Supporting Information

More effectively catalyzing the CO₂ fixation with aziridines: Computational screening of metal-substituted HKUST-1

Yan Jiang¹, Tian-ding Hu¹, Li-ying Yu¹ and Yi-hong Ding*²,¹

*Corresponding author

¹ Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, Changchun 130023, P. R. China.
² Key Laboratory of Carbon Materials of Zhejiang Province, College of Chemistry and Materials Engineering, Wenzhou University, Wenzhou 325035, P. R. China.

Tel: 86-13069218826
E-mail address: yhdd@jlu.edu.cn (Y.H. Ding)

1. Table S1. The energies (Hartrees) of M-HKUST-1 with different spin states. The minimum energies for each M-HKUST-1 are marked green. S2

2. Table S2. Relative Gibbs free energies (kcal/mol) for the stationary points along the reaction pathway for CO₂ fixation on M-HKUST-1 catalysts. S3

3. Table S3. The adsorption energies (kcal/mol) of M-HKUST-1 with NH₃, H₂O, aziridine and CO₂. S4

4. Table S4. The computed strain energies (in kcal/mol) of small-ring systems. S5

5. Table S5. The Coordinates of all stable intermediates and transition states. S7
**Table S1.** The energies (Hartrees) of M-HKUST-1 with different spin states. The minimum energies for each M-HKUST-1 are marked green.

| M-HKUST-1 | singlet  | triplet | quintet | septet   | nonet   | undecet | 13-et | 15-et |
|-----------|----------|---------|---------|----------|---------|---------|-------|-------|
| Fe        | -1003.5804 | -1003.6187 | -1003.6170 | -1003.6892 | -1003.6923 | -1003.5696 | -1003.4164 | -1003.2555 |
| Cr        | -929.3917 | -929.4450 | -929.4007 | -929.4821 | -929.5166 | -929.3483 | -929.1924 | -929.0746 |
| Ru        | -944.4922 | -944.5252 | -944.5034 | -944.4722 | -944.4307 | -944.2990 | -944.1413 | -943.9846 |
| Ti        | -873.0618 | -873.0812 | -873.0574 | -872.9157 | -872.7463 | -872.5847 | -872.4244 | -872.2652 |
| W         | -892.4703 | -892.4244 | -892.3563 | -892.3445 | -892.2906 | -892.1250 | -891.9583 | -891.7895 |
| V         | -899.50602 | -899.4972 | -899.5143 | -899.5266 | -899.4064 | -899.2487 | -899.0906 | -898.9115 |
| Mn        | -964.5513 | -964.6274 | -964.6200 | -964.6449 | -964.6894 | -964.7448 | -964.5840 | -964.4216 |
| Cu        | -1149.0179 | -1149.0489 | -1148.9111 | -1148.7332 | -1148.5716 | -1148.4067 | -1148.2438 | -1148.0614 |
| Sc        | -849.9176 | -849.9022 | -849.7432 | -849.5838 | -849.3848 | -849.2599 | -849.0714 | -848.8743 |
| Mo        | -891.9087 | -891.8843 | -891.7810 | -891.7754 | -891.8028 | -891.6396 | -891.4882 | -891.3106 |
| Zn        | -888.0134 | -887.8988 | -887.6896 | -887.5794 | -887.4066 | -887.2452 | -887.1133 | -886.9128 |
| Zr        | -850.0621 | -850.0544 | -850.0087 | -849.8605 | -849.6917 | -849.5231 | -849.3511 | -849.1643 |
| Tc        | -916.9132 | -916.9186 | -916.9120 | -916.8672 | -916.8616 | -916.8233 | -916.6643 | -916.5032 |
| Cd        | -852.9229 | -852.8036 | -852.6756 | -852.5230 | -852.3683 | -852.2208 | -852.0615 | -851.8721 |
| Rh        | -975.7757 | -975.7468 | -975.6921 | -975.6673 | -975.5087 | -975.3602 | -975.2032 | -975.0458 |
| Y         | -832.9032 | -832.8823 | -832.7232 | -832.5637 | -832.3788 | -832.2375 | -832.0185 | -831.8470 |
| Ag        | -1048.1770 | -1048.1723 | -1048.0162 | -1047.8594 | -1047.7167 | -1047.5386 | -1047.4069 | -1047.2742 |
| Nb        | -869.4452 | -869.4650 | -869.4161 | -869.4015 | -869.2421 | -869.0811 | -868.9212 | -868.7538 |
Table S2. Relative Gibbs free energies (kcal/mol) for the stationary points along the reaction pathway for CO$_2$ fixation on M-HKUST-1 catalysts.

|       | Cu  | Cr  | Mo  | W   | Ti  | Sc  | Ru  | Fe  | Zn  | Zr  | Cd  | Tc  | Y   | Rh  | Nb  | Ag  | Mn  | V   |
|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|       | 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00|
| cat+reactant |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Int$_0$ | -39.00| -34.57| -27.92| -27.89| -36.04| -28.68| -40.34| -79.88| -38.60| -31.84| -33.36| -41.16| -27.60| -40.98| -47.57| -34.96| -39.24| -72.05|
| Int$_1$ | -37.65| -32.66| -25.20| -25.07| -34.67| -26.32| -38.76| -78.80| -36.89| -30.79| -40.11| -25.23| -39.52| -45.70| -27.60| -40.98| -39.24| -63.72|
| Ts$_1$ | -4.75| 4.07| 12.58| 10.87| -5.35| 4.18| -5.51| -50.95| -8.60| -3.08| -0.99| -10.21| 5.79| -7.65| -12.42| 8.97| -7.48| -33.70|
| Int$_2$ | -10.53| -0.67| 12.18| 10.40| -5.52| -2.01| -15.23| -53.58| -12.27| -10.48| -3.46| -11.80| 1.77| -12.70| -20.97| -6.10| -10.33| -34.95|
| Int$_3$ | -7.34| 3.50| 15.50| 13.48| -1.90| 1.82| -11.52| -50.13| -8.61| -6.74| 0.38| -7.98| 4.19| -8.43| -11.37| -15.44| -6.64| -30.91|
| Ts$_2$ | -1.69| 6.08| 21.58| 20.01| 5.05| 11.13| 3.07| -39.57| -2.97| 4.36| 5.06| 0.80| 9.14| -1.52| -4.14| 10.67| -1.64| -29.64|
| Int$_4$ | -17.23| -18.81| -14.73| 0.43| -22.97| -18.30| -9.10| -73.53| -22.42| -23.39| -15.51| -28.59| -18.55| -11.04| -37.54| -9.16| -26.51| -58.52|
| Int$_5$ | -27.42| -25.01| -15.63| -15.94| -27.18| -24.61| -23.92| -74.63| -34.17| -28.62| -28.17| -28.97| -24.37| -24.01| -36.96| -21.37| -38.87| -54.38|
| Ts$_3$ | -12.17| -10.20| -1.47| -1.04| -7.06| -8.23| -9.11| -54.90| -17.23| -13.50| -10.85| -13.28| -9.65| -9.07| -21.21| -8.49| -21.28| -41.78|
| Int$_6$ | -48.19| -44.81| -37.88| -37.45| -46.28| -41.45| -44.93| -89.12| -46.49| -43.84| -41.59| -49.14| -41.87| -44.79| -55.55| -41.76| -48.75| -75.53|
| cat+product | -13.58| -13.58| -13.58| -13.58| -13.58| -13.58| -13.58| -13.58| -13.58| -13.58| -13.58| -13.58| -13.58| -13.58| -13.58| -13.58| -13.58| -13.58|
Table S3. The adsorption energies (kcal/mol) of M-HKUST-1 with NH$_3$, H$_2$O, aziridine and CO$_2$.

| M-HKUST-1 | NH$_3$-adsorption | H$_2$O-adsorption | aziridine-adsorption | CO$_2$-adsorption |
|-----------|-------------------|-------------------|----------------------|-------------------|
| Cu        | 40.06             | 30.19             | 39.00                | 23.87             |
| Sc        | 28.94             | 26.16             | 28.68                | 21.04             |
| Ti        | 34.04             | 28.58             | 36.04                | 22.24             |
| V         | 71.54             | 63.04             | 72.05                | 23.79             |
| Cr        | 34.76             | 28.21             | 34.57                | 22.78             |
| Mn        | 39.81             | 29.19             | 39.24                | 21.31             |
| Fe        | 80.20             | 70.97             | 79.88                | 17.64             |
| Zn        | 37.66             | 29.66             | 38.60                | 20.43             |
| Y         | 29.98             | 26.41             | 27.60                | 22.63             |
| Zr        | 31.25             | 28.59             | 31.84                | 23.18             |
| Nb        | 46.47             | 43.05             | 47.57                | 27.55             |
| Mo        | 28.62             | 22.61             | 27.92                | 21.21             |
| Tc        | 39.73             | 31.98             | 41.16                | 21.48             |
| Ru        | 40.47             | 29.05             | 40.34                | 21.49             |
| Rh        | 41.40             | 29.11             | 40.98                | 22.58             |
| Ag        | 34.62             | 28.26             | 34.96                | 22.39             |
| Cd        | 32.35             | 25.92             | 33.36                | 19.17             |
| W         | 27.76             | 22.59             | 27.89                | 21.54             |
### Table S4. The computed strain energies (in kcal/mol) of small-ring systems.

| systems | Ring strain energy (kcal/mol) |
|---------|-----------------------------|
|         | literature | this work |
|         | experiment | B3LYP/6-311++G(d,p)//B3LYP/6-31G(d) | B3LYP/6-311++G(d,p)//B3LYP/6-31G(d) |
| ![triangle](image1.png) | 54.5 | 54.0 | 54.16 |
| ![triangle](image2.png) | 27.5 | | 25.91 |
| ![square](image3.png) | 26.3 | | 25.64 |
| ![triangle](image4.png) | 26.3 | | 26.06 |
| ![triangle](image5.png) | 26.7 | | 25.34 |
| ![triangle](image6.png) | | | 25.15 |
| CH₃ |  | 23.68 |
|-----|---|-------|
| N   |   |       |
| CH₃ |   |       |
S5. The Coordinates of all stable intermediates and transition states.

**Aziridine**

| Atom | C1 | C2 | C3 | C4 | C5 | C6 |
|------|----|----|----|----|----|----|
| C    | -2.45349300 | 1.42176700 | 1.29537900 |
| C    | -2.58742700 | 1.94728400 | -0.08800700 |
| H    | -1.71110100 | 1.85536000 | 1.96132400 |
| H    | -3.32652400 | 0.96976900 | 1.75944500 |
| H    | -3.56912100 | 1.80579600 | -0.53833200 |
| C    | -1.78219200 | 3.12058600 | -0.59437900 |
| H    | -1.58026100 | 3.02147300 | -1.66786700 |
| H    | -2.33883100 | 4.05433400 | -0.43320500 |
| H    | -0.82050400 | 3.19407300 | -0.07724000 |
| N    | -1.88276500 | 0.66831600 | 0.15574700 |
| C    | -2.79543300 | -0.43723429 | -0.16936171 |
| H    | -2.71987572 | -0.66736602 | -1.21158553 |
| H    | -2.53063351 | -1.29938557 | 0.40637815 |
| H    | -3.80011250 | -0.14967119 | 0.06047860 |

**Oxazolidinone**

| Atom | C1 | C2 | C3 | C4 | C5 | C6 | C7 |
|------|----|----|----|----|----|----|----|
| C    | -3.97000400 | 0.82393800 | -0.59854500 |
| C    | -3.48050400 | -0.61106400 | -0.35558700 |
| H    | -4.20843200 | 1.00580100 | -1.65927200 |
| H    | -4.85551200 | 1.04504600 | 0.00237000 |
| H    | -3.74831800 | -0.92774500 | 0.65688300 |
| C    | -3.92332100 | -1.64193800 | -1.36976400 |
| H    | -3.63271900 | -1.34346500 | -2.38438700 |
| H    | -3.47529000 | -2.61702500 | -1.14890800 |
| H    | -5.01389200 | -1.72834600 | -1.30921300 |
| N    | -2.79135000 | 1.59168600 | -0.20107400 |
| C    | -1.68009400 | 0.81228300 | -0.21592100 |
| O    | -2.01138400 | -0.48020100 | -0.37680000 |
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| O       | -0.51710900 | 1.20970300 | -0.09749000 |
| C       | -2.74179400 | 3.03691600 | -0.23111000 |
| H       | -1.74524800 | 3.35781000 | 0.07907900  |
| H       | -2.94233000 | 3.41930300 | -1.24354700 |
| H       | -3.49115500 | 3.45023600 | 0.45307200  |

**Cu-HKUST-1**

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Cu     | 0.00180900 | -0.00236500 | -1.27354000 |
| Cu     | -0.00204600 | 0.00228300 | 1.27404200  |
| O       | -1.37562600 | 1.42589500 | -1.14024000 |
| O       | 1.37891200  | -1.42954600 | -1.13387900 |
| O       | -1.42678200 | -1.37926200 | -1.13599000 |
| O       | 1.42930000  | 1.37575000 | -1.13651500 |
| O       | 1.42629800  | 1.37854600 | 1.13643600  |
| O       | -1.42879200 | -1.37567400 | 1.13695700  |
| O       | 1.37593000  | -1.42576900 | 1.13903200  |
| O       | -1.37889100 | 1.42979600  | 1.13272800  |
| C       | -1.76375000 | 1.82820000 | -0.00504300 |
| C       | 1.76442600  | -1.82761700 | 0.00384000  |
| C       | -1.82811200 | -1.76404500 | 0.00073500  |
| C       | 1.82791600  | 1.76392100 | 0.00000800  |
| H       | -2.52805900 | 2.61929000 | -0.00752400 |
| H       | 2.61853200  | 2.52871800 | 0.00018700  |
| H       | -2.61901000 | -2.52857900 | 0.00132400  |
| H       | 2.52973200  | -2.61770400 | 0.00597900  |

**Cu-Int**

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Cu     | 0.00181100 | -0.00236400 | -1.27354000 |
| Cu     | -0.00204800 | 0.00228200 | 1.27404200  |
| O       | -1.37661800 | 1.42493800 | -1.14024000 |
| O       | 1.37990600  | -1.42858600 | -1.13387900 |
Cu-Int$_1$
Cu 0.48468200 0.23666600 -3.13758000
Cu 0.50244100 0.24293400 -0.42100400
O -1.00413900 1.54466700 -3.13703100
O 1.97262300 -1.07965000 -3.13995900
O -0.82054300 -1.24317000 -3.11611700
O 1.78935000 1.71029800 -3.06818500
O 2.08563900 1.54937800 -0.81188800
O -1.08043000 -1.04974800 -0.86194200
O 1.78658200 -1.31962500 -0.88572000
O -0.76663200 1.84938800 -0.89561100
C -1.26743600 2.08510800 -2.01777900
C 2.25893400 -1.58939600 -2.01436200
C -1.34164600 -1.52396200 -1.99520100
C 2.32532000 2.00660400 -1.95699800
H -2.03931000 2.86025100 -2.04795700
H 3.10734300 2.77326100 -2.04024600
H -2.12667900 -2.28768000 -2.03910900
H 3.02212400 -2.37322200 -2.03445400
C -1.09546900 -0.19387400 2.23911900
C 0.17674000 -0.84710200 2.63822200
H -1.72331800 -0.65440600 1.48157600
H -1.60202400 0.40469000 2.99330300
H 0.49131900 -0.61829400 3.65653400
C 0.61505500 -2.19356100 2.11617600
H 1.70881700 -2.26300500 2.06946400
H 0.24870900 -2.97614300 2.79318300
H 0.22225700 -2.38453800 1.11411700
N 0.19601800 0.32678300 1.72868900
Br -1.37904100 -0.02710900 5.96760600
|   |   |   |   |
|---|---|---|---|
| C | 0.64904900 | 1.59137800 | 2.32960000 |
| H | 1.73771400 | 1.66181800 | 2.23229300 |
| H | 0.19439000 | 2.42363100 | 1.78263500 |
| H | 0.37104600 | 1.65646900 | 3.39064700 |

**Cu-Ts₁**

|   |   |   |   |
|---|---|---|---|
| Cu | 0.00181100 | -0.00236400 | -1.27354000 |
| Cu | -0.00204800 | 0.00228200 | 1.27404200 |
| O  | -1.37661800 | 1.42493800 | -1.14024000 |
| O  | 1.37990600 | -1.42858600 | -1.13387900 |
| O  | -1.42582200 | -1.38025400 | -1.13599000 |
| O  | 1.42834200 | 1.37674400 | -1.13651500 |
| O  | 1.42533800 | 1.37953800 | 1.13643600 |
| O  | -1.42783400 | -1.37666800 | 1.13695700 |
| O  | 1.37692200 | -1.42481100 | 1.13903200 |
| O  | -1.37988600 | 1.42883600 | 1.13272800 |
| C  | -1.76502200 | 1.82697200 | -0.00504300 |
| C  | 1.76569700 | -1.82638900 | 0.00384000 |
| C  | -1.82688400 | -1.76531700 | 0.00073500 |
| C  | 1.82668800 | 1.76519300 | 0.00000800 |
| H  | -2.52988100 | 2.61753000 | -0.00752400 |
| H  | 2.61677200 | 2.53054000 | 0.00018700 |
| H  | -2.61725000 | -2.53040100 | 0.00132400 |
| H  | 2.53155300 | -2.61594300 | 0.00597900 |
| C  | -1.62425912 | 0.23965603 | 4.20454873 |
| C  | -0.36037412 | 0.95614606 | 4.61766992 |
| H  | -2.35417205 | -0.88284635 | 3.71053274 |
| H  | -2.08526277 | 0.39920819 | 4.96183405 |
| H  | 0.33841655 | -0.40330084 | 5.22939433 |
| C  | 0.10680755 | -2.22319800 | 3.95358971 |
| Atom | x      | y      | z      |
|------|--------|--------|--------|
| H    | 0.61595091 | -2.00698959 | 3.00681878 |
| H    | 0.80272959  | -2.74739794  | 4.61297772 |
| H    | -0.73837232 | -2.88591938 | 3.74615124 |
| N    | -0.72807971  | 0.45283396  | 3.24669658 |
| Br   | -1.065888694 | -1.99200048 | 6.97431528 |
| C    | -0.35910865  | 1.80964676  | 3.63944593 |
| H    | 0.52913691   | 2.12952140  | 3.08828523 |
| H    | -1.18629866  | 2.49262018  | 3.39852700 |
| H    | -0.15821883  | 1.87464208  | 4.71938177 |

**Cu-Int₂**

| Atom | x      | y      | z      |
|------|--------|--------|--------|
| Cu   | 0.48333000  | 0.26467500  | -3.04101500 |
| Cu   | 0.54975600  | 0.12016800  | -0.12779200 |
| O    | -1.03307500  | 1.52354500  | -3.12879300 |
| O    | 2.00533200   | -1.01190100 | -3.07045300 |
| O    | -0.76894300  | -1.24794000 | -3.02546400 |
| O    | 1.75063300   | 1.75781900  | -3.05544600 |
| O    | 2.23811100   | 1.40700500  | -0.85582900 |
| O    | -1.20302700  | -1.00543700 | -0.79999500 |
| O    | 1.67968400   | -1.46975600 | -0.86725100 |
| O    | -0.65859800  | 1.93797000  | -0.92737700 |
| C    | -1.23831600  | 2.11087200  | -2.01336500 |
| C    | 2.23180400   | -1.61760400 | -1.98034000 |
| C    | -1.36621900  | -1.50641400 | -1.93289200 |
| C    | 2.36549000   | 1.97144100  | -1.95990300 |
| H    | -2.03931000  | 2.86025100  | -2.04795700 |
| H    | 3.10734300   | 2.77326100  | -2.04024600 |
| H    | -2.12667900  | -2.28768000 | -2.03910900 |
| H    | 3.02212400   | -2.37322200 | -2.03445400 |
| C    | -0.92679500  | 0.19403600  | 2.41513200 |
|     | X     | Y     | Z     |    |
|-----|-------|-------|-------|----|
| C   | -0.42493300 | -0.77238600 | 3.50013000 |
| H   | -1.60276600 | -0.34377900 | 1.73907500 |
| H   | -1.48750100 | 1.01862700   | 2.88121200 |
| H   | 0.31597700  | -0.28670600  | 4.13666800 |
| C   | 0.05564400  | -2.11396600  | 2.98506200 |
| H   | 0.87069600  | -1.93779800  | 2.27266600 |
| H   | 0.42422700  | -2.74851000  | 3.79748600 |
| H   | -0.74521300 | -2.64102800  | 2.45607200 |
| N   | 0.23264700  | 0.66706300   | 1.68057500 |
| Br  | -1.97088700 | -1.10800500  | 4.86617500 |
| C   | 0.65131400  | 1.99577200   | 2.07870100 |
| H   | 1.55144400  | 2.28276100   | 1.52919800 |
| H   | -0.13678100 | 2.74105000   | 1.87082800 |
| H   | 0.86778100  | 2.03761300   | 3.16223500 |

**Cu-Int$_3$**

|     | X     | Y     | Z      |    |
|-----|-------|-------|--------|----|
| Cu  | 0.46237700 | 0.39494900 | -3.08933000 |
| Cu  | 0.56960500 | 0.29842200 | -0.17532400 |
| O   | -0.75002600 | 1.94884300 | -3.16926000 |
| O   | 1.68774000 | -1.16957400 | -3.12750600 |
| O   | -1.07026300 | -0.82577800 | -3.08803000 |
| O   | 2.01199000 | 1.59715400 | -3.08353200 |
| O   | 1.77400400 | 2.02909700 | -0.85750500 |
| O   | -0.76717600 | -1.31872600 | -0.88238900 |
| O   | 2.13046800 | -0.86666100 | -0.91907400 |
| O   | -1.19060300 | 1.58571100 | -0.97039100 |
| C   | -1.33553800 | 2.17291200 | -2.05677200 |
| C   | 2.27509300 | -1.41952300 | -2.03219600 |
| C   | -1.31891400 | -1.42982600 | -1.99733100 |
| C   | 2.28559800 | 2.18056100 | -1.98587800 |
H  -2.05417100  3.00146600  -2.09413100
H   3.09248200  2.91447600  -2.08642000
H  -2.14154000 -2.14646500  -2.08528300
H   3.00726300 -2.23200700  -2.08062800
C  -1.16533300  0.03143900  2.14757500
C  -0.72535900 -1.09535800  3.09250700
H  -1.74351900  0.72819500  2.69005500
H  -0.14161600 -0.70056500  3.92566600
H  -0.05327200 -2.27687500  2.42352000
H   0.89470200 -1.93888100  1.98896000
H   0.15543500 -3.07716200  3.13998100
H  -0.66827700 -2.66611000  1.60717900
N    0.01586700  0.70230800  1.62254900
Br  -2.42762700 -1.78312800  4.09182700
C    3.16361000  0.21294400  3.12161700
O    3.04391300  1.24418000  3.59912500
O    3.61520100 -0.82989800  2.68161600
C    0.09948500  2.09142400  2.03688300
H    0.28923900  2.16762100  3.12374800
H    0.91551500  2.59149200  1.50785200
H  -0.84077700  2.63003000  1.82268500

\textbf{Cu-Ts}_2

Cu   0.00181100 -0.00236400  -1.27354000
Cu  -0.00204800  0.00228200   1.27404200
O  -1.37661800  1.42493800  -1.14024000
O    1.37990600 -1.42858600  -1.13387900
O  -1.42582200 -1.38025400  -1.13599000
O    1.42834200  1.37674400  -1.13651500
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| O | 1.42533800 | 1.37953800 | 1.13643600 |
| O | -1.42783400 | -1.37666800 | 1.13695700 |
| O | 1.37692200  | -1.42481100 | 1.13903200 |
| O | -1.37988600 | 1.42883600  | 1.13272800 |
| C | -1.76502200 | 1.82697200  | -0.00504300 |
| C | 1.76569700  | -1.82638900 | 0.00384000 |
| C | -1.82688400 | -1.76531700 | 0.00073500 |
| C | 1.82668800  | 1.76519300  | 0.00000800 |
| H | -2.52988100 | 2.61753000  | -0.00752400 |
| H | 2.61677200  | 2.53054000  | 0.00018700 |
| H | -2.61725000 | -2.53040100 | 0.00132400 |
| H | 2.53155300  | -2.61594300 | 0.00597900 |
| C | -1.32601024 | -0.34963573 | 4.18037555 |
| C | -0.86160628 | -1.74014956 | 4.62378999 |
| H | -2.22181122 | -0.45299963 | 3.54949338 |
| H | -1.61908360 | 0.22276330  | 5.07167690 |
| H | -0.06595342 | -1.67400863 | 5.36432653 |
| C | -0.51210795 | -2.70980986 | 3.51582482 |
| H | 0.37031985  | -2.32739237 | 2.98778247 |
| H | -0.25803087 | -3.69515420 | 3.91919393 |
| H | -1.32937222 | -2.80893056 | 2.79595180 |
| N | -0.26917347 | 0.36792174  | 3.45788616 |
| Br| -2.40927520 | -2.54401820 | 5.75429730 |
| C | 1.54033980  | 0.48539828  | 4.48650958 |
| O | 1.44801205  | 1.56369134  | 4.99309418 |
| O | 2.10050663  | -0.54927090 | 4.28478523 |
| C | -0.63296418 | 1.79216781  | 3.46680037 |
| H | -0.75794490 | 2.12204603  | 4.47697866 |
| H | 0.14300430  | 2.36142242  | 2.99912302 |

s15
|   |    X     |    Y     |    Z     |
|---|---------|---------|---------|
| H | -1.54875192 | 1.92973064 | 2.93078798 |

**Cu-Int₄**

|   |    X     |    Y     |    Z     |
|---|---------|---------|---------|
| Cu | 0.18551400 | -0.74088400 | -3.84670500 |
| Cu | 0.18139600 | -0.70708200 | -1.11326800 |
| O  | -1.09388100 | 0.76906200 | -3.82499700 |
| O  | 1.46915300 | -2.24403000 | -3.80498500 |
| O  | -1.32271100 | -2.02262000 | -3.81071100 |
| O  | 1.68955700 | 0.54970900 | -3.84125000 |
| O  | 1.54745900 | 0.72878300 | -1.57712500 |
| O  | -1.17655600 | -2.23340000 | -1.54927400 |
| O  | 1.67500300 | -2.10142000 | -1.54190800 |
| O  | -1.31675700 | 0.60922800 | -1.56568700 |
| C  | -1.58470400 | 1.08193800 | -2.69577000 |
| C  | 1.95107000 | -2.56482000 | -2.67266300 |
| C  | -1.64185000 | -2.50881700 | -2.67901900 |
| C  | 2.00977500 | 1.01987000 | -2.70448300 |
| H  | -2.34765600 | 1.87415600 | -2.72263100 |
| H  | 2.79899700 | 1.78716000 | -2.71492000 |
| H  | -2.43502500 | -3.27377500 | -2.71378300 |
| H  | 2.71377800 | -3.35931700 | -2.70912800 |
| C  | 0.77451800 | 0.64247700 | 4.05973900 |
| C  | -0.05461400 | 1.93006200 | 4.18587600 |
| H  | 1.78069600 | 0.94565100 | 3.72678100 |
| H  | 0.88352400 | 0.16641000 | 5.03806000 |
| H  | -0.82525300 | 1.96719800 | 3.42262100 |
| C  | 0.75986000 | 3.20530000 | 4.24036600 |
| H  | 1.28159300 | 3.29133900 | 3.27865600 |
| H  | 0.12511600 | 4.08554700 | 4.37901700 |
| H  | 1.50196300 | 3.17832300 | 5.04753800 |
N 0.20793300 -0.32058800 3.13351300
Br -1.22920000 1.85202900 5.93531900
C 0.31409800 0.02852900 1.75857000
O 0.57958500 1.22217100 1.50293100
O 0.10708200 -0.92727900 0.92829000
C 0.19510100 -1.71709400 3.53446200
H -0.30103500 -2.29413300 2.75392100
H 1.21144400 -2.13137800 3.67076300
H -0.35462000 -1.83127700 4.47779300

Cu-Ts$_3$
Cu 0.00181100 -0.00236400 -1.27354000
Cu -0.00204800 0.00228200 1.27404200
O -1.37661800 1.42493800 -1.14024000
O 1.37990600 -1.42858600 -1.13387900
O -1.42582200 -1.38025400 -1.13599000
O 1.42834200 1.37674400 -1.13651500
O 1.42533800 1.37953800 1.13643600
O -1.42783400 -1.37666800 1.13695700
O 1.37692200 -1.42481100 1.13903200
O -1.37988600 1.42883600 1.13272800
C -1.76502200 1.82697200 -0.00504300
C 1.76569700 -1.82638900 0.00384000
C -1.82688400 -1.76531700 0.00073500
C 1.82668800 1.76519300 0.00000800
H -2.52988100 2.61753000 -0.00752400
H 2.61677200 2.53054000 0.00018700
H -2.61725000 -2.53040100 0.00132400
H 2.53155300 -2.61594300 0.00597900
C -0.17515370 0.32809417 6.98154920
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -0.55983745 | 1.77616895 | 6.74726491 |
| H       | 0.91279995  | 0.27609094 | 7.17487308 |
| H       | -0.68709370 | -0.06216886| 7.86145820 |
| H       | -1.53323434 | 1.97741138 | 6.33276329 |
| C       | 0.44383480  | 2.88607483 | 6.89785999 |
| H       | 1.12163019  | 2.86443265 | 6.03712829 |
| H       | -0.05212630 | 3.85781404 | 6.94164626 |
| H       | 1.02760563  | 2.75757980 | 7.81453370 |
| N       | -0.54562314 | -0.48010442| 5.82965044 |
| Br      | -1.75339293 | 2.23442044 | 8.99136483 |
| C       | -0.28456481 | 0.13543303 | 4.60354867 |
| O       | -0.07982801 | 1.38714223 | 4.68315940 |
| O       | -0.29171158 | -0.57623003| 3.55567370 |
| C       | -0.51097210 | -1.92155817| 5.96839357 |
| H       | -0.79936429 | -2.36536539| 5.01449403 |
| H       | 0.49564454  | -2.29126108| 6.23415502 |
| H       | -1.21302367 | -2.24058956| 6.74918985 |

**Cu-Int₅**

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Cu      | 0.18339400 | -0.74259700| -3.87486500|
| Cu      | 0.17344600 | -0.73570700| -1.21245900|
| O       | -1.09345600| 0.77644500 | -3.82808300|
| O       | 1.46412000 | -2.25982200| -3.81456000|
| O       | -1.33397800| -2.02177400| -3.81380800|
| O       | 1.70051600 | 0.53678200 | -3.82042900|
| O       | 1.53002600 | 0.75924400 | -1.56079800|
| O       | -1.16721600| -2.24861600| -1.55415800|
| O       | 1.68048200 | -2.09386400| -1.55391900|
| O       | -1.32997500| 0.59543100 | -1.57122000|
| C       | -1.58982200| 1.08002400 | -2.70047200|

S18
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 1.95154000 | -2.56840500 | -2.68460800 |
| C    | -1.64312700 | -2.51346700 | -2.68611700 |
| C    | 2.00743800  | 1.02688500  | -2.69144500 |
| H    | -2.34765600 | 1.87415600  | -2.72263100 |
| H    | 2.79899700  | 1.78716600  | -2.71492000 |
| H    | -2.43502500 | -3.27377500 | -2.71378300 |
| H    | 2.71377800  | -3.35931700 | -2.70912800 |
| C    | 0.34645600  | 0.85977300  | 3.99331100  |
| C    | -0.47118800 | 1.78403000  | 3.08058900  |
| H    | 1.36278500  | 1.24845200  | 4.17184500  |
| H    | -0.14932000 | 0.71884200  | 4.95727900  |
| H    | -1.53503200 | 1.69399900  | 3.32383100  |
| C    | -0.05307900 | 3.23748600  | 3.05435500  |
| H    | 1.00764400  | 3.33787500  | 2.79098800  |
| H    | -0.64919000 | 3.79628100  | 2.32677100  |
| H    | -0.22667800 | 3.65652600  | 4.05212200  |
| N    | 0.39603600  | -0.35455300 | 3.18367500  |
| Br   | -1.43473600 | 2.54659900  | 6.62080600  |
| C    | 0.14496700  | -0.07583300 | 1.87956000  |
| O    | -0.29651300 | 1.18482500  | 1.74437800  |
| O    | 0.28440000  | -0.85589000 | 0.93226900  |
| C    | 1.09710400  | -1.55123900 | 3.60758500  |
| H    | 1.07224300  | -2.28413900 | 2.79608700  |
| H    | 2.15081800  | -1.31854100 | 3.84955200  |
| H    | 0.61553700  | -1.97194300 | 4.49693100  |

**Cr-HKUST-1**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| Cr   | 0.001153  | 0.000016  | -1.227546 |
| Cr   | -0.001073 | 0.000007  | 1.227662  |
| O    | 0.661373  | 1.887448  | -1.128399 |
|      | 0.657030  | -1.888020  | -1.129762 |
|------|------------|------------|------------|
| O    | -1.886349  | 0.659893   | -1.130763  |
| O    | 1.889217   | -0.658485  | -1.127757  |
| O    | 1.886895   | -0.658365  | 1.130527   |
| O    | -1.889703  | 0.656761   | 1.127516   |
| O    | -0.659815  | -1.887984  | 1.128520   |
| O    | 0.655263   | 1.888711   | 1.129876   |
| C    | 0.846322   | 2.428668   | 0.000928   |
| C    | -0.846423  | -2.428591  | -0.000802  |
| C    | -2.428625  | 0.846301   | -0.002133  |
| C    | 2.428650   | -0.846415  | 0.001886   |
| H    | 1.207278   | 3.466225   | 0.001333   |
| H    | 3.466163   | -1.207495  | 0.003030   |
| H    | -3.466156  | 1.207332   | -0.003180  |
| H    | -1.207557  | -3.466086  | -0.001271  |

**Cr-Int<sub>0</sub>**

|      | 0.00142300 | -0.00056300 | -1.42449200 |
|------|------------|-------------|-------------|
| Cr   | -0.00142600| 0.00056800  | 1.42450700  |
| O    | 1.41783600 | 1.43657000 | -1.13278400 |
| O    | -1.41503700| -1.43786500| -1.13416300 |
| O    | -1.43589000| 1.41606900 | -1.13514200 |
| O    | 1.43856400 | -1.41680000| -1.13204600 |
| O    | 1.43694400 | -1.41497300| 1.13501600  |
| O    | -1.43963200| 1.41570900 | 1.13191400  |
| O    | -1.41674400| -1.43764600| 1.13289800  |
| O    | 1.41394000 | 1.43894700 | 1.13427300  |
| C    | 1.81109900 | 1.83946500 | 0.00099000  |
| C    | -1.81102900| -1.83953200| -0.00088000 |
| C    | -1.83952400| 1.81104300 | -0.00219600 |
|    |            |            |            |
|----|------------|------------|------------|
| C  | 1.83951800 | -1.81103700| 0.00207400 |
| H  | 2.58218600 | 2.62298100 | 0.00150500 |
| H  | 2.62286400 | -2.58229700| 0.00326900 |
| H  | -2.62287300| 2.58230000 |-0.00338100 |
| H  | -2.58234300| -2.62282500| -0.00139500|
| C  | 1.09947142 | 0.18367324 | 4.34105149 |
| C  | -0.13676431| 0.98165574 | 4.60408390 |
| H  | 1.86491278 | 0.56263855 | 3.66556485 |
| H  | 1.47362642 | -0.45420568| 5.14437840 |
| H  | -0.57887233| 0.83420523 | 5.59418048 |
| C  | -0.37773343| 2.34448124 | 3.99587563 |
| H  | -1.45126038| 2.53199631 | 3.86598469 |
| H  | 0.03055174 | 3.13523216 | 4.63827990 |
| H  | 0.09843079 | 2.41546085 | 3.01223530 |
| N  | -0.17431359| -0.17943147| 3.71711517 |
| C  | -0.82671820| -1.38074049| 4.22457706 |
| H  | -1.90175901| -1.32078129| 4.02014598 |
| H  | -0.42526816| -2.25675269| 3.70249601 |
| H  | -0.68651980| -1.52992238| 5.31143485 |

| Cr-Int_1 |
|----------|
| Cr       | 0.08731200 | 0.53568500 | -3.44254700 |
| Cr       | 0.12002100 | 0.61313700 | -0.50384500 |
| O        | 1.52195400 | 1.95525800 | -3.19101300 |
| O        | -1.35227600| -0.89689700| -3.34885100 |
| O        | -1.33787600| 1.96035900 | -3.21726700 |
| O        | 1.50392300 | -0.90524300| -3.28692600 |
| O        | 1.61410400 | -0.75958400| -1.02413800 |
| O        | -1.34577700| 2.04390800 | -0.94549900 |
| O        | -1.30409000| -0.82583200| -1.08487400 |

s21
| Atom |  X       |  Y       |  Z       |
|------|---------|---------|---------|
| O    | 1.52115700 | 2.09601700 | -0.92257900 |
| C    | 1.91055400 | 2.41920700 | -2.07575400 |
| C    | -1.71828400 | -1.26067200 | -2.18943400 |
| C    | -1.73697200 | 2.39009800  | -2.09116400 |
| C    | 1.95155600 | -1.22561900 | -2.14219000 |
| H    | 2.68287700 | 3.19922500  | -2.13557900 |
| H    | 2.72355500 | -2.00605300 | -2.13381500 |
| H    | -2.52218200 | 3.15854400  | -2.14046500 |
| H    | -2.48165200 | -2.04658100 | -2.13847900 |
| C    | -1.35771800 | -0.44607200 |  2.22384500 |
| C    | -0.09353600 | -1.20433600 |  2.35798300 |
| H    | -2.06077700 | -0.69073200 |  1.43089100 |
| H    | -1.77732500 | -0.03716900 |  3.14093900 |
| H    | 0.28094600  | -1.22641100 |  3.38393600 |
| C    | 0.24991800  | -2.41058300 |  1.51922900 |
| H    | 1.33294500  | -2.48702600 |  1.36369500 |
| H    | -0.07946900 | -3.30968600 |  2.05586500 |
| H    | -0.23862300 | -2.38938900 |  0.54130100 |
| N    | -0.08332900 |  0.16020000 |  1.74599400 |
| Br   | -0.36051900 | -1.00872300 |  5.93647400 |
| C    | 0.46702800  |  1.21451700 |  2.62429700 |
| H    | 1.54612600  |  1.29217600 |  2.44796600 |
| H    | -0.00002200 |  2.17361100 |  2.36798400 |
| H    | 0.29301700  |  0.99111900 |  3.68521900 |

**Cr-Ts**

| Cr   | 0.00142300 | -0.00056300 | -1.42449200 |
| Cr   | -0.00142600 |  0.00056800 |  1.42450700 |
| O    | 1.41783600  |  1.43657000 | -1.13278400 |
| O    | -1.41503700 | -1.43786500 | -1.13416300 |
| Atom | X             | Y             | Z             |
|------|---------------|---------------|---------------|
| O    | -1.43589000   | 1.41606900    | -1.13514200   |
| O    | 1.43856400    | -1.41680000   | -1.13204600   |
| O    | 1.43694400    | -1.41497300   | 1.13501600    |
| O    | -1.43963200   | 1.41570900    | 1.13191400    |
| O    | -1.41674400   | -1.43764600   | 1.13289800    |
| O    | 1.41394000    | 1.43894700    | 1.13427300    |
| C    | 1.81109900    | 1.83946500    | 0.00099000    |
| C    | -1.81102900   | -1.83953200   | -0.00080000   |
| C    | -1.83952400   | 1.81104300    | -0.00219600   |
| C    | 1.83951800    | -1.81103700   | 0.00207400    |
| H    | 2.58218600    | 2.62298100    | 0.00150500    |
| H    | 2.62286400    | -2.58229700   | 0.00326900    |
| H    | -2.62287300   | 2.58230000    | -0.00338100   |
| H    | -2.58234300   | -2.62282500   | -0.00139500   |
| C    | -1.13008064   | 0.06905772    | 4.22714351    |
| C    | 0.05174254    | -0.56738491   | 4.84767007    |
| H    | -1.80532175   | -0.62732209   | 3.72752057    |
| H    | -1.66931473   | 0.80094647    | 4.83354139    |
| H    | 0.67926597    | 0.05440597    | 5.47036055    |
| C    | 0.57172420    | -1.91069262   | 4.41198060    |
| H    | 1.20117132    | -1.81855083   | 3.51886557    |
| H    | 1.16708414    | -2.35127952   | 5.21529581    |
| H    | -0.25452753   | -2.58963198   | 4.18196148    |
| N    | -0.10128913   | 0.60101748    | 3.35078085    |
| Br   | -0.96863444   | -1.29352669   | 7.20480159    |
| C    | 0.24424535    | 1.99450351    | 3.61561141    |
| H    | 1.20181963    | 2.23733602    | 3.14746404    |
| H    | -0.53083409   | 2.64614518    | 3.18741412    |
| H    | 0.30817574    | 2.19420985    | 4.69583029    |
|     | X            | Y            | Z            |
|-----|--------------|--------------|--------------|
| Cr  | 0.09072500   | 0.63520100   | -3.29981500  |
| Cr  | 0.13565200   | 0.37235800   | -0.11826000  |
| O   | 1.42249500   | 2.12107900   | -3.20741600  |
| O   | -1.21399500  | -0.87435100  | -3.08685400  |
| O   | -1.44172300  | 1.97042300   | -3.36610600  |
| O   | 1.63840900   | -0.72779000  | -3.25810800  |
| O   | 1.40591800   | -1.01366900  | -1.02775000  |
| O   | -1.20422900  | 2.04671000   | -1.12296500  |
| O   | -1.44928200  | -0.93423600  | -0.81749100  |
| O   | 1.72036800   | 1.87169800   | -0.96254800  |
| C   | 1.94325500   | 2.39417000   | -2.07474900  |
| C   | -1.71372900  | -1.28159900  | -1.99299100  |
| C   | -1.72824900  | 2.39893700   | -2.19558200  |
| C   | 1.92770300   | -1.25189700  | -2.14425400  |
| H   | 2.68287700   | 3.19922500   | -2.13557900  |
| H   | 2.72355500   | -2.00605300  | -2.13381500  |
| H   | -2.52218200  | 3.15854400   | -2.14046500  |
| H   | -2.48165200  | -2.04658100  | -2.13847900  |
| C   | -1.02472900  | 0.02492600   | 2.60473200   |
| C   | -0.05810200  | -0.48061700  | 3.68604100   |
| H   | -1.40811100  | -0.84222100  | 2.04601700   |
| H   | -1.89275800  | 0.51062100   | 3.08599700   |
| H   | 0.38391800   | 0.35138500   | 4.23477200   |
| C   | 0.98438000   | -1.47466200  | 3.21332200   |
| H   | 1.58308600   | -0.99925000  | 2.42759300   |
| H   | 1.65024500   | -1.78029400  | 4.02695400   |
| H   | 0.51023900   | -2.36827200  | 2.79138700   |
| N   | -0.30780000  | 0.92210600   | 1.72630400   |
|     |        |        |         |
|-----|--------|--------|---------|
| Br  | -1.15890500 | -1.42534900 | 5.22648600 |
| C   | -0.39226900  | 2.31166000  | 2.13108400 |
| H   | 0.11817300   | 2.94274000  | 1.39538500 |
| H   | -1.44123600  | 2.66502700  | 2.20598000 |
| H   | 0.08264900   | 2.50770700  | 3.11247200 |
| Cr-Int<sub>3</sub> |        |        |         |
| Cr  | -0.27862400  | 0.66993000  | -3.43213100 |
| Cr  | -0.18591500  | 0.88214000  | -0.24869800 |
| O   | 0.28728300   | 2.65380000  | -3.37512000 |
| O   | -0.83870500  | -1.29396300 | -3.53249200 |
| O   | -2.18515300  | 1.24267500  | -3.27885500 |
| O   | 1.63751000   | 0.13947000  | -3.23808700 |
| O   | 1.72478200   | -0.04661000 | -0.96459900 |
| O   | -2.13277700  | 1.67147100  | -1.03632900 |
| O   | -1.07588200  | -1.02652700 | -1.30881000 |
| O   | 0.61556500   | 2.58093900  | -1.13886700 |
| C   | 0.62121100   | 3.14675300  | -2.25900900 |
| C   | -1.12927200  | -1.69854400 | -2.35511900 |
| C   | -2.67308800  | 1.61641500  | -2.16498200 |
| C   | 2.18961100   | -0.13074800 | -2.12448200 |
| H   | 0.95776200   | 4.19005800  | -2.24998500 |
| H   | 3.21664700   | -0.48366200 | -2.24828800 |
| H   | -3.71567200  | 1.93116500  | -2.25449800 |
| H   | -1.45707300  | -2.74225300 | -2.25258900 |
| C   | 0.10000600   | -1.23432400 | 1.79321100 |
| C   | 0.69214200   | -1.14497300 | 3.20638800 |
| H   | 0.92228500   | -1.39087700 | 1.08258100 |
| H   | -0.56202300  | -2.11400200 | 1.72221300 |
| H   | -0.06416800  | -0.85699600 | 3.93606200 |
| Atoms  | X       | Y       | Z       |
|--------|---------|---------|---------|
| C      | 1.951441 | -0.307260 | 3.321529 |
| H      | 1.732060 | 0.069791 | 2.941237 |
| H      | 2.296864 | -0.226321| 4.357691 |
| H      | 2.756927 | -0.727289| 2.709254 |
| N      | -0.607508| -0.001370| 1.486590 |
| Br     | 1.177340 | -3.081514| 3.886832 |
| C      | -0.453383| 2.638956| 3.257296 |
| O      | -0.073715| 3.258045| 2.340468 |
| O      | -0.832094| 2.087770| 4.219568 |
| C      | -2.011329| -0.087647| 1.866441 |
| H      | -2.157802| -0.178141| 2.958601 |
| H      | -2.544687| 0.814666| 1.542430 |
| H      | -2.515767| -0.954726| 1.396934 |

**Cr-Ts₂**

| Atoms  | X       | Y       | Z       |
|--------|---------|---------|---------|
| Cr     | 0.001153| 0.000016| -1.227546|
| Cr     | -0.001073| 0.000007| 1.227620|
| O      | 0.661373| 1.887448| -1.128399|
| O      | -0.657030| -1.888020| -1.129762|
| O      | -1.886349| 0.659893| -1.130763|
| O      | 1.889217| -0.658485| -1.127757|
| O      | 1.886895| -0.658356| 1.130527|
| O      | -1.889703| 0.656761| 1.127516|
| O      | -0.659815| -1.887984| 1.128520|
| O      | 0.655263| 1.888711| 1.129876|
| C      | 0.846322| 2.428668| 0.000928|
| C      | -0.846423| -2.428591| -0.000802|
| C      | -2.428625| 0.846301| -0.002133|
| C      | 2.428650| -0.846415| 0.001886|
| H      | 1.207278| 3.466225| 0.001333|
H                3.46616300   -1.20749500    0.00303000
H                -3.46615600    1.20733200   -0.00318000
H                -1.20755700   -3.46608600   -0.00127100
C                1.14968837   -0.91239133    3.84318188
C                2.02919119    0.26150236    4.28393638
H                1.72799763   -1.56315606    3.16996612
H                0.89039499   -1.50822921    4.72957622
H                1.54373026    0.84944613    5.06142096
C                2.57005993    1.14022934    3.17701412
H                1.72546931    1.64996309    2.69681743
H                3.24044275    1.90861484    3.57492853
H                3.09572653    0.55331913    2.41861186
N                -0.07660656   -0.45034674    3.18250104
Br               3.62710416   -0.56074045    5.32802523
C                -1.18049412    0.92410572    4.29538820
O                -1.98338937    0.20797075    4.81536725
O                -0.67219997    1.98681354    4.10223273
C                -1.02356395   -1.57458331    3.19874344
H                -1.17831931   -1.89601729    4.20752041
H                -1.95588904   -1.26172749    2.77709055
H                -0.62576508   -2.38432669    2.62344202

Cr-Int4
Cr               -0.65297400    0.15260200    1.24510200
Cr               -0.66527400    0.14790400    4.22585800
O                -2.01297100   -1.39810800    1.80386800
O                0.62438500    1.68583500    1.85802600
O                0.85668700   -1.19560600    1.80265900
O                -2.22067800    1.48980200    1.78708100
O                -2.00544600    1.64893000    4.04771400
O               0.67748600   -1.35321700    4.06583400 
O               0.84943200    1.49259300    4.10997900 
O               -2.17043600   -1.19787800    4.06357000 
C               -2.48208700   -1.68416400    2.92933800 
C                1.13004300    1.97539700    2.96659900 
C               1.15267400   -1.66387700    2.92804800 
C               -2.50013800    1.95610600    2.91682300 
H               -3.26381400   -2.45270600    2.95348400 
H               -3.27277200    2.73252300    2.95522300 
H                1.92091100   -2.44374300    2.94859900 
H                1.91227900    2.74115200    2.95057900 
C                0.36985300    1.06231200   -4.03035000 
C                1.68175300    0.36719700   -4.39068700 
H                0.66190700    2.03520700   -3.60479000 
H               -0.20935700    1.25397900   -4.94127700 
H                2.08426600   -0.14196400   -3.51785700 
C                2.70020700    1.27961200   -5.04766600 
H                2.98520600    2.05372700   -4.32219200 
H                3.60159100    0.73354100   -5.34059400 
H                2.28674000    1.77107000   -5.93692000 
N               -0.45478200    0.34896700   -3.07938000 
Br               1.30219400   -1.21525200   -5.68882900 
C               -0.07615500    0.44142700   -1.71776500 
O                1.05754700    0.90472600   -1.46868500 
O               -0.94502400    0.02238600   -0.86746400 
C                -1.81075100    0.00036300   -3.46338600 
H                -2.25633100   -0.57820800   -2.65462000 
H                -2.44149600    0.89144600   -3.63620700 
H                -1.80262500   -0.60213200   -4.38023800
|       | Cr    | Cr    | O     | O     | O     | O     | O     | O     | O     | O     | O     | C     | H     | H     | H     | C     | H     | H     | C     | H     | H     | C     | H     | H     | H     | C     | H     | H     | H     |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
|       | -0.00139400 | 0.00055800 | -1.41863400 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| Cr    | 0.00140700  | -0.00057200 | 1.41864600  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| O     | -1.41783700 | -1.41946100 | -1.13316000 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| O     | 1.41522300  | 1.42062900  | -1.13458900 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| O     | 1.41880600  | -1.41612700 | -1.13560500 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| O     | -1.42130600 | 1.41692900  | -1.13240700 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| O     | -1.41978700 | 1.41509700  | 1.13547200  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| O     | 1.42231800  | -1.41592600 | 1.13226300  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| O     | 1.41682600  | 1.42047200  | 1.13328600  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| O     | -1.41421000 | -1.42164200 | 1.13471200  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| C     | -1.81229600 | -1.81766100 | 0.00101700  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| C     | 1.81212200  | 1.81783400  | -0.00089400 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| C     | 1.81781100  | -1.81216100 | -0.00223300 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| C     | -1.81779500 | 1.81214200  | 0.00210300  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| H     | -2.58787200 | -2.59710300 | 0.00151300  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| H     | -2.59683000 | 2.58812600  | 0.00325200  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| H     | 2.59685300  | -2.58814000 | -0.00337200 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| H     | 2.58822100  | 2.59675500  | -0.00139400 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| C     | -0.40184069 | 0.47256009  | -6.93319635 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| C     | -0.42444262 | 1.98869654  | -6.89524680 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| H     | -1.44473516 | 0.11137650  | -6.96123715 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| H     | 0.10330640  | 0.12313044  | -7.83342770 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| H     | 0.49107066  | 2.49820978  | -6.64482357 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| C     | -1.70597342 | 2.75959320  | -7.04539834 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| H     | -2.26985085 | 2.68678240  | -6.10828704 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| H     | -1.50725002 | 3.80988759  | -7.26731305 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| H     | -2.31214142 | 2.34700105  | -7.85753653 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
N  0.31077404  -0.01012077  -5.76356116
Br  0.38016477  2.45314699  -9.33571840
C  -0.00611366  0.64669647  -4.58261894
O  -0.58570640  1.76759422  -4.76080400
O  0.30032146  0.14614728  -3.45943607
C  0.71311614  -1.42182249  -5.68533644
H  1.61236294  -1.50512951  -5.11147660
H  -0.06350542  -1.98853328  -5.2156805
H  0.88335204  -1.79936942  -6.67193567
Cr-Int
Cr  -0.67234400  0.14416800  1.34484200
Cr  -0.67031000  0.14165500  4.27784200
O  -2.06129200  -1.33940200  1.80571700
O  0.69406900  1.63701900  1.81143700
O  0.80128600  -1.23460800  1.81574100
O  -2.16822400  1.52655500  1.80284600
O  -2.04947500  1.61140100  4.07188600
O  0.70851400  -1.32651000  4.08443600
O  0.79872300  1.52009100  4.07882000
O  -2.13996200  -1.23652100  4.07554500
C  -2.48983600  -1.67846600  2.93801700
C  1.13723300  1.96843200  2.94051300
C  1.14639100  -1.67066000  2.94338200
C  -2.49867700  1.95822700  2.93640400
H  -3.26381400  -2.45270600  2.95348400
H  -3.27277200  2.73252300  2.95522300
H  1.92091100  -2.44374300  2.94859900
H  1.91227900  2.74115200  2.95057900
C  0.41950000  0.48720600  -4.11153700
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 1.64674500 | 0.09898100 | -3.27593000 |
| H       | 0.43839900 | 1.54718000 | -4.41412800 |
| H       | 0.35500400 | -0.13669400 | -5.00694100 |
| H       | 1.89181300 | -0.95281500 | -3.44870800 |
| C       | 2.87149700 | 0.96548900 | -3.45677000 |
| H       | 2.63993100 | 2.02202800 | -3.27310800 |
| H       | 3.67001700 | 0.65448100 | -2.77315200 |
| H       | 3.21626500 | 0.83240000 | -4.48845900 |
| N       | -0.66128700 | 0.25577400 | -3.15013000 |
| Br      | 2.23448500 | -1.19048200 | -6.57810000 |
| C       | -0.18458000 | 0.20807000 | -1.88768200 |
| O       | 1.15517300 | 0.19987200 | -1.87886000 |
| O       | -0.86871400 | 0.17351300 | -0.85186000 |
| C       | -2.06163900 | 0.41608000 | -3.47382200 |
| H       | -2.65612100 | 0.16598700 | -2.59194000 |
| H       | -2.28189000 | 1.45255000 | -3.77295200 |
| H       | -2.32951400 | -0.25207000 | -4.30094200 |
| Ru      | 0.00107500 | 0.00038300 | -1.17697600 |
| Ru      | -0.00084500 | -0.00021700 | 1.17744000 |
| O       | -0.00818500 | 2.06253000 | -1.13007600 |
| O       | 0.01044300 | -2.06185100 | -1.13104900 |
| O       | -2.07971700 | -0.00890800 | -1.13568200 |
| O       | 2.08159200 | 0.00955200 | -1.13271500 |
| O       | 2.08044600 | 0.00842000 | 1.13574500 |
| O       | -2.08191400 | -0.00979300 | 1.13278000 |
| O       | 0.00734300 | -2.06278200 | 1.12915300 |
| O       | -0.01059400 | 2.06239600 | 1.13012500 |
| C       | -0.01247500 | 2.63932800 | 0.00023200 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 0.01159500 | -2.63917800 | -0.00101000 |
| C    | -2.64761600 | -0.01215200 | -0.00189500 |
| C    | 2.64782900  | 0.01152100  | 0.00193000  |
| H    | -0.01829300 | 3.73544800  | 0.00012000  |
| H    | 3.74549400  | 0.01658400  | 0.00235800  |
| H    | -3.74528000 | -0.01766500 | -0.00307400 |
| H    | 0.01662800  | -3.73530300 | -0.00161700 |
| Ru   | 0.00011000  | 0.00004300  | -1.14147500 |
| Ru   | -0.00009300 | -0.00003300 | 1.14148100  |
| O    | -0.16971700 | 2.08592700  | -1.12834800 |
| O    | 0.16991500  | -2.08585700 | -1.12842900 |
| O    | -2.08593600 | -0.16974100 | -1.12853400 |
| O    | 2.08611100  | 0.16981200  | -1.12825300 |
| O    | 2.08597900  | 0.16970600  | 1.12853400  |
| O    | -2.08612300 | -0.16979800 | 1.12825200  |
| O    | 0.16960600  | -2.08593900 | 1.12833900  |
| O    | -0.16983900 | 2.08588100  | 1.12842100  |
| C    | -0.21696600 | 2.66148800  | 0.00005500  |
| C    | 0.21687300  | -2.66148900 | -0.00005200 |
| C    | -2.66155000 | -0.21695200 | -0.00019100 |
| C    | 2.66156600  | 0.21692400  | 0.00018600  |
| H    | -0.30668100 | 3.75474700  | 0.00005600  |
| H    | 3.75487800  | 0.30626800  | 0.00023800  |
| H    | -3.75484600 | -0.30648000 | -0.00028500 |
| H    | 0.30640000  | -3.75476300 | -0.00092000 |
| C    | 0.00275233  | 1.12318510  | 3.67364069  |
| C    | -1.12648465 | 0.37963898  | 4.31098199  |
| H    | -0.19459598 | 1.86927050  | 2.90539100  |

Ru-Int₀
| Atom | x        | y        | z        |
|------|----------|----------|----------|
| H    | 0.89194378 | 1.31336313 | 4.27811276 |
| H    | -0.94725737 | 0.06572169 | 5.34385463 |
| C    | -2.57569127 | 0.63698890 | 3.96623871 |
| H    | -3.17871143 | -0.26965624 | 4.10355204 |
| H    | -2.99427083 | 1.42425399 | 4.60629485 |
| H    | -2.67180578 | 0.95089053 | 2.92146767 |
| N    | -0.28709042 | -0.26291350 | 3.30163040 |
| C    | 0.65695499 | -1.27143058 | 3.76849685 |
| H    | 0.15208275 | -2.24297762 | 3.81645833 |
| H    | 1.48463790 | -1.34837989 | 3.05425044 |
| H    | 1.07895947 | -1.04844285 | 4.76617383 |

**Ru-Int**

| Atom | x        | y        | z        |
|------|----------|----------|----------|
| Ru   | 0.46654000 | 0.12686300 | -2.77522500 |
| Ru   | 0.46067600 | 0.12309100 | -0.34818500 |
| O    | 0.29907200 | 2.20623100 | -2.70641100 |
| O    | 0.63934100 | -1.94756100 | -2.70602900 |
| O    | -1.61870000 | -0.04171900 | -2.72232200 |
| O    | 2.55016000 | 0.29563800 | -2.70451500 |
| O    | 2.57440400 | 0.30078600 | -0.43205000 |
| O    | -1.63550700 | -0.04654800 | -0.45214400 |
| O    | 0.64183600 | -1.97568200 | -0.43755000 |
| O    | 0.29920900 | 2.22886600 | -0.43760800 |
| C    | 0.25184200 | 2.78214100 | -1.57233400 |
| C    | 0.68642100 | -2.52656700 | -1.57219700 |
| C    | -2.18920600 | -0.08938500 | -1.58682000 |
| C    | 3.12237000 | 0.34312900 | -1.56974800 |
| H    | 0.16074900 | 3.88260400 | -1.58831700 |
| H    | 4.22230800 | 0.43412500 | -1.58813500 |
| H    | -3.28741600 | -0.17862300 | -1.58865800 |
H  0.77383000  -3.62690600  -1.58846500
C  -0.90247000  0.70447700   2.52513800
C  -0.34913000  -0.62905200   2.83477300
H  -1.73925500  0.78312600   1.83858200
H  -0.84184000  1.47392400   3.29019700
H   0.12213300  -0.70408100   3.81263100
C  -0.97709800  -1.90892300   2.34859900
H  -0.22627300  -2.69741100   2.21997300
H  -1.69640600  -2.22053800   3.11449900
H  -1.49848900  -1.77022900   1.39873600
N   0.37748100   0.28523900   1.89193600
Br  -2.16961600  -0.43893600   5.83729200
C   1.58099900   0.92073300   2.44752000
H   2.44743700   0.28214500   2.25311400
H   1.73722500   1.88463500   1.95249700
H   1.48271800   1.08174800   3.53026200

Ru-Ts₁
Ru  0.00011000   0.00004300  -1.14147500
Ru -0.00009300  -0.00003300   1.14148100
O  -0.16971700   2.08592700  -1.12834800
O   0.16991500  -2.08585700  -1.12842900
O   -2.08593600  -0.16974100  -1.12853400
O   2.08611100   0.16981200  -1.12825300
O   2.08597900   0.16970600   1.12853400
O   -2.08612300  -0.16979800   1.12825200
O   0.16960600  -2.08593900   1.12833900
O  -0.16983900   2.08588100   1.12842100
C  -0.21696600   2.66148800   0.00005500
C   0.21687300  -2.66148900  -0.00005200
C  -2.66155000  -0.21695200  -0.00019100
C   2.66156600   0.21692400   0.00018600
H  -0.30668100   3.75474700   0.00005600
H   3.75487800   0.30626800   0.00023800
H  -3.75484600  -0.30648000  -0.00028500
H   0.30640000  -3.75476300  -0.00009200
C  -1.14275750   0.29503848   3.94606538
C  -0.65266726  -1.02468683   4.39878508
H  -2.05076079   0.25453446   3.34240329
H  -1.18316810   1.08823009   4.69664313
H   0.16083996  -1.03337438   5.11032111
C  -1.01373779  -2.30730799   3.69936184
H  -0.37609339  -2.47065185   2.82239169
H  -0.88584840  -3.14762753   4.38594249
H  -2.05600786  -2.28740562   3.36794614
N   0.07516346   0.22428965   3.15798681
Br  -2.12142755  -1.35896161   6.60231036
C   1.16678839   1.04480683   3.67416431
H   2.11481919   0.72537536   3.23339315
H   0.98917945   2.09489520   3.40120385
H   1.23612468   0.97772502   4.77030985

**Ru-Int₂**

Ru   0.47662700   0.12947400  -2.79277800
Ru   0.45280100   0.13045600  -0.28869500
O    0.34805800   2.22338800  -2.71803700
O    0.69107900  -1.95949600  -2.71623100
O   -1.61641700  -0.05582900  -2.69539600
O    2.57452300   0.28326800  -2.72428700
O    2.58264800   0.31425900  -0.43967000
O  -0.36529300  0.61937800  -1.86217700
O  -0.99661100  -0.33484800  2.22539300
O   0.26596700  -1.74685700  -0.12548400
O  -1.57434100  2.05467200  0.48508700
O  -3.58270700  1.10883500  -0.00144900
O  -1.77046400  -2.62212500  -0.62247400
O  -3.01509200  -1.25814900  1.71714500
O  -2.39622700  -0.28149700  -2.35957600
C  -1.30898200  0.29620500  -2.64261300
C  -2.07986000  -0.92462000  2.50042000
C  -0.51702600  -2.68066500  -0.45930200
C  -2.82818500  2.07059400  0.32481300
H  -1.16341200  0.55150900  -3.69885400
H  -3.32930200  -0.92462000  2.50042000
H  -0.05450600  -3.66007200  -0.63025200
H  -2.22024600  -1.17905900  3.55765000
C   2.44273000  0.13192000  0.91470500
C   3.44808200  0.63457400  -0.12950800
H   2.21406400  -0.91858900  0.71047800
H   2.89387100  0.19148500  1.91958600
H   3.64426800  1.70038900  -0.01403800
C   3.12914100  0.25840700  -1.56062300
H   2.12698900  0.63465000  -1.79828800
H   3.85352800  0.68705900  -2.26137200
H   3.11465200  -0.83014700  -1.68445600
N   1.24367100  0.94156800  0.82539200
Br  5.35842500  -0.16103400  0.32918400
C   0.86999500  3.99031800  -1.90155900
O   1.85820200  3.94085800  -1.27758800
|   |       |       |       |       |       |
|---|-------|-------|-------|-------|-------|
| O | -0.10089200 | 4.08219600 | -2.54714300 |       |       |
| C | 1.27930400  | 2.08604400 | 1.71517400  |       |       |
| H | 2.15714400  | 2.73103900 | 1.52739500  |       |       |
| H | 0.38146600  | 2.69355600 | 1.57958700  |       |       |
| H | 1.32618900  | 1.77693500 | 2.77819900  |       |       |

**Ru-Ts₂**

|   |       |       |       |       |       |
|---|-------|-------|-------|-------|-------|
| Ru| -0.60526900 | 0.22012700 | 0.24220800 |       |       |
| Ru| -2.71567800 | -0.74213300 | -0.29737500 |       |       |
| O | -0.38981400 | 0.66024900 | -1.81867200 |       |       |
| O | -0.98584200 | -0.30302200 | 2.26800400  |       |       |
| O | 0.23386400  | -1.71613200 | -0.06350500 |       |       |
| O | -1.59432800 | 2.07019800 | 0.52591900  |       |       |
| O | -3.59966800 | 1.13290000 | 0.03634200  |       |       |
| O | -1.78235600 | -2.59490400 | -0.61484400 |       |       |
| O | -2.98635100 | -1.23244000 | 1.73349400  |       |       |
| O | -2.41042100 | -0.23939500 | -2.31521400 |       |       |
| C | -1.32186800 | 0.33730800 | -2.60498300 |       |       |
| C | -2.06539100 | -0.83939400 | 1.14078200  |       |       |
| C | -0.53171900 | -2.65283900 | -0.42292200 |       |       |
| C | -2.84421400 | 2.09615300 | 0.36540400  |       |       |
| H | -1.16879600 | 0.58289600 | -3.66255500 |       |       |
| H | -3.33468600 | 3.06412500 | 0.52560600  |       |       |
| H | -0.05989000 | -3.62868500 | -0.59395300 |       |       |
| H | -2.22563000 | -1.14767200 | 3.59394900  |       |       |
| C | 2.47713100  | 0.16187000 | 0.85816500  |       |       |
| C | 3.35050200  | 0.03943200 | -0.39456400 |       |       |
| H | 2.13249700  | -0.83939400 | 1.14078200  |       |       |
| H | 3.13138800  | 0.51160200 | 1.66897800  |       |       |
| H | 3.82888700  | 0.97849000 | -0.64310400 |       |       |
| Atom | x       | y       | z       |
|------|---------|---------|---------|
| C    | 2.75544600 | -0.63831800 | -1.60799300 |
| H    | 1.87398400 | -0.06784200 | -1.91148900 |
| H    | 3.46899300 | -0.65400200 | -2.43846200 |
| H    | 2.44246600 | -1.65782000 | -1.37560800 |
| N    | 1.34409500 | 1.10895600 | 0.74061600 |
| Br   | 5.03050100 | -1.09081900 | 0.20300800 |
| C    | 1.49512588 | 2.56912237 | -0.49970222 |
| O    | 2.15971753 | 3.33951566 | 0.10431310 |
| O    | 0.82375306 | 2.24188246 | -1.41065073 |
| C    | 1.19260400 | 1.78609700 | 2.03722600 |
| H    | 2.08630900 | 2.38313600 | 2.27430600 |
| H    | 0.33601200 | 2.46251600 | 1.99937700 |
| H    | 1.03699700 | 1.06634900 | 2.85689800 |

**Ru-Int₄**

| Atom | x       | y       | z       |
|------|---------|---------|---------|
| Ru   | 0.42454000 | -0.57623400 | 0.99125500 |
| Ru   | 0.43355500 | -0.57959400 | 3.33380000 |
| O    | 0.26650700 | 1.52413300 | 1.06204400 |
| O    | 0.60829700 | -2.69310200 | 1.04889000 |
| O    | -1.66667400 | -0.78949100 | 1.06890200 |
| O    | 2.54608000 | -0.39969700 | 1.04745300 |
| O    | 2.53162700 | -0.41784000 | 3.31520100 |
| O    | -1.66331700 | -0.73572800 | 3.33511100 |
| O    | 0.59782300 | -2.67888400 | 3.31707000 |
| O    | 0.26854800 | 1.51642800 | 3.32939000 |
| C    | 0.22110500 | 2.07885400 | 2.19185400 |
| C    | 0.65002300 | -3.24394100 | 2.18253900 |
| C    | -2.22390800 | -0.80596800 | 2.19667500 |
| C    | 3.09747100 | -0.36376100 | 2.18060800 |
| H    | 0.13062700 | 3.17175500 | 2.19366000 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | 4.19218600 | -0.27672400| 2.19384200 |
| H    | -3.31753800| -0.88947200| 2.19331900 |
| H    | 0.74370800 | -4.33775500| 2.19351200 |
| C    | -1.09711000| -0.13232300| -4.28787100|
| C    | -1.39500800| 1.33072600 | -4.61484200|
| H    | -2.03467200| -0.53905900| -3.87817200|
| H    | -0.87039200| -0.68114500| -5.21043800|
| H    | -1.23052500| 1.94970500 | -3.73633300|
| C    | -2.76330100| 1.55442800 | -5.23071900|
| H    | -3.52404100| 1.27746100 | -4.48720000|
| H    | -2.91477100| 2.60247000 | -5.50607100|
| H    | -2.90902900| 0.93574200 | -6.12539000|
| N    | -0.02518000| -0.33682300| -3.33617700|
| Br   | 0.03485900 | 2.05744100 | -5.94167500|
| C    | -0.35854400| -0.12714500| -1.97559100|
| O    | -1.41171600| 0.48034900 | -1.72415500|
| O    | 0.51125300 | -0.60155500| -1.13983200|
| C    | 1.08977500 | -1.18591600| -3.72008100|
| H    | 1.84859000 | -1.13526500| -2.93758700|
| H    | 0.79460200 | -2.24469800| -3.84166500|
| H    | 1.51863900 | -0.83022300| -4.66560900|

**Ru-Ts₃**

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Ru   | 0.00011000 | 0.00004300 | -1.14147500|
| Ru   | -0.00009300| -0.00003300| 1.14148100 |
| O    | -0.16971700| 2.08592700 | -1.12834800|
| O    | 0.16991500 | -2.08585700| -1.12842900|
| O    | -2.08593600| -0.16974100| -1.12853400|
| O    | 2.08611100 | 0.16981200 | -1.12825300|
| O    | 2.08597900 | 0.16970600 | 1.12853400 |
### Ru-Int$_5$

| Element | x     | y     | z     |
|---------|-------|-------|-------|
| Ru      | 0.43507100 | -0.57901600 | 1.01324700 |
| Ru      | 0.43568500 | -0.58093000 | 3.33208500 |
| O       | 0.28214600 | 1.51932800  | 1.06027400 |
| O       | 0.60043000 | -2.68701900 | 1.05589700 |
| O       | -1.66441100| -0.75377500 | 1.05867600 |
| O       | 2.54093100 | -0.41769500 | 1.05647800 |
| O       | 2.52869300 | -0.41142200 | 3.32010800 |
| O       | -1.65529100| -0.74957100 | 3.32183400 |
| O       | 0.60595700 | -2.67474100 | 3.31973300 |
| O       | 0.26428700 | 1.50877900  | 3.32300900 |
| C       | 0.22506200 | 2.07935800  | 2.18960000 |
| C       | 0.65052500 | -3.24457300 | 2.18722000 |
| C       | -2.22464100| -0.79823500 | 2.18865900 |
| C       | 3.09891500 | -0.36746800 | 2.18758900 |
| H       | 0.13062700 | 3.17175500  | 2.19366000 |
| H       | 4.19218600 | -0.27672400 | 2.19384200 |
| H       | -3.31753800| -0.88947200 | 2.19331900 |
| H       | 0.74370800 | -4.33775500 | 2.19351200 |
| C       | -0.88110800| 0.32713500  | -4.26318900 |
| C       | -1.44939600| 1.34131300  | -3.26218300 |
| H       | -1.63561600| -0.40901600 | -4.58310100 |
| H       | -0.48795100| 0.83737500  | -5.14721600 |
| H       | -0.92212800| 2.29405600  | -3.36051400 |
| C       | -2.94473000| 1.55189800  | -3.30564400 |
| H       | -3.48068800| 0.60225700  | -3.18620300 |
| H       | -3.26154500| 2.23929200  | -2.51299400 |
| H       | -3.18272400| 1.99399200  | -4.28012500 |
N          0.14717500   -0.32453600   -3.44815000  
Br         -1.42568200    2.88690900   -6.55809800  
C          -0.08225300   -0.11722800   -2.13405900  
O          -1.05392200    0.77847300   -1.94514100  
O          0.52772700   -0.68221800   -1.20638000  
C          1.03704100   -1.34526700   -3.95655900  
H          1.69354000   -1.67266800   -3.14799700  
H          0.46977000   -2.21001400   -4.33153000  
H          1.63656100   -0.93812500   -4.77795700  

Ti-HKUST-1

Ti          -0.00005900    0.00077100    1.42413700  
Ti          0.00007500   -0.00055000   -1.32592100  
O          -1.41549700   -1.39490600    1.09307900  
O          1.41556400    1.39605500    1.09224500  
O          -1.41699600    1.39467400    1.09213700  
O          1.41677300   -1.39349700    1.09309100  
O          1.48012000   -1.43354800   -1.15225600  
O          -1.48016800    1.43233700   -1.15326000  
O          1.48065200    1.43189300   -1.15312300  
O          -1.48051400   -1.43299400   -1.15225100  
C          -1.87061100   -1.82252400   -0.01393000  
C          1.87103600    1.82223100   -0.01516300  
C          -1.87156400    1.82170100   -0.01533000  
C          1.87116800   -1.82197900   -0.01388100  
H          -2.65766600   -2.58629100    0.02895500  
H          2.65842100   -2.58553000    0.02908800  
H          -2.65933400    2.58476700    0.02677700  
H          2.65859700    2.58551000    0.02697600  

Ti-Int

0
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Ti      | 0.00001100 | -0.00025500| 1.43151600 |
| Ti      | 0.00000200 | 0.00017500 | -1.34116700|
| O       | 1.42439300 | 1.40235700 | 1.09473200 |
| O       | -1.42442000| -1.40275600| 1.09442400 |
| O       | 1.42509800 | -1.40252000| 1.09431900 |
| O       | -1.42505900| 1.40162000 | 1.09463500 |
| O       | -1.48987900| -1.44257400| -1.15165400|
| O       | -1.49013900| -1.44226100| -1.15154200|
| O       | 1.49006400 | 1.44269600 | -1.15121800|
| C       | 1.87977200 | 1.83115500 | -0.01184700|
| C       | -1.87996100| -1.83099900| -0.01230000|
| C       | 1.88011300 | -1.83086300| -0.01240400|
| C       | -1.88001300| 1.83090200 | -0.01193600|
| H       | 2.66675200 | 2.59497800 | 0.03146200 |
| H       | -2.66688800| 2.59483100 | 0.03141300 |
| H       | 2.66715700 | -2.59463300| 0.03065900 |
| H       | -2.66687100| -2.59490800| 0.03073900 |
| C       | -0.42829386| -1.37016730| -3.79644746|
| C       | -1.06166172| -0.18558270| -4.45207341|
| H       | -0.96869041| -1.93166824| -3.03586503|
| H       | 0.27820489 | -1.95960267| -4.38435993|
| H       | -0.73558341| 0.00191343 | -5.47969714|
| C       | -2.46774256| 0.27149817 | -4.13696947|
| H       | -2.56996968| 1.35460850 | -4.28159064|
| H       | -3.19513212| -0.22901984| -4.78893051|
| H       | -2.72074287| 0.04493627 | -3.09582619|
| N       | -0.03848624| -0.00908638| -3.42338105|
| C       | 1.27816536 | 0.43377692 | -3.86676955|
| Atoms | x         | y         | z         |
|-------|-----------|-----------|-----------|
| H     | 1.29131813| 1.52836013| -3.91982174|
| H     | 2.03043724| 0.11538848| -3.13612329|
| H     | 1.56485159| 0.03347759| -4.85709380|
| Ti    | 0.11983300| 0.53723400| -0.54790900|
| Ti    | 0.11588800| 0.55153000| -3.52036800|
| O     | 1.64336700| 2.02329400| -0.86453400|
| O     | -1.38698700| -0.92354500| -0.91151700|
| O     | 1.60648900| -0.88411700| -0.95436200|
| O     | -1.37346900| 1.99702900| -0.92382700|
| O     | -1.30163600| 1.95971400| -3.17565700|
| O     | 1.54630100| -0.85938900| -3.20556300|
| O     | -1.30674100| -0.84209000| -3.16518000|
| O     | 1.51542100| 1.94344900| -3.11697900|
| C     | 1.99511400| 2.38276500| -2.01681700|
| C     | -1.76236500| -1.28119300| -2.05678000|
| C     | 1.95120000| -1.27492900| -2.08604300|
| C     | -1.75713300| 2.38076200| -2.06041000|
| H     | 2.78313700| 3.14585800| -2.11340600|
| H     | -2.55050300| 3.14571100| -2.11345500|
| H     | 2.78354200| -2.04375300| -2.11420900|
| H     | -2.55048600| -2.04402800| -2.11412900|
| C     | -1.28899800| -0.28963700| 2.21545200|
| C     | -0.00418300| -0.99135600| 2.40575300|
| H     | -1.98947300| -0.63235700| 1.45885100|
| H     | -1.70708000| 0.20480700| 3.08950700|
| H     | 0.38497200| -0.89599300| 3.42146100|
| C     | 0.36211800| -2.26889200| 1.69217700|
| H     | 1.44432400| -2.33739800| 1.53324400|
|   |          x  |          y  |          z  |
|---|------------|------------|------------|
| H | 0.05799900 | -3.10874300| 2.33010400 |
| H | -0.13641000| -2.36655000| 0.72431700 |
| N | -0.03518500| 0.31584900 | 1.66230900 |
| Br| -0.37818800| -0.48933200| 5.91535600 |
| C | 0.47755400 | 1.46896900 | 2.43865100 |
| H | 1.54934500 | 1.57917700 | 2.24169200 |
| H | -0.03671400| 2.37767200 | 2.10479600 |
| H | 0.31884600 | 1.32579900 | 3.51535500 |

**Ti-Ts₁**

|   |          x  |          y  |          z  |
|---|------------|------------|------------|
| Ti| 0.62029411 | 2.98772608 | -9.01613415|
| Ti| 0.62028511 | 2.98815608 | -11.78881715|
| O | 2.04467611 | 4.39033808 | -9.35291815|
| O | -0.80413689| 1.58522508 | -9.35322615|
| O | 2.04538111 | 1.58592908 | -9.35333115|
| O | -0.80477589| 4.38960108 | -9.35301515|
| O | -0.86951989| 4.43099108 | -11.59897515|
| O | 2.11016211 | 1.54540708 | -11.59930415|
| O | -0.86985589| 1.54572008 | -11.59919215|
| O | 2.11034711 | 4.43067708 | -11.59886815|
| C | 2.50005511 | 4.81913608 | -10.45949715|
| C | -1.25967789| 1.15698208 | -10.45995015|
| C | 2.50039611 | 1.15711808 | -10.45005415|
| C | -1.25972989| 4.81888308 | -10.45958615|
| H | 3.28703511 | 5.58295908 | -10.41618815|
| H | -2.04660489| 5.58281208 | -10.41623715|
| H | 3.28744011 | 0.39334808 | -10.41699115|
| H | -2.04658789| 0.39307308 | -10.41691115|
| C | -0.84095604| 2.71092514 | -6.29922874 |
| C | 0.23391101 | 1.88536210 | -5.70768420 |
|     | X          | Y          | Z         |
|-----|------------|------------|-----------|
| H   | -1.50508757 | 2.16825093 | -6.97373039 |
| H   | -1.39153432 | 3.36329050 | -5.61700010 |
| H   | 0.83410672  | 2.33674551 | -4.93039975 |
| C   | 0.71167993  | 0.60435286 | -6.33651965 |
| H   | 1.42975838  | 0.80430138 | -7.14071626 |
| H   | 1.19797300  | -0.01613291| -5.57994707 |
| H   | -0.12773599 | 0.04271254 | -6.75663918 |
| N   | 0.29881073  | 3.30861363 | -6.97235936 |
| Br  | -1.05386496 | 0.83431425 | -3.61927536 |
| C   | 0.70054940  | 4.60229135 | -6.42799124 |
| H   | 1.71220137  | 4.84951691 | -6.76043357 |
| H   | 0.01186927  | 5.37731314 | -6.79377647 |
| H   | 0.67065084  | 4.60203806 | -5.32801463 |

**Ti-Int<sub>2</sub>**

|     | X          | Y          | Z         |
|-----|------------|------------|-----------|
| Ti  | 0.11493000 | 0.55124800 | -0.54635700 |
| Ti  | 0.11445900 | 0.55157700 | -3.52671000 |
| O   | 1.65128400 | 2.02667800 | -0.86348100 |
| O   | -1.40941000| -0.93375400| -0.86328400 |
| O   | 1.58018900 | -0.90077000| -0.95498000 |
| O   | -1.34359400| 2.00454300 | -0.96139600 |
| O   | -1.32735300| 1.96195100 | -3.21954400 |
| O   | 1.56102000 | -0.85281200| -3.21260900 |
| O   | -1.29119800| -0.84043200| -3.12379200 |
| O   | 1.51886700 | 1.94739300 | -3.12389900 |
| C   | 1.99663200 | 2.38115800 | -2.02330500 |
| C   | -1.76263100| -1.28112500| -2.02281700 |
| C   | 1.98958300 | -1.27639500| -2.09171700 |
| C   | -1.75416500| 2.38097300 | -2.09522000 |
| H   | 2.78313700 | 3.14585800 | -2.11340600 |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| H    | -2.55050300 | 3.14571100 | -2.11345500 |
| H    | 2.78354200  | -2.04375300 | -2.11420900 |
| H    | -2.55048600 | -2.04402800 | -2.11420900 |
| C    | -0.59445600 | -0.40025300 | 2.29053900   |
| C    | 0.47456300  | -1.19947900 | 3.04945000   |
| H    | -1.18295000 | -1.09263600 | 1.67598500   |
| H    | -1.28271800 | 0.06808800  | 3.01581400   |
| H    | 1.16104000  | -0.53850900 | 3.57829800   |
| C    | 1.20185100  | -2.24584600 | 2.23207300   |
| H    | 1.66020400  | -1.75180800 | 1.36697700   |
| H    | 1.98242400  | -2.74620800 | 2.81539200   |
| H    | 0.50360700  | -3.00182400 | 1.85520500   |
| N    | 0.03824800  | 0.59775900  | 1.44706700   |
| Br   | -0.43015400 | -2.18848400 | 4.69222400   |
| C    | 0.37418400  | 1.80922300  | 2.17976500   |
| H    | 0.81846200  | 2.54316400  | 1.49910400   |
| H    | -0.52202400 | 2.27057600  | 2.64179300   |
| H    | 1.10300900  | 1.64625900  | 2.99715000   |

**Ti-Int₃**

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| Ti   | 0.81501300 | 0.27863900 | -0.19390900 |
| Ti   | 3.49473700  | -0.91900200 | 0.21238600 |
| O    | 1.93709700  | 2.11441600  | -0.02197300 |
| O    | 0.23986000  | -1.79074200 | -0.23886600 |
| O    | 0.89809600  | 0.17373600  | 1.89826500 |
| O    | 1.47840300  | 0.06110300  | -2.16471000 |
| O    | 3.51045700  | -0.87004100 | -1.83638400 |
| O    | 2.95787000  | -0.70935200 | 2.17538400 |
| O    | 2.34206100  | -2.57257800 | 0.08060900 |
| O    | 3.92566300  | 1.05490400  | 0.21808200 |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | 3.19033800 | 2.09215300 | 0.12957400 |
| C    | 1.08785000 | -2.71386800 | -0.10435000 |
| C    | 1.85920000 | -0.24166500 | 2.61212700 |
| C    | 2.56738700 | -0.43659700 | -2.57159000 |
| H    | 3.71951600 | 3.05456700 | 0.18639000 |
| H    | 2.71156000 | -0.49608400 | -3.66388500 |
| H    | 1.73212800 | -0.19893000 | 3.70734200 |
| H    | 0.72393300 | -3.74986800 | -0.14314400 |
| C    | -2.21917700 | 0.20069900 | -0.64741500 |
| C    | -3.11096900 | 0.51172700 | 0.56157600 |
| H    | -1.97247100 | -0.86711300 | -0.63424400 |
| H    | -2.77991400 | 0.40304200 | -1.57589800 |
| H    | -3.29766100 | 1.58134700 | 0.65499000 |
| C    | -2.66509200 | -0.11204400 | 1.86740600 |
| H    | -1.63990200 | 0.21685100 | 2.07548400 |
| H    | -3.31267400 | 0.18208900 | 2.70080000 |
| H    | -2.65593700 | -1.20505600 | 1.79434800 |
| N    | -1.00437200 | 0.99624500 | -0.58579300 |
| Br   | -5.07317200 | -0.18139400 | 0.16511100 |
| C    | -0.29980900 | 3.66581900 | 2.69879000 |
| O    | -1.00896500 | 4.10730500 | 1.87830800 |
| O    | 0.39776500  | 3.25887500 | 3.54843200 |
| C    | -1.18320500 | 2.31578800 | -1.17434400 |
| H    | -1.94307600 | 2.93009500 | -0.65665500 |
| H    | -0.24042400 | 2.87150300 | -1.13497100 |
| H    | -1.49505300 | 2.24918600 | -2.23662100 |

**Ti-Ts**

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| Ti   | 0.80968000 | 0.28370800 | -0.14544200 |
| Ti   | 3.29590900 | -0.84913700 | 0.19976100 |
O   1.92735700  2.05844200  -0.05908700
O   0.23794400  -1.76895600  -0.18237500
O   0.84735300   0.21905400   1.92883300
O   1.39187800   0.04218700  -2.17372400
O   3.43834300  -0.85390700  -1.84088100
O   2.88151000  -0.71928200   2.20242500
O   2.31447900  -2.63740200   0.07347200
O   3.94254900   1.08942200   0.29493400
C   3.16862200   2.08957000   0.14216900
C   1.05286400  -2.72045900  -0.08322300
C   1.78901900  -0.22590000   2.63214000
C   2.48424300  -0.42964400  -2.57114400
H   3.64546600   3.06975800   0.19575700
H   2.63751000  -0.48089300  -3.65451800
H   1.65807800  -0.18373900   3.71670900
H   0.64988300  -3.73467700  -0.13377700
C  -2.28569500   0.12873400  -0.91170400
C  -3.08726700  -0.02628500   0.38425100
H  -1.97997500  -0.87081100  -1.25944900
H  -2.97369800   0.53472400  -1.66680800
H  -3.52817800   0.92265200   0.68924000
C  -2.41957300  -0.74412000   1.53479200
H  -1.55999700  -0.15024000   1.86533400
H  -3.10556800  -0.85641500   2.38102400
H  -2.05627100  -1.72876100   1.22758000
N  -1.12009700   1.02580100  -0.77583400
Br  -4.81944500  -1.10436200  -0.11491700
C  -1.70372100   2.72157400   0.59182900
O  -2.39977400   3.37658300  -0.12123200
O       -1.16257800  2.46317200  1.61923100
C       -0.96409200  1.76294200 -2.03884100
H       -1.84289300  2.39553100 -2.23863700
H       -0.08588600  2.41677900 -1.98443200
H       -0.81905800  1.08462200 -2.89448400

Ti-Int$_d$
Ti       -0.42358900 -0.37574900  4.38596800
Ti       -0.44491500 -0.56414800  1.42252400
O        0.95386800  1.02293500  3.91357800
O       -1.82390600 -1.80203500  4.11107500
O        1.00271300 -1.80625000  4.15738100
O       -1.85909600  1.00978200  3.99636100
O       -1.90843800  0.95215600  1.74086100
O        1.01132100 -1.98886600  1.90962200
O       -1.93134000 -2.04023400  1.86541000
O        1.05413100  0.96477900  1.65496600
C        1.41776600  1.38887800  2.77971700
C       -2.29203900 -2.31436600  3.03692300
C        1.42912300 -2.29289700  3.05568100
C       -2.30451100  1.37576900  2.85793300
H        2.21771800  2.14418600  2.81484800
H       -3.11563300  2.12399400  2.86659300
H        2.24053800 -3.03649400  3.11832900
H       -3.09319900 -3.05680700  3.17021400
C        1.55307000  1.08595400 -3.10759500
C        1.47053700  0.37529000 -4.45744100
H        2.48278400  0.72493600 -2.64095700
H        1.65218900  2.16692200 -3.26223200
H        1.05852400 -0.62059700 -4.32569200
| Atomic Symbol | X   | Y   | Z   |
|---------------|-----|-----|-----|
| C             | 2.77876600 | 0.36207000 | -5.22245500 |
| H             | 3.51739800 | -0.21163800 | -4.64222400 |
| H             | 2.66593900 | -0.11241500 | -6.20189000 |
| H             | 3.16954400 | 1.37580200  | -5.37220000 |
| N             | 0.44263100 | 0.83509300  | -2.21340000 |
| Br            | 0.03515600 | 1.29061400  | -5.64565800 |
| C             | 0.45124100 | -0.39303900 | -1.53015600 |
| O             | 1.24941800 | -1.26938700 | -1.89845100 |
| O             | -0.42989700 | -0.50813800 | -0.57889700 |
| C             | -0.34531600 | 1.97016300  | -1.75533700 |
| H             | -1.18587700 | 1.59843500  | -1.16567600 |
| H             | 0.24576100  | 2.65290800  | -1.11746200 |
| H             | -0.72956400 | 2.53122300  | -2.61875300 |

### Ti-Ts₃

| Atomic Symbol | X   | Y   | Z   |
|---------------|-----|-----|-----|
| Ti            | 0.50563861 | 1.30955089 | 14.37764581 |
| Ti            | 0.47936479 | 1.14729964 | 11.60983884 |
| O             | 1.92069323 | 2.69532893 | 13.94538709 |
| O             | -0.91584847 | -0.11565457 | 14.13721367 |
| O             | 1.93351106  | -0.10425060 | 14.10940117 |
| O             | -0.92860208 | 2.68388042 | 13.97299925 |
| O             | -1.01479522 | 2.59317927 | 11.72921109 |
| O             | 1.97718969  | -0.27623613 | 11.86914527 |
| O             | -1.00266710 | -0.28711481 | 11.89817217 |
| O             | 1.96491266  | 2.60406923 | 11.70040432 |
| C             | 2.36371332  | 3.06017049 | 12.81120074 |
| C             | -1.37999744 | -0.60980289 | 13.06197842 |
| C             | 2.37987121  | -0.59554438 | 13.02535949 |
| C             | -1.39586767 | 3.04578494  | 12.84763107 |
| H             | 3.14776071  | 3.82817044 | 12.80200642 |
H: -2.1859006  3.80797914  12.85375126  
H:  3.17058040 -1.35250921  13.10548758  
H: -2.16315657 -1.37282217  13.15737247  
C:  0.30887835  1.56060331  5.45790662  
C: -0.35404301  0.22235709  5.69293724  
H:  1.37710131  1.38654533  5.22915974  
H: -0.11089430  2.15618209  4.64691681  
H: -1.34224973  0.20045857  6.12046448  
C:  0.36570148 -1.06111023  5.38211987  
H:  1.04128727 -1.29377048  6.21289485  
H: -0.34081064 -1.88321051  5.25111034  
H:  0.95159938 -0.96292828  4.46305839  
N:  0.14881723  2.29253800  6.70528602  
Br: -1.64957592  0.31027858  3.46035625  
C:  0.27710503  1.49586352  7.84511730  
O:  0.14647972  0.24628383  7.47378101  
O:  0.44709791  2.06410579  8.96438513  
C:  0.51200849  3.69466323  6.72468220  
H:  0.34555067  4.07858245  7.73213298  
H:  1.57315848  3.85467392  6.46211081  
H: -0.10787281  4.25298471  6.01171336  

**Ti-IntS**

Ti: -0.42542700 -0.37372500  4.37773300  
Ti: -0.44928800 -0.56316800  1.46680000  
O:  0.95712500  1.02047800  3.91753500  
O: -1.82602000 -1.80139100  4.11893600  
O:  0.99627000  1.79588700  4.12963800  
O: -1.85232300  1.00719100  3.98265900  
O: -1.91741900  0.95378400  1.73058900  

883
### Nb-HKUST-1

|     | x    | y    | z     |
|-----|------|------|-------|
| O   | 1.46706200 | -1.46676300 | -1.07992900 |
| O   | -1.46692200 | 1.46756300 | -1.07894400 |
| O   | 1.46759500 | 1.46684900 | -1.07895700 |
| O   | -1.46779300 | -1.46605500 | -1.07987400 |
| O   | -1.53915300 | -1.53841400 | 1.15898900  |
| O   | 1.53935300 | 1.53760200 | 1.15990400  |
| O   | -1.53860900 | 1.53831400 | 1.15991800  |
| O   | 1.53847300 | -1.53910400 | 1.15893200  |
| C   | 1.93303900 | -1.93296800 | 0.01959800  |
| C   | -1.93298700 | 1.93302600 | 0.01957000  |
| C   | 1.93392700 | 1.93207800 | 0.01957000  |
| C   | -1.93391900 | -1.93209500 | 0.01836200  |
| H   | 2.70650100 | -2.70624400 | -0.04502000 |
| H   | -2.70776700 | -2.70498400 | -0.04494800 |
| H   | 2.70780300 | 2.70493900 | -0.04397000 |
| H   | -2.70650700 | 2.70624200 | -0.04334200 |
| Nb  | 0.00001400 | -0.00053200 | 1.23077900  |
| Nb  | -0.00002400 | 0.00052800 | -1.29396900 |

### Nb-Int₀

|     | x    | y    | z     |
|-----|------|------|-------|
| O   | 1.49982900 | 1.49968000 | 1.11671300 |
| O   | -1.49966700 | -1.49967800 | 1.11688400 |
| O   | 1.49981600 | -1.49969400 | 1.11673100 |
| O   | -1.49965200 | 1.49969400 | 1.11686600 |
| O   | -1.50340300 | 1.50328400 | -1.12222000 |
| O   | 1.50325500 | -1.50329100 | -1.12235500 |
| O   | -1.50341400 | -1.50329400 | -1.12220200 |
| O   | 1.50327300 | 1.50325400 | -1.12237300 |
| C   | 1.93336800 | 1.93343200 | -0.00161800 |
C    -1.93350100   -1.93330700   -0.00137300
C     1.93344200   -1.93336800   -0.00159100
C    -1.93340600    1.93339200   -0.00139900
H     2.70701100    2.70666800    0.00133100
H    -2.70692000    2.70675700    0.00166200
H     2.70693000   -2.70675900    0.00135900
H    -2.70686500   -2.70682200    0.00169000
Nb   -0.00008200   -0.00001600   -1.25980800
Nb    0.00008600    0.00000700    1.26482100
C    -0.18675731   -1.14403823   -3.94865064
C    -1.20651823   -0.06468662   -4.11990677
H    -0.39892284   -2.00542892   -3.31715302
H     0.48699325   -1.34442271   -4.78418750
H    -1.17063497   -1.34442271   -4.78418750
H    -2.57316325   -0.11836989   -3.47595317
H    -2.95233391    0.89178948   -3.27520131
H    -3.29211739   -0.62791306   -4.13027552
H    -2.52780331   -0.65700157   -2.52351568
N    -0.04847615    0.13573408   -3.25098959
C     0.99705391    1.02947518   -3.73512433
H     0.74495820    2.06045224   -3.46193211
H     1.94620692    0.76794280   -3.25362924
H     1.13966724    0.98434039   -4.83093223

Nb-Int_{1}
O     1.52106800    1.61845800   -0.59783400
O    -1.59533300   -1.44743200   -0.61317900
O     1.52829800   -1.45698600   -0.60553600
O    -1.56850100    1.63053500   -0.59347800
O    -1.56459300    1.61249000   -2.86013500
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| O    | 1.50338300 | -1.46285200| -2.87171900|
| O    | -1.57180400| -1.45752800| -2.87782500|
| O    | 1.50808800 | 1.60890300 | -2.86366000|
| C    | 1.91748400 | 2.01849800 | -1.73216300|
| C    | -1.98441100| -1.85830400| -1.74594900|
| C    | 1.91841700 | -1.86342800| -1.73874300|
| C    | -1.97121800| 2.02409900 | -1.72794800|
| H    | 2.67694900 | 2.78409600 | -1.74341200|
| H    | -2.73698200| 2.78418500 | -1.74308100|
| H    | 2.67686800 |-2.62931100 |-1.74384000 |
| H    | -2.73692700|-2.62934000 |-1.74305300|
| Nb   | -0.03032900| 0.07450400 |-2.82661800 |
| Nb   | -0.02741200| 0.07399300 |-0.57109400 |
| C    | -1.38680800| -0.50074600| 2.45098800 |
| C    | -0.15829900| -1.30941900| 2.63504100 |
| H    | -2.15759500| -0.83543300| 1.75700900 |
| H    | -1.71201700| 0.09556500 | 3.29990200 |
| H    | 0.30203800 | -1.16212400| 3.61373600 |
| C    | 0.05514800 | -2.66939200| 2.01618500 |
| H    | 1.11887700 | -2.84959600| 1.82682700 |
| H    | -0.29995100| -3.42945000| 2.72572300 |
| H    | -0.49068800| -2.78888000| 1.07666500 |
| N    | -0.12105400| -0.07056200| 1.79521200 |
| Br   | -0.19097400| -0.09324300| 6.04304800 |
| C    | 0.55180600 | 1.08267100 | 2.43409700 |
| H    | 1.61487400 | 1.05376200 | 2.17919600 |
| H    | 0.12030600 | 2.00761900 | 2.03762500 |
| H    | 0.43173100 | 1.05265800 | 3.52501200 |

**Nb-Ts**

857
|     | X         | Y         | Z         |
|-----|-----------|-----------|-----------|
| O   | 1.49982900 | 1.49968000 | 1.11671300 |
| O   | -1.49966700 | -1.49967800 | 1.11688400 |
| O   | 1.49981600  | -1.49969400 | 1.11673100 |
| O   | -1.49965200 | 1.49969400  | 1.11686600 |
| O   | -1.50340300 | 1.50328400  | -1.12220000|
| O   | 1.50325500  | -1.50329100 | -1.12235500|
| O   | -1.50341400 | -1.50329400 | -1.12220200|
| O   | 1.50327300  | 1.50325400  | -1.12237300|
| C   | 1.93336800  | 1.93343200  | -0.00161800|
| C   | -1.93350100 | -1.93330700 | -0.00137300|
| C   | 1.93344200  | -1.93336800 | -0.00159100|
| C   | -1.93340600 | 1.93339200  | -0.00139900|
| H   | 2.70701100  | 2.70666800  | 0.00133100 |
| H   | -2.70692000 | 2.70675700  | 0.00166200 |
| H   | 2.70693000  | -2.70675900 | 0.00135900 |
| H   | -2.70686500 | -2.70682200 | 0.00169000 |
| Nb  | -0.00008200 | -0.00001600 | -1.25980800|
| Nb  | 0.00008600  | 0.00000700  | 1.26482100 |
| C   | -1.71221650 | 0.00287242  | 3.91970590 |
| C   | -0.72667213 | -0.76202777 | 4.71419239 |
| H   | -2.32640622 | -0.60818146 | 3.25680127 |
| H   | -2.30496262 | 0.74536929  | 4.45955476 |
| H   | -0.19631001 | -0.22905949 | 5.49106807 |
| C   | -0.20235385 | -2.10512969 | 4.28441866 |
| H   | 0.71924785  | -1.99605341 | 3.70024202 |
| H   | 0.01540742  | -2.70912639 | 5.16847768 |
| H   | -0.93731422 | -2.63508422 | 3.67168453 |
| N   | -0.49856629 | 0.49286819  | 3.29057315 |
| Br  | -2.27164265 | -1.52441794 | 6.74903905 |

**s88**
C         -0.11546028    1.83933635    3.70387368
H          0.92777278    2.02935350    3.43820483
H       -0.74887022    2.57127716    3.18218471
H       -0.24466728    1.97896872    4.78774051

Nb-Int$_2$
O          1.53759600    1.55265100   -0.64882400
O       -1.53567900   -1.47010500   -0.61217300
O           1.44607200   -1.49690700   -0.60914100
O      -1.63228400    1.51994000   -0.63664200
O       -1.55482100    1.63469800   -2.89932800
O          1.50198200   -1.43364200   -2.87210900
O      -1.56038200   -1.42774600   -2.87573400
O          1.50733300    1.63333500   -2.91347300
C           1.92056200    1.99881600   -1.76591200
C       -1.96355600   -1.86254800   -1.74840800
C           1.89113100   -1.87341700   -1.74272600
C      -1.99085800    1.98802100   -1.75620400
H           2.67694900    2.78409600   -1.74341200
H       -2.73698200    2.78418500   -1.74308100
H           2.67686800   -2.62933100   -1.74338400
H      -2.73692700   -2.62939400   -1.74305300
Nb         -0.02404100    0.10616200   -2.98415800
Nb       -0.04584800    0.01861800   -0.33577500
C           -0.42463700    0.02014900    2.66497100
C         0.72477900   -0.39838600    3.59450600
H        -0.89405700   -0.89186500    2.26440400
H        -1.19974000    0.55006400    3.24378300
H           1.29031800    0.47090100    3.92917600
C           1.62455200   -1.49172200    3.05656900
S60

H    2.04805400   -1.15654900   2.10207300
H    2.44326400   -1.71625800   3.74788700
H    1.05869500   -2.41111500   2.86944800
N    0.09085600    0.84669600    1.58679600
Br   -0.08001600   -1.06635200    5.42307000
C    0.21494800    2.24507200    1.95685300
H    0.71376800    2.78831800    1.15149100
H   -0.77699900    2.70522000    2.12836400
H    0.80665900    2.39513200    2.87813000

Nb-Int$_3$

O    1.75329500    1.54167500   -0.69263600
O   -1.36312200   -1.44361400   -0.67294600
O    1.61048000   -1.49255100   -0.67016200
O   -1.44407700    1.54271500   -0.70202800
O   -1.37532100    1.65459000   -2.96342800
O    1.68600300   -1.41150900   -2.93106200
O   -1.37899900   -1.40879300   -2.93622100
O    1.68001400    1.65378800   -2.95538000
C    2.11240300    2.00822200   -1.81337200
C   -1.78545700   -1.84122200   -1.80913600
C    2.06741700   -1.85882400   -1.80122700
C   -1.80863400    2.00895400   -1.81995100
H    2.85820300    2.80353500   -1.80086000
H   -2.55572800    2.80362400   -1.80052900
H    2.85812200   -2.60989200   -1.80083200
H   -2.55567300   -2.60995500   -1.80050100
Nb    0.15608000    0.12397200   -3.04068500
Nb    0.13435000    0.03341200   -0.39941300
C   -0.58946400    0.11020100    2.48570900
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | 0.29093900 | -0.32886600 | 3.66298900 |
| H       | -0.99850100 | -0.79670600 | 2.01329500 |
| H       | -1.45178200 | 0.68756200  | 2.86032400 |
| H       | 0.76415200  | 0.52944800  | 4.14120300 |
| C       | 1.28471000  | -1.42849400 | 3.34722000 |
| H       | 1.93654500  | -1.08408800 | 2.53420300 |
| H       | 1.90276600  | -1.67783500 | 4.21544800 |
| H       | 0.77189900  | -2.33505700 | 3.00754600 |
| N       | 0.18856300  | 0.88148000  | 1.52761000 |
| Br      | -0.95794800 | -1.00502500 | 5.21165300 |
| C       | 3.95957300  | 1.47579400  | 1.32047000 |
| O       | 3.86306600  | 2.63255900  | 1.47950600 |
| O       | 4.12032600  | 0.32365600  | 1.19879800 |
| C       | 0.26276100  | 2.29108000  | 1.87399000 |
| H       | 0.69020400  | 2.46299200  | 2.87828100 |
| H       | 0.89705100  | 2.80944800  | 1.15138900 |
| H       | -0.73790400 | 2.76326900  | 1.85842400 |

**Nb-Ts₂**

| O       | 1.49982900  | 1.49968000  | 1.11671300 |
| O       | -1.49966700 | -1.49967800 | 1.11688400 |
| O       | 1.49981600  | -1.49969400 | 1.11673100 |
| O       | -1.49965200 | 1.49969400  | 1.11686600 |
| O       | -1.50340300 | 1.50328400  | -1.12222000|
| O       | 1.50325500  | -1.50329100 | -1.12235500|
| O       | -1.50341400 | -1.50329400 | -1.12220200|
| O       | 1.50327300  | 1.50325400  | -1.12237300|
| C       | 1.93336800  | 1.93343200  | -0.00161800|
| C       | -1.93350100 | -1.93330700 | -0.00137300|
| C       | 1.93344200  | -1.93336800 | -0.00159100|
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -1.9334 | 1.93339 | -0.0014 |
| H    | 2.7070  | 2.70666 | 0.00133 |
| H    | -2.7069 | 2.70675 | 0.00166 |
| H    | 2.7069  | -2.7068 | 0.00136 |
| H    | -2.7069 | -2.7068 | 0.00170 |
| Nb   | -0.0001 | 0.00001 | -1.2598 |
| Nb   | 0.0001  | 0.0000  | 1.2648  |
| C    | -1.3286 | -0.3546 | 4.3413  |
| C    | -0.8642 | -1.7451 | 4.7848  |
| H    | -2.2244 | -0.4579 | 3.7105  |
| H    | -1.6217 | 0.2178  | 5.2326  |
| H    | -0.0686 | -1.6789 | 5.5253  |
| C    | -0.5147 | -2.7148 | 3.6768  |
| H    | 0.3677  | -2.3323 | 3.1488  |
| H    | -0.2607 | -3.7001 | 4.0802  |
| H    | -1.3320 | -2.8139 | 2.9569  |
| N    | -0.2718 | 0.3629  | 3.6189  |
| Br   | -2.4119 | -2.5489 | 5.9153  |
| C    | 1.5408  | 0.5558  | 4.6608  |
| O    | 1.6044  | 1.2534  | 5.6288  |
| O    | 1.9358  | -0.3244 | 3.9578  |
| C    | -0.6356 | 1.7872  | 3.6278  |
| H    | -0.7606 | 2.1170  | 4.6379  |
| H    | 0.1404  | 2.3564  | 3.1601  |
| H    | -1.5514 | 1.9248  | 3.0918  |
| Nb-Int$_4$ |
| O    | 0.9178  | 1.4058  | -1.2014 |
| O    | -2.1795 | -1.6973 | -1.1929 |
| O    | 0.8841  | -1.7427 | -1.2092 |
O    -2.17248800   1.39900900  -1.19263500
O    -2.15514200   1.38988200  -3.46188000
O     0.91341200  -1.69154500  -3.47630600
O    -2.16294600  -1.68610300  -3.46249100
O     0.91655000   1.38505300  -3.46997400
C     1.31831700   1.79533900  -2.33276500
C    -2.57006100  -2.09277100  -2.32734600
C     1.30468900  -2.11269000  -2.33862500
C    -2.56486300   1.79370100  -2.32613500
H     2.08339800   2.55481500  -2.34172800
H    -3.33053300   2.55490400  -2.34139700
H     2.08331700  -2.85861200  -2.34170000
H    -3.33047800  -2.85867500  -2.34136900
Nb    -0.61787700  -0.15045800  -3.41339400
Nb    -0.60982800  -0.15546900  -1.15357200
C     0.68901300  -0.83811400   4.23411500
C     1.82892700   0.10047400   4.62749900
H     1.17117600  -1.73726500   3.82709900
H     0.13025600  -1.13626800   5.12841600
H     2.13315200   0.69552800   3.77076700
C     3.00129400  -0.60152500   5.28905400
H     3.44256000  -1.28681900   4.55657800
H     3.76929500   0.11077900   5.60653300
H     2.68209500  -1.18225700   6.16310200
N    -0.23181600  -0.30138400   3.25324100
Br    1.12287000   1.54984200   5.94276700
C     0.21176800  -0.32048300   1.91233800
O     1.41858300  -0.52571800   1.70081000
O    -0.71695700  -0.10485900   1.03303200
C  -1.64437300  -0.24492000  3.59019200
H  -2.17876100  0.21874300  2.75926900
H  -2.07493800 -1.24966300  3.75970700
H  -1.79070000  0.35560500  4.49876100

**Nb-Ts$_3$**

O  1.49982900  1.49968000  1.11671300
O  -1.49966700 -1.49967800  1.11688400
O  1.49981600 -1.49969400  1.11673100
O  -1.49965200  1.49969400  1.11686600
O  -1.50340300  1.50328400 -1.12220000
O  1.50325500 -1.50329100 -1.12235500
O  -1.50341400 -1.50329400 -1.12220200
O  1.50327300  1.50325400 -1.12237300
C  1.93336800  1.93343200 -0.00161800
C  -1.93350100 -1.93330700 -0.00137300
C  1.93344200 -1.93336800 -0.00159100
C  -1.93340600  1.93339200 -0.00139900
H  2.70701100  2.70666800  0.00133100
H  -2.70692000  2.70675700  0.00166200
H  2.70693000 -2.70675900  0.00135900
H  -2.70686500 -2.70682200  0.00169000
Nb  -0.00008200 -0.00001600 -1.25980800
Nb  0.00008600  0.00000700  1.26482100
C  -1.10408246 -0.51177732  6.89182296
C  -0.49405142 -1.87350394  6.65064524
H  -2.20361885 -0.59772840  6.80639305
H  -0.87972654  0.09478550  7.87383061
H  0.57042399 -1.94016010  6.50019510
C  -1.35379644 -3.10172605  6.52840059
| Atom | X    | Y    | Z    |
|------|------|------|------|
| H    | -1.77698470 | -3.13455841 | 5.51823196 |
| H    | -0.76835803  | -4.00657223  | 6.70339592  |
| H    | -2.17045674  | -3.07591156  | 7.25623214  |
| N    | -0.56451642  | 0.37750210   | 5.87358270  |
| Br   | 0.12207805   | -2.27068446  | 9.12509187  |
| C    | -0.43429891  | -0.22035237  | 4.61754796  |
| O    | -0.48278214  | -1.50997646  | 4.74402473  |
| O    | -0.26644059  | 0.52526455   | 3.60736678  |
| C    | -0.83083946  | 1.79573731   | 6.00275585  |
| H    | -0.37516953  | 2.30993236   | 5.15544422  |
| H    | -1.91293582  | 2.01848087   | 6.00391754  |
| H    | -0.39927491  | 2.17456946   | 6.93788771  |
| Nb-Int₅ |      |      |      |
| O    | 0.91410100   | 1.39682100   | -1.20482900 |
| O    | -2.16742700  | -1.69762200  | -1.20245500 |
| O    | 0.91344200   | -1.70231800  | -1.20400500 |
| O    | -2.16860700  | 1.39195200   | -1.20240200 |
| O    | -2.16041800  | 1.38306100   | -3.46802300 |
| O    | 0.91045600   | -1.68917500  | -3.46904000 |
| O    | -2.15971800  | -1.68807300  | -3.46838800 |
| O    | 0.91090300   | 1.38433100   | -3.46940200 |
| C    | 1.31829200   | 1.79481300   | -2.33554400 |
| C    | -2.56694800  | -2.09608500  | -2.33432800 |
| C    | 1.31742800   | -2.09911500  | -2.33522400 |
| C    | -2.56795300  | 1.79155400   | -2.33406800 |
| H    | 2.08339800   | 2.55481500   | -2.34172800 |
| H    | -3.33053300  | 2.55490400   | -2.34139700 |
| H    | 2.08331700   | -2.85861200  | -2.34170000 |
| H    | -3.33047800  | -2.85867500  | -2.34136900 |
| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| Nb      | -0.62240800 | -0.15140800 | -3.42712100 |
| Nb      | -0.61754300 | -0.15032200 | -1.18089200 |
| C       | 0.60125100  | -0.43297700  | 4.29868000  |
| C       | 1.80204500  | -0.06589400  | 3.41636700  |
| H       | 0.62874600  | -1.48441400  | 4.62613900  |
| H       | 0.56336600  | 0.21419800   | 5.18004500  |
| H       | 2.05552000  | 0.98774600   | 3.55840300  |
| C       | 3.02770000  | -0.93621600  | 3.56689200  |
| H       | 2.78385700  | -1.99374600  | 3.40580600  |
| H       | 3.80276100  | -0.63899700  | 2.85176400  |
| H       | 3.40763300  | -0.79150000  | 4.58461400  |
| N       | -0.51012900 | -0.22546600  | 3.36636100  |
| Br      | 2.48225400  | 1.23962700   | 6.69291000  |
| C       | -0.07051900 | -0.19751300  | 2.09351000  |
| O       | 1.26232100  | -0.18807400  | 2.03593400  |
| O       | -0.79990700 | -0.18166000  | 1.08137600  |
| C       | -1.90109900 | -0.36445200  | 3.73888000  |
| H       | -2.52095400 | -0.17832600  | 2.85952100  |
| H       | -2.10516000 | -1.37748500  | 4.11526900  |
| H       | -2.14854900 | 0.35718100   | 4.52505300  |

**W-HKUST-1**

| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| W       | -0.003164  | 0.001110  | 1.271896 |
| W       | 0.001913   | -0.001299 | -1.269200 |
| O       | -1.046597  | 1.675489  | 1.148105 |
| O       | 1.039738   | -1.674051 | 1.154540 |
| O       | 1.675432   | 1.047696  | 1.121798 |
| O       | -1.681887  | -1.044762 | 1.116716 |
| O       | -1.679603  | -1.033184 | -1.155560 |
| O       | 1.685622   | 1.028034  | -1.150456 |
| Atom | X       | Y       | Z        |
|------|---------|---------|----------|
| O    | 1.038409| -1.685585| -1.117715|
| O    | -1.028820| 1.686635| -1.124055|
| C    | -1.330388| 2.152200| 0.011713 |
| C    | 1.332621 | -2.150381| 0.020279 |
| C    | 2.151721 | 1.330324| -0.014582|
| C    | -2.151795| -1.331774| -0.021063|
| H    | -1.910248| 3.087124| 0.012365 |
| H    | -3.086253| -1.912413| -0.025184|
| H    | 3.086663 | 1.910235| -0.015538|
| H    | 1.914795 | -3.083882| 0.025107 |

**W-Int**

| Atom | X       | Y       | Z        |
|------|---------|---------|----------|
| W    | -0.09058100 | 0.33726400 | -0.18639500 |
| W    | -2.31957700 | 0.33929100 | -0.18892400 |
| O    | -0.09061100 | 1.81176500 | -1.69729100 |
| O    | -0.10210500 | -1.12589600 | 1.32174600 |
| O    | -0.09518700 | -1.15915100 | -1.66171500 |
| O    | -0.09715500 | 1.85320900 | 1.28424800 |
| O    | -2.35135300 | 1.84028100 | 1.27353000 |
| O    | -2.34857400 | -1.15734600 | -1.65010300 |
| O    | -2.35414400 | -1.12177500 | 1.31095800 |
| O    | -2.34551900 | 1.80038100 | -1.68701800 |
| C    | -1.21934300 | 2.22492400 | -2.12321600 |
| C    | -1.22711100 | -1.54325800 | 1.74849900 |
| C    | -1.21986200 | -1.59014500 | -2.07471200 |
| C    | -1.22517800 | 2.27768100 | 1.69681800 |
| H    | -1.23073000 | 2.98714700 | -2.90715300 |
| H    | -1.23492700 | 3.06217500 | 2.45832700 |
| H    | -1.22213800 | -2.37799200 | -2.83189900 |
| H    | -1.22636500 | -2.30333600 | 2.53277300 |

867
C       3.00147700  -0.14596300   1.27764000
C       3.32717700  -0.75183400  -0.02386200
H       2.31565700  -0.65619800   1.94767800
H       3.76176100   0.46419700   1.75807800
H       4.31292900  -0.49415400  -0.40542100
C       2.84415500  -2.11956000  -0.42899400
H       2.70838500  -2.19120300  -1.51545500
H       3.61869800  -2.82735800   0.11251500
H       1.89798500  -2.37853300   0.05553100
N       2.37067000   0.40791300   0.04323300
Br      6.21266500  -2.08929500   1.37367500
C       2.93024500   1.69194200  -0.40405100
H       2.76310500   1.80733300  -1.48035900
H       2.42386100   2.51125400   0.11893000
H       4.00927400   1.75599300  -0.20300900

W-Ts_1
W       1.09601200   0.00178600   0.00084200
W      -1.09601800  -0.00170900  -0.00080900
O       1.12218400   1.46088200  -1.49881800
O       1.12460000  -1.45742200   1.50036600
O       1.12701300  -1.49789800  -1.45826800
O       1.11995800   1.50145500   1.46005800
O      -1.12690600   1.49786200   1.45820600
O      -1.11986200  -1.50151000  -1.45988900
O      -1.12227100  -1.46098600   1.49879800
O      -1.12468300   1.45727400  -1.50060400
C      -0.00160400   1.88371200  -1.93672200
C       0.00150800  -1.88398700   1.93643500
C       0.00461000  -1.93667900  -1.88371900

\[ \text{S68} \]
| Symbol | X         | Y         | Z         |
|--------|-----------|-----------|-----------|
| C      | -0.00448500 | 1.93659500 | 1.88385200 |
| H      | -0.00218800 | 2.64495800 | -2.72024700 |
| H      | -0.00638500 | 2.71998600 | 2.64523300 |
| H      | 0.00640400  | -2.72018100 | -2.64499300 |
| H      | 0.00217700  | -2.64552500 | 2.71967900 |
| C      | 3.89391770  | -0.38790678 | 1.36380058 |
| C      | 4.36606896  | -1.44258847 | 0.44101231 |
| H      | 3.17577900  | -0.73176182 | 2.10982938 |
| H      | 4.65677752  | 0.26353897  | 1.79717829 |
| H      | 5.17724046  | -1.18941365 | -0.2268214 |
| C      | 3.58638308  | -2.70386285 | 0.18418801 |
| H      | 2.79569596  | -2.53417432 | -0.55633068 |
| H      | 4.25765292  | -3.47929016 | -0.19263407 |
| H      | 3.12232807  | -3.06660498 | 1.10594202 |
| N      | 3.27001869  | 0.08644740  | 0.14104026 |
| Br     | 6.34736255  | -2.49962267 | 1.88381324 |
| C      | 3.94942776  | 1.22430042  | -0.47135379 |
| H      | 3.62677026  | 1.33732805  | -1.50971546 |
| H      | 3.68797522  | 2.13953990  | 0.07884361 |
| H      | 5.04264867  | 1.10221022  | -0.44298906 |

**W-Int₂**

| Symbol | X         | Y         | Z         |
|--------|-----------|-----------|-----------|
| W      | -0.04563300 | 0.34255300 | -0.18499400 |
| W      | -2.30744500 | 0.34041300 | -0.18795300 |
| O      | -0.07914000 | 1.82285400 | -1.70468900 |
| O      | -0.07897200 | -1.13846200 | 1.32805500 |
| O      | -0.08245600 | -1.17683300 | -1.66482600 |
| O      | -0.09112000 | 1.86740700  | 1.29288100 |
| O      | -2.35207200 | 1.84451900  | 1.27630000 |
| O      | -2.34340200 | -1.16120100 | -1.65238100 |
| Symbol | X          | Y          | Z          |
|--------|------------|------------|------------|
| O      | -2.337740  | -1.120392  | 1.309296   |
| O      | -2.338783  | 1.800458   | -1.685110  |
| C      | -1.211948  | 2.226456   | -2.121883  |
| C      | -1.210396  | -1.544547  | 1.746144   |
| C      | -1.213126  | -1.594402  | -2.071106  |
| C      | -1.222524  | 2.280054   | 1.695831   |
| H      | -1.230730  | 2.987147   | -2.907153  |
| H      | -1.234927  | 3.062175   | 2.458327   |
| H      | -1.222138  | -2.377992  | -2.831899  |
| H      | -1.226365  | -2.303360  | 2.532773   |
| C      | 2.985394   | -0.454801  | 0.748171   |
| C      | 3.789343   | -1.416593  | -0.133119  |
| H      | 2.356620   | -1.045569  | 1.426570   |
| H      | 3.681019   | 0.135816   | 1.374171   |
| H      | 4.366530   | -0.881560  | -0.886457  |
| C      | 3.014805   | -2.580016  | -0.714656  |
| H      | 2.184005   | -2.175899  | -1.304724  |
| H      | 3.643860   | -3.204264  | -1.358509  |
| H      | 2.595554   | -3.205444  | 0.082117   |
| N      | 2.177673   | 0.384072   | -0.107781  |
| Br     | 5.402494   | -2.261300  | 1.013715   |
| C      | 2.913422   | 1.546829   | -0.567614  |
| H      | 2.277338   | 2.166821   | -1.208389  |
| H      | 3.264000   | 2.182604   | 0.275714   |
| H      | 3.818303   | 1.300553   | -1.160763  |

**W-Int**

| W  | X         | Y         | Z          |
|----|-----------|-----------|------------|
| W  | 2.419825  | 0.057087  | -0.368236  |
| W  | 0.159890  | 0.051396  | -0.364423  |
| O  | 2.444364  | 1.515436  | -1.870447  |
O  2.45359300  -1.40406800  1.13071100
O  2.46032100  -1.44337400 -1.83621600
O  2.45135500   1.55704200    1.09523800
O  0.19186600   1.55570500    1.12294900
O  0.20018100  -1.45788800 -1.85889600
O  0.19464500  -1.42523500    1.14831900
O  0.18378600   1.54213300  -1.87918500
C  1.31746700   1.94137300  -2.30296700
C  1.32652500  -1.82860100    1.56725200
C  1.33103400  -1.87547000  -2.25944600
C  1.32122500   1.98419200    1.52207400
H  1.33507400   2.70002200  -3.08996200
H  1.33087700   2.77505000    2.27551800
H  1.34366600  -2.66511700  -3.01470800
H  1.33943900  -2.59046100    2.34996400
C  -2.86234600  -0.69501000    0.58336600
C  -3.79345400   0.33622600    1.22744100
H  -2.22399600  -1.12625300    1.36604300
H  -3.46587000  -1.52162200    0.16307500
H  -4.38003100   0.86772500    0.47890300
C  -3.14715600   1.26646600    2.23299500
H  -2.30828700   1.77516600    1.74448800
H  -3.85463400   2.01427900    2.60939500
H  -2.74641700   0.70216800    3.08329200
N  -2.06648500  -0.03247600   -0.42701300
Br  -5.37600600  -0.68192000    2.26506400
C  -1.95392900   3.83994700  -1.08868400
O  -2.74723800   3.50782300  -1.88156700
O  -1.18182600   4.23046200  -0.30165500
C    -2.74825400  -0.00595200  -1.70941600
H    -3.71918900   0.52749000  -1.68673300
H    -2.12913500   0.50407300  -2.45677500
H    -2.96158000  -1.02828300  -2.09202600

W-Ts₂
W    1.09601200   0.00178600   0.00084200
W   -1.09601800  -0.00170900  -0.00080900
O    1.12218400  1.46088200  -1.49881800
O    1.12460000  -1.45742200   1.50036600
O    1.12701300  -1.49789800  -1.45826800
O    1.11995800  1.50145500   1.46005800
O   -1.12690600  1.49786200   1.45820600
O   -1.11986200  -1.50151000  -1.45988900
O   -1.12227100  -1.46098600  -1.49879800
O   -1.12468300   1.45727400  -1.50060400
C   -0.00160400  1.88371200  -1.93672200
C    0.00150800  -1.88398700   1.93643500
C    0.00461000  -1.93667900  -1.88371900
C   -0.00448500  1.93659500   1.88385200
H   -0.00218800  2.64495800  -2.72024700
H   -0.00638500  2.71998600   2.64523300
H    0.00640400  -2.72018100  -2.6449300
H    0.00217700  -2.64552500   2.71967900
C   -3.97826841  -1.16794857   0.62276232
C   -4.35523510  -0.51954058   1.95815713
H   -3.35804926  -2.05632542   0.81581815
H   -4.89746728  -1.51298863   0.12882756
H   -5.08503705   0.27665735   1.81926707
C   -3.20196097  -0.07218401   2.82982673
H         -2.67639634  0.74238605  2.31600952
H         -3.55935699  0.31482181  3.78933693
H         -2.49175977 -0.88513530  3.00500499
N         -3.26976618 -0.22762106 -0.25336118
Br        -5.47558290 -1.92674222  2.99937516
C          -4.27325516  1.57337401 -0.56260504
O          -4.82620668  1.35422582 -1.59898672
O          -4.01918392  2.25728829  0.38223831
C          -3.34447454 -0.77095036 -1.61722039
H          -4.36952138 -0.91565967 -1.88784593
H          -4.36952138 -0.91565967 -1.88784593
H          -2.88878837 -0.08462965 -2.3001905
H          -2.82949337 -1.70804620 -1.65653680
W-Int4
  W         -0.65120500  0.43649900  0.10216400
  W         -2.88870800  0.44056700  0.09775600
  O         -0.66633600  1.91818100 -1.41549700
  O         -0.67670600 -1.01743800  1.62285400
  O         -0.66973100 -1.06615000 -1.37591400
  O         -0.67004600  1.95739000  1.57702700
  O         -2.92855300  1.94325400  1.55990900
  O         -2.92688700 -1.05868100 -1.36535500
  O         -2.93302300 -1.02065600  1.59816000
  O         -2.92463700  1.90307700 -1.40367600
  C         -1.79414900  2.32644200 -1.83687100
  C         -1.80010100 -1.43518000  2.03805400
  C         -1.79393500 -1.49001500 -1.78608600
  C         -1.79903600  2.37822400  1.98330800
  H         -1.80891900  3.08953300 -2.62144200
  H         -1.81311600  3.16456100  2.74403800

S73
|     |           |           |           |
|-----|-----------|-----------|-----------|
| H   | -1.80032700 | -2.27560600 | -2.54618800 |
| H   | -1.80455400 | -2.20095000 | 2.81848400  |
| C   | 4.87953600  | -0.65576300 | 0.88852000  |
| C   | 5.35064200  | -1.78755700 | -0.02163700 |
| H   | 4.49580600  | -1.15125900 | 1.79447900  |
| H   | 5.73343000  | -0.03507600 | 1.18188000  |
| H   | 4.51914000  | -2.16102900 | -0.61450400 |
| C   | 6.08311600  | -2.89830900 | 0.70706000  |
| H   | 5.37881700  | -3.37602400 | 1.40125600  |
| H   | 6.45738100  | -3.65841900 | 0.01141100  |
| H   | 6.93378600  | -2.50887700 | 1.28294500  |
| N   | 3.84659800  | 0.18727300  | 0.32532000  |
| Br  | 6.62573200  | -1.02988700 | -1.48229700 |
| C   | 2.53065700  | -0.34149600 | 0.33156400  |
| O   | 2.40505000  | -1.55813200 | 0.56692600  |
| O   | 1.59910900  | 0.51295200  | 0.07347600  |
| C   | 4.08841100  | 1.61738100  | 0.24775100  |
| H   | 3.23028300  | 2.08364400  | -0.2369600  |
| H   | 4.21123800  | 2.07755700  | 1.24562600  |
| H   | 4.99260800  | 1.81818300  | -0.34129900 |

**W-Ts$_3$**

|     |           |           |           |
|-----|-----------|-----------|-----------|
| W   | 1.09601200 | 0.00178600 | 0.00084200 |
| W   | -1.09601800 | -0.00170900 | -0.00080900 |
| O   | 1.12218400  | 1.46088200  | -1.49881800 |
| O   | 1.12460000  | -1.45742200 | 1.50036600  |
| O   | 1.12701300  | -1.49789800 | -1.45826800 |
| O   | 1.11995800  | 1.50145500  | 1.46005800  |
| O   | -1.12690600 | 1.49786200  | 1.45820600  |
| O   | -1.11986200 | -1.50151000 | -1.45988900 |
| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| W       | -0.67447 | 0.44303 | 0.09862 |
| W       | -2.89455 | 0.44147 | 0.09759 |
| O       | -0.67550 | 1.91596 | -1.40869 |
| O       | -0.67443 | -1.02099 | 1.60926 |
| O       | -0.67340 | -1.05855 | -1.37124 |
| O       | -0.67719 | 1.95453 | 1.57005 |
| O       | -2.93175 | 1.94245 | 1.55986 |
| O       | -2.92635 | -1.05701 | -1.36306 |
| O       | -2.92798 | -1.01879 | 1.59778 |
| O       | -2.92967 | 1.90383 | -1.40221 |
| C       | -1.80156 | 2.32828 | -1.83653 |
| C       | -1.79895 | -1.43894 | 2.03472 |
| C       | -1.79647 | -1.48981 | -1.78639 |
| C       | -1.80428 | 2.37921 | 1.98308 |
| H       | -1.80891 | 3.08953 | -2.62144 |
| H       | -1.81311 | 3.16456 | 2.74404 |
| H       | -1.80033 | -2.27561 | -2.54619 |
| H       | -1.80455 | -2.20095 | 2.81848 |
| C       | 4.95598 | -0.79152 | 0.16083 |
| C       | 4.06647 | -1.99013 | -0.19597 |
| H       | 5.33104 | -0.84363 | 1.19533 |
| H       | 5.80726 | -0.72987 | -0.52361 |
| H       | 4.15724 | -2.20994 | -1.26315 |
| C       | 4.27888 | -3.24081 | 0.62513 |
| H       | 4.17586 | -3.03129 | 1.69774 |
| H       | 3.55628 | -4.01529 | 0.34474 |
| H       | 5.29039 | -3.60356 | 0.41190 |
| N       | 4.00612 | 0.31435 | 0.02293 |
| Br      | 7.31484 | -2.62973 | -1.64046 |
|      | X         | Y         | Z       |
|------|-----------|-----------|---------|
| C    | 2.73176600| -0.13384900| 0.05405300|
| O    | 2.69231600| -1.47230600| 0.01404200|
| O    | 1.71345300| 0.57592000 | 0.11207700|
| C    | 4.37254100| 1.70261500 | 0.19223400|
| H    | 3.48214600| 2.31949800 | 0.05482900|
| H    | 4.78259100| 1.88167700 | 1.19758500|
| H    | 5.13126500| 1.97994200 | -0.54825700|

**Sc-HKUST-1**

|      | X         | Y         | Z       |
|------|-----------|-----------|---------|
| Sc   | -0.00151300| -0.00016500| 1.44400300|
| Sc   | 0.00127500 | 0.00006100 | -1.44360700|
| O    | -1.49284800| 1.48320100 | 1.13179200|
| O    | 1.48927300 | -1.48426100| 1.13390100|
| O    | 1.47925000 | 1.48851200 | 1.11975200|
| O    | -1.48260300| -1.48826800| 1.11717200|
| O    | -1.49180800| -1.48201300| -1.13438300|
| O    | 1.49507600 | 1.48129700 | -1.13175300|
| O    | 1.48097400 | -1.48979200| -1.11765400|
| O    | -1.47709000| 1.49139100 | -1.11971600|
| C    | -1.89263500| 1.89465700 | 0.00480500|
| C    | 1.89295700 | -1.89421700| 0.00769000|
| C    | 1.89464200 | 1.89245200 | -0.00459900|
| C    | -1.89463500| -1.89273900| -0.00812500|
| H    | -2.67200800| 2.67144400 | 0.00195300|
| H    | -2.67121200| -2.67232300| -0.00689600|
| H    | 2.67138900 | 2.67186500 | -0.00138900|
| H    | 2.67307100 | -2.67026500| 0.00651000|

**Sc-Int**

|      | X         | Y         | Z       |
|------|-----------|-----------|---------|
| Sc   | -0.00000500| 0.00021800 | 1.44377700|
| Sc   | -0.00000500| -0.00017300| -1.44390400|

S77
| Atoms | X       | Y       | Z       |
|-------|---------|---------|---------|
| O     | -1.49911500 | -1.49387200 | 1.12624000 |
| O     | 1.49892700  | 1.49449900  | 1.12589000 |
| O     | -1.49413400 | 1.49931000  | 1.12595100 |
| O     | 1.49422800  | -1.49875700 | 1.12635600 |
| O     | 1.49367300  | -1.49966100 | -1.12579200 |
| O     | -1.49386100 | 1.49907900  | -1.12620200 |
| O     | 1.49955800  | 1.49339700  | -1.12626100 |
| O     | -1.49922600 | -1.49410900 | -1.12591000 |
| C     | -1.90820300 | -1.90109100 | 0.00022300 |
| C     | 1.90813300  | 1.90119000  | -0.00025800 |
| C     | -1.90125400 | 1.90806900  | -0.00020800 |
| C     | 1.90122400  | -1.90806900 | 0.00032900 |
| H     | -2.68735300 | -2.67771600 | 0.00034300 |
| H     | 2.67745500  | -2.68761300 | 0.00046300 |
| H     | -2.67760600 | 2.68749200  | -0.00038800 |
| H     | 2.68790900  | 2.67718700  | -0.00043200 |
| C     | -1.12323911 | 0.19212315  | -4.35364342 |
| C     | 0.09476997  | 1.01303475  | -4.63076959 |
| H     | -1.94460731 | 0.60668923  | -3.77116027 |
| H     | -1.41986310 | -0.54627983 | -5.10130033 |
| H     | 0.60465072  | 0.77902774  | -5.57031988 |
| C     | 0.24239592  | 2.44379974  | -4.16558698 |
| H     | 1.29719508  | 2.69390487  | -3.99429829 |
| H     | -0.15497638 | 3.13993135  | -4.91536233 |
| H     | -0.29801159 | 2.59959291  | -3.22590247 |
| N     | 0.12147414  | -0.04129886 | -3.61888298 |
| C     | 0.85188979  | -1.25930141 | -3.94942114 |
| H     | 1.90848047  | -1.12764519 | -3.68983936 |
| H     | 0.45285982  | -2.09074052 | -3.35729596 |
H  0.78735136  -1.53256707  -5.01915537
Sc-Inti
Sc  0.06546300  0.27526300  -0.65854200
Sc  0.00211400  0.27348700  -3.63836500
O  -1.49648200  -1.20673600  -1.04602300
O  1.60695500  1.70135300  -1.04133100
O  -1.38061000  1.87017400  -1.05008100
O  1.50830300  -1.24599200  -1.04825300
O  1.57777700  -1.18813400  -3.30486800
O  -1.53577200  1.73070800  -3.30286600
O  1.48349000  1.82050000  -3.29416000
O  -1.43743500  -1.28793500  -3.30562200
C  -1.87191300  -0.16989800  2.09220600
C  -1.86235400  2.19266500  -2.17138100
C  1.93756100  -1.62439500  -2.17816500
H  -2.66235400  -2.40572700  -2.16696500
H  2.70245400  -2.41562400  -2.16684500
H  -2.65260700  2.95948100  -2.16796000
H  2.71290800  2.94917600  -2.16774000
C  -1.87093600  -0.16989800  2.09220600
C  -0.57799100  -0.73617600  2.54181900
H  -2.45825900  -0.67780300  1.33136300
H  -2.43083800  0.43262200  2.80495400
H  -0.28997200  0.47389700  3.56561800
C  -0.04909800  -2.06183200  2.05111500
H  1.04709400  -2.05458300  2.00652700
H  -0.34235800  -2.83786500  2.76662000
H  -0.43898700  -2.33577700  1.06443700
N    -0.60434900    0.42415500    1.59227400
Br   -0.24090600   -0.09029000    6.04521500
C    -0.24347400    1.72589500    2.19636000
H    0.83114300    1.89744400    2.06295100
H   -0.79770000    2.52068600    1.68472500
H   -0.45935800    1.74272300    3.27163700

Sc-Ts₁
Sc   -0.00000500    0.00021800    1.44377700
Sc   -0.00000500   -0.00017300   -1.44390400
O   -1.49911500   -1.49387200    1.12624000
O    1.49892700    1.49449900    1.12589000
O   -1.49413400    1.49931000    1.12591000
O    1.49422800   -1.49875700    1.12635600
O    1.49367300   -1.49966100   -1.12579200
O   -1.49386100    1.49907900   -1.12620200
O    1.49955800    1.49339700   -1.12626100
O   -1.49922600   -1.49410900   -1.12591000
C   -1.90820300   -1.90109100    0.00022300
C    1.90813300    1.90119000   -0.00025800
C   -1.90125400    1.90806900   -0.00020800
C    1.90122400   -1.90806900    0.00032900
H   -2.68735300   -2.67771600    0.00034300
H    2.67745500   -2.68761300    0.00046300
H   -2.67760600    2.68749200   -0.00038800
H    2.68790900    2.67718700   -0.00043200
C   -0.88455211   -0.16376472    4.45573466
C    0.32114590   -0.80109841    5.02750081
H   -1.53965393   -0.84691036    3.91289757
H   -1.44377468    0.50751455    5.11209369
H  0.93173303  -0.20217811  5.68828127
C  0.88213754  -2.09418778  4.50034798
H  1.50286636  -1.92150331  3.61309150
H  1.49639068  -2.56786323  5.26989996
H  0.07715600  -2.78304563  4.22824699
N  0.12102381   0.45956318  3.61330717
Br -0.66078813  -1.71729395  7.33421089
C  0.42240476   1.84274999  3.97009340
H  1.36870329   2.14797841  3.51574465
H -0.37611710   2.49574554  3.58970206
H  0.48625279   1.97141530  5.06106141

Sc-Int$_2$
Sc  -0.00033900   0.25365600  -0.60166100
Sc  0.03971300   0.28931300  -3.68638300
O  -1.45888900  -1.28078800  -1.00916400
O  1.48550000   1.81577800  -1.05093800
O  -1.57759100  1.69143100  -1.04204600
O  1.51717900  -1.26270400  -1.02893200
O  1.49056900  -1.27151800  -3.29410900
O  -1.41752100  1.84116900  -3.29671100
O  1.58904300   1.74116800  -3.31384200
O  -1.51726000  -1.17458200  -3.26886700
C  -1.88387700  -1.62516600  -2.15194500
C  1.93101700   2.17158800  -2.17729500
C  -1.88532400  2.16762500  -2.17026900
C  1.90610800  -1.65315600  -2.16573400
H  -2.66235400  -2.40572700  -2.16696500
H  2.70245400  -2.41562400  -2.16684500
H  -2.65260700  2.95948100  -2.16769600
H  2.71290800  2.94917600  -2.16774000
C  -0.56259600  -0.25590300  2.37014500
C  0.27654000  -1.32866900  3.08528400
H  -1.37181800  -0.76740800  1.82555100
H  -1.04574700  0.38960700  3.12563500
H  1.12885400  -0.88266500  3.59663300
C  0.68111700  -2.51279600  2.23149400
H  1.26656900  -2.14535200  1.37976200
H  1.28914300  -3.22760700  2.79563700
H  -0.20049800  -3.03265400  1.83819200
N  0.25737700  0.51646400  1.45746900
Br  -0.81323000  -2.06508100  4.73190200
C  1.02958900  1.54602700  2.13215500
H  1.55088700  2.15861300  1.38967700
H  0.38142200  2.21647900  2.73340300
H  1.80062500  1.15165400  2.82366500

Sc-Int₃

Sc  3.59043000  -0.93353500  0.71238600
Sc  0.86981200  0.47907000  0.42192400
O  3.50379400  -0.76914600  -1.43645300
O  2.99158200  -0.71892800  2.78394100
O  2.31633300  -2.66485000  0.60495400
O  4.18335300  1.16217100  0.77415400
O  2.17169800  2.18461300  0.61716900
O  0.30686500  -1.65068500  0.35280400
O  0.98180300  0.31151800  2.59749900
O  1.54006600  0.34058600  -1.65722000
C  2.57801000  -0.22178000  -2.10020200
C  1.92994500  -0.21951600  3.24554900

S82
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| C       | 1.06382800 | -2.65559300 | 0.44465500 |
| C       | 3.43338700 | 2.17147100  | 0.71989400 |
| H       | 2.68535500 | -0.23743500 | -3.19592700 |
| H       | 3.92606300 | 3.15539100  | 0.77026000 |
| H       | 0.57646200 | -3.64111900 | 0.37521500 |
| H       | 1.81734800 | -0.24751500 | 4.34163800 |
| C       | -1.94489100 | 0.33279800  | -1.00577300 |
| C       | -3.28957700 | 0.03695400  | -0.32888700 |
| H       | -1.48187800 | -0.62373100 | -1.27936300 |
| H       | -2.12911400 | 0.88917800  | -1.94282200 |
| H       | -3.80222200 | 0.95323900  | -0.03268500 |
| C       | -3.24057700 | -0.97456100 | 0.79616100 |
| H       | -2.55937700 | -0.59147300 | 1.56487600 |
| H       | -4.22759100 | -1.13199800 | 1.24262700 |
| H       | -2.84522300 | -1.93328300 | 0.44471100 |
| N       | -1.06411200 | 1.07031000  | -0.12003500 |
| Br      | -4.62787000 | -0.68930200 | -1.79248400 |
| C       | -1.89498300 | 2.48223600  | 3.45880100 |
| O       | -2.77638500 | 1.71188600  | 3.46405200 |
| O       | -1.03560000 | 3.27605700  | 3.47706300 |
| C       | -1.35504700 | 2.49375400  | -0.08837300 |
| H       | -2.31497300 | 2.75047900  | 0.40040800 |
| H       | -0.57253500 | 3.03249300  | 0.46504000 |
| H       | -1.39603500 | 2.93703200  | -1.10390800 |

**Sc-Ts₂**

| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| Sc      | 3.49012100 | -1.00487100 | 0.16335900 |
| Sc      | 0.78963800 | 0.38807300  | -0.10789100 |
| O       | 3.42935400 | -0.84366700 | -1.98679500 |
| O       | 2.93404300 | -0.83600800 | 2.25663800 |
| Atom | X-Coord   | Y-Coord   | Z-Coord   |
|------|-----------|-----------|-----------|
| O    | 2.23612900| -2.74873300| 0.01612700|
| O    | 4.09800300| 1.07637100 | 0.24833700|
| O    | 2.09227700| 2.09604000 | 0.01211600|
| O    | 0.22230900| -1.73189400| -0.17621300|
| O    | 0.92259000| 0.17160600 | 2.02636600|
| O    | 1.43024400| 0.19821700 | -2.19958100|
| C    | 2.48665800| -0.32454600| -2.64886000|
| C    | 1.86582700| -0.33412900| 2.69930400|
| C    | 0.97992300| -2.73993900| -0.11358200|
| C    | 3.34900100| 2.08626200 | 0.16141000|
| H    | 2.59927100| -0.32247400| -3.74572600|
| H    | 3.83997900| 3.07035200 | 0.22046100|
| H    | 0.49037800| -3.72615800| -0.17458400|
| H    | 1.73126400| -0.33255400| 3.79183900|
| C    | -2.36403300| 0.15651300 | -0.95116700|
| C    | -3.14072800| -0.04354300| 0.35384500|
| H    | -2.06951000| -0.83032800| -1.34765300|
| H    | -3.06759600| 0.59464400 | -1.67599700|
| H    | -3.61234200| 0.88844900 | 0.66776600|
| C    | -2.41919500| -0.72786400| 1.49413000|
| H    | -1.58509300| -0.09450200| 1.81912900|
| H    | -3.08470300| -0.87404100| 2.35129500|
| H    | -2.01114400| -1.69261700| 1.18113400|
| N    | -1.21155800| 1.04492700 | -0.76909100|
| Br   | -4.82985600| -1.19065500| -0.11294600|
| C    | -1.78583700| 2.88755400 | 0.66441000|
| O    | -2.58658800| 3.41704300 | -0.02918900|
| O    | -1.08592800| 2.67182400 | 1.59384300|
| C    | -1.01443000| 1.82562000 | -1.99761800|
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| H       | -1.90110990 | 2.43776900 | -2.22765400 |
| H       | -0.16658100 | 2.51505200 | -1.88064400 |
| H       | -0.79448800 | 1.19113700 | -2.87172800 |
| Sc      | 1.60442200  | -0.23904200 | 0.14959900 |
| Sc      | 4.60674900  | 0.27933000  | 0.30113600 |
| O       | 2.37615100  | -2.24201900 | 0.32660800 |
| O       | 1.66059600  | 1.93663900  | 0.03797100 |
| O       | 2.16316500  | -0.26679600 | -1.95500200 |
| O       | 1.86437700  | -0.03333300 | 2.28196600 |
| O       | 4.09466400  | 0.33178300  | 2.41300800 |
| O       | 4.39427000  | 0.10793500  | -1.84297300 |
| O       | 3.88757300  | 2.31971000  | 0.15421700 |
| O       | 4.60738800  | -1.88626700 | 0.42422600 |
| C       | 3.57875700  | -2.61704800 | 0.40824600 |
| C       | 2.68249100  | 2.67888100  | 0.05653200 |
| C       | 3.31165200  | -0.11382000 | -2.45545700 |
| C       | 2.94385900  | 0.17927400  | 2.90586900 |
| H       | 3.74322400  | -3.70474500 | 0.47303500 |
| H       | 2.86810000  | 0.23790200  | 4.00445900 |
| H       | 3.37275200  | -0.17963000 | -3.55460300 |
| H       | 2.49770200  | 3.76329700  | -0.02239900 |
| C       | -3.63327200 | -0.46722100 | -1.68618000 |
| C       | -4.72095500 | -1.00841300 | -0.76004800 |
| H       | -3.35930900 | -1.30658400 | -2.34221000 |
| H       | -4.04252300 | 0.33215500  | -2.31409500 |
| H       | -4.26941500 | -1.56199000 | 0.06091900 |
| C       | -5.78479100 | -1.81735100 | -1.47929700 |
| H       | -5.30833400 | -2.70727000 | -1.91435300 |

Sc-Int₄
H    -6.56969800  -2.14942100  -0.79371300  
H    -6.25069800  -1.24232900  -2.28859800  
N    -2.44241500    0.01755200  -1.01805900  
Br   -5.65255200    0.56136700   0.22322800  
C    -1.53147000   -0.95019200  -0.57561500  
O    -1.86365300   -2.14407000  -0.60854200  
O    -0.38981300   -0.49087700  -0.14415700  
C    -2.10330700    1.42806200  -1.13614400  
H    -1.21736800    1.63326100  -0.53689200  
H    -1.88537200    1.70827500  -2.18020200  
H    -2.93268400    2.04682400  -0.77308500  

**Sc-Ts₃**

Sc    1.58302100   -0.26505800   0.00272000  
Sc    4.54320900    0.26153800   0.16265700  
O    2.32576600   -2.27361900   0.12030900  
O    1.62196400    1.91425700  -0.11076800  
O    2.10731800   -0.29072300  -2.09646400  
O    1.84531400   -0.10180500  2.13730100  
O    4.05970600    0.34421000  2.27430700  
O    4.33985000    0.05584400 -1.97962800  
O    3.85066000    2.30093200 -0.01891400  
O    4.54876100  -1.90265400   0.31020500  
C    3.52857400   -2.64159400   0.25531800  
C    2.64251000    2.65900600  -0.09725400  
C    3.25901000  -0.14560600  -2.59716500  
C    2.91154200    0.15369400  2.76663000  
H    3.69768200   -3.72568400   0.33417100  
H    2.82255800    0.21696300  3.86559500  
H    3.32721000  -0.20056900  -3.69346700  

S86
H 2.45216000  3.74235800  -0.16126300
C -3.88764000  0.53976400  -0.78704900
C -4.40919600 -0.71273600  -0.10593300
H -4.01786700  0.44103900  -1.87924500
H -4.46030500  1.40855700  -0.46237900
H -4.33013400 -0.77537500   0.96645200
C -4.98559100 -1.85539100  -0.89859200
H -4.17044400 -2.39746600  -1.39179400
H -5.53037200 -2.54330500  -0.25008500
H -5.67833800 -1.48393200  -1.65970200
N -2.48308400  0.75322900  -0.45103100
Br -6.76539600  0.26963500   0.53316500
C -1.76714400 -0.39795100  -0.22323800
O -2.45800700 -1.45259100  -0.09600200
O -0.49047300 -0.34730800  -0.13713000
C -1.86945300  2.01365500  -0.82901700
H -0.83856000  2.03843500  -0.47431900
H -1.87012500  2.15104000  -1.92206100
H -2.42638600  2.84260800  -0.37632100

Sc-Int_5
Sc  1.64721800 -0.24620800   0.15190600
Sc  4.57660200  0.28544700   0.30125600
O  2.36992700 -2.24733800   0.31451200
O  1.66628700  1.93562700   0.04128400
O  2.16782900 -0.29846600  -1.94916200
O  1.87872700 -0.06719500   2.27741500
O  4.09928400  0.33388600   2.41490700
O  4.39084900  0.10611900  -1.84066200
O  3.89111600  2.32370200   0.15252600
| Atom | X       | Y       | Z       | V         |
|------|---------|---------|---------|-----------|
| O    | 4.595360 | -1.880856 | 0.429492 | 0.42949200 |
| C    | 3.575440 | -2.620508 | 0.406517 | 0.40651700 |
| C    | 2.685014 | 2.684040 | 0.056870 | 0.05687000 |
| C    | 3.312112 | -0.124272 | -2.456526 | -2.45652600 |
| C    | 2.950227 | 0.169201 | 2.908844 | 2.90884400 |
| H    | 3.743224 | -3.704745 | 0.473035 | 0.47303500 |
| H    | 2.868100 | 0.237902 | 4.004459 | 4.00445900 |
| H    | 3.372752 | -0.179630 | -3.554603 | -3.55460300 |
| H    | 2.497702 | 3.763297 | -0.022399 | -0.02239900 |
| C    | -3.783533 | 0.656029 | -1.028423 | -1.02842300 |
| C    | -3.878058 | -0.851849 | -0.749152 | -0.74915200 |
| H    | -3.888737 | 0.895086 | -2.097617 | -2.09761700 |
| H    | -4.552374 | 1.194408 | -0.466299 | -0.46629900 |
| H    | -4.361446 | -1.019239 | 0.216284 | 0.21628400 |
| C    | -4.532487 | -1.686492 | -1.825117 | -1.82511700 |
| H    | -4.049598 | -1.530832 | -2.797983 | -2.79798300 |
| H    | -4.485472 | -2.751080 | -1.570825 | -1.57082500 |
| H    | -5.583738 | -1.382439 | -1.875837 | -1.87583700 |
| N    | -2.417085 | 0.952189 | -0.583414 | -0.58341400 |
| Br   | -7.050958 | 0.419645 | 0.102671 | 0.10267100 |
| C    | -1.705767 | -0.173176 | -0.427373 | -0.42737300 |
| O    | -2.455772 | -1.262177 | -0.590261 | -0.59026100 |
| O    | -0.485995 | -0.255589 | -0.159306 | -0.15930600 |
| C    | -1.865229 | 2.292322 | -0.558351 | -0.55835100 |
| H    | -0.819172 | 2.251579 | -0.249262 | -0.24926200 |
| H    | -1.926943 | 2.745394 | -1.557371 | -1.55737100 |
| H    | -2.435387 | 2.913003 | 0.142149 | 0.14214900 |
| Mo-HKUST-1 | Mo | -0.000000 | -0.000000 | -1.06100000 |
| Mo | -0.000012 | -0.000437 | 1.06101200 |
O   -1.49453300   1.50653800  -1.12012000
O    1.49551300  -1.50618600  -1.12032200
O   -1.50731100  -1.49470700  -1.12030000
O    1.50582300   1.49541400  -1.12045800
O    1.50580600   1.49520300   1.12013900
O   -1.50662100  -1.49517100   1.12028300
O    1.49613600  -1.50585200   1.12026200
O   -1.49462000   1.50667200   1.12047400
C   -1.91758100   1.93340800   0.00015600
C    1.91973600  -1.93195900  -0.00006000
C   -1.93386200  -1.91789400   0.00001400
C    1.93195300   1.91897500  -0.00013400
H   -2.68835700   2.71157900   0.00000200
H     2.70853700   2.69135000   0.00001800
H   -2.71187400  -2.68882000   0.00011700
H    2.69223300  -2.70841200  -0.00018100
Mo-Int
Mo   -0.00007800  -0.00019600  -1.06075600
Mo    0.00003800  -0.00021700   1.06075700
O   -1.50030900   1.50289300  -1.11967700
O    1.50072200  -1.50262700  -1.11986500
O   -1.50314200  -1.50039600  -1.11966700
O    1.50252200   1.50058600  -1.11980600
O    1.50262700   1.50052600   1.11970700
O   -1.50300000  -1.50040300   1.11983300
O    1.50086300  -1.50267200   1.11963600
O   -1.50020500   1.50290900   1.11983500
C   -1.92653700   1.93020300   0.00009900
C    1.92759000  -1.92946500  -0.00014300
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -1.93045100 | -1.92663600 | 0.00010400 |
| C    | 1.92952100  | 1.92718700  | -0.00006000 |
| H    | -2.69975500 | 2.70568500  | 0.00012200 |
| H    | 2.70404300  | 2.70136900  | -0.00006000 |
| C    | -1.05710643 | -0.15091895 | 4.01821682 |
| H    | -0.84501711 | 1.90221516 | 3.12226103 |
| C    | -2.39973919 | -0.50745426 | 3.42198147 |
| C    | 1.35433656  | -0.60300302 | 3.59214116 |
| H    | 1.39408604  | -1.67398876 | 3.36299177 |
| H    | 2.18012872  | -0.10796961 | 3.06855987 |
| H    | 1.50579994  | -0.47360388 | 4.68002230 |

**Mo-Int**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| Mo   | 0.21016000 | 0.44413600 | -2.67868900 |
| Mo   | 0.21598000 | 0.43883900 | -0.52647700 |
| O    | -1.29107300 | 1.94814900 | -2.75439500 |
| O    | 1.71205000  | -1.05631100 | -2.75615800 |
| O    | -1.29347800 | -1.05518900 | -2.76423300 |
| O    | 1.71275500  | 1.94671900  | -2.74821500 |
| O    | 1.73251600  | 1.95485700  | -0.50297500 |
| O    | -1.30024000 | -1.06601000 | -0.52131300 |
```
|     |          |          |          |
|-----|----------|----------|----------|
| O   | 1.73280300 | -1.06161800 | -0.51210400 |
| O   | -1.29683900 | 1.96335100  | -0.50935800 |
| C   | -1.71371200 | 2.37703400  | -1.63136400 |
| C   | 2.14351200  | -1.48104600 | -1.63420200 |
| C   | -1.71915800 | -1.48176000 | -1.64153900 |
| C   | 2.14333400  | 2.37189800  | -1.62750000 |
| H   | -2.48739200 | 3.15175000  | -1.64140100 |
| H   | 2.91640600  | 3.14743400  | -1.64159200 |
| H   | -2.49343000 | -2.25392400 | -1.64136600 |
| H   | 2.91415600  | -2.25789400 | -1.64174000 |
| C   | -1.31566200 | -0.03887600 | 2.56755600  |
| C   | -0.03060400 | -0.67054300 | 2.92532400  |
| H   | -1.97874200 | -0.52647600 | 1.85794100  |
| H   | -1.80189400 | 0.57505100  | 3.32240500  |
| H   | 0.31766000  | -0.43602700 | 3.92973500  |
| C   | 0.37049900  | -2.03876200 | 2.43785900  |
| H   | 1.45820800  | -2.11336200 | 2.31379700  |
| H   | 0.05484600  | -2.75486900 | 3.20512900  |
| H   | -0.10431700 | -2.29165900 | 1.48476400  |
| N   | -0.05673000 | 0.48995400  | 1.97664300  |
| Br  | -1.00514300 | -1.69997600 | 6.12370800  |
| C   | 0.40189000  | 1.76332100  | 2.54879300  |
| H   | 1.48369600  | 1.85821600  | 2.40354100  |
| H   | -0.09426600 | 2.59337900  | 2.03214900  |
| H   | 0.18251600  | 1.83056500  | 3.62416600  |

**Mo-Ts**

|     |          |          |          |
|-----|----------|----------|----------|
| Mo  | -0.00007800 | -0.00019600 | -1.06075600 |
| Mo  | 0.00003800  | -0.00021700 | 1.06075700  |
```
O       -1.50030900    1.50289300   -1.11967700
O        1.50072200   -1.50262700   -1.11986500
O       -1.50314200   -1.50039600   -1.11966700
O        1.50252200    1.50058600   -1.11980600
O        1.50262700    1.50052600    1.11970700
O       -1.50300000   -1.50040300    1.11983300
O        1.50086300   -1.50267200    1.11963600
O       -1.50020500    1.50290900    1.11983500
C       -1.92653700    1.93020300    0.00009900
C        1.92759000   -1.92946500   -0.00014300
C       -1.93045100   -1.92663600    0.00010400
C        1.92952100    1.92718700   -0.00006000
H       -2.69975500    2.70568500    0.00012200
H         2.70404300    2.70136900   -0.00006900
H       -2.70579300   -2.69998900    0.00015700
H         2.70179300   -2.70395900   -0.00021700
C       -0.84963673   -0.28796589    4.15708716
C        0.43207202   -0.90792477    4.55670212
H        0.15153178   -2.86291077    3.70477523
N        0.03250262    0.40158269    3.23201549
Br    -0.24684061   -1.94832068    6.91915298
C        0.33488360    1.77838051    3.61191829
H        1.21253140    2.13263632    3.06482118

S92
H    -0.52062619  2.41962502  3.35570275
H     0.52251209  1.86489618  4.69272962

Mo-Int$_2$
Mo   0.20801100  0.44731800   -2.66023600
Mo   0.21620600  0.44283800   -0.47035200
O    -1.29496800  1.95119600   -2.75367600
O     1.71424100  -1.05735500   -2.74712200
O    -1.29370600  -1.05199600   -2.74318200
O     1.70999800   1.94851600   -2.73927000
O     1.74337400   1.96784000   -0.48904800
O    -1.30460900  -1.08651900   -0.49367700
O     1.73873600  -1.08300700   -0.49616200
O    -1.30411800  -1.08651900   -0.49367700
C    -1.71226600  2.38106900   -1.62775100
C     2.14099200  -1.48518900   -1.62549100
C    -1.71611000  -1.48454000   -1.62103600
C     2.14252500   2.37404100   -1.61851600
H    -2.48742700   3.15177100   -1.64151000
H     2.91637100   3.14745500   -1.64170100
H    -2.49346500  -2.25390300   -1.64147500
H     2.91412100  -2.25787300   -1.64184900
C    -0.74183600  -0.36743100    2.57393800
C     0.18098300  -1.26764800    3.40156700
H    -1.37887900  -1.00243900    1.94475100
H    -1.40722900   0.19909000    3.25309600
H     0.89822500  -0.68424500    3.97776800
C     0.83061100  -2.41062600    2.65132400
H     1.40248500  -1.98968600    1.81632400
H     1.50363900  -2.98722600    3.29506200
| Atom | x     | y     | z     | E   |
|------|-------|-------|-------|-----|
| H    | 0.07201100 | -3.08637800 | 2.23942500 |     |
| N    | 0.08247200 | 0.49952300 | 1.76561500 |     |
| Br   | -0.93495200 | -2.15026200 | 5.02192900 |     |
| C    | 0.46017900 | 1.70220700 | 2.48096200 |     |
| H    | 1.07535600 | 2.34436700 | 1.84124900 |     |
| H    | -0.42453100 | 2.29527800 | 2.80334400 |     |
| H    | 1.05156900 | 1.51210500 | 3.40123600 |     |

**Mo-Int₃**

| Atom | x     | y     | z     | E   |
|------|-------|-------|-------|-----|
| Mo   | 0.09859400 | 0.45623100 | -2.76554100 |     |
| Mo   | 0.10657400 | 0.44243500 | -0.57734400 |     |
| O    | -1.40344000 | 1.96166400 | -2.85615900 |     |
| O    | 1.60433600 | -1.04681600 | -2.84642500 |     |
| O    | -1.40579000 | -1.04218400 | -2.84861200 |     |
| O    | 1.59911800 | 1.96221900 | -2.83863500 |     |
| O    | 1.64920800 | 1.96154100 | -0.58781700 |     |
| O    | -1.41616400 | -1.07608300 | -0.59905500 |     |
| O    | 1.60894300 | -1.09138900 | -0.59686200 |     |
| O    | -1.40636700 | 1.99391500 | -0.60524200 |     |
| C    | -1.81873000 | 2.39156900 | -1.72962500 |     |
| C    | 2.02508700 | -1.48326800 | -1.72519800 |     |
| C    | -1.82687100 | -1.47513500 | -1.72638400 |     |
| C    | 2.03774400 | 2.37883000 | -1.71863400 |     |
| H    | -2.59641900 | 3.16047300 | -1.74214200 |     |
| H    | 2.80737900 | 3.15615700 | -1.74233300 |     |
| H    | -2.60245700 | -2.24520100 | -1.74210700 |     |
| H    | 2.80512900 | -2.24917100 | -1.74248100 |     |
| C    | -0.71045700 | -0.46100800 | 2.45393800 |     |
| C    | 0.30872900 | -1.07023800 | 3.42053400 |     |
| H    | -1.10997700 | -1.26290700 | 1.81722300 |     |
H    -1.56032800  -0.04631100  3.02913000
H     0.80779600  -0.30401800  4.01189700
C     1.27624900  -2.06409700  2.81161600
H     1.79403000  -1.57692200  1.97773900
H     2.01293100  -2.41428600  3.54155700
H     0.74038000  -2.93148300  2.40971400
N    -0.04310200   0.54500200  1.65932700
Br    -0.72978800  -2.11220200  4.99148700
C     3.78518200   1.28485900  1.58296400
O     3.43520500   2.12017500  2.32365800
O     4.19605100   0.45667100  0.86606900
C    -0.06154400   1.84119000  2.31127600
H     0.45500400   1.85606800  3.29206400
H     0.43988300   2.58663700  1.68353900
H    -1.09665800   2.20198500  2.49701100

Mo-Ts2
Mo    -0.00007800  -0.00019600  -1.06075600
Mo     0.00003800  -0.00021700   1.06075700
O    -1.50030900   1.50289300  -1.11967700
O     1.50072200  -1.50262700  -1.11986500
O    -1.50314200  -1.50039600  -1.11966700
O     1.50252200   1.50058600  -1.11980600
O     1.50262200   1.50052600   1.11970700
O    -1.50300000  -1.50040300   1.11983300
O     1.50086300  -1.50267200   1.11963600
O    -1.50020500   1.50290900   1.11983500
C    -1.92653700   1.93020300  0.00009900
C     1.92759000  -1.92946500  -0.00014300
C    -1.93045100  -1.92663600   0.00010400
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | 1.92952100 | 1.92718700 | -0.00006000 |
| H       | -2.69975500 | 2.70568500 | 0.00012200 |
| H       | 2.70404300  | 2.70136900 | -0.00006900 |
| H       | -2.70579300 | -2.69989000 | 0.00015700 |
| H       | 2.70179300  | -2.70395900 | -0.00021700 |
| C       | -0.91114639 | -0.15764817 | 4.16004421 |
| C       | -0.32510851 | -1.48456618 | 4.65163787 |
| H       | -1.83696953 | -0.35806621 | 3.59983004 |
| H       | -1.83943444 | 0.45025147  | 5.03410973 |
| H       | 0.51068852  | -1.32067148 | 5.33017624 |
| C       | 0.01685591  | -2.49825350 | 3.58136905 |
| H       | 0.83490123  | -2.09439158 | 2.97190364 |
| H       | 0.36326217  | -3.43767587 | 4.02369651 |
| H       | -0.83686191 | -2.69506575 | 2.92685107 |
| N       | 0.04501639  | 0.57881155  | 3.32508109 |
| Br      | -1.73747355 | -2.31252000 | 5.93196912 |
| C       | 1.72711926  | 0.91354781  | 3.48626135 |
| O       | 1.89102031  | 2.04156141  | 3.84485589 |
| O       | 2.04775609  | -0.23365865 | 3.40797180 |
| C       | -0.41371640 | 1.97450323  | 3.27499133 |
| H       | -0.49489071 | 2.35919352  | 4.27014162 |
| H       | 0.28952928  | 2.56145274  | 2.72196711 |
| H       | -1.36969522 | 2.01877459  | 2.79640536 |

**Mo-Int\textsubscript{4}**

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Mo      | -0.12954600 | 0.53087900 | -3.39959000 |
| Mo      | -0.13148300 | 0.52917900 | -1.23806600 |
| O       | -1.63149500 | 2.03836900 | -3.48647000 |
| O       | 1.37123400  | -0.96876600 | -3.49574700 |
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| O    | -1.63089100 | -0.96796800 | -3.49929600 |
| O    | 1.37503100  | 2.03444600  | -3.48445800 |
| O    | 1.39312100  | 2.05658000  | -1.23590100 |
| O    | -1.66571300 | -0.96405000 | -1.25237000 |
| O    | 1.39383000  | -0.97832100 | -1.24812000 |
| O    | -1.64861700 | 2.06149000  | -1.23769200 |
| C    | -2.05618700 | 2.46773200  | -2.36285200 |
| C    | 1.79991000  | -1.39110000 | -2.36892900 |
| C    | -2.06549400 | -1.38429300 | -2.37171200 |
| C    | 1.80087500  | 2.46335500  | -2.36079900 |
| H    | -2.82930500 | 3.24353100  | -2.38061300 |
| H    | 2.57449300  | 3.23921500  | -2.38080400 |
| H    | -2.83534300 | -2.16214300 | -2.38057800 |
| H    | 2.57224300  | -2.16613300 | -2.38095200 |
| C    | -1.02844000 | -0.67358300 | 4.28147400 |
| C    | -0.08725000 | -1.76292300 | 4.79359500 |
| H    | -1.89509300 | -1.20875100 | 3.86084600 |
| H    | -1.38575800 | -0.06820400 | 5.12274500 |
| H    | 0.56341300  | -2.10004200 | 3.99032600 |
| C    | -0.79490900 | -2.91304500 | 5.48495900 |
| H    | -1.42824800 | -3.41873100 | 4.74331400 |
| H    | -0.08453700 | -3.64205300 | 5.88628000 |
| H    | -1.43229400 | -2.56066700 | 6.30525500 |
| N    | -0.45669600 | 0.19465600  | 3.27485600 |
| Br   | 1.26931800  | -0.93953100 | 6.14281200 |
| C    | -0.37787500 | -0.33617800 | 1.95768800 |
| O    | -0.53743000 | -1.56657900 | 1.83316100 |
| O    | -0.13173300 | 0.52620000  | 1.03573800 |
| C    | -0.49425600 | 1.62802000  | 3.50412400 |
|       | x       | y       | z       |
|-------|---------|---------|---------|
| H     | 0.02923300 | 2.11980300 | 2.68422200 |
| H     | -1.52609600 | 2.02447100 | 3.53735000 |
| H     | 0.00217400 | 1.87222400 | 4.45215800 |
| Mo-Ts3 |        |         |         |
| Mo    | -0.00007800 | -0.00019600 | -1.06075600 |
| Mo    | 0.00003800 | -0.00021700 | 1.06075700 |
| O     | -1.50030900 | 1.50289300 | -1.11967700 |
| O     | 1.50072200 | -1.50262700 | -1.11986500 |
| O     | -1.50314200 | -1.50039600 | -1.11966700 |
| O     | 1.50252200 | 1.50058600 | -1.11980600 |
| O     | 1.50262700 | 1.50052600 | 1.11970700 |
| O     | -1.50300000 | -1.50040300 | 1.11983300 |
| O     | 1.50086300 | -1.50267200 | 1.11963600 |
| O     | -1.50020500 | 1.50290900 | 1.11983500 |
| C     | -1.92653700 | 1.93020300 | 0.00009900 |
| C     | 1.92759000 | -1.92663600 | 0.00010400 |
| C     | -1.93045100 | -1.92521000 | -0.00006000 |
| H     | -2.69975500 | 2.70568500 | 0.00012200 |
| H     | 2.70404300 | -2.70136900 | -0.00006900 |
| H     | -2.70579300 | -2.69989000 | 0.00015700 |
| H     | 2.70179300 | -2.70395900 | -0.00021700 |
| C     | -0.20656710 | -0.04019050 | 6.78344667 |
| C     | 0.39927830 | -1.42474326 | 6.65792264 |
| H     | -1.29921489 | -0.14160555 | 6.92329448 |
| H     | 0.19368120 | 0.47033050 | 7.65968708 |
| H     | 1.41279823 | -1.50001622 | 6.30166016 |
| C     | -0.43675741 | -2.66280487 | 6.83163418 |
| H     | -1.06248758 | -2.79057506 | 5.94120139 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | 0.19372712 | -3.54514660| 6.95865411 |
| H    | -1.08210467| -2.57320805| 7.71088918 |
| N    | 0.10303143 | 0.74987782 | 5.60139586 |
| Br   | 1.52335304 | -1.57441358| 8.97839853 |
| C    | 0.00256257 | 0.03561521 | 4.40552870 |
| O    | -0.01970063| -1.22634922| 4.55378888 |
| O    | -0.03810921| 0.68155076 | 3.31664376 |
| C    | -0.15094451| 2.17520539 | 5.64805197 |
| H    | 0.12046033 | 2.60413816 | 4.68243540 |
| H    | -1.21397615| 2.40359993 | 5.84397575 |
| H    | 0.45294020 | 2.63850970 | 6.43860408 |

**Mo-Int5**

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Mo   | -0.12901300| 0.53546200 | -3.41280400|
| Mo   | -0.12900700| 0.53361400 | -1.26888100|
| O    | -1.63043300| 2.04055700 | -3.49330600|
| O    | 1.37078600 | -0.96482500| -3.49528600|
| O    | -1.63224600| -0.96308500| -3.49493300|
| O    | 1.37357600 | 2.03804000 | -3.49408000|
| O    | 1.38500800 | 2.05108400 | -1.24918500|
| O    | -1.64662600| -0.97142700| -1.25073700|
| O    | 1.38395800 | -0.97407700| -1.25152200|
| O    | -1.64304600| 2.05280400 | -1.24811200|
| C    | -2.05649400| 2.46773000 | -2.37035800|
| C    | 1.79903000 | -1.39148700| -2.37187300|
| C    | -2.06113000| -1.38830300| -2.37148300|
| C    | 1.80015800 | 2.46503500 | -2.37102200|
| H    | -2.82930500| 3.24353100 | -2.38061300|
| H    | 2.57449300 | 3.23921500 | -2.38080400|
| H    | -2.83534300| -2.16214300| -2.38057800|
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 2.57224300| -2.16611300| -2.38095200|
| C    | -0.20638200| -0.46291700| 4.48131600 |
| C    | -0.00858600| -1.74935700| 3.66987500 |
| H    | -1.23143200| -0.37316800| 4.87741600 |
| H    | 0.50016500 | -0.42313000| 5.31552600 |
| H    | 1.03136500 | -2.07703700| 3.74994700 |
| C    | -0.94927300| -2.88714100| 3.99306300 |
| H    | -1.99688400| -2.57150200| 3.90443700 |
| H    | -0.77626600| -3.73420200| 3.32060100 |
| H    | -0.74031000| -3.20073200| 5.02234300 |
| N    | 0.03064500 | 0.55374800 | 3.45560300 |
| Br   | 1.43964000 | -2.32468700| 6.94702300 |
| C    | -0.09526000| 0.03119100 | 2.21390500 |
| O    | -0.20799800| -1.30547500| 2.26970400 |
| O    | -0.10968900| 0.66941000 | 1.15176900 |
| C    | 0.02348300 | 1.97352200 | 3.72977400 |
| H    | 0.20069700 | 2.51116000 | 2.79579700 |
| H    | -0.94455200| 2.28888800 | 4.14617800 |
| H    | 0.80945900 | 2.21838800 | 4.45237200 |

**Zn-HKUST-1**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| Zn   | -1.39943500| -0.00022200| 0.01617700|
| Zn   | 1.40007800 | 0.00080700 | -0.01607200|
| O    | -1.70256800| 0.85033000 | 1.77486400 |
| O    | -1.74488300| -0.85335600| -1.73338800|
| O    | -0.52371000| -1.74850200| 0.85410200 |
| O    | -0.54645300| 1.74856300 | -0.84152000|
| O    | 1.71192300 | 1.75510100 | -0.87226900|
| O    | 1.73468500 | -1.75394600| 0.83024600 |
| O    | 0.51342500 | -0.84689800| -1.75405000|

S100
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| O       | 0.5557200 | 0.8479190 | 1.7419760 |
| C       | -0.5563980 | 1.0986640 | 2.2713980 |
| C       | -0.6103690 | -1.1002710 | -2.2567960 |
| C       | 0.5975210 | -2.2645250 | 1.0915360 |
| C       | 0.5685340 | 2.2647920 | -1.1064930 |
| H       | -0.5543920 | 1.5795240 | 3.2607900 |
| H       | 0.5720620 | 3.2538090 | -1.5881260 |
| H       | 0.6132410 | -3.2540190 | 1.5719450 |
| H       | -0.6310320 | -1.5825270 | -3.2452950 |

**Zn-Int$_0$**

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Zn      | -2.2975940 | -0.1738740 | 0.1106590 |
| Zn      | 0.6674710 | 0.1557440 | -0.1409810 |
| O       | -2.4467100 | -0.6785890 | 2.0223600 |
| O       | -2.8758840 | 0.2525870 | -1.7353760 |
| O       | -1.4105990 | -2.0015050 | -0.4387800 |
| O       | -1.7605120 | 1.8170000 | 0.5469550 |
| O       | 0.4888260 | 2.0886710 | 0.3525640 |
| O       | 0.8448140 | -1.7631030 | -0.6309310 |
| O       | -0.6418980 | 0.5051230 | -1.9397860 |
| O       | -0.2076850 | -0.4368590 | 1.8572850 |
| C       | -1.2631110 | -0.6940980 | 2.4913280 |
| C       | -1.8145990 | 0.5171180 | -2.3892870 |
| C       | -0.2452370 | -2.4183220 | -0.6714950 |
| C       | -0.6968990 | 2.4872910 | 0.5928190 |
| H       | -1.2022940 | -0.9640700 | 3.5607620 |
| H       | -0.7653120 | 3.5393030 | 0.8655900 |
| H       | -0.1227110 | -3.4650260 | -0.9455140 |
| H       | -1.9856850 | 0.7761630 | -3.4471510 |
| C       | 3.5134670 | 0.1766940 | 1.2355650 |
C   4.02595100  -0.41110900  -0.03352300
H   2.91263500  -0.43077100  1.90727000
H   4.07909200   0.97225300  1.71422500
H   4.93603500   0.05752300 -0.40634800
C   3.88312200 -1.86270500 -0.41781100
H   3.87416700 -1.97410900 -1.50837600
H   4.74335600 -2.41812300 -0.02330900
H   2.96496800 -2.30003000  0.00000000
N   2.87419800   0.53212700 -0.06262900
C   3.20198500   1.89182100 -0.56335600
H   3.09275200   1.89699300 -1.65317000
H   2.47505700   2.57032900 -0.11860400
H   4.23135300   2.17182400 -0.30707700

Zn-Int₁
Zn   -3.13175300   0.34496900  1.02359400
Zn    0.00124700   0.46787100  0.35546500
O   -3.85705400   0.06133800  2.92646900
O   -3.60970500   0.65706100 -0.93970100
O   -2.64981500 -1.63203000  0.57321200
O   -2.60379100  2.35577700  1.17863200
O   -0.33238000  2.32523200  1.12321700
O   -0.38397300 -1.52094800  0.59025100
O   -1.35831500   0.71148300 -1.16188900
O   -1.62822500   0.09145000  2.75996000
C   -2.68368300 -0.01890900  3.42687400
C   -2.53936700   0.77153000 -1.59744000
C   -1.49606100 -2.12294500  0.50817200
C   -1.46692300   2.87977200  1.26462500
H   -2.60194600 -0.19872900  4.50288900
H  -1.46658000  3.96264900  1.48104300
H  -1.44089000 -3.21025200  0.34214600
H  -2.62744800  0.94016000 -2.67013400
C   2.65967100 -1.02007300 -0.14602000
C   2.36786000 -0.47212000 -1.48539900
H   2.02681600 -1.79554900  0.27528000
H   3.70426000 -0.99994600  0.15784900
H   3.25876000 -0.07999000 -1.97946900
C   1.29583500 -1.00810800 -2.40055800
H   1.75478600 -1.75429700 -3.06127800
H   0.47930500 -1.48963100 -1.85590700
H   0.87502500 -0.21385000 -3.02869600
N   1.99133800  0.31758300 -0.26014200
Br  5.88861600 -0.41334200 -1.82364200
C   2.86658500  1.48157600  0.01821200
H   2.46012400  2.36011000 -0.49338400
H   2.87164800  1.67544700  1.09662400
H   3.88864000  1.29107100 -0.33113200

Zn-Ts

Zn  -1.42789900 -0.00545000  0.00413200
Zn   1.42804500  0.00560700 -0.00390900
O  -1.70521900 -0.31489500  1.94294100
O  -1.71954700  0.30064100 -1.93309100
O  -0.53922300 -1.93329500 -0.30506000
O  -0.55348800  1.92923300  0.30841100
O   1.70515000  1.94489700  0.30247500
O   1.71942500 -1.93112600 -0.31078000
O   0.53908100  0.30888400 -1.93257700
O   0.55339900 -0.30450800  1.92972400
| Atom | C     | H     | Br     | Zn  | N    |
|------|-------|-------|--------|-----|------|
|      | -0.56253100 | -0.39968400 | 2.50231500 |      |      |
|      | -0.58075400  | 0.39448300  | -2.49898300 |      |      |
|      | 0.58064000   | -2.49830000 | -0.39904300 |      |      |
|      | 0.56247800   | 2.50307500  | 0.39514500  |      |      |
|      | -0.56784000  | -0.57234600 | 3.58833800  |      |      |
|      | 0.56786900   | 3.58919300  | 0.56720600  |      |      |
|      | 0.59356300   | -3.58424900 | -0.57177800 |      |      |
|      | -0.59361700  | 0.56659700  | -3.58503000 |      |      |
|      | 4.34020215   | -1.20370801 | 0.50244489  |      |      |
|      | 4.87659999   | -0.89468338 | -0.84081977 |      |      |
|      | 3.67651825   | -2.06894848 | 0.53312056  |      |      |
|      | 5.05785357   | -1.20775348 | 1.32648763  |      |      |
|      | 5.65088480   | -0.14275550 | -0.90376802 |      |      |
|      | 4.18451601   | -1.31439838 | -2.10904568 |      |      |
|      | 3.51042841   | -0.52631226 | -2.46546655 |      |      |
|      | 4.93147801   | -1.50942555 | -2.88222387 |      |      |
|      | 3.59777681   | -2.22422339 | -1.95278552 |      |      |
|      | 3.64240213   | 0.04893787  | 0.27265339  |      |      |
|      | 6.95327338   | -2.56581572 | -0.90013162 |      |      |
|      | 4.20258660   | 1.18449760  | 0.99878115  |      |      |
|      | 3.83735750   | 2.12057161  | 0.56820615  |      |      |
|      | 3.88344005   | 1.13415969  | 2.04983608  |      |      |
|      | 5.30260887   | 1.17698795  | 0.96956531  |      |      |

**Zn-Int$_2$**

| Atom | Zn     | O     |
|------|--------|-------|
|      | -3.06084600 | 0.35483300 | 1.01712000 |
|      | 0.13608800 | 0.47423000 | 0.32616300 |
|      | -3.84992400 | 0.04842700 | 2.91774600 |
|      | -3.60139700 | 0.66666800 | -0.93880700 |
|      | -2.61669700 | -1.61807700 | 0.56775100 |
O  -2.64241800  2.37681100  1.20543300
O  -0.37238900  2.31501700  1.12514700
O  -0.34664300 -1.52964400  0.50324000
O  -1.34918900  0.69695500 -1.16139100
O  -1.61902200  0.08118100  2.77004400
C  -2.68094600 -0.02772900  3.42564400
C  -2.52720400  0.76887400 -1.59677700
C  -1.46430600 -2.11609700  0.47417900
C  -1.49081100  2.88059700  1.27250400
H  -2.60194600 -0.19872900  4.50288900
H  -1.46658000  3.96264900  1.48104300
H  -1.44089000 -3.21025200  0.34214600
H  -2.62744800  0.94016000 -2.67013400
C   2.87557400 -0.54209100 -0.44117100
C   3.12354100 -0.50053900 -1.95763600
H   2.37845400 -1.49019700 -0.1956900
H   3.84863700 -0.53621700  0.08353500
H   3.52595000  0.46476900 -2.26409200
C   1.95672300 -0.93472200 -2.82293100
H   2.19468300 -0.86545400 -3.88955500
H   1.66182900 -1.96492800 -2.59338500
H   1.10288200 -0.27921400 -2.61248100
N   2.05829400  0.58207300 -0.05684800
Br  4.76355300 -1.76005100 -2.44090000
C   2.82062900  1.79250400  0.17974100
H   2.15881600  2.58758800  0.53999800
H   3.61187000  1.64358000  0.94553800
H   3.33553800  2.18712400 -0.72044100

Zn-Int₃
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Zn      | -3.4622100 | 0.32124400 | 0.60411700 |
| Zn      | -0.26886300| 0.41716000 | -0.08133100|
| O       | -4.25792000| 0.00672100 | 2.49558500 |
| O       | -3.93776300| 0.62477500 | -1.35330000|
| O       | -3.01575800| -1.65539400| 0.14796800 |
| O       | -3.06168500| 2.34984500 | 0.78454700 |
| O       | -0.79497000| 2.27479700 | 0.66425200 |
| O       | -0.74548100| -1.57541500| 0.13233800 |
| O       | -1.68608400| 0.62993000 | -1.64783400|
| O       | -2.02798500| 0.06169200 | 2.33853500 |
| C       | -3.08653100| -0.06018400| 2.99824800 |
| C       | -2.88081300| 0.71941300 | -2.03721100|
| C       | -1.86442200| -2.15704400| 0.06730500 |
| C       | -1.90551600| 2.84679400 | 0.83466000 |
| H       | -3.00048800| -0.23547700| 4.07142400 |
| H       | -1.86500700| 3.92594100 | 1.04983800 |
| H       | -1.83931100| -3.24710600| -0.08903700|
| H       | -3.02608600| 0.90346500 | -3.10164000|
| C       | 2.54104800 | -0.44470500| 0.32373700 |
| C       | 3.54388100 | -1.07316600| -0.65699500|
| H       | 1.94855700 | -1.25677500| 0.76531600 |
| H       | 3.09762200 | 0.03815600 | 1.14863800 |
| H       | 4.06166300 | -0.30740700| 1.23431300 |
| C       | 2.98144800 | -2.17357200| -1.53306800|
| H       | 2.13105600 | -1.76383300| -2.09021800|
| H       | 3.72363600 | -2.55090800| -2.24450700|
| H       | 2.61748500 | -3.00905900| -0.92485900|
| N       | 1.68834200 | 0.49671500 | -0.37803100|
| Br      | 5.16086600 | -1.88974200| 0.43210800 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 0.63447800| 0.62210400| -3.71357800|
| O    | 0.72276300| 1.78542600| -3.62840800|
| O    | 0.55773000| -0.53553300| -3.86718400|
| C    | 2.30404000| 1.81278400| -0.47402900|
| H    | 3.23696000| 1.81303200| -1.07025400|
| H    | 1.62111600| 2.51792500| -0.95985300|
| H    | 2.56550100| 2.23809600| 0.51771100|

**Zn-Ts₂**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| Zn   | -1.42789900| -0.00545000| 0.00413200|
| Zn   | 1.42804500| 0.00560700| -0.00390900|
| O    | -1.70521900| -0.31489500| 1.94294100|
| O    | -1.71954700| 0.30064100| -1.93309100|
| O    | -0.53922300| -1.93329500| -0.30506000|
| O    | -0.55348800| 1.92923300| 0.30841100|
| O    | 1.70515000| 1.94489700| 0.30247500|
| O    | 1.71942500| -1.93112600| -0.31307800|
| O    | 0.53908100| 0.30888400| -1.93257700|
| O    | 0.55339900| -0.30450800| 1.92972400|
| C    | -0.56253100| -0.39968400| 2.50231500|
| C    | -0.58075400| 0.39448300| -2.49898300|
| C    | 0.58064000| -2.49830000| -0.39904300|
| C    | 0.56247800| 2.50307500| 0.39514500|
| H    | -0.56784000| -0.57234600| 3.58833800|
| H    | 0.56786900| 3.58919300| 0.56720600|
| H    | 0.59356300| -3.58424900| -0.57177800|
| H    | -0.59361700| 0.56659700| -3.58503000|
| C    | 4.65585607| 0.29662174| 1.40754691|
| C    | 5.16130764| -1.07541440| 1.86345442|
| H    | 3.97083034| 0.69956228| 2.16881854|
H      5.51244708  0.98229974  1.34392088
H      5.95011314 -1.44379324  1.20930201
C      4.10165046 -2.12821457  2.10576718
H      3.62303358 -2.36358824  1.14697847
H      4.54390242 -3.05159395  2.49299967
H      3.33283954 -1.77275766  2.79753529
N      3.98662082  0.21982937  0.10370233
Br     6.20779854 -0.75877140  3.63097377
C      4.31039930 -0.55789810 -1.64773668
O      5.12057649 -0.09280071 -2.39283108
O      3.85725915 -1.53182891 -1.12702308
C      3.93814378  1.58634763 -0.43590663
H      4.92998145  1.98427793 -0.48891142
H      3.50841223  1.56789998 -1.41564664
H      3.34075165  2.20154114  0.20406179

Zn-Int₄
Zn     3.82679400 -0.53913100  0.00856100
Zn     0.84126300  0.74166300  0.00458600
O      4.82903900  1.25824700 -0.18558300
O      4.15368600 -2.59131200  0.16792100
O      3.33790400 -0.50514800 -2.00854500
O      3.49074700 -0.16036100  2.01856100
O      1.29501200  0.43243300  1.97760400
O      1.14314900  0.08662100 -1.91487400
O      2.00737900 -1.96383500  0.19566600
O      2.66239700  1.88509600 -0.16474400
C      3.89544600  2.11430500 -0.22504500
C      2.90184600 -2.83900700  0.23492400
C      2.20132400 -0.27625400 -2.49907900
|   |   |   |   |
|---|---|---|---|
| C  | 2.38955900 | 0.15723600 | 2.54068200 |
| H  | 4.19125700 | 3.16650400 | -0.32148200 |
| H  | 2.39074100 | 0.20230300 | 3.64174100 |
| H  | 2.13029400 | -0.40967600 | -3.59109200 |
| H  | 2.59457700 | -3.88879800 | 0.33303300 |
| C  | -3.90031000 | 0.96779600 | 0.35252000 |
| C  | -4.21692000 | 0.06022700 | -0.84159000 |
| H  | -4.79553700 | 1.53434400 | 0.63241400 |
| H  | -3.60560500 | 0.34419500 | 1.20164100 |
| H  | -3.39177600 | -0.63025500 | -1.00975400 |
| C  | -4.64248100 | 0.76986600 | -2.11216300 |
| H  | -3.81659600 | 1.41145300 | -2.44505100 |
| H  | -4.86216400 | 0.05540400 | -2.91114800 |
| H  | -5.52907500 | 1.39383900 | -1.94882300 |
| N  | -2.84158900 | 1.92025500 | 0.04197600 |
| Br | -5.74700900 | -1.19901100 | -0.24399500 |
| C  | -1.52484300 | 1.48770500 | 0.03592000 |
| O  | -1.29027300 | 0.24310800 | 0.16127100 |
| O  | -0.57929000 | 2.33595700 | -0.10772900 |
| C  | -3.16306900 | 3.33455700 | -0.03960600 |
| H  | -2.24713200 | 3.87815600 | -0.27176000 |
| H  | -3.90520300 | 3.52563700 | -0.82714000 |
| H  | -3.56834000 | 3.71024400 | 0.91315500 |

**Zn-Ts₃**

|   |   |   |   |
|---|---|---|---|
| Zn | 4.04702200 | -0.47669900 | -0.01690100 |
| Zn | 1.17655500 | 0.29928800 | 0.10224100 |
| O  | 4.88399000 | 1.12254000 | -0.88642600 |
| O  | 4.04019800 | -2.29786500 | 0.81596300 |
| O  | 3.07205000 | -1.10643600 | -1.77054100 |
| At  | x    | y    | z    |
|-----|------|------|------|
| O   | 3.68001100 | 0.52015400 | 1.79652200 |
| O   | 1.47985800 | 1.10618400 | 1.90025900 |
| O   | 0.87452500 | -0.50422100 | -1.68822800 |
| O   | 1.86931200 | -1.70166700 | 0.90095800 |
| O   | 2.70944400 | 1.71333000 | -0.79502100 |
| C   | 3.90953000 | 1.92326300 | -1.08791400 |
| C   | 2.81272100 | -2.49667100 | 1.10832100 |
| C   | 1.89467100 | -1.03194300 | -2.22621700 |
| C   | 2.66541400 | 1.03984500 | 2.34387100 |
| H   | 4.17564600 | 2.88331700 | -1.56996900 |
| H   | 2.81233700 | 1.49977600 | 3.32520100 |
| H   | 1.71378000 | -1.47275100 | -3.21035400 |
| H   | 2.59007800 | -3.46451700 | 1.58376500 |
| C   | -4.09164400 | 0.88950300 | -0.68999200 |
| C   | -4.20093600 | -0.53816600 | -0.19163000 |
| H   | -4.03646300 | 0.88065500 | -1.79387200 |
| H   | -4.97555200 | 1.45864700 | -0.40224800 |
| H   | -4.11102500 | -0.71111100 | 0.86770600 |
| C   | -4.34867200 | -1.69445900 | -1.14219600 |
| H   | -3.37366300 | -1.90706000 | -1.59560400 |
| H   | -4.70603000 | -2.58384500 | -0.61979200 |
| H   | -5.06373800 | -1.45375200 | -1.93441100 |
| N   | -2.91121500 | 1.52368500 | -0.11440300 |
| Br  | -6.75912900 | -0.47887600 | 0.43553700 |
| C   | -1.81431600 | 0.68200900 | -0.03229400 |
| O   | -2.08007800 | -0.55543000 | -0.15764300 |
| O   | -0.67132600 | 1.19565200 | 0.18731700 |
| C   | -2.74958200 | 2.95461900 | -0.27360900 |
| H   | -1.81829200 | 3.25262400 | 0.21046500 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -2.70289500 | 3.25085900 | -1.33600000 |
| H    | -3.59045400 | 3.47841200 | 0.19661700  |
| Zn-Int_5 |        |         |         |
| Zn   | 3.91818100  | -0.58217400 | 0.00732400 |
| Zn   | 1.02675900  | 0.58515100  | 0.01336100  |
| O    | 4.78007400  | 1.25398500  | -0.18124500 |
| O    | 4.16158400  | -2.60753600 | 0.16968400  |
| O    | 3.34517900  | -0.49974900 | -2.00342900 |
| O    | 3.48960400  | -0.15998100 | 2.00925000  |
| O    | 1.27265300  | 0.33182000  | 1.98481200  |
| O    | 1.13530800  | 0.01385100  | -1.90561500 |
| O    | 2.02392700  | -1.95135500 | 0.18634700  |
| O    | 2.62117100  | 1.93698100  | -0.15362900 |
| C    | 3.86530100  | 2.12630800  | -0.21940900 |
| C    | 2.90596100  | -2.84169700 | 0.23253100  |
| C    | 2.20819400  | -0.30424600 | -2.50008500 |
| C    | 2.38866300  | 0.11907100  | 2.54606700  |
| H    | 4.19125700  | 3.16650400  | -0.32148200 |
| H    | 2.39074100  | 0.20230300  | 3.64174100  |
| H    | 2.13029400  | -0.40967600 | -3.59109200 |
| H    | 2.59457700  | -3.88879800 | 0.33303300  |
| C    | -4.20858700 | 0.94579200  | -0.17083300 |
| C    | -3.58032500 | -0.45822800 | -0.29528500 |
| H    | -4.89797500 | 1.16068100  | -0.99057200 |
| H    | -4.75792500 | 1.06915100  | 0.76698500  |
| H    | -3.90343600 | -1.10860700 | 0.51452400  |
| C    | -3.76405700 | -1.12396900 | -1.64368400 |
| H    | -3.44407100 | -0.46243000 | -2.45915700 |
| H    | -3.18336900 | -2.05161000 | -1.69630800 |

S111
H   -4.82896200 -1.35770200 -1.74898900
N   -3.02224200 1.81444600 -0.22854200
Br  -6.88810600 -0.96858400  0.41310800
C   -1.89217600 1.10530900 -0.10343300
O   -2.12196000 -0.20312600 -0.08223700
O   -0.73702400 1.58425300 -0.01554700
C   -3.08873900 3.25884400 -0.16407600
H   -2.07380500 3.66090300 -0.19522300
H   -3.66251400 3.64671700 -1.01377600
H   -3.57783100 3.58104100  0.76447200

Zr-HKUST-1
O   -1.39165300 -1.40021500  1.12088400
O    1.39197100  1.39703900  1.12273600
O   -1.42441500  1.36363600  1.10375400
O    1.42458800 -1.36680100  1.10163000
O    1.41429000 -1.37568500 -1.12337400
O   -1.41426100  1.37839700 -1.12123500
O    1.40145600  1.38907200 -1.10170100
O   -1.40224100 -1.38568900 -1.10350400
C   -1.82733100 -1.83146100  0.00802700
C    1.82664700  1.83197200  0.01087800
C   -1.86068300  1.79802700 -0.00804300
C    1.86179900 -1.79725800 -0.01126700
H   -2.60371100 -2.60233600  0.00630700
H    2.64637200 -2.55980100 -0.01154600
H   -2.64739700  2.55837200 -0.00618600
H    2.59944500  2.60644400  0.01109800
Zr    0.00018594 -0.00197611  1.52070415
Zr    0.00003061  0.00144382 -1.37929383
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| O    | -1.12153100 | 1.44627200 | -1.49767400 |
| O    | -1.12192400 | -1.44617100 | 1.49752300  |
| O    | -1.12291800 | 1.49850200 | 1.44620900  |
| O    | -1.12278300 | -1.49841600 | -1.44641900 |
| O    | 1.12155800  | -1.49799100 | -1.44569100 |
| O    | 1.12142400  | 1.49788600 | 1.44585600  |
| O    | 1.12243100  | -1.44656300 | 1.49813400  |
| O    | 1.12282200  | 1.44649900 | -1.49791400 |
| C    | 0.00062900  | 1.87415000 | -1.94001800 |
| C    | 0.00013600  | -1.87407500 | 1.94010600  |
| C    | -0.00054000 | 1.94128000 | 1.87286300  |
| C    | -0.00037200 | -1.94125100 | -1.87292700 |
| H    | 0.00034700  | 2.63356300 | -2.72548400 |
| H    | 0.00002100  | -2.72780300 | 2.63113900  |
| H    | -0.00020600 | 2.72785300 | 2.63113900  |
| H    | -0.00033600 | -2.63343000 | 2.72562700  |
| Zr   | -1.54114400 | 0.00004800 | -0.00013400 |
| Zr   | 1.54135500  | -0.00007200 | 0.00012400  |
| C    | 3.95084143  | -1.03123340 | 0.44377488  |
| C    | 4.20406718  | 0.28437744 | 1.10656122  |
| H    | 3.31219470  | 1.77308952 | 0.92082544  |
| H    | 4.74248398  | -1.14519812 | -0.18403950 |
| H    | 5.17472792  | 0.73582745 | 0.87961852  |
| C    | 3.63644215  | 0.64270344 | 2.46106521  |
| H    | 4.38091163  | 1.72568834 | 2.54736489  |
| H    | 4.31782239  | 0.33177201 | 3.26338039  |
| H    | 2.67060679  | 0.14998652 | 2.61504858  |
N       -3.27670089  0.18342273  -0.01862627
C       -3.72242430  0.72707670  -1.29614875
H       -3.48797003  1.79698029  -1.33406237
H       -3.18262814  0.22728563  -2.10852620
H       -4.80718787  0.60167251  -1.47145552

Zr-Int
O       -2.79283800  2.09813900  -1.78078700
O       -2.84525900  -0.81358600  1.22320700
O       -2.80089000  2.14826700  1.15626700
O       -2.81910200  -0.85132200  -1.75049400
O       -0.56409900  -0.82230000  -1.77735600
O       -0.54554000  2.16371300  1.14850800
O       -0.58976300  -0.78835400  1.23385200
O       -0.53641700  2.11280600  -1.79196400
C       -1.66934200  2.52639700  -2.22448400
C       -1.71046400  -1.21668100  1.65749700
C       -1.67444800  2.59259700  1.57566700
C       -1.68782200  -1.27361900  -2.17933700
H       -1.68474700  3.28298200  -3.01593400
H       -1.68507300  -2.07838400  -2.92167400
H       -1.68530000  3.37727200  2.34068900
H       -1.68543000  -1.98401100  2.43517700
Zr      -3.23983500  0.64383100  -0.28860000
Zr      -0.08300200  0.65554000  -0.29437300
C       2.45688500  -1.00719600  1.33106900
C       2.56902500  -1.70093400  0.03248600
H       1.60182700  -1.19851100  1.97192100
H       3.39763700  -0.72138600  1.79913000
H       3.60195300  -1.79527900  -0.30541100
C     1.62927400  -2.78762200  -0.42714500
H     1.54023600  -2.79934900  -1.51940200
H     2.04201700  -3.75380000  -0.10833200
H     0.62919700  -2.67671600  -0.00184700
N     2.10749600  -0.26993300    0.07218400
Br    6.05729000  -1.36812700    0.99317200
C     3.12805500   0.71546900  -0.36516700
H     3.04861800   0.85682200  -1.45060100
H     2.94478800   1.67540200    0.13705800
H     4.14412900   0.37614700  -0.11674300

Zr-Ts$_1$
O    -1.12153100   1.44627200  -1.49767400
O    -1.12192400  -1.44617100   1.49752300
O    -1.12291800   1.49850200   1.44620900
O    -1.12278300  -1.49841600  -1.44641900
O     1.12155800  -1.49799100  -1.44569100
O     1.12142400   1.49788600   1.44585600
O     1.12243100  -1.44656300   1.49813400
O     1.12282200   1.44649900  -1.49791400
C     0.00062900   1.87415000  -1.94001800
C     0.00013600  -1.87407500   1.94010600
C    -0.00054000   1.94128000   1.87286300
C    -0.00037200  -1.94125100  -1.87292700
H     0.00034700   2.63356300  -2.72548400
H     0.00002100  -2.72780300  -2.63122400
H    -0.00020600   2.72785300   2.63113900
H    -0.00033600  -2.63343000   2.72562700
Zr   -1.54114400   0.00004800  -0.00013400
Zr    1.54135500  -0.00007200   0.00012400
| Atom | x     | y     | z     |
|------|-------|-------|-------|
| C    | 4.27434828 | -0.36798777 | 1.51869370 |
| C    | 4.86752928 | -1.22378996 | 0.46830438 |
| H    | 3.55737765 | -0.87897024 | 2.16282756 |
| H    | 4.96626272 | 0.25628981 | 2.08932341 |
| H    | 5.68870281 | -0.81123095 | -0.10120775 |
| C    | 4.18751123 | -2.46040962 | -0.05312171 |
| H    | 3.57446461 | -2.22796613 | -0.93212884 |
| H    | 4.94286084 | -3.19580892 | -0.34022304 |
| H    | 3.54089709 | -2.90344893 | 0.70981209 |
| N    | 3.66296758 | 0.25625208 | 0.35878468 |
| Br   | 6.83676425 | -2.35981335 | 1.86126456 |
| C    | 4.27169862 | 1.52650099 | -0.02394009 |
| H    | 3.97815166 | 1.78957850 | 0.65661340 |
| H    | 3.91982630 | 2.31525805 | 0.65661340 |
| H    | 5.36949443 | 1.48038120 | 0.03669221 |

**Zr-Int₂**

| Atom | x     | y     | z     |
|------|-------|-------|-------|
| O    | -2.80156500 | 2.09701500 | -1.78553400 |
| O    | -2.81154800 | -0.80853000 | 1.21125600 |
| O    | -2.80360200 | 2.15180600 | 1.15682300 |
| O    | -2.80142400 | -0.84384200 | -1.74768300 |
| O    | -0.53614900 | -0.85819100 | -1.77171600 |
| O    | -0.53941500 | 2.18651800 | 1.15813200 |
| O    | -0.54782600 | -0.80868200 | 1.22158100 |
| O    | -0.53766400 | 2.11152100 | -1.79693000 |
| C    | -1.67567900 | 2.52297400 | -2.22518700 |
| C    | -1.67946700 | -1.22257400 | 1.64507100 |
| C    | -1.67551000 | 2.59606800 | 1.57210200 |
| C    | -1.67349100 | -1.28095200 | -2.16981300 |
| H    | -1.68474700 | 3.28298200 | -3.01593400 |
| Atoms | X     | Y     | Z     |
|-------|-------|-------|-------|
| H     | -1.68507300 | -2.07838400 | -2.92167400 |
| H     | -1.68530000 | 3.37727200  | 2.34068900  |
| H     | -1.68543000 | -1.98401100 | 2.43517700  |
| Zr    | -3.27652200 | 0.64561100  | -0.28792200 |
| Zr    | -0.05096700 | 0.66195800  | -0.29650100 |
| C     | 2.79484400  | -0.54682800 | 0.79723700  |
| C     | 3.39475000  | -1.70973100 | -0.00757100 |
| H     | 2.11051600  | -0.95916100 | 1.54879500  |
| H     | 3.60395200  | -0.02261800 | 1.33438300  |
| H     | 4.04126400  | -1.34745200 | -0.80746100 |
| C     | 2.39642100  | -2.73483400 | -0.50417800 |
| H     | 1.66364700  | -2.22807100 | -1.14418900 |
| H     | 2.88547900  | -3.52562200 | -1.08266900 |
| H     | 1.85371200  | -3.19049500 | 0.33115600  |
| N     | 2.07316500  | 0.36444700  | -0.07171100 |
| Br    | 4.79829200  | -2.70378500 | 1.20179000  |
| C     | 2.93907600  | 1.30720400  | -0.76804200 |
| H     | 2.33676300  | 2.02118100  | -1.34895500 |
| H     | 3.55749700  | 1.89710600  | -0.06395400 |
| H     | 3.63132800  | 0.82975100  | -1.48571900 |

**Zr-Int₃**

| Atoms | X     | Y     | Z     |
|-------|-------|-------|-------|
| O     | -2.82896900 | 2.13749800 | -1.85372800 |
| O     | -2.85525700 | -0.76919000 | 1.14318000 |
| O     | -2.84199800 | 2.19732200 | 1.08665300 |
| O     | -2.82583100 | -0.79610500 | -1.81654000 |
| O     | -0.56040800 | -0.81359800 | -1.84798100 |
| O     | -0.57805700 | 2.23463000 | 1.08363900 |
| O     | -0.59199400 | -0.76634600 | 1.15168200 |
| O     | -0.56517000 | 2.15622500 | -1.87043400 |
\[ Zr-Ts_2 \]
O  -1.12153100  1.44627200  -1.49767400
O  -1.12192400 -1.44617100   1.49752300
O  -1.12291800  1.49850200   1.44620900
O  -1.12278300 -1.49841600  -1.44641900
O   1.12155800 -1.49799100  -1.44569100
O   1.12142400  1.49788600   1.44585600
O   1.12243100 -1.44656300   1.49813400
O   1.12282200  1.44649900  -1.49791400
C   0.00062900  1.87415000  -1.94001800
C   0.00013600 -1.87407500   1.94010600
C  -0.00054000  1.94128000   1.87286300
C  -0.00037200 -1.94125100   1.87292700
H   0.00034700  2.63356300  -2.72548400
H   0.00002100 -2.72780300  -2.63122400
H  -0.00020600  2.72785300   2.63113900
H  -0.00033600 -2.63343000   2.72562700
Zr  -1.54114400  0.00004800  -0.00013400
Zr   1.54135500  0.00007200   0.00012400
C   4.55048544 -0.48629908   1.48888067
C   4.93430574 -1.91317523   1.08573981
H   3.87754280 -0.52621210   2.35877201
H   5.45936301  0.04543789   1.80375858
H   5.71031354 -1.91322115   0.32177360
C   3.78936843 -2.83129463   0.71675158
H   3.32135999 -2.44890773  -0.19894435
H   4.14712138 -3.84489687   0.50989753
H   3.03120842 -2.86460408   1.50418212
N   3.91469678  0.23563828   0.38056537
Br   5.95153685 -2.72793022   2.70467337
|   |   |   |   |
|---|---|---|---|
| C | 4.46695335 | 0.30624093 | -1.58337537 |
| O | 5.27262046 | 1.18845677 | -1.56183450 |
| O | 3.98210932 | -0.67861968 | -2.05241241 |
| C | 3.98822903 | 1.66815561 | 0.70210404 |
| H | 5.00916351 | 1.94596668 | 0.86152109 |
| H | 3.58643670 | 2.23709658 | -0.11015768 |
| H | 3.42261030 | 1.86411982 | 1.58899382 |

**Zr-Int**

|   |   |   |   |
|---|---|---|---|
| O | 1.58424600 | -1.05786800 | -1.68630900 |
| O | 1.53561600 | 0.70052500 | 2.11730200 |
| O | 1.22289700 | 1.70945500 | -0.67070500 |
| O | 1.88978300 | -2.04724300 | 1.07947200 |
| O | 4.12093500 | -1.71065900 | 0.97004800 |
| O | 3.45836500 | 2.03209600 | -0.77487700 |
| O | 3.76724900 | 1.04234600 | 1.99519200 |
| O | 3.81664200 | -0.71546400 | -1.80205000 |
| C | 2.70838200 | -1.13394600 | -2.29094900 |
| C | 2.64023400 | 1.11978100 | 2.60120500 |
| C | 2.24983700 | 2.40824700 | -0.96906700 |
| C | 3.09621800 | -2.41813900 | 1.27247600 |
| H | 2.72853200 | -1.58121300 | -3.29213000 |
| H | 3.26121400 | -3.40311200 | 1.72285400 |
| H | 2.08714800 | 3.39584200 | -1.41600400 |
| H | 2.61998900 | 1.57421200 | 3.59897600 |
| Zr | 1.08041700 | -0.24937300 | 0.24029200 |
| Zr | 4.23637000 | 0.22960800 | 0.07229900 |
| C | -4.47171400 | 0.76211100 | 0.11060100 |
| C | -5.24814400 | -0.24933500 | -0.74004200 |
| H | -4.81115900 | 1.77768300 | -0.12262300 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -4.67069100 | 0.56122800 | 1.16734600 |
| H    | -5.03300700 | -1.26020200 | -0.39659800 |
| C    | -5.09549100 | -0.10450500 | -2.24212300 |
| H    | -4.03987300 | -0.25337200 | -2.50220300 |
| H    | -5.68765400 | -0.85500500 | -2.77481700 |
| H    | -5.40312500 | 0.89018000 | -2.58485800 |
| N    | -3.03894000 | 0.69016300 | -0.14579600 |
| Br   | -7.25157300 | -0.03396300 | -0.26248900 |
| C    | -2.32172000 | -0.34478200 | 0.46071800 |
| O    | -2.92113700 | -1.21253100 | 1.10142100 |
| O    | -1.02353900 | -0.30855200 | 0.27271200 |
| C    | -2.41318800 | 1.80030700 | -0.85014900 |
| H    | -1.34234600 | 1.62867500 | -0.93367100 |
| H    | -2.83149200 | 1.90845500 | -1.86017700 |
| H    | -2.57063100 | 2.74710100 | -0.31225200 |
| Zr-Ts3 |          |           |           |
| O    | 1.62174100  | -1.06742000 | -1.81346900 |
| O    | 1.57492800  | 0.68065100  | 1.98900300  |
| O    | 1.25908500  | 1.70363600  | -0.78235100 |
| O    | 1.92115500  | -2.06047700 | 0.95419200  |
| O    | 4.15137000  | -1.73434500 | 0.81743500  |
| O    | 3.49424800  | 2.01591500  | -0.91136700 |
| O    | 3.80485800  | 1.01230500  | 1.85795400  |
| O    | 3.85070700  | -0.73260200 | -1.94602400 |
| C    | 2.74271900  | -1.14821000 | -2.42486300 |
| C    | 2.67918600  | 1.09939400  | 2.47257300  |
| C    | 2.28563100  | 2.39660800  | -1.09490500 |
| C    | 3.12869100  | -2.43720900 | 1.13670200  |
| H    | 2.76267700  | -1.59439100 | -3.41887000 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 3.2953900 | -3.4162900 | 1.5961400 |
| H    | 2.1212930 | 3.3826640 | -1.5427440 |
| H    | 2.6541340 | 1.5610340 | 3.4722360 |
| Zr   | 1.1294790 | -0.2612930 | 0.1164830 |
| Zr   | 4.2638620 | 0.2055730 | -0.0751690 |
| C    | -4.4386290 | 0.7953420 | -0.0019670 |
| C    | -4.9021580 | -0.6493870 | 0.0240010 |
| H    | -4.9690190 | 1.3451330 | -0.7837010 |
| H    | -4.6633210 | 1.2791580 | 0.9575780 |
| H    | -5.1573760 | -1.1033450 | 0.9650450 |
| C    | -5.0897670 | -1.4123700 | -1.2619620 |
| H    | -4.1193350 | -1.7615580 | -1.6334660 |
| H    | -5.7351440 | -2.2776890 | -1.1052130 |
| H    | -5.5500180 | -0.7754100 | -2.0226510 |
| N    | -2.9996000 | 0.8462220 | -0.2750510 |
| Br   | -7.4281800 | 0.0834870 | 0.2608410 |
| C    | -2.3119180 | -0.2715550 | 0.1098530 |
| O    | -3.0162750 | -1.2763520 | 0.4225540 |
| O    | -1.0243590 | -0.2677160 | 0.1123340 |
| C    | -2.3909980 | 2.1449150 | -0.5011650 |
| H    | -1.3208090 | 2.0238950 | -0.6741430 |
| H    | -2.8462720 | 2.6167270 | -1.3817380 |
| H    | -2.5385200 | 2.8093210 | 0.3631970 |

**Zr-Int**

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| O    | -1.3669480 | 0.5263080 | -1.8525320 |
| O    | -1.8772140 | -0.0427430 | 2.26078000 |
| O    | -1.0987840 | -1.7937510 | -0.00718800 |
| O    | -2.1368720 | 2.2437710 | 0.43100100 |
| O    | -4.3055640 | 1.7283360 | 0.08824000 |
O    -3.27331400  -2.30145900  -0.34153600
O    -4.04483700  -0.56721400   1.92630900
O    -3.53581900   0.00063500  -2.18608200
C    -2.37748000   0.34305300  -2.61143800
C    -3.03216000  -0.38744300   2.68927300
C    -2.03988800  -2.62616400  -0.23695700
C    -3.36886300   2.57005900   0.32088600
H    -2.24608900   0.48396500  -3.68923100
H    -3.63167700   3.62592700   0.42918500
H    -1.77413200  -3.68122200  -0.35295000
H    -3.15986900  -0.53953000   3.76551900
Zr   -1.18022100   0.34750500   0.28247100
Zr   -4.20822900  -0.38702300  -0.19647100
C    4.30354800  -0.22597500  -0.80183900
C    4.45714000   1.10691300  -0.05413800
H    4.40786400  -0.11520000  -1.89126800
H    5.04300700  -0.94786900  -0.44165100
H    4.93184700   0.93510000   0.91483500
C    5.15570200   2.21601900  -0.80439400
H    4.68034400   2.40157800  -1.77559100
H    5.14696600   3.14312300  -0.22068800
H    6.19510900   1.90252900  -0.95095800
N    2.92055400  -0.59309200  -0.47001000
Br   7.52268600  -0.53594500   0.39115900
C    2.25993700   0.44988600   0.03998400
O    3.04657900   1.50332200   0.23033200
O    1.03638200   0.49569400   0.33278900
C    2.32775300  -1.86257100  -0.84851500
H    1.29804300  -1.91282700  -0.49053100
|   | X          | Y          | Z          |
|---|------------|------------|------------|
| H | 2.33459700 | -1.97164700| -1.94107100|
| H | 2.91111600 | -2.67934300| -0.41016800|
|   | **Tc-HKUST-1** |         |            |
| O | 2.17330300 | -0.00236300| -1.13289500|
| O | -2.17330400|  0.00237600| -1.13289200|
| O |  0.00239000|  2.06325700| -1.10384300|
| O | -0.00239300| -2.06326000| -1.10384500|
| O | -0.00238800| -2.06315400|  1.10384300|
| O |  0.00238900|  2.06314700|  1.10384300|
| O | -2.17328100|  0.00237000|  1.13303700|
| O |  2.17328300| -0.00236100|  1.13303300|
| C |  2.75974500| -0.00297200|  0.00007400|
| C | -2.75974500|  0.00299300|  0.00007400|
| C |  0.00317600|  2.70373800| -0.00014300|
| C | -0.00317400| -2.70374300| -0.00014600|
| H |  3.85636300| -0.00408100|  0.00008500|
| H | -0.00450000| -3.79415000| -0.00007600|
| H |  0.00453300|  3.79414400| -0.00007000|
| H | -3.85636300|  0.00413200|  0.00009000|
| Tc| -0.00000200| -0.00000200| -1.27358600|
| Tc|  0.00000100| -0.00000400|  1.27368000|
|   | **Tc-Int_{1}** |         |            |
| O | -1.65211600|  0.10727400| -2.74355300|
| O |  2.57408400|  0.09933900| -2.72251500|
| O |  0.45766300| -1.99627800| -2.73256000|
| O |  0.46302600|  2.20337800| -2.74164100|
| O |  0.47612900|  2.21583400| -0.48668900|
| O |  0.46688200| -2.02709200| -0.47981700|
| O |  2.60565100|  0.07902200| -0.46491700|

S124
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| O    | -1.67130000 | 0.08528600 | -0.48806200 |
| C    | -2.23924300 | 0.09988300 | -1.61447300 |
| C    | 3.16607500  | 0.08785200 | -1.59675300 |
| C    | 0.46057100  | -2.59480200 | -1.60799400 |
| C    | 0.47073100  | 2.78916200  | -1.61020800 |
| H    | -3.33428700 | 0.10700400 | -1.62045300 |
| H    | 0.47364400  | 3.88326500  | -1.62039600 |
| H    | 0.45463500  | -3.68800900 | -1.62045600 |
| H    | 4.26257100  | 0.08824500  | -1.62039400 |
| Tc   | 0.45946800  | 0.10498000  | -2.70416400 |
| Tc   | 0.46285100  | 0.07895400  | -0.44287000 |
| C    | -0.93069200 | 0.92828400  | 2.46879400  |
| C    | -0.43121500 | -0.40308100 | 2.85416100  |
| H    | -1.75798100 | 1.00711600  | 1.77026400  |
| H    | -0.84673800 | 1.73247500  | 3.19532300  |
| H    | 0.02028100  | -0.44658700 | 3.84349400  |
| C    | -1.09195600 | -1.68415300 | 2.41782200  |
| H    | -0.36051800 | -2.49577700 | 2.31942200  |
| H    | -1.80975400 | -1.94628800 | 3.20338100  |
| H    | -1.61649400 | -1.57198600 | 1.46519900  |
| N    | 0.34155900  | 0.43860300  | 1.86760400  |
| Br   | -2.05199600 | -0.33559400 | 5.90632800  |
| C    | 1.55893100  | 1.05963200  | 2.41142600  |
| H    | 2.40560100  | 0.38119600  | 2.26756700  |
| H    | 1.75861300  | 1.99155800  | 1.87235300  |
| H    | 1.45214800  | 1.27885600  | 3.48291800  |

**Tc-Ts<sub>1</sub>**

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| O    | -2.11527600 | 0.00510200 | -1.12533500 |
| O    | 2.11528200  | -0.00514300 | -1.12529800 |
| Element | x        | y        | z        |
|---------|----------|----------|----------|
| O       | -0.005203 | -2.095829 | -1.122844 |
| O       | 0.005077  | 2.095858  | -1.122859 |
| O       | 0.005202  | 2.095830  | 1.122841  |
| O       | -0.005078 | -2.095858 | 1.122856  |
| O       | 2.115278  | -0.005103 | 1.125336  |
| O       | -2.115284 | 0.005142  | 1.125298  |
| C       | -2.702098 | 0.006598  | -0.000007 |
| C       | 2.702098  | -0.006601 | 0.000008  |
| C       | -0.006669 | -2.690743 | 0.000008  |
| C       | 0.006667  | 2.690743  | -0.000010 |
| H       | -3.798429 | 0.009376  | -0.000031 |
| H       | 0.009502  | 3.785637  | 0.000026  |
| H       | -0.009507 | -3.785637 | -0.000034 |
| H       | 3.798429  | -0.009383 | 0.000028  |
| Tc      | -0.000015 | 0.000002  | -1.102364 |
| Tc      | 0.000015  | -0.000010 | 1.102365  |
| C       | -0.956859 | 0.650383  | 4.101286  |
| H       | -1.922036 | 0.658574  | 3.592929  |
| H       | -0.850893 | 1.488900  | 4.793923  |
| H       | 0.329039  | -0.717699 | 5.239599  |
| C       | -1.056839 | -1.964748 | 4.014901  |
| H       | -0.389069 | -2.326851 | 3.224030  |
| H       | -1.112505 | -2.724385 | 4.798257  |
| H       | -2.054671 | -1.829882 | 3.587579  |
| N       | 0.163043  | 0.419143  | 3.206190  |
| Br      | -1.839276 | -0.712117 | 6.932475  |
| C       | 1.366912  | 1.168197  | 3.552863  |
| H       | 2.233664  | 0.739814  | 3.042716  |
H    1.24919423  2.21190881  3.22742053
H    1.54556185  1.16149402  4.63868037

Tc-Int$_2$

O    -1.65439000  0.10918200  -2.72319600
O     2.57921100  0.09881100  -2.71760300
O     0.46016100  -2.00943500  -2.73375000
O     0.46244200  2.21579100  -2.74738700
O     0.48943300  2.23603800  -0.48170200
O     0.45407200  -2.04573800  -0.46973700
O     2.62457400  0.08589900  -0.45156600
O    -1.69324500  0.07966600  -0.45755000
C    -2.23937100  0.09779700  -1.59285600
C     3.16724600  0.09112600  -1.58893500
C     0.45566800  -2.59591800  -1.60473300
C     0.47635200  2.79093400  -1.61012400
H    -3.33428700  0.10700400  -1.62045300
H     0.47364400  3.88326500  -1.62039600
H     0.45463500  -3.68800900  -1.62045600
H     4.26257100  0.08824500  -1.62039400
Tc    0.46102500  0.10688500  -2.71111800
Tc    0.46581500  0.08481100  -0.38149300
C    -0.76474100  0.20953700   2.51421000
C    -0.71039100  -1.06452700   3.36643400
H    -1.65535000  0.17325100   1.87807100
H    -0.85699300  1.08832500   3.17596600
H     0.21246800  -1.11981200   3.94375300
C    -1.00441900  -2.35171800   2.62684100
H    -0.29168500  -2.44338200   1.79894900
H    -0.91238500  -3.22439900   3.28228900
| Atom | X-coordinate | Y-coordinate | Z-coordinate |
|------|--------------|--------------|--------------|
| H    | -2.01332400  | -2.33378500  | 2.19980300   |
| N    | 0.43113400   | 0.28751600   | 1.69552800   |
| Br   | -2.12400100  | -0.90056100  | 4.94344400   |
| C    | 1.52940900   | 0.93020500   | 2.39503500   |
| H    | 2.42293500   | 0.93050400   | 1.76500500   |
| H    | 1.28839500   | 1.98146900   | 2.65265500   |
| H    | 1.79047400   | 0.42429500   | 3.34450100   |

**Te-Int₃**

| Atom | X-coordinate | Y-coordinate | Z-coordinate |
|------|--------------|--------------|--------------|
| O    | -1.63657700  | 0.20734200   | -2.80345800  |
| O    | 2.59594200   | 0.20029300   | -2.78709200  |
| O    | 0.47848600   | -1.90952100  | -2.80264500  |
| O    | 0.48029100   | 2.31467300   | -2.82763700  |
| O    | 0.51021700   | 2.33240300   | -0.56212800  |
| O    | 0.46442700   | -1.95023100  | -0.53882300  |
| O    | 2.64477700   | 0.16715500   | -0.52113500  |
| O    | -1.67477900  | 0.17683500   | -0.53837600  |
| C    | -2.22135800  | 0.19517100   | -1.67340100  |
| C    | 3.18584200   | 0.18365800   | -1.66028900  |
| C    | 0.47133000   | -2.49934900  | -1.67576500  |
| C    | 0.49548500   | 2.88826000   | -1.68962900  |
| H    | -3.31583500  | 0.20400400   | -1.69733200  |
| H    | 0.49209600   | 3.98026500   | -1.69727500  |
| H    | 0.47308700   | -3.59100900  | -1.69733500  |
| H    | 4.28102300   | 0.18524500   | -1.69727300  |
| Te   | 0.47905900   | 0.20606000   | -2.78538400  |
| Te   | 0.48097400   | 0.17834800   | -0.45643200  |
| C    | -0.80829900  | 0.48058000   | 2.39229200   |
| C    | -0.86191500  | -0.75099300  | 3.30380200   |
| H    | -1.67949200  | 0.46677100   | 1.72965300   |
H   -0.86544000   1.39451100   3.00771800
H   0.03169700  -0.83282800   3.92263800
C   -1.20467000  -2.05155100   2.60812200
H   -0.46984300  -2.22245800   1.81205500
H   -1.19227600  -2.89783400   3.30199200
H   -2.19424200  -1.99298800   2.13997600
N   0.41732800   0.44421000   1.61312300
Br  -2.33428900  -0.42964300   4.79726100
C   3.00059800  -2.76791500   2.14022300
O   2.82208100  -2.11207500   3.09123100
O   3.20581800  -3.45357100   1.2144900
C   1.51266900   1.10453700   2.30297700
H   1.71438700   0.66923600   3.2980500
H   2.42933200   1.02337200   1.71224200
H   1.30196600   2.18086300   2.46075700

\textbf{Tc-Ts}_2

\begin{align*}
\text{O} & : -2.11527600, 0.00510200, -1.12533500 \\
\text{O} & : 2.11528200, -0.00514300, -1.12529800 \\
\text{O} & : -0.00520300, -2.09582900, -1.12284400 \\
\text{O} & : 0.00507700, 2.09585800, -1.12285900 \\
\text{O} & : 0.00520200, 2.09583000, 1.12284100 \\
\text{O} & : -0.00507800, -2.09585800, 1.12285600 \\
\text{O} & : 2.11527800, -0.00510300, 1.12533600 \\
\text{O} & : -2.11528400, 0.00514200, 1.12529800 \\
\text{C} & : -2.70209800, 0.00659800, -0.00000700 \\
\text{C} & : 2.70209800, -0.00660100, 0.00000800 \\
\text{C} & : -0.00666900, -2.69074300, 0.00000800 \\
\text{C} & : 0.00666700, 2.69074300, -0.00001000 \\
\text{H} & : -3.79842900, 0.00937600, -0.00003100 \\
\end{align*}
|        |        |        |        |
|--------|--------|--------|--------|
| H      | 0.00950200 | 3.78563700 | 0.00002600 |
| H      | -0.00950700 | -3.78563700 | -0.00003400 |
| H      | 3.79842900 | -0.00938300 | 0.00002800 |
| Tc     | -0.00001500 | 0.00000200 | -1.10236400 |
| Tc     | 0.00001500 | -0.00000100 | 1.10236500 |
| C      | -1.11624117 | 0.72333640 | 4.36767259 |
| C      | -1.69260862 | -0.61192649 | 4.84797427 |
| H      | -1.86004694 | 1.22997700 | 3.73425008 |
| H      | -0.94194306 | 1.36493515 | 5.24284226 |
| H      | -1.04690944 | -1.07701711 | 5.59134210 |
| C      | -2.09250705 | -1.59178554 | 3.76633917 |
| H      | -1.18647094 | -1.90758671 | 3.23425002 |
| H      | -2.55572803 | -2.48594404 | 4.19537550 |
| H      | -2.77605586 | -1.13637004 | 3.04431374 |
| N      | 0.14093738 | 0.53636132 | 3.63396556 |
| Br     | -3.36804993 | -0.15263220 | 5.98879671 |
| C      | 1.66179924 | -0.60110898 | 4.37697090 |
| O      | 2.38164145 | 0.13872669 | 4.97891663 |
| O      | 1.25504684 | -1.68523462 | 4.08672277 |
| C      | 0.82020269 | 1.83970110 | 3.60560973 |
| H      | 0.95935069 | 2.19123244 | 4.60659103 |
| H      | 1.77231028 | 1.73538506 | 3.12863038 |
| H      | 0.22337806 | 2.54117494 | 3.06096782 |

**Tc-Int**

|        |        |        |        |
|--------|--------|--------|--------|
| O      | -1.68223300 | 0.49338100 | -3.41519000 |
| O      | 2.54926300 | 0.48683500 | -3.40374900 |
| O      | 0.42839400 | -1.61050100 | -3.42362600 |
| O      | 0.43582900 | 2.59818200 | -3.41071200 |
| O      | 0.44198500 | 2.62333000 | -1.15221400 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| O       | 0.43091700| -1.62987500| -1.16647600|
| O       | 2.57715400| 0.49239200 | -1.14287000|
| O       | -1.70778800| 0.51430400| -1.15584500|
| C       | -2.26774400| 0.50511800| -2.28135500|
| C       | 3.13508200| 0.48812400| -2.27150300|
| C       | 0.42856800| -2.19655500| -2.28821900|
| C       | 0.44033300| 3.18610400| -2.27915400|
| H       | -3.36414000| 0.50483700| -2.29578600|
| H       | 0.44379100| 4.28109800| -2.29572900|
| H       | 0.42478200| -3.29017600| -2.29578900|
| H       | 4.23271800| 0.48607800| -2.29572700|
| Tc      | 0.43233300| 0.49027900| -3.37369500|
| Tc      | 0.42493100| 0.48680500| -1.10806300|
| C       | -1.40866700| 0.12918500| 4.09392700|
| C       | -1.32019900| -1.28079900| 4.67539900|
| H       | -2.35778800| 0.15443100| 3.53276800|
| H       | -1.47864800| 0.86154700| 4.90546100|
| H       | -0.87738900| -1.95721600| 3.94713900|
| C       | -2.63558200| -1.80356100| 5.22103600|
| H       | -3.34253800| -1.89146700| 4.38440000|
| H       | -2.51813000| -2.79046700| 5.67785000|
| H       | -3.06321500| -1.12389600| 5.96720200|
| N       | -0.31952700| 0.49491200| 3.21375100|
| Br      | 0.07390400| -1.31752800| 6.21835500|
| C       | -0.37244000| -0.03260500| 1.90058700|
| O       | -1.17740400| -0.95430900| 1.68242400|
| O       | 0.46103200| 0.50604500| 1.06807500|
| C       | 0.45625500| 1.68198600| 3.52845200|
| H       | 1.25486200| 1.77444700| 2.79217400|
| Atom | x   | y   | z   |
|------|-----|-----|-----|
| Tc   | -0.00001500 | 0.00000200 | -1.10236400 |
| Tc   | 0.00001500 | -0.00000100 | 1.10236500 |
| C    | -0.23087506 | -0.69506604 | 6.75262269 |
| C    | -0.75604741 | -2.07798365 | 6.41928075 |
| H    | -1.08881658 | -0.03106332 | 6.96873109 |
| H    | 0.39189359 | -0.73320759 | 7.64663679 |
| H    | -0.06974699 | -2.78357914 | 5.98188742 |
| C    | -2.22249915 | -2.40196431 | 6.50407852 |
| H    | -2.73235775 | -1.94698680 | 5.64754680 |
| H    | -2.38494082 | -3.48153409 | 6.48827003 |

**H**

| Atom | x   | y   | z   |
|------|-----|-----|-----|
| H    | -0.15348900 | 2.60300000 | 3.49179200 |
| H    | 0.89287300 | 1.59264300 | 4.53160900 |

**Tc-Ts_3**

| Atom | x   | y   | z   |
|------|-----|-----|-----|
| O    | -2.11527600 | 0.00510200 | -1.12533500 |
| O    | 2.11528200 | -0.00514300 | -1.12529800 |
| O    | -0.00520300 | -2.09582900 | -1.12284400 |
| O    | 0.00507700 | 2.09585800 | -1.12285900 |
| O    | 0.00520200 | 2.09583000 | 1.12284100 |
| O    | -0.00507800 | -2.09588000 | 1.12285600 |
| O    | 2.11527800 | -0.00510300 | 1.12533600 |
| O    | -2.11528400 | 0.00514200 | 1.12529800 |
| C    | -2.70209800 | 0.00659800 | -0.00000700 |
| C    | 2.70209800 | -0.00660100 | 0.00000800 |
| C    | -0.00666900 | -2.69074300 | 0.00000800 |
| C    | 0.00666700 | 2.69074300 | -0.00001000 |
| H    | -3.79842900 | 0.00937600 | -0.00003100 |
| H    | 0.00950200 | 3.78563700 | 0.00002600 |
| H    | -0.00950700 | -3.78563700 | -0.00003400 |
| H    | 3.79842900 | -0.00938300 | 0.00002800 |

S132
| Atom | X         | Y         | Z         | Energy         |
|------|-----------|-----------|-----------|---------------|
| H    | -2.65347250 | -2.00412046 | 7.42783251 |
| N    | 0.56811580  | -0.18133183 | 5.64969323 |
| Br   | -0.13007049 | -3.27251372 | 8.61962273 |
| C    | 0.02542013  | -0.44934372 | 4.39046296 |
| O    | -0.86367714 | -1.35689730 | 4.38953552 |
| O    | 0.46364400  | 0.19698455  | 3.39306302 |
| C    | 1.36138651  | 1.00805415  | 5.88440009 |
| H    | 1.87826289  | 1.26505154  | 4.95878689 |
| H    | 0.74064226  | 1.87033644  | 6.18721092 |
| H    | 2.09747554  | 0.81761350  | 6.67568934 |
| Tc-Int$_5$ |
| O    | -1.67890600 | 0.49871700  | -3.41130300 |
| O    | 2.54694300  | 0.49007700  | -3.41013100 |
| O    | 0.42891200  | -1.60440500 | -3.41772000 |
| O    | 0.43806100  | 2.59650200  | -3.41470100 |
| O    | 0.44582000  | 2.61433800  | -1.16079500 |
| O    | 0.43002600  | -1.62090800 | -1.16547200 |
| O    | 2.56746700  | 0.49507200  | -1.15445000 |
| O    | -1.69825800 | 0.49588300  | -1.15605100 |
| C    | -2.26760000 | 0.50006400  | -2.28218100 |
| C    | 3.13581800  | 0.48977400  | -2.28099500 |
| C    | 0.42866900  | -2.19624300 | -2.28789000 |
| C    | 0.44227500  | 3.18665900  | -2.28553600 |
| H    | -3.36414000 | 0.50483700  | -2.29578600 |
| H    | 0.44379100  | 4.28109800  | -2.29572900 |
| H    | 0.42478200  | -3.29017600 | -2.29578900 |
| H    | 4.23271800  | 0.48607800  | -2.29572700 |
| Tc   | 0.43373500  | 0.49352900  | -3.37697900 |
| Tc   | 0.43452800  | 0.48983900  | -1.13842500 |
| Atom | C          | H          | N          | Br        |
|------|------------|------------|------------|-----------|
|      | -1.24870400 | -0.24213500 | 4.12433500 |           |
|      | -1.21648500 | -1.55660000 | 3.33172000 |           |
|      | -2.25336800 | 0.20969100  | 4.14378300 |           |
|      | -0.91208900 | -0.40713100 | 5.15195400 |           |
|      | -0.45252000 | -2.21782700 | 3.75124400 |           |
|      | -2.53349800 | -2.28557000 | 3.19809000 |           |
|      | -3.30407300 | -1.63512600 | 2.76519700 |           |
|      | -2.41955800 | -3.17040400 | 2.56179100 |           |
|      | -2.83401000 | -2.60610700 | 4.20178500 |           |
|      | -0.33860000 | 0.58696600  | 3.33018200 |           |
|      | -1.29499100 | -2.47172100 | 6.81478700 |           |
|      | -0.17055600 | 0.07176200  | 2.09308400 |           |
|      | -0.72853800 | -1.14008900 | 1.99500100 |           |
|      | 0.43408500  | 0.62364700  | 1.15585800 |           |
|      | 0.02221100  | 1.93945300  | 3.69145400 |           |
|      | 0.68056600  | 2.34389500  | 2.92045200 |           |
|      | -0.87214900 | 2.57492800  | 3.77097400 |           |
|      | 0.53837300  | 1.94281100  | 4.65808600 |           |

Ag-HKUST-1

| Atom | O          | O          | O          | C          |
|------|------------|------------|------------|------------|
|      | -1.51903400 | -1.51528500 | 1.24615200 | -1.93305100 |
|      | 1.51929700  | 1.51759900  | 1.24275900 | 1.93287000  |
|      | -1.51625800 | 1.52030300  | 1.24323100 | -1.93287000 |
|      | 1.51661700  | -1.51801200 | 1.24581100 | 1.93287000  |
|      | 1.61209900  | -1.61657900 | -1.05107800| 1.93287000  |
|      | -1.61244500 | 1.61425900  | -1.05366100| 1.93287000  |
|      | 1.61529200  | 1.61109400  | -1.05413200| 1.93287000  |
|      | -1.61553900 | -1.61342700 | -1.05073900| 1.93287000  |
|      | -1.93305100 | -1.92921000 | 0.11011900 |             |
|      | 1.93287000  | 1.92938900  | 0.10590900 |             |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | -1.92932200 | 1.93292700 | 0.10648300 |
| C       | 1.92935800  | -1.93291400 | 0.10968300 |
| H       | -2.71552900 | -2.71084400 | 0.21903500 |
| H       | 2.71059800  | -2.71578600 | 0.21840100 |
| H       | -2.71064700 | 2.71571300  | 0.21386900 |
| H       | 2.71585700  | 2.71051400  | 0.21307300 |
| Ag      | 0.00019400  | 0.00135900  | 1.31276900 |
| Ag      | -0.00018700 | -0.00136600 | -1.48086000 |
| Ag-Int0 |         |         |         |
| O       | -1.27675600 | -2.11527500 | -0.09318300 |
| O       | -1.28645000 | 2.10910500  | 0.10193000 |
| O       | -1.28911400 | 0.09443100  | -2.10776600 |
| O       | -1.27386600 | -0.10060800 | 2.11659200 |
| O       | 1.01114000  | -0.10243500 | 2.29109100 |
| O       | 0.99462400  | 0.10669600  | -2.29774800 |
| O       | 0.99749200  | 2.29716200  | 0.10104800 |
| O       | 1.00803500  | -2.29204100 | -0.10807900 |
| C       | -0.15182900 | -2.72922500 | -0.12469100 |
| C       | -0.16438300 | 2.72861600  | 0.12560500 |
| C       | -0.16772600 | 0.12452000  | -2.72823500 |
| C       | -0.14818000 | -0.12574400 | 2.72942300 |
| H       | -0.29125600 | -3.82521800 | -0.17458700 |
| H       | -0.28623600 | -0.17655400 | 3.82554900 |
| H       | -0.31342800 | 0.17433000  | -3.82341800 |
| H       | -0.30886900 | 3.82391500  | 0.17633400 |
| Ag      | -1.28000800 | -0.00305800 | 0.00437900 |
| Ag      | 1.57600100  | 0.00387200  | -0.00539200 |
| C       | 4.01542739  | 0.61015189  | 1.29633390 |
| C       | 4.39402953  | -0.79039163 | 0.93664076 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 3.27248592| 0.79715076| 2.07019874|
| H    | 4.77909319| 1.38444793| 1.19888749|
| H    | 5.42063822|-0.91297161| 0.57811443|
| C    | 3.81380724|-2.00079425| 1.63201430|
| H    | 3.78474175|-2.86515104| 0.95633968|
| H    | 4.41714818|-2.27333149| 2.50744003|
| H    | 2.79029434|-1.79835197| 1.96481641|
| N    | 3.51190257|-0.01129011| 0.06998061|
| C    | 4.07526389| 0.47622203|-1.18351396|
| H    | 3.97184795|-0.29933373|-1.95092411|
| H    | 3.51621992| 1.36049782|-1.51009363|
| H    | 5.14404472| 0.75003706|-1.10667951|
| Ag-Int1 |   |   |   |
| O    | -2.81585500|-2.58170200|-0.77641400|
| O    | -2.91887300| 1.70212600|-0.13168700|
| O    | -2.82304900|-0.15412200|-2.59604200|
| O    | -2.81844500|-0.77380400| 1.67860700|
| O    | -0.58931400|-0.27223800| 1.80752000|
| O    | -0.61249900|-0.75079100|-2.76133900|
| O    | -0.81703600| 1.77501200|-0.99352100|
| O    | -0.60170000|-2.77163200|-0.23232200|
| C    | -1.72772100|-3.19668900|-0.54423300|
| C    | -1.82523200| 2.27575300|-0.48652400|
| C    | -1.72476700|-0.40575400|-3.19333800|
| C    | -1.70840000|-0.55383400| 2.26810200|
| H    | -1.80806300|-4.28732000|-0.63608900|
| H    | -1.80304300|-0.63865600| 3.36404700|
| H    | -1.83023500|-0.28777200|-4.28492000|
| H    | -1.82567600| 3.36181300|-0.28516800|
Ag  -2.81541400  -0.43205900  -0.45786800
Ag   0.23177900  -0.66603000  -0.46567100
C    2.28454000  1.51747900  0.72040600
C    3.31144400  0.47720900  0.43999600
H    1.59831900  1.34863900  1.54518600
H    2.51318500  2.55867700  0.50640000
H    4.21855200  0.82633900 -0.04751100
C    3.47574200 -0.75361100  1.31177600
H    3.09198100 -1.64968000  0.80525000
H    4.53498400 -0.89891600  1.54074500
H    2.94795000 -0.64039000  2.26320700
N    2.10676700  0.62737000 -0.43538600
Br   5.06737400  2.01475300  2.34941000
C    2.31988800  1.25834700 -1.74393700
H    2.52365500  0.48554100 -2.49280400
H    1.40743400  1.79468600 -2.01749500
H    3.16543900  1.96376800 -1.71754800
Ag-Ts1
O    -1.27675600 -2.11527500 -0.09318300
O    -1.28645000  2.10910500  0.10193000
O    -1.28911400  0.09443100 -2.10776600
O    -1.27386600 -0.10060800  2.11659200
O    1.01114000 -0.10243500  2.29109100
O    0.99462400  0.10669600 -2.29774800
O    0.99749200  2.29716200  0.10104800
O    1.00803500 -2.29204100 -0.10807900
C    -0.15182900 -2.72922500 -0.12469100
C    -0.16438300  2.72861600  0.12560500
C    -0.16772600  0.12452000 -2.72823500
|   |  X     |  Y     |  Z     |
|---|--------|--------|--------|
| C | -0.14818000 | -0.12574400 | 2.72942300 |
| H | -0.29125600 | -3.82521800 | -0.17458700 |
| H | -0.28623600 | -0.17655400 | 3.82554900 |
| H | -0.31342800 | 0.17433000 | -3.82341800 |
| H | -0.30886900 | 3.82391500 | 0.17633400 |
| Ag | -1.28000800 | -0.00305800 | 0.00437900 |
| Ag | 1.57600100 | 0.00387200 | -0.00539200 |
| C | 4.67954068 | 0.64920025 | 0.72249707 |
| C | 5.17206577 | -0.67210285 | 0.27622812 |
| H | 4.20507961 | 0.64354737 | 1.70479699 |
| H | 5.36426605 | 1.49231238 | 0.60249931 |
| H | 5.77855142 | -0.69805195 | -0.61840967 |
| C | 4.60852307 | -1.96732002 | 0.79427250 |
| H | 3.79651920 | -2.32545528 | 0.15014633 |
| H | 5.39677160 | -2.72368139 | 0.81361344 |
| H | 4.21561197 | -1.84629177 | 1.80789704 |
| N | 3.74703563 | 0.42671138 | -0.36827501 |
| Br | 7.54588391 | -0.70957681 | 1.48963518 |
| C | 4.04817266 | 1.19155289 | -1.57446653 |
| H | 3.51008745 | 0.77086515 | -2.42799322 |
| H | 3.72230886 | 2.23219126 | -1.43308247 |
| H | 5.12712713 | 1.19230784 | -1.79083576 |

**Ag-Int₂**

|   |  X     |  Y     |  Z     |
|---|--------|--------|--------|
| O | -2.89900900 | -2.63638000 | -0.80533400 |
| O | -3.02266800 | 1.77201100 | -0.15711500 |
| O | -2.88081600 | -0.18224000 | -2.64104400 |
| O | -2.84092800 | -0.79771200 | 1.70700400 |
| O | -0.60695600 | -0.28352500 | 1.79499200 |
| O | -0.65191400 | -0.74758400 | -2.74035500 |
| Atom | x    | y    | z    |
|------|------|------|------|
| O    | -0.92334700 | 1.73988500 | -1.02487700 |
| O    | -0.69255000 | -2.72393700 | -0.20453300 |
| C    | -1.80284200 | -3.19648900 | -0.54790200 |
| C    | -1.90585900 | 2.28682700  | -0.50054600 |
| C    | -1.76837900 | -0.41197600 | -3.19494300 |
| C    | -1.73214300 | -0.56795800 | 2.26851000  |
| H    | -1.80806300 | -4.28732000 | -0.63608900 |
| H    | -1.80304300 | -0.63865600 | 3.36404700  |
| H    | -1.83023500 | -0.28777200 | -4.28492000 |
| H    | -1.82567600 | 3.36181300  | -0.28516800 |
| Ag   | -2.92867300 | -0.42281500 | -0.45971200 |
| Ag   | 0.11951500  | -0.67491100 | -0.45984800 |
| C    | 2.34474500  | 1.26565600  | 0.51093600  |
| C    | 3.72807600  | 0.70997200  | 0.90478800  |
| H    | 1.65155800  | 1.11590400  | 1.34860800  |
| H    | 2.41669500  | 2.34459900  | 0.30878900  |
| H    | 4.42283600  | 0.78328700  | 0.06735900  |
| C    | 3.70826700  | -0.67829200 | 1.51267700  |
| H    | 3.26566700  | -1.36665500 | 0.78322400  |
| H    | 4.71800500  | -1.02241100 | 1.75815300  |
| H    | 3.09428600  | -0.70128200 | 2.41912900  |
| N    | 1.91564400  | 0.50492000  | -0.64261300 |
| Br   | 4.61178200  | 2.01067100  | 2.28139600  |
| C    | 2.03045100  | 1.23924100  | -1.87893200 |
| H    | 1.87076300  | 0.57391200  | -2.73189800 |
| H    | 1.27278300  | 2.04308600  | -1.92464400 |
| H    | 3.02570200  | 1.71486800  | -1.96878600 |

**Ag-Int3**

| O    | -3.58407900 | 0.29875000 | -1.56089100 |
| Atom | X   | Y   | Z   | W   |
|------|-----|-----|-----|-----|
| O    | -2.56662700 | 4.24822000 | 0.51145000 |
| O    | -0.25499500  | 3.98372500  | 0.27126100  |
| C    | 1.42817000   | 0.21185000  | 2.53728300  |
| H    | 2.38291000   | 0.48347900  | 3.02465600  |
| H    | 0.62492800   | 0.81064600  | 2.96736900  |
| H    | 1.25698500   | -0.85673400 | 2.75589700  |
| Ag-Ts₂ |     |     |     |     |
| O    | -1.27675600  | -2.11527500 | -0.09318300 |
| O    | -1.28645000  | 2.10910500  | 0.10193000  |
| O    | -1.28911400  | 0.09443100  | -2.10776600 |
| O    | -1.27386600  | -0.10060800 | 2.11659200  |
| O    | 1.01114000   | -0.10243500 | 2.29109100  |
| O    | 0.99462400   | 0.10669600  | -2.29774800 |
| O    | 0.99749200   | 2.29716200  | 0.10104800  |
| O    | 1.00803500   | -2.29204100 | -0.10807900 |
| C    | -0.15182900  | -2.72922500 | -0.12469100 |
| C    | -0.16438300  | 2.72861600  | 0.12560500  |
| C    | -0.16772600  | 0.12452000  | -2.72823500 |
| C    | -0.14818000  | -0.12574400 | 2.72942300  |
| H    | -0.29125600  | -3.82521800 | -0.17458700 |
| H    | -0.28623600  | -0.17655400 | 3.82554900  |
| H    | -0.31342800  | 0.17433000  | -3.82341800 |
| H    | -0.30886900  | 3.82391500  | 0.17633400  |
| Ag   | -1.28000800  | -0.00305800 | 0.00437900  |
| Ag   | 1.57600100   | 0.00387200  | -0.00539200 |
| C    | 4.63439410   | 0.45318444  | 1.62092752  |
| C    | 4.89574936   | -0.93404449 | 2.21515428  |
| H    | 3.96877772   | 1.01415628  | 2.29429312  |
| H    | 5.58687134   | 0.99958543  | 1.57419623  |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 5.66180287 | -1.46691784 | 1.65386960 |
| C    | 3.67574179  | -1.79779505 | 2.45072485 |
| H    | 3.23203870  | -2.04163537 | 1.47736975 |
| H    | 3.94696664  | -2.73938777 | 2.93858295 |
| H    | 2.92495658  | -1.27737350 | 3.05192859 |
| N    | 4.04956290  | 0.36408882  | 0.27786459 |
| Br   | 5.85795536  | -0.62392439 | 4.03106061 |
| C    | 4.95052551  | -0.76422895 | -1.04496819 |
| O    | 5.74174626  | -0.05753370 | -1.59489532 |
| O    | 4.47350828  | -1.82846580 | -0.79026366 |
| C    | 4.24367647  | 1.67255422  | -0.36333603 |
| H    | 5.28546805  | 1.91658638  | -0.36764982 |
| H    | 3.88228557  | 1.63370204  | -1.36970928 |
| H    | 3.70456927  | 2.41979425  | 0.18062698 |
| Ag-Int₄ |      |         |          |
| O    | -3.77811600 | -1.83636500 | 0.75684000 |
| O    | -3.73423000 | 2.35805900  | 0.47581500 |
| O    | -3.73099700 | 0.11837400  | -1.48234900 |
| O    | -3.76226900 | 0.37828100  | 2.70696100 |
| O    | -1.55388800 | -0.15564000 | 2.86778900 |
| O    | -1.60657500 | 0.93094800  | -1.69675100 |
| O    | -1.54961900 | 2.60456600  | 1.09348900 |
| O    | -1.68066600 | -1.96920700 | -0.11810300 |
| C    | -2.71122200 | -2.44760800 | 0.33401100 |
| C    | -2.67669900 | 3.01042200  | 0.79115000 |
| C    | -2.68317900 | 0.51606000  | -2.12208000 |
| C    | -2.66380500 | 0.09665600  | 3.32997800 |
| H    | -2.83006300 | -3.54638100 | 0.43032900 |
| H    | -2.82504300 | 0.10228300  | 4.43046500 |
| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| H    | -2.85223500 | 0.45316700 | -3.21850200 |
| H    | -2.84767600 | 4.10275200 | 0.78125000 |
| Ag   | -3.61398100 | 0.24995800 | 0.61173200 |
| Ag   | -0.32631600 | 0.67585700 | 0.57370800 |
| C    | 4.05023300  | -1.45793600 | -0.06668300 |
| C    | 4.07232200  | -1.41774400 | -1.59373600 |
| H    | 3.26152900  | -2.17727000 | 0.19601400 |
| H    | 5.00364900  | -1.84837100 | 0.30952000 |
| H    | 3.28358100  | -0.76393800 | -1.96123400 |
| C    | 4.03040400  | -2.78821100 | -2.24284200 |
| H    | 3.07264400  | -3.26136800 | -1.98705200 |
| H    | 4.09882700  | -2.71931800 | -3.33226300 |
| H    | 4.84349100  | -3.42993300 | -1.88274000 |
| N    | 3.76504000  | -0.19221300 | 0.57532300 |
| Br   | 5.78822900  | -0.44292300 | -2.24674300 |
| C    | 2.43008600  | 0.22434000  | 0.66693400 |
| O    | 1.57784000  | -0.48516500 | 0.01890100 |
| O    | 2.13693500  | 1.24407200  | 1.34450000 |
| C    | 4.79806500  | 0.45686200  | 1.36270600 |
| H    | 4.39835200  | 1.40442100  | 1.72480400 |
| H    | 5.09195900  | -0.15271500 | 2.23471000 |
| H    | 5.68950300  | 0.64635700  | 0.75310600 |

**Ag-Ts₃**

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| O    | -1.27675600 | -2.11527500 | -0.09318300 |
| O    | -1.28645000 | 2.10910500  | 0.10193000 |
| O    | -1.28911400 | 0.09443100  | -2.10776600 |
| O    | -1.27386600 | -0.10060800 | 2.11659200 |
| O    | 1.01114000  | -0.10243500 | 2.29109100 |
| O    | 0.99462400  | 0.10669600  | -2.29774800 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| O    | 0.99749200 | 2.29716200 | 0.10104800 |
| O    | 1.00803500 | -2.29204100| -0.10807900|
| C    | -0.15182900| -2.72922500| -0.12469100|
| C    | -0.16438300| 2.72861600 | 0.12560500 |
| C    | -0.16772600| 0.12452000 | -2.72823500|
| C    | -0.14818000| -0.12574400| 2.72942300 |
| H    | -0.29125600| -3.82521800| -0.17458700|
| H    | -0.28623600| -0.17655400| 3.82554900 |
| H    | -0.31342800| 0.17433000 | -3.82341800|
| H    | -0.30886900| 3.82391500 | 0.17633400 |
| Ag   | -1.28000800| -0.00305800| 0.00437900 |
| Ag   | 1.57600100 | 0.00387200 | -0.00539200|
| C    | 7.35417649 | -0.67323495| -0.18975448|
| C    | 7.11472099 | -2.03968633| 0.42250009 |
| H    | 7.59220388 | 0.04256658 | 0.61934208 |
| H    | 8.20968912 | -0.70672379| -0.86468664|
| H    | 6.66825449 | -2.79721617| -0.19959507|
| C    | 7.30232615 | -2.28364627| 1.89488682 |
| H    | 6.45891967 | -1.83852880| 2.43446338 |
| H    | 7.34414787 | -3.35310810| 2.11078136 |
| H    | 8.23195397 | -1.82639380| 2.24709625 |
| N    | 6.18328672 | -0.24729950| -0.94232259|
| Br   | 9.32385076 | -3.17347393| -0.28072487|
| C    | 4.97228484 | -0.53845670| -0.30930461|
| O    | 5.06529520 | -1.39809330| 0.62156718 |
| O    | 3.92258670 | 0.04277751 | -0.71536821|
| C    | 6.31672746 | 0.90812385 | -1.80614851|
| H    | 5.35107958 | 1.09976358 | -2.27600702|
| H    | 6.61809250 | 1.81307311 | -1.24865902|

S144
H  7.06968631  0.71258424  -2.58013210

Ag-Int$_5$

O  3.91017800  -0.88468200  -1.93898800
O  3.61600700  -0.43995900   2.34923800
O  2.82806000  -2.57853700   0.36843500
O  4.62093800   1.22283300   0.09873200
O  2.71751400   2.22936000  -0.66213600
O  0.74376000  -1.70463300   0.60716100
O  1.78095900   0.91598900   2.18151300
O  1.70963200  -0.41851300  -2.27731800
C  2.84730900  -0.75749100  -2.62392400
C  2.66803700   0.30674500   2.79133000
C  1.55390000  -2.61212100   0.51255400
C  3.90689800   2.19080900  -0.36201200
H  3.02223700  -0.96930200  -3.66005700
H  4.52678000   3.13407900  -0.46432900
H  1.20891500  -3.67374800   0.66518800
H  2.71360900   0.42916200   3.86200800
Ag  3.66143500  -0.65918300   0.19391700
Ag  0.99034500   0.57409900  -0.13456700
C  -4.57327100   0.88906500  -0.51043200
C  -3.89287300  -0.49098300  -0.46790900
H  -4.91512200   1.15999400  -1.52343400
H  -5.43160800   0.92077300   0.15868900
H  -4.02829200  -0.94977300   0.51484200
C  -4.32352300  -1.44741900  -1.55613900
H  -4.17349000  -1.00562000  -2.54862100
H  -3.75317700  -2.37756700  -1.50323100
H  -5.38706900  -1.67014900  -1.41618300
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| N       | -3.47538900 | 1.74533300 | -0.08549700 |
| Br      | -7.64043900 | -0.76739000 | 0.52422200  |
| C       | -2.27628800 | 1.13713600 | -0.27270100 |
| O       | -2.46051800 | -0.16271700 | -0.57460900 |
| O       | -1.16299000 | 1.65687200 | -0.19330800 |
| C       | -3.60778700 | 3.17216200 | 0.05833300  |
| H       | -2.64191300 | 3.58213200 | 0.35646600  |
| H       | -3.91876200 | 3.64112300 | -0.88825800 |
| H       | -4.35541600 | 3.40361900 | 0.82382600  |

**Mn-HKUST-1**

| Mn      | 0.00592200 | -0.00068400 | -1.53285200 |
| Mn      | -0.00591500 | 0.00068300 | 1.53288600  |
| O       | 1.35467400 | 1.52430800 | -0.95894500 |
| O       | -1.34514500 | -1.52551800 | -0.96635200 |
| O       | -1.55662300 | 1.38586400 | -1.30154500 |
| O       | 1.56617800 | -1.38683400 | -1.29097300 |
| O       | 1.52242900 | -1.34684300 | 0.96792100  |
| O       | -1.53193700 | 1.34779500 | 0.95733700  |
| O       | -1.38856100 | -1.56306800 | 1.29254600  |
| O       | 1.37894200 | 1.56430500 | 1.29993200  |
| C       | 1.74227100 | 1.96975500 | 0.15965900  |
| C       | -1.74227400 | -1.96977800 | 0.14957700  |
| C       | -1.96974800 | 1.74226700 | -0.16185300 |
| C       | 1.96979100 | -1.74225500 | -0.14741500 |
| H       | 2.47154400 | 2.79482200 | 0.13203000  |
| H       | 2.79475300 | -2.47163900 | -0.11330300 |
| H       | -2.79474500 | 2.47161600 | -0.13536500 |
| H       | -2.47164300 | -2.79475900 | 0.11663000  |

**Mn-Int**
Mn  0.00592200  -0.00068400  -1.53285200
Mn  -0.00591500  0.00068300  1.53288600
O   1.37267400  1.54230800  -1.12094500
O   -1.36314500  -1.54351800  -1.12835200
O   -1.53862300  1.36786400  -1.13954500
O   1.54817800  -1.36883400  -1.12897300
O   1.54042900  -1.36484300  1.12992100
O   -1.54993700  1.36579500  1.11933700
O   -1.37056100  -1.54506800  1.13054600
O   1.36094200  1.54630500  1.13793200
C   1.74227100  1.96975500  0.00965900
C   -1.74227400 -1.96977800  -0.00042300
C   -1.96974800  1.74226700  -0.01185300
C   1.96979100 -1.74225500  0.00258500
H   2.47154400  2.79482200  0.01203000
H   2.79475300 -2.47163900  0.00669700
H   -2.79474500  2.47161600  -0.01536500
H   -2.47164300 -2.79475900  -0.00337000
C   0.01050257  0.11746400  4.98979203
C   1.21419555  -0.68483511  5.36619637
H   -0.79374272  -0.33603867  4.41245138
H   -0.30620152  0.90962577  5.67125652
H   1.69446291  -0.38423538  6.30239905
C   1.36888181  -2.14631228  5.01203058
H   2.42728620  -2.41168359  4.89433659
H   0.94336144  -2.78434098  5.79721771
H   0.85854792  -2.36882076  4.06896745
N   1.27981197  0.29241009  4.28133081
C   2.00588373  1.52901114  4.54577431
H  3.06962377  1.37529277  4.33146679
H  1.63105538  2.31609375  3.88159601
H  1.90802050  1.88014908  5.58994652

Mn-Int₁
Mn  -3.39184700  -0.46149300  0.11985100
Mn  -0.32887000   0.24391500  -0.27499000
O   -2.42030800  -1.56481700  1.65163400
O   -3.30685900   0.82943500 -1.56068400
O   -3.45620600  -2.16484200 -1.14226800
O   -4.26255400   0.95953000  1.42147500
O   -2.08960000  1.42394800  1.12885400
O   -1.31629900  -1.48678300 -1.27379000
O   -1.13767900  1.47915200 -1.70717100
O   -0.26707100 -0.88909600  1.44345200
C   -1.20602900 -1.54188800  1.97815600
C   -2.35404100  1.48324500 -2.05608700
C   -2.26934900 -2.26147800 -1.57070300
C   -3.21811000  1.65451900  1.64089800
H   -0.90342900 -2.16407900  2.82358900
H   -3.32872500  2.51065700  2.33027300
H   -2.05147900 -3.09488800 -2.25994800
H   -2.60281400  2.13552100 -2.89910400
C   2.67767300  -0.15214000  0.63561500
C   2.74693700 -0.59618300 -0.77193100
H   2.11153800 -0.72519800  1.36334400
H   3.53684900  0.41352100  0.99251000
H   3.65298000 -0.26025200 -1.27819500
C   2.14325100 -1.88587600 -1.27079400
H   1.82277400 -1.79881400 -2.31682800
H   2.90152000  -2.67762800  -1.21576800
H   1.28056700  -2.20222500  -0.67504000
N   1.83037900   0.52967200  -0.39513300
Br  6.03548100   0.85160600  -0.30916200
C   2.29270100   1.88009000  -0.79578600
H   1.91325900   2.09956000  -1.79944900
H   1.88293100   2.61813600  -0.09553500
H   3.38853900   1.94015700  -0.78653100

Mn-Ts$_1$

Mn   -3.29831400  -0.53199300   0.07862800
Mn   -0.30031600   0.56373400   0.02366500
O   -2.34715500  -1.52901000  1.68761200
O   -3.29772600   0.86659800  -1.50418600
O   -3.50571100  -2.25335200  -1.15634800
O   -4.08755000   0.92222400  1.40434300
O   -1.92974300   1.53854800  1.21348800
O   -1.41125600  -1.46055100  -1.18093200
O   -1.11824400   1.48237500 -1.65273400
O   -0.17707800  -0.88917700  1.49245900
C   -1.13101200  -1.53273800  2.01133300
C   -2.32787200   1.49010300  -2.00925300
C   -2.29130400  -2.28780400  -1.53921200
C   -3.09889200   1.66763300  1.66924400
H   -0.85844200  -2.17015400  2.85540000
H   -3.28373800   2.50458200  2.36208400
H   -2.00649200  -3.10096300 -2.22813700
H   -2.55782700   2.12944600  -2.86729300
C   2.73934000   0.83396300   0.78437900
C   3.14056400   0.19444000  -0.47176900
| Atom | x     | y     | z     |
|------|-------|-------|-------|
| H    | 2.43708800 | 0.14209400 | 1.57401300 |
| H    | 3.42337800 | 1.59422500 | 1.17290400 |
| H    | 3.61243400 | 0.82398600 | -1.21269900 |
| C    | 2.62504700 | -1.14975000 | -0.90773900 |
| H    | 1.77328000 | -1.04971400 | -1.59278500 |
| H    | 3.41991400 | -1.68471200 | -1.43287600 |
| H    | 2.31390700 | -1.75161400 | -0.04842900 |
| N    | 1.61866400 | 1.34902800 | -0.00497600 |
| Br   | 5.68290900 | -0.51396900 | 0.10996100 |
| C    | 1.81911500 | 2.71934400 | -0.47082500 |
| H    | 1.08582400 | 2.95871300 | -1.24803100 |
| H    | 1.69468400 | 3.43939700 | -0.35785300 |
| H    | 2.82505100 | 2.88452900 | -0.88971400 |

**Mn-Int_2**

| Atom | x     | y     | z     |
|------|-------|-------|-------|
| Mn   | -3.27844600 | -0.51594600 | 0.03677200 |
| Mn   | -0.25271200 | 0.71074400 | 0.06926200 |
| O    | -2.39127300 | -1.52641400 | 1.65963400 |
| O    | -3.34886700 | 0.88012600 | -1.54110800 |
| O    | -3.56694500 | -2.26220700 | -1.19083900 |
| O    | -4.12475900 | 0.92472000 | 1.37049100 |
| O    | -1.96537300 | 1.54243100 | 1.21081500 |
| O    | -1.47887600 | -1.45773400 | -1.21418900 |
| O    | -1.17536600 | 1.53306900 | -1.63956100 |
| O    | -0.22779700 | -0.86188800 | 1.46778800 |
| C    | -1.17294800 | -1.51763800 | 1.98114800 |
| C    | -2.37359700 | 1.51414900 | -2.02599100 |
| C    | -2.35181800 | -2.28910000 | -1.57257200 |
| C    | -3.14094600 | 1.67068300 | 1.64645100 |
| H    | -0.90342900 | -2.16407900 | 2.82358900 |
|  | x     | y     | z     |
|---|-------|-------|-------|
| H | -3.32872500 | 2.51065700 | 2.33027300 |
| H | -2.05147900 | -3.09488800 | -2.25994800 |
| H | -2.60281400 | 2.13552100 | -2.89910400 |
| C | 2.73774900 | 0.79192900 | 0.74078800 |
| C | 3.57772900 | -0.15000300 | -0.13621400 |
| H | 2.35425500 | 0.21603500 | 1.59347100 |
| H | 3.39192300 | 1.58614600 | 1.14611500 |
| H | 3.92370400 | 0.35394200 | -1.03892900 |
| C | 2.95030900 | -1.49625900 | -0.43792200 |
| H | 2.00113300 | -1.32918900 | -0.96131900 |
| H | 3.59626300 | -2.10986000 | -1.07450800 |
| H | 2.73425900 | -2.04484100 | 0.48539900 |
| N | 1.64756700 | 1.33932900 | -0.03390000 |
| Br | 5.43184300 | -0.52377500 | 0.82284000 |
| C | 2.03683700 | 2.49665500 | -0.81802200 |
| H | 1.17085700 | 2.88672400 | -1.36549100 |
| H | 2.43301600 | 3.31754900 | -0.18264300 |
| H | 2.81919600 | 2.28680600 | -1.57543500 |

**Mn-Int₃**

|  | x     | y     | z     |
|---|-------|-------|-------|
| Mn | -3.20823200 | -0.81869100 | -0.37337600 |
| Mn | -0.11906300 | -0.18183800 | 0.60630900 |
| O | -2.06436800 | -1.97675300 | -1.70286400 |
| O | -3.51411900 | 0.46886800 | 1.26540400 |
| O | -4.07867500 | 0.45093700 | -1.88846300 |
| O | -3.48624300 | -2.53339900 | 0.91504000 |
| O | -1.41787600 | -1.76138300 | 1.31910000 |
| O | -2.00507900 | 1.03720800 | -1.28833100 |
| O | -1.39324200 | 1.19653300 | 1.63161200 |
| O | 0.03382400 | -1.25337000 | -1.22080200 |
|    |        |        |        |        |
|----|--------|--------|--------|--------|
| C  | -0.81534300 | -1.92656200 | -1.86508800 |
| C  | -2.64028100  | 1.17519100  | 1.83285900  |
| C  | -3.04874700  | 1.19338700  | -1.97329800 |
| C  | -2.37085100  | -2.56696000 | 1.50489500  |
| H  | -0.42723700  | -2.56098800 | -2.67433300 |
| H  | -2.19919400  | -3.35848700 | 2.24529200  |
| H  | -3.06938500  | 2.02654600  | -2.69108300 |
| H  | -3.02315800  | 1.85747600  | 2.60409400  |
| C  | 2.90642100   | -0.57598600 | 0.78080200  |
| C  | 3.76082000   | 0.38645200  | -0.06022000 |
| H  | 2.61425600   | -1.41920700 | 0.14031100  |
| H  | 3.53115600   | -0.98502800 | 1.59729500  |
| H  | 4.05450400   | 1.26446800  | 0.51546800  |
| C  | 3.18944800   | 0.75900900  | -1.41273100 |
| H  | 2.23171000   | 1.26842900  | -1.25519900 |
| H  | 3.85615300   | 1.43242800  | -1.96059300 |
| H  | 3.00307700   | -0.13293600 | -2.02059700 |
| N  | 1.73637900   | 0.09821600  | 1.29335100  |
| Br | 5.65310600   | -0.49984500 | -0.39174200 |
| C  | -0.83375900  | 3.52620300  | -0.27805600 |
| O  | -1.88589300  | 4.01441800  | -0.11506300 |
| O  | 0.24484900   | 3.10869500  | -0.44533000 |
| C  | 2.00422300   | 0.88064400  | 2.48470500  |
| H  | 2.67019900   | 1.75096900  | 2.31684200  |
| H  | 1.06655500   | 1.28044900  | 2.88840400  |
| H  | 2.48335300   | 0.27387900  | 3.28264100  |

**Mn-Ts₂**

|    |        |        |        |
|----|--------|--------|--------|
| Mn | -0.03184900 | -0.00136700 | -1.48968400 |
| Mn | 0.03218100  | 0.00204400  | 1.48971200  |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| O       | 1.20841700   | -1.53726600  | -0.59975100  |
| O       | -1.23044100  | 1.53918100   | -0.55670400  |
| O       | 1.56414500   | 1.26501500   | -1.70518900  |
| O       | -1.63223900  | -1.27088600  | -1.64201700  |
| O       | -1.52574100  | -1.21727100  | 0.60826200   |
| O       | 1.55000600   | 1.22211000   | 0.54810200   |
| O       | -1.23499300  | 1.59858300   | 1.69618300   |
| O       | 1.30069200   | -1.59826400  | 1.65104100   |
| C       | 1.61190000   | -2.02054100  | 0.49359500   |
| C       | -1.59295300  | 2.01985300   | 0.55214600   |
| C       | 2.00987700   | 1.60151500   | -0.56394000  |
| C       | -2.02971100  | -1.60385000  | -0.48182000  |
| H       | 2.29366300   | -2.88279600  | 0.44712900   |
| H       | -2.88875400  | -2.28924300  | -0.42970400  |
| H       | 2.87263900   | 2.28409900   | -0.55019300  |
| H       | -2.27927900  | 2.87952600   | 0.53277700   |
| C       | -1.86033407  | -0.15174051  | 4.58897073   |
| C       | -1.78449720  | -0.78091161  | 5.99229253   |
| H       | -2.40077083  | -0.85237532  | 3.93854437   |
| H       | -2.46288574  | 0.77222619   | 4.63680948   |
| H       | -1.04556431  | -0.27446240  | 6.61155913   |
| C       | -1.61228137  | -2.28824198  | 6.00520592   |
| H       | -0.72499334  | -2.55053769  | 5.41716150   |
| H       | -1.48335579  | -2.67732174  | 7.02003598   |
| H       | -2.47363720  | -2.78233817  | 5.54264508   |
| N       | -0.52434562  | 0.11348086   | 4.06250716   |
| Br      | -3.54967977  | -0.36270125  | 7.05163026   |
| C       | 1.49082475   | -1.28427835  | 4.66050508   |
| O       | 1.79701242   | -0.77442434  | 5.67639521   |

S153
O 1.59546244 -2.04200421  3.76064086
C -0.03928567  1.41465500  4.51226147
H  0.12580325  1.45564174  5.60514720
H  0.92319473  1.64491321  4.03920146
H -0.73800634  2.23921046  4.26462193

Mn-Int$_4$
Mn  0.63218200  0.39569400  -3.72466900
Mn  0.55420300  0.28519700   -0.49868800
O  1.88201800 -1.25126100  -3.28721000
O -0.66210900  1.99135900  -3.23192300
O  2.24345600  1.67418000  -4.38356000
O -1.01180600  0.89025700  -4.24296700
O -0.87791800  0.81460300  -2.00402400
O  2.11881100  1.54550300  -2.15223800
O -0.62032200  1.94447900  -0.95909500
O  1.88956800  1.22450600  -1.01438400
C  2.23089700  1.65712500  -2.14577700
C -0.97422600  2.39617900  -2.07991700
C  2.64110700  1.97576700  -3.21230300
C -1.39728400  1.21672000  -3.07825000
H  2.92526700  2.39329500  -2.1308500
H -2.25715200  1.90974000  -3.00918000
H  3.50424000  2.66360000  -3.13040700
H -1.64767500  3.25902600  -2.04743700
C  0.17847400 -0.77811900   4.13430000
C -1.61534200  0.25400900  4.23815500
H  0.22689600 -0.94223700   5.13887000
H -0.18722600  1.73412100   3.60318300
H -2.07351100  0.23309600  -2.50143000
C    -1.78469600  1.05870200  4.97898200
H    -1.22874600  1.83772400  4.44148400
H    -2.83632500  1.35723300  5.01982700
H    -1.39968200  0.99547500  6.00322300
N     0.68593200  0.16836500  3.44212100
Br   -2.71733900 -1.70673700  5.21691200
C     0.64781100  0.23239500  2.05562900
O    -0.24925000 -0.44307500  1.44528200
O     1.48464400  0.95813600  1.42960700
C     1.73328100  0.84658700  4.18649600
H     2.27787200  1.48996200  3.49456500
H     1.31129000  1.46060200  4.99511100
H     2.43833700  0.12689400  4.63312400

Mn-Ts₃

Mn    -0.03184900 -0.00136700 -1.48968400
Mn     0.03218100  0.00204400  1.48971200
O     1.20841700 -1.53726600 -0.59975100
O    -1.23044100  1.53918100 -0.55670400
O     1.56414500  1.26501500 -1.70518900
O    -1.63223900 -1.27088600 -1.64201700
O    -1.52574100 -1.21727100  0.60826200
O     1.55006000  1.22211000  0.54810200
O    -1.23499300  1.59858300  1.69618300
O     1.30069200 -1.59826400  1.65104100
C     1.61190000 -2.02054100  0.49359500
C    -1.59295300  2.01985300  0.55214600
C     2.00987700  1.60151500 -0.56394000
C    -2.02971100 -1.60385000 -0.48182000
H     2.29366300 -2.88279600  0.44712900
H       -2.88875400  -2.28924300  -0.42970400
H        2.87263900   2.28409900   -0.55019300
H       -2.27927900   2.87952600   0.53277700
C       0.06708766  -0.79568672   7.41743033
C       0.77043288  -2.10258487   7.10645336
H       -1.01347915  -0.99473169   7.54558098
H        0.44051440  -0.37948342   8.35331710
H        1.78482748  -2.05367646   6.74756933
C       0.02886031  -3.41128311   7.10272952
H       -0.58188502  -3.46580567   6.19464123
H        0.72368017  -4.25330957   7.12075494
H       -0.62479280  -3.48766770   7.97693899
N        0.30252549   0.16788164   6.35212865
Br       1.90357738  -2.48804186   9.39286112
C       0.23798345  -0.38476890   5.07055870
O        0.32049257  -1.65233670   5.04581130
O        0.12678268   0.39674197   4.07987097
C      -0.07111382   1.54705216   6.59147591
H       0.15356187   2.12507306   5.69404551
H      -1.14782960   1.65481345   6.81422953
H        0.49874767   1.94813007   7.43919506

Mn-Int$_5$
Mn      0.59766900   0.36994800  -3.82632800
Mn      0.66354900   0.37673100  -0.70686700
O      1.88410300  -1.22675800  -3.27578800
O     -0.64150300   1.98728500  -3.22655400
O      2.20579500   1.64594000  -4.29471700
O     -1.02608900  -0.90500600  -4.26372800
O     -0.85847500  -0.79878800  -2.02881400
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| O       | 2.16542600   | 1.57568400   | -2.04719800  |
| O       | -0.59861900  | 1.97137600   | -0.95816500  |
| O       | 1.90625100   | -1.22260200  | -1.00710800  |
| C       | 2.23971700   | -1.65370300  | -2.14576900  |
| C       | -0.96492600  | 2.40790900   | -2.08470800  |
| C       | 2.63979500   | 1.97301700   | -3.14634500  |
| C       | -1.39818200  | -1.21854500  | -3.08970400  |
| H       | 2.92526700   | -2.50329500  | -2.13308500  |
| H       | -2.25715200  | -1.90974000  | -3.00991800  |
| H       | 3.50424000   | 2.66360000   | -3.13040700  |
| H       | -1.64767500  | 3.25902600   | -2.04743700  |
| C       | -0.60847000  | -0.26433800  | 4.45950100   |
| C       | -1.62448100  | -0.77307600  | 3.41381200   |
| H       | -1.06566700  | 0.42538300   | 5.17359600   |
| H       | -0.16089500  | -1.08364400  | 5.02910400   |
| H       | -1.77468900  | -1.84725800  | 3.50102000   |
| C       | -2.94784800  | -0.03570600  | 3.39586800   |
| H       | -2.79636500  | 1.04895900   | 3.31593700   |
| H       | -3.56217700  | -0.36779800  | 2.55136000   |
| H       | -3.46462000  | -0.27146500  | 4.33241300   |
| N       | 0.38039700   | 0.42150200   | 3.61470600   |
| Br      | -2.52136700  | -2.22262900  | 6.39331100   |
| C       | 0.17648600   | 0.16937700   | 2.31409400   |
| O       | -0.92836200  | -0.54381600  | 2.11202000   |
| O       | 0.91050900   | 0.54199600   | 1.37142900   |
| C       | 1.55408100   | 1.08443200   | 4.14053300   |
| H       | 2.13077000   | 1.49234600   | 3.30792900   |
| H       | 1.25711400   | 1.89777300   | 4.81320100   |
| H       | 2.17799200   | 0.37649200   | 4.70252500   |
### Cd-HKUST-1

|    | X     | Y     | Z     |
|----|-------|-------|-------|
| Cd | -1.50986600 | -0.00198000 | -0.00036500 |
| Cd | 1.51071900 | 0.00200100 | 0.00018400 |
| O  | -1.78629100 | -1.33462200 | -1.68608400 |
| O  | -1.79260800 | 1.32826700 | 1.68637600 |
| O  | -0.47476100 | 1.62690200 | -1.28702100 |
| O  | -0.46878900 | -1.62811400 | 1.28574600 |
| O  | 1.79157800 | -1.68398500 | 1.33139500 |
| O  | 1.78554300 | 1.69009400 | -1.32930500 |
| O  | 0.46755400 | 1.28747600 | 1.62542600 |
| O  | 0.47385500 | -1.28617500 | -1.62626900 |
| C  | -0.62661000 | -1.66099800 | -2.09787700 |
| C  | -0.63393400 | 1.65843800 | 2.09784900 |
| C  | 0.62601200 | 2.10094400 | -1.65762900 |
| C  | 0.63298900 | -2.09835700 | 1.65846700 |
| H  | -0.60576900 | -2.34573900 | -2.96134000 |
| H  | 0.61455800 | -2.96264300 | 2.34223700 |
| H  | 0.60583500 | 2.96566500 | -2.34081800 |
| H  | -0.61495200 | 2.34281200 | 2.96163700 |

### Cd-Int₀

|    | X     | Y     | Z     |
|----|-------|-------|-------|
| Cd | -1.50986600 | -0.00198100 | -0.00036500 |
| Cd | 1.51071900 | 0.00200200 | 0.00018400 |
| O  | -1.78629100 | -1.33462300 | -1.68608400 |
| O  | -1.79260800 | 1.32826700 | 1.68637600 |
| O  | -0.47476200 | 1.62690200 | -1.28702100 |
| O  | -0.46878800 | -1.62811400 | 1.28574600 |
| O  | 1.79157900 | -1.68398400 | 1.33139500 |
| O  | 1.78554200 | 1.69009500 | -1.32930500 |

S158
O  0.46755300  1.28747600  1.62542600
O  0.47385500 -1.28617500 -1.62626900
C -0.62660900 -1.66099800 -2.09787700
C -0.63393500  1.65843800  2.09784900
C  0.62601100  2.10094400 -1.65762900
C  0.63299000 -2.09835700  1.65846700
H -0.60576800 -2.34573900 -2.96134000
H  0.61455900 -2.96264300  2.34223700
H  0.60583400  2.96566500 -2.34081800
H -0.61495300  2.34281200  2.96163700
C  4.25892782 -0.12967710  0.20678179
C  4.85656270 -0.60163618 -1.07942506
H  3.51917693 -0.73797445  0.72499056
H  4.87809083  0.49070351  0.85791977
H  5.87768851 -0.25614840 -1.26766073
C  4.50982988 -1.93367678 -1.70450183
H  4.60591328 -1.89139604 -2.79696418
H  5.17695449 -2.72280036 -1.33450756
H  3.47753007 -2.21189350 -1.46728605
N  3.82980225  0.43853807 -1.07253543
C  4.26444408  1.80123854 -1.35613132
H  4.26952188  1.95963326 -2.44055986
H  3.55485850  2.50637359 -0.90846964
H  5.27376836  2.02964816 -0.96592086

Cd-Int

Cd -3.00806400  0.81333000  0.42162400
Cd  0.31309200  0.46654700 -0.05631400
O -3.56975400 -0.52978600 -1.30084900
O -3.70512000  2.16067500  2.09392900
O  -2.35211100  2.42514000  -1.04024200
O  -2.42082800 -0.97889600  1.68267600
O  -0.14836400 -0.84219600  1.65389600
O  -0.07345700  2.39044400  -1.03074700
O  -1.47357900  2.02733300  1.91140700
O  -1.31970500 -0.52236900  -1.27824300
C  -2.43846800 -0.87896000  -1.73814100
C  -2.51988500  2.45400300  2.46084700
C  -1.21537000  2.85355500  -1.34414500
C  -1.26240500 -1.32665400  2.01551200
H  -2.41097400 -1.55953100  -2.59779500
H  -1.19064700 -2.17643500  2.70578200
H  -1.19937200  3.75187300  -1.97727300
H  -2.42015900  3.12902000  3.32518200
C  2.98921300 -1.27628400  1.43274400
C  2.66958800 -1.76573900  -0.75232200
H  2.31553800 -1.48457000  1.43274400
H  4.04814500 -1.16371600  0.83118800
H  3.55937400 -1.91547900  -1.36734900
C  1.48937700 -2.65187600  -1.06369600
H  1.10692200 -2.46712500  -2.07507800
H  1.81395900 -3.69880100  -1.01357500
H  0.66736200 -2.52022700  -0.35258300
N  2.43746000 -0.32438300  -0.40990900
Br  6.24311700 -1.96184400  -0.96745000
C  3.41624100  0.62969500  -0.98566800
H  3.05525900  0.95635700  -1.96734700
H  3.48901400  1.50397100  -0.32810300
H  4.40477800  0.16410700  -1.09127700
| Cd-Ts₁       |          |          |          |
|--------------|----------|----------|----------|
| Cd           | -1.50986600 | -0.00198100 | -0.00036500 |
| Cd           | 1.51071900  | 0.00200200  | 0.00018400  |
| O            | -1.78629100 | -1.33462300 | -1.68608400 |
| O            | -1.79260900 | 1.32826600  | 1.68637600  |
| O            | -0.47476200 | 1.62690200  | -1.28702100 |
| O            | -0.46878800 | -1.62811400 | 1.28574600  |
| O            | 1.79157900  | -1.68398400 | 1.33139500  |
| O            | 1.78554200  | 1.69009500  | -1.32930500 |
| O            | 0.46755300  | 1.28747600  | 1.62542600  |
| O            | 0.47385500  | -1.28617500 | -1.62626900 |
| C            | -0.62660900 | -1.66099800 | -2.09787700 |
| C            | -0.63393500 | 1.65843800  | 2.09784900  |
| C            | 0.62601100  | 2.10094400  | -1.65762900 |
| C            | 0.63299000  | -2.09835700 | 1.65846700  |
| H            | -0.60576800 | -2.34573900 | -2.96134000 |
| H            | 0.61455900  | -2.96264300 | 2.34223700  |
| H            | 0.60583400  | 2.96566500  | -2.34081800 |
| H            | -0.61495300 | 2.34281200  | 2.96163700  |
| C            | 4.66685784  | -0.40118769 | 0.96583737  |
| C            | 5.16174991  | -1.15067761 | -0.20929050 |
| H            | 4.06244868  | -0.99325863 | 1.65445916  |
| H            | 5.39527500  | 0.22163459  | 1.49080137  |
| H            | 5.88353251  | -0.65576846 | -0.84408953 |
| C            | 4.48035156  | -2.38612377 | -0.73169547 |
| H            | 3.75037661  | -2.13055687 | -1.50908327 |
| H            | 5.22710577  | -3.05728064 | -1.16262345 |
| H            | 3.95751393  | -2.91445440 | 0.07078147  |
| N            | 3.88433067  | 0.26344785  | -0.06117847 |
| Atoms | X (Å) | Y (Å) | Z (Å) |
|-------|-------|-------|-------|
| Br    | 7.343 | 2.264 | 0.843 |
| C     | 4.379 | 1.588 | -0.422 |
| H     | 3.946 | 1.901 | -1.376 |
| H     | 4.079 | 2.309 | 0.352 |
| H     | 5.476 | 1.600 | -0.501 |

**Cd-Int₂**

| Atoms | X (Å) | Y (Å) | Z (Å) |
|-------|-------|-------|-------|
| Cd    | -2.911 | 0.819 | 0.403 |
| Cd    | 0.469 | 0.401 | -0.124 |
| O     | -3.574 | -0.530 | -1.309 |
| O     | -3.698 | 2.146 | 2.094 |
| O     | -2.423 | 2.482 | -1.049 |
| O     | -2.406 | -0.988 | 1.667 |
| O     | -0.130 | -0.923 | 1.565 |
| O     | -0.147 | 2.361 | -1.002 |
| O     | -1.463 | 2.021 | 1.936 |
| O     | -1.326 | -0.506 | -1.278 |
| C     | -2.439 | -0.874 | -1.740 |
| C     | -2.518 | 2.445 | 2.469 |
| C     | -1.258 | 2.860 | -1.337 |
| C     | -1.245 | -1.356 | 1.975 |
| H     | -2.411 | -1.559 | -2.598 |
| H     | -1.191 | -2.176 | 2.706 |
| H     | -1.199 | 3.752 | -1.977 |
| H     | -2.421 | 3.129 | 3.325 |
| C     | 3.412 | -0.881 | -0.089 |
| C     | 3.659 | -1.959 | -1.158 |
| H     | 2.957 | -1.364 | 0.787 |
| H     | 4.386 | -0.472 | 0.236 |
| H     | 4.047 | -1.519 | -2.076 |
| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| C    | 2.49593  | -2.89562 | -1.42179 |
| H    | 1.64058  | -2.29905 | -1.76141 |
| H    | 2.73426  | -3.63259 | -2.19547 |
| H    | 2.20419  | -3.42597 | -0.50796 |
| N    | 2.55205  | 0.14848  | -0.61978 |
| Br   | 5.30548  | -3.15511 | -0.57643 |
| C    | 3.26751  | 1.16139  | -1.37291 |
| H    | 2.58533  | 1.96678  | -1.66897 |
| H    | 4.08692  | 1.62296  | -0.78068 |
| H    | 3.73692  | 0.78584  | -2.30618 |

**Cd-Int₃**

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| Cd   | -0.14759 | -0.00656 | -0.45725 |
| Cd   | 3.19153  | -0.67069 | 0.13352  |
| O    | 1.01978  | 1.91079  | -0.61672 |
| O    | -0.01830 | -1.88640 | 0.73002  |
| O    | 2.00871  | 0.34277  | 1.99030  |
| O    | 1.45302  | -0.91636 | -1.84873 |
| O    | 3.60234  | -1.56426 | -1.93045 |
| O    | 4.18302  | -0.18599 | 2.14147  |
| O    | 2.15270  | -2.57563 | 0.77362  |
| O    | 3.24030  | 1.41708  | -0.74269 |
| C    | 2.23955  | 2.16889  | -0.84057 |
| C    | 0.91803  | -2.70160 | 0.96857  |
| C    | 3.09664  | 0.28086  | 2.61436  |
| C    | 2.45137  | -1.42571 | -2.42790 |
| H    | 2.45160  | 3.19723  | -1.16623 |
| H    | 2.29392  | -1.77538 | -3.45657 |
| H    | 3.11607  | 0.65850  | 3.64806  |
| H    | 0.60650  | -3.66188 | 1.40519  |
C  -3.29186900  -0.44876700  -0.76084200
C  -4.25153300   0.08436600   0.31885300
H  -2.93056300  -1.43427500  -0.43634300
H  -3.86321700  -0.60660900  -1.69618800
H  -4.60870700   1.08444500   0.06997700
C  -3.74263900   0.00032100   1.74546400
H  -2.82290200   0.59330400   1.82237200
H  -4.47218700   0.39466500   2.46011900
H  -3.50537500  -1.03451600   2.01711200
N  -2.19397100  -0.94992500  -0.10934500
Br -6.05793600  -1.00442400   0.22529000
C  -0.34558300   4.15540600   0.59386200
O   0.08131500   4.89332500  -0.21058100
O  -0.78847700   3.47193800   1.43163000
C  -2.51666900   1.56432600  -1.84370200
H  -3.30092800   2.24708600  -1.45688700
H  -1.62906700   2.18316200  -2.02609500
H  -2.87828000   1.20657800  -2.83271200

Cd-Ts₂

Cd  -1.50986600  -0.00198100  -0.00036500
Cd   1.51071900   0.00200200   0.00018400
O  -1.78629100  -1.33462300  -1.68608400
O  -1.79260900   1.32826600   1.68637600
O  -0.47476200   1.62690200  -1.28702100
O  -0.46878800  -1.62811400   1.28574600
O   1.79157900  -1.68398400   1.33139500
O   1.78554200   1.69009500  -1.32930500
O   0.46755300   1.28747600   1.62542600
O   0.47385500  -1.28617500  -1.62626900

S164
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | -0.62660900 | -1.66099800 | -2.09787700 |
| C    | -0.63393500 | 1.65843800  | 2.09784900  |
| C    | 0.62601100  | 2.10094400  | -1.65762900 |
| C    | 0.63299000  | -2.09835700 | 1.65846700  |
| H    | -0.60576800 | -2.34573900 | -2.96134000 |
| H    | 0.61455900  | -2.96264300 | 2.34223700  |
| H    | 0.60583400  | 2.96566500  | -2.34081800 |
| H    | -0.61495300 | 2.34281200  | 2.96163700  |
| C    | -4.49780773 | -0.18079731 | 1.89326597  |
| C    | -5.76939850 | 0.68086755  | 2.07080028  |
| H    | -3.73326665 | 0.20247139  | 2.57881260  |
| H    | -4.71753967 | -1.21659522 | 2.20117744  |
| H    | -6.34942264 | 0.71566911  | 1.14937456  |
| C    | -5.53352801 | 2.06153839  | 2.65394539  |
| H    | -4.81209260 | 2.59170209  | 2.02162429  |
| H    | -6.45723770 | 2.64715734  | 2.70555640  |
| H    | -5.10720215 | 1.98931409  | 3.66080343  |
| N    | -3.98800537 | -0.14900828 | 0.51860644  |
| Br   | -7.12812135 | -0.34722543 | 3.29848303  |
| C    | -4.08892401 | 1.96743828  | -0.59460487 |
| O    | -4.81894968 | 1.67477966  | -1.47902158 |
| O    | -3.37650742 | 2.61635367  | 0.09272058  |
| C    | -4.77017674 | -1.03816982 | -0.34184180 |
| H    | -5.81895006 | -0.71150967 | -0.44203216 |
| H    | -4.34488179 | -1.05723536 | -1.34901048 |
| H    | -4.78385482 | -2.07698616 | 0.03666078  |

**Cd-Int₄**

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Cd   | -3.42938200 | 0.23465700 | 0.19514100 |
| Cd   | -0.05907000 | 0.57705400 | 0.62913200 |
| Atoms | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| O     | -4.196596 | -1.105417 | -1.496872 |
| O     | -4.088527 | 1.577646  | 1.910352  |
| O     | -2.925714 | 2.033376  | -1.082862 |
| O     | -2.906778 | -1.433941 | 1.633565  |
| O     | -0.629525 | -1.303487 | 1.635382  |
| O     | -0.649351 | 1.994865  | -0.953474 |
| O     | -1.840137 | 1.541006  | 1.866897  |
| O     | -1.963372 | -0.966857 | -1.333644 |
| C     | -3.014168 | -1.398199 | -1.869224 |
| C     | -2.946883 | 1.917462  | 2.336761  |
| C     | -1.763118 | 2.411938  | -1.375779 |
| C     | -1.746911 | -1.805802 | 1.942644  |
| H     | -2.911902 | -2.083173 | -2.726890 |
| H     | -1.691575 | -2.700077 | 2.576698  |
| H     | -1.700300 | 3.228231  | -2.106357 |
| H     | -2.921087 | 2.605378  | 3.196098  |
| C     | 4.745105  | 0.287708  | -0.369326 |
| C     | 4.889427 | -1.234116 | -0.262752 |
| H     | 5.737761  | 0.752261  | -0.364313 |
| H     | 4.252854  | 0.531927  | -1.315892 |
| H     | 3.919284  | -1.706901 | -0.408369 |
| C     | 5.598060  | -1.737840 | 0.978976  |
| H     | 5.669278  | -2.829953 | 0.981233  |
| H     | 6.608814  | -1.323113 | 1.061659  |
| H     | 5.018723  | -1.430898 | 1.859326  |
| N     | 3.981428  | 0.833719  | 0.747571  |
| Br    | 5.951559  | -1.856362 | -1.923806 |
| C     | 2.595698  | 0.742659  | 0.722108  |
| O     | 2.062414  | 0.027131  | -0.187737 |
O  1.90949600  1.35914500  1.60484500
C  4.65124700  1.71423100  1.69116700
H  3.93233900  2.00229700  2.45942200
H  5.50271200  1.20417800  2.16457500
H  5.02600600  2.62704100  1.19746700

Cd-Ts₃
Cd  -1.50986600  -0.00198100  -0.00036500
Cd   1.51071900   0.00200200   0.00018400
O   -1.78629100  -1.33462300  -1.68608400
O   -1.79260900   1.32826600   1.68637600
O   -0.47476200  1.62690200  -1.28702100
O   -0.46878800 -1.62811400   1.28574600
O    1.79157900 -1.68398400   1.33139500
O    1.78554200  1.69009500 -1.32930500
O    0.46755300  1.28747600   1.62542600
O    0.47385500 -1.28617500  -1.62626900
C   -0.62660900 -1.66099800 -2.09787700
C   -0.63393500   1.65843800   2.09784900
C    0.62601100   2.10094400 -1.65762900
C    0.63299000 -2.09835700   1.65846700
H   -0.60576800 -2.34573900 -2.96134000
H    0.61455900 -2.96264300   2.34223700
H    0.60583400  2.96566500 -2.34081800
H   -0.61495300   2.34281200   2.96163700
C    6.94434212 -0.62517487   0.99971155
C    6.45812666 -2.06238455   0.90169556
H    7.63559063 -0.52558277   1.84043222
H    7.48772545 -0.35069912   0.08577619
H    6.48126191 -2.55963979  -0.05121005
|     |   x   |    y   |    z   |
|-----|-------|-------|-------|
| C   | 6.03854159 | -2.81978832 | 2.13413538 |
| H   | 5.00174928  | -2.57195862  | 2.38776047  |
| H   | 6.10896820  | -3.89602943  | 1.96331985  |
| H   | 6.68225582  | -2.56442597  | 2.98083554  |
| N   | 5.80215186  | 0.26629518   | 1.21775276  |
| Br  | 8.95234676  | -2.95711380  | 0.87592993  |
| C   | 4.61810035  | -0.19095934  | 0.70647225  |
| O   | 4.61170585  | -1.41378616  | 0.34221848  |
| O   | 3.60056635  | 0.57860393   | 0.64442756  |
| C   | 6.04719742  | 1.66936306   | 1.48073024  |
| H   | 5.08738748  | 2.17084536   | 1.61298315  |
| H   | 6.64672229  | 1.78083004   | 2.39282994  |
| H   | 6.58784092  | 2.14968773   | 0.64931790  |

**Cd-IntS**

|     |     x   |     y   |     z   |
|-----|--------|--------|--------|
| Cd  | -3.57475500 | 0.22625700 | 0.19386100 |
| Cd  | -0.32679300 | 0.40418500 | 0.40576900 |
| O   | -4.18567000 | -1.10842500 | -1.49645300 |
| O   | -4.05975400 | 1.57351500 | 1.89893700 |
| O   | -2.87765600 | 1.98916900 | -1.06870800 |
| O   | -2.87867800 | -1.41317400 | 1.61094500 |
| O   | -0.60120500 | -1.40350500 | 1.55139200 |
| O   | -0.59985200 | 1.93730100 | -1.08410600 |
| O   | -1.80290500 | 1.55545300 | 1.87469500 |
| O   | -1.95247200 | -0.96340800 | -1.32230900 |
| C   | -3.00041200 | -1.39832800 | -1.86576600 |
| C   | -2.91855100 | 1.91877600 | 2.33237900 |
| C   | -1.73903200 | 2.38033200 | -1.41935700 |
| C   | -1.73672300 | -1.83744100 | 1.90866200 |
| H   | -2.91190200 | -2.08317300 | -2.72687900 |
| Atom | x          | y          | z          |
|------|------------|------------|------------|
| H    | -1.691575  | -2.700077  | 2.576698   |
| H    | -1.700300  | 3.228231   | -2.106357  |
| H    | -2.921087  | 2.605378   | 3.196098   |
| C    | 4.905138   | -0.521299  | -0.215553  |
| C    | 3.855752   | -1.306703  | -1.032244  |
| H    | 5.589422   | -1.184976  | 0.318546   |
| H    | 5.507926   | 0.135666   | -0.848501  |
| H    | 3.974913   | -1.131356  | -2.099180  |
| C    | 3.780185   | -2.787972  | -0.724093  |
| H    | 2.929898   | -3.246360  | -1.241446  |
| H    | 4.709419   | -3.242609  | -1.083713  |
| H    | 3.672499   | -2.963097  | 0.354423   |
| N    | 4.060353   | 0.239049   | 0.718066   |
| Br   | 6.891678   | -1.816879  | -2.564021  |
| C    | 2.764480   | 0.163293   | 0.385271   |
| O    | 2.562178   | -0.667263  | -0.638074  |
| O    | 1.821642   | 0.772770   | 0.937352   |
| C    | 4.590217   | 1.136081   | 1.722518   |
| H    | 3.757466   | 1.584645   | 2.268301   |
| H    | 5.229879   | 0.583380   | 2.420900   |
| H    | 5.188516   | 1.929687   | 1.255040   |

**Rh-HKUST-1**

| Atom | x          | y          | z          |
|------|------------|------------|------------|
| O    | -1.121531  | 1.446272   | -1.497674  |
| O    | -1.121924  | -1.446171  | 1.497523   |
| O    | -1.122918  | 1.498502   | 1.446209   |
| O    | -1.122783  | -1.498416  | -1.446419  |
| O    | 1.121558   | -1.497991  | -1.445691  |
| O    | 1.121424   | 1.497886   | 1.445856   |
| O    | 1.122431   | -1.446563  | 1.498134   |

S169
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| O    | 1.12282200 | 1.44649900 | -1.49791400 |
| C    | 0.00062900  | 1.87415000 | -1.94001800 |
| C    | 0.00013600  | -1.87407500 | 1.94010600 |
| C    | -0.00054000 | 1.94128000  | 1.87286300  |
| C    | -0.00037200 | -1.94125100 | -1.87292700 |
| H    | 0.00034700  | 2.63356300  | -2.72548400 |
| H    | 0.00002100  | -2.72780300 | -2.63122400 |
| H    | -0.00020600 | 2.72785300  | 2.63113900  |
| H    | -0.00033600 | -2.63343000 | 2.72562700  |
| Rh   | 1.54135500  | -0.00007200 | 0.00012400  |
| Rh   | -1.54114400 | 0.00004800  | -0.00013400 |

**Rh-Int**

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| O    | 1.46229400 | -1.46182500 | -1.13833900 |
| O    | -1.46229300 | 1.46183000  | -1.13833600 |
| O    | 1.46190800  | 1.46220400  | -1.13839000 |
| O    | -1.46190900 | -1.46220500 | -1.13839000 |
| O    | -1.46192100 | -1.46220400 | 1.13839000  |
| O    | 1.46192000  | 1.46220100  | 1.13832900  |
| O    | -1.46227300 | 1.46184100  | 1.13838300  |
| O    | 1.46227600  | -1.46183800 | 1.13838000  |
| C    | 1.85720400  | -1.85650600 | 0.00001800  |
| C    | -1.85719300 | 1.85651800  | 0.00002200  |
| C    | 1.85675000  | 1.85695900  | -0.00002600 |
| C    | -1.85674600 | -1.85696700 | -0.00002600 |
| H    | 2.63381900  | -2.63267900 | 0.00002200  |
| H    | -2.63318100 | -2.63332000 | -0.00003600 |
| H    | 2.63319200  | 2.63330500  | -0.00003400 |
| H    | -2.63379500 | 2.63270400  | 0.00002700  |
| Rh   | -0.00000100 | -0.00000100 | 1.20306600  |
Rh       -0.00000200    0.00000000   -1.20305800
C        -0.46852954    1.33715229    3.63963147
C        -0.95892610    0.01120905    4.12504535
H        -1.05500551    1.91178141    2.92433803
H         0.13503371    1.93758380    4.32330465
H       -0.64263815   -0.25468153    5.13833530
C       -2.28151420   -0.58128435    3.69494182
H       -2.24346228   -1.67802264    3.70946219
H       -3.08863229   -0.25987924    4.36570718
H       -2.53017541   -0.26594629    2.67609527
N        0.10980498    0.09184770    3.13128568
C       1.45931199   -0.22847475    3.58130465
H       1.61600967    0.26893909    2.92756194
H       1.65969649    0.08373038    4.62319940

Rh-Int$_1$

O       -2.62557100   -1.21354900   -1.76458300
O       -2.69554900    0.23171200    2.13515100
O       -3.45025800    1.31004000   -0.49440600
O       -1.88279700   -2.29718700    0.86457000
O        0.22841400   -1.46990200    0.60421600
O       -1.33582700    2.14256600   -0.73934100
O        -0.57250700    1.03780000    1.88799000
O        -0.52260600   -0.36050000   -2.03238500
C       -1.56553000   -0.97136500   -2.41080200
C       -1.64610100    0.81844000    2.52534800
C       -2.60149800    2.19907900   -0.78967400
C       -0.62170100   -2.36009200    0.90795900
H       -1.54298700   -1.34324300   -3.44394800
| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| H    | -0.1877600 | -3.30691800 | 1.25165400 |
| H    | -3.01694600 | 3.15534500 | -1.13727500 |
| H    | -1.66164100 | 1.19175200 | 3.55831900 |
| Rh   | -0.44774500 | 0.36506800 | -0.08058000 |
| Rh   | -2.74696400 | -0.52337000 | 0.19510700 |
| C    | 2.65172800 | 0.48443100 | 0.64401700 |
| C    | 2.79206000 | 0.45523800 | -0.82495500 |
| H    | 2.31954600 | -0.41220600 | 1.15654600 |
| H    | 3.31514900 | 1.13713200 | 1.20388800 |
| H    | 3.52893100 | 1.15478300 | -1.21514400 |
| C    | 2.63612100 | -0.79850300 | -1.64417100 |
| H    | 2.28687400 | -0.57058900 | -2.65812800 |
| H    | 3.62935300 | -1.25827900 | -1.70159000 |
| H    | 1.93914700 | -1.50387400 | -1.18683000 |
| N    | 1.60951200 | 1.13611000 | -0.19503800 |
| Br   | 6.11617600 | 0.27545600 | 0.02727600 |
| C    | 1.64365300 | 2.60531600 | -0.21875200 |
| H    | 1.18135800 | 2.96309700 | -1.14314300 |
| H    | 1.07721700 | 2.99209600 | 0.63393600 |
| H    | 2.67802900 | 2.96867800 | -0.16177600 |

**Rh-Ts**

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| O    | -2.64622600 | -1.20531500 | -1.79329600 |
| O    | -2.70807900 | 0.22079400 | 2.13011600 |
| O    | -3.48189700 | 1.30578700 | -0.50960200 |
| O    | -1.88824700 | -2.31097000 | 0.84397700 |
| O    | 0.22851700 | -1.47960700 | 0.59211000 |
| O    | -1.36257000 | 2.13582900 | -0.74705600 |
| O    | -0.58348100 | 1.04003700 | 1.87605900 |
| O    | -0.51497700 | -0.40427300 | -2.04088200 |
C      -1.57293500  -0.98206200  -2.42590800
C      -1.65799600   0.81160800   2.50912000
C      -2.62684500   2.18821900  -0.80047600
C      -0.62812500  -2.36537600   0.88909600
H      -1.55575000  -1.35161200  -3.46012500
H      -0.20053900  -3.31528700   1.23547700
H      -3.02970900   3.14697600  -1.15345200
H      -1.67440400   1.18338300   3.54214200
Rh     -0.44931200   0.37095700  -0.09296600
Rh     -2.78119200  -0.53877500   0.18106300
C      2.73856004   1.00925234   0.64589787
C      3.31888519   0.94900653  -0.71320918
H      2.51625300   0.03176860   1.07620419
H      3.24587100   1.66504610   1.35769594
H      3.70202912   1.87042256  -1.12922385
C      3.09993156  -0.21580193  -1.63993374
H      2.22963623  -0.04394365  -2.28457351
H      3.98118008  -0.34648012  -2.27248145
H      2.93407238  -1.13884807  -1.07696107
N      1.60406940   1.59458704  -0.04631955
Br     5.88193383   0.54584807  -0.09919087
C      1.49601944   3.04226362   0.10573889
H      0.82471400   3.44903961  -0.65511849
H      1.08097535   3.27128216   1.09790510
H      2.47885284   3.52974398   0.01994623

Rh-Int₂
O      -2.62476900  -1.20492100  -1.77286100
O      -2.69538400   0.22798200   2.14443200
O      -3.46565200   1.31422300  -0.49082800
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| O    | -1.87556500 | -2.30234800 | 0.86114600 |
| O    | 0.24068200  | -1.46969400 | 0.60772900 |
| O    | -1.34686400 | 2.14469800  | -0.74083300|
| O    | -0.57425400 | 1.05437300  | 1.89153200 |
| O    | -0.50232900 | -0.38155700 | -2.03448000|
| C    | -1.55591000 | -0.97368100 | 2.52479000 |
| C    | -1.64707100 | 0.82065400  | -2.03448000|
| C    | -2.61159300 | 2.19633700  | -0.78723200|
| C    | -0.61506700 | -2.35634300 | 0.90550500 |
| H    | -1.54298700 | -1.34324300 | -3.44394800|
| H    | -0.18777600 | -3.06918000 | 1.25165400 |
| H    | -3.01694600 | 3.15534500  | -1.13727500|
| H    | -1.66164100 | 1.19175200  | 3.55831900 |
| Rh   | -0.43051700 | 0.38673100  | -0.07755000|
| Rh   | -2.76450600 | -0.53163400 | 0.19707800 |
| C    | 2.59180200  | 0.47161100  | 0.29735600 |
| C    | 3.67649700  | 0.23695500  | -0.75885500|
| H    | 2.25916000  | -0.49867500 | 0.67910400 |
| H    | 3.00361300  | 1.04127700  | 1.14950300 |
| H    | 3.98942100  | 1.17287300  | -1.22112400|
| C    | 3.35489100  | -0.83548200 | -1.77968000|
| H    | 2.40794600  | -0.56235800 | -2.26006900|
| H    | 4.13895700  | -0.92047900 | -2.53998600|
| H    | 3.22498500  | -1.80896700 | -1.29375100|
| N    | 1.52252900  | 1.16516200  | -0.39930200|
| Br   | 5.48698900  | -0.32783400 | 0.20895900 |
| C    | 1.59379300  | 2.59545600  | -0.15795400|
| H    | 0.81718300  | 3.11425300  | -0.72632600|
| H    | 1.48208900  | 2.87020800  | 0.91224100 |
Rh-Int₃

|     | X         | Y         | Z         |
|-----|-----------|-----------|-----------|
| O   | -2.401768| -0.318496| -2.296706|
| O   | -3.073132| -0.932644|  1.775829|
| O   | -3.522308|  1.297091|-0.099713 |
| O   | -1.949588| -2.554693|-0.425196 |
| O   |  0.123283| -1.739885|  0.100124|
| O   | -1.428623|  2.128492|  0.310940|
| O   | -1.001683| -0.075137|  2.243749|
| O   | -0.287436|  0.433050|-1.836079 |
| C   | -1.257323|  0.134421| -2.592412|
| C   | -2.127844| -0.578600|  2.535611|
| C   | -2.682785|  2.209047|  0.141230|
| C   | -0.710620| -2.646267|-0.199635 |
| H   | -1.076618|  0.295138| -3.664500|
| H   | -0.281447| -3.654189|-0.271593 |
| H   | -3.098343|  3.223159|  0.217498|
| H   | -2.303082| -0.726093|  3.610450|
| Rh  | -0.541033|  0.233602|  0.229930|
| Rh  | -2.833082| -0.667620|-0.284843 |
| C   |  2.467296|  0.123221|  0.575652|
| C   |  3.649174|  0.792339|-0.136152 |
| H   |  2.186843| -0.772248|  0.012557|
| H   |  2.770068| -0.208101|  1.584845|
| H   |  3.887231|  1.759066|  0.306456|
| C   |  3.528970|  0.856612|-1.645947 |
| H   |  2.581638|  1.351188|-1.890668 |
| H   |  4.358169|  1.410937|-2.097118 |
| H   |  3.500510| -0.150056|-2.076850 |
|       | x            | y            | z            |
|-------|--------------|--------------|--------------|
| N     | 1.37906600   | 1.08984900   | 0.59649800   |
| Br    | 5.42295000   | -0.27713000  | 0.30922000   |
| C     | 1.06083700   | 3.91904800   | -1.13742000  |
| O     | 1.41070400   | 4.44173500   | -0.15032500  |
| O     | 0.72486000   | 3.47478200   | -2.16429400  |
| C     | 1.38050800   | 1.82261500   | 1.85518000   |
| H     | 2.31869700   | 2.39391000   | 1.97556200   |
| H     | 0.55934200   | 2.54486600   | 1.86906800   |
| H     | 1.28070200   | 1.16648700   | 2.74163400   |
| **Rh-Ts** |       |              |              |
| O     | -2.39692600  | -0.38668000  | -2.28793100  |
| O     | -3.09564100  | -0.92515700  | 1.78672700   |
| O     | -3.52338000  | 1.27435000   | -0.13681600  |
| O     | -1.95724600  | -2.58062400  | -0.36726300  |
| O     | 0.12858900   | -1.75394300  | 0.07453100   |
| O     | -1.44663700  | 2.09514700   | 0.36349500   |
| O     | -0.99900900  | -0.13958800  | 2.24697500   |
| O     | -0.33023500  | 0.47314500   | -1.81803700  |
| C     | -1.27459900  | 0.11779300   | -2.58158700  |
| C     | -2.13718100  | -0.60912200  | 2.54595800   |
| C     | -2.69253000  | 2.18353700   | 0.14950100   |
| C     | -0.71116600  | -2.66782400  | -0.18355600  |
| H     | -1.08413500  | 0.27009700   | -3.65298500  |
| H     | -0.28896400  | -3.67923000  | -0.26007800  |
| H     | -3.10586000  | 3.19811800   | 0.22901300   |
| H     | -2.31059900  | -0.75113400  | 3.62196500   |
| Rh    | -0.54624900  | 0.22098700   | 0.23875400   |
| Rh    | -2.82902800  | -0.68761300  | -0.27196400  |
| C     | 2.39580175   | 0.28216232   | 0.97176849   |
C          3.41674979  -0.15406753  -0.08680023
H          1.94084463  -0.61543778   1.41517316
H          2.95560157   0.78154070   1.77417790
H          3.92731250   0.69938390  -0.52692097
C          2.96557084  -1.14387248  -1.13427500
H          2.12959236  -0.69646399  -1.68088263
H          3.77291584  -1.35965521  -1.84234991
H          2.62360113  -2.07617666  -0.67669931
N          1.36254558   1.21296106   0.46855564
Br         5.00634038  -1.04128672   0.97510202
C          1.97490362   2.50948728  -1.11915120
O          2.61944314   3.31641704  -0.52729990
O          1.42769438   2.07197491  -2.08173969
C          1.04381268   2.16286645   1.54094317
H          1.91939386   2.79324289   1.76325936
H          0.23502848   2.82129623   1.22002810
H          0.73936350   1.65678695   2.46935596

Rh-Int₄
O          2.24000700  -1.28274000  -3.27545000
O          -0.73172500   1.62845300  -3.29570300
O          2.21842000   1.65830800  -3.27557600
O          -0.70681600  -1.29835100  -3.28813200
O          -0.71075300  -1.29340600  -1.00222200
O          2.24493700   1.63972100  -0.98943600
O          -0.66975800   1.68555800  -1.01161400
O          2.21603300  -1.31557200  -0.98992000
C          2.61407800  -1.68212300  -2.13197600
C          -1.08735300   2.03839100  -2.14798300
C          2.61623700   2.03285400  -2.13190000
|  | X       | Y       | Z       |
|---|---------|---------|---------|
| C | -1.093197 | -1.679918 | -2.141569 |
| H | 3.396437  | -2.456359 | -2.135755 |
| H | -1.870563 | -2.457000 | -2.135813 |
| H | 3.395810  | 2.809625  | -2.135811 |
| H | -1.871177 | 2.809024  | -2.135750 |
| Rh| 0.750313  | 0.177397  | -0.891208 |
| Rh| 0.756261  | 0.177320  | -3.360937 |
| C | -0.915227 | 0.621492  | 4.280982  |
| C | -2.179681 | -0.255199 | 4.284888  |
| H | -1.225566 | 1.634557  | 3.976554  |
| H | -0.502622 | 0.696155  | 5.289934  |
| H | -2.098013 | -1.051974 | 3.552450 |
| C | -3.483758 | 0.504333  | 4.165501  |
| H | -3.470698 | 1.001902  | 3.187820  |
| H | -4.347472 | -0.165540 | 4.212971  |
| H | -3.584633 | 1.261740  | 4.952244  |
| N | 0.125873  | 0.122536  | 3.397565  |
| Br| -2.261130 | -1.374330 | 6.072214  |
| C | -0.156224 | 0.258341  | 2.011765  |
| O | -1.339229 | 0.460619  | 1.688473  |
| O | 0.876280  | 0.137983  | 1.244857  |
| C | 1.498161  | 0.176074  | 3.876278  |
| H | 2.143441  | -0.299587 | 3.137445  |
| H | 1.857963  | 1.210407  | 4.026308  |
| H | 1.578983  | -0.362128 | 4.829203  |

**Rh-Ts₃**

|   | X       | Y       | Z       |
|---|---------|---------|---------|
| O | 1.462294 | -1.461825 | -1.138339 |
| O | -1.462293 | 1.461830  | -1.138336 |
| O | 1.461908  | 1.462204  | -1.138390 |
O   -1.46190900  -1.46220500  -1.13839000
O   -1.46192100  -1.46220400  1.13838300
O    1.46192000   1.46220100  1.13832900
O   -1.46227300   1.46184100  1.13838300
O    1.46227600  -1.46183800  1.13838000
C    1.85720400  -1.85650600  0.00001800
C   -1.85719300   1.85651800  0.00002200
C    1.85675000   1.85695900 -0.00002600
C   -1.85674600  -1.85696700 -0.00002600
H    2.63381900  -2.63267900  0.00002200
H   -2.63318100  -2.63332000 -0.00003600
H    2.63319200   2.63330500 -0.00003400
H   -2.63379500   2.63270400  0.00002700
Rh  -0.00000100  -0.00000100  1.20306600
Rh  -0.00000200   0.00000000 -1.20305800
C    0.64525777  -0.88824324  6.91905485
C    1.34430146  -2.16797540  6.50311320
H   -0.41494471  -1.11648533  7.13709696
H    1.09323657  -0.49267298  7.83086402
H    2.32081771  -2.08413914  6.05637650
C    0.63252161  -3.49297311  6.52274375
H   -0.05667581  -3.53357181  5.67188207
H    1.34329736  -4.31861036  6.45043141
H    0.06240796  -3.61181056  7.44912772
N    0.76340822   0.11322583  5.86935833
Br   2.68747761  -2.59759158  8.66449280
C    0.59449181  -0.40069490  4.58119585
O    0.70048478  -1.66459514  4.50723650
O    0.37800173   0.40839896  3.63088737
|  |  |  |  |
|---|---|---|---|
| C | 0.38467455 | 1.47514116 | 6.18677322 |
| H | 0.51523998 | 2.08588592 | 5.29239515 |
| H | -0.66944152 | 1.55062312 | 6.50878308 |
| H | 1.02056882 | 1.86294857 | 6.99267474 |
| Rh-Int\textsubscript{5} |  |  |  |
| O | 2.22787400 | -1.29180900 | -3.27883400 |
| O | -0.70946800 | 1.64035000 | -3.28163000 |
| O | 2.22807000 | 1.64447200 | -3.27833700 |
| O | -0.70904900 | -1.28763700 | -3.28182200 |
| O | -0.69722800 | -1.29963500 | -0.99968800 |
| O | 2.23140400 | 1.64692300 | -0.99570900 |
| O | -0.69824400 | 1.65182700 | -0.99924100 |
| O | 2.23141100 | -1.29385700 | -0.99637700 |
| C | 2.61780200 | -1.68051400 | -2.13706500 |
| C | -1.09276400 | 2.03338900 | -2.13844300 |
| C | 2.61762000 | 2.03321400 | -2.13655500 |
| C | -1.09230800 | -1.68156900 | -2.13873200 |
| H | 3.39643700 | -2.45635900 | -2.13575500 |
| H | -1.87056300 | -2.45700000 | -2.13581300 |
| H | 3.39581000 | 2.80962500 | -2.13581100 |
| H | -1.87117700 | 2.80902400 | -2.13575000 |
| Rh | 0.75974500 | 0.17514900 | -0.90752600 |
| Rh | 0.75864200 | 0.17597700 | -3.35143600 |
| C | -0.93565400 | 0.21580800 | 4.26851700 |
| C | -1.99661300 | -0.04070600 | 3.19118300 |
| H | -0.97771900 | 1.24632300 | 4.65709200 |
| H | -1.05724400 | -0.48118000 | 5.10316000 |
| H | -2.28947000 | -1.09441600 | 3.20231300 |
| C | -3.21423100 | 0.85282800 | 3.23297000 |
| Atoms | X           | Y           | Z           |
|-------|-------------|-------------|-------------|
| H     | -2.92792400 | 1.91134100  | 3.18649900  |
| H     | -3.88575500 | 0.63049700  | 2.39587900  |
| H     | -3.73516600 | 0.64837900  | 4.17584300  |
| N     | 0.29637800  | 0.01271900  | 3.50200100  |
| Br    | -3.24616100 | -1.34401400 | 6.36036700  |
| C     | 0.05588000  | 0.12288600  | 2.17666200  |
| O     | -1.25373900 | 0.17239500  | 1.92307700  |
| O     | 0.93642000  | 0.17556600  | 1.29722300  |
| C     | 1.61694900  | 0.10505000  | 4.08522000  |
| H     | 2.35910100  | -0.07761600 | 3.30536300  |
| H     | 1.78875800  | 1.10269300  | 4.51759000  |
| H     | 1.72359800  | -0.64275000 | 4.87904600  |

**Y-HKUST-1**

| Atoms | X           | Y           | Z           |
|-------|-------------|-------------|-------------|
| O     | -1.49911500 | -1.49387200 | 1.12624000  |
| O     | 1.49892700  | 1.49449900  | 1.12589000  |
| O     | -1.49413400 | 1.49931000  | 1.12595100  |
| O     | 1.49422800  | -1.49875700 | 1.12635600  |
| O     | 1.49367300  | -1.49966100 | -1.12579200 |
| O     | -1.49386100 | 1.49907900  | -1.12620200 |
| O     | 1.49955800  | 1.49339700  | -1.12626100 |
| O     | -1.49922600 | -1.49410900 | -1.12591000 |
| C     | -1.90820300 | -1.90109100 | 0.00022300  |
| C     | 1.90813300  | 1.90119000  | -0.00025800 |
| C     | -1.90125400 | 1.90806900  | -0.00020800 |
| C     | 1.90122400  | -1.90806900 | 0.00032900  |
| H     | -2.68735300 | -2.67771600 | 0.00034300  |
| H     | 2.67745500  | -2.68761300 | 0.00046300  |
| H     | -2.67760600 | 2.68749200  | -0.00038800 |
| H     | 2.68790900  | 2.67718700  | -0.00043200 |
|   | X  | Y  | Z  |
|---|----|----|----|
| Y | -0.00000500 | -0.00017300 | -1.44390400 |
| Y | -0.00000500 | 0.00021800 | 1.44377700 |
| Y-Int0 | 0 | 0 | 0 |
| O | -1.59210600 | 1.59187700 | -1.12926100 |
| O | 1.59202800 | -1.59321000 | -1.12756900 |
| O | -1.59257200 | -1.59272100 | -1.12751700 |
| O | 1.59254400 | 1.59141500 | -1.12936700 |
| O | 1.59245900 | 1.59283600 | 1.12746300 |
| O | -1.59239800 | -1.59147500 | 1.12931900 |
| O | 1.59222300 | -1.59174400 | 1.12926500 |
| O | -1.59212200 | 1.59311000 | 1.12757100 |
| C | -1.99761900 | 1.99745600 | -0.00106800 |
| C | 1.99726900 | -1.99780000 | 0.00107500 |
| C | -1.99772600 | -1.99732200 | 0.00115400 |
| C | 1.99780600 | 1.99728900 | -0.00119000 |
| H | -2.77547300 | 2.77650000 | -0.00150600 |
| H | 2.77607800 | 2.77591600 | -0.00165700 |
| H | -2.77616200 | -2.77578400 | 0.00165200 |
| H | 2.77606300 | -2.77590300 | 0.00151900 |
| Y | 0.00004700 | 0.00091600 | 1.60465300 |
| Y | -0.00003000 | -0.00089400 | -1.60463000 |
| C | 0.58219324 | 1.62524108 | 4.12346050 |
| C | 1.14237446 | -0.34423224 | 4.65209481 |
| H | 1.12125968 | -2.18859742 | 3.36330631 |
| H | -0.02368783 | -2.23253857 | 4.79897030 |
| H | 0.86980554 | -0.11382791 | 5.68655719 |
| C | 2.47403947 | 0.21449224 | 4.20513619 |
| H | 2.48199699 | 1.30997998 | 4.27099161 |
| H | 3.28807365 | -0.17007716 | 4.83292737 |
|   |   |   |   |
|---|---|---|---|
| H | 2.67684608 | -0.06230177 | 3.16514901 |
| N | 0.04012546 | -0.33530729 | 3.69229564 |
| C | -1.27992203 | 0.01718540 | 4.20172302 |
| H | -1.39381277 | 1.10705791 | 4.18420882 |
| H | -2.04585905 | -0.41956688 | 3.55078827 |
| H | -1.45981617 | -0.33538098 | 5.23444065 |
| Y-Int<sub>0</sub> |   |   |   |
| O | -1.59210600 | 1.59187700 | -1.12926100 |
| O | 1.59202800 | -1.59321000 | -1.12756900 |
| O | -1.59257200 | -1.59272100 | -1.12751700 |
| O | 1.59254400 | 1.59141500 | -1.12936700 |
| O | 1.59245900 | 1.59283600 | 1.12746300 |
| O | -1.59239800 | -1.59147500 | 1.12931900 |
| O | 1.59222300 | -1.59174400 | 1.12926500 |
| O | -1.59212200 | 1.59311000 | 1.12757100 |
| C | -1.99761900 | 1.99745600 | -0.00106800 |
| C | 1.99726900 | -1.99780000 | 0.00107500 |
| C | -1.99772600 | -1.99732200 | 0.00115400 |
| C | 1.99780600 | 1.99728900 | -0.00119000 |
| H | -2.77547300 | 2.77650000 | -0.00150600 |
| H | 2.77607800 | 2.77591600 | -0.00165700 |
| H | -2.77616200 | -2.77578400 | 0.00165200 |
| H | 2.77606300 | -2.77590300 | 0.00151900 |
| Y | 0.00004700 | 0.00091600 | 1.60465300 |
| Y | -0.00003000 | -0.00089400 | -1.60463000 |
| C | 0.58219324 | -1.62524108 | 4.12346050 |
| C | 1.14237446 | -0.34423224 | 4.65209481 |
| H | 1.12125968 | -2.18859742 | 3.36330631 |
| H | -0.02368783 | -2.23253857 | 4.79897030 |
| Element | X         | Y          | Z          |
|---------|-----------|------------|------------|
| H       | 0.86980554| -0.11382791| 5.68655719 |
| C       | 2.47403947| 0.21449224 | 4.20513619 |
| H       | 2.48199699| 1.30997998 | 4.27099161 |
| H       | 3.28807365| -0.17007716| 4.83292737 |
| H       | 2.67684608| -0.06230177| 3.16514901 |
| N       | 0.04012546| -0.33530729| 3.69229564 |
| C       | -1.27992203| 0.01718540| 4.20172302 |
| H       | -1.39381277| 1.10705791| 4.18420882 |
| H       | -2.04585905| -0.41956688| 3.55078827 |
| H       | -1.45981617| -0.33538098| 5.23444065 |

**Y-Int**

| Element | X         | Y          | Z          |
|---------|-----------|------------|------------|
| O       | -2.65159700| 1.83253100| 1.61362800 |
| O       | -3.33575800| -1.01455100| -1.83878300|
| O       | -3.61149900| -1.21290600| 1.31370100 |
| O       | -2.36420500| 2.03526500 | -1.58110100|
| O       | -0.23630600| 1.26160300 | -1.49846200|
| O       | -1.47326900| -1.94351500| 1.44410200 |
| O       | -1.20288800| -1.75534000| -1.68480100|
| O       | -0.52620400| 1.06765900| 1.79363300 |
| C       | -1.49277900| 1.80931700| 2.12136400 |
| C       | -2.36064900| -1.72789700| -2.19994800|
| C       | -2.70413100| -1.97347900| 1.74680800 |
| C       | -1.13757000| 2.05697700 | -1.88940100|
| H       | -1.30646300| 2.51446600| 2.94556600 |
| H       | -0.81543000| 2.85573700| -2.57368600|
| H       | -3.01797200| -2.74582800| 2.46814300 |
| H       | -2.52671800| -2.40407900| -3.05173700|
| Y       | -0.36007400| -0.47896800| 0.03598400 |
| Y       | -3.45913400| 0.58996600| -0.15259300|
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | 2.59229300 | -0.80192900 | 1.69424800 |
| C    | 3.14096700  | -1.01903300 | 0.33144000 |
| H    | 1.89620700  | -1.52402200 | 2.13245200 |
| H    | 3.19504100  | -0.26132600 | 2.42227300 |
| H    | 4.12772600  | -0.57998400 | 0.13147600 |
| C    | 2.81499700  | -2.24251700 | -0.49213000 |
| H    | 2.70705200  | -1.96973800 | -1.55374100 |
| H    | 3.64211000  | -2.95348800 | -0.43630700 |
| H    | 1.89773400  | -2.75437500 | -0.16728800 |
| N    | 2.06203400  | -0.01115200 | 0.55882900 |
| Br   | 6.27912300  | 0.37725700  | -0.30450000 |
| C    | 2.52473000  | 1.39382500  | 0.51961500 |
| H    | 2.41297400  | 1.76407800  | -0.50286500 |
| H    | 1.89765100  | 1.98747500  | 1.19298100 |
| H    | 3.58232000  | 1.47866400  | 0.79886600 |
| Y-Ts1 |      |       |      |
| O    | -1.59210600 | 1.59187700  | -1.12926100 |
| O    | 1.59202800  | -1.59321000 | -1.12756900 |
| O    | -1.59257200 | -1.59272100 | -1.12751700 |
| O    | 1.59254400  | 1.59141500  | -1.12936700 |
| O    | 1.59245900  | 1.59283600  | 1.12746300 |
| O    | -1.59239800 | -1.59147500 | 1.12931900 |
| O    | 1.59222300  | -1.59174400 | 1.12926500 |
| O    | -1.59212200 | 1.59311000  | 1.12757100 |
| C    | -1.99761900 | 1.99745600  | -0.00106800 |
| C    | 1.99726900  | -1.99780000 | 0.00107500 |
| C    | -1.99772600 | -1.99732200 | 0.00115400 |
| C    | 1.99780600  | 1.99728900  | -0.00119000 |
| H    | -2.77547300 | 2.77650000  | -0.00150600 |
|     | x        | y        | z        |
|-----|----------|----------|----------|
| H   | 2.77607800 | 2.77591600 | -0.00165700 |
| H   | -2.77616200 | -2.77578400 | 0.00165200 |
| H   | 2.77606300 | -2.77590300 | 0.00151900 |
| Y   | 0.00004700 | 0.00091600 | 1.60465300 |
| Y   | -0.00003000 | -0.00089400 | -1.60463000 |
| C   | -1.17431222 | -0.23228312 | 4.85067767 |
| C   | -0.01817136 | -1.02388428 | 5.32426476 |
| H   | -1.90763837 | -0.80466068 | 4.28087501 |
| H   | -1.64738159 | 0.42781421 | 5.58181600 |
| C   | -0.66089870 | -0.54380670 | 5.40014961 |
| C   | 0.29062036 | 1.68686555 | 4.47697368 |
| H   | 1.19069628 | -2.08896487 | 3.89393557 |
| H   | 0.85138595 | -2.96974188 | 5.40014961 |
| H   | -0.41482832 | -2.79680004 | 4.16712770 |
| N   | -0.14466512 | 0.36988480 | 4.02238343 |
| Br  | -1.04837795 | -2.04577018 | 7.56104753 |
| C   | 0.29062036 | 1.68686555 | 4.47697368 |
| H   | 1.24281661 | 1.94840078 | 4.00799257 |
| H   | -0.46040247 | 2.43568142 | 4.18659919 |
| H   | 0.40517845 | 1.71667852 | 5.5710242 |

**Y-Int$_2$**

|     | x        | y        | z        |
|-----|----------|----------|----------|
| O   | -1.71520500 | 1.66933300 | -2.99719000 |
| O   | 1.56753900 | -1.40258500 | -2.98774000 |
| O   | -1.71698000 | -1.40570500 | -2.99461400 |
| O   | 1.57054200 | 1.67210500 | -2.99995800 |
| O   | 1.52145200 | 1.72710400 | -0.73737300 |
| O   | -1.66323100 | -1.46429800 | -0.73258800 |
| O   | 1.53334400 | -1.46268200 | -0.72474100 |
| O   | -1.67043700 | 1.73103900 | -0.73460100 |
| Element | X              | Y              | Z              |
|---------|----------------|----------------|----------------|
| C       | -2.08908100    | 2.10410300     | -1.87143500    |
| C       | 1.94593300     | -1.83737400    | -1.86386500    |
| C       | -2.08826200    | -1.83947300    | -1.86852800    |
| C       | 1.94341200     | 2.10352200     | -1.87335200    |
| H       | -2.84808600    | 2.90872800     | -1.87353900    |
| H       | 2.70346500     | 2.90814400     | -1.87369000    |
| H       | -2.84877500    | -2.64355600    | -1.87038100    |
| H       | 2.70345000     | -2.64367500    | -1.87051400    |
| Y       | -0.07691200    | 0.13444100     | -0.16404700    |
| Y       | -0.07299100    | 0.13232800     | -3.59076300    |
| C       | -0.46058700    | -0.82341900    | 3.03870400     |
| C       | 0.75392500     | -1.47382900    | 3.72215600     |
| H       | -1.02615800    | -1.61510900    | 2.52396000     |
| H       | -1.12906000    | -0.40416900    | 3.81209200     |
| H       | 1.40162100     | -0.71974600    | 4.16930700     |
| C       | 1.52861800     | -2.45666400    | 2.86775300     |
| H       | 1.87189600     | -1.94388000    | 1.96128300     |
| H       | 2.40069300     | -2.85377700    | 3.39737100     |
| H       | 0.89311000     | -3.29558600    | 2.56153000     |
| N       | -0.03798500    | 0.19131700     | 2.09585700     |
| Br      | 0.10810300     | -2.49829400    | 5.44500200     |
| C       | 0.26138000     | 1.46299900     | 2.73818800     |
| H       | 0.49955700     | 2.22441900     | 1.98140600     |
| H       | -0.59641500    | 1.84503200     | 3.32756400     |
| H       | 1.13047700     | 1.43143000     | 3.42357500     |
| Y-Int   |               |                |                |
| O       | -1.36212700    | 1.90248100     | -3.02957700    |
| O       | 2.32871500     | -0.68217400    | -2.97585700    |
| O       | -0.78622100    | -1.26765800    | -3.07764000    |
O   1.77067000  2.45467100  -2.94931200
O   1.82929400  2.43740800  -0.68526100
O  -0.82509600 -1.25037000  -0.80964100
O   2.36670600 -0.72655900  -0.70948100
O  -1.28843200  2.00231800  -0.76570300
C  -1.78989200  2.25983800  -1.89659300
C   2.80128500 -1.02931000  -1.85937200
C  -1.12884200 -1.71179200  -1.94556600
C   2.12253500  2.90392000  -1.82586300
H  -2.71088300  2.86481200  -1.88925800
H   2.76050900  3.80311600  -1.83294600
H  -1.77197500  2.60719600  -1.94799600
H   3.70003000 -1.66832000  -1.89165500
Y   0.49402700  0.60459800  -0.19210700
Y   0.48644000  0.60371100  -3.57053700
C  -1.19913800 -0.60502500   2.45344200
C  -0.70362100 -1.73531200   3.36610100
H  -1.72178200 -1.06055800  -1.60229800
H  -1.93729800  0.00374100   3.00587800
H  -0.11481900  1.35093600   4.19668700
C  -0.01472100 -2.88184700   2.65685000
H   0.87797100 -2.49038600   2.15320900
H   0.29404100 -3.66812000   3.35484800
H  -0.67213400 -3.31656100   1.89352500
N  -0.09373900  0.21213700   1.98015300
Br  -2.35565300 -2.53499300   4.41022300
C   3.46568800 -0.35505800   2.59564800
O   3.39591400 -1.37778500   3.16116100
O   3.56408400  0.67449200   2.05177700
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 0.29136000 | 1.22339500 | 2.94955400 |
| H       | 0.77788700 | 0.82344000 | 3.86074900 |
| H       | 1.01403700 | 1.92767600 | 2.51131300 |
| H       | -0.57091300| 1.82306500 | 3.29782200 |
| Y-Ts₂   |            |            |            |
| O       | -1.82928617| 1.31390621 | -1.12758345|
| O       | 1.84781305 | -1.28656118| -1.1290616 |
| O       | -1.29083032| -1.82465928| -1.16134178|
| O       | 1.30940235 | 1.85204007 | -1.09530101|
| O       | 1.29070904 | 1.82474899 | 1.16128700 |
| O       | -1.30923882| -1.85207909| 1.09525291 |
| O       | 1.82938804 | -1.31376060| 1.12758920 |
| O       | -1.84787969| 1.28644151 | 1.12900517 |
| C       | -2.30675550| 1.63069375 | 0.00087712 |
| C       | 2.30647782 | -1.63109724| -0.00087844|
| C       | -1.63084303| -2.30626048| -0.04139388|
| C       | 1.63093685 | 2.30623675 | 0.04139388 |
| H       | -3.20519806| 2.26690712 | 0.00121069 |
| H       | 2.26619416 | 3.20521147 | 0.05752239 |
| H       | -2.26629015| -3.20510072| -0.05752769|
| H       | 3.20568749 | -2.26622435| -0.0018596 |
| Y       | -0.01316493| -0.01948194| 1.60448052 |
| Y       | 0.01318688 | 0.01950101 | -1.60445802|
| C       | -1.29980536| -0.31584378| 4.79691211 |
| C       | -0.81748945| -1.68081825| 5.29694428 |
| H       | -2.19120147| -0.45710260| 4.16713856 |
| H       | -1.60504220| 0.28709548 | 5.66365629 |
| H       | -0.02618652| -1.57385935| 6.03737112 |
| C       | -0.44916645| -2.68842798| 4.22968714 |
|   | X        | Y        | Z        |
|---|----------|----------|----------|
| H| 0.43003704 | -2.31464049 | 3.69033547 |
| H| -0.18278683 | -3.65323178 | 4.67281330 |
| H| -1.26169766 | -2.82783246 | 3.51113138 |
| N| -0.25015076 | 0.38779464 | 4.05065358 |
| Br| -2.35850709 | -2.46165281 | 6.45240637 |
| C| 1.67816525 | 0.80565905 | 4.76967146 |
| O| 1.68161180 | 1.37285119 | 5.82140788 |
| O| 2.14117696 | 0.05340724 | 3.96670367 |
| C| -0.63437123 | 1.80584710 | 4.00164483 |
| H| -0.76858697 | 2.17362907 | 4.99744729 |
| H| 0.13543482 | 2.36733149 | 3.51478356 |
| H| -1.54963217 | 1.90876811 | 3.45703058 |

**Y-Int**

| O| 3.51494600 | 2.21765600 | 0.06133700 |
| O| 4.15675000 | -2.24531800 | 0.46709800 |
| O| 3.93676500 | -0.24239700 | -1.99289100 |
| O| 3.72978000 | 0.21766900 | 2.50958600 |
| O| 1.49658600 | -0.16340500 | 2.44064400 |
| O| 1.69570900 | -0.57682500 | -2.05624700 |
| O| 1.91701600 | -2.57224300 | 0.39736400 |
| O| 1.27351700 | 1.88627600 | -0.01990800 |
| C| 2.31685500 | 2.60207400 | -0.03046600 |
| C| 3.11941400 | -2.96184500 | 0.48259300 |
| C| 2.84019600 | -0.44946300 | -2.58227000 |
| C| 2.59179800 | 0.07400700 | 3.03248300 |
| H| 2.15846600 | 3.68897100 | -0.13731800 |
| H| 2.54582500 | 0.16121100 | 4.13170800 |
| H| 2.87693500 | -0.52280900 | -3.68310100 |
| H| 3.26426200 | -4.05064700 | 0.58674000 |
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| Y    | 1.05657800 | -0.43908400 | 0.18095700 |
| Y    | 4.38096800  | 0.07200800  | 0.26943700 |
| C    | -4.57407600 | 0.80941300  | 0.28031400 |
| C    | -5.30413500 | 0.40655900  | -1.00501800 |
| H    | -4.90452200 | 1.80599200  | 0.59545100 |
| H    | -4.82395100 | 0.09334000  | 1.06868600 |
| H    | -5.07781200 | -0.63164000 | -1.24394300 |
| C    | -5.10787400 | 1.33181000  | -2.19054600 |
| H    | -4.04021900 | 1.35210600  | -2.44367800 |
| H    | -5.66097500 | 0.97953600  | -3.06646100 |
| H    | -5.43240400 | 2.35336800  | -1.96103500 |
| N    | -3.13153700 | 0.84406900  | 0.07863000 |
| Br   | -7.32783000 | 0.33212400  | -0.56177500 |
| C    | -2.43595400 | -0.37354200 | 0.13070000 |
| O    | -3.07556900 | -1.43094800 | 0.19561000 |
| O    | -1.13586200 | -0.27501400 | 0.08919900 |
| C    | -2.46619300 | 2.13787900  | 0.12115200 |
| H    | -1.40527500 | 2.01031100  | -0.08905700 |
| H    | -2.89511300 | 2.81757900  | -0.62814300 |
| H    | -2.57047300 | 2.61257500  | 1.11090200 |

**Y-Ts<sub>3</sub>**

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| O    | 3.58164900 | 2.37304500 | -0.12739300 |
| O    | 4.21863400 | -2.09348700 | 0.28360100 |
| O    | 3.99216400 | -0.06012800 | -2.17874500 |
| O    | 3.81808000 | 0.33661400  | 2.33545900 |
| O    | 1.57845500 | -0.02498000 | 2.26960100 |
| O    | 1.75662700 | -0.41061600 | -2.22551900 |
| O    | 1.97947800 | -2.41494400 | 0.20393700 |
| O    | 1.33656200 | 2.04561100  | -0.20900000 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 2.38215600 | 2.75960700 | -0.21549800|
| C    | 3.18150200 | -2.80705600| 0.30184400 |
| C    | 2.89934600 | -0.27810100| -2.76281500|
| C    | 2.67322900 | 0.21138100 | 2.85744200 |
| H    | 2.22369400 | 3.84392700 | -0.32197900|
| H    | 2.61105300 | 0.31616700 | 3.94704700 |
| H    | 2.94216300 | -0.36785300| -3.86776200|
| H    | 3.32949000 | -3.89569100| 0.40207900 |
| Y    | 1.14670300 | -0.27362400| 0.01131800 |
| Y    | 4.43976100 | 0.22451600 | 0.09101600 |
| C    | -4.55087900| 0.72394200 | -0.54486500|
| C    | -5.00623700| -0.65086800| -0.07158200|
| H    | -4.80474700| 0.84638600 | -1.61063800|
| H    | -5.08295700| 1.49893600 | 0.00948100 |
| H    | -5.00334900| -0.85270200| 0.98660500 |
| C    | -5.45667600| -1.70914200| -1.04671700|
| H    | -4.58069300| -2.14572900| -1.54001700|
| H    | -6.00636500| -2.50107200| -0.53284200|
| H    | -6.11371700| -1.27626100| -1.80585500|
| N    | -3.11390900| 0.90833700 | -0.33946400|
| Br   | -7.45013600| 0.13094000 | 0.47280900 |
| C    | -2.37171000| -0.22600700| -0.14767300|
| O    | -3.02851700| -1.30049700| -0.01028200|
| O    | -1.09299400| -0.14143000| -0.10286400|
| C    | -2.54475900| 2.20773500 | -0.63710800|
| H    | -1.48091700| 2.20074800 | -0.39723200|
| H    | -2.66681800| 2.46339100 | -1.70175000|
| H    | -3.04373800| 2.98126800 | -0.03877500|
| Y-Int₅ |       |       |       |
|-------|-------|-------|-------|
| O     | 3.51051300 | 2.21695600 | 0.05368500 |
| O     | 4.15326600 | -2.24369000 | 0.48542200 |
| O     | 3.94554200 | -0.22469600 | -2.00220500 |
| O     | 3.72747700 | 0.18506000 | 2.50640800 |
| O     | 1.49466800 | -0.18081800 | 2.44379900 |
| O     | 1.71149200 | -0.60693900 | -2.04894600 |
| O     | 1.91523500 | -2.56957100 | 0.43629300 |
| O     | 1.26725300 | 1.89385500 | 0.04344300 |
| C     | 2.31128500 | 2.60562300 | -0.01318000 |
| C     | 3.11814600 | -2.96263200 | 0.50361100 |
| C     | 2.84563600 | -0.45230900 | -2.58403400 |
| C     | 2.59164600 | 0.05652000 | 3.03598700 |
| H     | 2.15846600 | 3.68897100 | -0.13731800 |
| H     | 2.54582500 | 0.16121100 | 4.13170800 |
| H     | 2.87693500 | -0.52280900 | -3.68310100 |
| H     | 3.26426200 | -4.05064700 | 0.58674000 |
| Y     | 1.08384800 | -0.44221500 | 0.19737000 |
| Y     | 4.34241100 | 0.06968200 | 0.25268900 |
| C     | -4.24954800 | 1.26326000 | -1.36207900 |
| C     | -4.50603900 | -0.24984800 | -1.29475100 |
| H     | -4.26254100 | 1.64689000 | -2.39433900 |
| H     | -4.99627700 | 1.80083900 | -0.76954300 |
| H     | -5.05060900 | -0.49082700 | -0.38016400 |
| C     | -5.18992700 | -0.86352400 | -2.49603500 |
| H     | -4.65377400 | -0.63076900 | -3.42364300 |
| H     | -5.25608500 | -1.95242100 | -2.38439900 |
| H     | -6.20563200 | -0.45314500 | -2.53543000 |
| N     | -2.89067700 | 1.35424700 | -0.81336000 |
| Atoms  | X         | Y         | Z         |
|--------|-----------|-----------|-----------|
| Br     | -7.57348300 | 1.14918000 | -0.34565700 |
| C      | -2.30083600 | 0.14980700 | -0.78684400 |
| O      | -3.14043600 | -0.82337900 | -1.14098900 |
| O      | -1.11640300 | -0.09585700 | -0.46662500 |
| C      | -2.21163300 | 2.61500700 | -0.58741900 |
| H      | -1.18144500 | 2.42739700 | -0.27987600 |
| H      | -2.20597500 | 3.20929100 | -1.51070800 |
| H      | -2.73465300 | 3.18528000 | 0.18899800 |

**V-HKUST-1**

| Atoms  | X         | Y         | Z         |
|--------|-----------|-----------|-----------|
| V      | 0.00009800 | 0.00002700 | -1.29144900 |
| V      | -0.00010400 | -0.00002600 | 1.29145000 |
| O      | -0.00274900 | 2.02630000 | -1.12197800 |
| O      | 0.00292700 | -2.02625400 | -1.12206000 |
| O      | -2.05682600 | -0.00279800 | -1.12900300 |
| O      | 2.05699200 | 0.00284100 | -1.12869900 |
| O      | 2.05682000 | 0.00276300 | 1.12899100 |
| O      | -2.05699600 | -0.00280800 | 1.12868700 |
| O      | 0.00272600 | -2.02629900 | 1.12198800 |
| O      | -0.00288500 | 2.02625500 | 1.12207100 |
| C      | -0.00345000 | 2.61161200 | 0.00005800 |
| C      | 0.00346200 | -2.61161100 | -0.00004800 |
| C      | -2.62896600 | -0.00338300 | -0.00020200 |
| C      | 2.62896100 | 0.00337900 | 0.00019000 |
| H      | -0.00505200 | 3.70939300 | 0.00008100 |
| H      | 3.72867800 | 0.00506100 | 0.00027500 |
| H      | -3.72868300 | -0.00505600 | -0.00028600 |
| H      | 0.00507500 | -3.70939200 | -0.00007000 |

**V-Int**

| Atoms  | X         | Y         | Z         |
|--------|-----------|-----------|-----------|
| V      | 0.00009800 | 0.00002700 | -1.29549400 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| V    | -0.000102 | -0.000026 | 1.295496  |
| O    | -0.001281 | 2.035277  | -1.122270 |
| O    | 0.001459  | -2.035231 | -1.122352 |
| O    | -2.066170 | -0.001345 | -1.129087 |
| O    | 2.066340  | 0.001390  | -1.128781 |
| O    | 2.066166  | 0.001314  | 1.129081  |
| O    | -2.066340 | -0.001360 | 1.128775  |
| O    | 0.001258  | -2.035274 | 1.122274  |
| O    | -0.001423 | 2.035230  | 1.122357  |
| C    | -0.001610 | 2.621864  | 0.000056  |
| C    | 0.001615  | -2.621864 | -0.000051 |
| C    | -2.640471 | -0.001549 | -0.000200 |
| C    | 2.640469  | 0.001545  | 0.000194  |
| H    | -0.002451 | 3.719411  | 0.000079  |
| H    | 3.739742  | 0.002523  | 0.000279  |
| H    | -3.739744 | -0.002517 | -0.000282 |
| H    | 0.002461  | -3.719410 | -0.000072 |
| C    | -0.481180 | 1.099482  | -3.807416 |
| C    | 0.864427  | 0.694859  | -4.317182 |
| H    | -0.569277 | 1.854370  | -3.027557 |
| H    | -1.321493 | 1.060908  | -4.503549 |
| H    | 0.882687  | 0.367186  | -5.361111 |
| C    | 2.149810  | 1.318590  | -3.823191 |
| H    | 2.982479  | 0.606783  | -3.890165 |
| H    | 2.408561  | 2.202172  | -4.420684 |
| H    | 2.050647  | 1.624021  | -2.776196 |
| N    | 0.125693  | -0.168425 | -3.397803 |
| C    | -0.463626 | 1.380250  | -3.955072 |
| H    | 0.282918  | -2.182515 | -3.943056 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| H       | -1.31056586 | -1.68869788 | -3.33156384 |
| H       | -0.82409563  | -1.25518041  | -4.99307766 |
| V-Int₁  |         |         |         |
| V       | 0.62119000   | 0.42404100   | -3.21747000 |
| V       | 0.63757400   | 0.45776000   | -0.35797900 |
| O       | 0.61630300   | 2.56318300   | -3.17962200 |
| O       | 0.61477000   | -1.68482600  | -3.17982200 |
| O       | -1.45595200  | 0.43220700   | -3.06415600 |
| O       | 2.68888000   | 0.43752400   | -2.97995800 |
| O       | 2.75774100   | 0.46749300   | -0.70757900 |
| O       | -1.43315300  | 0.51489400   | -0.79706700 |
| O       | 0.69346500   | -1.53496000  | -0.93092500 |
| O       | 0.69339500   | 2.40035800   | -0.94256200 |
| C       | 0.64685700   | 3.06114200   | -2.02511700 |
| C       | 0.64990300   | -2.17836400  | -2.01772100 |
| C       | -2.00368900  | 0.46353100   | -1.92409100 |
| C       | 3.27816100   | 0.44950000   | -1.85894200 |
| H       | 0.63563600   | 4.16058200   | -1.91684400 |
| H       | 4.37782900   | 0.44369400   | -1.91664400 |
| H       | -3.10165700  | 0.43865400   | -1.91720500 |
| H       | 0.64054800   | -3.27823900  | -1.91699500 |
| C       | -0.62545900  | 0.34557300   | 2.47325500  |
| C       | -0.52526300  | -1.11416700  | 2.32454500  |
| H       | -1.35557500  | 0.88835200   | 1.87762700  |
| H       | -0.38985400  | 0.77139500   | 3.44435200  |
| H       | -0.16314700  | -1.61414100  | 3.22044000  |
| C       | -1.47838400  | -1.93648600  | 1.49962700  |
| H       | -0.99735300  | -2.85334800  | 1.13824800  |
| H       | -2.30847400  | -2.20619200  | 2.16261800  |
|   | X          | Y          | Z          |
|---|------------|------------|------------|
| H | -1.86256400| -1.37990900| 0.64229100 |
| N | 0.51357000 | -0.23531900| 1.67916900 |
| Br| -2.22812800| -1.15736600| 5.29014900 |
| C | 1.82239100 | -0.24468600| 2.35596600 |
| H | 2.42346900 | -1.06542100| 1.95209400 |
| H | 2.34914000 | 0.69750800 | 2.16546900 |
| H | 1.70950800 | -0.37657500| 3.43988200 |

| V-Ts₁ |
| V   | 0.00009800 | 0.00002700 | -1.29549400 |
| V   | -0.00010200| -0.00002600| 1.29549600  |
| O   | -0.00128100| 2.03527700 | -1.12227000 |
| O   | 0.00145900 | -2.03523100| -1.12235200 |
| O   | -2.06617000| -0.00134500| -1.12908700 |
| O   | 2.06634000 | 0.00139000 | -1.12878100 |
| O   | 2.06616600 | 0.00131400 | 1.12908100  |
| O   | -2.06634000| -0.00136000| 1.12877500  |
| O   | 0.00125800 | -2.03527400| 1.12227400  |
| O   | -0.00142300| 2.03523000 | 1.12235700  |
| C   | -0.00161000| 2.62186400 | 0.00005600  |
| C   | 0.00161500 | -2.62186400| -0.00005100 |
| C   | -2.64047100| -0.00154900| -0.00020000 |
| C   | 2.64046900 | 0.00154500 | 0.00019400  |
| H   | -0.00245100| 3.71941100 | 0.00007900  |
| H   | 3.73974200 | 0.00252300 | 0.00027900  |
| H   | -3.73974400| -0.00251700| -0.00028200 |
| H   | 0.00246100 | -3.71941000| -0.00007200 |
| C   | -0.60160803| 0.39446040 | 4.32476084  |
| C   | -0.62580655| -1.01709907| 4.76577458  |
| H   | -1.47513923| 0.69974234 | 3.74700261  |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -0.32775074 | 1.13739955 | 5.07784115 |
| H    | 0.13881135  | -1.33125196 | 5.46258332 |
| C    | -1.42422514 | -2.07693807 | 4.05668579 |
| H    | -0.81604525 | -2.58063352 | 3.29581932 |
| H    | -1.76219212 | -2.82171566 | 4.78116974 |
| H    | -2.30072957 | -1.6450971  | 3.56555712 |
| N    | 0.48479094  | -0.10867684 | 3.50290872 |
| Br   | -2.08523694 | -0.77867061 | 6.98433005 |
| C    | 1.81389507  | 0.24971104  | 3.98829966 |
| H    | 2.56800072  | -0.38626717 | 3.51726032 |
| H    | 2.02437752  | 1.29644849  | 3.72534957 |
| H    | 1.88386444  | 0.14591856  | 5.08159302 |

**V-Int**

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| V    | 0.63922700 | 0.44405600 | -3.23640500 |
| V    | 0.63125000 | 0.44145400 | -0.42657200 |
| O    | 0.64510400 | 2.57304400 | -3.16693700 |
| O    | 0.63377300 | -1.68862700 | -3.16538700 |
| O    | -1.45478700 | 0.44695200 | -3.04405600 |
| O    | 2.73170200 | 0.43637200 | -3.04250200 |
| O    | 2.73574600 | 0.46444000 | -0.76394400 |
| O    | -1.46030300 | 0.41174100 | -0.76604700 |
| O    | 0.66325000 | -1.55632100 | -0.90671900 |
| O    | 0.61524200 | 2.43720600 | -0.90780700 |
| C    | 0.63243300 | 3.06349000 | -2.00870000 |
| C    | 0.64559600 | -2.18155400 | -2.00970500 |
| C    | -2.00485800 | 0.43240700 | -1.90902700 |
| C    | 3.28034700 | 0.44856300 | -1.90636300 |
| H    | 0.63563600 | 4.16058200 | -1.91684400 |
| H    | 4.37782900 | 0.44369400 | -1.91664400 |
H  -3.10165700  0.43865400  -1.91720500
H   0.64054800 -3.27823900  -1.91699500
C  -0.60005300  0.38142400  2.33057600
C  -0.70287700 -0.99940600  2.99616700
H  -1.48021700  0.53286800  1.69647800
H  -0.60626800  1.16141900  3.11015700
H   0.18628900 -1.22498300  3.58397000
C  -1.07526700 -2.13783900  2.07014200
H  -0.32690800 -2.19331400  1.27054600
H  -1.10266100 -3.09592900  2.60146400
H  -2.04980700 -1.96014400  1.60278300
N   0.60720300  0.46607000  1.52449200
Br -2.15102300 -0.90718200  4.52354500
C   1.79593900  0.75926400  2.30912400
H   2.65864400  0.86621300  1.64490100
H   1.68032000  1.70193600  2.87803700
H   2.04331900 -0.02837200  3.04482200
V-Int₃
V   3.20789700 -1.74440200  0.71516800
V   0.60780400  0.04677200  0.51342400
O   3.84134100  0.07904900  1.20173500
O   1.77485300 -3.02524300  0.20078200
O   3.47339100 -1.25435000 -1.33774900
O   2.77209600 -2.12001700  2.78047800
O   0.95533600 -0.82831000  2.47327500
O   1.58278700 -0.00811300 -1.37486300
O  -0.21560300 -1.97554500 -0.00047200
O   2.13364100  1.55800000  1.14077000
C   3.33039400  1.24302000  1.31523900

S199
C  0.52373100 -2.98155800 -0.04796500
C  2.60844500 -0.50818500 -1.89844900
C  1.70823900 -1.54701600  3.17635000
H  4.06754800  2.02157400  1.59876100
H  1.40240300 -1.68435100  4.24118100
H  2.75896200 -0.25726200 -2.97449000
H  0.09380400 -3.96318800 -0.33206000
C -1.72798500  0.68880700 -1.26747400
C -3.18599400  1.11231500 -1.03483300
H -1.67709700 -0.40544900 -1.20236900
H -1.42193100  0.96488400 -2.29153600
H -3.26559500  2.18380700 -0.85766100
C -3.93712100  0.29163300 -0.00334600
H -3.37433500  0.30372300  0.93738400
H -4.94223800  0.68461400  0.18196800
H -4.01907600 -0.75265800 -0.32445900
N -0.85904300  1.30059200 -0.26761700
Br -4.28453800  0.94184300 -2.83997000
C -1.81500100  2.17527700  2.06365300
O -1.44732400  1.24869600  2.68720400
O -2.26506000  3.18735900  1.66650200
C -0.39804900  2.60290900 -0.73784200
H -1.21988700  3.33159900 -0.86714500
H  0.30376300  3.03782500 -0.01685900
H  0.12710500  2.52791700 -1.71119600

V-Ts$_2$
V  3.23995600 -1.18983100  0.08411700
V  0.67178800  0.53789500 -0.09056100
O  3.92241600  0.60220800  0.57958200
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| O    | 1.83566500 | -2.52006900 | -0.42457200 |
| O    | 3.41959600  | -0.67081400 | -1.94802400 |
| O    | 2.72201900  | -1.50552000 |  2.09871200  |
| O    | 0.87374800  | -0.20798700 |  1.91395900  |
| O    | 1.54469700  |  0.60796500 | -2.06035200  |
| O    | -0.10772900 | -1.41305800 | -0.66539300  |
| O    | 2.19166600  |  2.03651500 |  0.46541200  |
| C    | 3.38782100  |  1.76458900 |  0.67158600  |
| C    | 0.59214900  | -2.45017800 | -0.69267900  |
| C    | 2.57979200  |  0.07832500 | -2.53966400  |
| C    | 1.67063000  | -0.94776800 |  2.54575700  |
| H    | 4.08712300  |  2.57335900 |  0.96531400  |
| H    | 1.42197800  | -1.13256600 |  3.60773400  |
| H    | 2.77853700  |  0.29452300 | -3.60793700  |
| H    | 0.11337900  | -3.41140300 | -0.96550700  |
| C    | -2.50705200 |  0.64162400 | -0.69602600  |
| C    | -3.21059600 |  0.09274500 |  0.55064700  |
| H    | -2.18271800 | -0.19751200 | -1.31682500  |
| H    | -3.26001200 |  1.20739300 | -1.26139700  |
| H    | -3.86185200 |  0.82725400 |  1.00397300  |
| C    | -2.40532500 | -0.67550800 |  1.56904400  |
| H    | -1.68712900 |  0.01098000 |  2.02971800  |
| H    | -3.05743100 | -1.06497800 |  2.35782400  |
| H    | -1.85385700 | -1.50082000 |  1.11404000  |
| N    | -1.30501200 |  1.52057300 | -0.51313600  |
| Br   | -4.65973000 | -1.24843900 | -0.24469800  |
| C    | -1.45533585 |  3.14599261 |  0.96179242  |
| O    | -0.86522916 |  2.73451356 |  1.96831455  |
| O    | -2.25696552 |  3.96607440 |  0.48043219  |
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| C       | -1.05018800 | 2.15886100 | -1.83385600 |
| H       | -1.91663100 | 2.76709300 | -2.13721700 |
| H       | -0.17857800 | 2.80661500 | -1.75119100 |
| H       | -0.86537800 | 1.38994400 | -2.58971900 |
| V       | -0.82190600 | -0.65992400 | -3.97320300 |
| V       | -0.86806200 | -0.66621900 | -1.11619100 |
| O       | -0.83485300 | 1.40842600 | -3.83950100 |
| O       | -0.82591300 | -2.72444300 | -3.77810500 |
| O       | -2.97503000 | -0.66592800 | -3.92932100 |
| O       | 1.30216300  | -0.63902200 | -3.98732600 |
| O       | 1.11762200  | -0.74264900 | -1.74394100 |
| O       | -2.85236800 | -0.69815800 | -1.68456000 |
| O       | -0.91501500 | -2.78139200 | -1.50233000 |
| O       | -0.93617300 | 1.39544500 | -1.56699800 |
| C       | -0.87710900 | 1.95148500 | -2.69429700 |
| C       | -0.86563100 | -3.29963700 | -2.64883800 |
| C       | -3.48930100 | -0.67963800 | -2.77938800 |
| C       | 1.77836200  | -0.68348500 | -2.81509600 |
| H       | -0.86016200 | 3.04480500 | -2.69842200 |
| H       | 2.88203100  | -0.67208300 | -2.69822200 |
| H       | -4.59745500 | -0.67712300 | -2.69878300 |
| H       | -0.85525000 | -4.39401600 | -2.69857300 |
| C       | 1.96702900  | 0.04459600  | 3.49199000  |
| C       | 1.82911300  | 1.47960400  | 3.99369000  |
| H       | 2.82835800  | 0.05125400  | 2.80732300  |
| H       | 2.20956700  | -0.61801000 | 4.32997300  |
| H       | 1.26236600  | 2.07180600  | 3.27994500  |
| C       | 3.14971400  | 2.13141500  | 4.36091900  |
| Atom | X    | Y    | Z    |
|------|------|------|------|
| H    | 3.75835600 | 2.21388400 | 3.44943800 |
| H    | 2.99980000 | 3.13705300 | 4.77244300 |
| H    | 3.70421100 | 1.53654200 | 5.09635600 |
| N    | 0.80542500 | -0.46968100 | 2.79587300 |
| Br   | 0.60048900 | 1.51682900 | 5.67063800 |
| C    | 0.64506100 | -0.04792000 | 1.45929100 |
| O    | 1.34017200 | 0.89622600 | 1.05572300 |
| O    | -0.24757000 | -0.71155500 | 0.78738100 |
| C    | 0.18224100 | -1.68375200 | 3.29628900 |
| H    | -0.73320300 | -1.86504200 | 2.73088500 |
| H    | 0.83502200 | -2.56958200 | 3.18362600 |
| H    | -0.06646000 | -1.56329300 | 4.35930000 |

**V-Ts₃**

| Atom | X    | Y    | Z    |
|------|------|------|------|
| V    | 0.00009800 | 0.00002700 | -1.29549400 |
| V    | -0.00010200 | -0.00002600 | 1.29549600 |
| O    | -0.00128100 | 2.03527700 | -1.12227000 |
| O    | 0.00145900 | -2.03523100 | -1.12235200 |
| O    | -2.06617000 | -0.00134500 | -1.12908700 |
| O    | 2.06634000 | 0.00139000 | -1.12878100 |
| O    | 2.06616600 | 0.00131400 | 1.12908100 |
| O    | -2.06634000 | -0.00136000 | 1.12877500 |
| O    | 0.00125800 | -2.03527400 | 1.12227400 |
| O    | -0.00142300 | 2.03523000 | 1.12235700 |
| C    | -0.00161000 | 2.62186400 | 0.00005600 |
| C    | 0.00161500 | -2.62186400 | -0.00005100 |
| C    | -2.64047100 | -0.00154900 | -0.00020000 |
| C    | 2.64046900 | 0.00154500 | 0.00019400 |
| H    | -0.00245100 | 3.71941100 | 0.00007900 |
| H    | 3.73974200 | 0.00252300 | 0.00027900 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -3.73974400 | -0.00251700 | -0.00028200 |
| H    | 0.00246100  | -3.71941000 | -0.00007200 |
| C    | -0.62833276 | -0.16929951 | 7.04091101  |
| C    | -0.89945887 | -1.62108076 | 6.71964204  |
| H    | -1.59521248 | 0.36495759  | 7.09904082  |
| H    | -0.10270414 | -0.00628512 | 7.98202611  |
| H    | -0.07209039 | -2.24858171 | 6.43347749  |
| C    | -2.30013432 | -2.16948097 | 6.72021539  |
| H    | -2.78225436 | -1.90123928 | 5.77352982  |
| H    | -2.29344715 | -3.25616548 | 6.82595178  |
| H    | -2.87980348 | -1.74832441 | 7.54722808  |
| N    | 0.19246866  | 0.34373411  | 5.95378445  |
| Br   | -0.32910852 | -2.44736860 | 9.09707824  |
| C    | -0.17003994 | -0.14651298 | 4.69670245  |
| O    | -0.90499546 | -1.20855458 | 4.85473145  |
| O    | 0.26504345  | 0.44905247  | 3.66685233  |
| C    | 0.76645848  | 1.66547195  | 6.10394948  |
| H    | 1.33083928  | 1.90014365  | 5.20041634  |
| H    | -0.00648786 | 2.44249626  | 6.24300249  |
| H    | 1.43731068  | 1.68642733  | 6.97213815  |

**V-Int$_5$**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| V    | -0.84422500 | -0.66941000 | -4.00443500 |
| V    | -0.87426700 | -0.66948000 | -1.14679400 |
| O    | -0.85310800 | 1.39056800  | -3.81320100 |
| O    | -0.85692700 | -2.73149500 | -3.79734000 |
| O    | -3.00225000 | -0.66959900 | -3.97722100 |
| O    | 1.27856300  | -0.66997800 | -3.95961700 |
| O    | 1.12337900  | -0.68182200 | -1.71354600 |
| O    | -2.81652300 | -0.68403100 | -1.74365100 |
O  -0.88797100  -2.76274200  -1.52277700
O  -0.90457200  1.40196200  -1.54026800
C  -0.87270400  1.95023200  -2.67653300
C  -0.86699500  -3.29894800  -2.66499400
C  -3.49263100  -0.67640700  -2.81944400
C  1.77481500  -0.67402600  -2.79817500
H  -0.86016200  3.04480500  -2.69842200
H  2.88203100  -0.67208300  -2.69822200
H  -4.59745500  -0.67712300  -2.69878300
H  -0.85525000  -4.39401600  -2.69857300
C  1.60839700  0.16120000  3.65044100
C  1.63654900  1.40358900  2.75021900
H  2.57766800  -0.36081400  3.67657200
H  1.32285900  0.43837700  4.67013900
H  0.94394500  2.15502300  3.13803300
C  2.99598000  2.01021200  2.49522100
H  3.69268800  1.26603200  2.08989400
H  2.92076700  2.84631400  1.79130800
H  3.36906100  2.38614000  3.45451700
N  0.61258700  -0.66546800  2.96179800
Br  1.82569500  2.54903800  6.14736600
C  0.41755300  -0.23281600  1.70391700
O  1.05165300  0.91410600  1.47174400
O  -0.27764700  -0.81747400  0.84419100
C  0.14857100  -1.94041300  3.46527000
H  -0.56397800  -2.36225400  2.75390100
H  0.98946300  -2.63759500  3.58833000
H  -0.33667400  -1.80147100  4.43744100
| Atom  | X       | Y       | Z       |
|-------|---------|---------|---------|
| Fe    | 0.00000400 | 0.00000500 | -1.21633500 |
| Fe    | 0.00000500 | 0.00001900 | 1.21676100 |
| O     | -0.00099300 | 2.02372700 | -1.12416800 |
| O     | 0.00099600 | -2.02370800 | -1.12418000 |
| O     | -2.04877200 | -0.00085600 | -1.13025500 |
| O     | 2.04878000 | 0.00087300 | -1.13024900 |
| O     | 2.04741900 | 0.00020400 | 1.12977300 |
| O     | -2.04741300 | -0.00030000 | 1.12976700 |
| O     | 0.00011300 | -2.02465000 | 1.12409800 |
| O     | -0.00014600 | 2.02466600 | 1.12411100 |
| C     | -0.00094300 | 2.60182200 | -0.00020800 |
| C     | 0.00091900 | -2.60180300 | -0.00021700 |
| C     | -2.61849000 | -0.00089100 | 0.00001100 |
| C     | 2.61849700 | 0.00083600 | 0.00001700 |
| H     | -0.00133000 | 3.70067700 | -0.00073300 |
| H     | 3.71843500 | 0.00149900 | 0.00081400 |
| H     | -3.71842800 | -0.00158200 | 0.00080600 |
| H     | 0.00130500 | -3.70065900 | -0.00074700 |

| Atom  | X       | Y       | Z       |
|-------|---------|---------|---------|
| Fe    | 2.08189600 | 0.17900800 | 0.11497100 |
| Fe    | -0.40849200 | -0.12431200 | -0.10423600 |
| O     | 1.73140400 | 1.11307400 | 1.86571500 |
| O     | 2.24637200 | -0.77047500 | -1.65419200 |
| O     | 1.92777000 | 1.94485100 | -0.89810600 |
| O     | 2.20048900 | -1.58366900 | 1.12762600 |
| O     | -0.06113300 | -1.61255300 | 1.24936300 |
| O     | -0.21272800 | 1.40876000 | -1.40789400 |
| O     | 0.06908400 | -1.40250800 | -1.64065300 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| O    | -0.50018500 | 1.20651300 | 1.47498200 |
| C    | 0.55432400  | 1.49109200 | 2.11093300 |
| C    | 1.25172400  | -1.41638100| -2.08385000|
| C    | 0.82722200  | 2.12770000 | -1.47967100|
| C    | 1.09628800  | -2.04739500| 1.51643600 |
| H    | 0.43969900  | 2.13664100 | 2.96787800 |
| H    | 1.13018700  | -2.91871500| 2.15490900 |
| H    | 0.74774400  | 2.99628900 | -2.11763800|
| H    | 1.44155100  | -2.05839400| -2.93001700|
| C    | -3.12515900 | -0.20517610| 1.15939467 |
| C    | -3.47263100 | 0.43634790 | -0.13884933|
| H    | -2.56658200 | 0.35962490 | 1.90013567 |
| H    | -3.77127800 | -0.98817010| 1.55213867 |
| H    | -4.35743100 | 0.03875390 | -0.63824033|
| C    | -3.16856700 | 1.88324590 | -0.44572933|
| H    | -2.96656200 | 2.02506590 | -1.51316233|
| H    | -4.03275600 | 2.50192090 | -0.17317733|
| H    | -2.30063900 | 2.23661290 | 0.11658967 |
| N    | -2.36336500 | -0.54468910| -0.06234733|
| C    | -2.63905200 | -1.87464310| -0.63369933|
| H    | -2.38692700 | -1.86654810| -1.69721933|
| H    | -2.01042600 | -2.61263310| -0.12817033|
| H    | -3.69526800 | -2.15521910| -0.51097833|

Fe-Int

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Fe   | 0.41363200  | 0.38750400 | -3.40221400|
| Fe   | 0.43476100  | 0.37554500 | -0.32656900|
| O    | 0.43027400  | 2.38701500 | -3.16538700|
| O    | 0.38077600  | -1.62675500| -3.21714400|
| O    | -1.61384400 | 0.40640000 | -3.25390200|
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| O    | 2.41333600 | 0.35951800 | -3.14917200 |
| O    | 2.44529600 | 0.73484900 | -0.91078500 |
| O    | -1.53858400 | 0.07693700 | -1.01468000 |
| O    | 0.86089500 | -1.58140900 | -1.00232800 |
| O    | 0.16586100 | 2.41016000 | -0.91206800 |
| C    | 0.25229100 | 2.94980500 | -2.03766100 |
| C    | 0.64506700 | -2.15709100 | -2.09189200 |
| C    | -2.12942100 | 0.20658000 | -2.11134300 |
| C    | 2.97995500 | 0.58483400 | -2.03290000 |
| H    | 0.16676800 | 4.04024100 | -2.08194300 |
| H    | 4.07038600 | 0.65494100 | -2.08214700 |
| H    | -3.21841300 | 0.13651000 | -2.07931300 |
| H    | 0.68529200 | -3.24854700 | -2.08292200 |
| C    | -1.29493900 | 0.45761500 | 2.22708500 |
| C    | -0.69086900 | -0.88366300 | 2.37621300 |
| H    | -2.01877200 | 0.64304200 | 1.43809100 |
| H    | -1.37627200 | 1.05344800 | 3.13383900 |
| H    | -0.36304000 | -1.08418200 | 3.39812800 |
| C    | -1.11107400 | -2.08819600 | 1.57201000 |
| H    | -0.27036300 | -2.77563800 | 1.42216200 |
| H    | -1.88808000 | -2.61891400 | 2.13722400 |
| H    | -1.51613800 | -1.81674200 | 0.59399400 |
| N    | 0.09683200 | 0.22192500 | 1.73141900 |
| Br   | -0.68888000 | -0.16600800 | 5.86520000 |
| C    | 1.17652900 | 0.79984500 | 2.56718400 |
| H    | 2.10104000 | 0.24325200 | 2.37959900 |
| H    | 1.32541900 | 1.84639500 | 2.27831700 |
| H    | 0.91939200 | 0.73848000 | 3.63277500 |
|          | x       | y       | z       |
|----------|---------|---------|---------|
| Fe       | -0.00054000 | 0.00014700 | -1.19374800 |
| Fe       | 0.00043500  | -0.00007400 | 1.38086100  |
| O        | -0.13713400 | 1.95079900  | -1.17840300 |
| O        | 0.13623600  | -1.95043800 | -1.17885200 |
| O        | -1.95153200 | -0.13651000 | -1.17669200 |
| O        | 1.95024600  | 0.13690000  | -1.17787000 |
| O        | 2.01767200  | 0.14682800  | 1.08565800  |
| O        | -2.01670200 | -0.14757100 | 1.08688500  |
| O        | 0.14807200  | -2.01741900 | 1.08457700  |
| O        | -0.14636900 | 2.01725700  | 1.08504600  |
| C        | -0.18192700 | 2.54923900  | -0.06284000 |
| C        | 0.18197500  | -2.54915300 | -0.06344900 |
| C        | -2.54928000 | -0.18205000 | -0.06084300 |
| C        | 2.54909600  | 0.18186500  | -0.06253000 |
| H        | -0.25933300 | 3.64443700  | -0.10280800 |
| H        | 3.64428500  | 0.25913700  | -0.10301200 |
| H        | -3.64451400 | -0.25929400 | -0.10017800 |
| H        | 0.25919100  | -3.64435100 | -0.10378700 |
| C        | -0.84370735 | -0.04461675 | 4.50088603  |
| C        | -0.71590529 | -1.48361221 | 4.77568157  |
| H        | -1.77685350 | 0.23249229  | 4.00647297  |
| H        | -0.64401658 | 0.61849042  | 5.35003678  |
| H        | 0.13306269  | -1.78896987 | 5.37035130  |
| C        | -1.43218598 | -2.52786627 | 3.96746680  |
| H        | -0.94633046 | -2.66217146 | 2.99442120  |
| H        | -1.42452809 | -3.48024623 | 4.50373850  |
| H        | -2.47370171 | -2.23617832 | 3.79854518  |
| N        | 0.26951819  | -0.21705300 | 3.57222128  |
Br               -2.08602279   -1.79161606    7.05185281  
C                 1.54863978    0.16454665    4.15971108  
H                 2.37025304   -0.18506969    3.52841449  
H                 1.62838323    1.26401735    4.24854339  
H                 1.69020987   -0.25066436    5.17146290  

Fe-Int$_2$
Fe                 0.42636200    0.39872400   -3.36359500  
Fe                 0.42044300    0.40231400   -0.21084300  
O                  0.46876600    2.41873400   -3.21177500  
O                  0.38776900   -1.62174900   -3.20331800  
O                 -1.57911000    0.43789600   -3.16728700  
O                  2.43415300    0.35312700   -3.17523100  
O                  2.43234500    0.74688700   -0.93766800  
O                 -1.58296100    0.03632800   -0.93111300  
O                  0.77459300  -1.59979300   -0.96482100  
O                  0.06809400    2.38567200   -0.97606000  
C                 0.23243400    2.94886400   -2.07627100  
C                 -2.12774800    0.20134400   -2.04203900  
C                  2.97948300    0.58743400   -2.04807300  
H                  0.16676800    4.04024100   -2.08194300  
H                  4.07038600    0.65491400   -2.08214700  
H                 -3.21841300    0.13651000   -2.07931300  
H                 0.68529200   -3.24854700   -2.08292200  
C                -0.67412500    0.05055500    2.56764000  
C                -0.41544700   -1.33018100    3.18844100  
H                -1.59807000   -0.00092600    1.97557700  
H                -0.83954300    0.78864500    3.37349100  
H                 0.54099500   -1.35423100    3.71045500  

S210
|       | x             | y             | z             |
|-------|---------------|---------------|---------------|
| C     | -0.58636700   | -2.50610900   | 2.24985700    |
| H     | 0.08945400    | -2.36898100   | 1.39663000    |
| H     | -0.35061500   | -3.45455800   | 2.74375300    |
| H     | -1.61159400   | -2.55317900   | 1.86519200    |
| N     | 0.44396600    | 0.41676300    | 1.73197800    |
| Br    | -1.73835100   | -1.61730100   | 4.82266500    |
| C     | 1.53416000    | 1.04295100    | 2.45259200    |
| H     | 2.31568400    | 1.35434500    | 1.74985100    |
| H     | 1.20116700    | 1.94392800    | 3.00793300    |
| H     | 2.01969300    | 0.37756000    | 3.19375700    |

**Fe-Int₃**

|       | x             | y             | z             |
|-------|---------------|---------------|---------------|
| Fe    | 0.33123200    | 0.35773200    | -3.41705800   |
| Fe    | 0.34991200    | 0.34017300    | -0.38703200   |
| O     | 0.40954900    | 2.40697000    | -3.36194800   |
| O     | 0.26744700    | -1.67653700   | -3.28718900   |
| O     | -1.63631900   | 0.44763100    | -3.17185000   |
| O     | 2.29331300    | 0.28909100    | -3.12434800   |
| O     | 2.45588300    | 0.71778500    | -0.89175100   |
| O     | -1.73526900   | -0.04762400   | -0.95043500   |
| O     | 0.73917200    | -1.64641700   | -1.06408900   |
| O     | -0.00874500   | 2.29907600    | -1.13371600   |
| C     | 0.16086300    | 2.90034700    | -2.21716100   |
| C     | 0.53817700    | -2.20823800   | -2.16392000   |
| C     | -2.22324100   | 0.15579100    | -2.07710400   |
| C     | 2.91116300    | 0.54115200    | -2.03933800   |
| H     | 0.08389800    | 3.98867200    | -2.17269500   |
| H     | 3.98751600    | 0.60337200    | -2.17289900   |
| H     | -3.30128300   | 0.08494100    | -2.17006500   |
| H     | 0.60242200    | -3.30011600   | -2.17367400   |

S211
| Element | x       | y       | z       |
|---------|---------|---------|---------|
| C       | -1.08623800 | 0.27930100 | 2.24378700 |
| C       | -0.89928900 | -0.91254800 | 3.18664100 |
| H       | -1.87689700 | 0.03378300 | 1.52470900 |
| H       | -1.42969300 | 1.15384400 | 2.82434600 |
| H       | -0.07583500 | -0.74534000 | 3.88233900 |
| C       | -0.82807700 | -2.26691600 | 2.51008400 |
| H       | 0.00006600 | -2.25288400 | 1.79193800 |
| H       | -0.65956200 | -3.07419700 | 3.23132500 |
| H       | -1.75177800 | -2.47394300 | 1.95697200 |
| N       | 0.16679300 | 0.53889400 | 1.56411100 |
| Br      | -2.53397100 | -0.98370100 | 4.55302100 |
| C       | 3.16840700 | -1.43822700 | 2.35109000 |
| O       | 3.51699400 | -0.53989600 | 3.01579500 |
| O       | 2.85995900 | -2.36761500 | 1.71241200 |
| C       | 0.98824600 | 1.49772600 | 2.28104500 |
| H       | 1.24358400 | 1.18543000 | 3.31178400 |
| H       | 1.93487300 | 1.65115500 | 1.75137800 |
| H       | 0.49017900 | 2.48667900 | 2.36969500 |

**Fe-Ts₂**

| Element | x       | y       | z       |
|---------|---------|---------|---------|
| Fe      | -0.00054000 | 0.00014700 | -1.19374800 |
| Fe      | 0.00043500 | -0.00007400 | 1.38086100 |
| O       | -0.13713400 | 1.95079900 | -1.17840300 |
| O       | 0.13623600 | -1.95043800 | -1.17885200 |
| O       | -1.95153200 | -0.13651000 | -1.17669200 |
| O       | 1.95024600 | 0.13690000 | -1.17787000 |
| O       | 2.01767200 | 0.14682800 | 1.08565800 |
| O       | -2.01670200 | -0.14757100 | 1.08688500 |
| O       | 0.14807200 | -2.01741900 | 1.08457700 |
| O       | -0.14636900 | 2.01725700 | 1.08504600 |
C    -0.18192700    2.54923900   -0.06284000
C     0.18197500   -2.54915300   -0.06344900
C    -2.54928000   -0.18205000   -0.06084300
C     2.54909600    0.18186500   -0.06253000
H    -0.25933300    3.64443700   -0.10280800
H     3.64428500    0.25913700   -0.10301200
H    -3.64451400   -0.25929400   -0.10017800
H     0.25919100   -3.64435100   -0.10378700
C    -1.12298391    0.36312497    4.39020238
C    -1.37220752   -1.07755720    4.84549566
H    -2.03342770    0.73713938    3.88899411
H    -0.99203983    0.97439312    5.29642969
H    -0.56553959   -1.43891035    5.48133987
C    -1.74440312   -2.08355568    3.78160191
H    -0.88645389   -2.22392821    3.11404872
H    -1.98816934   -3.05437762    4.22558416
H    -2.59035999   -1.73628275    3.18122847
N     0.06582503    0.51622176    3.53688521
Br   -2.94389774   -0.98453252    6.22571264
C     1.82267617   -0.62138833    4.46716708
O     2.33759068    0.24139375    5.10187846
O     1.66778366   -1.71846019    4.04101553
C     0.51019323    1.91520285    3.61531058
H     0.83212448    2.16544583    4.63875418
H     1.36467210    2.07494967    2.94984571
H    -0.28368178    2.62103855    3.31835858

Fe-Int₄

Fe     1.12086800   -0.00840000   -0.18289700
Fe     4.21467100    0.03957200    0.33342600
O  1.81075700  2.02972700  -0.01808900
O  1.88489300  -1.98657300  -0.12310800
O  1.44577000  -0.05655500   1.94041800
O  2.14332100   0.06074800  -2.08572600
O  4.33705600   0.46614500  -1.63750600
O  3.67858800  -0.39075800   2.23957800
O  4.15473000  -1.95242800  -0.09559200
O  3.96153800   2.02351000   0.72952100
C  2.85223100   2.56657400   0.41460800
C  3.01474900  -2.51395900  -0.17888800
C  2.46542500  -0.28832600   2.62346500
C  3.32089800   0.33246900  -2.39854600
H  2.81370000   3.65073800   0.55571300
H  3.53493600   0.47284200  -3.45418500
H  2.31918600  -0.42324900   3.69524400
H  3.03707600  -3.60093300  -0.31530400
C  -4.14747600  -0.68589000  -1.14743500
C  -4.90824300  -0.92675000   0.16406900
H  -3.84334600  -1.67894200  -1.50794400
H  -4.82610600  -0.25272300  -1.89214400
H  -4.20329600  -1.04766000   0.98623400
C  -5.90393000  -2.06878700   0.08342700
H  -5.34889000  -2.99749000  -0.10700700
H  -6.45890500  -2.18677500   1.01883000
H  -6.62421300  -1.91235400  -0.72896900
N  -2.96893300   0.14582000  -1.01393100
Br  -5.92975000   0.79847800   0.69798400
C  -1.80712900  -0.47576000  -0.52896200
O  -1.89703200  -1.61838600  -0.06632900
O       -0.73989200  0.26315600  -0.61464700
C       -2.93405800  1.42736700  -1.70073300
H       -2.00122800  1.92826100  -1.44333300
H       -2.97194900  1.30937300  -2.79876500
H       -3.77983900  2.05067300  -1.38821700

Fe-Ts$_3$
Fe      -0.00054000  0.00014700  -1.19374800
Fe      0.00043500 -0.00007400  1.38086100
O       -0.13713400  1.95079900  -1.17840300
O       0.13623600 -1.95043800  -1.17885200
O       -1.95153200 -0.13651000  -1.17669200
O       1.95024600  0.13690000  -1.17787000
O       2.01767200  0.14682800  1.08565800
O       -2.01670200 -0.14757100  1.08688500
O       0.14807200  2.01741900  1.08457700
O       -0.14636900  2.01725700  1.08504600
C       -0.18192700  2.54923900  -0.06284000
C       0.18197500 -2.54915300  -0.06344900
C       -2.54928000 -0.18205000  -0.06084300
C       2.54909600  0.18186500  -0.06253000
H       -0.25933300  3.64443700  -0.10280800
H       0.25919100 -3.64435100  -0.10378700
H       -3.64451400 -0.25929400  -0.10017800
H       -0.00054000 -0.00007400  -0.10378700
C       -2.25004568 -1.62145767  -6.22783997
H       -0.25888142  3.64443700  -0.10017800
H       0.25919100  3.64443700  -0.10017800
C       -1.11228683  0.54202685  -7.81088504
H       2.99323866 -0.96522000  -5.80682000
|   | x     | y     | z     |
|---|-------|-------|-------|
| C | -2.41538269 | -3.11251134 | -6.11612085 |
| H | -1.88581791 | -3.45397789 | -5.21983720 |
| H | -3.47021503 | -3.38427577 | -6.03793778 |
| H | -1.99543778 | -3.61581496 | -6.99271913 |
| N | -0.57556742 | -0.02760888 | -5.87134793 |
| Br | -3.56939848 | -1.37466074 | -8.38975472 |
| C | -0.70980957 | -0.44723469 | -4.53299711 |
| O | -1.57179699 | -1.45381809 | -4.56896212 |
| O | -0.07752461 | 0.18271053 | -3.64240963 |
| C | 0.51157584 | 0.84809724 | -6.25804862 |
| H | 0.22024190 | 1.44738510 | -7.13051056 |
|...|...|...|...|

Fe-Int$_5$

|   | x     | y     | z     |
|---|-------|-------|-------|
| Fe | 0.47524900 | 0.43435600 | 1.22564400 |
| Fe | 0.48181900 | 0.44958100 | 4.15248500 |
| O  | 0.52230600 | 2.55906100 | 1.61324500 |
| O  | 0.47066400 | -1.67341900 | 1.59877900 |
| O  | -1.50486700 | 0.46858200 | 1.79144500 |
| O  | 2.48098800 | 0.39856400 | 1.78202500 |
| O  | 2.49231000 | 0.79861600 | 4.01441100 |
| O  | -1.52612300 | 0.08807600 | 4.02565500 |
| O  | 0.83244800 | -1.47828100 | 3.83628400 |
| O  | 0.12892600 | 2.37488200 | 3.84670300 |
| C  | 0.29700100 | 3.01111000 | 2.75345200 |
| C  | 0.67872600 | -2.12035300 | 2.74645100 |
| C  | -2.06967800 | 0.24725300 | 2.89164600 |
| C  | 3.03870500 | 0.63413500 | 2.88247800 |
| H  | 0.22571900 | 4.09020300 | 2.86410000 |
H  4.12933700  0.70490300  2.86389600
H  -3.15946200  0.18647200  2.86673000
H   0.74424300 -3.19858500  2.86312100
C   0.31524200 -0.61851200 -4.00751300
C  -0.89349500 -1.20249100 -3.25919100
H   1.11068300 -1.36404400 -4.16903500
H   0.00749500 -0.20890900 -4.96749200
H  -1.80058200 -0.68017800 -3.56657800
C  -1.07624600 -2.70249400 -3.33142000
H  -0.23784000 -3.21584900 -2.84869500
H  -2.00658100 -2.99827700 -2.81352800
H  -1.15494400 -2.98554800 -4.38556700
N   0.76597500  0.40440500 -3.06064900
Br  -2.01620000 -1.14852500 -6.32107200
C   0.27668900  0.15830800 -1.83171700
O  -0.63311300 -0.81168300 -1.84620600
O   0.61296900  0.76513100 -0.79449700
C   1.85052600  1.32418300 -3.32516100
H   1.97086800  1.98296100 -2.46287200
H  2.79245600  0.78327200 -3.49794800
H   1.62021600  1.91992300 -4.21508900