 5.5374410
H -1.9490530 13.1757860 6.4085270
H -1.9715780 14.7687210 6.5565870
C -2.7662670 15.4277080 4.0676990
H -2.9832340 16.1726590 4.6663550
H -3.3841550 15.4289270 3.3066710
H -1.8481050 15.5286580 3.7409810
C -0.2627190 11.2530350 0.7642360
H 0.0711470 10.2926780 0.8291360
H 0.6983840 11.5542420 1.5891760
H 0.8579910 11.4162080 0.0024680
C -0.6455600 13.4373000 0.2230770
H -0.1229740 13.4425360 0.0024680
H -0.1088760 13.8159900 0.0024680
H -1.4563530 13.9735180 0.1011740
C -1.8343670 11.4497620 0.5367170
H -1.9382540 10.4844050 0.4071650
H -1.3818470 11.6171180 1.3892960
H -2.7172200 11.8748430 0.453540
C -6.9578000 11.6412830 1.6355690
C -7.7553820 11.8012750 2.9350410
H -7.1493120 12.0507540 3.6620150
H -8.1960150 10.9527560 3.1536760
H -8.4327940 12.500570 2.8180740
C -6.2852940 12.9721230 1.3090960
H -5.696470 13.2325960 2.0506300
H -6.9703640 13.6610940 1.1746090
H -5.7529140 12.8773090 0.4910650
C -7.8939900 11.2482780 0.4866240
H -8.5644640 11.9491840 0.3578110
H -8.3419060 10.4047100 0.7032850
H -7.3717700 11.1378900 0.3356020
C -4.6378980 7.1894500 0.5473280
C -3.3587570 7.3113790 0.2504680
H -3.2558990 6.5234800 0.8242000
H -2.5966990 7.3716210 0.3627470
H -3.3967850 8.1181490 0.8069270
C -5.7973520 7.0080520 0.4046970
H -5.6425030 6.2145670 0.9599220
H -5.8739400 7.7971800 0.9796630
H -6.6252050 6.8930530 0.1061100
C -4.5360060 5.9952570 1.4724560
H -5.3346400 5.9497380 2.0382910
H -3.7407940 6.0876590 2.0382910
H -4.4653080 5.1749540 0.9401800
| C | -0.6088380 | 4.7796520 | 9.1703380 |
| H | 0.2929140 | 4.4451490 | 9.3598540 |
| H | -0.8751850 | 5.4124850 | 9.8681930 |
| H | -0.6138040 | 5.2292930 | 8.3012260 |
| C | -2.1925090 | 8.1122400 | 11.9703970 |
| C | -3.4263110 | 7.4318330 | 11.4267710 |
| H | -3.1656330 | 6.6178610 | 10.9490310 |
| H | -0.8427900 | 7.6735040 | 13.4685170 |
| H | -1.4245890 | 6.3651400 | 12.7528940 |
| C | -2.4525830 | 9.4939120 | 12.5552340 |
| H | -2.9268580 | 10.0426140 | 11.8966140 |
| H | -1.5989510 | 9.9196620 | 12.7800380 |
| H | -2.9998750 | 9.4077510 | 13.3648750 |
| C | 2.5848370 | 7.8697710 | 10.1924450 |
| C | 2.8319660 | 7.0162110 | 11.4136920 |
| H | 3.7876330 | 6.8083330 | 11.4771110 |
| H | 2.3209450 | 6.1836720 | 11.3389220 |
| H | 2.5497030 | 7.5031410 | 12.2149430 |
| C | 3.3582200 | 9.1164420 | 10.2852290 |
| H | 3.0827540 | 9.6126040 | 11.0847520 |
| H | 3.1940560 | 9.6633800 | 9.4881730 |
| H | 4.3123700 | 8.9032780 | 10.3469200 |
| C | 3.0030470 | 7.0516600 | 8.9467670 |
| H | 2.9052420 | 7.5969440 | 8.1432950 |
| H | 2.4297890 | 6.2535010 | 8.8712570 |
| H | 3.9368100 | 6.7646930 | 9.0390580 |
| C | -0.4236590 | 13.4169510 | 9.9476520 |
| C | -0.0661490 | 12.8475100 | 11.3194270 |
| H | -0.3039370 | 13.4969840 | 12.0150620 |
| H | 0.8972880 | 12.6665500 | 11.3561950 |
| H | -0.5601850 | 12.0145630 | 11.4672400 |
| C | 0.3320960 | 14.7045550 | 9.6836120 |
| H | 0.1399160 | 15.0151270 | 8.7750180 |
| H | 1.2939660 | 14.5428310 | 9.7768900 |
| H | 0.0510880 | 15.3871680 | 10.3271790 |
| C | -1.9215420 | 13.7120830 | 9.9029870 |
| H | -2.1403690 | 14.3922350 | 10.5739460 |
| H | -2.4219400 | 12.8904080 | 10.0952190 |
| H | -2.1630610 | 14.0420480 | 9.0119130 |
| C | 2.0678030 | 11.7242550 | 5.7896360 |
| C | 3.1296730 | 10.6458480 | 6.0075310 |
| H | 3.5541140 | 10.7766650 | 6.8823180 |
| H | 3.8087420 | 10.7075340 | 5.3030130 |
| H | 2.7078260 | 9.7615580 | 5.9791530 |
Complex 14: DUFNUO structure

Nuclear Repulsion Energy = 16928.38338359 hartrees

$end

$molecule
0 21

Fe  -0.1719730 10.4359500 4.4004910
Fe  -0.1719730 7.3684350 4.4004910
Fe  -1.9672190 11.9497340 2.4315350
C   2.0523380 10.4053140 2.3829540
C   1.2899450 9.0691890 2.2526990
O   0.2876110 8.8924310 3.2421060
C   1.1322130 11.6086820 2.0798480
O   -0.0639960 11.6333110 2.8277550
C   2.6913630 10.5529380 3.7694610
O   1.7187980 10.7822580 4.7842140
C   3.1643380 10.4282910 1.3037770
C   4.3982330 9.5948090 1.5736160
O   -4.2871140 6.4125580 3.5450350
C   -2.7927950 6.3059320 3.4668830
O   -2.1484700 7.2290700 4.0363060
C   -2.1977520 5.2396760 2.7825180
C   -0.8203140 5.1279440 2.5612620
O   0.0448320 5.9596240 2.9801880
C   -0.2866990 3.9631710 1.7689970
C   -6.1458520 11.0920730 2.1016740
C   -4.6603680 10.9524090 1.8608800
O   -3.9533520 11.9327640 2.2467150
C   -4.1593150 9.7870350 1.2779030
C   -2.8218930 9.5963100 0.9383610
O   -1.9141800 10.4448100 1.1175490
C   -2.3768570 8.3032860 0.3009940
C   -2.1129630 15.7700870 4.4427360
C   -2.0340680 14.7924340 3.2926230
O  -2.1241900 13.5776530 3.6069940
C  -1.8733400 15.2579830 2.0066240
| Atoms | C   | O   | H   |
|-------|-----|-----|-----|
| 1.853806  | 5.2396760 | 6.0184630 |
| 0.476380 | 5.1279440 | 6.2397200 |
| -0.3887780 | 5.9596240 | 6.5542670 |
| -0.0572460 | 3.9631710 | 7.0319870 |
| 5.8019070  | 11.0920730 | 6.6993070 |
| 4.3164230  | 10.9520730 | 6.9401020 |
| 3.8153690  | 9.7870350 | 7.5230790 |
| 2.4779470  | 9.5631000  | 7.8626210 |
| 1.5702350  | 10.4481000 | 7.6834330 |
| 2.0329110  | 8.3032860  | 8.4999880 |
| 1.7690180  | 15.7700870 | 4.3582460 |
| 1.6901230  | 14.7924340 | 5.5083580 |
| 1.7802450  | 13.5776530 | 5.1939870 |
| 1.5293950  | 15.2579830 | 6.7943580 |
| 1.4235830  | 14.4575400 | 7.9277480 |
| 1.3521370  | 13.1975550 | 7.9082100 |
| 1.3696830  | 15.0882830 | 9.2973570 |
| 1.1978590  | 9.0346480  | 7.4227480 |
| -2.2750080 | 8.3318200  | 6.4775230 |
| -1.9539050 | 12.4286490 | 6.5637720 |
| -1.2330600 | 11.5576220 | 7.6515740 |
| -3.6322120 | 11.3113320 | 5.0676050 |
| -3.5134550 | 9.7404800  | 4.8123770 |
| -3.8110930 | 11.3398650 | 7.5811660 |
| -3.0898250 | 10.1294390 | 8.3222080 |
| -5.3394670 | 9.6203390  | 7.9596080 |
| -5.2019480 | 9.9026710  | 6.4564000 |
| -4.5190710 | 8.6757250  | 7.0759890 |
| 4.3869850  | 5.8223620  | 5.8544130 |
| 4.2035840  | 7.3046090  | 5.4601290 |
| 4.2048330  | 6.2008080  | 4.3723280 |
| 2.4030400  | 4.5698860  | 6.3719110 |
| -0.5925420 | 4.2620230  | 7.7712670 |
| 0.6534470  | 3.4390530  | 7.3717020 |
| -0.5963040 | 3.4180290  | 6.4757620 |
| 6.2984820  | 10.5829730 | 7.3347380 |
| 6.0456110  | 12.0186650 | 6.7503530 |
| 6.0035710  | 10.7812070 | 5.8104080 |
| 4.4255530  | 9.1142420  | 7.6990990 |
| 1.5621790  | 8.4970150  | 9.3149590 |
| 2.8010740  | 7.7746630  | 8.7129720 |
| 1.4732720  | 7.8257230  | 7.8944810 |
| 1.5550370  | 16.6636400 | 4.6504390 |
| 2.6511640  | 15.7640800 | 4.0062070 |
| 1.1673920  | 15.4937610 | 3.6752900 |
| 1.4962390  | 16.1770660 | 6.9228520 |
| 0.7890260  | 14.5701730 | 9.8535790 |
Complex 15: VIVDAF structure

Nuclear Repulsion Energy = 13889.88152012 hartrees

$end
$comment
Complex 16: YAYPOD structure
Nuclear Repulsion Energy = 16376.86928265 hartrees
$end

$molecule
1 21
  Fe  9.7252780  4.4946290  1.4622260
  Fe  8.6326970  2.1230090  2.5777060
  Fe 10.9029100  4.2460180  4.4429000
  Fe  8.7831720  1.5669050  -0.6117140
  O  9.6925660  3.5165400  3.2842850
  O  9.0644950  2.8524860  0.7458340
  O  9.8332270  5.5970230  0.1275770
  O  8.2139830  1.1972590  4.1609660
  O 10.7655190  6.0877030  3.7291680
  O  7.2293520  0.7752740  0.2257130
  N 10.3140940  6.2447210  2.4370440
  N  7.4910480  0.6705960  1.6748540
  C  6.9055030  4.3997640  2.3356370
  C  5.5643110  5.0932580  2.6300450
  O  7.8050830  5.1750380  1.8743980
  O  6.9251300  3.2973700  2.6889260
  C 12.5515940  3.6048620  2.2375010
  C 13.8568030  3.0749280  1.7239220
  O 12.5417810  3.6762920  3.4053190
  O 11.7174380  3.9287110  1.2823100
  C 10.6117730  0.3074930  1.4687690
  C 12.1034400  -0.5430190  1.5636340
  O 10.2061440  0.8635970  2.3879760
  O 10.1210930  0.2257130  0.1897300
  C 10.2977380  7.4877770  2.1131950
  C  9.8822950  7.7592860  0.8145290
  C  9.7743460  9.1299190  0.5724600
