Single metal four-electron reduction by U(II) and masked “U(II)” compounds

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Experimental Details

General considerations
All manipulations were carried out under inert atmospheres using an MBraun glovebox equipped with a purifier unit and Schlenk line techniques. The water and oxygen levels were always kept at less than 1 ppm. Anhydrous solvents were purchased from Sigma Aldrich and vacuum distilled under potassium/benzophenone (THF, toluene) or sodium sand/benzophenone (hexane). Depleted uranium turnings were purchased from IBILABS, Florida (USA). Azobenzene and diphenylacetylene were purchased from Sigma Aldrich and dried under vacuum.

\[ \text{[U\{N(SiMe}_3\}_2\}_3]}^{1}, \text{ KC}_8^{2}, \text{ [K(2.2.2-cryptand)][\{(Me}_3Si\}_2N\}_2U\}_2(\mu-O)]^{3} \] (complex 1) and \[ \text{[K(2.2.2-cryptand)][U\{N(SiMe}_3\}_2\}_3]}^{4} \] (complex 2) were synthesized according to their respective literature procedures. Elemental analyses were performed under nitrogen by the “Analytische Laboratorien Prof. Dr. H. Malissa und G. Reuter GmbH” in Lindlar, Germany and with a Thermo Scientific Flash 2000 Organic Elemental Analyzer at EPFL.

$^1$H NMR experiments were carried out using NMR tubes adapted with J. Young valves. $^1$H NMR spectra were recorded on a Bruker 400 MHz spectrometer and the chemical shifts are reported in ppm with residual proteo-solvent signals used as an internal reference.

Caution: Depleted uranium (primary isotope $^{238}$U) is a weak α-emitter (4.197 MeV) with a half-life of $4.47 \times 10^9$ years. Manipulations and reactions should be carried out in monitored fume hoods or in an inert atmosphere glovebox in a radiation laboratory equipped with α- and β-counting equipment.

Synthesis [K(2.2.2-cryptand)][U(η$^2$-C$_2$Ph$_2$){N(SiMe$_3$)$_2$}$_3$], 3.

From complex 1 NMR scale. A cold (−80 °C) solution of diphenylacetylene (1.2 mg, 6.7 µmol, 1.0 eq) in THF-d$_8$ (0.5 mL) was added to cold (−80 °C) purple crystals of 1 (15.1 mg, 6.60 µmol, 1.0 eq), resulting in a brown solution. The $^1$H-NMR spectrum at −80 °C immediately showed full conversion of complex 1 and the appearance of signals corresponding to [K(2.2.2-cryptand)][U(O){N(SiMe$_3$)$_2$}$_3$]. At 0 °C and 25 °C additional paramagnetic signals were observed, assigned to complex 3. TMS$_2$O (1.5 µL, 6.7 µmol, 1.0 eq) was added and used as internal standard to determine a conversion of 66%.

From complex 1 preparatory scale. A cold (−80 °C) solution of diphenylacetylene (4.0 mg, 22.4 µmol, 1.0 eq) in THF (1 mL) was added to cold (−80 °C) purple crystals of 1 (49.9 mg, 21.8 µmol, 1.0 eq), resulting in a brown solution, which was left to react for 15 min at −80 °C. Slow diffusion of hexane into the THF reaction mixture at −40 °C gave a mixture of X-ray quality copper and pink colored crystals, consisting of complex 3 and [K(2.2.2-cryptand)][U(O){N(SiMe$_3$)$_2$}$_3$]. The crystals were washed with toluene until [K(2.2.2-cryptand][U(O){N(SiMe$_3$)$_2$}$_3$] was fully removed. This resulted in significant loss of complex 3. The final pure, copper-colored residue of 3 was dried and collected (7.3 mg, 25%).

Anal. Calcd. for C$_{50}$H$_{100}$KN$_3$O$_5$Si$_6$: C, 45.74; H, 7.68; N, 5.33. Found: C, 44.29; H, 7.45; N, 4.97.
From in situ complex 2 preparatory scale. A cold (−80 °C) solution of [U(N(SiMe₃)₂)₃] (50.0 mg, 69.5 µmol, 1.0 eq) and 2.2.2-cryptand (26.2 mg, 69.6 µmol, 1.0 eq) in THF (0.5 mL) was added to KC₈ (9.4 mg, 70 µmol, 1.0 eq). After a few minutes, the black mixture was filtered and added to cold (−80 °C) diphenylacetylene (12.4 mg, 69.6 µmol, 1.0 eq), resulting in a brown solution, which was left to react for 15 min at −80 °C. Slow diffusion of hexane into the THF reaction mixture at −4 °C, resulting in a red/brown solution. The THF reaction mixture was later assigned to complex 2, among other products. After 3 h, approximately 60% remains, after 12 h approximately 25% remains and after 40 h nearly all 3 was consumed.

Anal. Calcd. for C₅₀H₁₀₀KN₅O₆Si₆U: C, 45.74; H, 7.68; N, 5.33. Found: C, 44.82; H, 7.56; N, 5.29. The elemental analyses were reproduced several times in different places and conditions always giving low values of carbon probably due to combustion issues that could not be solved.

¹H-NMR (400 MHz, THF-d₈, 233K): δ 29.3 (s, 12H, CPh), 17.1 (s, 4H, CPh), 11.6 (s, 2H, CPh-p), 3.9 (s, 12H, 2.2.2-cryptand), 3.8 (s, 12H, 2.2.2-cryptand), 2.8 (s, 12H, 2.2.2-cryptand), −12.3 (s, 54H, NSiMe₃). ¹H-NMR (400 MHz, THF-d₈, 298K): δ 29.3 (s, 4H, CPh), 17.1 (s, 4H, CPh), 11.6 (s, 2H, CPh-p), 3.9 (s, 12H, 2.2.2-cryptand), 3.8 (s, 12H, 2.2.2-cryptand), 2.8 (s, 12H, 2.2.2-cryptand), −12.3 (s, 54H, NSiMe₃).

Synthesis [K(2.2.2-cryptand)][U(NPh)₂(N(SiMe₃)₂)₃], 4.

From complex 1 NMR scale. A cold (−80 °C) solution of azobenzene (1.3 mg, 7.1 µmol, 1.1 eq) in THF-d₈ (0.5 mL) was added to cold (−80 °C) purple crystals of 1 (15.0 mg, 6.56 µmol, 1.0 eq), resulting in a red/brown solution. The ¹H-NMR spectrum at −80 °C immediately showed full conversion of complex 1 and the appearance of signals corresponding to [K(2.2.2-cryptand)][U(O)(N(SiMe₃)₂)₃]. At −40 °C an additional paramagnetic signal was observed that was later assigned to complex 5. Upon warming up to room temperature, complex 5 immediately starts to transform into complex 4 and the color slowly changed to yellow/brown. After 2h at room temperature, the paramagnetic signals assigned to 5 had completely disappeared and a set of diamagnetic signals assigned to complex 4 was observed in the ¹H-NMR spectrum of the solution.

From complex 1 preparatory scale. A cold (−80 °C) solution of azobenzene (4.0 mg, 22 µmol, 1.0 eq) in THF (1 mL) was added to cold (−80 °C) purple crystals of 1 (50.0 mg, 21.9 µmol, 1.0 eq), resulting in a red/brown solution. It was left at low temperature for 5 min and then stirred at room temperature for 2h, causing the color to change to yellow/brown. Slow diffusion of hexane into the THF reaction mixture at −40 °C gave a mixture of X-ray quality brown and pink crystals, consisting of complex 4 and the terminal oxo complex [K(2.2.2-cryptand)][U(O)(N(SiMe₃)₂)₃]. Washing with toluene (6 x 0.5 mL) removed [K(2.2.2-cryptand)][U(O)(N(SiMe₃)₂)₃]. The final pure, brown residue of 4 was dried and collected (19.8 mg, 69%).

Anal. Calcd for C₄₈H₁₀₀KN₇O₆Si₆U: C, 43.78; H, 7.65; N, 7.44. Found: C, 43.27; H, 7.61; N, 7.51.
From complex 2 NMR scale. A cold (−80°C) solution of [U{N(SiMe$_3$)$_2$)$_3$] (10.0 mg, 13.9 µmol, 1.0 eq) and 2.2.2-cryptand (5.3 mg, 14 µmol, 1.0 eq) in THF-$d_8$ (0.5 mL) was added to KC$_8$ (1.9 mg, 14 µmol, 1.0 eq). After a few minutes, the black mixture was filtered and added to cold (−80°C) azobenzene (2.6 mg, 14 µmol, 1.0 eq), resulting in a red/brown solution. At −40 °C an additional paramagnetic signal was observed that was later assigned to complex 5. Upon warming up to room temperature, complex 5 immediately starts to transform into complex 4 and the color slowly changed to yellow/brown. After 2h at room temperature, the paramagnetic signals assigned to 5 had completely disappeared and a set of diamagnetic signals assigned to complex 4 was observed in the $^1$H-NMR spectrum of the solution.

From complex 2 preparatory scale. A cold (−80°C) solution of [U{N(SiMe$_3$)$_2$)$_3$] (50.0 mg, 69.5 µmol, 1.0 eq) and 2.2.2-cryptand (26.3 mg, 69.9 µmol, 1.0 eq) in THF-$d_8$ (0.5 mL) was added to KC$_8$ (9.4 mg, 70 µmol, 1.0 eq). After a few minutes, the black mixture was filtered and added to cold (−80 °C) azobenzene (12.7 mg, 69.9 µmol, 1.0 eq), resulting in a red/brown solution. It was left at low temperature for 5 min and then stirred at room temperature for 2h, causing the color to change to yellow/brown. Slow diffusion of hexane into the THF reaction mixture at −40 °C gave X-ray quality brown crystals consisting of 4 (33.8 mg, 37%).

Anal. Calcd for C$_{48}$H$_{100}$KN$_7$O$_6$Si$_8$U: C, 43.78; H, 7.65; N, 7.44. Found: C, 43.11; H, 7.66; N, 7.45. The elemental analyses were reproduced several times in different places and conditions always giving low values of carbon probably due to combustion issues and/or the formation of silicon carbides that could not be solved.

$^1$H-NMR (400 MHz, THF-$d_8$, 298K): δ 6.97 (dd, 4H, NPh-o), 5.52 (m, 4H, NPh-m), 5.44 (dd, 2H, NPh-p), 3.57 (s, 12H, 2.2.2-cryptand), 3.53 (t, 12H, 2.2.2-cryptand), 2.54 (t, 12H, 2.2.2-cryptand), 0.45 (s, 54H, NSiMe$_3$). IR (Nujol mull): 1579 (m), 1464 (br s), 1377 (s), 1362 (m), 1355 (m), 1298 (m), 1245 (br s), 1164 (w), 1133 (m), 1104 (s), 1079 (m), 1059 (w), 1022 (w), 996 (s), 939 (s), 852 (m), 843 (br s), 773 (w), 753 (m), 722 (m), 695 (m), 665 (m), 600 (m), 565 (w), 522 (w).

Isolation of [K(2.2.2-cryptand)][U(N$_2$Ph$_2$)(N(SiMe$_3$)$_2$)$_3$], 5.

From complex 1. A cold (−80 °C) solution of azobenzene (1.3 mg, 7.1 µmol, 1.1 eq) in THF-$d_8$ (0.5 mL) was added to cold (−80 °C) purple crystals of 1 (15.1 mg, 6.6 µmol, 1.0 eq), resulting in a red/brown solution. Slow diffusion of cold hexane into the reaction mixture at −40 °C resulted in a mixture of pink and dark red crystals, characterized as [K(2.2.2-cryptand)][U(O)(N(SiMe$_3$)$_2$)$_3$] by NMR and complex 5 by X-ray crystallography, respectively. Complex 5 has a similar solubility as [K(2.2.2-cryptand)][U(O)(N(SiMe$_3$)$_2$)$_3$], and is temperature sensitive rendering separation impossible.

From complex 2. A cold (−80 °C) solution of [U(N(SiMe$_3$)$_2$)$_3$] (25.0 mg, 34.8 µmol, 1.0 eq) and 2.2.2-cryptand (13.1 mg, 34.8 µmol, 1.0 eq) in THF (0.5 mL) was added to KC$_8$ (4.7 mg, 35 µmol, 1.0 eq). After a few minutes, the black mixture was filtered and added to cold (−80 °C) azobenzene (6.4 mg, 35 µmol, 1.0 eq), resulting in a red/brown solution, which was left to react for 15 min at −80 °C. Slow diffusion of hexane into the THF reaction mixture at −40 °C

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allowed to isolate a few crystals of complex 5. Upon warming up a THF solution of complex 5 to room temperature, it immediately starts to transform into complex 4.

$^1$H-NMR (400 MHz, THF-d$_8$, 233K): $\delta$ 28.5 (s, 2H, NPh), 19.2 (s, 2H, NPh), 17.8 (s, 2H, NPh), 10.2 (s, 2H, NPh), 3.8 (s, 12H, 2.2.2-cryptand), 3.7 (s, 12H, 2.2.2-cryptand), 2.8 (s, 12H, 2.2.2-cryptand), –14 (br s, 54H, NSiMe$_3$). $^1$H-NMR (400 MHz, THF-d$_8$, 273K): $\delta$ 38.7 (s, 2H, NPh), 23.8 (s, 2H, NPh), 16.1 (s, 4H, NPh), 9.1 (s, 2H, NPh), 3.7 (s, 12H, 2.2.2-cryptand), 3.6 (s, 12H, 2.2.2-cryptand), 2.7 (s, 12H, 2.2.2-cryptand), –12.0 (s, 54H, NSiMe$_3$). $^1$H-NMR (400 MHz, THF-d$_8$, 298K): $\delta$ 15.1 (s, 4H, NPh), 8.6 (s, 2H, NPh), 3.6 (s, 12H, 2.2.2-cryptand), 3.5 (s, 12H, 2.2.2-cryptand), 2.6 (s, 12H, 2.2.2-cryptand), –10.7 (s, 54H, NSiMe$_3$).
NMR Spectroscopy

Figure S1 Variable temperature $^1$H-NMR spectra of the reaction mixture of 1 and diphenylacetylene in 1:1 ratio in THF-$d_8$.

Figure S2 Variable temperature $^1$H-NMR spectra of the reaction mixture of 2 and diphenylacetylene in 1:1 ratio in THF-$d_8$. 

Complex 3
THF
$[K(2.2.2$-cryptand)$][U(O)[N(SiMe$_3$)$_3$]]$
Figure S3 Variable temperature $^1$H-NMR spectra of complex 3 in THF-$d_8$.

Figure S4 $^1$H-NMR spectra of complex 3 at room temperature in THF-$d_8$ over time.
Figure S5 Variable temperature $^1$H-NMR spectra of the reaction mixture of 1 and azobenzene in 1:1 ratio in THF-$d_8$.

Figure S6 Variable temperature $^1$H-NMR spectra of the reaction mixture of [K(2.2.2-cryptand)][U(O){N(SiMe$_3$)$_2$}] and azobenzene in 1:1 ratio in THF-$d_8$. 
Figure S7 \(^1^H\)-NMR spectrum of complex 4 in THF-\(d_8\) at room temperature.

Figure S8 Variable temperature \(^1^H\)-NMR spectra of complex 5 in THF-\(d_8\).
IR spectroscopy

The imido substituents in 4 show a band at 1245 cm\(^{-1}\) in the infrared spectrum, consistent with a U=N-C moiety. The energy of this absorption is similar to that found in previously reported uranium(VI) imido complexes.\(^6\)

X-ray Structure and Refinement Details

The diffraction data for the analysed crystal structures were collected at low temperature using Cu \(K\alpha\) radiation on a Rigaku SuperNova dual system in combination with Atlas type CCD detector. The data reduction and correction were carried out by CrysAlis\(^\text{Pro}\).\(^7\)

The solutions and refinements were performed by SHELXT\(^8\) and SHELXL\(^9\), respectively. The crystal structures were refined using full-matrix least-squares based on \(F^2\) with all non-H atoms defined in anisotropic manner. Hydrogen atoms were placed in calculated positions by means of the “riding” model.

The refinement of the crystal structure of compound 3 was quite straightforward, although the anisotropic behaviour of the \([\text{K}(2.2.2\text{-cryptand})]^+\) was far from being ideal and some restraints were needed (SIMU card) to get reasonable ADPs. The raw data of the crystal structure of 4 were treated for twinning (2 major domains were found) and the refinement was completed by using the HKLF 5 format (MREG 0, BASF = 0.192(2)).
The crystal structure of compound 5 displayed several problems; the data were treated for twinning (2 major domains were observed) and the final model showed disordered solvent (1 THF per ionic pair). The solvent was removed by using the SQUEEZE algorithm of PLATON and the refinement was completed by employing the HKLF 5 format (MERG 0, BASF = 0.342(2)). Some geometries and ADPS were corrected by restraints (SADI and RIGU cards, respectively).

| Compound | Formula | 3 | 4 | 5 |
|----------|---------|---|---|---|
|          |         | C₅₀H₁₀₀KN₃O₆Si₆U | C₄₈H₁₀₀KN₃O₆Si₆U | C₄₈H₁₀₀KN₃O₆Si₆U |
| Dₐₑₑₑ / g cm⁻³ | 1.321 | 1.351 | 1.264 |
| μ / mm⁻¹ | 9.065 | 8.476 |
| Formula Weight | 1313.01 | 1317.01 | 1317.01 |
| Colour | clear intense orange | lustrous intense black | clear dark brown |
| Shape | plate | needle | prism |
| Size / mm³ | 0.20×0.20×0.04 | 0.14×0.09×0.04 | 0.28×0.18×0.11 |
| T / K | 140.00(10) | 139.9(6) | 140.00(10) |
| Crystal System | monoclinic | monoclinic | triclinic |
| Space Group | P 2₁ / c | I 2 / a |
| a / Å | 15.66789(14) | 22.6297(5) | 11.4770(3) |
| b / Å | 17.47136(16) | 23.9733(5) | 16.6790(8) |
| c / Å | 24.16489(19) | 23.9063(5) | 19.0067(8) |
| α / ° | 90 | 90 | 103.478(4) |
| β / ° | 93.6596(8) | 92.9909(18) | 101.463(3) |
| γ / ° | 90 | 90 | 90.908(3) |
| V / Å³ | 6601.39(10) | 12951.7(5) | 3460.2(3) |
| Z | 4 | 8 | 2 |
| Z' | 1 | 1 | 1 |
| Wavelength / Å | 1.54184 | 1.54184 | 1.54184 |
| Radiation type | Cu Kα | Cu Kα | Cu Kα |
| θₘᵢₙ / | 3.123 | 3.688 | 3.938 |
| θₘₐₓ / | 72.677 | 72.788 | 72.725 |
| Measured Refl's. | 33861 | 14444 | 14136 |
| Ind't Refl's | 12806 | 14444 | 14136 |
| Refl's with I > 2σ(I) | 11775 | 7639 | 13270 |
| Rₑₑₑ | 0.0210 | . | . |
| Parameters | 640 | 642 | 617 |
| Restraints | 162 | 0 | 934 |
| Largest Peak | 1.943 | 4.553 | 5.937 |
| Deepest Hole | -1.067 | -1.422 | -5.122 |
| GoOF | 1.040 | 0.841 | 1.147 |
| wR₂ (all data) | 0.0665 | 0.1328 | 0.2818 |
| wR₂ | 0.0648 | 0.1186 | 0.2799 |
| R₁ (all data) | 0.0306 | 0.0934 | 0.1104 |
| R₁ | 0.0273 | 0.0502 | 0.1069 |
Computational details

All calculations were performed using the Becke’s 3-parameter hybrid functional\textsuperscript{11} combined with the non-local correlation functional provided by Perdew/Wang\textsuperscript{12} using Gaussian09 suite of programs.\textsuperscript{13} The U and Si atoms were represented with a small-core Stuttgart-Dresden relativistic effective core potential associated with their adapted basis set.\textsuperscript{14-16} Additionally, the Si basis set was augmented by a d-polarization function ($\alpha = 0.284$)\textsuperscript{17} to represent the valence orbitals. All the other atoms C, H, O and N were described with a 6-31G (d,p), double $\zeta$ quality basis set.\textsuperscript{18} The nature of the extrema (minimum) was established with analytical frequencies calculations and geometry optimizations were computed without any symmetry constraints. Intrinsic Reaction Paths (IRPs)\textsuperscript{19} were traced from the various transition structures to obtain the connected intermediates and the enthalpy energies were computed at $T = 298$ K in the gas phase.

Spin density

\begin{align*}
U_1 &= 3.129196 \\
U_2 &= 3.128229 \\
\end{align*}

Figure S10 Frontier molecular orbitals of complex 1.
Figure S1 Frontier molecular orbitals of azobenzene.
Spin Density
U1 = 2.393774
U2 = 2.954623
N-N = 0.79449

Figure S12 Frontier molecular orbitals of the transition state TS1 in the reaction of complex 1 with azobenzene.
Spin Density
U1 = 2.196227

Figure S13 Frontier molecular orbitals of complex 5.
Spin Density
\( U_1 = 2.158650 \)

**Figure S14** Frontier molecular orbitals of [K(2.2.2-cryptand)][U(O)(N(SiMe$_3$)$_2$)$_2$].
Figure S15 Frontier molecular orbitals of the transition state TS2 in the reaction of complex 1 or 2 with azobenzene.
Figure S16 Frontier molecular orbitals of complex 4.
Figure S17 Molecular orbital diagram of complex 2.
Figure S18 Unpaired spin density plot of complex 2 showing spin density centered on the uranium: U = 4.10.
Figure S19 Molecular orbital diagram of the transition state TS1 in the reaction of complex 2 with azobenzene.
Figure S20 Unpaired spin density plot of the transition state TS1 in the reaction of complex 2 with azobenzene, showing spin density shared between the uranium and the nitrogen: U1 = 3.10, N-N=0.70.
Cartesian coordinates of all optimized structures

| Complex | U-O-U |
|---------|-------|
| C       | 10.05322000  | 14.994433000 | 1.204168000 |
| Si      | 10.194999000 | 13.507342000 | 2.403679000 |
| C       | 10.062687000 | 11.972387000 | 1.270273000 |
| N       | 9.078062000  | 13.531901000 | 3.751316000 |
| U       | 9.976519000  | 13.860897000 | 6.005537000 |
| O       | 11.625026000 | 12.495802000 | 6.422622000 |
| U       | 13.269898000 | 11.127162000 | 6.857563000 |
| N       | 14.137411000 | 11.434268000 | 9.133345000 |
| Si      | 15.837659000 | 11.644321000 | 9.500265000 |
| C       | 16.362390000 | 13.480830000 | 9.537389000 |
| Si      | 7.386705000  | 13.256469000 | 1.689958000 |
| C       | 6.938966000  | 11.400788000 | 3.359410000 |
| Si      | 7.357627000  | 14.798166000 | 8.506679000 |
| C       | 7.374928000  | 16.455695000 | 7.579739000 |
| Si      | 10.668050000 | 16.205552000 | 6.215312000 |
| C       | 11.613270000 | 16.705594000 | 7.603790000 |
| C       | 13.222591000 | 17.643617000 | 7.166425000 |
| C       | 5.492885000  | 14.535507000 | 8.885007000 |
| C       | 8.156487000  | 15.080423000 | 10.218878000 |
| C       | 5.507069500  | 11.887520000 | 7.928951000 |
| C       | 7.475430000  | 11.430501000 | 9.785309000 |
| C       | 8.070594000  | 10.604639000 | 7.122353000 |
| C       | 5.824467000  | 11.458919000 | 7.263143000 |
| Si      | 10.336351000 | 17.432024000 | 5.009605000 |
| C       | 11.747176000 | 17.630573000 | 3.735573000 |
| C       | 8.733518000  | 17.086299000 | 4.050437000 |
| C       | 10.065667000 | 19.208394000 | 5.687288000 |
| N       | 15.120291000 | 11.442906000 | 5.282645000 |
| Si      | 15.693555000 | 13.068839000 | 4.977562000 |
| C       | 17.449473000 | 13.463846000 | 5.637240000 |
| N       | 12.545329000 | 8.786671000  | 6.651976000 |
| Si      | 12.820251000 | 7.565406000  | 7.875160000 |
| C       | 11.379423000 | 7.415236000  | 9.121591000 |
| C       | 14.406166000 | 7.882433000  | 8.871232000 |
| C       | 13.067916000 | 5.778665000  | 7.215627000 |
| Si      | 15.884483000 | 10.153959000 | 4.375685000 |
| C       | 15.847253000 | 8.499596000  | 5.307496000 |
| C       | 17.751273000 | 10.405282000 | 4.003474000 |
| C       | 15.092898000 | 9.883531000  | 2.658718000 |
| Si      | 11.621584000 | 8.295793000  | 5.246853000 |
| C       | 9.990519000  | 7.378510000  | 5.644610000 |
| C       | 11.156289000 | 9.792795000  | 4.181767000 |
| C       | 12.531203000 | 7.114188000  | 4.042299000 |
| C       | 12.115924000 | 15.219900000 | 8.667130000 |
| C       | 10.712953000 | 17.875506000 | 8.826145000 |
| C       | 16.966018000 | 10.747847000 | 8.263298000 |
| C       | 16.412663000 | 10.949422000 | 11.195868000 |
| C       | 15.774911000 | 13.552619000 | 3.128357000 |
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C  14.576459000  14.343878000  5.822350000
Si  13.028579000  11.541155000  10.485436000
C  13.272836000  12.073507000  11.607305000
C  13.083509000  10.056328000  11.694710000
C  11.226759000  11.609411000  10.905629000
H  9.112202000  14.995658000  0.647171000
H  10.872630000  14.947951000  0.475001000
C  12.239430000  12.708233000  3.654849000
H  12.653048000  13.537710000  2.143718000
H  9.077517000  11.885495000  0.799716000
H  10.253850000  11.051760000  1.832265000
H  7.278904000  13.446021000  0.835270000
H  5.708423000  13.711940000  1.602390000
H  7.160824000  10.925987000  4.319564000
H  7.517663000  10.875983000  2.592176000
C  9.760264000  10.763592000  0.631575000
H  9.411430000  9.608381000  7.480700000
C  5.738029000  11.658764000  6.191278000
H  5.640367000  10.387941000  7.418909000
H  7.181002000  10.378498000  9.888808000
H  10.722526000  10.609758000  4.764878000
H  12.020723000  12.195655000  3.641013000
H  10.417213000  9.479522000  3.434929000
H  11.929290000  7.000169000  3.131387000
H  10.164689000  6.437852000  6.178325000
C  9.328532000  7.998218000  6.254316000
H  9.463533000  7.136463000  4.712876000
C  10.452025000  7.129951000  8.614541000
H  10.131485000  15.948017000  1.733239000
H  12.214212000  14.476350000  3.568901000
H  6.922280000  15.000444000  1.609968000
H  6.275958000  15.208602000  4.470235000
H  6.532020000  13.920434000  5.659286000
H  5.199569000  13.797402000  4.484478000
H  5.030008000  12.010736000  7.773773000
H  6.739266000  12.033563000  10.327579000
H  8.445662000  11.557322000  10.271930000
C  5.290795000  13.671993000  9.526426000
H  4.916751000  14.415322000  7.961600000
H  5.113842000  15.427269000  9.401028000
H  9.220899000  15.314301000  10.127013000
H  8.807115000  14.183194000  10.840210000
H  7.673462000  15.910165000  10.750562000
H  8.071946000  16.405480000  6.716887000
H  8.376676000  16.699232000  7.217499000
H  7.028903000  17.265016000  8.235299000
H  9.744410000  17.469671000  9.131359000
H  10.544652000  18.873374000  8.411174000
H  7.868035000  17.268807000  4.695379000
H  8.688178000  16.049158000  3.706503000
H  8.655758000  17.749123000  3.179292000
H  10.952389000  19.634822000  6.166936000
H  9.240271000  19.241617000  6.405929000
|   |        |        |        |
|---|--------|--------|--------|
| H | 9.800180000 | 19.861400000 | 4.845581000 |
| H | 11.940138000 | 16.697496000 | 3.198988000 |
| H | 11.498500000 | 9.873695000 | 8.400380000 |
| H | 12.934713000 | 11.940138000 | 7.230456000 |
| H | 10.885411000 | 11.498500000 | 8.425089000 |
| H | 16.225130000 | 12.934713000 | 5.094147000 |
| H | 16.884288000 | 10.885411000 | 2.576490000 |
| H | 16.931070000 | 12.934713000 | 3.360294000 |
| H | 18.012946000 | 15.931070000 | 6.163441000 |
| H | 18.234287000 | 17.012946000 | 5.681330000 |
| H | 16.510289000 | 18.234287000 | 4.652727000 |
| H | 14.801833000 | 16.510289000 | 2.647855000 |
| H | 17.957683000 | 10.326432000 | 3.489606000 |
| H | 18.126879000 | 9.511399000 | 2.042209000 |
| H | 14.027314000 | 18.126879000 | 2.741063000 |
| H | 15.187078000 | 14.027314000 | 6.702331000 |
| H | 15.577413000 | 15.187078000 | 6.528748000 |
| H | 16.528870000 | 15.577413000 | 8.067678000 |
| H | 14.844048000 | 16.528870000 | 6.933016000 |
| H | 16.170606000 | 14.844048000 | 6.657565000 |
| H | 13.507741000 | 16.170606000 | 8.079076000 |
| H | 12.684735000 | 13.507741000 | 4.467067000 |
| H | 15.284708000 | 12.684735000 | 8.245090000 |
| H | 14.453812000 | 15.284708000 | 9.226796000 |
| H | 14.454923000 | 14.453812000 | 9.737352000 |
| H | 12.190069000 | 14.454923000 | 6.702331000 |
| H | 13.918871000 | 12.190069000 | 6.528748000 |
| H | 13.284497000 | 13.918871000 | 8.067678000 |
| H | 11.195928000 | 13.284497000 | 6.933016000 |
| H | 11.596961000 | 11.195928000 | 9.885170000 |
| H | 12.529845000 | 11.596961000 | 8.079076000 |
| H | 11.268475000 | 12.529845000 | 9.238640000 |
| H | 12.878266000 | 11.268475000 | 9.387739000 |
| H | 11.327445000 | 12.878266000 | 9.728813000 |
| H | 13.020030000 | 11.327445000 | 6.658354000 |
| H | 13.866740000 | 13.020030000 | 6.519183000 |
| H | 13.782719000 | 13.866740000 | 8.081849000 |
| H | 12.678321000 | 13.782719000 | 4.230131000 |
| H | 14.027601000 | 12.678321000 | 12.242936000 |
| H | 12.275424000 | 14.027601000 | 12.430106000 |
| H | 11.055744000 | 12.275424000 | 9.142706000 |
| H | 10.593799000 | 11.055744000 | 10.769429000 |
| H | 14.246604000 | 10.593799000 | 12.108504000 |
| H | 13.180837000 | 14.246604000 | 11.032315000 |
| H | 12.500680000 | 13.180837000 | 12.386320000 |
| H | 15.940383000 | 12.500680000 | 12.052896000 |
| H | 17.496145000 | 15.940383000 | 11.282712000 |
| H | 16.172378000 | 17.496145000 | 8.574791000 |
| H | 15.801191000 | 16.172378000 | 10.299016000 |
| H | 17.431812000 | 15.801191000 | 9.761319000 |
| H | 13.523014000 | 17.431812000 | 5.557757000 |
| H | 14.654043000 | 13.523014000 | 6.914104000 |
| H | 14.890965000 | 14.654043000 | 5.513550000 |
| H | 17.548660000 | 14.890965000 | 6.698851000 |
| H | 17.637447000 | 17.548660000 | 5.522675000 |
Complex Azobenzene

H 16.063465000 14.606801000 3.031897000

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TS U-O-U-Azo

U 10.091145364 13.723010080 5.904935245
U 13.507500000 10.766400000 7.307600000
Si 13.716100000 6.953400000 7.761100000
Si 15.775300000 13.011000000 5.699500000
Si 11.441271790 16.651469945 7.584732535
Si 7.366198830 15.058115609 8.146487810
Si 16.786350941 10.364158607 9.139045216
Si 10.939420837 13.108059813 2.451994697
Si 15.622500000 10.512900000 4.100300000
Si 14.765779250 11.584751753 10.857444151
Si 6.726362513 12.462793442 7.002138161
Si 7.979696870 13.106786635 2.813205261
Si 10.846990057 17.219971906 4.717062944
Si 11.810100000 8.048400000 5.759400000
O 11.522300000 12.449600000 6.700800000
N 15.083200000 11.404200000 5.513500000
N 15.123471423 10.929568149 9.262517550
N 7.932110260 13.716937825 7.178216430
N 9.567500864 13.301126861 3.512436535
N 10.817820440 16.090550973 6.053485653
N 13.058600000 8.369200000 6.960100000
N 11.731900000 10.750900000 9.354700000
N 11.303912737 9.701582261 8.781503476
C 14.334000000 7.348800000 9.516500000
C 12.475400000 5.514300000 8.053200000
| Element | X    | Y    | Z    |
|---------|------|------|------|
| C       | 15.136900000 | 6.080500000 | 6.825900000 |
| C       | 15.623000000 | 14.201200000 | 4.214800000 |
| C       | 17.662600000 | 13.045700000 | 6.048000000 |
| C       | 14.925400000 | 13.878400000 | 7.157600000 |
| C       | 11.457506178 | 15.224209388 | 8.829372048 |
| C       | 13.224182280 | 17.340844407 | 7.505632947 |
| C       | 10.426862964 | 18.021156924 | 8.462396264 |
| C       | 5.464330270  | 15.163526782 | 8.408411858 |
| C       | 17.085629575 | 9.431176420  | 7.379287756 |
| C       | 11.14631437 | 11.747713422 | 9.227828867 |
| C       | 13.66864593 | 9.132044489  | 10.497110674 |
| C       | 9.08641535  | 11.45587668 | 1.489387651  |
| C       | 11.49938312 | 14.43922623 | 1.086210911  |
| C       | 12.519687096 | 13.25068561 | 3.476174207  |
| C       | 13.983078389 | 10.303154060 | 12.034267981 |
| C       | 16.245727226 | 12.285115348 | 11.869166724 |
| C       | 11.438400000 | 9.627100000  | 4.789100000  |
| C       | 10.154700000 | 7.411900000  | 6.473000000  |
| C       | 17.439900000 | 10.838300000 | 3.565600000  |
| C       | 9.461824699  | 16.88884896 | 3.460841876  |
| C       | 12.508136968 | 17.229911736 | 3.771536360  |
| C       | 7.357893636 | 10.807424089 | 6.331992508  |
| C       | 6.146572353 | 11.645094174 | 8.637186986  |
| C       | 8.118398604 | 13.436057355 | 0.924655550  |
| C       | 6.841128663 | 14.489722603 | 3.445611654  |
| C       | 14.646600000 | 10.865500000 | 2.497900000  |
| C       | 13.651110096 | 13.11830346 | 10.824114645 |
| C       | 5.111940050  | 13.001686403 | 6.120139274  |
| C       | 7.311591402  | 11.328630452 | 3.038642908  |
| C       | 10.585529118 | 19.063430939 | 5.191568563  |
| C       | 12.264700000 | 6.738700000  | 4.355000000  |
| C       | 10.20278212 | 9.038405455  | 9.38772989  |
| C       | 8.899452380  | 9.354126677  | 9.002845634  |
| C       | 10.427541560 | 8.016027530  | 10.311427952 |
| C       | 7.822320398  | 8.648052039  | 9.538081245  |
| C       | 9.350180256  | 7.308861661  | 10.846128189 |
| C       | 8.047784366  | 7.624755331  | 10.459660166 |
| C       | 11.003600000 | 11.004300000 | 10.548700000 |
| C       | 10.898700000 | 10.048200000 | 11.559300000 |
| C       | 10.446500000 | 12.270700000 | 10.726100000 |
| C       | 10.236400000 | 10.358300000 | 12.746900000 |
| C       | 9.784700000  | 12.581300000 | 11.914500000 |
| C       | 9.679500000  | 11.625400000 | 12.924700000 |
| H       | 16.197900000 | 15.109900000 | 4.435700000  |
| H       | 17.909300000 | 13.945800000 | 6.625000000  |
| H       | 18.009500000 | 12.180600000 | 6.615700000  |
| H       | 15.314200000 | 14.897800000 | 7.263300000  |
| H       | 15.109600000 | 13.352900000 | 8.101500000  |
| H       | 13.843700000 | 13.948800000 | 6.993000000  |
| H       | 18.997947778 | 11.456588875 | 8.646335351  |
| H       | 18.440164610 | 11.922461074 | 10.257371456 |
| H       | 17.747874774 | 12.694185324 | 8.823564967  |
| H       | 18.438890070 | 8.942450714  | 10.352282515 |
| X  | Y  | Z  |
|----|----|----|
| 17.237107561 | 9.514587025 | 11.513815598 |
| 15.828955714 | 12.663698306 | 12.811779609 |
| 16.717584134 | 13.129194060 | 11.356749583 |
| 17.025420623 | 11.562418056 | 12.123144638 |
| 14.160035108 | 13.948292000 | 10.319395784 |
| 12.694903857 | 12.663698306 | 10.328071808 |
| 13.920981676 | 10.747684534 | 13.018427856 |
| 14.653677442 | 9.448080163 | 12.172056917 |
| 13.356883594 | 17.463952219 | 4.448144380 |
| 15.963829898 | 17.560343285 | 8.514010249 |
| 13.899321217 | 16.613975730 | 7.046947899 |
| 12.776555130 | 18.266826041 | 6.922509412 |
| 10.834834759 | 18.17311177 | 9.470791042 |
| 11.877471551 | 15.552431322 | 9.786583350 |
| 10.426078973 | 14.850038289 | 9.020452540 |
| 12.555619960 | 14.388173994 | 8.458742073 |
| 12.990500000 | 4.743800000 | 9.816533500 |
| 11.593400000 | 5.829200000 | 8.620500000 |
| 15.482000000 | 5.197000000 | 7.392800000 |
| 16.008300000 | 6.722100000 | 6.676300000 |
| 14.805900000 | 5.745600000 | 5.837800000 |
| 13.535300000 | 7.204200000 | 10.252000000 |
| 14.673000000 | 8.384500000 | 9.606100000 |
| 15.159600000 | 6.681800000 | 9.791100000 |
| 12.429700000 | 5.742700000 | 4.860300000 |
| 13.159100000 | 7.020500000 | 3.873100000 |
| 15.542200000 | 8.110600000 | 3.401300000 |
| 14.727200000 | 8.323900000 | 4.970100000 |
| 16.487600000 | 8.306600000 | 4.887200000 |
| 15.024500000 | 10.224600000 | 1.690900000 |
| 14.769900000 | 11.906900000 | 2.185200000 |
| 13.574500000 | 10.680800000 | 2.600600000 |
| 17.677000000 | 10.148100000 | 2.745500000 |
| 18.147800000 | 10.648300000 | 4.377400000 |
| 17.607200000 | 11.855200000 | 3.197200000 |
| 14.586000000 | 14.491800000 | 4.027800000 |
| 16.029000000 | 13.772900000 | 3.291900000 |
| 18.236000000 | 13.082000000 | 5.115300000 |
| 18.144250537 | 9.155633064 | 7.435544147 |
| 16.80739384 | 10.04533009 | 6.65775354 |
| 16.496643690 | 8.510928994 | 7.480047292 |
| 16.847678449 | 8.172690352 | 10.43207622 |
| 13.439178307 | 13.432226133 | 11.853931627 |
| 13.035732576 | 9.921715141 | 11.646185498 |
| 12.498372645 | 17.984585215 | 2.974549906 |
| 12.721842784 | 16.261362336 | 3.311573815 |
| 10.555419782 | 19.657698767 | 4.26867959 |
| 9.634406162 | 19.209996737 | 5.713705251 |
| 11.385952935 | 19.470397635 | 5.818420341 |
| 9.617620842 | 17.479059624 | 2.54980520 |
| 9.416893821 | 15.829116372 | 3.19206980 |
| 8.494814598 | 17.172103993 | 3.88916668 |
| 10.461766115 | 18.982316614 | 7.94267328 |
| 9.376741724 | 17.732756542 | 8.567242153 |
| 7.576147425 | 17.555238454 | 8.09491561 |
| 8.817523649 | 16.800648089 | 7.060909141 |
|     | X         | Y         | Z         |
|-----|-----------|-----------|-----------|
| H   | 7.142439939 | 16.910911243 | 6.498954588 |
| H   | 7.671898046 | 15.877547163 | 10.516469119 |
| H   | 7.810418575 | 14.111331183 | 10.436778398 |
| H   | 9.163761095 | 15.131349666 | 9.926021304  |
| H   | 5.248922590 | 16.054217215 | 9.013927113  |
| H   | 4.941180798 | 15.278611610 | 7.453307596  |
| H   | 5.036891763 | 14.300588191 | 8.928362856  |
| H   | 6.977412730 | 11.182382959 | 9.174002689  |
| H   | 5.665161957 | 12.364186256 | 9.308917347  |
| H   | 4.522055266 | 13.700627408 | 6.719670886  |
| H   | 5.808182206 | 14.337400437 | 3.108560406  |
| H   | 6.852450340 | 14.51879358  | 4.537508143  |
| H   | 7.189057470 | 15.452588542 | 3.056306336  |
| H   | 8.464275014 | 14.454418313 | 0.719602686  |
| H   | 12.531117640 | 14.191896061 | 4.039975025  |
| H   | 11.137592980 | 15.450908662 | 1.502512731  |
| H   | 12.130100000 | 5.044200000  | 7.127000000  |
| H   | 9.366000000 | 7.548100000  | 5.723800000  |
| H   | 9.852800000 | 7.961200000  | 3.768000000  |
| H   | 10.199200000 | 6.347600000  | 6.720900000  |
| H   | 11.432200000 | 6.658200000  | 3.724900000  |
| H   | 10.560600000 | 9.453100000  | 4.156100000  |
| H   | 12.271600000 | 9.891300000  | 4.130600000  |
| H   | 11.208000000 | 10.500700000 | 5.413200000  |
| H   | 5.414317158 | 10.858063497 | 8.415502135  |
| H   | 4.494255145 | 12.111283772 | 5.942774386  |
| H   | 5.306711121 | 13.469511572 | 5.152529208  |
| H   | 6.578378383 | 10.04624700  | 6.441865305  |
| H   | 7.602915034 | 10.870111022 | 5.266298334  |
| H   | 8.253629827 | 10.459781764 | 6.852296426  |
| H   | 6.275503065 | 11.242595549 | 2.687113430  |
| H   | 7.923087358 | 10.624498214 | 2.46326741   |
| H   | 7.341117377 | 11.010856165 | 4.084341506  |
| H   | 7.120547579 | 13.32647623  | 0.479845729  |
| H   | 8.786890459 | 12.738730180 | 0.408719292  |
| H   | 11.925708812 | 11.36054393 | 0.930127042  |
| H   | 10.913278590 | 10.600347749 | 2.166218351  |
| H   | 10.163383557 | 11.387801474 | 0.768737069  |
| H   | 13.387094812 | 13.264499194 | 2.809590389  |
| H   | 12.656283852 | 12.439326839 | 4.194626254  |
| H   | 12.122378401 | 14.290077702 | 0.599252383  |
| H   | 10.378878663 | 14.383846957 | 0.312800920  |
| H   | 8.722020427 | 10.160838884 | 8.276884666  |
| H   | 11.454182369 | 7.766885620 | 10.616317354 |
| H   | 6.795405936 | 8.897249581  | 9.233606595  |
| H   | 9.528232032 | 6.502507237  | 11.572401903 |
| H   | 7.198315387 | 7.068089762  | 10.881427741 |
| H   | 11.314200000 | 9.104000000 | 11.42700000  |
| H   | 10.529100000 | 13.024500000 | 9.929800000  |
| H   | 10.153200000 | 9.604500000  | 13.54330000  |
| H   | 9.345900000 | 13.580100000 | 12.05430000  |
| H   | 9.157300000 | 11.869600000 | 13.86110000  |

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Complex U=O
C    7.332285000  16.905065000  0.339528000
| Element | x-coordinate | y-coordinate | z-coordinate |
|---------|--------------|--------------|-------------|
| Si      | 7.261324000  | 15.664398000 | 1.791334000 |
| C       | 7.158158000  | 13.928017000 | 1.002242000 |
| N       | 5.964445000  | 15.988134000 | 2.928063000 |
| U       | 6.571012000  | 16.483392000 | 5.643261000 |
| O       | 8.963106000  | 15.761368000 | 2.631214000 |
| Si      | 4.292983000  | 15.786733000 | 2.453141000 |
| C       | 3.149955000  | 16.700296000 | 3.669487000 |
| C       | 3.862096000  | 16.483518000 | 0.725776000 |
| N       | 4.891073000  | 15.859525000 | 6.781992000 |
| Si      | 8.747792000  | 18.906723000 | 4.280734000 |
| C       | 4.901691000  | 13.637421000 | 8.942030000 |
| C       | 5.716690000  | 13.061387000 | 6.014680000 |
| Si      | 2.803416000  | 13.622520000 | 6.718530000 |
| C       | 7.361302000  | 19.894161000 | 4.280734000 |
| C       | 8.721547000  | 19.986712000 | 2.945119000 |
| C       | 5.720198000  | 19.616523000 | 3.357896000 |
| C       | 7.235248000  | 21.663225000 | 4.996130000 |
| C       | 9.107917000  | 17.332928000 | 7.779070000 |
| C       | 8.107733000  | 20.169620000 | 8.069300000 |
| H       | 7.341408000  | 13.246962000 | 6.231330000 |
| H       | 5.570612000  | 13.231256000 | 4.941796000 |
| H       | 5.484594000  | 12.007651000 | 6.213766000 |
| H       | 2.541666000  | 13.892311000 | 5.643317000 |
| H       | 2.070587000  | 12.533995000 | 6.767713000 |
| H       | 4.794803000  | 12.551404000 | 9.005080000 |
| H       | 2.341408000  | 17.936874000 | 0.705335000 |
| H       | 9.107733000  | 16.754643000 | 3.043157000 |
| H       | 4.180170000  | 17.525926000 | 0.624192000 |
| H       | 3.287880000  | 17.784565000 | 3.601104000 |
| H       | 3.328059000  | 16.390901000 | 4.706011000 |
| H       | 2.101865000  | 16.482113000 | 3.431550000 |
| H       | 2.066528000  | 14.084645000 | 7.335199000 |
| H       | 4.196547000  | 14.110943000 | 9.586358000 |
| H       | 5.915613000  | 13.911064000 | 9.204077000 |
| H       | 2.205148000  | 15.900945000 | 8.889267000 |
| Atom | x          | y          | z          |
|------|------------|------------|------------|
| H    | 1.728077000| 16.644168000| 7.353474000|
| H    | 1.946840000| 17.647682000| 8.798320000|
| H    | 6.124248000| 18.117380000| 10.074382000|
| H    | 5.053062000| 19.050460000| 10.058596000|
| H    | 6.124248000| 19.550320000| 9.314406000|
| H    | 5.053062000| 19.879213000| 8.431208000|
| H    | 8.031171000| 21.183849000| 7.665157000|
| H    | 4.865627000| 19.724651000| 4.034273000|
| H    | 5.674997000| 18.624960000| 2.893204000|
| H    | 5.610929000| 22.013624000| 5.419667000|
| H    | 6.470546000| 21.726975000| 5.777156000|
| H    | 6.956098000| 23.580600000| 4.194581000|
| H    | 8.081656000| 19.042938000| 2.397099000|
| H    | 8.497217000| 20.778316000| 2.194280000|
| H    | 9.482628000| 16.526184000| 7.145293000|
| H    | 8.215970000| 19.950707000| 8.286997000|
| H    | 9.852140000| 17.570390000| 8.550200000|
| H    | 8.783771000| 20.200323000| 8.930494000|
| H    | 10.375812000| 20.544512000| 5.726126000|
| H    | 10.896406000| 18.870817000| 5.469665000|
| H    | 11.134535000| 19.645382000| 7.046086000|
| H    | 9.701433000| 20.199372000| 3.835610000|

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Complex U-Azo

| Atom | x          | y          | z          |
|------|------------|------------|------------|
| U    | 13.732880000| 9.962291000| 8.010746000|
| Si   | 13.965937000| 6.391523000| 8.007384000|
| Si   | 14.580289000| 13.262829000| 7.223609000|
| Si   | 17.160995000| 9.530890000| 8.930505000|
| Si   | 14.746586000| 11.491467000| 4.805929000|
| Si   | 15.579376000| 10.690300000| 11.184238000|
| Si   | 12.139154000| 7.473534000| 5.892195000|
| N    | 14.396835000| 11.642604000| 6.527017000|
| N    | 15.580196000| 10.065457000| 9.523968000|
| N    | 13.311074000| 7.812565000| 7.182132000|
| N    | 11.688170000| 10.570404000| 8.079920000|
| N    | 11.872030000| 10.067861000| 9.306979000|
| C    | 14.267353000| 6.763609000| 9.845644000|
| C    | 12.845303000| 4.845915000| 8.060415000|
| C    | 15.574922000| 5.770004000| 7.192862000|
| C    | 13.887354000| 14.675529000| 6.146080000|
| C    | 16.400799000| 13.690624000| 7.578551000|
| C    | 16.656382000| 13.431297000| 8.872987000|
| C    | 17.138599000| 9.367557000| 7.047680000|
| C    | 18.624066000| 10.703960000| 9.303979000|
| C    | 17.747547000| 7.843690000| 9.610123000|
| C    | 13.851892000| 10.758280000| 11.968466000|
| C    | 16.597214000| 9.622818000| 12.403428000|
| C    | 11.540162000| 9.052343000| 5.030668000|
| C    | 10.531500000| 6.631711000| 6.468962000|
| C    | 16.326919000| 12.407010000| 4.238815000|
| C    | 15.048946000| 9.675600000| 4.300517000|
|   | 13.364887000 | 12.173140000 | 3.680462000 |
|---|--------------|--------------|-------------|
| C | 16.313902000 | 12.445267000 | 11.341793000 |
| C | 12.882420000 | 6.360429000  | 4.530180000  |
| C | 10.820460000 | 9.212739000  | 9.765973000  |
| C | 9.613573000  | 9.078887000  | 9.158315000  |
| C | 11.119541000 | 6.360429000  | 4.530180000  |
| C | 10.630749000 | 8.465468000  | 10.942519000 |
| C | 9.226829000  | 7.492400000  | 10.150240000 |
| C | 10.805297000 | 11.468072000 | 10.078340000 |
| C | 9.775840000  | 13.397105000 | 9.613573000  |
| C | 9.059166000  | 14.069467000 | 9.078887000  |
| H | 13.985060000 | 15.616131000 | 7.853660000  |
| H | 14.777580000 | 16.935420000 | 8.015695000  |
| H | 16.810109000 | 12.977936000 | 8.299209000  |
| H | 13.813652000 | 12.601390000 | 9.569117000  |
| H | 12.580654000 | 13.535475000 | 8.715915000  |
| H | 19.518110000 | 10.297384000 | 8.814563000  |
| H | 18.845195000 | 10.785593000 | 10.372390000 |
| H | 18.460781000 | 11.711321000 | 8.911047000  |
| H | 18.696950000 | 7.581045000  | 9.126457000  |
| H | 17.921018000 | 7.865797000  | 10.689280000 |
| H | 16.444540000 | 10.015668000 | 13.416459000 |
| H | 17.673598000 | 9.639969000  | 12.205884000 |
| H | 16.262314000 | 8.580387000  | 12.397551000 |
| H | 17.361478000 | 12.488381000 | 11.032273000 |
| H | 15.758303000 | 13.174296000 | 10.747019000 |
| H | 13.852797000 | 11.505526000 | 12.771004000 |
| H | 13.609669000 | 9.791197000  | 12.421484000 |
| H | 13.374064000 | 4.079999000  | 8.643231000  |
| H | 11.897114000 | 5.051982000  | 8.562212000  |
| H | 15.968527000 | 4.901188000  | 7.734385000  |
| H | 16.358164000 | 6.531439000  | 7.166730000  |
| H | 15.379636000 | 5.460744000  | 6.160429000  |
| H | 13.299172000 | 6.816479000  | 10.353954000 |
| H | 14.802457000 | 7.700019000  | 10.030331000 |
| H | 14.845666000 | 5.950647000  | 10.301275000 |
| H | 13.175954000 | 5.375776000  | 4.913320000  |
| H | 13.775288000 | 6.818914000  | 4.082342000  |
| H | 14.651959000 | 9.493653000  | 3.295200000  |
| H | 14.583653000 | 8.951589000  | 4.975347000  |
| H | 16.122002000 | 9.462184000  | 4.282459000  |
| H | 13.623126000 | 11.993876000 | 2.629277000  |
| H | 13.235067000 | 13.250580000 | 3.814097000  |
| H | 12.401050000 | 11.694713000 | 3.873839000  |
| H | 16.490078000 | 12.193951000 | 3.174814000  |
| H | 17.211882000 | 12.063588000 | 4.784347000  |
| H | 16.259538000 | 13.493461000 | 4.350381000  |
| H | 12.823943000 | 14.519856000 | 5.941967000  |
| H | 14.414022000 | 14.799909000 | 5.194960000  |
| H | 17.021955000 | 13.665219000 | 6.679046000  |
| H | 18.094570000 | 8.947356000  | 6.712416000  |
| Atom | Cartesian Coordinates (Å) |
|------|--------------------------|
| H    | 17.009368000 10.346306000 6.579282000  |
| H    | 16.351413000 8.705254000 6.679064000  |
| H    | 17.035303000 7.042691000 9.401366000  |
| H    | 16.262084000 12.760462000 12.391498000 |
| H    | 13.052672000 10.997265000 5.692190000  |
| H    | 12.633867000 8.705254000 5.692190000  |
| H    | 12.343170000 9.620513000 5.692190000  |
| H    | 11.021617000 9.701999000 5.740780000  |
| H    | 10.641724000 5.560047000 6.648020000  |
| H    | 10.832869000 11.261854000 11.439269000 |
| H    | 10.327220000 7.060051000 12.373666000 |
| H    | 8.141224000 10.549058000 11.310745000 |
| H    | 14.921653000 12.196088000 10.119490000 |
| H    | 11.191653000 7.276070000 9.946852000  |
| H    | 10.832869000 8.765642000 5.692190000  |
| H    | 10.641724000 5.560047000 6.648020000  |
| H    | 10.327220000 7.060051000 12.373666000 |
| H    | 8.141224000 10.549058000 11.310745000 |
| H    | 14.921653000 12.196088000 10.119490000 |
| H    | 11.191653000 7.276070000 9.946852000  |
| H    | 10.832869000 8.765642000 5.692190000  |
| H    | 10.641724000 5.560047000 6.648020000  |
| H    | 10.327220000 7.060051000 12.373666000 |
| H    | 8.141224000 10.549058000 11.310745000 |
| H    | 14.921653000 12.196088000 10.119490000 |
| H    | 11.191653000 7.276070000 9.946852000  |
| H    | 10.832869000 8.765642000 5.692190000  |
| H    | 10.641724000 5.560047000 6.648020000  |
| H    | 10.327220000 7.060051000 12.373666000 |
| H    | 8.141224000 10.549058000 11.310745000 |
| H    | 14.921653000 12.196088000 10.119490000 |
| H    | 11.191653000 7.276070000 9.946852000  |
| H    | 10.832869000 8.765642000 5.692190000  |
| H    | 10.641724000 5.560047000 6.648020000  |
| H    | 10.327220000 7.060051000 12.373666000 |
| H    | 8.141224000 10.549058000 11.310745000 |
| H    | 14.921653000 12.196088000 10.119490000 |
| H    | 11.191653000 7.276070000 9.946852000  |
| H    | 10.832869000 8.765642000 5.692190000  |
| H    | 10.641724000 5.560047000 6.648020000  |
| H    | 10.327220000 7.060051000 12.373666000 |
| H    | 8.141224000 10.549058000 11.310745000 |
| H    | 14.921653000 12.196088000 10.119490000 |
| H    | 11.191653000 7.276070000 9.946852000  |
| H    | 10.832869000 8.765642000 5.692190000  |
| H    | 10.641724000 5.560047000 6.648020000  |
| H    | 10.327220000 7.060051000 12.373666000 |
| H    | 8.141224000 10.549058000 11.310745000 |
| H    | 14.921653000 12.196088000 10.119490000 |
| H    | 11.191653000 7.276070000 9.946852000  |
| C       | 11.446336000 | 9.631518000 | 5.435604000 
| C       | 16.397539000 | 10.419930000 | 12.599768000 
| C       | 13.675990000 | 9.387368000 | 12.046509000 
| C       | 18.097646000 | 8.703699000 | 10.304064000 
| C       | 18.107472000 | 11.671796000 | 9.537104000 
| C       | 17.442944000 | 9.508207000 | 7.499025000 
| C       | 14.634553000 | 13.476194000 | 8.075941000 
| C       | 16.931922000 | 13.538471000 | 6.152704000 
| C       | 14.108859000 | 14.088515000 | 5.135326000 
| C       | 15.613548000 | 5.829831000 | 6.378133000 
| C       | 12.986943000 | 4.961514000 | 7.775264000 
| C       | 14.840401000 | 6.651416000 | 9.236351000 
| H       | 8.915726000 | 14.970590000 | 10.051646000 
| H       | 9.607836000 | 14.915732000 | 7.657680000 
| H       | 9.768248000 | 13.214640000 | 11.600134000 
| H       | 11.117332000 | 13.107960000 | 6.835028000 
| H       | 11.298115000 | 11.457541000 | 10.783507000 
| H       | 7.575792000 | 7.253477000 | 10.207044000 
| H       | 9.729791000 | 6.395807000 | 11.137018000 
| H       | 7.617967000 | 9.264825000 | 8.734173000 
| H       | 11.851744000 | 7.537095000 | 10.625311000 
| H       | 9.729561000 | 10.386403000 | 8.200154000 
| H       | 10.755913000 | 9.935924000 | 6.225133000 
| H       | 12.223355000 | 10.398931000 | 5.353190000 
| H       | 10.895172000 | 9.630392000 | 4.487093000 
| H       | 11.680404000 | 7.039560000 | 3.437888000 
| H       | 10.694520000 | 5.808348000 | 6.235680000 
| H       | 10.281549000 | 7.117803000 | 5.360230000 
| H       | 9.718475000 | 7.174844000 | 5.685309000 
| H       | 12.651828000 | 4.605767000 | 6.599054000 
| H       | 12.720846000 | 9.475087000 | 11.527933000 
| H       | 14.029640000 | 12.506046000 | 12.534881000 
| H       | 17.536268000 | 7.765089000 | 10.348588000 
| H       | 17.005344000 | 8.525655000 | 7.293645000 
| H       | 17.016308000 | 10.221510000 | 6.790922000 
| H       | 18.521429000 | 9.431946000 | 7.314069000 
| H       | 17.223464000 | 13.750163000 | 5.121393000 
| H       | 14.422903000 | 13.979460000 | 4.091834000 
| H       | 13.039171000 | 13.862352000 | 5.191203000 
| H       | 16.523092000 | 12.624159000 | 3.297419000 
| H       | 17.649088000 | 11.577405000 | 4.182549000 
| H       | 16.967837000 | 11.047966000 | 2.638458000 
| H       | 13.071015000 | 10.148612000 | 3.259687000 
| H       | 13.417536000 | 11.879462000 | 3.183389000 
| H       | 14.273591000 | 10.755668000 | 2.114312000 
| H       | 16.834633000 | 8.754211000 | 4.748767000 
| H       | 15.155858000 | 8.238633000 | 4.976195000 
| H       | 15.797299000 | 8.489843000 | 3.336766000 
| H       | 13.342923000 | 7.644030000 | 3.563776000 
| H       | 12.922252000 | 6.057849000 | 4.222982000 
| H       | 15.528102000 | 5.829792000 | 9.468453000 
| H       | 15.363323000 | 7.596290000 | 9.409722000 
| H       | 14.010755000 | 6.609882000 | 9.949029000 
| H       | 15.284769000 | 5.656353000 | 5.348160000 
| H       | 16.448398000 | 6.535935000 | 6.341291000 
| H       | 15.991901000 | 4.879689000 | 6.775264000 

S34
H  12.103484000  5.197401000  8.178427000
H  13.518022000  4.134057000  8.065694000
H  14.006467000  8.345376000  11.979820000
H  13.528065000  9.627325000  13.106666000
H  13.521119000  12.557523000  10.839099000
H  15.159522000  9.382554000  12.779900000
H  17.294346000  10.998428000  12.362330000
H  17.694230000  9.382554000  12.779900000
H  17.294346000  10.998428000  12.362330000
H  15.996746000  10.813274000  13.542652000
H  18.326507000  9.011979000  11.326412000
H  19.048916000  8.495786000  9.798416000
H  17.674021000  12.463613000  8.919281000
H  18.091311000  12.015767000  10.575755000
H  19.157303000  11.551351000  9.242853000
H  13.556530000  13.549659000  8.227796000
H  15.044565000  12.795508000  8.820775000
H  15.069757000  14.465113000  8.266381000
H  17.628668000  12.793816000  6.549598000
H  17.067183000  14.460498000  6.730872000
H  14.245320000  15.140212000  5.415418000

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Final product U-N5
H  20.530536000  20.954786000  -0.289173000
U  20.386110000  24.033844000  6.171136000
Si  17.254709000  22.333049000  6.754148000
Si  22.038558000  20.812526000  6.608492000
N  20.770049000  23.295464000  4.456987000
N  18.072743000  23.589933000  5.836529000
N  21.833054000  22.480938000  7.149494000
C  20.713980000  22.692511000  3.214887000
C  21.832770000  22.663210000  2.355980000
H  22.751658000  23.141436000  2.681022000
C  21.759491000  22.048107000  1.114740000
C  22.637400000  22.041060000  0.468837000
C  20.580678000  21.436739000  0.683738000
C  19.468128000  21.450745000  1.526698000
H  18.651373000  20.974773000  1.213384000
C  19.529573000  22.065576000  2.772350000
H  18.672741000  22.076010000  3.438035000
C  18.297213000  21.816062000  8.257837000
H  18.208609000  22.561786000  9.053672000
H  17.932596000  20.857494000  8.646934000
H  19.364282000  21.709020000  8.040034000
C  15.544993000  22.817163000  7.463507000
H  14.806537000  23.007393000  6.677827000
H  15.169528000  21.982883000  8.069364000
H  15.592188000  23.698984000  8.108681000
C  16.881284000  20.770860000  5.720383000
H  17.766345000  20.401484000  5.196976000
H  16.516198000  19.967488000  6.372317000
H  16.106225000  20.968617000  4.973525000
C  15.970221000  23.472705000  3.559593000
H  15.162108000  23.005149000  4.132187000
H  16.497808000  22.683710000  3.012387000
C  22.038478000  22.543301000  10.184771000
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| H       | 21.923740000 | 21.459956000 | 10.294742000 |
| H       | 21.044798000 | 22.992560000 | 10.264544000 |
| C       | 20.534910000 | 20.983150000 | 5.700017000  |
| H       | 20.220683000 | 20.688213000 | 4.837992000  |
| H       | 19.866692000 | 19.983813000 | 6.380040000  |
| C       | 22.209739000 | 19.570100000 | 8.060290000  |
| H       | 21.305043000 | 19.596749000 | 8.677982000  |
| H       | 22.293092000 | 18.557194000 | 7.646347000  |
| Si      | 17.136315000 | 24.509891000 | 4.667808000  |
| Si      | 20.824527000 | 27.648684000 | 6.034531000  |
| N       | 19.983517000 | 24.776700000 | 7.878305000  |
| C       | 19.375024000 | 26.049659000 | 5.553231000  |
| H       | 17.972156000 | 25.401289000 | 9.019748000  |
| H       | 17.392797000 | 25.113859000 | 8.214525000  |
| H       | 17.356233000 | 25.897032000 | 10.229456000 |
| C       | 18.279333000 | 25.440795000 | 3.464817000  |
| H       | 18.650180000 | 24.756780000 | 2.694824000  |
| C       | 17.114703000 | 26.239722000 | 2.968968000  |
| H       | 15.901850000 | 25.643143000 | 12.141600000 |
| C       | 18.123840000 | 25.651015000 | 10.147444000 |
| C       | 15.958530000 | 25.555350000 | 10.112196000 |
| H       | 16.466301000 | 26.407190000 | 6.211171000  |
| H       | 15.536572000 | 26.438513000 | 4.706114000  |
| H       | 15.123623000 | 25.279633000 | 5.976659000  |
| C       | 18.279333000 | 25.440795000 | 3.464817000  |
| H       | 18.119330000 | 26.273281000 | 11.340704000 |
| C       | 17.627520000 | 26.661420000 | 12.232896000 |
| C       | 17.356233000 | 25.897032000 | 10.229456000 |
| H       | 17.972156000 | 25.401289000 | 9.019748000  |
| H       | 17.392797000 | 25.113859000 | 8.214525000  |
| H       | 17.356233000 | 25.897032000 | 10.229456000 |
| C       | 19.500185000 | 26.146655000 | 11.286329000 |
| C       | 19.155240000 | 25.897404000 | 3.940882000  |
| H       | 15.504364000 | 24.136838000 | 2.820565000  |
| C       | 18.968441000 | 27.719304000 | 6.419962000  |
| H       | 18.734629000 | 28.727790000 | 6.783797000  |
| H       | 18.370633000 | 27.549597000 | 5.519121000  |
| H       | 18.655945000 | 27.011370000 | 7.188647000  |
| C       | 20.961087000 | 28.953000000 | 4.636390000  |
| H       | 20.354734000 | 28.644598000 | 3.777716000  |
| H       | 20.549635000 | 29.901769000 | 5.004123000  |
| H       | 21.974106000 | 29.149543000 | 4.278048000  |
| C       | 21.714394000 | 28.340040000 | 7.567325000  |
| H       | 21.369119000 | 29.364455000 | 7.773692000  |
| C       | 21.485504000 | 27.730643000 | 8.444243000  |
| H       | 22.481251000 | 26.244932000 | 2.714453000  |
| H       | 22.048272000 | 27.231615000 | 2.522754000  |
| H       | 21.767063000 | 25.490731000 | 2.372440000  |
| Si      | 22.841514000 | 22.976962000 | 8.514261000  |
| H       | 23.326486000 | 23.532324000 | 4.874780000  |
| H       | 22.647591000 | 22.907967000 | 11.020926000 |
| C       | 24.591615000 | 22.192135000 | 8.524847000  |
| H       | 25.145758000 | 22.485665000 | 7.626863000  |
| H       | 25.136270000 | 22.592939000 | 9.389526000  |
| C       | 24.614967000 | 21.102409000 | 8.596036000  |
| H       | 23.529799000 | 20.567355000 | 5.450120000  |
| H       | 24.461200000 | 20.940294000 | 5.884673000  |
| H  | 5.623286 13.607006 1.196170 |
| H  | 7.045567 10.974769 4.179072 |
| H  | 7.482220 10.843149 2.472197 |
| H  | 5.799970 11.160337 2.932765 |
| H  | 10.094861 11.250802 7.205202 |
| H  | 8.968506 11.158210 5.849279 |
| H  | 8.913532 9.923649 7.116832 |
| H  | 5.858814 11.430973 6.430257 |
| H  | 6.108910 10.154310 7.631276 |
| H  | 8.116949 10.431054 9.876002 |
| H  | 10.222261 15.779570 1.498108 |
| H  | 11.913568 14.574037 3.960686 |
| H  | 6.825723 14.907844 1.255867 |
| H  | 5.899233 15.152257 4.182976 |
| H  | 6.090225 13.835896 5.350162 |
| H  | 4.891825 13.695115 4.050714 |
| H  | 5.285717 11.655039 8.086907 |
| H  | 7.327018 11.914177 10.428067 |
| H  | 9.069329 11.909067 10.107790 |
| H  | 4.682756 14.184718 8.138923 |
| H  | 106.015961 17.572344 9.212312 |
| H  | 11.044396 18.825898 8.509492 |
| H  | 7.868087 17.710729 4.560267 |
| H  | 8.714333 16.637179 3.439263 |
| H  | 8.760783 18.391721 3.183738 |
| H  | 11.154749 19.788027 6.326606 |
| H  | 9.413200 19.552539 6.547115 |
| H  | 10.031560 20.264763 5.046194 |
| H  | 11.889214 16.953893 3.201873 |
| H  | 11.653769 18.704846 3.081439 |
| H  | 12.134789 14.102292 7.750010 |
| H  | 10.762471 14.511260 8.783881 |
| H  | 12.399369 14.977618 9.275115 |
| H  | 11.699654 17.731683 9.738505 |
| H  | 13.415585 18.068908 6.655235 |
| H  | 13.759932 16.372911 6.278800 |
| H  | 14.020917 16.991073 7.920407 |
| H  | 12.754293 18.035467 4.298702 |

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TS UII- Azo

| U  | 9.797122674 13.950015155 6.309662270 |
| Si | 7.672461674 13.040319155 3.460092070 |
| Si | 7.679860674 12.174402155 8.684301270 |
| Si | 6.865680674 15.013206155 8.259859270 |
| Si | 11.257452674 16.588405155 8.065392270 |
| Si | 10.565943674 17.435107155 5.244624270 |

S38
| Element | X              | Y              | Z              |
|---------|----------------|----------------|----------------|
| Si      | 10.576346674   | 13.481406155   | 2.867356270    |
| N       | 7.970376674    | 13.703266155   | 7.854871270    |
| N       | 10.563711674   | 16.201519155   | 6.499325270    |
| N       | 9.245868674    | 13.579966155   | 4.018983270    |
| N       | 12.011208326   | 12.542501845   | 6.895282730    |
| N       | 11.228759326   | 11.669947845   | 6.258561730    |
| N       | 5.018058674    | 14.521326155   | 8.187300270    |
| N       | 10.5417994674  | 14.841601155   | 1.525633270    |
| C       | 6.273310674    | 13.751659155   | 4.526111270    |
| C       | 7.228426674    | 13.564839155   | 1.674080270    |
| C       | 7.466253674    | 11.144584155   | 3.508828270    |
| C       | 12.176994674   | 17.458920155   | 4.223525270    |
| C       | 6.273310674    | 13.751659155   | 4.056988270    |
| C       | 7.228426674    | 13.564839155   | 1.674080270    |
| C       | 7.466253674    | 11.144584155   | 3.508828270    |
| C       | 12.176994674   | 17.458920155   | 4.223525270    |
| C       | 6.273310674    | 13.751659155   | 4.056988270    |
| C       | 7.228426674    | 13.564839155   | 1.674080270    |
| C       | 7.466253674    | 11.144584155   | 3.508828270    |
| C       | 12.176994674   | 17.458920155   | 4.223525270    |
| C       | 6.273310674    | 13.751659155   | 4.056988270    |
| C       | 7.228426674    | 13.564839155   | 1.674080270    |
| C       | 7.466253674    | 11.144584155   | 3.508828270    |
| C       | 12.176994674   | 17.458920155   | 4.223525270    |
| C       | 6.273310674    | 13.751659155   | 4.056988270    |
| C       | 7.228426674    | 13.564839155   | 1.674080270    |
| C       | 7.466253674    | 11.144584155   | 3.508828270    |
| C       | 12.176994674   | 17.458920155   | 4.223525270    |
| C       | 6.273310674    | 13.751659155   | 4.056988270    |
| C       | 7.228426674    | 13.564839155   | 1.674080270    |
| C       | 7.466253674    | 11.144584155   | 3.508828270    |
| C       | 12.176994674   | 17.458920155   | 4.223525270    |
| C       | 6.273310674    | 13.751659155   | 4.056988270    |
| C       | 7.228426674    | 13.564839155   | 1.674080270    |
| C       | 7.466253674    | 11.144584155   | 3.508828270    |
| C       | 12.176994674   | 17.458920155   | 4.223525270    |
| C       | 6.273310674    | 13.751659155   | 4.056988270    |
| C       | 7.228426674    | 13.564839155   | 1.674080270    |
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| C       | 12.176994674   | 17.458920155   | 4.223525270    |
| C       | 6.273310674    | 13.751659155   | 4.056988270    |
| C       | 7.228426674    | 13.564839155   | 1.674080270    |
| C       | 7.466253674    | 11.144584155   | 3.508828270    |
| C       | 12.176994674   | 17.458920155   | 4.223525270    |
| C       | 6.273310674    | 13.751659155   | 4.056988270    |
| C       | 7.228426674    | 13.564839155   | 1.674080270    |
| C       | 7.466253674    | 11.144584155   | 3.508828270    |
| C       | 12.176994674   | 17.458920155   | 4.223525270    |
| C       | 6.273310674    | 13.751659155   | 4.056988270    |
| C       | 7.228426674    | 13.564839155   | 1.674080270    |
| C       | 7.466253674    | 11.144584155   | 3.508828270    |
| H  | 8.222543674 | 10.637750155 | 2.903005270 |
| H  | 6.476456674 | 10.850204155 | 3.138860270 |
| H  | 10.037967674 | 11.719141555 | 9.476582270 |
| H  | 9.754599674 | 10.916281555 | 7.928772270 |
| H  | 9.070022674 | 10.236016155 | 9.415016270 |
| H  | 6.806510674 | 10.838939155 | 6.752452270 |
| H  | 6.313034674 | 10.109306155 | 8.291498270 |
| H  | 6.936840674 | 11.310224155 | 10.889178270 |
| H  | 10.632050674 | 15.840631555 | 1.962532270 |
| H  | 12.307438674 | 14.430025155 | 4.494230270 |
| H  | 7.264267674 | 14.653192155 | 1.558608270 |
| H  | 6.174044674 | 14.831283155 | 4.374502270 |
| H  | 6.44742674 | 13.565874155 | 5.590602270 |
| H  | 5.320609674 | 13.284486155 | 4.249167270 |
| H  | 5.476267674 | 11.544951155 | 7.671043270 |
| H  | 6.058789674 | 12.804500155 | 10.550842270 |
| H  | 7.737987674 | 12.870862155 | 11.12106270 |
| H  | 4.764756674 | 13.709742155 | 8.876375270 |
| H  | 4.73352674 | 14.207423155 | 7.178128270 |
| H  | 4.399427674 | 15.387084155 | 8.454712270 |
| H  | 8.194234674 | 15.986438155 | 10.171500270 |
| H  | 6.820067674 | 15.067854155 | 10.797043270 |
| H  | 6.566519674 | 16.676935155 | 10.107316270 |
| H  | 6.747137674 | 16.208375155 | 6.048566270 |
| H  | 8.056810674 | 16.862952155 | 7.043802270 |
| H  | 6.367637674 | 17.289729155 | 7.397282270 |
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| H  | 8.176627674 | 17.561910155 | 4.535383270 |
| H  | 8.96035674 | 16.171837155 | 3.764590270 |
| H  | 9.250550674 | 17.813062155 | 3.149050270 |
| H  | 11.258317674 | 19.568357155 | 6.461746270 |
| H  | 9.496316674 | 19.369520155 | 6.487748270 |
| H  | 10.310463674 | 19.895364155 | 5.007264270 |
| H  | 12.342143674 | 16.521668155 | 3.686569270 |
| H  | 12.148194674 | 18.269519155 | 3.484862270 |
| H  | 11.837601674 | 14.262661155 | 8.899573270 |
| H  | 10.150356674 | 14.673420155 | 9.288358270 |
| H  | 11.473149674 | 15.374010155 | 10.22156270 |
| H  | 10.715296674 | 17.973003155 | 10.07133270 |
| H  | 13.183746674 | 18.107378155 | 7.477927270 |
| H  | 13.684988674 | 16.413837155 | 7.403559270 |
| H  | 13.518447674 | 17.222082155 | 8.972534270 |
| H  | 13.043271674 | 17.627473155 | 4.872282270 |
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