Supporting Information

Computational screening of metal-substituted HKUST-1 catalysts for chemical fixation of carbon dioxide into epoxides

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S1. Supercage-based calculations for HKUST-1

Calculations based on a supercage model with 408 atoms obtained from previous publication[1] were also performed with two-layer ONIOM(QM/MM) method[2] to verify the reliability of cluster-based calculations. The inner layer included a Cu_2 paddle-wheel unit and reactant molecules, and the remainder was the outer layer fixed at the crystal positions. Previous publications have demonstrated that this methodology can reproduce experimental results well in the MOF-catalyzed system.[3] For all geometry optimization and vibrational frequency calculations, the B3LYP was used in conjunction with the LANL2DZ effective core potential basis set and the 6-31+G* basis set to describe the QM atoms. The Universal Force Field (UFF) parameter set was used for describing the extended framework of MM atoms. Single-point energy calculations were subsequently performed at the ONIOM (M06-2X/6-311+G (2d,p)&&SDD :UFF).

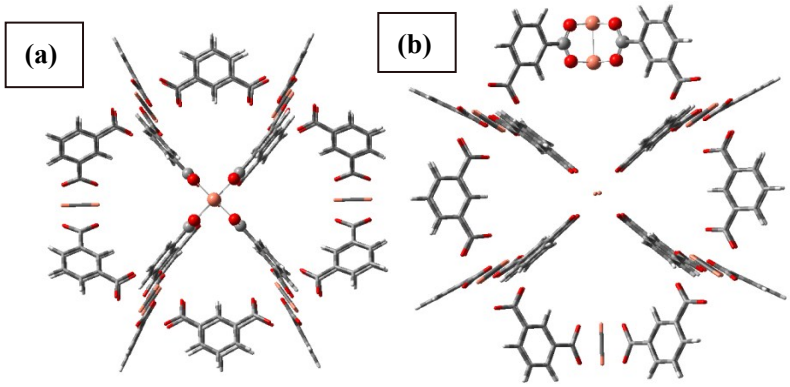

Figure S1. The top view (a) and side view (b) of the supercage model for HKUST-1.

A. From the geometrical point of view, the supercage-based calculations give the similar geometrical parameters with the cluster-based calculations (Table S1), suggesting that our cluster-based calculations are able to replicate the HKUST-1 structure very well.

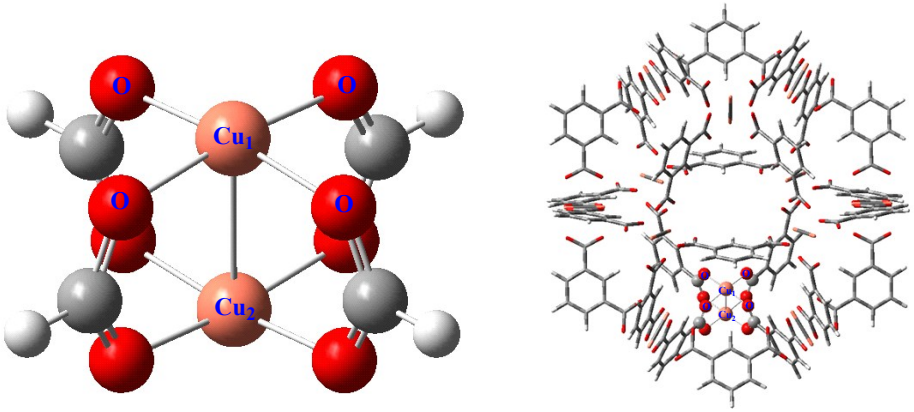

Figure S2. Optimized geometry of cluster model and supercage model for HKUST-1

Table S1. The key bond lengths and bond angles and its deviations of the optimized supercage model and cluster model for HKUST-1 (The supercage model is taken as reference).

	Supercage model	Cluster model	Deviation
Bond lengths(Å)			
Cu(1)-O	1.9673	1.9885	1.08%
Cu(1)-Cu(2)	2.5227	2.5486	1.03%
Bond angles(°)			
∠O-Cu(1)-Cu(2)	85.6452	86.0221	0.44%

B. The stability of the catalytic center of HKUST-1 in cluster model is investigated compared with the supercage model. It was shown that the two model calculations give the same energy ordering in different spin states for Cu-HKUST-1.

Table S2. The energies (Hartrees) of Cu-HKUST-1 with different spin states.

	Cluster Model			Supercage Model		
Spin state	**Total Energy (Hartree)**	**Relative Energy (Hartree)**	**Relative Energy (kcal/mol)**	**Total Energy (Hartree)**	**Relative Energy (Hartree)**	**Energy Barrier (kcal/mol)**
singlet	-1151.4500	0.1085	68.08	-1146.6024	0.1086	68.15
triplet	-1151.5585	0.0000	0.00	-1146.7110	0.0000	0.00
quintet	-1151.3829	0.1756	110.19	-1146.4972	0.2138	134.15
septet	-1151.2072	0.3513	220.44	-1146.3167	0.3942	247.38
nonet	-1151.0266	0.5319	333.77	-1146.1812	0.5297	332.42
undectet	-1150.8400	0.7185	450.87	-1146.0039	0.7071	443.71
13-et	-1150.6674	0.8911	559.17	-1145.8333	0.8777	550.74
15-et	-1150.4635	1.0950	687.12	-1145.7023	1.0086	632.92

C. The key reaction pathway has been investigated with the supercage model. The energy profiles along the reaction catalyzed by the HKUST-1/TBAB obtained with the cluster model and supercage model are shown in Figure S3. (the corresponding energies are listed in the table S3) As can be seen in Figure S3, the energy profiles obtained with the cluster and supercage models show that the cluster-based calculation can capture the relative trends from the supercage-based calculation and present the same reaction mechanism with supercage-based calculation. Specifically, the CO_2 insertion is also the lowest-barrier step in the three steps.

Figure S3. The energy profile along the reaction catalyzed by the HKUST-1/TBAB obtained with the cluster model and supercage model.

Table S3. The energies along the reaction catalyzed by the Cu-HKUST-1/TBAB obtained with the cluster and supercage model.

	Supercage Model			Cluster Model		
Structures	**Total Energy (Hartree)**	**Relative Energy (kcal/mol)**	**Energy Barrier (kcal/mol)**	**Total Energy (Hartree)**	**Relative Energy (kcal/mol)**	**Energy Barrier (kcal/mol)**
Cat+reactant	-1541.8108	0.00		-1546.6568	0.00	
Int0	-1541.8801	-43.48		-1546.7036	-29.34	
Int1	-1541.8871	-47.87		-1546.7040	-29.56	
TS1	-1541.8513	-25.42	22.45	-1546.6785	-13.57	15.99
Int2	-1541.8604	-31.10		-1546.6891	-20.24	
Int3	-1541.8470	-22.71		-1546.6856	-18.03	
TS2	-1541.8450	-21.46	9.64	-1546.6788	-13.77	6.48
Int4	-1541.8494	-24.20		-1546.6977	-25.63	
TS3	-1541.8195	-5.44	18.76	-1546.6779	-13.22	12.40
Int5	-1541.8592	-30.36		-1546.7216	-40.64	
Cat+product	-1541.8229	-7.60		-1546.6690	-7.60	

Based on these evidences, we believe that the cluster-based calculations would not affect the conclusion in a significant way. As stated by Donald G. Truhlar et al, "Intuitively, one would expect that calculations based on periodic unit cells or on larger and relaxed cluster models would provide better results than those based on small clusters. The studies that we describe in the following show that when the phenomena under investigation are localized, smaller clusters can be also be quantitatively accurate." [4, 5] The present work provides a similar case that the small model study can act as a very effective strategy to investigate systematically the mechanism of chemical fixation of CO_2 on metal-substituted HKUST-1.

S2. The reliability of single-point energy calculations

For modeling the CO_2 cycloaddition reactions, the inclusion of dispersion corrections is necessary since the adsorbates have the dispersion interaction with the HKUST-1. Thus, several dispersion-containing functionals including M06,[6] PBE0-D3[7, 8], and B3LYP-D3[7, 9] were chosen for the single-point energy calculation. One can see that M06-2X captures a similar trend with the M06, PBE0-D3, and B3LYP-D3 in the single-point energy calculation. In addition, we also test the basis set for this reaction and result showed that the activation energies change little as the basis set increased from 6-311+G(2df, p) to 6-311++G(3df,3p). For this reason, we believe that the M06-2X/6-311+(2df,p)&&SDD is reliable enough for our systems.

Table S4. Free energy barriers for ring-opening step (ΔG_1), CO_2-insertion step (ΔG_2) and ring-closing step (ΔG_3) of the CO_2 cycloaddition catalyzed by HKUST-1/TBAB calculated with different functionals.

Single-point calculation level	ΔG_1 (kcal mol^{-1})	ΔG_2 (kcal mol^{-1})	ΔG_3 (kcal mol^{-1})
M06-2X/6-311+G(2df, p)&&SDD	15.9900	6.4760	12.4033
PBE0-D3/6-311+G(2df, p)&&SDD	17.3003	7.1616	10.6911
B3LYP-D3/6-311+G(2df, p)&&SDD	15.3920	5.6685	14.4750
M06/6-311+G(2df, p)&&SDD	15.8602	5.9525	11.1889

Table S5. Free energy barriers for ring-opening step (ΔG_1), CO_2-insertion step (ΔG_2) and ring-closing step (ΔG_3) of the CO_2 cycloaddition catalyzed by HKUST-1/TBAB calculated with different basis sets.

Single-point calculation	ΔG_1 (kcal mol^{-1})	ΔG_2 (kcal mol^{-1})	ΔG_3 (kcal mol^{-1})
M06-2X/6-311+G(2df, p)&&LANL2DZ	16.8494	6.3218	13.5546
M06-2X/6-311+G(2df, p)&&SDD	15.9900	6.4760	12.4033
M06-2X/6-311+G(2df, 2p) &&SDD	15.9724	6.4683	12.3772
M06-2X/6-311+G(3df, 3p) &&SDD	16.1988	6.7883	11.8723
M06-2X/6-311++G(3df, 3p) &&SDD	16.2128	6.7874	11.8720

S3. The effects of electronic properties of different M-HKUST-1 on catalytic performance.

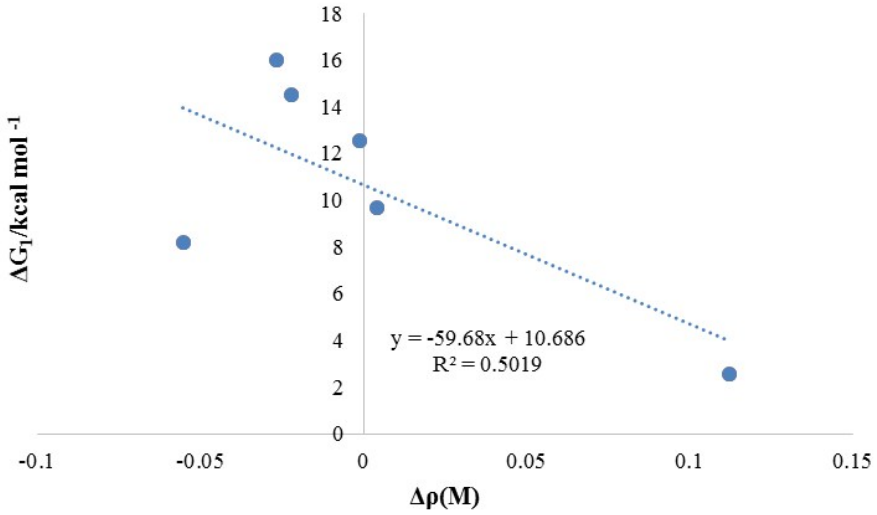

Figure S4. Relationship of the activation energy for ring-opening step ΔG_1 and the spin density difference $\Delta\rho$(M) for the active metal center between the **Int$_1$** (shown in Figure 2 of the main text) and all high spin M-HKUST-1.

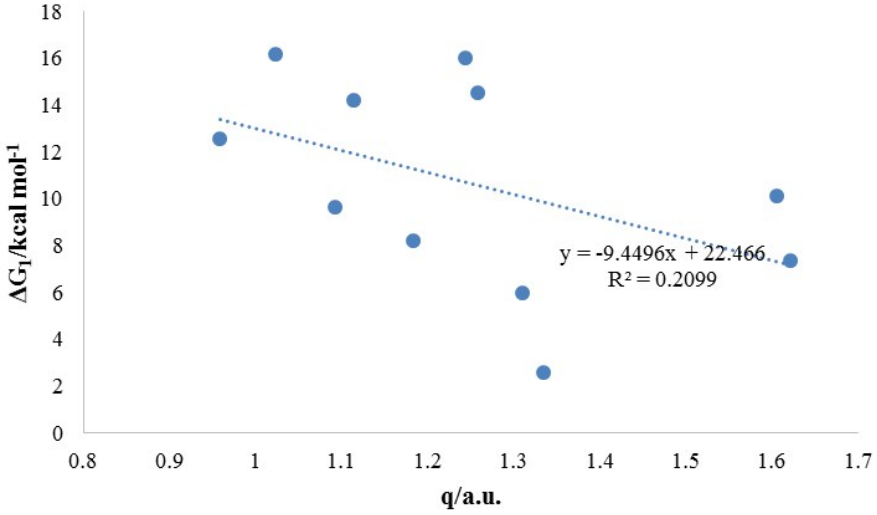

Figure S6. Relationship of NPA charge for the metal center in M-HKUST-1 and the activation energy for ring-opening step ΔG_1.

The moderate (spin density difference $\Delta\rho$(M)) and bad (NPA) correlation implies that the energy barriers for the reaction catalyzed by M-HKUST-1/TBAB are likely to be influenced by several factors (are not limited to the electronic properties of metal in the M-HKUST-1), e.g., coordination geometry. These factors lead synergistically to the deviation of the scaling line. When changing the original Cu atoms in HKUST-1 into other metal atoms in M-HKUST-1, the optimized M-HKUST-1 structures are significantly different from the Cu-HKUST-1 (i.e., the coordination number, M-M

bond interaction and/or oxidation state of the metal), which influences the activity of M-HKUST-1 to a different degree. Such deviation from the scaling line has also been mentioned by a very recent report.[10]

S4. Table S6. The energies (Hartrees) of M-HKUST-1 with different spin states. The minimum-energies for each M-HKUST-1 are marked green.

HKUST-1	singlet	triplet	quintet	septet	nonet	undectet	13-et	15-et
Cu	-1151.4500	-1151.5585	-1151.3829	-1151.2072	-1151.0266	-1150.8400	-1150.6674	-1150.4635
Fe	-1004.4615	-1004.4573	-1004.6153	-1004.6768	-1004.6841	-1004.6063	-1004.4671	-1004.2858
Cr	-930.5827	-930.8091	-930.6387	-930.7805	-930.8774	-930.6369	-930.5193	-930.3682
Ru	-946.2891	-946.3126	-946.3002	-946.2943	-946.2813	-946.1205	-945.9439	-945.7751
Ti	-873.3770	-873.4501	-873.4067	-873.2794	-873.0909	-872.9141	-872.7384	-872.5596
W	-890.8206	-890.7992	-890.7003	-890.7517	-890.7192	-890.5377	-890.3554	-890.1693
Sc	-850.3961	-850.3707	-850.2127	-849.8803	-849.8549	-849.6767	-849.4625	-849.2683
Mo	-893.0475	-892.9631	-892.9643	-893.0149	-892.9999	-892.8158	-892.6390	-892.4550
Zn	-1211.2742	-1211.1097	-1210.9161	-1210.7798	-1210.6043	-1210.4264	-1210.2611	-1210.0532
V	-900.0848	-900.0522	-900.0883	-900.1410	-900.0096	-899.7942	-899.6643	-899.4878
Cd	1092.1368	1091.9957	1091.8293	1091.6894	1091.5180	1091.3533	1091.1921	1090.9764

S5. Table S7. Relative Gibbs free energies (kcal mol^{-1}) for the stationary points along the reaction pathway for CO_2 fixation on M-HKUST-1 catalysts.

Structures	Mo	Cr	Fe	Ti	Cu	W	Sc	Ru	Zn	Cd	V
Cat+reactant	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Int0	-23.96	-28.34	-72.87	-40.54	-29.34	-23.21	-26.14	-40.49	-29.59	-24.54	-60.50
Int1	-20.46	-26.13	-66.12	-57.46	-29.56	-19.29	-21.78	-38.08	-26.25	-21.19	-57.57
TS1	-4.29	-11.63	-63.56	-47.79	-13.57	-5.11	-15.79	-25.54	-18.90	-11.08	-49.39
Int2	-7.56	-18.60	-71.23	-50.42	-20.24	-8.72	-24.28	-29.39	-26.09	-16.38	-51.52
Int3	-5.05	-16.08	-67.84	-47.14	-18.03	-5.43	-19.42	-26.00	-22.30	-11.40	-49.09
TS2	-1.56	-13.01	-62.25	-39.42	-13.77	-2.91	-14.05	-24.45	-17.09	-5.86	-48.57
Int4	-14.26	-24.92	-73.52	-62.58	-25.63	-14.26	-27.12	-31.92	-29.74	-21.82	-63.14
TS3	-3.36	-11.06	-58.47	-34.25	-13.22	-2.73	-9.14	-14.89	-15.13	-7.25	-41.92
Int5	-32.48	-38.71	-82.00	-69.60	-40.64	-31.49	-34.59	-47.50	-38.05	-33.61	-67.30
Cat+product	-7.60	-7.60	-7.60	-7.60	-7.60	-7.60	-7.60	-7.60	-7.60	-7.60	-7.60

S6. Table S8. The key geometrical parameters for the transition state of ring-opening step.

M-HKUST-1	Energy Barriers (kcal mol^{-1})	$d_{C(2)\text{-}Br}$ (Å)	$\theta_{OC(1)C(2)}$ (deg)
Zn	7.35	2.83	69.94
V	8.18	2.83	70.57
Ti	9.66	2.80	71.67
Cd	10.11	2.81	70.73
Sc	12.54	2.77	73.33
Fe	12.54	2.77	73.33
Ru	12.54	2.77	73.33
W	14.18	2.75	74.64
Cr	14.50	2.73	75.58
Pb	14.55	2.78	73.41
Cu	15.99	2.66	77.98
Mo	16.17	2.72	76.00

S7. Table S9. The Gibbs free energy (kcal mol^{-1}) of the key steps for CO_2 fixation catalyzed by M-HKUST-1.

M-HKUST-1	PO-adsorption	Ring-opening	CO_2-insertion	Ring-closing
Mo	-23.96	16.17	6.01	10.90
Cr	-28.34	14.50	5.59	13.86
Ti	-68.54	9.66	11.00	28.34
Cu	-29.34	15.99	6.48	12.40
W	-23.21	14.18	5.81	11.53
Sc	-26.14	5.99	10.23	17.98
Ru	-40.49	12.54	4.94	17.03
Zn	-29.59	7.35	9.00	14.62
Cd	-24.54	10.11	10.52	14.57
V	-60.50	8.18	2.95	21.22
Fe	-72.87	2.56	5.59	15.05

S8. The Coordinates of all stable intermediates and transition states.

Catalyst: Cu-HKUST-1; Co-catalyst: X^- (X = F, Cl, Br, I)

Cu-HKUST-1/F^-

Cu-HKUST-1

Cu	-0.000845	0.000072	-1.273814
Cu	0.001419	-0.000084	1.274814
O	-0.331103	-1.955835	-1.137057
O	0.328968	1.956093	-1.137254
O	1.955459	-0.330105	-1.137144
O	-1.956996	0.330170	-1.134876
O	-1.955957	0.322801	1.137654
O	1.958186	-0.323260	1.135367
O	0.323353	1.957379	1.135270
O	-0.323024	-1.957200	1.135459
C	-0.418298	-2.505718	-0.000795
C	0.416957	2.506008	-0.001076
C	2.506060	-0.417743	-0.001308
C	-2.505706	0.417457	0.001945
H	-0.598611	-3.590763	-0.000795
H	-3.590778	0.597623	0.003049
H	3.591099	-0.598070	-0.002001
H	0.596456	3.591188	-0.001221

F-Int_1

Cu	-0.290358	0.182531	-0.330736
Cu	2.267509	-0.199064	0.351285
O	-0.317042	-1.841289	0.075532
O	0.395801	2.096212	-0.560071
O	0.539734	-0.260977	-2.165946
O	-0.362989	0.516400	1.710765
O	1.867942	0.476520	2.169658
O	2.625921	-0.868084	-1.477480
O	2.613763	1.653487	-0.259777
O	1.789625	-2.030767	0.925914
C	0.630995	-2.452123	0.626204

C	1.616547	2.387729	-0.533152
C	1.697372	-0.712356	-2.328391
C	0.641575	0.642109	2.449760
H	0.449123	-3.497922	0.890978
H	0.442853	0.936482	3.482423
H	1.953596	-1.018397	-3.344977
H	1.873295	3.422765	-0.778721
O	-2.384445	0.388990	-0.783360
C	-3.459046	0.443349	0.227676
C	-4.475770	1.534157	0.051771
C	-3.387296	-0.692729	-0.671624
H	-3.078316	0.299210	1.237028
H	-5.371084	1.248165	0.612370
H	-4.091318	2.497726	0.412134
H	-4.751756	1.635558	-1.003638
F	-5.716648	-1.179301	0.413200
H	-4.062121	-0.739125	-1.519302
H	-2.984561	-1.636054	-0.318380

F-TS$_1$

Cu	0.347320	-0.164481	-0.296221
Cu	-2.252531	0.200594	0.307319
O	-0.367311	0.422400	-2.130960
O	0.365422	-0.672926	1.695452
O	-0.470212	-2.038129	-0.687118
O	0.326260	1.801494	0.279408
O	-1.911758	2.143030	0.507843
O	-2.582177	-1.739544	0.109871
O	-1.775115	-0.075375	2.203835
O	-2.589974	0.458806	-1.619029
C	-1.587763	0.549038	-2.393452
C	-0.604592	-0.484069	2.471168
C	-1.622223	-2.415210	-0.377792
C	-0.694384	2.499805	0.483362
H	-1.847498	0.770771	-3.435576
H	-0.513599	3.561793	0.664499
H	-1.842199	-3.472827	-0.546501
H	-0.434583	-0.698811	3.532665
O	2.371924	-0.472380	-0.750786
C	3.411597	-0.567934	0.256881
C	4.391895	-1.698151	0.077899

C	3.511361	0.645595	-0.526494
H	3.030497	-0.458791	1.273936
H	5.264760	-1.517362	0.715809
H	3.934764	-2.658605	0.351017
H	4.729505	-1.751771	-0.963141
F	5.332370	1.462311	0.319062
H	4.115586	0.664861	-1.419594
H	3.050717	1.559210	-0.184061

F-Int$_2$

Cu	0.456001	-0.461504	-0.667399
Cu	-2.117112	0.389779	0.484550
O	0.478463	1.727991	-0.496740
O	-0.669916	-2.261424	-0.262035
O	-0.875472	-0.175127	-2.182865
O	0.440053	-0.242383	1.631181
O	-1.700001	-0.085909	2.358109
O	-2.685151	0.916583	-1.359414
O	-2.756667	-1.428366	0.151657
O	-1.383520	2.183385	0.745040
C	-0.277088	2.458908	0.180630
C	-1.903419	-2.344171	-0.085515
C	-1.941641	0.477237	-2.282738
C	-0.445187	-0.280506	2.502105
H	0.023446	3.502472	0.327500
H	-0.132741	-0.510656	3.529059
H	-2.271552	0.692260	-3.304372
H	-2.358711	-3.340317	-0.134710
O	2.244993	-0.981423	-0.636225
C	3.245619	-0.448132	0.175421
C	4.340662	-1.496232	0.416654
C	3.790455	0.809442	-0.508682
H	2.818320	-0.154562	1.147999
H	5.150028	-1.087386	1.034509
H	3.908125	-2.367458	0.920941
H	4.761991	-1.829412	-0.541452
F	4.826239	1.419933	0.272946
H	4.238878	0.557404	-1.477009
H	2.999602	1.552380	-0.633269

F-Int$_3$

Cu	0.277321	0.375498	-0.107099
Cu	-2.594036	-0.269848	0.035410
O	-0.551653	1.642143	1.425983
O	-0.116614	-1.247524	-1.529699
O	-0.710894	1.559838	-1.409369
O	-0.299876	-1.316511	1.360989
O	-2.537543	-1.344724	1.699095
O	-2.830006	0.790424	-1.650238
O	-2.262165	-1.863935	-1.043657
O	-2.794142	1.368979	1.080815
C	-1.760359	1.917056	1.584137
C	-1.125529	-1.984055	-1.602364
C	-1.831683	1.495887	-1.969116
C	-1.327354	-1.650451	1.973897
H	-2.012102	2.751477	2.250520
H	-1.198084	-2.282677	2.862318
H	-1.952713	2.139973	-2.846288
H	-1.062578	-2.875403	-2.238235
O	2.084160	0.139443	0.330450
O	2.410661	3.059209	-0.247866
C	2.682942	-1.118819	0.476047
C	3.423012	2.483375	-0.154670
C	3.314916	-1.482245	-0.870949
H	1.913064	-1.870947	0.705095
C	3.704066	-1.106845	1.620066
O	4.488171	1.996984	-0.086330
H	2.549086	-1.529806	-1.648979
H	4.100238	-0.766687	-1.139054
F	3.940945	-2.770128	-0.818869
H	4.481341	-0.355327	1.433446
H	3.194733	-0.852903	2.556525
H	4.182396	-2.088443	1.729804

F-TS$_2$

Cu	0.219751	0.607162	-0.151849
Cu	-2.512012	-0.514620	0.058552
O	-0.662500	1.539160	1.563398
O	0.011975	-0.868224	-1.722878

O	-0.944261	1.761101	-1.229775
O	-0.094786	-1.302458	1.136768
O	-2.247969	-1.868552	1.497225
O	-2.985223	0.785868	-1.405878
O	-2.022015	-1.824133	-1.302956
O	-2.843136	0.875988	1.384732
C	-1.874664	1.542040	1.874550
C	-0.905827	-1.705274	-1.898131
C	-2.107300	1.643781	-1.691626
C	-0.989411	-1.956423	1.698559
H	-2.197437	2.207337	2.688981
H	-0.668603	-2.690174	2.450764
H	-2.366561	2.402188	-2.438239
H	-0.765255	-2.465403	-2.680074
O	2.105513	0.367984	0.226763
O	1.929915	2.705618	-0.278899
C	2.817075	-0.846986	0.403348
C	2.892064	2.024175	-0.061743
C	3.631844	-1.109752	-0.864758
H	2.070797	-1.644317	0.489214
C	3.662786	-0.830910	1.678680
O	4.080353	1.906788	0.043199
H	2.977403	-1.096982	-1.740775
H	4.453135	-0.397879	-0.979796
F	4.221600	-2.411675	-0.800511
H	4.406907	-0.028711	1.647043
H	3.009285	-0.670513	2.543563
H	4.179190	-1.791216	1.802655

F-Int$_4$

Cu	0.281064	-0.502003	-0.084346
Cu	2.765722	0.624265	0.063795
O	0.109697	0.602400	1.621682
O	1.211003	-1.286476	-1.750032
O	1.366833	-1.872094	1.031160
O	0.042881	1.225464	-1.155975
O	2.177583	2.014936	-1.212624
O	3.333602	-0.769793	1.340963
O	3.334165	-0.520020	-1.440925
O	2.091883	1.725228	1.561888
C	0.944170	1.447013	2.028170

C	2.428594	-1.189870	-2.030741
C	2.514583	-1.728571	1.509157
C	0.942374	2.024073	-1.508203
H	0.651775	2.033442	2.910402
H	0.625201	2.847742	-2.160686
H	2.872514	-2.534442	2.163569
H	2.776519	-1.756748	-2.906153
O	-1.431122	-1.634114	-0.235448
C	-2.649218	-1.305041	-0.137635
O	-2.807417	0.076656	0.098388
O	-3.660809	-2.013126	-0.233163
C	-4.118370	0.589221	0.347025
C	-5.097105	0.288460	-0.793128
H	-3.966468	1.675682	0.330601
C	-4.655115	0.183059	1.721082
H	-4.587751	0.313402	-1.759996
H	-5.636243	-0.648868	-0.668177
F	-6.081921	1.335409	-0.813022
H	-4.785575	-0.901828	1.773363
H	-3.953773	0.494170	2.503789
H	-5.621577	0.670641	1.904804

F-TS$_3$

Cu	-0.359803	-0.446710	-0.106483
Cu	-2.855787	0.524812	0.150305
O	-0.148163	1.326906	-1.066856
O	-1.238059	-1.980316	0.908392
O	-1.243770	-1.173250	-1.806249
O	-0.213142	0.540374	1.668214
O	-2.265484	1.521174	1.749249
O	-3.387599	-0.491751	-1.456959
O	-3.280110	-1.042754	1.280593
O	-2.308342	2.044698	-0.991795
C	-1.084875	2.124157	-1.320108
C	-2.399516	-1.951566	1.383939
C	-2.462802	-1.089205	-2.090361
C	-1.089403	1.287488	2.167334
H	-0.816341	3.013816	-1.904434
H	-0.809081	1.812575	3.089229
H	-2.783016	-1.597765	-3.009172
H	-2.704465	-2.828613	1.970273
O	1.507945	-1.369272	-0.373803

C	2.673278	-0.961538	-0.218380
O	2.895920	0.288530	0.233513
O	3.738482	-1.646401	-0.452285
C	4.328226	0.612053	0.245683
C	5.097034	-0.691587	0.113737
H	4.522329	1.052392	1.221476
C	4.619599	1.606397	-0.868103
H	5.291319	-1.285843	0.992458
H	5.717959	-0.872338	-0.748228
F	6.688598	0.349512	0.723486
H	4.417318	1.158522	-1.849886
H	3.992202	2.498649	-0.760397
H	5.675838	1.877364	-0.802103

F-Int$_5$

Cu	-0.407996	-0.425292	-0.089976
Cu	-2.899992	0.515621	0.125293
O	-0.182330	1.330342	-1.076288
O	-1.254502	-1.964312	0.937058
O	-1.235079	-1.199352	-1.791261
O	-0.264261	0.586334	1.670432
O	-2.435328	1.230742	1.907558
O	-3.290414	-0.226433	-1.664931
O	-3.405478	-1.213514	0.950105
O	-2.258429	2.193015	-0.710355
C	-1.066912	2.219941	-1.144782
C	-2.481044	-2.047505	1.194198
C	-2.389128	-0.935304	-2.208826
C	-1.223196	1.131450	2.270176
H	-0.776270	3.149351	-1.648191
H	-0.989421	1.586127	3.239612
H	-2.665270	-1.373340	-3.175260
H	-2.806397	-2.964898	1.699484
O	1.532279	-1.301058	-0.303675
C	2.677270	-0.882106	-0.144876
O	2.973350	0.341298	0.269970
O	3.748631	-1.630366	-0.379167
C	4.454670	0.539463	0.258993
C	4.973276	-0.877883	0.008849
H	4.720079	0.895324	1.249953
C	4.814194	1.551945	-0.808769

H	5.381911	-1.356761	0.893810
H	5.674574	-0.951745	-0.815701
F	6.963139	0.406381	0.631120
H	4.532322	1.189925	-1.806901
H	4.309646	2.508480	-0.628342
H	5.899938	1.666971	-0.738055

Cu-HKUST-1/Cl^-

Cl-Int_0

Cu	0.035443	0.248010	-0.330121
Cu	2.541835	-0.334101	0.361056
O	-0.158142	-1.769450	-0.009581
O	0.838621	2.115822	-0.477464
O	0.826527	-0.177381	-2.171780
O	-0.066300	0.514983	1.712343
O	2.143193	0.263206	2.206573
O	2.876344	-0.915438	-1.501917
O	3.015560	1.526264	-0.137063
O	1.928300	-2.161090	0.819612
C	0.742577	-2.479363	0.503035
C	2.073832	2.331854	-0.403558
C	1.964048	-0.675966	-2.349677
C	0.930163	0.516361	2.475247
H	0.478996	-3.520457	0.709411
H	0.734676	0.771119	3.519466
H	2.212746	-0.944772	-3.378953
H	2.395416	3.359867	-0.594577
O	-2.049502	0.632725	-0.787967
C	-3.112201	0.751937	0.220501
C	-4.036652	1.927148	0.069007
C	-3.121887	-0.368196	-0.713294
H	-2.743026	0.555200	1.225734
H	-4.966328	1.711465	0.606196
H	-3.577067	2.840792	0.468014
H	-4.286118	2.087033	-0.985225
Cl	-6.227615	-0.878227	0.202743
H	-3.803209	-0.343629	-1.557962
H	-2.793764	-1.349902	-0.385472

Cl-TS$_1$

Cu	-0.066758	0.325464	-0.275567
Cu	2.462841	-0.424604	0.293295
O	0.601350	-0.141079	-2.153178
O	-0.059517	0.612109	1.745749
O	0.961975	2.110657	-0.437164
O	-0.289632	-1.674491	0.062022
O	1.800296	-2.229789	0.765145
O	3.103660	1.385098	-0.178633
O	2.140011	0.173469	2.147917
O	2.643857	-0.981908	-1.588986
C	1.704239	-0.691288	-2.392356
C	0.964389	0.523162	2.469880
C	2.205663	2.254262	-0.408918
C	0.577837	-2.459656	0.514936
H	1.901589	-0.965918	-3.437007
H	0.235064	-3.477793	0.721472
H	2.576522	3.265018	-0.608826
H	0.839299	0.780704	3.529576
O	-2.003015	0.909764	-0.729775
C	-3.073744	0.941743	0.216659
C	-3.962004	2.163979	0.142975
C	-3.357281	-0.217688	-0.615898
H	-2.756363	0.711876	1.239179
H	-4.865477	1.999202	0.740617
H	-3.427744	3.044306	0.523312
H	-4.259837	2.357317	-0.894088
Cl	-5.558927	-1.175465	0.175668
H	-3.858839	-0.081390	-1.560257
H	-2.915367	-1.173087	-0.382899

Cl-Int$_2$

Cu	-0.162350	0.640752	-0.627408
Cu	2.275813	-0.587156	0.460203
O	-0.412065	-1.529849	-0.735262
O	1.108809	2.265186	0.017067
O	1.175987	0.418305	-2.139013
O	-0.244009	0.147900	1.621915
O	1.842951	-0.315177	2.370586
O	2.854090	-0.929796	-1.425221

O	3.090964	1.187554	0.377711
O	1.363496	-2.315673	0.467551
C	0.253774	-2.410731	-0.145801
C	2.337018	2.204633	0.236430
C	2.183199	-0.311828	-2.299923
C	0.608759	-0.014818	2.510773
H	-0.145733	-3.430917	-0.141721
H	0.282334	0.113236	3.550869
H	2.523369	-0.424585	-3.334301
H	2.885648	3.149533	0.327717
O	-1.895982	1.329659	-0.558475
C	-2.967752	0.815207	0.171087
C	-3.969487	1.937225	0.473116
C	-3.552160	-0.315218	-0.680677
H	-2.606103	0.392119	1.120906
H	-4.824892	1.567665	1.050123
H	-3.463452	2.723465	1.043698
H	-4.337977	2.377688	-0.462939
Cl	-5.015097	-1.204221	0.152929
H	-3.963545	0.056890	-1.619773
H	-2.817454	-1.099321	-0.850312

Cl-Int$_4$

Cu	0.045030	0.518779	-0.065316
Cu	-2.691818	-0.553809	-0.011705
O	-1.026501	1.689726	1.389465
O	-0.022415	-1.173129	-1.449134
O	-1.047356	1.504972	-1.442966
O	-0.322757	-1.194264	1.432909
O	-2.539941	-1.571356	1.681831
O	-3.016665	0.420536	-1.734870
O	-2.069311	-2.098247	-1.032926
O	-3.183579	1.056245	0.978701
C	-2.268694	1.773720	1.498868
C	-0.904310	-2.057530	-1.540625
C	-2.123514	1.259803	-2.039895
C	-1.310403	-1.674044	2.014279
H	-2.673985	2.574186	2.130267
H	-1.120722	-2.256449	2.925321
H	-2.303384	1.857155	-2.939589
H	-0.677720	-2.943205	-2.145921

O	1.849587	0.587028	0.450979
O	1.773660	3.512383	-0.288466
C	2.635363	-0.543820	0.711158
C	2.850252	3.058863	-0.295315
C	3.264089	-0.925767	-0.631648
H	1.993960	-1.371417	1.046298
C	3.657913	-0.236191	1.811487
O	3.964075	2.693373	-0.333087
H	2.497355	-1.168079	-1.364452
H	3.946237	-0.158035	-0.996991
Cl	4.335765	-2.494594	-0.533768
H	4.320785	0.581719	1.503017
H	3.122471	0.075226	2.715217
H	4.269303	-1.115459	2.045149

Cl-TS$_2$

Cu	-0.039693	0.724583	-0.156219
Cu	-2.590223	-0.761295	0.052205
O	-1.129919	1.655914	1.438958
O	0.052948	-0.874994	-1.600367
O	-1.297749	1.610305	-1.369541
O	-0.145134	-1.095740	1.278916
O	-2.203495	-1.957346	1.600241
O	-3.176707	0.348194	-1.525040
O	-1.848617	-2.075180	-1.185911
O	-3.177563	0.655559	1.254204
C	-2.340594	1.498050	1.714009
C	-0.731737	-1.844737	-1.743906
C	-2.413964	1.295684	-1.854406
C	-0.958031	-1.837171	1.856699
H	-2.793602	2.167558	2.460178
H	-0.567157	-2.455849	2.676161
H	-2.742272	1.950849	-2.668678
H	-0.448322	-2.632667	-2.456100
O	1.844868	0.785375	0.335514
O	1.360933	2.976550	-0.488242
C	2.712755	-0.301799	0.627609
C	2.404909	2.465073	-0.190827
C	3.488262	-0.593625	-0.658047
H	2.074147	-1.162276	0.849423
C	3.584933	-0.004789	1.849603

O	3.597726	2.529240	-0.088147
H	2.804624	-0.787433	-1.482590
H	4.208093	0.184899	-0.903355
Cl	4.521261	-2.172149	-0.514168
H	4.241080	0.851750	1.667512
H	2.934123	0.227797	2.699791
H	4.197899	-0.876609	2.105841

Cl-Int$_4$

Cu	0.566297	-0.519353	-0.169906
Cu	2.977367	0.714042	0.156639
O	0.362660	0.241329	1.711100
O	1.499410	-0.929285	-1.959089
O	1.744983	-2.003327	0.662937
O	0.198180	1.354806	-0.905980
O	2.278532	2.276918	-0.830734
O	3.651037	-0.856560	1.144423
O	3.577690	-0.094283	-1.542171
O	2.274468	1.474285	1.841753
C	1.154872	1.045566	2.259484
C	2.701394	-0.703032	-2.233318
C	2.894063	-1.878595	1.144045
C	1.039546	2.261452	-1.109808
H	0.846816	1.439662	3.237799
H	0.659918	3.170210	-1.594386
H	3.314646	-2.766661	1.634155
H	3.060642	-1.076561	-3.202697
O	-1.090929	-1.697810	-0.509444
C	-2.321726	-1.470945	-0.331913
O	-2.553149	-0.165082	0.157250
O	-3.293115	-2.210942	-0.538825
C	-3.879322	0.214234	0.539207
C	-4.843257	0.081465	-0.643129
H	-3.772198	1.282877	0.755190
C	-4.354113	-0.506323	1.802562
H	-4.381552	0.408276	-1.573029
H	-5.288460	-0.901655	-0.746317
Cl	-6.314831	1.261868	-0.405150
H	-4.447435	-1.580030	1.617382
H	-3.628560	-0.348096	2.608330
H	-5.324827	-0.109099	2.123314

Cl-TS$_3$

Cu	-0.632343	-0.488893	-0.059771
Cu	-3.084415	0.612458	0.150133
O	-0.391641	1.150101	-1.234822
O	-1.543111	-1.847114	1.159844
O	-1.606919	-1.373015	-1.632723
O	-0.392249	0.702329	1.576825
O	-2.519640	1.470038	1.835838
O	-3.594673	-0.266917	-1.542388
O	-3.654507	-0.993125	1.154939
O	-2.396308	2.165596	-0.864207
C	-1.227646	2.079938	-1.351755
C	-2.762015	-1.843853	1.458788
C	-2.757590	-1.083025	-2.039263
C	-1.297299	1.348516	2.158121
H	-0.912286	2.939658	-1.957367
H	-1.000071	1.884468	3.068427
H	-3.096199	-1.599767	-2.946874
H	-3.114142	-2.688432	2.066167
O	1.177071	-1.524342	-0.251730
C	2.368167	-1.150450	-0.234112
O	2.616022	0.172939	0.012545
O	3.399700	-1.871621	-0.409906
C	4.008713	0.530951	-0.173011
C	4.883970	-0.670110	0.145532
H	4.190925	1.313190	0.562925
C	4.221713	1.062399	-1.587164
H	4.861779	-1.107748	1.130183
H	5.496532	-1.138147	-0.605163
Cl	6.774209	0.547412	0.774416
H	4.026357	0.277003	-2.326925
H	3.538912	1.896809	-1.778831
H	5.254593	1.408413	-1.694610

Cl-Int$_5$

Cu	-0.732698	-0.446836	-0.067725
Cu	-3.181774	0.576492	0.146235
O	-0.453868	1.262794	-1.120555

O	-1.598578	-1.926561	1.022753
O	-1.592969	-1.258326	-1.731998
O	-0.518376	0.618035	1.653337
O	-2.667926	1.328165	1.900980
O	-3.611662	-0.209313	-1.617425
O	-3.726924	-1.113129	1.029568
O	-2.493676	2.206280	-0.748636
C	-1.310065	2.179289	-1.202450
C	-2.824873	-1.964598	1.293446
C	-2.742417	-0.967127	-2.145907
C	-1.454005	1.207469	2.249056
H	-0.997243	3.081774	-1.739020
H	-1.194082	1.685506	3.199746
H	-3.044800	-1.426856	-3.093547
H	-3.170702	-2.854107	1.832223
O	1.210643	-1.376563	-0.261308
C	2.363409	-0.973964	-0.185127
O	2.711290	0.268505	0.134417
O	3.416957	-1.758626	-0.421626
C	4.174368	0.434316	-0.015749
C	4.648727	-1.022976	-0.106431
H	4.534002	0.915778	0.890206
C	4.459521	1.280968	-1.241764
H	5.045457	-1.404917	0.833147
H	5.363765	-1.202495	-0.905447
Cl	7.298947	0.447526	0.631039
H	4.115284	0.781505	-2.156801
H	3.956824	2.251276	-1.163197
H	5.541774	1.434206	-1.288280

Cu-HKUST-1/Br^-

Br-Int_1

Cu	0.634589	0.259837	-0.342498
Cu	3.112656	-0.396530	0.368252
O	0.292656	-1.642883	0.347603
O	1.569819	1.998558	-0.848354
O	1.300245	-0.553489	-2.099382
O	0.634639	0.894419	1.622452
O	2.840126	0.555410	2.083554
O	3.315012	-1.328638	-1.366872

O	3.708081	1.297550	-0.475095
O	2.377889	-2.054028	1.170499
C	1.158603	-2.322721	0.953211
C	2.820166	2.118756	-0.854070
C	2.387463	-1.169333	-2.216497
C	1.663468	0.951318	2.339457
H	0.824315	-3.283463	1.353090
H	1.537647	1.405040	3.324999
H	2.569651	-1.638216	-3.185823
H	3.210149	3.064681	-1.239376
O	-1.451699	0.727755	-0.789156
C	-2.454922	0.997031	0.243828
C	-3.321598	2.205905	0.023000
C	-2.564165	-0.202111	-0.586142
H	-2.048541	0.872077	1.246584
H	-4.241499	2.100662	0.608988
H	-2.796771	3.121527	0.323977
H	-3.605391	2.288669	-1.030925
Br	-6.097004	-0.491838	0.081632
H	-3.284083	-0.215442	-1.399419
H	-2.268707	-1.167407	-0.184798

Br-TS$_1$

Cu	0.484011	0.435976	-0.401046
Cu	2.867680	-0.583070	0.392508
O	-0.093767	-1.373336	0.406311
O	1.699577	1.952696	-0.982486
O	1.045879	-0.572767	-2.068219
O	0.683527	1.142722	1.551898
O	2.603296	0.119108	2.217047
O	3.119109	-1.277568	-1.445823
O	3.663524	1.139560	-0.155519
O	1.950187	-2.250350	0.896369
C	0.682192	-2.269360	0.819574
C	2.930141	1.999523	-0.730120
C	2.149297	-1.141744	-2.250917
C	1.572354	0.844508	2.381248
H	0.220371	-3.202494	1.165003
H	1.453418	1.261401	3.386014
H	2.295492	-1.581158	-3.241824
H	3.458869	2.907346	-1.047293
O	-1.406979	1.184463	-0.769431

C	-2.453717	1.213318	0.192545
C	-3.215871	2.520142	0.266016
C	-2.903523	0.160121	-0.715074
H	-2.145336	0.856257	1.181471
H	-4.120327	2.391859	0.871132
H	-2.583689	3.296641	0.715100
H	-3.509165	2.847670	-0.738259
Br	-5.286605	-0.702159	0.091521
H	-3.385379	0.432711	-1.641041
H	-2.532195	-0.844194	-0.586777

Br-Int$_2$

Cu	0.349540	0.752012	-0.617712
Cu	2.642213	-0.737437	0.454204
O	-0.112578	-1.375936	-0.786829
O	1.767902	2.226672	0.078411
O	1.672176	0.442807	-2.125237
O	0.198221	0.207725	1.617921
O	2.223616	-0.472524	2.368962
O	3.197484	-1.087802	-1.437370
O	3.630497	0.948979	0.422001
O	1.561248	-2.366143	0.410490
C	0.454243	-2.333985	-0.213767
C	2.982375	2.039194	0.303137
C	2.600868	-0.382457	-2.299490
C	1.023162	-0.056857	2.508464
H	-0.046490	-3.308334	-0.238258
H	0.701403	0.079455	3.548953
H	2.935745	-0.502542	-3.334791
H	3.621422	2.922400	0.422275
O	-1.309805	1.605495	-0.532024
C	-2.434413	1.161304	0.164028
C	-3.324012	2.360325	0.516414
C	-3.108815	0.139585	-0.756555
H	-2.125831	0.657001	1.092401
H	-4.217403	2.051064	1.070849
H	-2.748291	3.063673	1.127624
H	-3.637837	2.880364	-0.398396
Br	-4.774273	-0.764761	0.075164
H	-3.490183	0.597846	-1.669780
H	-2.444325	-0.693856	-0.973840

Br-Int$_3$

Cu	-0.422568	0.649688	-0.093589
Cu	-2.890176	-0.944241	0.005212
O	-1.756790	1.699460	1.232892
O	-0.098612	-1.128918	-1.318439
O	-1.637758	1.278413	-1.569860
O	-0.499653	-0.972250	1.545300
O	-2.604199	-1.766718	1.786120
O	-3.337972	-0.202355	-1.804990
O	-1.934070	-2.410236	-0.861895
O	-3.727425	0.611524	0.837873
C	-2.994081	1.539702	1.310041
C	-0.782598	-2.177857	-1.348122
C	-2.619559	0.771842	-2.165019
C	-1.391694	-1.590858	2.149408
H	-3.574643	2.291411	1.859601
H	-1.121882	-2.043795	3.112434
H	-2.879489	1.244303	-3.117870
H	-0.361794	-3.046888	-1.867668
O	1.312267	1.112169	0.463432
O	0.629744	3.854737	-0.556329
C	2.293488	0.174301	0.812893
C	1.772630	3.709696	-0.362094
C	3.033175	-0.136826	-0.491715
H	1.814072	-0.745848	1.175567
C	3.188920	0.736097	1.923264
O	2.933365	3.657038	-0.203065
H	2.353954	-0.546105	-1.236413
H	3.583305	0.724148	-0.872131
Br	4.480517	-1.599973	-0.299349
H	3.687621	1.653691	1.587975
H	2.565322	0.979917	2.790425
H	3.952169	0.010773	2.227980

Br-TS$_2$

Cu	-0.528460	0.827980	-0.179099
Cu	-2.796821	-1.058368	0.063144

O	-1.825517	1.653687	1.320554
O	-0.108884	-0.818341	-1.505305
O	-1.871912	1.405293	-1.482938
O	-0.380340	-0.890899	1.375710
O	-2.273807	-2.070787	1.699690
O	-3.500941	-0.169460	-1.603105
O	-1.793263	-2.299254	-1.060531
O	-3.665409	0.307667	1.147180
C	-3.001833	1.308430	1.571679
C	-0.711239	-1.916112	-1.602547
C	-2.898590	0.872855	-1.975484
C	-1.077597	-1.722527	1.981170
H	-3.590985	1.935591	2.257150
H	-0.619584	-2.211292	2.852043
H	-3.301789	1.409334	-2.841310
H	-0.270590	-2.686877	-2.250640
O	1.297577	1.237578	0.368149
O	0.478886	3.247768	-0.628145
C	2.325406	0.328487	0.741870
C	1.583094	2.947294	-0.265842
C	3.163838	0.089736	-0.515562
H	1.828886	-0.607482	1.014738
C	3.107970	0.846207	1.951059
O	2.741732	3.226148	-0.135973
H	2.536704	-0.251325	-1.337077
H	3.767342	0.950961	-0.796205
Br	4.527903	-1.426758	-0.273871
H	3.622258	1.783035	1.716529
H	2.406923	1.028865	2.772975
H	3.846126	0.105527	2.279622

Br-Int$_4$

Cu	-1.097604	0.541175	-0.209480
Cu	-3.428561	-0.815823	0.200820
O	-0.874346	-0.038613	1.733022
O	-2.027463	0.732770	-2.036449
O	-2.382838	2.009900	0.479749
O	-0.596843	-1.361559	-0.774232
O	-2.614321	-2.408229	-0.640179
O	-4.218174	0.786535	1.040917
O	-4.053296	-0.198226	-1.567749

O	-2.703452	-1.379852	1.952217
C	-1.620703	-0.843336	2.341733
C	-3.207983	0.404792	-2.301162
C	-3.528753	1.852139	0.958771
C	-1.374708	-2.335601	-0.907097
H	-1.302356	-1.130171	3.353561
H	-0.929782	-3.255826	-1.307180
H	-4.013153	2.749781	1.365460
H	-3.576178	0.668359	-3.302821
O	0.485107	1.792130	-0.635257
C	1.724632	1.666620	-0.421544
O	2.031883	0.426294	0.184597
O	2.647927	2.450577	-0.679330
C	3.371860	0.169332	0.620439
C	4.338392	0.242855	-0.564888
H	3.320818	-0.875074	0.946674
C	3.779642	1.044229	1.807587
H	3.915638	-0.219131	-1.455126
H	4.712432	1.238877	-0.774379
Br	6.030217	-0.876484	-0.187059
H	3.821647	2.095713	1.510842
H	3.043399	0.932928	2.611491
H	4.760976	0.736276	2.188187

Br-TS$_3$

Cu	-1.181162	0.507770	-0.047976
Cu	-3.594717	-0.698246	-0.048297
O	-0.949080	-0.756454	1.525095
O	-2.073065	1.463115	-1.614123
O	-2.250136	1.735752	1.200125
O	-0.837978	-1.061355	-1.301926
O	-2.928520	-1.955283	-1.416883
O	-4.209047	0.582333	1.322981
O	-4.157203	0.555576	-1.470470
O	-2.915869	-1.895213	1.373183
C	-1.770401	-1.645859	1.859275
C	-3.274633	1.331502	-1.951742
C	-3.413294	1.526883	1.620269
C	-1.697518	-1.875255	-1.718254
H	-1.463370	-2.301556	2.684486
H	-1.345115	-2.622750	-2.440209

H	-3.805720	2.253870	2.343242
H	-3.619165	1.970887	-2.775471
O	0.585843	1.628694	-0.061014
C	1.789835	1.317027	0.055616
O	2.088909	-0.020065	0.137711
O	2.786113	2.101093	0.093470
C	3.475068	-0.277253	0.468209
C	4.350969	0.815756	-0.123474
H	3.695702	-1.224482	-0.023646
C	3.633233	-0.410541	1.980540
H	4.329615	1.006070	-1.184484
H	4.913105	1.488863	0.500583
Br	6.431546	-0.498039	-0.423320
H	3.395949	0.537743	2.476629
H	2.952364	-1.180129	2.358712
H	4.663699	-0.692433	2.220458

Br-Int$_5$

Cu	1.340568	-0.463776	0.024375
Cu	3.757799	0.637778	-0.131740
O	1.065693	1.075336	1.318797
O	2.187206	-1.756694	-1.295383
O	2.278054	-1.479990	1.527179
O	1.035394	0.826754	-1.521142
O	3.161163	1.613606	-1.745511
O	4.270679	-0.376118	1.488910
O	4.298892	-0.900390	-1.261439
O	3.072007	2.109447	1.007200
C	1.908263	1.991155	1.495625
C	3.403121	-1.727056	-1.610553
C	3.436941	-1.220803	1.936087
C	1.936934	1.514218	-2.061939
H	1.601385	2.802772	2.163573
H	1.631772	2.113483	-2.925993
H	3.784255	-1.800184	2.798300
H	3.744855	-2.523655	-2.280199
O	-0.591390	-1.454945	0.166857
C	-1.752159	-1.077033	0.179065
O	-2.142831	0.183871	0.004371
O	-2.781812	-1.908193	0.373822
C	-3.594643	0.295005	0.238207

C	-4.034867	-1.176269	0.184526
H	-4.008138	0.865672	-0.591071
C	-3.839891	0.993667	1.562992
H	-4.460856	-1.461242	-0.777549
H	-4.718005	-1.458381	0.983072
Br	-7.008851	0.339815	-0.398931
H	-3.445028	0.404892	2.400808
H	-3.359052	1.977762	1.570777
H	-4.920698	1.120527	1.681095

Cu-HKUST-1/I^-

I-Int_1

Cu	1.230295	0.276448	-0.334200
Cu	3.689315	-0.447047	0.363531
O	1.857505	-0.465473	-2.125338
O	1.185531	0.843773	1.637825
O	2.224189	2.015964	-0.754101
O	0.873615	-1.656918	0.285594
O	2.950522	-2.132091	1.094128
O	4.345614	1.262514	-0.390123
O	3.379714	0.446208	2.111211
O	3.860943	-1.298025	-1.421519
C	2.938453	-1.089389	-2.265044
C	2.208050	0.852026	2.368420
C	3.475819	2.115010	-0.741340
C	1.728298	-2.373997	0.862845
H	3.118140	-1.517141	-3.253730
H	1.379804	-3.345399	1.220107
H	3.885274	3.069617	-1.079344
H	2.076973	1.267256	3.370103
O	-0.858761	0.788348	-0.790319
C	-1.844165	1.096523	0.245348
C	-2.688161	2.318960	0.009103
C	-1.981914	-0.116533	-0.563944
H	-1.429677	0.982285	1.246076
H	-3.601761	2.253681	0.611031
H	-2.138559	3.228628	0.281618
H	-2.984978	2.385354	-1.042375
I	-6.040288	-0.328581	0.049926
H	-2.709444	-0.131311	-1.371083

H	-1.698463	-1.080787	-0.150308

I-TS$_1$

Cu	0.917621	0.447834	-0.268387
Cu	3.326070	-0.645417	0.289061
O	1.644517	0.176783	-2.163885
O	0.841989	0.438337	1.771454
O	2.143746	2.111620	-0.139197
O	0.467757	-1.540244	-0.223052
O	2.540579	-2.443498	0.021190
O	4.089142	1.156886	0.556665
O	2.776506	-0.691672	2.185652
O	3.742827	-0.540470	-1.634791
C	2.815993	-0.188615	-2.428568
C	1.692726	-0.119480	2.510782
C	3.332878	2.132115	0.252303
C	1.284013	-2.490396	-0.145030
H	3.095687	-0.214647	-3.490116
H	0.854669	-3.492848	-0.232678
H	3.789929	3.122558	0.348629
H	1.482669	-0.117568	3.588101
O	-0.897530	1.336544	-0.711119
C	-1.990961	1.397990	0.185855
C	-2.703871	2.736445	0.217396
C	-2.474323	0.349347	-0.720111
H	-1.750885	1.039519	1.194383
H	-3.636702	2.657525	0.786894
H	-2.056666	3.489534	0.684256
H	-2.939253	3.066528	-0.801298
I	-5.045880	-0.504425	0.057554
H	-2.887182	0.638235	-1.675173
H	-2.122625	-0.663114	-0.591989

I-Int$_2$

Cu	0.794166	0.811574	-0.606346
Cu	2.989833	-0.828067	0.446389
O	0.215103	-1.280378	-0.834167
O	2.284034	2.188609	0.139740

O	2.111742	0.468440	-2.109271
O	0.590068	0.222094	1.613200
O	2.567044	-0.588707	2.363571
O	3.543843	-1.161057	-1.449018
O	4.069801	0.801329	0.465491
O	1.820351	-2.391751	0.350803
C	0.722951	-2.282760	-0.281544
C	3.484065	1.928492	0.369951
C	2.995565	-0.401987	-2.297349
C	1.390066	-0.110736	2.503620
H	0.169736	-3.227030	-0.335841
H	1.065702	0.016457	3.544437
H	3.333456	-0.513188	-3.332626
H	4.169661	2.771609	0.517943
O	-0.815255	1.756282	-0.510192
C	-1.970314	1.359366	0.163569
C	-2.791317	2.601307	0.534799
C	-2.688782	0.398834	-0.792579
H	-1.699983	0.817625	1.082728
H	-3.704778	2.337385	1.079927
H	-2.178909	3.257965	1.161958
H	-3.068406	3.155883	-0.371477
I	-4.540952	-0.559690	0.048661
H	-3.042615	0.903292	-1.692879
H	-2.056658	-0.452117	-1.038517

I-Int$_3$

Cu	-0.841662	0.697275	-0.103378
Cu	-3.106819	-1.174818	0.011059
O	-2.305799	1.611245	1.187444
O	-0.295104	-1.054779	-1.283461
O	-2.103383	1.146782	-1.602684
O	-0.750381	-0.888647	1.570704
O	-2.745241	-1.928331	1.809006
O	-3.621709	-0.523008	-1.816204
O	-1.975536	-2.531787	-0.820626
O	-4.128690	0.285795	0.808040
C	-3.515246	1.304799	1.263607
C	-0.853541	-2.176033	-1.300846
C	-3.016938	0.519908	-2.191979
C	-1.566746	-1.600746	2.178860

H	-4.185697	1.991432	1.795811
H	-1.253085	-2.001171	3.151757
H	-3.322322	0.942155	-3.154796
H	-0.330379	-2.999149	-1.801828
O	0.817740	1.372940	0.468683
O	-0.179835	3.969648	-0.663084
C	1.896645	0.568852	0.859646
C	0.959318	3.996034	-0.404942
C	2.684937	0.305460	-0.429637
H	1.521869	-0.387655	1.250241
C	2.701045	1.272749	1.959200
O	2.104787	4.114672	-0.183503
H	2.058696	-0.186324	-1.171332
H	3.142523	1.211900	-0.827822
I	4.413820	-1.109890	-0.201322
H	3.096924	2.228131	1.593927
H	2.036750	1.476750	2.806108
H	3.536562	0.654481	2.307269

I-TS$_2$

Cu	-0.952153	0.865017	-0.191375
Cu	-3.026396	-1.232936	0.070135
O	-2.357127	1.596005	1.262913
O	-0.345003	-0.768357	-1.458514
O	-2.323702	1.265521	-1.531820
O	-0.663854	-0.788617	1.417137
O	-2.439175	-2.138212	1.747008
O	-3.782081	-0.469390	-1.635396
O	-1.880262	-2.398577	-0.996721
O	-4.050634	0.069396	1.094942
C	-3.498552	1.142524	1.502249
C	-0.831832	-1.923941	-1.531941
C	-3.280422	0.618049	-2.027409
C	-1.288380	-1.666068	2.037100
H	-4.161558	1.726175	2.158097
H	-0.802134	-2.081342	2.930567
H	-3.716946	1.086747	-2.916176
H	-0.303025	-2.664484	-2.148432
O	0.811153	1.470265	0.382555
O	-0.186990	3.344216	-0.708379
C	1.919696	0.678046	0.791934

C	0.933391	3.176154	-0.310924
C	2.786706	0.480797	-0.455615
H	1.510994	-0.289936	1.096655
C	2.634471	1.314343	1.986997
O	2.051858	3.581912	-0.166235
H	2.194152	0.067081	-1.269740
H	3.306220	1.388200	-0.759452
I	4.415524	-1.018965	-0.182236
H	3.065106	2.283676	1.718801
H	1.906986	1.466388	2.791907
H	3.431438	0.659564	2.357975

I-Int$_4$

Cu	-1.574579	0.555812	-0.222345
Cu	-3.848361	-0.886258	0.217889
O	-1.325294	0.023009	1.730143
O	-2.515960	0.674972	-2.050216
O	-2.916167	1.984847	0.442441
O	-0.999146	-1.336509	-0.751958
O	-2.973860	-2.459335	-0.598697
O	-4.697999	0.698009	1.033346
O	-4.502848	-0.325405	-1.558662
O	-3.095703	-1.390357	1.976083
C	-2.036060	-0.802012	2.354118
C	-3.683297	0.296461	-2.305558
C	-4.053200	1.789247	0.928661
C	-1.738103	-2.342539	-0.867772
H	-1.704282	-1.057780	3.370024
H	-1.257492	-3.251251	-1.252611
H	-4.572955	2.673736	1.320274
H	-4.063608	0.526899	-3.310901
O	-0.043954	1.857952	-0.683828
C	1.198512	1.791865	-0.459521
O	1.548984	0.585406	0.192988
O	2.089728	2.604059	-0.739399
C	2.894415	0.386741	0.645853
C	3.846953	0.400619	-0.554214
H	2.861023	-0.632903	1.045040
C	3.282323	1.348954	1.770889
H	3.432377	-0.158988	-1.391296
H	4.148160	1.397064	-0.860965

I	5.764061	-0.664271	-0.112492
H	3.320844	2.376625	1.400637
H	2.535137	1.289497	2.570253
H	4.259288	1.077195	2.188196

I-TS$_3$

Cu	-1.680825	0.508577	-0.132153
Cu	-4.057756	-0.754021	0.047955
O	-1.435151	-0.464600	1.634534
O	-2.576041	1.159693	-1.845119
O	-2.802195	1.895079	0.883213
O	-1.277128	-1.238167	-1.102043
O	-3.224610	-2.360052	-0.741821
O	-4.838596	0.878588	0.837093
O	-4.483961	-0.081574	-1.762332
O	-3.515844	-1.366268	1.849710
C	-2.330502	-1.115836	2.227388
C	-3.673197	0.741769	-2.288892
C	-4.034749	1.825241	1.104644
C	-2.034100	-2.236994	-1.166383
H	-2.058122	-1.529200	3.207356
H	-1.618474	-3.128129	-1.653693
H	-4.489690	2.695293	1.596112
H	-3.983222	1.137543	-3.265263
O	0.054400	1.664562	-0.312391
C	1.263897	1.415798	-0.121347
O	1.594196	0.114494	0.177466
O	2.236041	2.225266	-0.185930
C	2.971186	-0.052049	0.589589
C	3.854197	0.925937	-0.170498
H	3.210466	-1.072771	0.290904
C	3.084948	0.099141	2.104861
H	3.830002	0.942082	-1.248685
H	4.382255	1.717489	0.333213
I	6.138758	-0.435513	-0.252584
H	2.827624	1.120175	2.408732
H	2.396624	-0.594639	2.598241
H	4.108250	-0.121986	2.426557

I-Int$_5$

Cu	-1.910524	0.471594	-0.016400
Cu	-4.303866	-0.681451	-0.104240
O	-1.619170	-0.948956	1.405883
O	-2.761591	1.635405	-1.449562
O	-2.881005	1.594352	1.387655
O	-1.559763	-0.938076	-1.445217
O	-3.672486	-1.769525	-1.631742
O	-4.849398	0.447411	1.428091
O	-4.861160	0.753290	-1.356290
O	-3.600750	-2.045691	1.153701
C	-2.446738	-1.864432	1.645140
C	-3.974889	1.561069	-1.767680
C	-4.037604	1.344205	1.808645
C	-2.445710	-1.678686	-1.939817
H	-2.133928	-2.613093	2.379893
H	-2.121860	-2.340771	-2.748987
H	-4.404615	1.985031	2.617014
H	-4.323500	2.293610	-2.502977
O	0.016061	1.504142	0.070450
C	1.178875	1.146474	0.140497
O	1.593992	-0.118309	0.061552
O	2.194468	2.004203	0.307749
C	3.034112	-0.190578	0.348991
C	3.457362	1.280940	0.204794
H	3.481239	-0.813121	-0.424923
C	3.246996	-0.791125	1.726989
H	3.908493	1.504305	-0.763060
H	4.114874	1.626715	1.000868
I	6.786935	-0.274022	-0.277612
H	2.818635	-0.151224	2.508588
H	2.778210	-1.778829	1.788930
H	4.324169	-0.896743	1.893140

Catalyst: M-HKUST-1 (M = Mo, Cr, Ti, Cu, W, Sc, Fe, Ru, Zn, Cd and V); Co-catalyst: Br^-

Cu-HKUST-1

Cu-HKUST-1

Cu	-0.000845	0.000072	-1.273814
Cu	0.001419	-0.000084	1.274814
O	-0.331103	-1.955835	-1.137057
O	0.328968	1.956093	-1.137254
O	1.955459	-0.330104	-1.137144
O	-1.956996	0.330169	-1.134876
O	-1.955957	0.322800	1.137654
O	1.958186	-0.323260	1.135367
O	0.323352	1.957379	1.135270
O	-0.323023	-1.957200	1.135459
C	-0.418297	-2.505718	-0.000795
C	0.416957	2.506008	-0.001076
C	2.506060	-0.417742	-0.001308
C	-2.505706	0.417457	0.001945
H	-0.598610	-3.590763	-0.000795
H	-3.590779	0.597622	0.003049
H	3.591099	-0.598069	-0.002001
H	0.596455	3.591188	-0.001221

PO

C	1.045532	0.618438	-0.058795
C	-0.153400	-0.036372	0.488109
O	0.829685	-0.790173	-0.242933
H	0.961329	1.217787	-0.965972
H	1.878173	0.875102	0.596442
H	-0.154300	-0.261705	1.557102
C	-1.513810	0.099789	-0.148751
H	-2.081234	-0.833758	-0.051389
H	-2.088544	0.897881	0.338548
H	-1.422838	0.334952	-1.214647

PC

C	-2.299350	-0.562585	-0.264468
H	-2.567309	-1.562282	0.090954
H	-2.158027	-0.604602	-1.349902
H	-3.134690	0.113538	-0.044825
C	-1.040952	-0.070358	0.423612
O	0.071393	-0.949067	0.127319
C	-0.506182	1.286954	-0.057074
H	-0.809324	1.512023	-1.086753
H	-0.768896	2.120800	0.596687
H	-1.167957	-0.073790	1.513590
C	1.210683	-0.219455	-0.019738
O	0.919640	1.112722	-0.024243
O	2.311592	-0.677782	-0.129794

Cu-Int$_0$

Cu	-0.522738	-0.085332	-0.275052
Cu	2.027482	0.134211	0.279923
O	-0.479155	-1.481331	1.180370
O	-0.116916	1.346561	-1.604020
O	0.145988	-1.462924	-1.572033
O	-0.685169	1.328771	1.162352
O	1.540070	1.530638	1.588463
O	2.354814	-1.276146	-1.059041
O	2.106683	1.502401	-1.145676
O	1.732196	-1.255923	1.662713
C	0.581521	-1.756473	1.809718
C	1.045762	1.810708	-1.762555
C	1.367502	-1.756766	-1.688300
C	0.319461	1.818929	1.749646
H	0.494704	-2.527562	2.583093
H	0.112698	2.593559	2.496440
H	1.609341	-2.527547	-2.428121
H	1.152272	2.580856	-2.533870
O	-2.703362	-0.289104	-0.610538
C	-3.693463	0.090141	0.386476
C	-4.840335	0.923912	-0.119300
C	-3.509053	-1.320833	0.013674
H	-3.231875	0.421231	1.315937
H	-5.656925	0.922668	0.613589

H	-4.522048	1.961371	-0.271856
H	-5.220455	0.533990	-1.069158
H	-4.213942	-1.789917	-0.670826
H	-2.950902	-1.987380	0.666641

Cu-Int$_1$

Cu	0.634589	0.259837	-0.342498
Cu	3.112656	-0.396530	0.368252
O	0.292656	-1.642883	0.347603
O	1.569819	1.998558	-0.848354
O	1.300245	-0.553489	-2.099382
O	0.634639	0.894419	1.622452
O	2.840126	0.555410	2.083554
O	3.315012	-1.328638	-1.366872
O	3.708081	1.297550	-0.475095
O	2.377889	-2.054028	1.170499
C	1.158603	-2.322721	0.953211
C	2.820166	2.118756	-0.854070
C	2.387463	-1.169333	-2.216497
C	1.663468	0.951318	2.339457
H	0.824315	-3.283463	1.353090
H	1.537647	1.405040	3.324999
H	2.569651	-1.638216	-3.185823
H	3.210149	3.064681	-1.239376
O	-1.451699	0.727755	-0.789156
C	-2.454922	0.997031	0.243828
C	-3.321598	2.205905	0.023000
C	-2.564165	-0.202111	-0.586142
H	-2.048541	0.872077	1.246584
H	-4.241499	2.100662	0.608988
H	-2.796771	3.121527	0.323977
H	-3.605391	2.288669	-1.030925
Br	-6.097004	-0.491838	0.081632
H	-3.284083	-0.215442	-1.399419
H	-2.268707	-1.167407	-0.184798

Cu-TS$_1$

Cu	0.484011	0.435976	-0.401046

Cu	2.867680	-0.583070	0.392508
O	-0.093767	-1.373336	0.406311
O	1.699577	1.952696	-0.982486
O	1.045879	-0.572767	-2.068219
O	0.683527	1.142722	1.551898
O	2.603296	0.119108	2.217047
O	3.119109	-1.277568	-1.445823
O	3.663524	1.139560	-0.155519
O	1.950187	-2.250350	0.896369
C	0.682192	-2.269360	0.819574
C	2.930141	1.999523	-0.730120
C	2.149297	-1.141744	-2.250917
C	1.572354	0.844508	2.381248
H	0.220371	-3.202494	1.165003
H	1.453418	1.261401	3.386014
H	2.295492	-1.581158	-3.241824
H	3.458869	2.907346	-1.047293
O	-1.406979	1.184463	-0.769431
C	-2.453717	1.213318	0.192545
C	-3.215871	2.520142	0.266016
C	-2.903523	0.160121	-0.715074
H	-2.145336	0.856257	1.181471
H	-4.120327	2.391859	0.871132
H	-2.583689	3.296641	0.715100
H	-3.509165	2.847670	-0.738259
Br	-5.286605	-0.702159	0.091521
H	-3.385379	0.432711	-1.641041
H	-2.532195	-0.844194	-0.586777

Cu-Int$_2$

Cu	0.349540	0.752012	-0.617712
Cu	2.642213	-0.737437	0.454204
O	-0.112578	-1.375936	-0.786829
O	1.767902	2.226672	0.078411
O	1.672176	0.442807	-2.125237
O	0.198221	0.207725	1.617921
O	2.223616	-0.472524	2.368962
O	3.197484	-1.087802	-1.437370
O	3.630497	0.948979	0.422001
O	1.561248	-2.366143	0.410490
C	0.454243	-2.333985	-0.213767

C	2.982375	2.039194	0.303137
C	2.600868	-0.382457	-2.299490
C	1.023162	-0.056857	2.508464
H	-0.046490	-3.308334	-0.238258
H	0.701403	0.079455	3.548953
H	2.935745	-0.502542	-3.334791
H	3.621422	2.922400	0.422275
O	-1.309805	1.605495	-0.532024
C	-2.434413	1.161304	0.164028
C	-3.324012	2.360325	0.516414
C	-3.108815	0.139585	-0.756555
H	-2.125831	0.657001	1.092401
H	-4.217403	2.051064	1.070849
H	-2.748291	3.063673	1.127624
H	-3.637837	2.880364	-0.398396
Br	-4.774273	-0.764761	0.075164
H	-3.490183	0.597846	-1.669780
H	-2.444325	-0.693856	-0.973840

Cu-Int$_3$

Cu	-0.422568	0.649688	-0.093589
Cu	-2.890176	-0.944241	0.005212
O	-1.756790	1.699460	1.232892
O	-0.098612	-1.128918	-1.318439
O	-1.637758	1.278413	-1.569860
O	-0.499653	-0.972250	1.545300
O	-2.604199	-1.766718	1.786120
O	-3.337972	-0.202355	-1.804990
O	-1.934070	-2.410236	-0.861895
O	-3.727425	0.611524	0.837873
C	-2.994081	1.539702	1.310041
C	-0.782598	-2.177857	-1.348122
C	-2.619559	0.771842	-2.165019
C	-1.391694	-1.590858	2.149408
H	-3.574643	2.291411	1.859601
H	-1.121882	-2.043795	3.112434
H	-2.879489	1.244303	-3.117870
H	-0.361794	-3.046888	-1.867668
O	1.312267	1.112169	0.463432
O	0.629744	3.854737	-0.556329
C	2.293488	0.174301	0.812893

C	1.772630	3.709696	-0.362094
C	3.033175	-0.136826	-0.491715
H	1.814072	-0.745848	1.175567
C	3.188920	0.736097	1.923264
O	2.933365	3.657038	-0.203065
H	2.353954	-0.546105	-1.236413
H	3.583305	0.724148	-0.872131
Br	4.480517	-1.599973	-0.299349
H	3.687621	1.653691	1.587975
H	2.565322	0.979917	2.790425
H	3.952169	0.010773	2.227980

Cu-TS$_2$

Cu	-0.528460	0.827980	-0.179099
Cu	-2.796821	-1.058368	0.063144
O	-1.825517	1.653687	1.320554
O	-0.108884	-0.818341	-1.505305
O	-1.871912	1.405293	-1.482938
O	-0.380340	-0.890899	1.375710
O	-2.273807	-2.070787	1.699690
O	-3.500941	-0.169460	-1.603105
O	-1.793263	-2.299254	-1.060531
O	-3.665409	0.307667	1.147180
C	-3.001833	1.308430	1.571679
C	-0.711239	-1.916112	-1.602547
C	-2.898590	0.872855	-1.975484
C	-1.077597	-1.722527	1.981170
H	-3.590985	1.935591	2.257150
H	-0.619584	-2.211292	2.852043
H	-3.301789	1.409334	-2.841310
H	-0.270590	-2.686877	-2.250640
O	1.297577	1.237578	0.368149
O	0.478886	3.247768	-0.628145
C	2.325406	0.328487	0.741870
C	1.583094	2.947294	-0.265842
C	3.163838	0.089736	-0.515562
H	1.828886	-0.607482	1.014738
C	3.107970	0.846207	1.951059
O	2.741732	3.226148	-0.135973
H	2.536704	-0.251325	-1.337077
H	3.767342	0.950961	-0.796205

Br	4.527903	-1.426758	-0.273871
H	3.622258	1.783035	1.716529
H	2.406923	1.028865	2.772975
H	3.846126	0.105527	2.279622

Cu-Int$_4$

Cu	-1.097604	0.541175	-0.209480
Cu	-3.428561	-0.815823	0.200820
O	-0.874346	-0.038613	1.733022
O	-2.027463	0.732770	-2.036449
O	-2.382838	2.009900	0.479749
O	-0.596843	-1.361559	-0.774232
O	-2.614321	-2.408229	-0.640179
O	-4.218174	0.786535	1.040917
O	-4.053296	-0.198226	-1.567749
O	-2.703452	-1.379852	1.952217
C	-1.620703	-0.843336	2.341733
C	-3.207983	0.404792	-2.301162
C	-3.528753	1.852139	0.958771
C	-1.374708	-2.335601	-0.907097
H	-1.302356	-1.130171	3.353561
H	-0.929782	-3.255826	-1.307180
H	-4.013153	2.749781	1.365460
H	-3.576178	0.668359	-3.302821
O	0.485107	1.792130	-0.635257
C	1.724632	1.666620	-0.421544
O	2.031883	0.426294	0.184597
O	2.647927	2.450577	-0.679330
C	3.371860	0.169332	0.620439
C	4.338392	0.242855	-0.564888
H	3.320818	-0.875074	0.946674
C	3.779642	1.044229	1.807587
H	3.915638	-0.219131	-1.455126
H	4.712432	1.238877	-0.774379
Br	6.030217	-0.876484	-0.187059
H	3.821647	2.095713	1.510842
H	3.043399	0.932928	2.611491
H	4.760976	0.736276	2.188187

Cu-TS_3

Cu	-1.181162	0.507770	-0.047976
Cu	-3.594717	-0.698246	-0.048297
O	-0.949080	-0.756454	1.525095
O	-2.073065	1.463115	-1.614123
O	-2.250136	1.735752	1.200125
O	-0.837978	-1.061355	-1.301926
O	-2.928520	-1.955283	-1.416883
O	-4.209047	0.582333	1.322981
O	-4.157203	0.555576	-1.470470
O	-2.915869	-1.895213	1.373183
C	-1.770401	-1.645859	1.859275
C	-3.274633	1.331502	-1.951742
C	-3.413294	1.526883	1.620269
C	-1.697518	-1.875255	-1.718254
H	-1.463370	-2.301556	2.684486
H	-1.345115	-2.622750	-2.440209
H	-3.805720	2.253870	2.343242
H	-3.619165	1.970887	-2.775471
O	0.585843	1.628694	-0.061014
C	1.789835	1.317027	0.055616
O	2.088909	-0.020065	0.137711
O	2.786113	2.101093	0.093470
C	3.475068	-0.277253	0.468209
C	4.350969	0.815756	-0.123474
H	3.695702	-1.224482	-0.023646
C	3.633233	-0.410541	1.980540
H	4.329615	1.006070	-1.184484
H	4.913105	1.488863	0.500583
Br	6.431546	-0.498039	-0.423320
H	3.395949	0.537743	2.476629
H	2.952364	-1.180129	2.358712
H	4.663699	-0.692433	2.220458

Cu-Int_5

Cu	1.340568	-0.463776	0.024375
Cu	3.757799	0.637778	-0.131740
O	1.065693	1.075336	1.318797
O	2.187206	-1.756694	-1.295383

O	2.278054	-1.479990	1.527179
O	1.035394	0.826754	-1.521142
O	3.161163	1.613606	-1.745511
O	4.270679	-0.376118	1.488910
O	4.298892	-0.900390	-1.261439
O	3.072007	2.109447	1.007200
C	1.908263	1.991155	1.495625
C	3.403121	-1.727056	-1.610553
C	3.436941	-1.220803	1.936087
C	1.936934	1.514218	-2.061939
H	1.601385	2.802772	2.163573
H	1.631772	2.113483	-2.925993
H	3.784255	-1.800184	2.798300
H	3.744855	-2.523655	-2.280199
O	-0.591390	-1.454945	0.166857
C	-1.752159	-1.077033	0.179065
O	-2.142831	0.183871	0.004371
O	-2.781812	-1.908193	0.373822
C	-3.594643	0.295005	0.238207
C	-4.034867	-1.176269	0.184526
H	-4.008138	0.865672	-0.591071
C	-3.839891	0.993667	1.562992
H	-4.460856	-1.461242	-0.777549
H	-4.718005	-1.458381	0.983072
Br	-7.008851	0.339815	-0.398931
H	-3.445028	0.404892	2.400808
H	-3.359052	1.977762	1.570777
H	-4.920698	1.120527	1.681095

Zn-HKUST-1

Zn-HKUST-1

Zn	-1.427603	0.013269	-0.002662
Zn	1.427628	-0.013411	0.002920
O	-1.695293	1.431170	-1.361975
O	-1.728351	-1.399448	1.355657
O	-0.536363	1.359023	1.409607
O	-0.557253	-1.349903	-1.412952
O	1.701401	-1.375418	-1.411183
O	1.722221	1.343841	1.418000
O	0.530257	-1.415798	1.355332
O	0.563343	1.406549	-1.353914

C	-0.550368	1.832371	-1.754455
C	-0.592333	-1.820779	1.752812
C	0.584431	1.748733	1.826965
C	0.558215	-1.759846	-1.824993
H	-0.551557	2.626269	-2.515413
H	0.562786	-2.522308	-2.617431
H	0.599045	2.510733	2.619711
H	-0.610408	-2.613426	2.514844

Zn-Int$_0$

Zn	-2.092629	-0.138995	0.456805
Zn	0.697817	0.119465	-0.536692
O	-1.761104	0.007792	2.416476
O	-3.132674	-0.349920	-1.226228
O	-1.182194	-2.040711	0.338668
O	-1.624692	1.892465	0.120238
O	0.482557	2.083758	-0.687733
O	0.924680	-1.848696	-0.470390
O	-1.016495	-0.153309	-1.980323
O	0.366672	0.203051	1.677147
C	-0.509622	0.156459	2.582592
C	-2.254726	-0.302465	-2.149542
C	-0.074298	-2.499128	-0.032000
C	-0.641199	2.541230	-0.311835
H	-0.187435	0.251049	3.630133
H	-0.734459	3.627482	-0.375000
H	0.075791	-3.579303	0.026000
H	-2.644942	-0.403729	-3.173190
O	2.829616	0.339834	-0.601008
C	3.713418	-0.178510	0.441834
C	4.891169	-0.974594	-0.047939
C	3.577208	1.271287	0.225227
H	3.153594	-0.602211	1.274380
H	5.626718	-1.084731	0.758471
H	4.570969	-1.975371	-0.357518
H	5.373877	-0.482220	-0.898264
H	4.345868	1.807595	-0.327312
H	2.961775	1.867546	0.894115

Zn-Int$_1$

Zn	-3.152070	-0.428903	-0.373044
Zn	-0.225613	0.291269	0.390578
O	-2.620430	-2.195566	-1.223347
O	-4.624046	0.892471	0.121922
O	-2.377417	0.601446	-2.018503
O	-2.840009	-1.243726	1.525765
O	-0.836031	-0.392272	2.169942
O	-0.384593	1.397617	-1.278091
O	-2.591791	1.592252	0.750201
O	-0.555027	-1.517259	-0.595326
C	-1.365866	-2.324778	-1.124285
C	-3.833638	1.738919	0.664336
C	-1.317398	1.266069	-2.126380
C	-1.902056	-1.056039	2.339915
H	-0.935755	-3.238200	-1.543702
H	-2.008914	-1.534075	3.323014
H	-1.168915	1.793900	-3.078070
H	-4.288001	2.648120	1.076811
O	1.695083	0.755855	0.832812
C	2.815718	1.044639	-0.102814
C	3.508894	2.357932	0.109630
C	2.972447	-0.069627	0.811690
H	2.561442	0.800672	-1.132208
H	4.498214	2.289292	-0.355921
H	2.939516	3.180932	-0.339343
H	3.645167	2.554692	1.178254
Br	5.871811	-0.577435	-0.215673
H	3.548515	0.058681	1.719080
H	2.831293	-1.083987	0.459082

Zn-TS$_1$

Zn	3.095090	0.513294	-0.324507
Zn	0.172178	-0.387497	0.389738
O	2.512388	2.418929	-0.736477
O	4.631566	-0.834884	-0.212098
O	2.273058	-0.125040	-2.133428
O	2.884991	0.896366	1.715900
O	0.921082	-0.119197	2.235494
O	0.325135	-1.100918	-1.495002
O	2.639888	-1.698294	0.332848
O	0.479531	1.588328	-0.187181
C	1.263596	2.503081	-0.557370

C	3.877357	-1.797164	0.161778
C	1.214115	-0.769876	-2.334938
C	1.986731	0.509817	2.504901
H	0.809079	3.478414	-0.743637
H	2.138265	0.757160	3.565503
H	1.027829	-1.078533	-3.373665
H	4.355494	-2.766581	0.340976
O	-1.708453	-0.940999	0.793959
C	-2.779648	-1.161560	-0.170217
C	-3.483790	-2.487102	-0.045374
C	-3.113445	-0.048439	0.698727
H	-2.489463	-0.904007	-1.189861
H	-4.430631	-2.435368	-0.593446
H	-2.864065	-3.292474	-0.458424
H	-3.702212	-2.709221	1.004743
Br	-5.708689	0.664692	-0.188594
H	-3.648204	-0.219369	1.619953
H	-2.872977	0.964943	0.414534

Zn-Int$_2$

Zn	2.984301	-0.629851	-0.001260
Zn	0.034554	0.704880	-0.172377
O	2.567570	-1.987963	-1.480743
O	4.472310	0.008503	1.298309
O	1.897081	-1.775119	1.345513
O	3.210857	0.845759	-1.446214
O	1.258396	1.981682	-1.197170
O	-0.004068	-0.539095	1.476601
O	2.532582	1.114679	1.418973
O	0.580116	-0.907439	-1.405933
C	1.376541	-1.776110	-1.846529
C	3.712142	0.910608	1.787690
C	0.759596	-1.489518	1.803959
C	2.408728	1.787337	-1.679888
H	0.986814	-2.419631	-2.637268
H	2.762779	2.533679	-2.410750
H	0.387016	-2.169352	2.588464
H	4.118690	1.544941	2.580675
O	-1.717176	1.488347	-0.235276
C	-2.856286	1.012838	0.414215
C	-3.722329	2.185860	0.887838

C	-3.548797	0.142542	-0.638816
H	-2.614640	0.377051	1.284102
H	-4.638329	1.848129	1.387458
H	-3.141187	2.797912	1.587158
H	-3.994182	2.818109	0.032209
Br	-5.279789	-0.802789	0.019500
H	-3.880016	0.727915	-1.496663
H	-2.918890	-0.688199	-0.952053

Zn-Int$_3$

Zn	-3.138912	-0.758980	-0.007925
O	-1.408388	1.937109	0.998756
O	-0.028584	-0.938959	-1.221956
O	-2.492339	0.769762	-1.586850
O	-0.877368	-0.930336	1.622136
O	-2.906597	-1.929516	1.662620
O	-4.481806	-0.246556	-1.507819
O	-1.979347	-2.096510	-1.094426
O	-3.417722	0.897381	1.215798
C	-2.602450	1.838310	1.398797
C	-0.799318	-1.905319	-1.486941
C	-3.643129	0.560565	-2.034459
C	-1.741905	-1.708723	2.101121
H	-2.987073	2.681809	1.996314
H	-1.444300	-2.253116	2.999817
H	-3.950334	1.102833	-2.934179
H	-0.389207	-2.693201	-2.140589
O	1.658434	1.095351	0.522574
O	0.781157	3.229032	-1.180889
C	2.698759	0.212994	0.843627
C	1.859815	3.396970	-0.759461
C	3.321716	-0.162991	-0.503752
H	2.325099	-0.714125	1.315353
C	3.685350	0.879812	1.808493
O	2.943688	3.680862	-0.413107
H	2.587648	-0.617848	-1.165698
H	3.818278	0.684643	-0.976726
Br	4.812252	-1.598122	-0.373664
H	4.092245	1.793632	1.358832
H	3.153538	1.161374	2.724725
H	4.514098	0.211308	2.070951

Zn	-0.166117	0.497856	0.257598

Zn-TS_2

Zn	-3.057210	-0.892205	0.023439
O	-1.377213	1.582831	1.558691
O	-0.273856	-0.193243	-1.729738
O	-2.910874	1.150308	-1.024516
O	-0.502036	-1.210243	1.042971
O	-2.363327	-2.490832	1.112612
O	-4.735779	-0.138146	-0.940627
O	-2.057068	-1.600945	-1.653812
O	-3.191791	0.229149	1.767152
C	-2.438501	1.176674	2.110666
C	-1.012314	-1.122169	-2.165226
C	-4.109863	0.916369	-1.299948
C	-1.153595	-2.232791	1.377244
H	-2.748973	1.715573	3.020951
H	-0.606877	-2.978080	1.961847
H	-4.658438	1.662063	-1.886378
H	-0.701008	-1.585764	-3.115875
O	1.655050	1.163268	0.425540
O	0.436522	2.891178	-0.827422
C	2.749663	0.361284	0.794278
C	1.618050	2.897577	-0.667584
C	3.387933	-0.096653	-0.520592
H	2.384038	-0.530678	1.327517
C	3.705630	1.130558	1.711600
O	2.730208	3.291381	-0.760375
H	2.665551	-0.609973	-1.152560
H	3.867052	0.722247	-1.056404
Br	4.891143	-1.480123	-0.261700
H	4.094965	2.018485	1.201001
H	3.157638	1.460538	2.601522
H	4.548025	0.504856	2.028405
Zn	-0.241213	0.686948	0.123996

Zn-Int_4

Zn	-3.031279	-1.000037	0.061319

O	-4.502753	0.398831	-0.239445
O	-2.693141	-3.011570	0.405258
O	-2.795972	-0.333454	2.013424
O	-2.600022	-0.987584	-1.968597
O	-0.695966	0.251909	-2.011657
O	-0.875665	0.868298	1.836250
O	-0.844387	-1.756209	0.294753
O	-2.662706	1.706124	-0.360542
C	-3.903279	1.502746	-0.388665
C	-1.425777	-2.855884	0.442497
C	-1.836160	0.342943	2.465999
C	-1.597026	-0.469048	-2.524509
H	-4.529281	2.381834	-0.561567
H	-1.500946	-0.670426	-3.603527
H	-1.842963	0.497372	3.557072
H	-0.811371	-3.745623	0.615273
O	0.564774	2.790585	-0.361036
C	1.741566	2.349053	-0.153126
O	1.651442	0.926670	0.007095
O	2.827228	2.910768	-0.092747
C	2.753678	0.132076	0.495534
C	3.875408	0.190717	-0.540777
H	2.332973	-0.877477	0.503469
C	3.157856	0.533210	1.912045
H	3.493369	0.005794	-1.543480
H	4.447838	1.112916	-0.500021
Br	5.235492	-1.301840	-0.233546
H	3.581928	1.541130	1.926459
H	2.274477	0.509827	2.558587
H	3.898057	-0.172350	2.305029
Zn	-0.640939	1.150424	-0.178627

Zn-TS$_3$

Zn	3.644553	0.651115	-0.038705
O	4.670652	-1.115746	-0.041975
O	3.773697	2.704562	-0.029891
O	3.189188	0.362076	1.977487
O	3.200446	0.378603	-2.058553
O	1.032768	-0.296911	-1.996964
O	1.020110	-0.307116	1.896431
O	1.687266	1.901048	-0.037450

O	2.570485	-1.960167	-0.049772
C	3.826009	-2.056307	-0.047385
C	2.503644	2.851724	-0.032513
C	2.085944	0.039078	2.485649
C	2.101121	0.057329	-2.576576
H	4.226322	-3.073443	-0.050202
H	2.066802	0.076688	-3.677015
H	2.045131	0.049054	3.586157
H	2.112212	3.875203	-0.030119
O	-0.806496	-1.961000	-0.043462
C	-1.972094	-1.495674	0.054668
O	-2.096546	-0.144882	0.043196
O	-3.044650	-2.158281	0.151992
C	-3.455344	0.300459	0.351432
C	-4.422778	-0.797803	-0.065381
H	-3.600488	1.178266	-0.275722
C	-3.539557	0.659766	1.829289
H	-4.543700	-1.047803	-1.107093
H	-5.044072	-1.303177	0.653861
Br	-6.439936	0.744878	-0.382139
H	-3.375439	-0.226703	2.453315
H	-2.776023	1.404043	2.076282
H	-4.529576	1.072188	2.044970
Zn	0.838099	-0.805914	-0.054061

Zn-Int$_5$

Zn	3.858214	0.539004	-0.062106
O	4.736177	-1.284971	0.134610
O	4.052360	2.560108	-0.253808
O	3.296868	0.477342	1.954303
O	3.381231	0.088287	-2.049527
O	1.171127	-0.427745	-1.988640
O	1.088355	-0.046255	1.900441
O	1.918119	1.888253	-0.233523
O	2.581342	-1.978061	0.157978
C	3.827301	-2.162454	0.201476
C	2.793790	2.783249	-0.302242
C	2.170498	0.281686	2.473972
C	2.277181	-0.210027	-2.568735
H	4.160387	-3.199990	0.309542
H	2.263146	-0.308090	-3.662613

H	2.110343	0.396001	3.564822
H	2.476430	3.828446	-0.410813
O	-0.804061	-1.611738	0.064034
C	-1.954462	-1.160134	0.105857
O	-2.237871	0.124713	0.005198
O	-3.012236	-1.932438	0.257257
C	-3.700191	0.331867	0.235136
C	-4.236094	-1.104098	0.125610
H	-4.058697	0.954497	-0.580953
C	-3.892452	1.000835	1.580792
H	-4.690224	-1.325532	-0.838098
H	-4.912081	-1.387597	0.927733
Br	-6.972582	0.540015	-0.387636
H	-3.540252	0.358867	2.398408
H	-3.348072	1.950455	1.619012
H	-4.963798	1.192518	1.696761
Zn	0.990402	-0.631857	-0.009705

Cr-HKUST-1

Cr-HKUST-1

Cr	0.001422	-0.000559	-1.424832
Cr	-0.001425	0.000563	1.424845
O	1.413974	1.440357	-1.132841
O	-1.411198	-1.441622	-1.134226
O	-1.439670	1.412217	-1.135206
O	1.442329	-1.412952	-1.132096
O	1.440726	-1.411113	1.135083
O	-1.443396	1.411854	1.131968
O	-1.412874	-1.441436	1.132952
O	1.410094	1.442704	1.134334
C	1.806196	1.844249	0.000992
C	-1.806140	-1.844304	-0.000884
C	-1.844297	1.806152	-0.002200
C	1.844293	-1.806146	0.002081
H	2.575205	2.629779	0.001506
H	2.629692	-2.575287	0.003275
H	-2.629697	2.575293	-0.003382
H	-2.575326	-2.629661	-0.001398

Cr-Int$_0$

Cr	2.235684	0.105140	0.403339
Cr	-0.537038	-0.053910	-0.382178
O	1.771240	-1.598103	1.414955
O	2.214015	1.779132	-0.744194
O	1.463797	1.189520	1.942175
O	2.520584	-1.005897	-1.270707
O	0.339614	-1.143744	-1.884579
O	-0.726132	1.064747	1.357620
O	0.030438	1.662655	-1.353467
O	-0.417101	-1.738575	0.828133
C	0.625688	-2.135418	1.422662
C	1.179195	2.188108	-1.349336
C	0.231514	1.431985	2.096784
C	1.572862	-1.379121	-2.023735
H	0.530084	-3.052566	2.016769
H	1.859412	-1.976779	-2.897321
H	-0.032719	2.030657	2.977342
H	1.296512	3.106171	-1.937206
O	-2.834607	-0.277710	-0.668252
C	-3.810104	0.113961	0.342405
C	-4.974340	0.927612	-0.155959
C	-3.622505	-1.302319	-0.006585
H	-3.330230	0.467261	1.254545
H	-5.773818	0.935925	0.595468
H	-4.668943	1.964341	-0.337407
H	-5.373248	0.514489	-1.088122
H	-4.338590	-1.789099	-0.666728
H	-3.044617	-1.954937	0.643952

Cr-Int$_1$

Cr	3.296726	-0.549897	0.374004
Cr	0.625200	0.380659	-0.324894
O	2.462750	-2.397986	0.355722
O	3.759406	1.429159	0.294174
O	2.672032	-0.303985	2.289222
O	3.545895	-0.662748	-1.639048
O	1.469739	0.073078	-2.197518
O	0.586591	0.423631	1.760478
O	1.679452	2.169951	-0.244030

O	0.379891	-1.684288	-0.197990
C	1.232509	-2.564714	0.085558
C	2.900821	2.322441	0.018611
C	1.502999	0.109101	2.563428
C	2.628069	-0.345227	-2.456517
H	0.877583	-3.602483	0.102788
H	2.883198	-0.450367	-3.518583
H	1.270687	0.201610	3.631667
H	3.276199	3.353759	0.009754
O	-1.480706	0.938199	-0.739932
C	-2.613810	1.055274	0.207731
C	-3.405160	2.329361	0.145194
C	-2.679974	0.056057	-0.842536
H	-2.349797	0.703203	1.203741
H	-4.394033	2.125719	0.571487
H	-2.910614	3.134168	0.704639
H	-3.540881	2.647903	-0.893964
Br	-5.756038	-0.599225	0.101860
H	-3.282737	0.253116	-1.721844
H	-2.487611	-0.985891	-0.610849

Cr-TS$_1$

Cr	3.174990	-0.643565	0.343560
Cr	0.543068	0.467463	-0.319201
O	2.226507	-2.431286	0.428173
O	3.795325	1.284428	0.176716
O	2.647902	-0.286492	2.268704
O	3.367198	-0.857400	-1.665169
O	1.333444	0.008836	-2.195738
O	0.607262	0.584501	1.778435
O	1.762608	2.163587	-0.337318
O	0.181579	-1.586751	-0.084746
C	0.977590	-2.514540	0.204893
C	2.997638	2.229103	-0.113127
C	1.523407	0.227518	2.561169
C	2.448230	-0.504027	-2.467681
H	0.550784	-3.521958	0.275070
H	2.663506	-0.670895	-3.530256
H	1.338696	0.375073	3.632299
H	3.451302	3.226155	-0.173566
O	-1.461834	1.153937	-0.694379

C	-2.561589	1.254385	0.215266
C	-3.328764	2.556749	0.158418
C	-2.921440	0.155490	-0.668709
H	-2.302936	0.960997	1.238576
H	-4.269270	2.453197	0.710764
H	-2.733928	3.367416	0.598641
H	-3.560460	2.818079	-0.880485
Br	-5.396765	-0.714169	0.082224
H	-3.389970	0.366067	-1.616970
H	-2.584713	-0.846695	-0.455310

Cr-Int$_2$

Cr	2.695475	-1.032507	0.341078
Cr	0.518772	1.163079	-0.419208
O	1.427710	-2.395098	1.185556
O	4.007309	0.325296	-0.500529
O	2.800567	-0.026323	2.067402
O	2.368448	-1.801463	-1.473267
O	0.921465	-0.183171	-2.177924
O	1.115671	1.469694	1.703189
O	2.403242	1.886170	-0.826470
O	-0.123182	-0.939211	0.451576
C	0.226962	-1.991262	1.020528
C	3.583157	1.455941	-0.871204
C	2.020015	0.929213	2.379942
C	1.591857	-1.231944	-2.307318
H	-0.575569	-2.628952	1.416448
H	1.537575	-1.769886	-3.260012
H	2.202433	1.301859	3.393837
H	4.315364	2.160868	-1.283130
O	-1.325959	1.649243	-0.521787
C	-2.462141	1.222428	0.162480
C	-3.415777	2.399814	0.396821
C	-3.047428	0.128594	-0.731398
H	-2.202185	0.771593	1.134961
H	-4.326081	2.090396	0.924158
H	-2.902543	3.163716	0.992338
H	-3.698003	2.851458	-0.563637
Br	-4.728590	-0.807529	0.060129
H	-3.393372	0.518579	-1.688726
H	-2.340942	-0.687638	-0.856677

Cr-Int$_3$

Cr	-2.908866	-1.175006	-0.312024
O	-1.737765	-2.829837	-0.596537
O	-4.135030	0.469651	-0.032465
O	-2.638570	-0.613812	-2.209052
O	-2.929857	-1.496747	1.662706
O	-1.133620	-0.219706	2.257279
O	-1.078723	0.999156	-1.789068
O	-2.420101	1.771125	0.655805
O	-0.096761	-1.320636	-0.304095
C	-0.512789	-2.474838	-0.524270
C	-3.628300	1.545064	0.394783
C	-1.826743	0.315478	-2.524453
C	-2.077615	-1.014314	2.474969
H	0.249415	-3.254620	-0.668661
H	-2.231527	-1.371711	3.499345
H	-1.820230	0.512234	-3.602273
H	-4.301015	2.395147	0.566269
Cr	-0.589450	0.883947	0.404600
O	1.313955	1.185663	0.536854
O	0.433229	3.792255	-0.256350
C	2.331680	0.289920	0.885656
C	1.555509	3.597657	-0.527509
C	2.955493	-0.116825	-0.449764
H	1.915486	-0.612896	1.360177
C	3.320028	0.949645	1.854348
O	2.681455	3.527795	-0.845070
H	2.213750	-0.584553	-1.091595
H	3.460852	0.712927	-0.943143
Br	4.429440	-1.567059	-0.279416
H	3.767041	1.840373	1.394393
H	2.782057	1.262986	2.756713
H	4.124069	0.262592	2.143886

Cr-TS$_2$

Cr	-2.830538	-1.268938	-0.133756
O	-1.591427	-2.901289	-0.094061

O	-4.112055	0.351755	-0.169543
O	-2.603670	-1.101327	-2.110933
O	-2.847114	-1.200490	1.872344
O	-1.168382	0.306077	2.216261
O	-1.131204	0.632883	-1.969896
O	-2.501780	1.885415	0.251190
O	-0.058186	-1.260528	-0.033338
C	-0.392962	-2.461906	-0.060778
C	-3.686255	1.522184	0.036179
C	-1.828443	-0.205147	-2.582570
C	-2.053806	-0.504988	2.579606
H	0.418763	-3.204952	-0.056179
H	-2.196308	-0.663054	3.655001
H	-1.805680	-0.204044	-3.679038
H	-4.420600	2.337972	0.032665
Cr	-0.647283	1.059681	0.226979
O	1.314622	1.313318	0.405196
O	0.280363	3.303742	-0.588662
C	2.361252	0.449217	0.788045
C	1.455542	3.099540	-0.539167
C	2.986336	-0.039008	-0.519033
H	1.925539	-0.417919	1.301259
C	3.338668	1.156329	1.732075
O	2.604505	3.328094	-0.714747
H	2.237787	-0.525616	-1.139468
H	3.512234	0.749547	-1.055768
Br	4.414506	-1.497541	-0.238017
H	3.805435	2.016303	1.239302
H	2.789293	1.516812	2.609402
H	4.126152	0.472552	2.069400

Cr-Int$_4$

Cr	-2.898149	-1.255967	-0.009187
O	-1.562745	-2.725200	-0.283941
O	-4.118494	0.332886	0.288255
O	-3.262307	-1.169814	-2.002941
O	-2.523022	-1.283760	2.002076
O	-1.030183	0.425019	2.118264
O	-1.612468	0.362903	-1.902363
O	-2.583763	2.016547	0.336463
O	0.070414	-1.175655	-0.014328

C	-0.349079	-2.328359	-0.236686
C	-3.746016	1.536411	0.371203
C	-2.451765	-0.323357	-2.517026
C	-1.731918	-0.502738	2.599876
H	0.386428	-3.117748	-0.419331
H	-1.649871	-0.651129	3.684566
H	-2.518379	-0.208339	-3.609338
H	-4.554444	2.258404	0.495050
Cr	-0.718118	1.188538	0.213310
O	1.441681	1.389505	0.294709
O	0.202836	2.707802	-0.918964
C	2.629882	0.647931	0.660311
C	1.425213	2.451744	-0.706334
C	3.171004	-0.017499	-0.602410
H	2.234753	-0.131384	1.316093
C	3.617523	1.531474	1.417565
O	2.474065	2.890492	-1.147133
H	2.380504	-0.571528	-1.104247
H	3.677919	0.675381	-1.269191
Br	4.568768	-1.429026	-0.140280
H	4.008278	2.321794	0.771420
H	3.111458	1.992943	2.272853
H	4.449706	0.926368	1.793176

Cr-TS$_3$

Cr	-3.952503	-0.693014	-0.089957
O	-3.178453	-1.911804	-1.515284
O	-4.401359	0.669968	1.344517
O	-4.341215	0.699822	-1.512298
O	-3.235110	-1.940073	1.340727
O	-1.156551	-1.023687	1.412041
O	-2.270555	1.635953	-1.469360
O	-2.329405	1.601264	1.417516
O	-1.101766	-0.990414	-1.476277
C	-1.967850	-1.802452	-1.886547
C	-3.529141	1.490125	1.771598
C	-3.452664	1.531014	-1.880231
C	-2.041695	-1.841919	1.765927
H	-1.646852	-2.509356	-2.662388

H	-1.757000	-2.566973	2.539276
H	-3.767234	2.242757	-2.654650
H	-3.877037	2.184914	2.547362
O	0.631814	1.564568	0.033514
C	1.841004	1.262329	0.127945
O	2.154217	-0.072337	0.101664
O	2.826862	2.052509	0.233029
C	3.544964	-0.338730	0.415777
C	4.402314	0.822118	-0.063494
H	3.784398	-1.230477	-0.162858
C	3.693947	-0.612102	1.909595
H	4.402775	1.097529	-1.105840
H	4.952870	1.440046	0.624623
Br	6.518758	-0.438767	-0.444850
H	3.438775	0.281266	2.491534
H	3.023000	-1.424376	2.207661
H	4.727026	-0.899737	2.129759
Cr	-1.262930	0.501047	-0.019479

Cr-Int$_5$

Cr	-4.111930	0.618453	0.160219
O	-3.376802	1.655786	1.742141
O	-4.472502	-0.566920	-1.450496
O	-4.427954	-0.976865	1.377064
O	-3.418702	2.064740	-1.084331
O	-1.312989	1.232585	-1.264429
O	-2.322084	-1.816363	1.230336
O	-2.370510	-1.412956	-1.616313
O	-1.267151	0.829162	1.590013
C	-2.164202	1.546513	2.103581
C	-3.571901	-1.294996	-1.971029
C	-3.511069	-1.814285	1.641946
C	-2.223282	2.065191	-1.512499
H	-1.868806	2.153375	2.969176
H	-1.958197	2.895275	-2.180032
H	-3.797811	-2.634811	2.312781
H	-3.886865	-1.892629	-2.836741
O	0.634586	-1.350916	-0.216966
C	1.809527	-0.996659	-0.218732
O	2.212581	0.248865	-0.000581
O	2.815106	-1.836742	-0.444442

C	3.677866	0.347210	-0.220860
C	4.092483	-1.131440	-0.233397
H	4.094606	0.869161	0.637603
C	3.937434	1.103384	-1.509318
H	4.518252	-1.466804	0.711138
H	4.760080	-1.394968	-1.050065
Br	6.989492	0.286416	0.420061
H	3.535889	0.561794	-2.375827
H	3.476248	2.096455	-1.471166
H	5.021972	1.211712	-1.610867
Cr	-1.402961	-0.449105	-0.042812

Ti-HKUST-1

Ti-HKUST-1

Ti	0.000456	0.000483	1.279484
Ti	-0.000459	-0.000266	-1.278246
O	-2.058875	-0.047743	1.126889
O	2.059649	0.049129	1.125874
O	-0.047622	2.018059	1.114898
O	0.048925	-2.017412	1.115911
O	0.047538	-2.017168	-1.116256
O	-0.048870	2.016879	-1.117262
O	2.057506	0.047105	-1.126559
O	-2.058226	-0.049106	-1.125537
C	-2.647072	-0.062002	0.000771
C	2.647097	0.061490	-0.000641
C	-0.063527	2.621393	-0.001267
C	0.063495	-2.621198	-0.000008
H	-3.744352	-0.086816	0.000226
H	0.090836	-3.716637	-0.000330
H	-0.090949	3.716826	-0.001973
H	3.744388	0.085811	-0.001959

Ti-Int$_0$

Ti	-0.369953	-0.061009	-0.480603
Ti	2.052163	0.133029	0.552695
O	0.264968	1.421720	-1.755455
O	-0.607027	-1.548085	1.003064
O	-0.835644	1.403851	0.962656
O	0.493717	-1.475203	-1.716985

O	2.554783	-1.286506	-0.821414
O	1.256458	1.533107	1.799636
O	1.465402	-1.313721	1.846072
O	2.330562	1.541025	-0.878978
C	1.424187	1.914994	-1.690633
C	0.315751	-1.854909	1.805028
C	0.034023	1.881252	1.741718
C	1.710425	-1.799748	-1.623730
H	1.672798	2.726382	-2.375136
H	2.074249	-2.589507	-2.279718
H	-0.280514	2.665382	2.430240
H	0.120731	-2.650890	2.525721
O	-2.586141	-0.308846	-0.687476
C	-3.634941	0.034813	0.272886
C	-4.719658	0.936402	-0.249482
C	-3.463382	-1.354151	-0.178267
H	-3.214116	0.295332	1.242043
H	-5.580336	0.915127	0.430665
H	-4.360663	1.969621	-0.310844
H	-5.050861	0.620909	-1.244150
H	-4.130277	-1.755815	-0.938742
H	-2.954664	-2.071647	0.459836

Ti-Int$_1$

Ti	0.714106	0.315180	-0.383162
Ti	3.346076	-0.528533	0.490539
O	1.676127	2.182138	-0.510293
O	0.313457	-1.742883	-0.052299
O	0.470107	0.633267	1.713247
O	1.499028	-0.168910	-2.280162
O	3.516920	-0.813200	-1.505206
O	2.545879	-0.044196	2.279040
O	2.393928	-2.306228	0.605332
O	3.692659	1.443152	0.174535
C	2.887412	2.354346	-0.209639
C	1.176519	-2.574346	0.327332
C	1.385021	0.416180	2.547354
C	2.662638	-0.624824	-2.434075
H	3.292137	3.374312	-0.272637
H	2.978597	-0.895482	-3.450602
H	1.185284	0.644697	3.603070
H	0.871489	-3.625404	0.424938

O	-1.316141	0.693614	-0.708661
C	-2.480481	1.002200	0.162109
C	-3.170173	2.307923	-0.102732
C	-2.578852	-0.122898	-0.752378
H	-2.265915	0.769918	1.202691
H	-4.183768	2.234235	0.306887
H	-2.633476	3.142078	0.366393
H	-3.249837	2.492358	-1.179353
Br	-5.639361	-0.510612	0.107185
H	-3.120864	-0.003757	-1.682755
H	-2.448231	-1.133285	-0.384465

Ti-TS$_1$

Ti	0.662261	0.364678	-0.381756
Ti	3.273365	-0.605689	0.472933
O	1.725357	2.167342	-0.490765
O	0.201347	-1.676160	-0.042221
O	0.446484	0.687523	1.729307
O	1.417866	-0.138371	-2.296081
O	3.404122	-0.885387	-1.524176
O	2.495461	-0.097579	2.263385
O	2.256266	-2.352797	0.588636
O	3.721784	1.351338	0.165013
C	2.947201	2.293083	-0.206372
C	1.024279	-2.554599	0.322745
C	1.361508	0.418608	2.547242
C	2.556766	-0.651793	-2.449966
H	3.386565	3.299274	-0.274056
H	2.859356	-0.939037	-3.465878
H	1.190294	0.649631	3.607512
H	0.662813	-3.588979	0.415520
O	-1.305993	0.836166	-0.698128
C	-2.424599	1.138413	0.166107
C	-3.070286	2.482778	-0.059672
C	-2.779839	-0.006923	-0.658727
H	-2.206715	0.920382	1.213203
H	-4.044968	2.497892	0.439867
H	-2.438790	3.283915	0.344005
H	-3.225604	2.660678	-1.129611
Br	-5.416054	-0.584864	0.093358
H	-3.233828	0.144693	-1.625535

H	-2.562728	-1.009968	-0.326340

Ti-Int$_2$

Ti	0.586191	0.551062	-0.405218
Ti	3.095021	-0.767675	0.481835
O	1.831473	2.224578	-0.175757
O	0.031594	-1.506320	-0.533437
O	0.325005	0.525578	1.709255
O	1.539099	0.284496	-2.248270
O	3.430725	-0.748620	-1.565943
O	2.218134	-0.541506	2.342118
O	1.936261	-2.462576	0.231361
O	3.698895	1.212306	0.602996
C	3.007390	2.220985	0.285250
C	0.749593	-2.490460	-0.202339
C	1.110796	0.027461	2.561135
C	2.651804	-0.281776	-2.443935
H	3.477913	3.200800	0.428667
H	2.972006	-0.381283	-3.488179
H	0.800854	0.099615	3.610923
H	0.294678	-3.482703	-0.306155
O	-1.188011	1.160102	-0.598861
C	-2.437915	1.061787	0.027417
C	-3.186352	2.393411	-0.070685
C	-3.132887	-0.093036	-0.693960
H	-2.305528	0.793552	1.087394
H	-4.165571	2.343822	0.419895
H	-2.589020	3.177342	0.407685
H	-3.329644	2.669437	-1.123521
Br	-4.953847	-0.600424	0.135781
H	-3.371866	0.151658	-1.729124
H	-2.545803	-1.006446	-0.630480

Ti-Int$_3$

Ti	-3.098176	-1.040715	-0.393445
O	-1.514714	1.700634	-0.977950
O	-0.562259	-1.472298	1.488160
O	-0.090998	-0.796461	-1.405114
O	-1.989387	1.038394	1.751121

O	-3.937193	0.018722	1.205869
O	-1.997492	-1.911330	-1.923820
O	-2.440215	-2.569117	0.838477
O	-3.452980	0.670671	-1.542447
C	-2.601770	1.604459	-1.615291
C	-1.366883	-2.438936	1.505057
C	-0.780081	-1.594557	-2.092164
C	-3.207885	0.762973	1.926758
H	-2.826011	2.411871	-2.317061
H	-3.678613	1.209208	2.806929
H	-0.272800	-2.060387	-2.942195
H	-1.125240	-3.263161	2.182217
O	1.113656	0.705881	0.721144
O	0.432514	4.041260	0.545653
C	2.324737	0.046767	0.985564
C	1.009525	3.669063	-0.400674
C	3.028490	-0.028183	-0.368240
H	2.122538	-0.976778	1.339037
C	3.119295	0.799627	2.056271
O	1.608102	3.360522	-1.358334
H	2.413615	-0.542024	-1.102974
H	3.342304	0.950633	-0.730400
Br	4.781195	-1.128287	-0.320196
H	3.347778	1.818067	1.714986
H	2.514802	0.874548	2.966891
H	4.060189	0.289804	2.294863
Ti	-0.708424	0.293259	0.314753

Ti-TS$_2$

Ti	-2.964482	-1.198017	0.015662
O	-1.742376	1.030441	-1.832110
O	-0.558536	-0.352684	1.853938
O	0.013106	-1.098060	-1.005297
O	-2.285106	1.745786	0.884084
O	-4.053540	0.335702	0.903705
O	-1.704047	-2.569741	-0.875592
O	-2.258030	-1.850521	1.845385
O	-3.506916	-0.384477	-1.820982
C	-2.766182	0.504790	-2.343231
C	-1.242616	-1.279786	2.355048
C	-0.527011	-2.215725	-1.200727

C	-3.470620	1.431819	1.169997
H	-3.040168	0.843019	-3.347055
H	-4.056073	2.178613	1.713847
H	0.076714	-2.969339	-1.715571
H	-0.939040	-1.633615	3.345753
O	1.154144	1.122433	0.222398
O	0.101349	3.147594	-0.555093
C	2.254564	0.343161	0.663122
C	1.265719	2.943942	-0.363236
C	3.142305	0.151654	-0.566030
H	1.862616	-0.637193	0.961383
C	2.950448	0.983073	1.866826
O	2.410147	3.279028	-0.359623
H	2.574785	-0.291910	-1.380884
H	3.648502	1.065287	-0.871755
Br	4.669695	-1.190436	-0.242495
H	3.374170	1.957750	1.604443
H	2.213840	1.123667	2.665314
H	3.753230	0.337250	2.241468
Ti	-0.813205	0.619388	-0.029604

Ti-Int$_4$

Ti	-3.275254	-1.098784	0.119546
O	-1.905235	0.876327	-1.966336
O	-0.666334	-0.251233	1.784909
O	-0.265937	-1.241839	-0.913075
O	-2.346090	1.856539	0.769926
O	-4.205625	0.573499	0.924908
O	-2.073301	-2.589356	-0.712600
O	-2.471866	-1.603628	1.969057
O	-3.771406	-0.388284	-1.760133
C	-2.988596	0.399806	-2.382598
C	-1.402942	-1.066316	2.396624
C	-0.879500	-2.329370	-1.060359
C	-3.540857	1.647730	1.087612
H	-3.300922	0.683509	-3.395819
H	-4.074010	2.479909	1.564405
H	-0.325071	-3.142206	-1.546778
H	-1.097989	-1.345650	3.413856
O	1.403412	0.914600	0.029708
O	0.135760	2.581102	-0.575721

C	2.590400	0.268055	0.528159
C	1.349563	2.322365	-0.340602
C	3.641680	0.297647	-0.580167
H	2.261549	-0.765001	0.672874
C	3.037855	0.861410	1.861655
O	2.383304	2.974401	-0.377848
H	3.220154	-0.032699	-1.528040
H	4.133551	1.261202	-0.678920
Br	5.144264	-1.036675	-0.203857
H	3.353471	1.901223	1.737912
H	2.203116	0.822827	2.569083
H	3.871067	0.280142	2.272172
Ti	-0.855347	0.649484	-0.137276

Ti-TS$_3$

Ti	-3.788084	0.852994	0.208123
O	-0.971040	1.017432	-1.180021
O	-2.674433	-1.998102	1.007024
O	-2.567730	-1.312503	-1.736921
O	-1.097138	0.281459	1.728971
O	-2.914631	1.613639	1.921230
O	-4.454558	-0.086003	-1.533205
O	-4.563570	-0.782768	1.253088
O	-2.799213	2.314004	-0.866485
C	-1.640054	2.070357	-1.330087
C	-3.839777	-1.803702	1.452634
C	-3.696835	-0.909041	-2.130110
C	-1.790102	1.159381	2.303893
H	-1.182892	2.861245	-1.932491
H	-1.390248	1.570247	3.236577
H	-4.052312	-1.303147	-3.087938
H	-4.259598	-2.594454	2.081435
O	0.459696	-1.321814	-0.270860
C	1.682922	-1.020575	-0.334232
O	2.066831	0.155769	0.207572
O	2.595902	-1.732643	-0.844007
C	3.460067	0.478867	-0.080832
C	4.238693	-0.814690	-0.260412
H	3.805624	0.994558	0.813850
C	3.521944	1.395778	-1.296820

H	4.347203	-1.501692	0.563345
H	4.703897	-1.067732	-1.197596
Br	6.505536	0.119660	0.398630
H	3.153941	0.878293	-2.190443
H	2.899473	2.280237	-1.128368
H	4.557031	1.709102	-1.463282
Ti	-1.509097	-0.695757	-0.075507

Ti-Int$_4$

Ti	-4.270998	0.471642	0.319930
O	-1.346510	1.680330	-0.720663
O	-2.296859	-2.216461	0.500119
O	-2.311118	-0.770482	-2.076170
O	-1.341911	0.232516	1.869877
O	-3.491646	0.851682	2.143679
O	-4.413640	-0.101529	-1.615869
O	-4.398589	-1.477672	0.844246
O	-3.496714	2.223872	-0.316180
C	-2.306643	2.489797	-0.698413
C	-3.491662	-2.376281	0.858357
C	-3.508886	-0.555189	-2.393805
C	-2.296765	0.669903	2.558840
H	-2.123662	3.518409	-1.040483
H	-2.102953	0.915376	3.612766
H	-3.813130	-0.765159	-3.429503
H	-3.792289	-3.368561	1.223959
O	0.518077	-0.833219	-0.442836
C	1.723477	-0.593289	-0.382177
O	2.236048	0.460536	0.230208
O	2.634860	-1.381523	-0.935461
C	3.702568	0.512742	-0.017976
C	3.979149	-0.897474	-0.559401
H	4.180763	0.669307	0.946154
C	4.000541	1.646715	-0.978923
H	4.388781	-1.574276	0.188620
H	4.600690	-0.914589	-1.451011
Br	6.990815	-0.040012	0.395672
H	3.533801	1.472154	-1.957091
H	3.631411	2.596897	-0.577677
H	5.087976	1.699679	-1.092136
Ti	-1.520665	-0.361404	-0.158053

W-HKUST-1

W-HKUST-1

W	1.093228	0.055361	-0.054800
W	-1.093068	-0.057296	0.053549
O	1.154981	-1.710922	-1.175103
O	1.086944	1.823344	1.064503
O	1.265935	-1.058866	1.708047
O	0.974101	1.171477	-1.820947
O	-1.267012	1.064081	-1.704278
O	-0.975393	-1.164692	1.825155
O	-1.154418	1.710454	1.172836
O	-1.086110	-1.825600	-1.064436
C	0.044769	-2.283446	-1.445488
C	-0.044045	2.281708	1.444532
C	0.187498	-1.434160	2.282037
C	-0.188845	1.444660	-2.275316
H	0.063194	-3.206751	-2.029085
H	-0.264320	2.030487	-3.194295
H	0.262767	-2.011805	3.206205
H	-0.062013	3.204517	2.029000

W-Int$_0$

W	-1.618528	-0.083914	0.243989
W	0.529485	0.056920	-0.247896
O	-1.793644	-1.815392	-0.913228
O	-1.491351	1.648151	1.417058
O	-2.100375	1.080694	-1.422709
O	-1.183413	-1.253056	1.928630
O	1.008418	-1.110376	1.439366
O	0.087074	1.228594	-1.926907
O	0.700133	1.797308	0.927907
O	0.395558	-1.677706	-1.413803
C	-0.743525	-2.248796	-1.500141
C	-0.355616	2.223605	1.510193
C	-1.140417	1.493243	-2.159665
C	0.041702	-1.519709	2.169262
H	-0.824873	-3.153975	-2.106007
H	0.276925	-2.129447	3.044994

H	-1.383914	2.103370	-3.032292
H	-0.282677	3.127529	2.119771
O	3.060387	0.283135	-0.534141
C	4.042910	-0.130799	0.456732
C	5.187162	-0.960416	-0.062512
C	3.872596	1.290746	0.119690
H	3.572081	-0.482223	1.374403
H	5.997115	-0.987746	0.677304
H	4.861673	-1.990455	-0.247330
H	5.579853	-0.547627	-0.997522
H	4.586848	1.772286	-0.546605
H	3.315052	1.947795	0.783625

W-Int$_1$

W	2.360171	-0.368002	0.268052
W	0.293551	0.266224	-0.240206
O	3.051624	1.595819	0.034605
O	1.724091	-2.350291	0.514213
O	2.768732	-0.750235	-1.749976
O	2.005618	0.000793	2.301822
O	-0.092730	0.644707	1.795079
O	0.673069	-0.108986	-2.274431
O	-0.373840	-1.714205	0.000050
O	0.956706	2.249199	-0.479610
C	2.193495	2.489132	-0.291348
C	0.481784	-2.598864	0.326223
C	1.829198	-0.537500	-2.594248
C	0.845253	0.430897	2.629993
H	2.545625	3.516841	-0.415011
H	0.648814	0.624604	3.687851
H	2.033483	-0.735718	-3.649775
H	0.137172	-3.628250	0.454202
O	-1.978718	0.840420	-0.671603
C	-3.112740	0.972154	0.274331
C	-3.876770	2.263070	0.216865
C	-3.193149	-0.021453	-0.780819
H	-2.853596	0.611653	1.268157
H	-4.871663	2.078656	0.637986
H	-3.366018	3.052790	0.783051
H	-4.001899	2.591045	-0.820618
Br	-6.306345	-0.598426	0.107432

H	-3.788976	0.188760	-1.661711
H	-3.015077	-1.066262	-0.551996

W-TS_1

W	2.287190	-0.422982	0.261391
W	0.242267	0.310090	-0.243298
O	3.092868	1.475282	-0.110082
O	1.538919	-2.344275	0.648349
O	2.619670	-0.953835	-1.736234
O	2.009267	0.091484	2.276751
O	-0.060715	0.833777	1.779673
O	0.553653	-0.215102	-2.258401
O	-0.531714	-1.613755	0.140417
O	1.028897	2.229142	-0.621123
C	2.281835	2.398450	-0.473149
C	0.279211	-2.524957	0.502545
C	1.673240	-0.733749	-2.571738
C	0.885556	0.611916	2.601863
H	2.693322	3.392710	-0.666311
H	0.730568	0.880608	3.650325
H	1.840370	-1.009584	-3.616315
H	-0.121875	-3.521943	0.701441
O	-1.906273	0.983021	-0.644162
C	-3.002308	1.121733	0.274536
C	-3.701853	2.461241	0.242989
C	-3.398177	0.062317	-0.640274
H	-2.751133	0.793565	1.287491
H	-4.649487	2.389946	0.788287
H	-3.070433	3.230540	0.705275
H	-3.915329	2.757556	-0.790289
Br	-5.937696	-0.690862	0.091482
H	-3.862627	0.312451	-1.580934
H	-3.115405	-0.959248	-0.441874

W-Int_2

W	2.224886	-0.479043	0.230633
W	0.197012	0.386401	-0.217004
O	3.076458	1.436052	0.235111
O	1.433083	-2.426940	0.242051

O	2.634985	-0.656781	-1.816315
O	1.872458	-0.325407	2.296049
O	-0.170384	0.537797	1.866949
O	0.601388	0.211636	-2.283146
O	-0.611769	-1.577465	-0.205132
O	1.045943	2.320305	-0.215917
C	2.292828	2.425361	0.009037
C	0.177939	-2.548082	0.019821
C	1.725254	-0.269679	-2.633072
C	0.742342	0.152710	2.663450
H	2.729139	3.427215	0.013011
H	0.554200	0.234399	3.737522
H	1.932593	-0.363876	-3.702280
H	-0.241887	-3.557154	0.023306
O	-1.783588	1.147274	-0.555435
C	-2.967794	0.964997	0.147726
C	-3.717935	2.292299	0.319776
C	-3.724443	-0.056125	-0.702203
H	-2.794361	0.527542	1.148603
H	-4.663515	2.164809	0.862022
H	-3.080703	2.991206	0.873817
H	-3.927414	2.733438	-0.663984
Br	-5.557531	-0.678847	0.105935
H	-4.002760	0.343623	-1.677131
H	-3.169840	-0.986697	-0.792111

W-Int$_3$

W	-2.385349	-0.547400	-0.184784
O	-2.791824	1.128356	-1.375688
O	-2.031994	-2.243924	0.997395
O	-3.065704	0.491143	1.505280
O	-1.770073	-1.609453	-1.891620
O	0.345791	-0.898940	-1.545131
O	-0.960011	1.220339	1.877268
O	0.080309	-1.533674	1.361517
O	-0.686969	1.870660	-1.028927
C	-1.847575	1.978607	-1.539955
C	-0.867452	-2.368773	1.516144
C	-2.194040	1.153539	2.172993
C	-0.528379	-1.550643	-2.199274
H	-2.057337	2.852088	-2.162743

H	-0.199198	-2.096553	-3.087236
H	-2.536722	1.697135	3.057075
H	-0.679009	-3.252436	2.131844
O	1.747467	0.864056	0.462170
O	1.353891	3.952607	0.449836
C	2.879266	0.151245	0.853188
C	1.870004	3.512923	-0.503577
C	3.589587	-0.163674	-0.464623
H	2.611950	-0.803665	1.340900
C	3.737509	0.967836	1.828317
O	2.414196	3.190804	-1.490135
H	2.955412	-0.742407	-1.131493
H	3.971374	0.730335	-0.956578
Br	5.285380	-1.368729	-0.257016
H	4.067781	1.902104	1.354073
H	3.131514	1.229459	2.703168
H	4.623311	0.411684	2.159936
W	-0.287510	0.174908	0.171697

W-TS$_2$

W	-2.315539	-0.690146	-0.051932
O	-2.738027	0.163470	-1.913186
O	-1.963163	-1.587451	1.812524
O	-3.283699	0.899383	0.899485
O	-1.417854	-2.329471	-1.011490
O	0.565052	-1.259578	-0.923883
O	-1.312754	1.989519	1.017981
O	0.016462	-0.512590	1.927215
O	-0.759887	1.244196	-1.835734
C	-1.857372	0.955381	-2.406923
C	-0.861730	-1.301061	2.400449
C	-2.561675	1.907303	1.231702
C	-0.159798	-2.255525	-1.238849
H	-2.070604	1.409609	-3.378032
H	0.320134	-3.104409	-1.733515
H	-3.056213	2.747225	1.725851
H	-0.665726	-1.767999	3.370123
O	1.800652	1.180146	0.207066
O	1.078799	3.432327	-0.437258
C	2.852590	0.339894	0.656149
C	2.167039	2.943970	-0.374806

C	3.701736	0.015135	-0.574261
H	2.403358	-0.599190	1.006981
C	3.628489	0.955709	1.825924
O	3.357226	3.045548	-0.514048
H	3.085361	-0.403725	-1.366119
H	4.297095	0.855838	-0.920611
Br	5.089946	-1.474018	-0.212261
H	4.134708	1.876992	1.522827
H	2.922737	1.191248	2.630740
H	4.374787	0.251069	2.212474
W	-0.361379	0.388053	0.043996

W-Int$_4$

W	-2.700037	-0.629921	0.160302
O	-2.135804	-1.146699	2.111667
O	-3.330791	-0.150873	-1.780212
O	-1.879146	-2.422096	-0.550342
O	-3.588443	1.126446	0.883034
O	-1.637867	2.214799	0.563246
O	0.082004	-1.359775	-0.889772
O	-1.378979	0.928315	-2.122998
O	-0.177817	-0.069101	1.802828
C	-0.984462	-0.748261	2.511619
C	-2.523466	0.531423	-2.506413
C	-0.652745	-2.395661	-0.924314
C	-2.854637	2.177347	0.926665
H	-0.679417	-1.013776	3.527813
H	-3.309005	3.099632	1.300377
H	-0.214581	-3.327397	-1.293104
H	-2.845319	0.786479	-3.520334
O	1.131127	1.627978	-0.550426
C	2.381767	1.539318	-0.354838
O	2.734918	0.308838	0.230563
O	3.268902	2.359230	-0.619575
C	4.089846	0.091901	0.646065
C	5.038181	0.207746	-0.550493
H	4.075289	-0.956655	0.961991
C	4.483810	0.967245	1.837220
H	4.618577	-0.258211	-1.440220
H	5.376886	1.217557	-0.754472
Br	6.767437	-0.859488	-0.204363

H	4.491692	2.022583	1.551536
H	3.760467	0.825926	2.647974
H	5.478028	0.684813	2.203585
W	-0.761956	0.433142	-0.162594

W-TS$_3$

W	-2.822431	-0.523851	-0.073284
O	-2.259082	-1.955692	1.348874
O	-3.451605	0.879706	-1.496354
O	-2.215103	-1.809978	-1.611883
O	-3.495742	0.732467	1.463583
O	-1.451347	1.679944	1.551215
O	-0.165293	-0.874373	-1.548210
O	-1.406574	1.827323	-1.430540
O	-0.208256	-1.023450	1.437268
C	-1.060764	-1.894746	1.799678
C	-2.598181	1.760452	-1.869627
C	-1.004207	-1.704870	-2.020009
C	-2.654769	1.570332	1.947132
H	-0.755615	-2.640580	2.539085
H	-2.997491	2.230370	2.749261
H	-0.674715	-2.372245	-2.821102
H	-2.917678	2.499103	-2.610435
O	1.267887	1.475423	0.092681
C	2.480666	1.178052	0.181115
O	2.814067	-0.143750	0.055188
O	3.451598	1.972905	0.361790
C	4.203054	-0.414082	0.371288
C	5.052208	0.789047	-0.007016
H	4.463172	-1.257562	-0.267766
C	4.333612	-0.796003	1.842966
H	5.059790	1.144412	-1.024880
H	5.583198	1.361394	0.733928
Br	7.188582	-0.410060	-0.453511
H	4.056924	0.047955	2.485538
H	3.669372	-1.636469	2.068994
H	5.367281	-1.085938	2.057535
W	-0.799309	0.402884	0.001671

W-Int$_5$

W	-2.918844	-0.494541	-0.091785
O	-2.376037	-2.020427	1.236785
O	-3.521972	1.007120	-1.422226
O	-2.346993	-1.696492	-1.709065
O	-3.551326	0.682886	1.522191
O	-1.486556	1.575117	1.648363
O	-0.279626	-0.811174	-1.600067
O	-1.457296	1.901154	-1.311710
O	-0.308122	-1.137889	1.362168
C	-1.174735	-2.013946	1.681641
C	-2.653207	1.890106	-1.748546
C	-1.137368	-1.595119	-2.119301
C	-2.690419	1.471213	2.049617
H	-0.878800	-2.807390	2.373235
H	-3.010609	2.089732	2.892771
H	-0.825727	-2.218498	-2.961607
H	-2.958612	2.679016	-2.441549
O	1.333565	1.385791	0.167035
C	2.503576	1.016484	0.182523
O	2.896256	-0.237227	-0.008830
O	3.519368	1.850445	0.397284
C	4.357306	-0.345947	0.223791
C	4.788177	1.127598	0.203316
H	4.774830	-0.893236	-0.618427
C	4.601242	-1.073322	1.532023
H	5.218613	1.436021	-0.748452
H	5.459072	1.401494	1.013948
Br	7.677719	-0.347708	-0.407909
H	4.201051	-0.506392	2.382782
H	4.128385	-2.061527	1.515360
H	5.683843	-1.191988	1.642510
W	-0.884531	0.378132	0.023413

Mo-HKUST-1

Mo-HKUST-1

Mo	-0.000416	-0.000089	1.060859

Mo	0.000060	0.000007	-1.060839
O	1.492004	-1.510356	1.120310
O	-1.492951	1.510141	1.119728
O	-1.510942	-1.492617	1.119079
O	1.509962	1.492507	1.119943
O	1.510992	1.491847	-1.119606
O	-1.509858	-1.492701	-1.120467
O	-1.491661	1.511201	-1.119817
O	1.493282	-1.509825	-1.119237
C	1.917148	-1.939213	0.000627
C	-1.916432	1.940177	-0.000108
C	-1.939645	-1.917052	-0.000824
C	1.939952	1.916321	0.000267
H	2.687300	-2.717710	0.000935
H	2.719120	2.685796	0.000371
H	-2.718358	-2.686984	-0.001237
H	-2.685867	2.719382	-0.000160

Mo-Int$_0$

Mo	1.733362	0.087480	0.311538
O	-0.909666	1.086033	1.462697
O	0.183815	-1.168055	-1.991283
O	-0.559993	-1.848782	0.857325
O	-0.165928	1.760953	-1.383490
O	1.989943	1.886887	-0.783091
O	1.598916	-1.707764	1.445228
O	2.337762	-1.031296	-1.386821
O	1.250279	1.215425	2.049558
C	0.019819	1.468662	2.241484
C	1.416028	-1.417654	-2.174528
C	0.467171	-2.285194	1.466997
C	0.968488	2.333029	-1.397060
H	-0.254683	2.048972	3.127825
H	1.073368	3.260452	-1.967512
H	0.371813	-3.210321	2.043840
H	1.701298	-1.996756	-3.057660
Mo	-0.318290	-0.037923	-0.262032
O	-2.863244	-0.277968	-0.661620
C	-3.884512	0.067189	0.312277
C	-5.019075	0.916514	-0.197509
C	-3.687349	-1.329885	-0.103712
H	-3.453706	0.366146	1.267609
H	-5.855785	0.892580	0.512096

H	-4.698504	1.958684	-0.308954
H	-5.373028	0.557189	-1.169410
H	-4.373146	-1.775631	-0.823080
H	-3.149149	-2.022134	0.540260

Mo-Int$_1$

Mo	2.652099	-0.401935	0.340545
O	0.216931	0.724898	1.776505
O	1.114772	-0.251416	-2.289727
O	-0.054369	-1.754684	0.056480
O	1.387730	2.221484	-0.572449
O	3.440080	1.553730	0.045786
O	2.003289	-2.398185	0.675204
O	3.167900	-0.905697	-1.660994
O	2.274032	0.063400	2.381374
C	1.117925	0.530558	2.645096
C	2.266731	-0.714028	-2.541731
C	0.768896	-2.630170	0.454367
C	2.615482	2.440861	-0.350450
H	0.891883	0.777523	3.687154
H	2.994689	3.455751	-0.507983
H	0.399998	-3.647051	0.619764
H	2.505324	-0.964988	-3.580203
Mo	0.688440	0.226132	-0.251444
O	-1.601962	0.801543	-0.770718
C	-2.748348	1.035629	0.133418
C	-3.502258	2.319678	-0.061447
C	-2.817876	-0.052376	-0.825492
H	-2.514878	0.768791	1.162663
H	-4.506849	2.181336	0.354429
H	-2.997744	3.157512	0.437647
H	-3.603491	2.548959	-1.127810
Br	-5.977251	-0.512028	0.102440
H	-3.398952	0.078656	-1.731837
H	-2.659373	-1.073314	-0.495746

Mo-TS$_1$

Mo	2.547615	-0.466558	0.341908

O	0.241701	0.950059	1.737254
O	0.963319	-0.402758	-2.268532
O	-0.257213	-1.634607	0.217044
O	1.465338	2.170741	-0.754910
O	3.475696	1.393250	-0.119633
O	1.765154	-2.378281	0.847409
O	2.976844	-1.161403	-1.622304
O	2.261250	0.180235	2.348509
C	1.149607	0.752934	2.595921
C	2.071283	-0.969741	-2.499138
C	0.511810	-2.531851	0.667625
C	2.709935	2.307238	-0.570487
H	0.971928	1.094969	3.620235
H	3.161517	3.274365	-0.812574
H	0.075732	-3.502603	0.920820
H	2.267996	-1.319958	-3.517154
Mo	0.613721	0.265785	-0.267155
O	-1.530576	0.965072	-0.739815
C	-2.639369	1.200762	0.130570
C	-3.321082	2.540857	-0.041235
C	-3.057897	0.060056	-0.672431
H	-2.415740	0.972905	1.177998
H	-4.275336	2.539846	0.497395
H	-2.681859	3.343054	0.349188
H	-3.518298	2.736542	-1.101567
Br	-5.586632	-0.594657	0.083596
H	-3.489067	0.225117	-1.647219
H	-2.778695	-0.938757	-0.377744

Mo-Int$_2$

Mo	2.466216	-0.515442	0.345801
O	0.121649	0.784106	1.795083
O	1.020298	-0.115409	-2.325503
O	-0.350873	-1.614136	-0.043221
O	1.491273	2.260206	-0.498447
O	3.451828	1.361547	0.146308
O	1.634720	-2.461349	0.592869
O	2.983244	-0.994928	-1.662793
O	2.099946	-0.100445	2.401386
C	0.986391	0.466244	2.657807
C	2.127504	-0.681356	-2.554801

C	0.389861	-2.563438	0.337318
C	2.725155	2.337519	-0.235720
H	0.769887	0.691411	3.706257
H	3.206928	3.313242	-0.341050
H	-0.066795	-3.549429	0.459270
H	2.373220	-0.923842	-3.592667
Mo	0.563025	0.338719	-0.278155
O	-1.415542	1.081683	-0.696042
C	-2.614442	1.026618	-0.003240
C	-3.330817	2.384272	-0.016812
C	-3.385174	-0.075100	-0.731263
H	-2.471439	0.717325	1.049431
H	-4.287634	2.351881	0.520029
H	-2.682430	3.131892	0.454687
H	-3.513351	2.700549	-1.052737
Br	-5.249895	-0.547739	0.114404
H	-3.638971	0.204113	-1.753750
H	-2.854422	-1.022703	-0.691600

Mo-Int$_3$

Mo	-2.619338	-0.710638	-0.216568
O	-1.414667	1.165521	1.872004
O	0.108043	-0.943483	-1.560607
O	-1.118908	1.814601	-1.082317
O	-0.183218	-1.572890	1.404853
O	-2.229795	-2.412876	0.999221
O	-3.152700	0.931625	-1.461202
O	-1.945738	-1.783590	-1.930706
O	-3.450193	0.298532	1.464007
C	-2.640941	1.018885	2.137744
C	-0.709876	-1.650405	-2.214021
C	-2.267113	1.835452	-1.613250
C	-1.077080	-2.455868	1.542255
H	-3.039126	1.546430	3.009031
H	-0.850691	-3.322079	2.171126
H	-2.523396	2.686781	-2.250376
H	-0.332215	-2.187796	-3.088677
O	1.375962	0.868090	0.490972
O	0.821121	3.909716	0.513808
C	2.533970	0.205488	0.881551
C	1.390973	3.512414	-0.427612

C	3.264656	-0.064534	-0.435288
H	2.306467	-0.765825	1.358097
C	3.353487	1.046263	1.870839
O	1.982140	3.239464	-1.402131
H	2.658584	-0.661136	-1.112101
H	3.614099	0.849311	-0.914625
Br	5.009838	-1.204143	-0.232777
H	3.648608	1.998171	1.408316
H	2.731986	1.273859	2.744450
H	4.259241	0.522983	2.202610
Mo	-0.648347	0.124934	0.161873

Mo-TS_2

Mo	-2.551213	-0.832470	-0.062604
O	-1.767584	1.899208	1.027304
O	0.317055	-1.302371	-0.949966
O	-1.155978	1.181124	-1.871470
O	-0.294369	-0.573455	1.960652
O	-2.201470	-1.754104	1.822756
O	-3.059029	-0.010316	-1.953670
O	-1.599970	-2.470533	-1.034241
O	-3.663273	0.700293	0.898534
C	-3.003385	1.740851	1.233012
C	-0.352981	-2.327605	-1.258915
C	-2.228299	0.828411	-2.438896
C	-1.127106	-1.407206	2.415825
H	-3.547995	2.549201	1.729232
H	-0.915196	-1.868759	3.385661
H	-2.466321	1.270254	-3.411003
H	0.169701	-3.152916	-1.751937
O	1.408822	1.176230	0.226989
O	0.581997	3.441927	-0.405357
C	2.487347	0.382437	0.673521
C	1.699862	3.037860	-0.346715
C	3.357965	0.122433	-0.557641
H	2.089353	-0.586553	1.009069
C	3.230029	1.017644	1.855980
O	2.883521	3.179165	-0.463427
H	2.769877	-0.324096	-1.355603
H	3.902603	1.001651	-0.892756
Br	4.841647	-1.285930	-0.218684

H	3.689612	1.968384	1.568209
H	2.510242	1.206298	2.660813
H	4.010972	0.347472	2.236010
Mo	-0.726141	0.320335	0.037708

Mo-Int$_4$

Mo	-3.077584	-0.655720	0.260490
O	-0.600794	0.137769	1.840072
O	-1.851151	0.559411	-2.249940
O	-2.126022	2.238945	0.270937
O	-0.327608	-1.544112	-0.689612
O	-2.264097	-2.567992	-0.188695
O	-4.046115	1.173943	0.750715
O	-3.775376	-0.484721	-1.742217
O	-2.535082	-0.909559	2.300358
C	-1.393462	-0.444999	2.631819
C	-2.985055	0.096326	-2.558659
C	-3.333432	2.227042	0.641763
C	-1.045704	-2.575791	-0.569401
H	-1.083880	-0.564393	3.675080
H	-0.595971	-3.545716	-0.804598
H	-3.805762	3.183877	0.887695
H	-3.316831	0.198522	-3.597189
O	0.691735	1.488520	-0.756300
C	1.942489	1.462744	-0.569970
O	2.338149	0.338723	0.188606
O	2.810877	2.253082	-0.963665
C	3.701974	0.224879	0.611668
C	4.637034	0.195654	-0.600689
H	3.725175	-0.767059	1.075822
C	4.080471	1.274405	1.658837
H	4.223187	-0.400141	-1.412082
H	4.950792	1.174056	-0.947105
Br	6.397627	-0.773590	-0.129028
H	4.049348	2.277134	1.223995
H	3.371364	1.228833	2.492969
H	5.087818	1.079484	2.046162
Mo	-1.223944	0.345658	-0.205229

Mo-TS_3

Mo	-3.219084	-0.552028	-0.146033
O	-0.655186	-1.208320	1.353966
O	-1.882370	1.931160	-1.297754
O	-1.948926	1.505259	1.707072
O	-0.590146	-0.781470	-1.656381
O	-2.621941	-1.723695	-1.815674
O	-3.971595	0.548358	1.512395
O	-3.905367	0.969934	-1.463971
O	-2.686777	-2.144667	1.157914
C	-1.498675	-2.111021	1.621494
C	-3.063178	1.885298	-1.747243
C	-3.147936	1.344151	2.074280
C	-1.414736	-1.569949	-2.200085
H	-1.192815	-2.919486	2.293301
H	-1.074391	-2.162540	-3.055238
H	-3.507205	1.924590	2.930646
H	-3.388252	2.681961	-2.424521
O	0.817903	1.424336	0.224257
C	2.035878	1.156716	0.291499
O	2.404423	-0.147715	0.066170
O	2.990738	1.956515	0.531879
C	3.796659	-0.408370	0.364775
C	4.625262	0.829547	0.060192
H	4.072550	-1.206958	-0.323860
C	3.940635	-0.876919	1.810519
H	4.604775	1.259493	-0.928357
H	5.142873	1.367665	0.835505
Br	6.770949	-0.280124	-0.483820
H	3.647853	-0.079734	2.503606
H	3.295173	-1.743822	1.985969
H	4.980814	-1.157567	2.006057
Mo	-1.276490	0.354563	0.024581

Mo-Int_5

Mo	-3.345955	0.515653	0.149233
O	-0.784812	1.288681	-1.297370
O	-1.947037	-1.970827	1.214368
O	-1.999560	-1.435862	-1.762952
O	-0.733527	0.753111	1.684308

O	-2.787637	1.635493	1.866347
O	-4.048690	-0.544400	-1.556692
O	-3.996032	-1.075572	1.402703
O	-2.838652	2.166632	-1.089372
C	-1.647015	2.182523	-1.542832
C	-3.132722	-1.977949	1.658566
C	-3.200170	-1.296035	-2.140005
C	-1.580457	1.500565	2.255415
H	-1.354046	3.021561	-2.182040
H	-1.259702	2.067343	3.135330
H	-3.532979	-1.854435	-3.021446
H	-3.438150	-2.809313	2.302536
O	0.867388	-1.329874	-0.269679
C	2.042820	-0.988226	-0.259986
O	2.466365	0.238206	0.033625
O	3.043842	-1.822074	-0.547931
C	3.926597	0.334037	-0.196683
C	4.326049	-1.144896	-0.300084
H	4.360496	0.801145	0.684777
C	4.184220	1.160848	-1.442047
H	4.753270	-1.538929	0.621270
H	4.990403	-1.363552	-1.132797
Br	7.258945	0.224871	0.413649
H	3.769717	0.674295	-2.334762
H	3.733025	2.154444	-1.342855
H	5.268945	1.264952	-1.546711
Mo	-1.387453	-0.328542	-0.036706

V-HKUST-1

V-HKUST-1

V	-0.000098	-0.000026	-1.295868
V	0.000102	0.000026	1.295869
O	-0.000238	-2.035393	-1.122334
O	0.000062	2.035348	-1.122416
O	2.066326	-0.000184	-1.129138
O	-2.066495	0.000140	-1.128833
O	-2.066322	0.000214	1.129130
O	2.066498	-0.000169	1.128825
O	0.000258	2.035394	1.122341
O	-0.000097	-2.035348	1.122423

C	-0.000190	-2.621783	0.000057
C	0.000180	2.621783	-0.000050
C	2.640480	-0.000124	-0.000201
C	-2.640476	0.000120	0.000193
H	-0.000557	-3.719368	0.000079
H	-3.739758	0.000676	0.000278
H	3.739761	-0.000668	-0.000285
H	0.000544	3.719368	-0.000072

V-Int$_0$

V	2.085813	0.103686	0.586723
V	-0.526920	-0.052280	-0.582080
O	1.167049	-0.448472	2.418147
O	2.887079	0.655625	-1.322211
O	1.525965	2.079331	0.909830
O	2.163529	-1.895540	0.031493
O	0.086124	-2.062427	-0.867657
O	-0.560995	1.983546	0.022378
O	0.766544	0.465275	-2.004239
O	-0.840319	-0.537630	1.403092
C	-0.074244	-0.642072	2.412958
C	2.001377	0.709182	-2.208017
C	0.406016	2.572685	0.593974
C	1.219207	-2.521049	-0.530441
H	-0.574957	-0.930236	3.357484
H	1.421525	-3.582578	-0.741478
H	0.272362	3.634394	0.853563
H	2.268833	0.982002	-3.245402
O	-2.650492	-0.323006	-0.724744
C	-3.652771	0.125792	0.247088
C	-4.787373	0.929182	-0.325209
C	-3.465672	-1.307124	-0.025547
H	-3.181377	0.510480	1.148906
H	-5.605535	0.983826	0.403630
H	-4.459498	1.951237	-0.544355
H	-5.168908	0.477313	-1.246422
H	-4.158643	-1.824505	-0.685517
H	-2.903460	-1.917449	0.675271

V-Int$_1$

V	2.999903	-0.662864	0.626051
V	0.690255	0.502655	-0.562727
O	1.746757	-1.831655	1.864398
O	4.212946	0.554957	-0.662354
O	2.845410	0.933110	1.955124
O	2.818473	-2.066044	-0.899028
O	0.977550	-1.151736	-1.866901
O	0.999192	1.882306	1.030867
O	2.279045	1.356728	-1.469511
O	0.005734	-0.830216	0.848403
C	0.513390	-1.638098	1.680956
C	3.546530	1.297061	-1.426985
C	1.929783	1.804662	1.882497
C	1.893593	-2.015704	-1.763037
H	-0.211203	-2.210499	2.287412
H	1.904271	-2.827861	-2.504872
H	1.963080	2.580725	2.661668
H	4.078534	1.963328	-2.130645
O	-1.288881	0.907766	-0.943944
C	-2.413801	1.130919	0.010879
C	-3.175604	2.409618	-0.174446
C	-2.517920	0.022766	-0.917960
H	-2.121956	0.879570	1.027616
H	-4.152685	2.282138	0.304610
H	-2.643272	3.256181	0.276569
H	-3.341029	2.612647	-1.237885
Br	-5.438587	-0.574529	0.161193
H	-3.115098	0.130676	-1.814900
H	-2.309365	-0.982631	-0.575658

V-TS$_1$

V	2.950273	-0.700227	0.594299
V	0.650414	0.527077	-0.542557
O	1.694492	-1.931667	1.765833
O	4.167120	0.581687	-0.622350
O	2.793860	0.824172	2.007273
O	2.786371	-2.029984	-0.997504
O	0.955593	-1.058907	-1.930682
O	0.949994	1.819728	1.126612
O	2.241384	1.436435	-1.399548

O	-0.046788	-0.882504	0.794962
C	0.461780	-1.730151	1.585203
C	3.507238	1.366656	-1.349562
C	1.877172	1.696746	1.976016
C	1.868021	-1.929155	-1.864423
H	-0.261735	-2.336409	2.157711
H	1.881622	-2.700235	-2.648120
H	1.905156	2.430356	2.794848
H	4.048492	2.066497	-2.011014
O	-1.281061	0.981115	-0.917289
C	-2.359682	1.230004	0.028178
C	-3.076515	2.543295	-0.150071
C	-2.688226	0.074028	-0.785559
H	-2.062057	1.012665	1.054723
H	-4.018480	2.508465	0.407755
H	-2.460103	3.371109	0.221371
H	-3.306974	2.717145	-1.206919
Br	-5.272480	-0.622839	0.141591
H	-3.217235	0.198537	-1.717659
H	-2.414148	-0.915469	-0.455619

V-Int$_2$

V	2.929626	-0.794103	0.288615
V	0.553681	0.635021	-0.234633
O	1.866624	-2.608292	0.021428
O	3.917364	1.088565	0.534311
O	2.278692	-0.695174	2.279357
O	3.267953	-0.689655	-1.771066
O	1.364522	0.481424	-2.207636
O	0.355546	0.452625	1.873609
O	1.931758	2.080234	0.134738
O	0.011324	-1.368089	-0.348530
C	0.643112	-2.458275	-0.240462
C	3.172935	2.091445	0.389664
C	1.197084	-0.132083	2.612635
C	2.436096	-0.103715	-2.524247
H	0.038170	-3.365932	-0.397738
H	2.690727	-0.113221	-3.592453
H	0.968095	-0.159752	3.686260
H	3.620631	3.092937	0.491499
O	-1.199147	1.221264	-0.716549

C	-2.392325	1.077326	0.000593
C	-3.151734	2.407230	0.041131
C	-3.130622	-0.027907	-0.755216
H	-2.206172	0.737241	1.033380
H	-4.102709	2.316238	0.579441
H	-2.532134	3.160403	0.541156
H	-3.351976	2.755883	-0.980522
Br	-4.922224	-0.598003	0.125384
H	-3.419952	0.282964	-1.759012
H	-2.547238	-0.945121	-0.773929

V-Int$_3$

V	-3.051650	-0.909490	-0.489941
O	-4.032820	0.054568	1.151231
O	-1.997353	-1.816686	-2.090174
O	-2.532937	-2.502431	0.767045
O	-3.238593	0.844065	-1.611461
O	-1.304263	1.766584	-0.846519
O	-0.564597	-1.636287	1.512772
O	-0.108610	-0.905623	-1.244498
O	-2.006144	0.798886	1.797824
C	-3.263883	0.696056	1.911930
C	-0.757584	-1.590425	-2.086877
C	-1.466757	-2.518651	1.446056
C	-2.356591	1.747297	-1.544874
H	-3.700923	1.228756	2.771773
H	-2.538992	2.622927	-2.180861
H	-1.314991	-3.420410	2.053459
H	-0.153047	-2.026211	-2.899193
O	1.153964	0.869506	0.640354
O	0.467952	3.963818	0.610569
C	2.311196	0.137564	0.944677
C	0.979238	3.597293	-0.375593
C	3.036347	0.014717	-0.396041
H	2.059603	-0.874793	1.302995
C	3.126491	0.857809	2.023276
O	1.521954	3.329883	-1.378327
H	2.412713	-0.486064	-1.132168
H	3.393450	0.975871	-0.764667
Br	4.743716	-1.155760	-0.310683
H	3.407082	1.861806	1.678463

H	2.513696	0.968262	2.924994
H	4.038113	0.304887	2.278668
V	-0.629477	0.192810	0.439272

V-TS_2

V	-3.003876	-1.134241	-0.097700
O	-4.383968	0.510982	-0.310621
O	-1.723990	-2.821502	0.100200
O	-3.089228	-0.947272	1.958539
O	-2.628666	-1.081469	-2.131419
O	-0.802172	0.275695	-2.038698
O	-1.300081	0.443860	2.187403
O	-0.031631	-1.345783	0.257721
O	-2.470614	1.659236	-0.127690
C	-3.723376	1.584407	-0.270912
C	-0.505330	-2.514003	0.235692
C	-2.261688	-0.244834	2.617283
C	-1.660014	-0.431538	-2.630452
H	-4.254745	2.554681	-0.367632
H	-1.583458	-0.515044	-3.723729
H	-2.432419	-0.261008	3.703538
H	0.238887	-3.330730	0.347411
O	1.272370	1.119576	0.357925
O	0.052626	3.135795	-0.452340
C	2.385810	0.372060	0.770467
C	1.238703	3.081037	-0.412262
C	3.122512	0.024040	-0.523833
H	2.042690	-0.564802	1.230921
C	3.234496	1.144029	1.787167
O	2.365748	3.415442	-0.528432
H	2.473330	-0.520042	-1.206164
H	3.565739	0.896469	-1.002766
Br	4.722836	-1.261312	-0.249627
H	3.623595	2.070419	1.350020
H	2.606362	1.405418	2.646684
H	4.078306	0.539596	2.140591
V	-0.679923	0.650038	0.097633

V-Int_4

V	-3.201860	-1.018387	0.116830
O	-4.503074	0.612062	-0.350718
O	-1.998855	-2.729639	0.599001
O	-3.159254	-0.428926	2.096929
O	-2.936005	-1.399965	-1.894801
O	-1.045888	-0.157240	-2.158415
O	-1.281096	0.853245	1.972491
O	-0.263703	-1.321542	0.371689
O	-2.549135	1.705834	-0.508927
C	-3.805827	1.645009	-0.563874
C	-0.768155	-2.454067	0.609683
C	-2.262409	0.334617	2.568276
C	-1.969484	-0.913848	-2.558493
H	-4.314392	2.596634	-0.823919
H	-1.966719	-1.212312	-3.617257
H	-2.385555	0.552024	3.639551
H	-0.037862	-3.256925	0.846182
O	1.414801	0.872751	-0.060912
O	0.120849	2.557982	-0.540364
C	2.589266	0.232704	0.475637
C	1.341117	2.299391	-0.344003
C	3.690198	0.320998	-0.580189
H	2.270925	-0.808349	0.573338
C	2.962219	0.793598	1.845731
O	2.367845	2.963703	-0.361588
H	3.320010	0.023726	-1.559950
H	4.170637	1.294560	-0.618773
Br	5.193862	-1.005711	-0.182490
H	3.271370	1.839866	1.767488
H	2.095267	0.729318	2.511696
H	3.781105	0.209796	2.280630
V	-0.797417	0.646867	-0.144810

V-TS$_3$

V	-3.822725	0.707271	0.421490
O	-3.193645	2.163726	-0.911134
O	-4.125218	-0.940517	1.638290
O	-2.807181	1.705358	2.002084
O	-4.805839	-0.327052	-1.200785
O	-2.810319	-1.268697	-1.603507

O	-0.970216	0.583748	1.343078
O	-2.202064	-2.018716	1.075387
O	-1.257590	1.124984	-1.501798
C	-2.100324	2.062973	-1.542175
C	-3.289737	-1.891186	1.700365
C	-1.584678	1.396733	2.090542
C	-4.042985	-1.090193	-1.847765
H	-1.871247	2.905074	-2.203280
H	-4.456607	-1.665079	-2.705498
H	-0.976868	1.872448	2.891547
H	-3.562218	-2.697702	2.389294
O	0.525287	-1.297676	-0.435172
C	1.744116	-0.989704	-0.463897
O	2.118095	0.158039	0.151189
O	2.669259	-1.667316	-1.001494
C	3.512667	0.499474	-0.096849
C	4.303943	-0.779417	-0.320728
H	3.839279	0.975671	0.826560
C	3.595288	1.471967	-1.268065
H	4.384066	-1.512085	0.466083
H	4.787104	-0.987357	-1.259844
Br	6.543416	0.112527	0.439054
H	3.249243	0.994334	-2.192156
H	2.964802	2.345204	-1.072474
H	4.631882	1.797512	-1.398726
V	-1.393070	-0.610635	-0.293926

V-Int$_5$

V	-3.958640	0.691093	0.386291
O	-3.737400	1.551702	-1.484459
O	-3.818602	-0.382375	2.150398
O	-2.863944	2.292043	1.262841
O	-5.006798	-0.968764	-0.521754
O	-2.974139	-1.817371	-0.929798
O	-1.008546	1.156226	0.696831
O	-1.862070	-1.432060	1.659990
O	-1.778764	0.526118	-2.016070
C	-2.748874	1.304207	-2.235915
C	-2.852098	-1.162952	2.396105
C	-1.610833	2.143968	1.211088
C	-4.243701	-1.857208	-0.978823

H	-2.750351	1.839140	-3.191976
H	-4.684639	-2.755099	-1.467419
H	-0.960953	2.935376	1.647426
H	-2.895235	-1.658874	3.371949
O	0.528641	-1.106735	-0.480909
C	1.719321	-0.793296	-0.413207
O	2.162610	0.334747	0.107100
O	2.679144	-1.583358	-0.870174
C	3.633732	0.435415	-0.105333
C	3.991084	-1.000899	-0.514307
H	4.072813	0.696658	0.854727
C	3.907916	1.496614	-1.152322
H	4.415584	-1.588808	0.297535
H	4.631271	-1.065534	-1.390345
Br	6.922729	0.069019	0.432963
H	3.477947	1.217976	-2.123161
H	3.485628	2.459081	-0.843501
H	4.994709	1.590769	-1.242467
V	-1.494517	-0.605998	-0.251603

Cd-HKUST-1

Cd-HKUST-1

Cd	-1.536856	-0.002448	-0.000242
Cd	1.537725	0.002473	-0.000136
O	-1.783991	-1.385795	-1.652568
O	-1.791115	1.378589	1.652976
O	-0.476725	1.596038	-1.334732
O	-0.468948	-1.596900	1.333746
O	1.790533	-1.651338	1.380074
O	1.782733	1.658653	-1.378636
O	0.468175	1.334531	1.594778
O	0.475259	-1.333895	-1.595098
C	-0.624319	-1.724960	-2.059491
C	-0.632472	1.721358	2.060039
C	0.623189	2.063971	-1.720413
C	0.632093	-2.060321	1.721475
H	-0.602504	-2.431553	-2.903986
H	0.613356	-2.905325	2.427557
H	0.602035	2.909952	-2.425263

H	-0.612950	2.426384	2.905893

Cd-Int$_0$

Cd	-0.850718	0.054140	-0.579345
Cd	2.115017	-0.020412	0.462731
O	-0.554271	-1.773043	-1.691680
O	-1.187796	1.946888	0.427071
O	0.996539	1.065954	-1.790129
O	-0.381833	-1.026784	1.522160
O	1.738059	-1.116157	2.309360
O	3.152901	1.049956	-1.131560
O	0.937331	1.815608	1.207657
O	1.542823	-1.833016	-0.831129
C	0.596204	-2.283975	-1.520383
C	-0.186053	2.359295	1.093479
C	2.213531	1.349004	-1.938509
C	0.491534	-1.358423	2.366764
H	0.754632	-3.233120	-2.039476
H	0.167703	-1.918285	3.259636
H	2.523621	1.905356	-2.837988
H	-0.351452	3.299037	1.628173
O	-3.173734	-0.305021	-0.474424
C	-4.050471	0.227386	0.565323
C	-5.336308	0.837451	0.077345
C	-3.774162	-1.215470	0.489028
H	-3.498493	0.800129	1.308808
H	-6.037389	0.946522	0.914058
H	-5.153211	1.832717	-0.342801
H	-5.802342	0.212693	-0.691466
H	-4.511788	-1.881247	0.045320
H	-3.063421	-1.669432	1.176303

Cd-Int$_1$

Cd	0.007509	0.236274	0.306309
Cd	-3.139217	-0.232619	-0.230579
O	-0.399672	-0.791459	2.155735
O	-0.007674	0.940513	-1.736062
O	-1.685130	1.862137	0.848063
O	-1.231696	-1.871410	-0.760577

O	-3.411549	-2.248529	-1.151161
O	-3.915284	1.700981	0.550725
O	-2.252484	0.771952	-2.074756
O	-2.651044	-0.975615	1.869922
C	-1.576202	-1.110278	2.502294
C	-1.078184	1.068311	-2.401743
C	-2.862079	2.303692	0.925423
C	-2.182357	-2.584439	-1.175315
H	-1.638767	-1.558651	3.496513
H	-1.962208	-3.582693	-1.597851
H	-3.013731	3.310152	1.357581
H	-0.935042	1.503843	-3.393338
O	2.169124	0.691617	0.628719
C	3.291486	0.853877	-0.331935
C	3.953047	2.200735	-0.340755
C	3.458913	-0.083135	0.762508
H	3.059379	0.431425	-1.307701
H	4.948945	2.077858	-0.780513
H	3.371501	2.922966	-0.927168
H	4.073344	2.579082	0.679964
Br	6.402560	-0.670206	-0.162071
H	4.026889	0.211059	1.636470
H	3.357603	-1.147323	0.585740

Cd-TS$_1$

Cd	0.085576	0.315833	0.326969
Cd	-3.104138	-0.243776	-0.225647
O	-0.508684	-0.336970	2.307087
O	0.068087	0.351376	-1.850516
O	-1.540151	2.005250	0.366680
O	-1.390915	-2.058609	-0.277284
O	-3.578687	-2.400039	-0.643083
O	-3.768367	1.872468	0.031306
O	-2.173121	0.252821	-2.240045
O	-2.765477	-0.438146	2.016785
C	-1.707132	-0.490629	2.688209
C	-0.970160	0.374625	-2.575599
C	-2.696641	2.498419	0.285607
C	-2.372549	-2.799829	-0.539410
H	-1.816552	-0.689846	3.759215
H	-2.198691	-3.878361	-0.695136
H	-2.796675	3.583641	0.450518

H	-0.773475	0.530857	-3.641192
O	2.206399	0.826496	0.604420
C	3.259973	0.907158	-0.392981
C	3.914401	2.258575	-0.528157
C	3.660224	-0.016770	0.652982
H	2.978862	0.454969	-1.346278
H	4.853607	2.144682	-1.079984
H	3.256614	2.952711	-1.066110
H	4.140062	2.676761	0.458876
Br	6.248251	-0.785461	-0.110329
H	4.183877	0.342843	1.524761
H	3.453185	-1.072351	0.566668

Cd-Int$_2$

Cd	-0.246248	0.835220	-0.178745
Cd	2.850281	-0.536954	0.239663
O	1.192029	2.223823	-1.126402
O	-0.520201	-1.353291	0.206796
O	1.072107	0.884813	1.713865
O	1.834694	-0.856500	-1.947128
O	3.870757	-1.665545	-1.465069
O	3.094223	0.160901	2.386646
O	1.471229	-2.202561	0.911087
O	3.280895	1.561930	-0.502773
C	2.445975	2.345943	-1.019750
C	0.232050	-2.240696	0.701952
C	1.996001	0.758456	2.562396
C	2.882728	-1.480525	-2.247075
H	2.863308	3.275829	-1.436147
H	2.958019	-1.902407	-3.261197
H	1.822716	1.213342	3.547237
H	-0.269643	-3.175486	0.994759
O	-2.193457	1.630814	-0.357469
C	-3.373434	1.128859	0.191646
C	-4.467657	2.201377	0.120703
C	-3.708022	-0.124639	-0.622034
H	-3.254936	0.824096	1.249652
H	-5.415980	1.852623	0.546790
H	-4.134228	3.088740	0.671018
H	-4.632724	2.495257	-0.924219
Br	-5.398170	-1.138044	0.034559

H	-3.932092	0.113096	-1.662267
H	-2.926154	-0.878038	-0.542710

Cd-Int$_3$

Cd	-3.010793	-0.787955	-0.014095
O	-1.215842	1.735645	1.623333
O	-0.008022	-0.423626	-1.760561
O	-2.705134	1.298454	-1.230771
O	-0.645600	-1.324931	1.176110
O	-2.513713	-2.571777	1.303106
O	-4.666217	0.209658	-1.236698
O	-1.886794	-1.712457	-1.749601
O	-3.152075	0.549099	1.811338
C	-2.335905	1.448106	2.134735
C	-0.785027	-1.316272	-2.206481
C	-3.904720	1.171694	-1.579517
C	-1.305932	-2.321460	1.575981
H	-2.635808	2.073582	2.989715
H	-0.775436	-3.035567	2.221931
H	-4.336272	1.948107	-2.231725
H	-0.444355	-1.821962	-3.123097
O	2.137232	1.120106	0.502641
O	0.851525	3.083288	-0.848361
C	3.181187	0.255112	0.840614
C	2.008737	3.267537	-0.754445
C	3.731059	-0.246657	-0.498686
H	2.822684	-0.621030	1.411764
C	4.229816	0.986019	1.687859
O	3.128260	3.610464	-0.759798
H	2.961441	-0.741017	-1.089093
H	4.209162	0.550861	-1.068035
Br	5.206096	-1.689203	-0.321331
H	4.625002	1.847953	1.135818
H	3.753831	1.358632	2.602241
H	5.063143	0.329208	1.964632
Cd	0.074106	0.645819	0.192974

Cd-TS$_2$

Cd	-3.050783	-0.798065	0.022867
O	-1.121363	1.566697	1.760253
O	-0.228896	-0.164564	-1.958678
O	-2.877421	1.423424	-0.964362
O	-0.563586	-1.415189	0.907927
O	-2.401734	-2.703806	1.068496
O	-4.819685	0.302608	-0.914919
O	-2.083587	-1.487164	-1.906849
O	-3.017027	0.323681	1.992872
C	-2.182249	1.196285	2.340077
C	-1.037694	-1.018726	-2.422607
C	-4.103712	1.313837	-1.211719
C	-1.174506	-2.462894	1.250551
H	-2.401150	1.710328	3.288185
H	-0.579105	-3.237770	1.755091
H	-4.604084	2.151696	-1.724104
H	-0.784528	-1.411008	-3.419124
O	2.118459	1.033113	0.349474
O	0.947473	2.980948	-0.752771
C	3.179344	0.212603	0.756810
C	2.127174	2.967515	-0.616109
C	3.891235	-0.195817	-0.536798
H	2.793867	-0.702978	1.237263
C	4.088649	0.939487	1.754768
O	3.256113	3.302176	-0.661820
H	3.208513	-0.692697	-1.223884
H	4.387329	0.646997	-1.017666
Br	5.395962	-1.578434	-0.257472
H	4.511318	1.842261	1.298807
H	3.493799	1.242453	2.624085
H	4.909313	0.297717	2.096015
Cd	0.005089	0.681171	0.078175

Cd-Int$_4$

Cd	-3.017813	-0.937643	0.129625
O	-1.047351	1.453051	1.813518
O	-0.687587	0.280516	-2.219558
O	-3.263943	1.400788	-0.573513
O	-0.337036	-1.294123	0.477317
O	-1.962485	-2.826631	0.773022
O	-5.024721	0.031566	-0.331575

O	-2.359779	-1.254133	-2.016420
O	-2.736741	-0.029692	2.188188
C	-1.943201	0.890754	2.506022
C	-1.482769	-0.607290	-2.641282
C	-4.495967	1.155950	-0.612264
C	-0.755863	-2.445287	0.771813
H	-2.031527	1.264379	3.535087
H	-0.000868	-3.195186	1.056661
H	-5.180137	1.967913	-0.910364
H	-1.383509	-0.844129	-3.709114
O	2.158399	0.896560	0.069516
O	1.111685	2.728967	-0.566133
C	3.290014	0.144444	0.559237
C	2.272254	2.292763	-0.309992
C	4.337786	0.063638	-0.551342
H	2.866336	-0.852760	0.711295
C	3.805327	0.692051	1.888486
O	3.379893	2.814642	-0.341814
H	3.883175	-0.204173	-1.503922
H	4.939307	0.963239	-0.641295
Br	5.668700	-1.441560	-0.185234
H	4.218487	1.696063	1.760480
H	2.981857	0.736692	2.609450
H	4.581942	0.032300	2.290752
Cd	-0.259015	0.982561	-0.182965

Cd-TS$_3$

Cd	3.318687	0.734372	-0.004966
O	0.649161	-0.487258	2.055847
O	0.662852	-0.338326	-2.176161
O	2.504417	-1.915718	-0.107521
O	1.178364	1.973415	0.039465
O	3.178967	2.987502	0.078336
O	4.607170	-1.102914	-0.071406
O	2.789729	0.476832	-2.200392
O	2.780565	0.309382	2.162963
C	1.696886	-0.095143	2.649721
C	1.712951	0.105922	-2.727666
C	3.757936	-2.040934	-0.109627
C	1.904109	2.998962	0.076760
H	1.639159	-0.122614	3.745069
H	1.417065	3.988297	0.111197

H	4.158057	-3.066567	-0.148396
H	1.664367	0.164649	-3.822024
O	-1.225269	-2.418042	-0.100153
C	-2.322402	-1.820322	0.005914
O	-2.252309	-0.452807	0.013782
O	-3.483761	-2.311439	0.097901
C	-3.533250	0.183832	0.340265
C	-4.641526	-0.774718	-0.074063
H	-3.560608	1.074911	-0.283900
C	-3.549342	0.541084	1.819990
H	-4.820154	-0.978198	-1.117604
H	-5.325219	-1.187138	0.647889
Br	-6.437184	1.054341	-0.338616
H	-3.505575	-0.363633	2.437827
H	-2.686618	1.169082	2.062835
H	-4.469555	1.086902	2.047413
Cd	0.421297	-0.880721	-0.079571

Cd-Int$_5$

Cd	3.701396	0.528631	-0.044585
O	0.777950	-0.111264	2.087453
O	0.881530	-0.503426	-2.163357
O	2.536643	-2.011850	0.160603
O	1.605603	1.959001	-0.226421
O	3.705086	2.754015	-0.248089
O	4.719397	-1.438455	0.161243
O	3.089413	0.050349	-2.190393
O	2.984901	0.445731	2.121289
C	1.866242	0.225638	2.644001
C	1.996746	-0.266965	-2.718304
C	3.767016	-2.275496	0.214340
C	2.439122	2.899178	-0.292511
H	1.799925	0.325883	3.731213
H	2.071846	3.936744	-0.396945
H	4.062003	-3.335108	0.317868
H	1.983615	-0.365832	-3.807477
O	-1.302026	-1.677400	0.058896
C	-2.442917	-1.207859	0.102271
O	-2.701336	0.087001	0.015087
O	-3.520845	-1.956763	0.241551
C	-4.159193	0.322201	0.242760

C	-4.724677	-1.100832	0.114298
H	-4.502841	0.961669	-0.566747
C	-4.343962	0.979044	1.595567
H	-5.179675	-1.300327	-0.853878
H	-5.410999	-1.378187	0.909868
Br	-7.422440	0.618486	-0.389332
H	-4.007714	0.320921	2.407092
H	-3.782198	1.917949	1.647257
H	-5.411855	1.190234	1.709608
Cd	0.664489	-0.573338	-0.018512

Sc-HKUST-1

Sc-HKUST-1

Sc	0.000239	0.001180	-1.442960
Sc	-0.000324	-0.001402	1.443507
O	-1.479163	1.515185	-1.124877
O	1.480540	-1.511893	-1.126548
O	-1.513411	-1.478291	-1.128010
O	1.513319	1.481336	-1.125560
O	1.507238	1.484151	1.126643
O	-1.507564	-1.487292	1.124179
O	1.485250	-1.508750	1.125659
O	-1.486141	1.505674	1.127302
C	-1.886914	1.922215	0.001632
C	1.887396	-1.921870	-0.000724
C	-1.922302	-1.887022	-0.002389
C	1.921964	1.887103	0.001144
H	-2.657579	2.707251	0.002625
H	2.706754	2.658019	0.002313
H	-2.707344	-2.657679	-0.003485
H	2.658522	-2.706454	-0.001231

Sc-Int$_0$

Sc	-0.373792	-0.122716	-0.679176
Sc	2.142870	0.198657	0.788757
O	0.726327	-1.707267	-1.578269
O	-0.908481	1.556574	0.611921
O	0.592480	1.244929	-1.983414

O	-0.753737	-1.462522	1.020025
O	1.199089	-1.183007	2.122324
O	2.546243	1.495941	-0.883188
O	1.054513	1.796379	1.705337
O	2.678437	-1.464954	-0.473037
C	1.924607	-2.026497	-1.313192
C	-0.142373	2.110759	1.451819
C	1.752494	1.733915	-1.833291
C	0.045307	-1.674206	1.977578
H	2.342438	-2.874820	-1.870841
H	-0.301654	-2.354682	2.766139
H	2.093344	2.431688	-2.607980
H	-0.560826	2.950804	2.022699
O	-2.687114	-0.307868	-0.805539
C	-3.683144	0.002586	0.222982
C	-4.763306	0.963720	-0.191326
C	-3.572083	-1.358725	-0.316904
H	-3.213426	0.188152	1.186653
H	-5.591848	0.925693	0.527040
H	-4.374674	1.987751	-0.208491
H	-5.150688	0.718871	-1.185669
H	-4.284576	-1.698784	-1.066128
H	-3.059808	-2.124368	0.260093

Sc-Int$_1$

Sc	0.769521	0.329047	-0.569150
Sc	3.294047	-0.560906	0.718316
O	1.671165	-0.653184	-2.240910
O	0.527463	1.164998	1.430702
O	2.008309	2.020968	-1.028973
O	0.189819	-1.631549	0.162244
O	2.101637	-2.284111	1.177005
O	3.938879	1.357958	-0.058023
O	2.446924	0.464990	2.402061
O	3.591023	-1.357338	-1.278596
C	2.784401	-1.255814	-2.242315
C	1.324595	1.048348	2.401851
C	3.219943	2.173544	-0.697186
C	0.891302	-2.433076	0.839428
H	3.073685	-1.739020	-3.186670
H	0.397841	-3.357999	1.170167

H	3.693829	3.118983	-1.000441
H	1.008079	1.504017	3.351092
O	-1.347476	0.754251	-0.819704
C	-2.491536	1.064068	0.084714
C	-3.185393	2.370424	-0.167103
C	-2.634376	-0.068602	-0.805727
H	-2.242004	0.845186	1.120379
H	-4.181894	2.308892	0.284400
H	-2.626196	3.206017	0.271737
H	-3.308064	2.543800	-1.241491
Br	-5.598470	-0.531963	0.108771
H	-3.196954	0.042354	-1.724082
H	-2.482357	-1.073701	-0.432996

Sc-TS$_1$

Sc	0.725248	0.371538	-0.539665
Sc	3.260662	-0.628359	0.672157
O	1.563312	-0.601089	-2.253491
O	0.556611	1.163780	1.488610
O	2.009178	2.035830	-0.986719
O	0.107158	-1.589527	0.169778
O	2.022552	-2.322616	1.122719
O	3.941302	1.288365	-0.080697
O	2.479991	0.388478	2.395095
O	3.480322	-1.387546	-1.348882
C	2.656454	-1.237965	-2.291519
C	1.375149	1.002602	2.435213
C	3.232745	2.140687	-0.682118
C	0.800957	-2.426743	0.810229
H	2.910463	-1.708538	-3.252431
H	0.287815	-3.344854	1.130210
H	3.729050	3.077838	-0.975369
H	1.096504	1.445944	3.402290
O	-1.334800	0.875475	-0.771477
C	-2.461204	1.182294	0.111803
C	-3.134670	2.505510	-0.137074
C	-2.746657	0.023710	-0.709005
H	-2.218072	0.984866	1.156012
H	-4.109802	2.499501	0.362042
H	-2.526136	3.329562	0.255222
H	-3.296907	2.661311	-1.209150

Br	-5.449577	-0.590662	0.092838
H	-3.245654	0.142542	-1.658928
H	-2.537835	-0.971516	-0.346244

Sc-Int$_2$

Sc	-0.564804	0.477880	-0.046517
Sc	-3.406669	-0.699475	0.058416
O	-0.860153	0.269989	2.101134
O	-1.075058	0.388530	-2.162595
O	-1.746421	2.290320	0.062444
O	-0.165082	-1.682781	-0.120709
O	-2.267649	-2.526745	-0.046046
O	-3.838176	1.424448	0.139042
O	-3.160240	-0.494442	-2.082190
O	-2.949525	-0.603400	2.172892
C	-1.878094	-0.186789	2.693061
C	-2.143674	-0.042921	-2.678638
C	-3.006244	2.371705	0.124491
C	-1.009753	-2.620119	-0.108302
H	-1.820485	-0.225356	3.793149
H	-0.600689	-3.641947	-0.156853
H	-3.423152	3.390344	0.170619
H	-2.192546	-0.021199	-3.779599
O	1.312192	0.997385	-0.159169
C	2.686769	1.035160	-0.377251
C	3.288726	2.341247	0.151894
C	3.228191	-0.213000	0.320944
H	2.904084	0.952548	-1.456762
H	4.369133	2.394287	-0.027833
H	2.803808	3.188453	-0.345969
H	3.102033	2.429782	1.229844
Br	5.239053	-0.547780	-0.029468
H	3.152874	-0.144003	1.406239
H	2.744406	-1.115243	-0.046959

Sc-Int$_3$

Sc	-3.480996	-0.762709	-0.555468
O	-1.924442	1.009843	1.917254

O	-0.212915	-1.143873	-1.353416
O	-1.148317	1.718044	-0.891937
O	-1.008010	-1.822493	1.509657
O	-3.068559	-2.411514	0.772754
O	-3.198794	1.098704	-1.628219
O	-2.283113	-1.735162	-2.061456
O	-3.988019	0.430259	1.187184
C	-3.187067	0.998891	1.977657
C	-1.021826	-1.721333	-2.130625
C	-2.198926	1.863304	-1.582128
C	-2.016546	-2.579376	1.450692
H	-3.633359	1.550390	2.819852
H	-1.974226	-3.493308	2.063784
H	-2.242898	2.762579	-2.216183
H	-0.572965	-2.277480	-2.968731
O	1.197134	0.327426	0.887496
O	0.585638	4.024087	0.484160
C	2.510843	-0.102128	1.089798
C	1.136090	3.566290	-0.440524
C	3.096314	-0.261147	-0.313721
H	2.515019	-1.089635	1.582950
C	3.281207	0.889415	1.967824
O	1.724199	3.166119	-1.370089
H	2.500003	-0.941886	-0.917218
H	3.230854	0.694892	-0.819310
Br	4.983012	-1.109403	-0.321520
H	3.327727	1.871812	1.479946
H	2.756110	1.009621	2.921942
H	4.303956	0.547141	2.165165
Sc	-0.691126	0.047469	0.431661

Sc-TS$_1$

Sc	-3.198359	-1.276754	0.005282
O	-2.288101	1.818811	0.983132
O	-0.010612	-1.199377	-1.030739
O	-1.730155	1.060248	-1.922551
O	-0.583052	-0.449507	1.912929
O	-2.367671	-1.844978	1.899525
O	-3.540801	-0.297633	-1.888342
O	-1.799956	-2.586498	-0.955548
O	-4.089147	0.447824	0.953534

C	-3.492731	1.528130	1.220305
C	-0.602742	-2.291072	-1.239162
C	-2.793813	0.581180	-2.402536
C	-1.315439	-1.350762	2.399272
H	-4.089755	2.306649	1.718316
H	-1.006159	-1.756597	3.375031
H	-3.104922	0.974083	-3.382548
H	-0.012106	-3.081608	-1.726357
O	1.220246	1.065513	0.254043
O	0.032389	3.056726	-0.551747
C	2.331861	0.315379	0.693215
C	1.212836	2.999311	-0.389352
C	3.187105	0.102419	-0.555638
H	1.975076	-0.665294	1.039489
C	3.056974	1.009786	1.849648
O	2.331838	3.384439	-0.389332
H	2.610711	-0.390161	-1.335585
H	3.648400	1.022665	-0.911799
Br	4.779344	-1.170795	-0.243893
H	3.451426	1.982654	1.536378
H	2.345553	1.169442	2.667482
H	3.885795	0.396125	2.221647
Sc	-0.796174	0.610520	-0.016688

Sc-Int$_4$

Sc	-3.351424	-1.192652	0.143801
O	-2.409951	1.942685	0.748845
O	-0.149531	-1.290647	-0.869637
O	-1.870846	0.800870	-2.092492
O	-0.649647	-0.167440	1.889259
O	-2.468845	-1.500350	2.085618
O	-3.709128	-0.499913	-1.857632
O	-1.950438	-2.641322	-0.636847
O	-4.247415	0.625175	0.866138
C	-3.623249	1.717965	0.998984
C	-0.753438	-2.394784	-0.955410
C	-2.952880	0.292157	-2.490457
C	-1.403841	-0.968724	2.507053
H	-4.204618	2.571998	1.379588
H	-1.102201	-1.236348	3.532412
H	-3.277961	0.564534	-3.506694

H	-0.166333	-3.236413	-1.355502
O	1.361019	0.938365	0.045285
O	0.088549	2.575343	-0.629923
C	2.559153	0.305814	0.540783
C	1.303425	2.329896	-0.383096
C	3.586735	0.295672	-0.589384
H	2.231800	-0.721087	0.725713
C	3.032293	0.943421	1.844323
O	2.334093	2.983068	-0.445991
H	3.146057	-0.070965	-1.514916
H	4.075464	1.255097	-0.733812
Br	5.098114	-1.022940	-0.193650
H	3.346783	1.977838	1.679775
H	2.211436	0.929565	2.568680
H	3.872553	0.374646	2.257834
Sc	-0.919006	0.627835	-0.139663

Sc-TS$_3$

Sc	-4.438213	0.194712	0.190677
O	-1.786103	1.428613	-1.463565
O	-1.938147	-1.734470	1.357809
O	-2.196371	-1.540859	-1.606250
O	-1.547777	1.227811	1.534251
O	-3.777692	1.542693	1.746527
O	-4.432077	-1.254465	-1.421594
O	-4.170662	-1.449811	1.579571
O	-4.018657	1.736531	-1.264087
C	-2.878126	2.002106	-1.736664
C	-3.072445	-2.011041	1.844434
C	-3.396884	-1.764140	-1.932988
C	-2.571074	1.754247	2.054636
H	-2.827099	2.823990	-2.468027
H	-2.387360	2.476649	2.865766
H	-3.551179	-2.482474	-2.753768
H	-3.099768	-2.831642	2.578360
O	0.630447	-0.340692	-0.302334
C	1.884605	-0.266092	-0.371880
O	2.499792	0.566920	0.499261
O	2.635244	-0.902398	-1.166676
C	3.925993	0.715887	0.220388

C	4.427323	-0.549372	-0.457100
H	4.382913	0.813158	1.203850
C	4.145236	1.974682	-0.610357
H	4.425465	-1.487292	0.074637
H	4.822354	-0.534475	-1.458406
Br	6.853676	-0.308515	0.287771
H	3.668475	1.878130	-1.592986
H	3.713536	2.840414	-0.097720
H	5.218583	2.136343	-0.747355
Sc	-1.476851	-0.204781	-0.080318

Sc-Int$_5$

Sc	-4.155496	0.871577	0.093884
O	-1.118806	1.043781	-1.256892
O	-2.762907	-1.984630	1.225708
O	-2.608349	-1.522843	-1.681486
O	-1.307208	0.541669	1.786612
O	-3.224799	1.737966	1.828481
O	-4.543983	-0.356978	-1.647239
O	-4.707977	-0.838489	1.314277
O	-3.046819	2.221183	-1.151876
C	-1.851423	2.035229	-1.523091
C	-3.958971	-1.810843	1.602383
C	-3.748868	-1.209344	-2.130466
C	-2.078654	1.422462	2.259552
H	-1.401040	2.821807	-2.145757
H	-1.714798	1.972368	3.140391
H	-4.080320	-1.737906	-3.037368
H	-4.383908	-2.593508	2.247807
O	0.525417	-1.197481	-0.150269
C	1.715509	-0.867432	-0.176055
O	2.168373	0.285448	0.275381
O	2.659355	-1.657806	-0.659700
C	3.623386	0.403393	-0.027529
C	3.981263	-1.040498	-0.409369
H	4.113090	0.703571	0.895925
C	3.814287	1.433600	-1.122542
H	4.467366	-1.592835	0.392690
H	4.564518	-1.125835	-1.322583
Br	6.936006	0.099957	0.338866
H	3.331593	1.116473	-2.055895

H	3.393859	2.398567	-0.819322
H	4.891754	1.542562	-1.281348
Sc	-1.614973	-0.651467	0.012016

Fe-HKUST-1

Fe-HKUST-1

Fe	0.000022	-0.000024	-1.219656
Fe	-0.000007	0.000049	1.221138
O	0.000638	2.029860	-1.124446
O	-0.000546	-2.029909	-1.124386
O	-2.057721	0.000601	-1.130984
O	2.057789	-0.000682	-1.130918
O	2.055572	-0.003654	1.129627
O	-2.055617	0.003619	1.129560
O	-0.003800	-2.031284	1.124006
O	0.003649	2.031359	1.123951
C	0.002644	2.610202	-0.000573
C	-0.002660	-2.610191	-0.000481
C	-2.629045	0.002685	-0.000297
C	2.629057	-0.002631	-0.000208
H	0.003993	3.708793	-0.001337
H	3.728636	-0.004014	0.001098
H	-3.728625	0.003698	0.000948
H	-0.004092	-3.708782	-0.001186

Fe-Int$_0$

Fe	-0.535186	-0.073810	-0.372282
Fe	2.136710	0.134095	0.401355
O	-0.674342	1.945646	0.351968
O	0.002369	-2.077724	-0.914073
O	-0.680687	-0.719889	1.624015
O	0.296842	0.616395	-2.120461
O	2.466798	0.792039	-1.526680
O	1.483021	-0.548637	2.242216
O	2.146769	-1.751330	-0.263651
O	1.523262	1.972664	0.897856
C	0.364314	2.490627	0.797221

C	1.191137	-2.441222	-0.747034
C	0.266566	-0.820521	2.454811
C	1.508767	0.889675	-2.348230
H	0.291222	3.529765	1.144608
H	1.751712	1.248553	-3.364784
H	0.002573	-1.181922	3.466399
H	1.462841	-3.463054	-1.042968
O	-2.637695	-0.290952	-0.660339
C	-3.636137	0.079565	0.340518
C	-4.772865	0.924271	-0.165241
C	-3.448627	-1.328519	-0.045904
H	-3.172851	0.394020	1.274104
H	-5.592193	0.919977	0.564365
H	-4.445096	1.960414	-0.303397
H	-5.151507	0.546271	-1.120342
H	-4.143836	-1.792540	-0.742537
H	-2.892122	-1.997868	0.604974

Fe-Int$_1$

Fe	0.472998	0.420878	-0.377079
Fe	3.154602	-0.577571	0.405789
O	0.566850	0.787987	1.728056
O	1.340586	-0.205734	-2.214306
O	0.168516	-1.649890	0.073424
O	1.741243	2.130017	-0.570514
O	3.771945	1.343108	0.035444
O	2.219281	-2.374306	0.682749
O	3.357439	-1.000921	-1.569171
O	2.608425	-0.014724	2.277370
C	1.480272	0.514147	2.540122
C	2.449424	-0.747322	-2.425686
C	0.972178	-2.526098	0.469159
C	2.969510	2.251875	-0.354108
H	1.303152	0.754079	3.602564
H	3.415348	3.253468	-0.516093
H	0.567847	-3.540192	0.654248
H	2.679820	-1.040767	-3.464336
O	-1.422974	0.949698	-0.768260
C	-2.534041	1.091272	0.216932
C	-3.289932	2.385088	0.148157
C	-2.675789	0.058801	-0.790763

H	-2.230991	0.765299	1.209939
H	-4.260766	2.226529	0.630310
H	-2.744154	3.188471	0.657869
H	-3.469135	2.674200	-0.892505
Br	-5.568153	-0.610651	0.096200
H	-3.272544	0.250392	-1.672570
H	-2.461047	-0.973108	-0.544096

Fe-TS$_1$

Fe	0.434581	0.449427	-0.374938
Fe	3.118612	-0.603692	0.393790
O	0.147201	-1.632810	-0.020809
O	1.728567	2.136778	-0.461699
O	1.333009	-0.113663	-2.240178
O	0.516626	0.698003	1.768488
O	2.549881	-0.136122	2.298060
O	3.346473	-0.926681	-1.608779
O	3.751250	1.318625	0.135462
O	2.188446	-2.404216	0.568101
C	0.942266	-2.532332	0.334823
C	2.952782	2.244016	-0.221538
C	2.448451	-0.635693	-2.464994
C	1.420903	0.384065	2.576451
H	0.530816	-3.548627	0.461853
H	1.234335	0.575015	3.651236
H	2.696722	-0.875082	-3.517479
H	3.400037	3.248530	-0.328168
O	-1.423771	1.033840	-0.764033
C	-2.512431	1.184029	0.209761
C	-3.255205	2.490027	0.136657
C	-2.773998	0.108356	-0.726969
H	-2.209034	0.884559	1.213096
H	-4.203638	2.377762	0.672743
H	-2.667286	3.296655	0.591314
H	-3.475802	2.751133	-0.903748
Br	-5.436859	-0.666757	0.094938
H	-3.323962	0.303102	-1.635054
H	-2.513200	-0.910513	-0.480829

Fe-Int$_2$

Fe	0.313987	0.664353	-0.264165
Fe	3.001292	-0.726501	0.259309
O	0.005599	-1.491196	-0.440725
O	1.785993	2.200914	0.123530
O	1.337111	0.471238	-2.184416
O	0.450690	0.266220	1.887404
O	2.456237	-0.726592	2.231611
O	3.288580	-0.597760	-1.760873
O	3.760899	1.147793	0.478924
O	1.997522	-2.478215	-0.006973
C	0.755399	-2.480064	-0.293881
C	3.008953	2.173076	0.373076
C	2.425119	-0.042473	-2.519194
C	1.332531	-0.251735	2.605150
H	0.305270	-3.479496	-0.425281
H	1.133087	-0.313661	3.693418
H	2.687943	-0.023238	-3.595592
H	3.515572	3.142618	0.523001
O	-1.383537	1.437473	-0.534518
C	-2.574923	1.141809	0.130448
C	-3.452652	2.394838	0.220961
C	-3.199196	0.015849	-0.697514
H	-2.390112	0.762867	1.151001
H	-4.399499	2.195681	0.736971
H	-2.906815	3.173569	0.765525
H	-3.668112	2.773784	-0.786767
Br	-4.966017	-0.733098	0.092370
H	-3.479803	0.350337	-1.696361
H	-2.548338	-0.854973	-0.738585

Fe-Int$_3$

Fe	-3.156871	-0.849810	-0.338010
O	-1.323117	1.684516	-0.995677
O	-0.613835	-1.609854	1.437415
O	-0.173301	-1.015837	-1.403621
O	-1.799993	1.027841	1.825992
O	-3.832485	0.180441	1.300221
O	-2.239625	-1.780072	-1.921285
O	-2.652297	-2.409906	0.857637

O	-3.365745	0.824320	-1.463782
C	-2.440527	1.696671	-1.554650
C	-1.534066	-2.454395	1.468842
C	-0.982486	-1.665646	-2.101031
C	-3.027619	0.879536	2.001917
H	-2.674209	2.554439	-2.208469
H	-3.481819	1.409963	2.861983
H	-0.573884	-2.207099	-2.976912
H	-1.381322	-3.351446	2.093500
O	1.332704	0.958924	0.687061
O	0.614008	4.031515	0.380479
C	2.488636	0.223289	0.972915
C	1.175321	3.583146	-0.542066
C	3.086601	-0.112268	-0.395879
H	2.246288	-0.722841	1.487414
C	3.425561	1.041177	1.868206
O	1.758433	3.226525	-1.493379
H	2.390784	-0.685229	-1.005125
H	3.433223	0.775849	-0.923587
Br	4.762827	-1.324090	-0.293902
H	3.714419	1.971696	1.361729
H	2.896543	1.307062	2.790173
H	4.333844	0.483635	2.125531
Fe	-0.396563	0.261762	0.364253

Fe-TS$_2$

Fe	-3.070297	-1.067317	-0.014596
O	-1.702202	1.161284	-1.709399
O	-0.505847	-0.654255	1.731354
O	-0.039293	-1.140541	-1.137909
O	-2.056861	1.759985	1.124656
O	-3.914795	0.472121	1.012040
O	-1.917579	-2.398589	-1.035969
O	-2.411230	-1.872539	1.756956
O	-3.552245	-0.138879	-1.777526
C	-2.771308	0.765772	-2.222046
C	-1.286340	-1.499379	2.223379
C	-0.709436	-2.169613	-1.373787
C	-3.257149	1.508080	1.362404
H	-3.081546	1.251249	-3.167145
H	-3.834924	2.256259	1.941065

H	-0.218414	-2.987618	-1.938927
H	-0.971638	-1.982491	3.169184
O	1.351578	1.248118	0.264418
O	0.421635	3.210410	-0.608791
C	2.414819	0.392800	0.689693
C	1.561278	2.883331	-0.391898
C	3.223524	0.065418	-0.565499
H	1.943071	-0.528527	1.049615
C	3.211467	1.024147	1.832091
O	2.727590	3.178809	-0.438541
H	2.581741	-0.361973	-1.333385
H	3.792290	0.915553	-0.936084
Br	4.627479	-1.389834	-0.225856
H	3.703719	1.944744	1.505830
H	2.526157	1.263848	2.652706
H	3.968983	0.325295	2.204444
Fe	-0.541178	0.687206	0.013878

Fe-Int$_4$

Fe	-3.635220	-0.894521	0.209759
O	-0.688282	-1.383888	-0.834469
O	-2.498885	2.028836	0.551612
O	-0.967158	-0.125464	1.791892
O	-2.183530	0.785096	-2.079271
O	-4.104444	-0.351131	-1.705135
O	-2.893065	-1.279107	2.077869
O	-4.410013	0.865109	0.892584
O	-2.621774	-2.514561	-0.507423
C	-1.401795	-2.409732	-0.862939
C	-3.690674	1.918429	0.910089
C	-1.762240	-0.825705	2.455284
C	-3.304948	0.347084	-2.413652
H	-0.933801	-3.340404	-1.235899
H	-3.660977	0.581848	-3.438146
H	-1.465188	-1.092614	3.490518
H	-4.192147	2.829652	1.288247
Fe	-1.033401	0.653518	-0.235404
O	0.492135	1.815981	-0.597208
C	1.749200	1.682865	-0.380585
O	2.036366	0.438187	0.173857
O	2.643260	2.492781	-0.616902

C	3.375085	0.141376	0.611383
C	4.334464	0.206126	-0.578963
H	3.290321	-0.904355	0.922696
C	3.795011	0.991674	1.810050
H	3.906453	-0.269980	-1.459684
H	4.687901	1.207221	-0.803606
Br	6.030429	-0.880519	-0.197459
H	3.880133	2.044557	1.528415
H	3.045776	0.896606	2.603480
H	4.759172	0.644312	2.198558

Fe-TS$_3$

Fe	3.856115	0.700950	-0.160101
O	1.018829	0.826396	-1.563403
O	2.323606	-1.475138	1.572385
O	1.063067	1.146417	1.346234
O	2.243515	-1.806456	-1.328215
O	4.278232	-0.827290	-1.451170
O	3.113453	2.080704	1.154815
O	4.359044	-0.501727	1.408497
O	3.067587	1.773532	-1.704187
C	1.855380	1.611548	-2.062615
C	3.513368	-1.306460	1.920063
C	1.925383	2.013765	1.611597
C	3.417983	-1.719745	-1.750290
H	1.517199	2.239339	-2.907833
H	3.763533	-2.496444	-2.463059
H	1.638888	2.818215	2.319413
H	3.885004	-1.917569	2.764152
Fe	1.123598	-0.571377	0.044532
O	-0.599272	-1.539198	0.208557
C	-1.813101	-1.200130	0.256882
O	-2.110059	0.101093	0.053522
O	-2.787852	-1.978008	0.466959
C	-3.515656	0.403003	0.312616
C	-4.335237	-0.853089	0.059735
H	-3.767116	1.162819	-0.425363
C	-3.656874	0.946460	1.729071
H	-4.403623	-1.265774	-0.934002
H	-4.891820	-1.330952	0.847556
Br	-6.521395	0.354356	-0.462811

H	-3.389154	0.180175	2.466195
H	-2.993103	1.805931	1.865810
H	-4.692214	1.258173	1.896010

Fe-Int$_5$

Fe	-3.951484	0.607957	0.068239
O	-1.163871	1.200080	1.272665
O	-2.365075	-1.758541	-1.196646
O	-1.121491	0.932437	-1.644650
O	-2.043304	-1.528105	1.769648
O	-4.114613	-0.617247	1.652805
O	-3.269996	1.639665	-1.515113
O	-4.475182	-0.948036	-1.178183
O	-3.237527	2.094743	1.316791
C	-2.011030	2.056549	1.637062
C	-3.576273	-1.772129	-1.531630
C	-2.101633	1.606279	-2.029443
C	-3.226118	-1.388833	2.149118
H	-1.643788	2.856480	2.304936
H	-3.567407	-1.988480	3.010195
H	-1.968552	2.255690	-2.911141
H	-3.891952	-2.589255	-2.205853
Fe	-1.288214	-0.452062	0.031179
O	0.551252	-1.389518	-0.194362
C	1.723242	-1.007815	-0.208330
O	2.113363	0.198992	0.160967
O	2.717684	-1.793021	-0.592840
C	3.570213	0.354738	-0.105989
C	3.999973	-1.100378	-0.345135
H	4.015204	0.756831	0.801205
C	3.758449	1.290839	-1.283085
H	4.473141	-1.559136	0.521344
H	4.626424	-1.237581	-1.222771
Br	6.891217	0.240064	0.380299
H	3.321952	0.871455	-2.198670
H	3.287990	2.259363	-1.081928
H	4.835640	1.432043	-1.416728

Ru-HKUST-1

Ru-HKUST-1

Ru	-0.000441	0.000375	-1.178876
Ru	0.000322	-0.000229	1.179064
O	-2.007212	-0.515428	-1.131624
O	2.006258	0.516531	-1.132655
O	0.515538	-2.005806	-1.132772
O	-0.516708	2.006455	-1.131363
O	-0.515476	2.006228	1.132569
O	0.516924	-2.006487	1.131160
O	2.007418	0.515120	1.131485
O	-2.006425	-0.516978	1.132512
C	-2.563181	-0.659609	0.000595
C	2.563269	0.658949	-0.000712
C	0.659390	-2.562821	-0.000984
C	-0.659178	2.563037	0.000799
H	-3.625277	-0.933040	0.000717
H	-0.932539	3.625097	0.000988
H	0.933229	-3.624758	-0.001536
H	3.625506	0.931831	-0.001149

Ru-Int$_0$

Ru	1.802791	0.130183	0.220254
Ru	-0.461277	-0.079519	-0.198042
O	1.837597	1.839048	-0.961547
O	1.720989	-1.589507	1.396164
O	2.195811	-1.037486	-1.459012
O	1.359631	1.297057	1.896273
O	-0.859004	1.092514	1.502369
O	-0.018652	-1.252341	-1.872852
O	-0.497906	-1.801476	1.000223
O	-0.381277	1.645324	-1.370503
C	0.745229	2.207957	-1.486094
C	0.600747	-2.161286	1.519292
C	1.203455	-1.462826	-2.122169
C	0.141514	1.513163	2.156954
H	0.781023	3.104254	-2.099505
H	-0.070267	2.122914	3.035632

H	1.427616	-2.074163	-2.996493
H	0.577183	-3.055411	2.136601
O	-2.729097	-0.297296	-0.594488
C	-3.737335	0.084271	0.390146
C	-4.881375	0.902937	-0.144016
C	-3.533478	-1.329518	0.037254
H	-3.285127	0.431734	1.317717
H	-5.707432	0.904626	0.578202
H	-4.567817	1.940428	-0.304653
H	-5.246081	0.498413	-1.093693
H	-4.220170	-1.814644	-0.654152
H	-2.972817	-1.982231	0.701743

Ru-Int$_1$

Ru	2.641758	-0.473756	0.296356
Ru	0.502077	0.285761	-0.228432
O	3.331022	1.498704	0.243550
O	1.912366	-2.432624	0.339171
O	3.044365	-0.666699	-1.748985
O	2.192266	-0.263611	2.331521
O	0.111044	0.479542	1.829097
O	0.962841	0.069741	-2.266399
O	-0.168087	-1.694841	-0.176715
O	1.248866	2.247988	-0.261893
C	2.478226	2.398005	-0.022275
C	0.679225	-2.590633	0.094266
C	2.116448	-0.352470	-2.554226
C	1.036219	0.161600	2.628166
H	2.851745	3.418886	-0.046255
H	0.815141	0.265645	3.690947
H	2.341725	-0.458738	-3.615930
H	0.306350	-3.611126	0.119634
O	-1.521505	1.007871	-0.754895
C	-2.645471	1.136475	0.203866
C	-3.402703	2.431580	0.144908
C	-2.742047	0.131997	-0.840345
H	-2.374147	0.784035	1.196426
H	-4.384320	2.265748	0.602698
H	-2.869639	3.226306	0.682076
H	-3.556930	2.743558	-0.893558

Br	-5.702854	-0.618833	0.097308
H	-3.332242	0.336525	-1.725813
H	-2.551372	-0.907773	-0.606440

Ru-TS_1

Ru	2.612017	-0.472475	0.291894
Ru	0.460156	0.285853	-0.233051
O	3.306668	1.498846	0.198668
O	1.880312	-2.428858	0.373293
O	2.996949	-0.704319	-1.748871
O	2.177870	-0.224261	2.327751
O	0.092299	0.510844	1.825527
O	0.917093	0.036432	-2.272568
O	-0.205468	-1.699351	-0.141027
O	1.218790	2.243759	-0.295227
C	2.450046	2.394513	-0.066487
C	0.646659	-2.589284	0.133722
C	2.069274	-0.391834	-2.555851
C	1.021397	0.200336	2.623205
H	2.821895	3.416167	-0.099436
H	0.800048	0.311341	3.686003
H	2.299594	-0.507643	-3.616480
H	0.278969	-3.611635	0.167307
O	-1.508916	0.990228	-0.750641
C	-2.588425	1.164837	0.190719
C	-3.288501	2.500316	0.110457
C	-2.972033	0.067549	-0.684373
H	-2.312578	0.876476	1.207214
H	-4.228619	2.447613	0.670368
H	-2.653320	3.289035	0.532412
H	-3.517348	2.752033	-0.931081
Br	-5.530107	-0.627282	0.091992
H	-3.454693	0.272993	-1.626751
H	-2.691047	-0.945287	-0.441959

Ru-Int_2

Ru	2.553499	-0.585883	0.269997
Ru	0.369460	0.422116	-0.223319

O	3.413442	1.291989	0.048549
O	1.594840	-2.424632	0.477416
O	2.789055	-0.945736	-1.768544
O	2.216299	-0.176835	2.290035
O	0.175910	0.740462	1.856477
O	0.772312	-0.001280	-2.257917
O	-0.441811	-1.505501	0.031541
O	1.399787	2.249324	-0.431074
C	2.643973	2.264854	-0.249231
C	0.333451	-2.458885	0.310712
C	1.853328	-0.573240	-2.551729
C	1.118530	0.382915	2.612130
H	3.136864	3.237121	-0.357507
H	0.982322	0.577054	3.684693
H	2.019692	-0.783390	-3.617274
H	-0.133629	-3.442854	0.423174
O	-1.443213	1.307920	-0.705079
C	-2.583065	1.057042	0.058747
C	-3.366395	2.355740	0.289037
C	-3.343086	0.020657	-0.769873
H	-2.336128	0.612445	1.038389
H	-4.279448	2.185302	0.872893
H	-2.727079	3.066119	0.825316
H	-3.638581	2.805406	-0.675058
Br	-5.112857	-0.661786	0.109734
H	-3.674289	0.421312	-1.727648
H	-2.763294	-0.890404	-0.891473

Ru-Int$_3$

Ru	-2.709666	-0.711007	-0.247318
O	-3.383176	0.298298	1.438337
O	-1.956196	-1.678268	-1.928412
O	-2.239439	-2.370635	0.928046
O	-3.063645	0.985365	-1.404632
O	-0.984039	1.821240	-0.982996
O	-0.140466	-1.596001	1.367284
O	0.144038	-0.914540	-1.499944
O	-1.298192	1.095727	1.883590
C	-2.528201	0.963124	2.111898
C	-0.710456	-1.559818	-2.163903
C	-1.082087	-2.428626	1.456030

C	-2.130463	1.847898	-1.502466
H	-2.914662	1.481027	2.996987
H	-2.365375	2.722287	-2.123053
H	-0.887333	-3.321022	2.064951
H	-0.338574	-2.080770	-3.053181
O	1.423762	0.991485	0.514377
O	0.852355	4.008596	0.482766
C	2.525343	0.211193	0.877223
C	1.389114	3.587337	-0.467544
C	3.250502	-0.046313	-0.445218
H	2.214302	-0.757605	1.301665
C	3.382747	0.950369	1.912546
O	1.952174	3.288965	-1.451129
H	2.612187	-0.567824	-1.153601
H	3.664204	0.864145	-0.877650
Br	4.904627	-1.303344	-0.273997
H	3.735971	1.905477	1.501104
H	2.769610	1.167824	2.794308
H	4.252788	0.356778	2.219098
Ru	-0.459458	0.148595	0.212536

Ru-TS$_2$

Ru	-2.673055	-0.894167	0.026380
O	-3.697497	0.678309	0.883151
O	-1.612952	-2.448206	-0.856455
O	-2.117767	-1.574960	1.916111
O	-3.195764	-0.174838	-1.840816
O	-1.289747	1.058992	-1.948776
O	-0.223164	-0.321896	1.881864
O	0.280725	-1.195226	-0.922396
O	-1.810401	1.946096	0.907836
C	-3.028516	1.738767	1.131279
C	-0.384172	-2.245869	-1.124154
C	-1.025259	-1.139987	2.405904
C	-2.381939	0.635478	-2.402211
H	-3.591134	2.560497	1.587406
H	-2.681980	1.003098	-3.393065
H	-0.755540	-1.528181	3.398612
H	0.153048	-3.085510	-1.579715
O	1.577063	1.169474	0.111913
O	0.579811	3.023192	-0.597082

C	2.696188	0.406227	0.585784
C	1.707810	2.591119	-0.346256
C	3.681924	0.246849	-0.571285
H	2.265728	-0.575098	0.805263
C	3.295016	0.992323	1.864371
O	2.861404	3.031258	-0.394944
H	3.169498	-0.064990	-1.479264
H	4.299999	1.123823	-0.737853
Br	5.013555	-1.279424	-0.209292
H	3.716113	1.982734	1.672661
H	2.507119	1.079710	2.620256
H	4.079943	0.332701	2.253300
Ru	-0.663699	0.463804	-0.031067

Ru-Int$_4$

Ru	-3.014819	-0.775774	0.229141
O	-2.336012	-1.159874	2.166489
O	-3.679275	-0.385448	-1.713360
O	-2.056639	-2.511133	-0.442528
O	-3.959019	0.969638	0.901381
O	-2.078663	2.172700	0.492024
O	-0.172965	-1.324657	-0.883781
O	-1.795837	0.808133	-2.143591
O	-0.454733	0.048235	1.768084
C	-1.214693	-0.658171	2.482120
C	-2.915010	0.314791	-2.444584
C	-0.859400	-2.380223	-0.842009
C	-3.270981	2.035491	0.875209
H	-0.867871	-0.865973	3.492423
H	-3.773161	2.939345	1.226104
H	-0.367496	-3.291138	-1.188055
H	-3.271982	0.512232	-3.453685
O	0.613452	1.709562	-0.672417
C	1.864692	1.600170	-0.454987
O	2.195509	0.399522	0.176857
O	2.752356	2.407885	-0.750598
C	3.544437	0.183159	0.614344
C	4.501055	0.229739	-0.579998
H	3.510230	-0.849225	0.977699
C	3.939580	1.106976	1.767451
H	4.082452	-0.278940	-1.446566

H	4.846253	1.226117	-0.833928
Br	6.219016	-0.827387	-0.167587
H	3.970512	2.147529	1.433373
H	3.203654	1.016435	2.573947
H	4.923877	0.824045	2.159030
Ru	-1.068942	0.455548	-0.201154

Ru-TS$_3$

Ru	-3.191132	0.668946	0.211469
O	-2.344734	2.273043	-0.821179
O	-4.022094	-0.944189	1.243501
O	-2.462619	1.444644	2.012387
O	-3.904019	-0.116751	-1.592180
O	-1.984659	-1.291700	-1.868997
O	-0.540864	0.268754	1.761324
O	-2.100499	-2.123701	0.990311
O	-0.421799	1.103225	-1.105190
C	-1.157575	2.117566	-1.239315
C	-3.283816	-1.964684	1.393319
C	-1.304583	1.066806	2.368078
C	-3.137899	-0.915912	-2.211809
H	-0.724538	2.958998	-1.775916
H	-3.524674	-1.322749	-3.148226
H	-0.927233	1.480689	3.304655
H	-3.726662	-2.799183	1.933294
O	0.793871	-1.291645	-0.507442
C	2.007729	-0.970318	-0.509101
O	2.341041	0.267213	-0.050634
O	2.971231	-1.701200	-0.889242
C	3.737159	0.596817	-0.272019
C	4.568404	-0.675043	-0.219563
H	3.996511	1.236735	0.570764
C	3.885052	1.353006	-1.588743
H	4.571596	-1.281256	0.672007
H	5.107283	-1.033504	-1.079744
Br	6.822127	0.099426	0.538692
H	3.608885	0.712198	-2.434207
H	3.229237	2.229543	-1.589443
H	4.923246	1.678304	-1.709730
Ru	-1.213272	-0.534642	-0.059288

Ru-Int$_5$

Ru	-3.286304	-0.611475	-0.100319
O	-2.667963	-1.995241	1.332922
O	-3.884711	0.782301	-1.533333
O	-2.579135	-1.867624	-1.613822
O	-3.975277	0.654727	1.416690
O	-1.946609	1.657338	1.531298
O	-0.551107	-0.863084	-1.524279
O	-1.855759	1.789184	-1.434943
O	-0.636666	-0.996420	1.448883
C	-1.486597	-1.869257	1.775856
C	-3.032772	1.659434	-1.869175
C	-1.374423	-1.704519	-1.977323
C	-3.147571	1.495845	1.881923
H	-1.171993	-2.595738	2.521048
H	-3.516679	2.151573	2.672181
H	-1.011935	-2.364108	-2.766617
H	-3.356097	2.381093	-2.615921
O	0.769334	1.484844	0.147356
C	1.932934	1.085130	0.171772
O	2.303446	-0.170198	-0.021878
O	2.953501	1.905339	0.400869
C	3.764347	-0.302456	0.209454
C	4.216079	1.165902	0.221950
H	4.172881	-0.837265	-0.645233
C	3.996714	-1.062136	1.500764
H	4.672435	1.484295	-0.713921
H	4.870696	1.416898	1.053425
Br	7.093933	-0.311356	-0.385780
H	3.601954	-0.509256	2.363377
H	3.511399	-2.043744	1.461312
H	5.078089	-1.195540	1.608760
Ru	-1.208767	0.410389	0.006557

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