

Supporting Information

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

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

M-HKUST-1	singlet	triplet	quintet	septet	nonet	undectet	13-et	15-et
Fe	-1003.5804	-1003.6187	-1003.6170	-1003.6892	-1003.6923	-1003.5696	-1003.4164	-1003.2555
Cr	-929.3917	-929.4450	-929.4007	-929.4821	-929.5166	-929.3483	-929.1924	-929.0746
Ru	-944.4922	-944.5252	-944.5034	-944.4722	-944.4307	-944.2990	-944.1413	-943.9846
Ti	-873.0618	-873.0812	-873.0574	-872.9157	-872.7463	-872.5847	-872.4244	-872.2652
W	-892.4703	-892.4244	-892.3563	-892.3445	-892.2906	-892.1250	-891.9583	-891.7895
V	-899.50602	-899.4972	-899.5143	-899.5266	-899.4064	-899.2487	-899.0906	-898.9115
Mn	-964.5513	-964.6274	-964.6200	-964.6449	-964.6894	-964.7448	-964.5840	-964.4216
Cu	-1149.0179	-1149.0489	-1148.8911	-1148.7332	-1148.5716	-1148.4067	-1148.2438	-1148.0614
Sc	-849.9176	-849.9022	-849.7432	-849.5838	-849.3848	-849.2599	-849.0714	-848.8743
Mo	-891.9087	-891.8843	-891.7810	-891.7754	-891.8028	-891.6396	-891.4882	-891.3106
Zn	-888.0134	-887.8988	-887.6896	-887.5794	-887.4066	-887.2452	-887.1133	-886.9128
Zr	-850.0621	-850.0544	-850.0087	-849.8605	-849.6917	-849.5231	-849.3511	-849.1643
Tc	-916.9132	-916.9186	-916.9120	-916.8672	-916.8616	-916.8233	-916.6643	-916.5032
Cd	-852.9229	-852.8036	-852.6756	-852.5230	-852.3683	-852.2208	-852.0615	-851.8721
Rh	-975.7757	-975.7468	-975.6921	-975.6673	-975.5087	-975.3602	-975.2032	-975.0458
Y	-832.9032	-832.8823	-832.7232	-832.5637	-832.3788	-832.2375	-832.0185	-831.8470
Ag	-1048.1770	-1048.1723	-1048.0162	-1047.8594	-1047.7167	-1047.5386	-1047.4069	-1047.2742
Nb	-869.4452	-869.4650	-869.4161	-869.4015	-869.2421	-869.0811	-868.9212	-868.7538

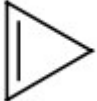
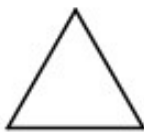


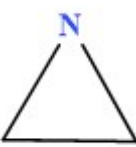
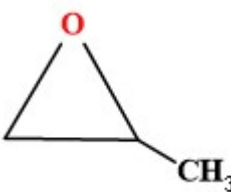
Table S2. Relative Gibbs free energies (kcal/mol) for the stationary points along the reaction pathway for CO₂ fixation on M-HKUST-1 catalysts.

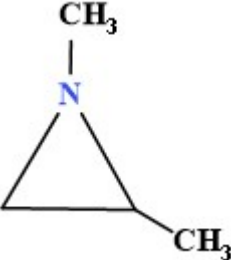
	Cu	Cr	Mo	W	Ti	Sc	Ru	Fe	Zn	Zr	Cd	Tc	Y	Rh	Nb	Ag	Mn	V
cat+reactant	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Int₀	-39.00	-34.57	-27.92	-27.89	-36.04	-28.68	-40.34	-79.88	-38.60	-31.84	-33.36	-41.16	-27.60	-40.98	-47.57	-34.96	-39.24	-72.05
Int₁	-37.65	-32.66	-25.20	-25.07	-34.67	-26.32	-38.76	-78.80	-36.89	-28.17	-30.79	-40.11	-25.23	-39.52	-45.70	-31.79	-36.53	-63.72
Ts₁	-4.75	4.07	12.58	10.87	-5.35	4.18	-5.51	-50.95	-8.60	-3.08	-0.99	-10.21	5.79	-7.65	-12.42	8.97	-7.48	-33.70
Int₂	-10.53	-0.67	12.18	10.40	-5.52	-2.01	-15.23	-53.58	-12.27	-10.48	-3.46	-11.80	1.77	-12.70	-20.97	-6.10	-10.33	-34.95
Int₃	-7.34	3.50	15.50	13.48	-1.90	1.82	-11.52	-50.13	-8.61	-6.74	0.38	-7.98	4.19	-8.43	-11.37	-15.44	-6.64	-30.91
Ts₂	-1.69	6.08	21.58	20.01	5.05	11.13	3.07	-39.57	-2.97	4.36	5.06	0.80	9.14	-1.52	-4.14	10.67	-1.64	-29.64
Int₄	-17.23	-18.81	-14.73	0.43	-22.97	-18.30	-9.10	-73.53	-22.42	-23.39	-15.51	-28.59	-18.55	-11.04	-37.54	-9.16	-26.51	-58.52
Int₅	-27.42	-25.01	-15.63	-15.94	-27.18	-24.61	-23.92	-74.63	-34.17	-28.62	-28.17	-28.97	-24.37	-24.01	-36.96	-21.37	-38.87	-54.38
Ts₃	-12.17	-10.20	-1.47	-1.04	-7.06	-8.23	-9.11	-54.90	-17.23	-13.50	-10.85	-13.28	-9.65	-9.07	-21.21	-8.49	-21.28	-41.78
Int₆	-48.19	-44.81	-37.88	-37.45	-46.28	-41.45	-44.93	-89.12	-46.49	-43.84	-41.59	-49.14	-41.87	-44.79	-55.55	-41.76	-48.75	-75.53
cat+product	-13.58	-13.58	-13.58	-13.58	-13.58	-13.58	-13.58	-13.58	-13.58	-13.58	-13.58	-13.58	-13.58	-13.58	-13.58	-13.58	-13.58	-13.58

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

M-HKUST-1	NH₃-adsorption	H₂O-adsorption	aziridine-adsorption	CO₂-adsorption
Cu	40.06	30.19	39.00	23.87
Sc	28.94	26.16	28.68	21.04
Ti	34.04	28.58	36.04	22.24
V	71.54	63.04	72.05	23.79
Cr	34.76	28.21	34.57	22.78
Mn	39.81	29.19	39.24	21.31
Fe	80.20	70.97	79.88	17.64
Zn	37.66	29.66	38.60	20.43
Y	29.98	26.41	27.60	22.63
Zr	31.25	28.59	31.84	23.18
Nb	46.47	43.05	47.57	27.55
Mo	28.62	22.61	27.92	21.21
Tc	39.73	31.98	41.16	21.48
Ru	40.47	29.05	40.34	21.49
Rh	41.40	29.11	40.98	22.58
Ag	34.62	28.26	34.96	22.39
Cd	32.35	25.92	33.36	19.17
W	27.76	22.59	27.89	21.54

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

systems	Ring strain energy (kcal/mol)		
	literature		this work
	experiment	B3LYP/6-311++G(d,p)// B3LYP/6-31G(d)	B3LYP/6-311++G(d,p)// B3LYP/6-31G(d)
	54.5	54.0	54.16
	27.5		25.91
	26.3		25.64
	26.3		26.06
	26.7		25.34
			25.15

			23.68
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S5. The Coordinates of all stable intermediates and transition states.

Aziridine

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

Oxazolidinone

C	-3.97000400	0.82393800	-0.59854500
C	-3.48050400	-0.61106400	-0.35558700
H	-4.20843200	1.00580100	-1.65927200
H	-4.85551200	1.04504600	0.00237000
H	-3.74831800	-0.92774500	0.65688300
C	-3.92332100	-1.64193800	-1.36976400
H	-3.63271900	-1.34346500	-2.38438700
H	-3.47529000	-2.61702500	-1.14890800
H	-5.01389200	-1.72834600	-1.30921300
N	-2.79135000	1.59168600	-0.20107400
C	-1.68009400	0.81228300	-0.21592100
O	-2.01138400	-0.48020100	-0.37680000

O	-0.51710900	1.20970300	-0.09749000
C	-2.74179400	3.03691600	-0.23111000
H	-1.74524800	3.35781000	0.07907900
H	-2.94233000	3.41930300	-1.24354700
H	-3.49115500	3.45023600	0.45307200

Cu-HKUST-1

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

Cu-Int₀

Cu	0.00181100	-0.00236400	-1.27354000
Cu	-0.00204800	0.00228200	1.27404200
O	-1.37661800	1.42493800	-1.14024000
O	1.37990600	-1.42858600	-1.13387900

O	-1.42582200	-1.38025400	-1.13599000
O	1.42834200	1.37674400	-1.13651500
O	1.42533800	1.37953800	1.13643600
O	-1.42783400	-1.37666800	1.13695700
O	1.37692200	-1.42481100	1.13903200
O	-1.37988600	1.42883600	1.13272800
C	-1.76502200	1.82697200	-0.00504300
C	1.76569700	-1.82638900	0.00384000
C	-1.82688400	-1.76531700	0.00073500
C	1.82668800	1.76519300	0.00000800
H	-2.52988100	2.61753000	-0.00752400
H	2.61677200	2.53054000	0.00018700
H	-2.61725000	-2.53040100	0.00132400
H	2.53155300	-2.61594300	0.00597900
C	-0.08122929	0.44876615	4.37187289
C	-0.92097591	-0.76227629	4.12198750
H	-0.44453697	1.43664543	4.09276818
H	0.58796250	0.43451355	5.23454016
H	-0.76954210	-1.58261119	4.83023240
C	-2.30498243	-0.68988735	3.51819736
H	-2.53700527	-1.60458539	2.95785232
H	-3.06514242	-0.56799315	4.30047968
H	-2.37855312	0.15662540	2.82731221
N	0.21833674	-0.45495348	3.25956860
C	1.40395215	-1.29147831	3.40391196
H	1.29768950	-2.17965019	2.77069881
H	2.28348308	-0.73133043	3.06658745
H	1.58192695	-1.62405544	4.44356964

Cu-Int₁

Cu	0.48468200	0.23666600	-3.13758000
Cu	0.50244100	0.24293400	-0.42100400
O	-1.00413900	1.54466700	-3.13703100
O	1.97262300	-1.07965000	-3.13995900
O	-0.82054300	-1.24317000	-3.11611700
O	1.78935000	1.71029800	-3.06818500
O	2.08563900	1.54937800	-0.81188800
O	-1.08043000	-1.04974800	-0.86194200
O	1.78658200	-1.31962500	-0.88572000
O	-0.76663200	1.84938800	-0.89561100
C	-1.26743600	2.08510800	-2.01777900
C	2.25893400	-1.58939600	-2.01436200
C	-1.34164600	-1.52396200	-1.99520100
C	2.32532000	2.00660400	-1.95699800
H	-2.03931000	2.86025100	-2.04795700
H	3.10734300	2.77326100	-2.04024600
H	-2.12667900	-2.28768000	-2.03910900
H	3.02212400	-2.37322200	-2.03445400
C	-1.09546900	-0.19387400	2.23911900
C	0.17674000	-0.84710200	2.63822200
H	-1.72331800	-0.65440600	1.48157600
H	-1.60202400	0.40469000	2.99330300
H	0.49131900	-0.61829400	3.65653400
C	0.61505500	-2.19356100	2.11617600
H	1.70881700	-2.26300500	2.06946400
H	0.24870900	-2.97614300	2.79318300
H	0.22225700	-2.38453800	1.11411700
N	0.19601800	0.32678300	1.72868900
Br	-1.37904100	-0.02710900	5.96760600

C	0.64904900	1.59137800	2.32960000
H	1.73771400	1.66181800	2.23229300
H	0.19439000	2.42363100	1.78263500
H	0.37104600	1.65646900	3.39064700
Cu-Ts₁			
Cu	0.00181100	-0.00236400	-1.27354000
Cu	-0.00204800	0.00228200	1.27404200
O	-1.37661800	1.42493800	-1.14024000
O	1.37990600	-1.42858600	-1.13387900
O	-1.42582200	-1.38025400	-1.13599000
O	1.42834200	1.37674400	-1.13651500
O	1.42533800	1.37953800	1.13643600
O	-1.42783400	-1.37666800	1.13695700
O	1.37692200	-1.42481100	1.13903200
O	-1.37988600	1.42883600	1.13272800
C	-1.76502200	1.82697200	-0.00504300
C	1.76569700	-1.82638900	0.00384000
C	-1.82688400	-1.76531700	0.00073500
C	1.82668800	1.76519300	0.00000800
H	-2.52988100	2.61753000	-0.00752400
H	2.61677200	2.53054000	0.00018700
H	-2.61725000	-2.53040100	0.00132400
H	2.53155300	-2.61594300	0.00597900
C	-1.62425912	-0.23965603	4.20454873
C	-0.36037412	-0.95614606	4.61766992
H	-2.35417205	-0.88284635	3.71053274
H	-2.08526277	0.39920819	4.96183405
H	0.33841655	-0.40330084	5.22939433
C	0.10680755	-2.22319800	3.95358971

H	0.61595091	-2.00698959	3.00681878
H	0.80272959	-2.74739794	4.61297772
H	-0.73837232	-2.88591938	3.74615124
N	-0.72807971	0.45283396	3.24669658
Br	-1.06588694	-1.99200048	6.97431528
C	-0.35910865	1.80964676	3.63944593
H	0.52913691	2.12952140	3.08828523
H	-1.18629866	2.49262018	3.39852700
H	-0.15821883	1.87464208	4.71938177

Cu-Int₂

Cu	0.48333000	0.26467500	-3.04101500
Cu	0.54975600	0.12016800	-0.12779200
O	-1.03307500	1.52354500	-3.12879300
O	2.00533200	-1.01190100	-3.07045300
O	-0.76894300	-1.24794000	-3.02546400
O	1.75063300	1.75781900	-3.05544600
O	2.23811000	1.40700500	-0.85582900
O	-1.20302700	-1.00543700	-0.79999500
O	1.67968400	-1.46975600	-0.86725100
O	-0.65859800	1.93797000	-0.92737700
C	-1.23831600	2.11087200	-2.01336500
C	2.23180400	-1.61760400	-1.98034000
C	-1.36621900	-1.50641400	-1.93289200
C	2.36549000	1.97144100	-1.95990300
H	-2.03931000	2.86025100	-2.04795700
H	3.10734300	2.77326100	-2.04024600
H	-2.12667900	-2.28768000	-2.03910900
H	3.02212400	-2.37322200	-2.03445400
C	-0.92679500	0.19403600	2.41513200

C	-0.42493300	-0.77238600	3.50013000
H	-1.60276600	-0.34377900	1.73907500
H	-1.48750100	1.01862700	2.88121200
H	0.31597700	-0.28670600	4.13666800
C	0.05564400	-2.11396600	2.98506200
H	0.87069600	-1.93779800	2.27266600
H	0.42422700	-2.74851000	3.79748600
H	-0.74521300	-2.64102800	2.45607200
N	0.23264700	0.66706300	1.68057500
Br	-1.97088700	-1.10800500	4.86617500
C	0.65131400	1.99577200	2.07870100
H	1.55144400	2.28276100	1.52919800
H	-0.13678100	2.74105000	1.87082800
H	0.86778100	2.03761300	3.16223500

Cu-Int₃

Cu	0.46237700	0.39494900	-3.08933000
Cu	0.56960500	0.29842200	-0.17532400
O	-0.75002600	1.94884300	-3.16926000
O	1.68774000	-1.16957400	-3.12750600
O	-1.07026300	-0.82577800	-3.08880300
O	2.01199000	1.59715400	-3.08353200
O	1.77400400	2.02909700	-0.85750500
O	-0.76717600	-1.31872600	-0.88238900
O	2.13046800	-0.86666100	-0.91907400
O	-1.19060300	1.58571100	-0.97039100
C	-1.33553800	2.17291200	-2.05677200
C	2.27509300	-1.41952300	-2.03219600
C	-1.31891400	-1.42982600	-1.99733100
C	2.28559800	2.18056100	-1.98587800

H	-2.05417100	3.00146600	-2.09413100
H	3.09248200	2.91447600	-2.08642000
H	-2.14154000	-2.14646500	-2.08528300
H	3.00726300	-2.23200700	-2.08062800
C	-1.16533300	0.03143900	2.14757500
C	-0.72535900	-1.09535800	3.09250700
H	-1.74351900	-0.40422800	1.32211500
H	-1.82031800	0.72819500	2.69005500
H	-0.14161600	-0.70056500	3.92566600
C	-0.05327200	-2.27687500	2.42352000
H	0.89470200	-1.93888100	1.98896000
H	0.15543500	-3.07716200	3.13998100
H	-0.66827700	-2.66611000	1.60717900
N	0.01586700	0.70230800	1.62254900
Br	-2.42762700	-1.78312800	4.09182700
C	3.31636100	0.21294400	3.12161700
O	3.04391300	1.24418000	3.59912500
O	3.61520100	-0.82989800	2.68161600
C	0.09948500	2.09142400	2.03688300
H	0.28923900	2.16762100	3.12374800
H	0.91551500	2.59149200	1.50785200
H	-0.84077700	2.63003000	1.82268500
Cu-Ts₂			
Cu	0.00181100	-0.00236400	-1.27354000
Cu	-0.00204800	0.00228200	1.27404200
O	-1.37661800	1.42493800	-1.14024000
O	1.37990600	-1.42858600	-1.13387900
O	-1.42582200	-1.38025400	-1.13599000
O	1.42834200	1.37674400	-1.13651500

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

H	-1.54875192	1.92973064	2.93078798
Cu-Int₄			
Cu	0.18551400	-0.74088400	-3.84670500
Cu	0.18139600	-0.70708200	-1.11326800
O	-1.09388100	0.76906200	-3.82499700
O	1.46915300	-2.24403000	-3.80498500
O	-1.32271100	-2.02296200	-3.81071100
O	1.68955700	0.54970900	-3.84125000
O	1.54745900	0.72878300	-1.57712500
O	-1.17655600	-2.23340000	-1.54927400
O	1.67500300	-2.10104200	-1.54190800
O	-1.31675700	0.60922800	-1.56568700
C	-1.58470400	1.08193800	-2.69577000
C	1.95107000	-2.56482000	-2.67266300
C	-1.64185000	-2.50881700	-2.67901900
C	2.00977500	1.01987000	-2.70448300
H	-2.34765600	1.87415600	-2.72263100
H	2.79899700	1.78716600	-2.71492000
H	-2.43502500	-3.27377500	-2.71378300
H	2.71377800	-3.35931700	-2.70912800
C	0.77451800	0.64247700	4.05973900
C	-0.05461400	1.93006200	4.18587600
H	1.78069600	0.94565100	3.72678100
H	0.88352400	0.16641000	5.03806000
H	-0.82525300	1.96719800	3.42262100
C	0.75986000	3.20530000	4.24036600
H	1.28159300	3.29133900	3.27865600
H	0.12511600	4.08554700	4.37901700
H	1.50196300	3.17832300	5.04753800

N	0.20793300	-0.32058800	3.13351300
Br	-1.22920000	1.85202900	5.93531900
C	0.31409800	0.02852900	1.75857000
O	0.57958500	1.22217100	1.50293100
O	0.10708200	-0.92727900	0.92829000
C	0.19510100	-1.71709400	3.53446200
H	-0.30103500	-2.29413300	2.75392100
H	1.21144400	-2.13137800	3.67076300
H	-0.35462000	-1.83127700	4.47779300
Cu-Ts₃			
Cu	0.00181100	-0.00236400	-1.27354000
Cu	-0.00204800	0.00228200	1.27404200
O	-1.37661800	1.42493800	-1.14024000
O	1.37990600	-1.42858600	-1.13387900
O	-1.42582200	-1.38025400	-1.13599000
O	1.42834200	1.37674400	-1.13651500
O	1.42533800	1.37953800	1.13643600
O	-1.42783400	-1.37666800	1.13695700
O	1.37692200	-1.42481100	1.13903200
O	-1.37988600	1.42883600	1.13272800
C	-1.76502200	1.82697200	-0.00504300
C	1.76569700	-1.82638900	0.00384000
C	-1.82688400	-1.76531700	0.00073500
C	1.82668800	1.76519300	0.00000800
H	-2.52988100	2.61753000	-0.00752400
H	2.61677200	2.53054000	0.00018700
H	-2.61725000	-2.53040100	0.00132400
H	2.53155300	-2.61594300	0.00597900
C	-0.17515370	0.32809417	6.98154920

C	-0.55983745	1.77616895	6.74726491
H	0.91279995	0.27609094	7.17487308
H	-0.68709370	-0.06216886	7.86145820
H	-1.53323434	1.97741138	6.33276329
C	0.44383480	2.88607483	6.89785999
H	1.12163019	2.86443265	6.03712829
H	-0.05212630	3.85781404	6.94164626
H	1.02760563	2.75757980	7.81453370
N	-0.54562314	-0.48010442	5.82965044
Br	-1.75339293	2.23442044	8.99136483
C	-0.28456481	0.13543303	4.60354867
O	-0.07982801	1.38714223	4.68315940
O	-0.29171158	-0.57623003	3.55567370
C	-0.51097210	-1.92155817	5.96839357
H	-0.79936429	-2.36536539	5.01449403
H	0.49564454	-2.29126108	6.23415502
H	-1.21302367	-2.24058956	6.74918985

Cu-Int₅

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

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

Cr-HKUST-1

Cr	0.001153	0.000016	-1.227546
Cr	-0.001073	0.000007	1.227662
O	0.661373	1.887448	-1.128399

O	-0.657030	-1.888020	-1.129762
O	-1.886349	0.659893	-1.130763
O	1.889217	-0.658485	-1.127757
O	1.886895	-0.658365	1.130527
O	-1.889703	0.656761	1.127516
O	-0.659815	-1.887984	1.128520
O	0.655263	1.888711	1.129876
C	0.846322	2.428668	0.000928
C	-0.846423	-2.428591	-0.000802
C	-2.428625	0.846301	-0.002133
C	2.428650	-0.846415	0.001886
H	1.207278	3.466225	0.001333
H	3.466163	-1.207495	0.003030
H	-3.466156	1.207332	-0.003180
H	-1.207557	-3.466086	-0.001271

Cr-Int₀

Cr	0.00142300	-0.00056300	-1.42449200
Cr	-0.00142600	0.00056800	1.42450700
O	1.41783600	1.43657000	-1.13278400
O	-1.41503700	-1.43786500	-1.13416300
O	-1.43589000	1.41606900	-1.13514200
O	1.43856400	-1.41680000	-1.13204600
O	1.43694400	-1.41497300	1.13501600
O	-1.43963200	1.41570900	1.13191400
O	-1.41674400	-1.43764600	1.13289800
O	1.41394000	1.43894700	1.13427300
C	1.81109900	1.83946500	0.00099000
C	-1.81102900	-1.83953200	-0.00088000
C	-1.83952400	1.81104300	-0.00219600

C	1.83951800	-1.81103700	0.00207400
H	2.58218600	2.62298100	0.00150500
H	2.62286400	-2.58229700	0.00326900
H	-2.62287300	2.58230000	-0.00338100
H	-2.58234300	-2.62282500	-0.00139500
C	1.09947142	0.18367324	4.34105149
C	-0.13676431	0.98165574	4.60408390
H	1.86491278	0.56263855	3.66556485
H	1.47362642	-0.45420568	5.14437840
H	-0.57887233	0.83420523	5.59418048
C	-0.37773343	2.34448124	3.99587563
H	-1.45126038	2.53199631	3.86598469
H	0.03055174	3.13523216	4.63827990
H	0.09843079	2.41546085	3.01223530
N	-0.17431359	-0.17943147	3.71711517
C	-0.82671820	-1.38074049	4.22457706
H	-1.90175901	-1.32078129	4.02014598
H	-0.42526816	-2.25675269	3.70249601
H	-0.68651980	-1.52992238	5.31143485

Cr-Int₁

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

O	1.52115700	2.09601700	-0.92257900
C	1.91055400	2.41920700	-2.07575400
C	-1.71828400	-1.26067200	-2.18943400
C	-1.73697200	2.39009800	-2.09116400
C	1.95155600	-1.22561900	-2.14219000
H	2.68287700	3.19922500	-2.13557900
H	2.72355500	-2.00605300	-2.13381500
H	-2.52218200	3.15854400	-2.14046500
H	-2.48165200	-2.04658100	-2.13847900
C	-1.35771800	-0.44607200	2.22384500
C	-0.09353600	-1.20433600	2.35798300
H	-2.06077700	-0.69073200	1.43089100
H	-1.77732500	-0.03716900	3.14093900
H	0.28094600	-1.22641100	3.38393600
C	0.24991800	-2.41058300	1.51922900
H	1.33294500	-2.48702600	1.36369500
H	-0.07946900	-3.30968600	2.05586500
H	-0.23862300	-2.38938900	0.54130100
N	-0.08332900	0.16020000	1.74599400
Br	-0.36051900	-1.00872300	5.93647400
C	0.46702800	1.21451700	2.62429700
H	1.54612600	1.29217600	2.44796600
H	-0.00002200	2.17361100	2.36798400
H	0.29301700	0.99111900	3.68521900
Cr-Ts₁			
Cr	0.00142300	-0.00056300	-1.42449200
Cr	-0.00142600	0.00056800	1.42450700
O	1.41783600	1.43657000	-1.13278400
O	-1.41503700	-1.43786500	-1.13416300

O	-1.43589000	1.41606900	-1.13514200
O	1.43856400	-1.41680000	-1.13204600
O	1.43694400	-1.41497300	1.13501600
O	-1.43963200	1.41570900	1.13191400
O	-1.41674400	-1.43764600	1.13289800
O	1.41394000	1.43894700	1.13427300
C	1.81109900	1.83946500	0.00099000
C	-1.81102900	-1.83953200	-0.00088000
C	-1.83952400	1.81104300	-0.00219600
C	1.83951800	-1.81103700	0.00207400
H	2.58218600	2.62298100	0.00150500
H	2.62286400	-2.58229700	0.00326900
H	-2.62287300	2.58230000	-0.00338100
H	-2.58234300	-2.62282500	-0.00139500
C	-1.13008064	0.06905772	4.22714351
C	0.05174254	-0.56738491	4.84767007
H	-1.80532175	-0.62732209	3.72752057
H	-1.66931473	0.80094647	4.83354139
H	0.67926597	0.05440597	5.47036055
C	0.57172420	-1.91069262	4.41198060
H	1.20117132	-1.81855083	3.51886557
H	1.16708414	-2.35127952	5.21529581
H	-0.25452753	-2.58963198	4.18196148
N	-0.10128913	0.60101748	3.35078085
Br	-0.96863444	-1.29352669	7.20480159
C	0.24424535	1.99450351	3.61561141
H	1.20181963	2.23733602	3.14746404
H	-0.53083409	2.64614518	3.18741412
H	0.30817574	2.19420985	4.69583029

Cr-Int₂

Cr	0.09072500	0.63520100	-3.29981500
Cr	0.13565200	0.37235800	-0.11826000
O	1.42249500	2.12107900	-3.20741600
O	-1.21399500	-0.87435100	-3.08685400
O	-1.44172300	1.97042300	-3.36610600
O	1.63840900	-0.72779000	-3.25810800
O	1.40591800	-1.01366900	-1.02775000
O	-1.20422900	2.04671000	-1.12296500
O	-1.44928200	-0.93423600	-0.81749100
O	1.72036800	1.87169800	-0.96254800
C	1.94325500	2.39417000	-2.07474900
C	-1.71372900	-1.28159900	-1.99299100
C	-1.72824900	2.39893700	-2.19558200
C	1.92770300	-1.25189700	-2.14425400
H	2.68287700	3.19922500	-2.13557900
H	2.72355500	-2.00605300	-2.13381500
H	-2.52218200	3.15854400	-2.14046500
H	-2.48165200	-2.04658100	-2.13847900
C	-1.02472900	0.02492600	2.60473200
C	-0.05810200	-0.48061700	3.68604100
H	-1.40811100	-0.84222100	2.04601700
H	-1.89275800	0.51062100	3.08599700
H	0.38391800	0.35138500	4.23477200
C	0.98438000	-1.47466200	3.21332200
H	1.58308600	-0.99925000	2.42759300
H	1.65024500	-1.78029400	4.02695400
H	0.51023900	-2.36827200	2.79138700
N	-0.30780000	0.92210600	1.72630400

Br	-1.15890500	-1.42534900	5.22648600
C	-0.39226900	2.31166000	2.13108400
H	0.11817300	2.94274000	1.39538500
H	-1.44123600	2.66502700	2.20598000
H	0.08264900	2.50770700	3.11247200
Cr-Int₃			
Cr	-0.27862400	0.66993000	-3.43213100
Cr	-0.18591500	0.88214000	-0.24869800
O	0.28728300	2.65380000	-3.37512000
O	-0.83870500	-1.29396300	-3.53249200
O	-2.18515300	1.24267500	-3.27885500
O	1.63751000	0.13947000	-3.23808700
O	1.72478200	-0.04661000	-0.96459900
O	-2.13277700	1.67147100	-1.03632900
O	-1.07588200	-1.02652700	-1.30881000
O	0.61556500	2.58093900	-1.13886700
C	0.62121100	3.14675300	-2.25900900
C	-1.12927200	-1.69854400	-2.35511900
C	-2.67308800	1.61641500	-2.16498200
C	2.18961100	-0.13074800	-2.12448200
H	0.95776200	4.19005800	-2.24998500
H	3.21664700	-0.48366200	-2.24828800
H	-3.71567200	1.93116500	-2.25449800
H	-1.45707300	-2.74225300	-2.25258900
C	0.10000600	-1.23432400	1.79321100
C	0.69214200	-1.14497300	3.20638800
H	0.92228500	-1.39087700	1.08258100
H	-0.56202300	-2.11400200	1.72221300
H	-0.06416800	-0.85699600	3.93606200

C	1.95144100	-0.30726000	3.32152900
H	1.73205900	0.69791900	2.94123700
H	2.29686400	-0.22632100	4.35769100
H	2.75692700	-0.72728900	2.70925400
N	-0.60750800	-0.00137000	1.48659000
Br	1.17734000	-3.08151400	3.88683200
C	-0.45338300	2.63895600	3.25729600
O	-0.07371500	3.25804500	2.34046800
O	-0.83209400	2.08777000	4.21956800
C	-2.01132900	-0.08764700	1.86644100
H	-2.15780200	-0.17814100	2.95860100
H	-2.54468700	0.81466600	1.54243000
H	-2.51576700	-0.95472600	1.39693400
Cr-Ts₂			
Cr	0.00115300	0.00001600	-1.22754600
Cr	-0.00107300	0.00000700	1.22766200
O	0.66137300	1.88744800	-1.12839900
O	-0.65703000	-1.88802000	-1.12976200
O	-1.88634900	0.65989300	-1.13076300
O	1.88921700	-0.65848500	-1.12775700
O	1.88689500	-0.65836500	1.13052700
O	-1.88970300	0.65676100	1.12751600
O	-0.65981500	-1.88798400	1.12852000
O	0.65526300	1.88871100	1.12987600
C	0.84632200	2.42866800	0.00092800
C	-0.84642300	-2.42859100	-0.00080200
C	-2.42862500	0.84630100	-0.00213300
C	2.42865000	-0.84641500	0.00188600
H	1.20727800	3.46622500	0.00133300

H	3.46616300	-1.20749500	0.00303000
H	-3.46615600	1.20733200	-0.00318000
H	-1.20755700	-3.46608600	-0.00127100
C	1.14968837	-0.91239133	3.84318188
C	2.02919119	0.26150236	4.28393638
H	1.72799763	-1.56315606	3.16996612
H	0.89039499	-1.50822921	4.72957622
H	1.54373026	0.84944613	5.06142096
C	2.57005993	1.14022934	3.17701412
H	1.72546931	1.64996309	2.69681743
H	3.24044275	1.90861484	3.57492853
H	3.09572653	0.55331913	2.41861186
N	-0.07660656	-0.45034674	3.18250104
Br	3.62710416	-0.56074045	5.32802523
C	-1.18049412	0.92410572	4.29538820
O	-1.98338937	0.20797075	4.81536725
O	-0.67219997	1.98681354	4.10223273
C	-1.02356395	-1.57458331	3.19874344
H	-1.17831931	-1.89601729	4.20752041
H	-1.95588904	-1.26172749	2.77709055
H	-0.62576508	-2.38432669	2.62344202
Cr-Int₄			
Cr	-0.65297400	0.15260200	1.24510200
Cr	-0.66527400	0.14790400	4.22585800
O	-2.01297100	-1.39810800	1.80386800
O	0.62438500	1.68583500	1.85802600
O	0.85668700	-1.19560600	1.80265900
O	-2.22067800	1.48980200	1.78708100
O	-2.00544600	1.64893000	4.04771400

O	0.67748600	-1.35321700	4.06583400
O	0.84943200	1.49259300	4.10997900
O	-2.17043600	-1.19787800	4.06357000
C	-2.48208700	-1.68416400	2.92933800
C	1.13004300	1.97539700	2.96659900
C	1.15267400	-1.66387700	2.92804800
C	-2.50013800	1.95610600	2.91682300
H	-3.26381400	-2.45270600	2.95348400
H	-3.27277200	2.73252300	2.95522300
H	1.92091100	-2.44374300	2.94859900
H	1.91227900	2.74115200	2.95057900
C	0.36985300	1.06231200	-4.03035000
C	1.68175300	0.36719700	-4.39068700
H	0.66190700	2.03520700	-3.60479000
H	-0.20935700	1.25397900	-4.94127700
H	2.08426600	-0.14196400	-3.51785700
C	2.70020700	1.27961200	-5.04766600
H	2.98520600	2.05372700	-4.32219200
H	3.60159100	0.73354100	-5.34059400
H	2.28674000	1.77107000	-5.93692000
N	-0.45478200	0.34896700	-3.07938000
Br	1.30219400	-1.21525200	-5.68882900
C	-0.07615500	0.44142700	-1.71776500
O	1.05754700	0.90472600	-1.46868500
O	-0.94502400	0.02238600	-0.86746400
C	-1.81075100	0.00036300	-3.46338600
H	-2.25633100	-0.57820800	-2.65462000
H	-2.44149600	0.89144600	-3.63620700
H	-1.80262500	-0.60213200	-4.38023800

Cr-Ts₃

Cr	-0.00139400	0.00055800	-1.41863400
Cr	0.00140700	-0.00057200	1.41864600
O	-1.41783700	-1.41946100	-1.13316000
O	1.41522300	1.42062900	-1.13458900
O	1.41880600	-1.41612700	-1.13560500
O	-1.42130600	1.41692900	-1.13240700
O	-1.41978700	1.41509700	1.13547200
O	1.42231800	-1.41592600	1.13226300
O	1.41682600	1.42047200	1.13328600
O	-1.41421000	-1.42164200	1.13471200
C	-1.81229600	-1.81766100	0.00101700
C	1.81212200	1.81783400	-0.00089400
C	1.81781100	-1.81216100	-0.00223300
C	-1.81779500	1.81214200	0.00210300
H	-2.58787200	-2.59710300	0.00151300
H	-2.59683000	2.58812600	0.00325200
H	2.59685300	-2.58814000	-0.00337200
H	2.58822100	2.59675500	-0.00139200
C	-0.40184069	0.47256009	-6.93319635
C	-0.42444262	1.98869654	-6.89524680
H	-1.44473516	0.11137650	-6.96123715
H	0.10330640	0.12313044	-7.83342770
H	0.49107066	2.49820978	-6.64482357
C	-1.70597342	2.75959320	-7.04539834
H	-2.26985085	2.68678240	-6.10828704
H	-1.50725002	3.80988759	-7.26731305
H	-2.31214142	2.34700105	-7.85753653

N	0.31077404	-0.01012077	-5.76356116
Br	0.38016477	2.45314699	-9.33571840
C	-0.00611366	0.64669647	-4.58261894
O	-0.58570640	1.76759422	-4.76080400
O	0.30032146	0.14614728	-3.45943607
C	0.71311614	-1.42182249	-5.68533644
H	1.61236294	-1.50512951	-5.11147660
H	-0.06350542	-1.98853328	-5.21565805
H	0.88335204	-1.79936942	-6.67193567

Cr-Int₅

Cr	-0.67234400	0.14416800	1.34484200
Cr	-0.67031000	0.14165500	4.27784200
O	-2.06129200	-1.33940200	1.80571700
O	0.69406900	1.63701900	1.81143700
O	0.80128600	-1.23460800	1.81574100
O	-2.16822400	1.52655500	1.80284600
O	-2.04947500	1.61140100	4.07188600
O	0.70851400	-1.32651000	4.08443600
O	0.79872300	1.52009100	4.07882000
O	-2.13996200	-1.23652100	4.07554500
C	-2.48983600	-1.67846600	2.93801700
C	1.13723300	1.96843200	2.94051300
C	1.14639100	-1.67066000	2.94338200
C	-2.49867700	1.95822700	2.93640400
H	-3.26381400	-2.45270600	2.95348400
H	-3.27277200	2.73252300	2.95522300
H	1.92091100	-2.44374300	2.94859900
H	1.91227900	2.74115200	2.95057900
C	0.41950000	0.48720600	-4.11153700

C	1.64674500	0.09898100	-3.27593000
H	0.43839900	1.54718000	-4.41412800
H	0.35500400	-0.13669400	-5.00694100
H	1.89181300	-0.95281500	-3.44870800
C	2.87149700	0.96548900	-3.45677000
H	2.63993100	2.02202800	-3.27310800
H	3.67001700	0.65448100	-2.77315200
H	3.21626500	0.83240000	-4.48845900
N	-0.66128700	0.25577400	-3.15013000
Br	2.23448500	-1.19048200	-6.57810000
C	-0.18458000	0.20807000	-1.88768200
O	1.15517300	0.19987200	-1.87886000
O	-0.86871400	0.17351300	-0.85186000
C	-2.06163900	0.41608000	-3.47382200
H	-2.65612100	0.16598700	-2.59194000
H	-2.28189000	1.45255000	-3.77295200
H	-2.32951400	-0.25207000	-4.30094200

Ru-HKUST-1

Ru	0.00107500	0.00038300	-1.17697600
Ru	-0.00084500	-0.00021700	1.17744000
O	-0.00818500	2.06253000	-1.13007600
O	0.01044300	-2.06185100	-1.13104900
O	-2.07971700	-0.00890800	-1.13568200
O	2.08159200	0.00955200	-1.13271500
O	2.08044600	0.00842000	1.13574500
O	-2.08191400	-0.00979300	1.13278000
O	0.00734300	-2.06278200	1.12915300
O	-0.01059400	2.06239600	1.13012500
C	-0.01247500	2.63932800	0.00023200

C	0.01159500	-2.63917800	-0.00101000
C	-2.64761600	-0.01215200	-0.00189500
C	2.64782900	0.01152100	0.00193000
H	-0.01829300	3.73544800	0.00012000
H	3.74549400	0.01658400	0.00235800
H	-3.74528000	-0.01766500	-0.00307400
H	0.01662800	-3.73530300	-0.00161700
Ru-Int₀			
Ru	0.00011000	0.00004300	-1.14147500
Ru	-0.00009300	-0.00003300	1.14148100
O	-0.16971700	2.08592700	-1.12834800
O	0.16991500	-2.08585700	-1.12842900
O	-2.08593600	-0.16974100	-1.12853400
O	2.08611100	0.16981200	-1.12825300
O	2.08597900	0.16970600	1.12853400
O	-2.08612300	-0.16979800	1.12825200
O	0.16960600	-2.08593900	1.12833900
O	-0.16983900	2.08588100	1.12842100
C	-0.21696600	2.66148800	0.00005500
C	0.21687300	-2.66148900	-0.00005200
C	-2.66155000	-0.21695200	-0.00019100
C	2.66156600	0.21692400	0.00018600
H	-0.30668100	3.75474700	0.00005600
H	3.75487800	0.30626800	0.00023800
H	-3.75484600	-0.30648000	-0.00028500
H	0.30640000	-3.75476300	-0.00009200
C	0.00275233	1.12318510	3.67364069
C	-1.12648465	0.37963898	4.31098199
H	-0.19459598	1.86927050	2.90539100

H	0.89194378	1.31336313	4.27811276
H	-0.94725737	0.06572169	5.34385463
C	-2.57569127	0.63698890	3.96623871
H	-3.17871143	-0.26965624	4.10355204
H	-2.99427083	1.42425399	4.60629485
H	-2.67180578	0.95089053	2.92146767
N	-0.28709042	-0.26291350	3.30163040
C	0.65695499	-1.27143058	3.76849685
H	0.15208275	-2.24297762	3.81645833
H	1.48463790	-1.34837989	3.05425044
H	1.07895947	-1.04844285	4.76617383
Ru-Int₁			
Ru	0.46654000	0.12686300	-2.77522500
Ru	0.46067600	0.12309100	-0.34818500
O	0.29907200	2.20623100	-2.70641100
O	0.63934100	-1.94756100	-2.70602900
O	-1.61870000	-0.04171900	-2.72232200
O	2.55016000	0.29563800	-2.70451500
O	2.57440400	0.30078600	-0.43205000
O	-1.63550700	-0.04654800	-0.45214400
O	0.64183600	-1.97568200	-0.43755000
O	0.29920900	2.22886600	-0.43760800
C	0.25184200	2.78214100	-1.57233400
C	0.68642100	-2.52656700	-1.57219700
C	-2.18920600	-0.08938500	-1.58682000
C	3.12237000	0.34312900	-1.56974800
H	0.16074900	3.88260400	-1.58831700
H	4.22230800	0.43412500	-1.58813500
H	-3.28741600	-0.17862300	-1.58865800

H	0.77383000	-3.62690600	-1.58846500
C	-0.90247000	0.70447700	2.52513800
C	-0.34913000	-0.62905200	2.83477300
H	-1.73925500	0.78312600	1.83858200
H	-0.84184000	1.47392400	3.29019700
H	0.12213300	-0.70408100	3.81263100
C	-0.97709800	-1.90892300	2.34859900
H	-0.22627300	-2.69741100	2.21997300
H	-1.69640600	-2.22053800	3.11449900
H	-1.49848900	-1.77022900	1.39873600
N	0.37748100	0.28523900	1.89193600
Br	-2.16961600	-0.43893600	5.83729200
C	1.58099900	0.92073300	2.44752000
H	2.44743700	0.28214500	2.25311400
H	1.73722500	1.88463500	1.95249700
H	1.48271800	1.08174800	3.53026200
Ru-Ts₁			
Ru	0.00011000	0.00004300	-1.14147500
Ru	-0.00009300	-0.00003300	1.14148100
O	-0.16971700	2.08592700	-1.12834800
O	0.16991500	-2.08585700	-1.12842900
O	-2.08593600	-0.16974100	-1.12853400
O	2.08611100	0.16981200	-1.12825300
O	2.08597900	0.16970600	1.12853400
O	-2.08612300	-0.16979800	1.12825200
O	0.16960600	-2.08593900	1.12833900
O	-0.16983900	2.08588100	1.12842100
C	-0.21696600	2.66148800	0.00005500
C	0.21687300	-2.66148900	-0.00005200

C	-2.66155000	-0.21695200	-0.00019100
C	2.66156600	0.21692400	0.00018600
H	-0.30668100	3.75474700	0.00005600
H	3.75487800	0.30626800	0.00023800
H	-3.75484600	-0.30648000	-0.00028500
H	0.30640000	-3.75476300	-0.00009200
C	-1.14275750	0.29503848	3.94606538
C	-0.65266726	-1.02468683	4.39878508
H	-2.05076079	0.25453446	3.34240329
H	-1.18316810	1.08823009	4.69664313
H	0.16083996	-1.03337438	5.11032111
C	-1.01373779	-2.30730799	3.69936184
H	-0.37609339	-2.47065185	2.82239169
H	-0.88584840	-3.14762753	4.38594249
H	-2.05600786	-2.28740562	3.36794614
N	0.07516346	0.22428965	3.15798681
Br	-2.12142755	-1.35896161	6.60231036
C	1.16678839	1.04480683	3.67416431
H	2.11481919	0.72537536	3.23339315
H	0.98917945	2.09489520	3.40120385
H	1.23612468	0.97772502	4.77030985
Ru-Int₂			
Ru	0.47662700	0.12947400	-2.79277800
Ru	0.45280100	0.13045600	-0.28869500
O	0.34805800	2.22338800	-2.71803700
O	0.69107900	-1.95949600	-2.71623100
O	-1.61641700	-0.05582900	-2.69539600
O	2.57452300	0.28326800	-2.72428700
O	2.58264800	0.31425900	-0.43967000

O	-1.66503200	-0.04259400	-0.41480200
O	0.59815900	-1.98712300	-0.44150800
O	0.27593200	2.23926600	-0.44255300
C	0.25951200	2.78315900	-1.57918300
C	0.68486300	-2.52660100	-1.57854700
C	-2.18895800	-0.09194400	-1.56145000
C	3.12355600	0.34462600	-1.57909700
H	0.16074900	3.88260400	-1.58831700
H	4.22230800	0.43412500	-1.58813500
H	-3.28741600	-0.17862300	-1.58865800
H	0.77383000	-3.62690600	-1.58846500
C	-0.72378900	0.08613500	2.58417900
C	-0.55446500	-1.17923100	3.43510100
H	-1.60604600	-0.02811200	1.94543300
H	-0.89381300	0.95349400	3.24569300
H	0.36119500	-1.14108300	4.02559100
C	-0.70163800	-2.48529900	2.68460700
H	0.02765800	-2.49611000	1.86618800
H	-0.52886700	-3.34769700	3.33754000
H	-1.70042300	-2.57027000	2.24185800
N	0.46227200	0.26195600	1.77031300
Br	-2.00199000	-1.16300700	4.98384200
C	1.49429200	1.02978200	2.43736800
H	2.39135700	1.06411000	1.81365000
H	1.16881700	2.07184600	2.63303500
H	1.77840400	0.59750100	3.41558200
Ru-Int₃			
Ru	-0.57390900	0.18157300	0.21177900
Ru	-2.73982300	-0.78383300	-0.32977200

O	-0.36529300	0.61937800	-1.86217700
O	-0.99661100	-0.33484800	2.22539300
O	0.26596700	-1.74685700	-0.12548400
O	-1.57434100	2.05467200	0.48508700
O	-3.58270700	1.10883500	-0.00144900
O	-1.77046400	-2.62212500	-0.62247400
O	-3.01509200	-1.25814900	1.71714500
O	-2.39622700	-0.28149700	-2.35957600
C	-1.30898200	0.29620500	-2.64261300
C	-2.07986000	-0.92462000	2.50042000
C	-0.51702600	-2.68066500	-0.45930200
C	-2.82818500	2.07059400	0.32481300
H	-1.16341200	0.55150900	-3.69885400
H	-3.32930200	3.03273800	0.48930700
H	-0.05450600	-3.66007200	-0.63025200
H	-2.22024600	-1.17905900	3.55765000
C	2.44273000	0.13192000	0.91470500
C	3.44808200	0.63457400	-0.12950800
H	2.21406400	-0.91858900	0.71047800
H	2.89387100	0.19148500	1.91958600
H	3.64426800	1.70038900	-0.01403800
C	3.12914100	0.25840700	-1.56062300
H	2.12698900	0.63465000	-1.79828800
H	3.85352800	0.68705900	-2.26137200
H	3.11465200	-0.83014700	-1.68445600
N	1.24367100	0.94156800	0.82539200
Br	5.35842500	-0.16103400	0.32918400
C	0.86999500	3.99031800	-1.90155900
O	1.85820200	3.94085800	-1.27758800

O	-0.10089200	4.08219600	-2.54714300
C	1.27930400	2.08604400	1.71517400
H	2.15714400	2.73103900	1.52739500
H	0.38146600	2.69355600	1.57958700
H	1.32618900	1.77693500	2.77819900
Ru-Ts₂			
Ru	-0.60526900	0.22012700	0.24220800
Ru	-2.71567800	-0.74213300	-0.29737500
O	-0.38981400	0.66024900	-1.81867200
O	-0.98584200	-0.30302200	2.26800400
O	0.23386400	-1.71613200	-0.06350500
O	-1.59432800	2.07019800	0.52591900
O	-3.59966800	1.13290000	0.03634200
O	-1.78235600	-2.59490400	-0.61484400
O	-2.98635100	-1.23244000	1.73349400
O	-2.41042100	-0.23939500	-2.31521400
C	-1.32186800	0.33730800	-2.60498300
C	-2.06539100	-0.89778600	2.53798300
C	-0.53171900	-2.65283900	-0.42292200
C	-2.84421400	2.09615300	0.36540400
H	-1.16879600	0.58289600	-3.66255500
H	-3.33468600	3.06412500	0.52560600
H	-0.05989000	-3.62868500	-0.59395300
H	-2.22563000	-1.14767200	3.59394900
C	2.47713100	0.16187000	0.85816500
C	3.35050200	0.03943200	-0.39456400
H	2.13249700	-0.83939400	1.14078200
H	3.13138800	0.51160200	1.66897800
H	3.82888700	0.97849000	-0.64310400

C	2.75544600	-0.63831800	-1.60799300
H	1.87398400	-0.06784200	-1.91148900
H	3.46899300	-0.65400200	-2.43846200
H	2.44246600	-1.65782000	-1.37560800
N	1.34409500	1.10895600	0.74061600
Br	5.03050100	-1.09081900	0.20300800
C	1.49512588	2.56912237	-0.49970222
O	2.15971753	3.33951566	0.10431310
O	0.82375306	2.24188246	-1.41065073
C	1.19260400	1.78609700	2.03722600
H	2.08630900	2.38313600	2.27430600
H	0.33601200	2.46251600	1.99937700
H	1.03699700	1.06634900	2.85689800

Ru-Int₄

Ru	0.42454000	-0.57623400	0.99125500
Ru	0.43355500	-0.57959400	3.33388000
O	0.26650700	1.52413300	1.06204400
O	0.60829700	-2.69310200	1.04888900
O	-1.66667400	-0.78949100	1.06890200
O	2.54608000	-0.39969700	1.04745300
O	2.53162700	-0.41784000	3.31520100
O	-1.66331700	-0.73572800	3.33511100
O	0.59782300	-2.67888400	3.31707000
O	0.26854800	1.51642800	3.32939000
C	0.22110500	2.07885400	2.19185400
C	0.65002300	-3.24394100	2.18253900
C	-2.22390800	-0.80596800	2.19667500
C	3.09747100	-0.36376100	2.18060800
H	0.13062700	3.17175500	2.19366000

H	4.19218600	-0.27672400	2.19384200
H	-3.31753800	-0.88947200	2.19331900
H	0.74370800	-4.33775500	2.19351200
C	-1.09711000	-0.13232300	-4.28787100
C	-1.39500800	1.33072600	-4.61484200
H	-2.03467200	-0.53905900	-3.87817200
H	-0.87039200	-0.68114500	-5.21043800
H	-1.23052500	1.94970500	-3.73633300
C	-2.76330100	1.55442800	-5.23071900
H	-3.52404100	1.27746100	-4.48720000
H	-2.91477100	2.60247000	-5.50607100
H	-2.90902900	0.93574200	-6.12533900
N	-0.02518000	-0.33682300	-3.33617700
Br	0.03485900	2.05744100	-5.94167500
C	-0.35854400	-0.12714500	-1.97559100
O	-1.41171600	0.48034900	-1.72415500
O	0.51125300	-0.60155500	-1.13983200
C	1.08977500	-1.18591600	-3.72008100
H	1.84859000	-1.13526500	-2.93758700
H	0.79460200	-2.24469800	-3.84166500
H	1.51863900	-0.83022300	-4.66560900

Ru-Ts₃

Ru	0.00011000	0.00004300	-1.14147500
Ru	-0.00009300	-0.00003300	1.14148100
O	-0.16971700	2.08592700	-1.12834800
O	0.16991500	-2.08585700	-1.12842900
O	-2.08593600	-0.16974100	-1.12853400
O	2.08611100	0.16981200	-1.12825300
O	2.08597900	0.16970600	1.12853400

O	-2.08612300	-0.16979800	1.12825200
O	0.16960600	-2.08593900	1.12833900
O	-0.16983900	2.08588100	1.12842100
C	-0.21696600	2.66148800	0.00005500
C	0.21687300	-2.66148900	-0.00005200
C	-2.66155000	-0.21695200	-0.00019100
C	2.66156600	0.21692400	0.00018600
H	-0.30668100	3.75474700	0.00005600
H	3.75487800	0.30626800	0.00023800
H	-3.75484600	-0.30648000	-0.00028500
H	0.30640000	-3.75476300	-0.00009200
C	-1.03003682	0.19033380	-6.54826767
C	-1.62795075	1.55139589	-6.24860080
H	-1.84796447	-0.55213387	-6.60707008
H	-0.52413591	0.20320742	-7.51394163
H	-0.95911814	2.33888329	-5.94472886
C	-3.11673265	1.75407288	-6.18243115
H	-3.48820905	1.31871038	-5.24798009
H	-3.36786428	2.81630997	-6.20994485
H	-3.61156996	1.26291082	-7.02592739
N	-0.06443321	-0.16861532	-5.52061573
Br	-1.34931403	2.62585469	-8.58064999
C	-0.47316098	0.15895335	-4.22601011
O	-1.43785620	0.98487083	-4.17852934
O	0.14083617	-0.36144140	-3.24787201
C	0.80800908	-1.29790126	-5.76920567
H	1.44995630	-1.43422861	-4.89778277
H	0.24345314	-2.23291856	-5.93535530
H	1.42686194	-1.10641405	-6.65501268

Ru-Int₅

Ru	0.43507100	-0.57901600	1.01324700
Ru	0.43568500	-0.58059300	3.33208500
O	0.28214600	1.51932800	1.06027400
O	0.60043000	-2.68701900	1.05589700
O	-1.66441100	-0.75377500	1.05867600
O	2.54093100	-0.41769500	1.05647800
O	2.52869300	-0.41142200	3.32010800
O	-1.65529100	-0.74957100	3.32183400
O	0.60595700	-2.67474100	3.31973300
O	0.26428700	1.50877900	3.32300900
C	0.22506200	2.07935800	2.18960000
C	0.65052500	-3.24457300	2.18722000
C	-2.22464100	-0.79823500	2.18865900
C	3.09891500	-0.36746800	2.18758900
H	0.13062700	3.17175500	2.19366000
H	4.19218600	-0.27672400	2.19384200
H	-3.31753800	-0.88947200	2.19331900
H	0.74370800	-4.33775500	2.19351200
C	-0.88110800	0.32713500	-4.26318900
C	-1.44939600	1.34113100	-3.26218300
H	-1.63561600	-0.40901600	-4.58310100
H	-0.48795100	0.83737500	-5.14721600
H	-0.92212800	2.29405600	-3.36051400
C	-2.94473000	1.55189800	-3.30564400
H	-3.48068800	0.60225700	-3.18620300
H	-3.26154500	2.23929200	-2.51299400
H	-3.18272400	1.99399200	-4.28012500

N	0.14717500	-0.32453600	-3.44815000
Br	-1.42568200	2.88690900	-6.55809800
C	-0.08225300	-0.11722800	-2.13405900
O	-1.05392200	0.77847300	-1.94514100
O	0.52772700	-0.68221800	-1.20638000
C	1.03704100	-1.34526700	-3.95655900
H	1.69354000	-1.67266800	-3.14799700
H	0.46977000	-2.21001400	-4.33153000
H	1.63656100	-0.93812500	-4.77795700

Ti-HKUST-1

Ti	-0.00005900	0.00077100	1.42413700
Ti	0.00007500	-0.00055000	-1.32592100
O	-1.41549700	-1.39490600	1.09307900
O	1.41556400	1.39605500	1.09224500
O	-1.41699600	1.39467400	1.09213700
O	1.41677300	-1.39349700	1.09309100
O	1.48012000	-1.43354800	-1.15225600
O	-1.48016800	1.43233700	-1.15326000
O	1.48065200	1.43189300	-1.15312300
O	-1.48051400	-1.43299400	-1.15225100
C	-1.87061100	-1.82252400	-0.01393000
C	1.87103600	1.82223100	-0.01516300
C	-1.87156400	1.82170100	-0.01533000
C	1.87116800	-1.82197900	-0.01388100
H	-2.65766000	-2.58629100	0.02895500
H	2.65842100	-2.58553000	0.02908800
H	-2.65933400	2.58476700	0.02677700
H	2.65859700	2.58551000	0.02697600

Ti-Int₀

Ti	0.00001100	-0.00025500	1.43151600
Ti	0.00000200	0.00017500	-1.34116700
O	1.42439300	1.40235700	1.09473200
O	-1.42442000	-1.40275600	1.09442400
O	1.42509800	-1.40205200	1.09431900
O	-1.42505900	1.40162000	1.09463500
O	-1.48980300	1.44301000	-1.15132500
O	1.48987900	-1.44257400	-1.15165400
O	-1.49013900	-1.44226100	-1.15154200
O	1.49006400	1.44269600	-1.15121800
C	1.87977200	1.83115500	-0.01184700
C	-1.87996100	-1.83099900	-0.01230000
C	1.88011300	-1.83086300	-0.01240400
C	-1.88001300	1.83090200	-0.01193600
H	2.66675200	2.59497800	0.03146200
H	-2.66688800	2.59483100	0.03141300
H	2.66715700	-2.59463300	0.03065900
H	-2.66687100	-2.59490800	0.03073900
C	-0.42829386	-1.37016730	-3.79644746
C	-1.06166172	-0.18558270	-4.45207341
H	-0.96869041	-1.93166824	-3.03586503
H	0.27820489	-1.95960267	-4.38435993
H	-0.73558341	0.00191343	-5.47969714
C	-2.46774256	0.27149817	-4.13696947
H	-2.56996968	1.35460850	-4.28159064
H	-3.19513212	-0.22901984	-4.78893051
H	-2.72074287	0.04493627	-3.09582619
N	-0.03848624	-0.00908638	-3.42338105
C	1.27816536	0.43377692	-3.86676955

H	1.29131813	1.52836013	-3.91982174
H	2.03043724	0.11538848	-3.13612329
H	1.56485159	0.03347759	-4.85709380
Ti-Int₁			
Ti	0.11983300	0.53723400	-0.54790900
Ti	0.11588800	0.55153000	-3.52036800
O	1.64336700	2.02329400	-0.86453400
O	-1.38698700	-0.92354500	-0.91151700
O	1.60648900	-0.88411700	-0.95436200
O	-1.37346900	1.99702900	-0.92382700
O	-1.30163600	1.95971400	-3.17565700
O	1.54630100	-0.85938900	-3.20556300
O	-1.30674100	-0.84209000	-3.16518000
O	1.51542100	1.94344900	-3.11697900
C	1.99511400	2.38276500	-2.01681700
C	-1.76236500	-1.28119300	-2.05678000
C	1.99512000	-1.27492900	-2.08604300
C	-1.75713300	2.38076200	-2.06041000
H	2.78313700	3.14585800	-2.11340600
H	-2.55050300	3.14571100	-2.11345500
H	2.78354200	-2.04375300	-2.11420900
H	-2.55048600	-2.04402800	-2.11412900
C	-1.28899800	-0.28963700	2.21545200
C	-0.00418300	-0.99135600	2.40575300
H	-1.98947300	-0.63235700	1.45885100
H	-1.70708000	0.20480700	3.08950700
H	0.38497200	-0.89599300	3.42146100
C	0.36211800	-2.26889200	1.69217700
H	1.44432400	-2.33739800	1.53324400

H	0.05799900	-3.10874300	2.33010400
H	-0.13641000	-2.36655000	0.72431700
N	-0.03518500	0.31584900	1.66230900
Br	-0.37818800	-0.48933200	5.91535600
C	0.47755400	1.46896900	2.43865100
H	1.54934500	1.57917700	2.24169200
H	-0.03671400	2.37767200	2.10479600
H	0.31884600	1.32579900	3.51535500
Ti-Ts₁			
Ti	0.62029411	2.98772608	-9.01613415
Ti	0.62028511	2.98815608	-11.78881715
O	2.04467611	4.39033808	-9.35291815
O	-0.80413689	1.58522508	-9.35322615
O	2.04538111	1.58592908	-9.35333115
O	-0.80477589	4.38960108	-9.35301515
O	-0.86951989	4.43099108	-11.59897515
O	2.11016211	1.54540708	-11.59930415
O	-0.86985589	1.54572008	-11.59919215
O	2.11034711	4.43067708	-11.59886815
C	2.50005511	4.81913608	-10.45949715
C	-1.25967789	1.15698208	-10.45995015
C	2.50039611	1.15711808	-10.46005415
C	-1.25972989	4.81888308	-10.45958615
H	3.28703511	5.58295908	-10.41618815
H	-2.04660489	5.58281208	-10.41623715
H	3.28744011	0.39334808	-10.41699115
H	-2.04658789	0.39307308	-10.41691115
C	-0.84095604	2.71092514	-6.29922874
C	0.23391101	1.88536210	-5.70768420

H	-1.50508757	2.16825093	-6.97373039
H	-1.39153432	3.36329050	-5.61700010
H	0.83410672	2.33674551	-4.93039975
C	0.71167993	0.60435286	-6.33651965
H	1.42975838	0.80430138	-7.14071626
H	1.19797300	-0.01613291	-5.57994707
H	-0.12773599	0.04271254	-6.75663918
N	0.29881073	3.30861363	-6.97235936
Br	-1.05386496	0.83431425	-3.61927536
C	0.70054940	4.60229135	-6.42799124
H	1.71220137	4.84951691	-6.76043357
H	0.01186927	5.37731314	-6.79377647
H	0.67065084	4.60203806	-5.32801463

Ti-Int₂

Ti	0.11493000	0.55124800	-0.54635700
Ti	0.11445900	0.55157700	-3.52671000
O	1.65128400	2.02667800	-0.86348100
O	-1.40941000	-0.93375400	-0.86328400
O	1.58018900	-0.90077000	-0.95498000
O	-1.34359400	2.00454300	-0.96139600
O	-1.32735300	1.96195100	-3.21954400
O	1.56102000	-0.85281200	-3.21260900
O	-1.29119800	-0.84043200	-3.12379200
O	1.51886700	1.94739300	-3.12389900
C	1.99663200	2.38115800	-2.02330500
C	-1.76263100	-1.28112500	-2.02281700
C	1.98958300	-1.27639500	-2.09171700
C	-1.75416500	2.38097300	-2.09522000
H	2.78313700	3.14585800	-2.11340600

H	-2.55050300	3.14571100	-2.11345500
H	2.78354200	-2.04375300	-2.11420900
H	-2.55048600	-2.04402800	-2.11412900
C	-0.59445600	-0.40025300	2.29053900
C	0.47456300	-1.19947900	3.04945000
H	-1.18295000	-1.09263600	1.67598500
H	-1.28271800	0.06808800	3.01581400
H	1.16104000	-0.53850900	3.57829800
C	1.20185100	-2.24584600	2.23207300
H	1.66020400	-1.75180800	1.36697700
H	1.98242400	-2.74620800	2.81539200
H	0.50360700	-3.00182400	1.85520500
N	0.03824800	0.59775900	1.44706700
Br	-0.43015400	-2.18848400	4.69222400
C	0.37418400	1.80922300	2.17976500
H	0.81846200	2.54316400	1.49910400
H	-0.52202400	2.27057600	2.64179300
H	1.10300900	1.64625900	2.99715000

Ti-Int₃

Ti	0.81501300	0.27863900	-0.19390900
Ti	3.49473700	-0.91900200	0.21238600
O	1.93709700	2.11441600	-0.02197300
O	0.23986000	-1.79074200	-0.23886600
O	0.89809600	0.17373600	1.89826500
O	1.47840300	0.06110300	-2.16471000
O	3.51045700	-0.87004100	-1.83638400
O	2.95787000	-0.70935200	2.17538400
O	2.34206100	-2.57257800	0.08060900
O	3.92566300	1.05490400	0.21808200

C	3.19033800	2.09215300	0.12957400
C	1.08785000	-2.71386800	-0.10435000
C	1.85920000	-0.24166500	2.61212700
C	2.56738700	-0.43659700	-2.57159000
H	3.71951600	3.05456700	0.18639000
H	2.71156000	-0.49608400	-3.66388500
H	1.73212800	-0.19893000	3.70734200
H	0.72393300	-3.74986800	-0.14314400
C	-2.21917700	0.20069900	-0.64741500
C	-3.11096900	0.51172700	0.56157600
H	-1.97247100	-0.86711300	-0.63424400
H	-2.77991400	0.40304200	-1.57589800
H	-3.29766100	1.58134700	0.65499000
C	-2.66509200	-0.11204400	1.86740600
H	-1.63990200	0.21685100	2.07548400
H	-3.31267400	0.18208900	2.70080000
H	-2.65593700	-1.20505600	1.79434800
N	-1.00437200	0.99624500	-0.58579300
Br	-5.07317200	-0.18139400	0.16511100
C	-0.29980900	3.66581900	2.69879000
O	-1.00896500	4.10730500	1.87830800
O	0.39776500	3.25887500	3.54843200
C	-1.18320500	2.31578800	-1.17434400
H	-1.94307600	2.93009500	-0.65665500
H	-0.24042400	2.87150300	-1.13497100
H	-1.49505300	2.24918600	-2.23662100
Ti-Ts₂			
Ti	0.80968000	0.28370800	-0.14544200
Ti	3.29590900	-0.84913700	0.19976100

O	1.92735700	2.05844200	-0.05908700
O	0.23794400	-1.76895600	-0.18237500
O	0.84735300	0.21905400	1.92883300
O	1.39187800	0.04218700	-2.17372400
O	3.43834300	-0.85390700	-1.84088100
O	2.88151000	-0.71928200	2.20242500
O	2.31447900	-2.63740200	0.07347200
O	3.94254900	1.08942200	0.29493400
C	3.16862200	2.08957000	0.14216900
C	1.05286400	-2.72045900	-0.08322300
C	1.78901900	-0.22590000	2.63214000
C	2.48424300	-0.42964400	-2.57114400
H	3.64546600	3.06975800	0.19575700
H	2.63751000	-0.48089300	-3.65451800
H	1.65807800	-0.18373900	3.71670900
H	0.64988300	-3.73467700	-0.13377700
C	-2.28569500	0.12873400	-0.91170400
C	-3.08726700	-0.02628500	0.38425100
H	-1.97997500	-0.87081100	-1.25944900
H	-2.97369800	0.53472400	-1.66680800
H	-3.52817800	0.92265200	0.68924000
C	-2.41957300	-0.74412000	1.53479200
H	-1.55999700	-0.15024000	1.86533400
H	-3.10556800	-0.85641500	2.38102400
H	-2.05627100	-1.72876100	1.22758000
N	-1.12009700	1.02580100	-0.77583400
Br	-4.81944500	-1.10436200	-0.11491700
C	-1.70372100	2.72157400	0.59182900
O	-2.39977400	3.37658300	-0.12123200

O	-1.16257800	2.46317200	1.61923100
C	-0.96409200	1.76294200	-2.03884100
H	-1.84289300	2.39553100	-2.23863700
H	-0.08588600	2.41677900	-1.98443200
H	-0.81905800	1.08462200	-2.89448400
Ti-Int₄			
Ti	-0.42358900	-0.37574900	4.38596800
Ti	-0.44491500	-0.56414800	1.42252400
O	0.95386800	1.02293500	3.91357800
O	-1.82390600	-1.80203500	4.11107500
O	1.00271300	-1.80625000	4.15738100
O	-1.85909600	1.00978200	3.99636100
O	-1.90843800	0.95215600	1.74086100
O	1.01132100	-1.98886600	1.90962200
O	-1.93134000	-2.04023400	1.86541000
O	1.05413100	0.96477900	1.65496600
C	1.41776600	1.38887800	2.77971700
C	-2.29203900	-2.31436600	3.03692300
C	1.42912300	-2.29289700	3.05568100
C	-2.30451100	1.37576900	2.85793300
H	2.21771800	2.14418600	2.81484800
H	-3.11563300	2.12399400	2.86659300
H	2.24053800	-3.03649400	3.11832900
H	-3.09319900	-3.05680700	3.17021400
C	1.55307000	1.08595400	-3.10759500
C	1.47053700	0.37529000	-4.45744100
H	2.48278400	0.72493600	-2.64095700
H	1.65218900	2.16692200	-3.26223200
H	1.05852400	-0.62059700	-4.32569200

C	2.77876600	0.36207000	-5.22245500
H	3.51739800	-0.21163800	-4.64222400
H	2.66593900	-0.11241500	-6.20189000
H	3.16954400	1.37580200	-5.37220000
N	0.44263100	0.83509300	-2.21340000
Br	0.03515600	1.29061400	-5.64565800
C	0.45124100	-0.39303900	-1.53015600
O	1.24941800	-1.26938700	-1.89845100
O	-0.42989700	-0.50813800	-0.57889700
C	-0.34531600	1.97016300	-1.75533700
H	-1.18587700	1.59843500	-1.16567600
H	0.24576100	2.65290800	-1.11746200
H	-0.72956400	2.53122300	-2.61875300
Ti-Ts₃			
Ti	0.50563861	1.30955089	14.37764581
Ti	0.47936479	1.14729964	11.60983884
O	1.92069323	2.69532893	13.94538709
O	-0.91584847	-0.11565457	14.13721367
O	1.93351106	-0.10425060	14.10940117
O	-0.92860208	2.68388042	13.97299925
O	-1.01479522	2.59317927	11.72921109
O	1.97718969	-0.27623613	11.86914527
O	-1.00266710	-0.28711481	11.89817217
O	1.96491266	2.60406923	11.70040432
C	2.36371332	3.06017049	12.81120074
C	-1.37999744	-0.60980289	13.06197842
C	2.37987121	-0.59554438	13.02535949
C	-1.39586767	3.04578494	12.84763107
H	3.14776071	3.82817044	12.80200642

H	-2.18559006	3.80797914	12.85375126
H	3.17058040	-1.35250921	13.10548758
H	-2.16315657	-1.37282217	13.15737247
C	0.30887835	1.56060331	5.45790662
C	-0.35404301	0.22235709	5.69293724
H	1.37710131	1.38654533	5.22915974
H	-0.11089430	2.15618209	4.64691681
H	-1.34224973	0.20045857	6.12046448
C	0.36570148	-1.06111023	5.38211987
H	1.04128727	-1.29377048	6.21289485
H	-0.34081064	-1.88321051	5.25111034
H	0.95159938	-0.96292828	4.46305839
N	0.14881723	2.29253800	6.70528602
Br	-1.64957592	0.31027858	3.46035625
C	0.27710503	1.49586352	7.84511730
O	0.14647972	0.24628383	7.47378101
O	0.44709791	2.06410579	8.96438513
C	0.51200849	3.69466323	6.72468220
H	0.34555067	4.07858245	7.73213298
H	1.57315848	3.85467392	6.46211081
H	-0.10787281	4.25298471	6.01171336

Ti-Int₅

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

O	1.02859200	-1.99188200	1.88601800
O	-1.92539300	-2.03228600	1.87717800
O	1.04552500	0.96316500	1.66327400
C	1.41883800	1.38958200	2.78510000
C	-2.29369100	-2.31333900	3.04565200
C	1.43519600	-2.29164200	3.03854400
C	-2.30786900	1.37674500	2.85000000
H	2.21771800	2.14418600	2.81484800
H	-3.11563300	2.12399400	2.86659300
H	2.24053800	-3.03649400	3.11832900
H	-3.09319900	-3.05680700	3.17021400
C	0.98611600	1.19766400	-3.38841400
C	1.07703300	-0.28893300	-3.76081800
H	1.96872600	1.63086000	-3.14601400
H	0.53541200	1.76636400	-4.20725400
H	0.30155100	-0.53380000	-4.49123300
C	2.42647700	-0.77397100	-4.23615200
H	3.21325300	-0.53603500	-3.50956300
H	2.41167700	-1.85709400	-4.40205000
H	2.63254400	-0.27415300	-5.18915900
N	0.15098500	1.14195800	-2.18459500
Br	0.72966700	1.41765500	-6.85672800
C	0.11370800	-0.10406700	-1.68438900
O	0.70604300	-0.98095000	-2.49838800
O	-0.41506900	-0.46162200	-0.61185500
C	-0.31917400	2.32269900	-1.48889900
H	-0.96212100	2.02177700	-0.65911800
H	0.52585600	2.90270300	-1.09193900
H	-0.88607800	2.95126800	-2.18472100

Nb-HKUST-1

O	1.46706200	-1.46676300	-1.07992900
O	-1.46692200	1.46756300	-1.07894400
O	1.46759500	1.46684900	-1.07895700
O	-1.46779300	-1.46605500	-1.07987400
O	-1.53915300	-1.53841400	1.15898900
O	1.53935300	1.53760200	1.15990400
O	-1.53860900	1.53831400	1.15991800
O	1.53847300	-1.53910400	1.15893200
C	1.93303900	-1.93296800	0.01829700
C	-1.93298700	1.93302600	0.01959800
C	1.93392700	1.93207800	0.01957000
C	-1.93391900	-1.93209500	0.01836200
H	2.70650100	-2.70624400	-0.04502000
H	-2.70776700	-2.70498400	-0.04494800
H	2.70780300	2.70493900	-0.04339700
H	-2.70650700	2.70624200	-0.04334200
Nb	0.00001400	-0.00053200	1.23077900
Nb	-0.00002400	0.00052800	-1.29396900

Nb-Int₀

O	1.49982900	1.49968000	1.11671300
O	-1.49966700	-1.49967800	1.11688400
O	1.49981600	-1.49969400	1.11673100
O	-1.49965200	1.49969400	1.11686600
O	-1.50340300	1.50328400	-1.12222000
O	1.50325500	-1.50329100	-1.12235500
O	-1.50341400	-1.50329400	-1.12220200
O	1.50327300	1.50325400	-1.12237300
C	1.93336800	1.93343200	-0.00161800

C	-1.93350100	-1.93330700	-0.00137300
C	1.93344200	-1.93336800	-0.00159100
C	-1.93340600	1.93339200	-0.00139900
H	2.70701100	2.70666800	0.00133100
H	-2.70692000	2.70675700	0.00166200
H	2.70693000	-2.70675900	0.00135900
H	-2.70686500	-2.70682200	0.00169000
Nb	-0.00008200	-0.00001600	-1.25980800
Nb	0.00008600	0.00000700	1.26482100
C	-0.18675731	-1.14403823	-3.94865064
C	-1.20651823	-0.06468662	-4.11990677
H	-0.39892284	-2.00542892	-3.31715302
H	0.48699325	-1.34442271	-4.78418750
H	-1.17063497	0.45517485	-5.08216912
C	-2.57316325	-0.11836989	-3.47595317
H	-2.95233391	0.89178948	-3.27520131
H	-3.29211739	-0.62791306	-4.13027552
H	-2.52780331	-0.65700157	-2.52351568
N	-0.04847615	0.13573408	-3.25098959
C	0.99705391	1.02947518	-3.73512433
H	0.74495820	2.06045224	-3.46193211
H	1.94620692	0.76794280	-3.25362924
H	1.13966724	0.98434039	-4.83093223
Nb-Int₁			
O	1.52106800	1.61845800	-0.59783400
O	-1.59533300	-1.44743200	-0.61317900
O	1.52829800	-1.45698600	-0.60553600
O	-1.56850100	1.63053500	-0.59347800
O	-1.56459300	1.61249000	-2.86013500

O	1.50338300	-1.46285200	-2.87171900
O	-1.57180400	-1.45752800	-2.87782500
O	1.50808800	1.60890300	-2.86366000
C	1.91748400	2.01849800	-1.73216300
C	-1.98441100	-1.85830400	-1.74594900
C	1.91841700	-1.86342800	-1.73874300
C	-1.97121800	2.02409900	-1.72794800
H	2.67694900	2.78409600	-1.74341200
H	-2.73698200	2.78418500	-1.74308100
H	2.67686800	-2.62933100	-1.74338400
H	-2.73692700	-2.62939400	-1.74305300
Nb	-0.03032900	0.07450400	-2.82661800
Nb	-0.02741200	0.07399300	-0.57109400
C	-1.38680800	-0.50074600	2.45098800
C	-0.15829900	-1.30941900	2.63504100
H	-2.15759500	-0.83543300	1.75700900
H	-1.71201700	0.09556500	3.29990200
H	0.30203800	-1.16212400	3.61373600
C	0.05514800	-2.66939200	2.01618500
H	1.11887700	-2.84959600	1.82682700
H	-0.29998100	-3.42945000	2.72572300
H	-0.49068800	-2.78888000	1.07666500
N	-0.12105400	-0.07056200	1.79521200
Br	-0.19097400	-0.09324300	6.04304800
C	0.55180600	1.08267100	2.43409700
H	1.61487400	1.05376200	2.17919600
H	0.12030600	2.00761900	2.03762500
H	0.43173100	1.05265800	3.52501200

Nb-Ts₁

O	1.49982900	1.49968000	1.11671300
O	-1.49966700	-1.49967800	1.11688400
O	1.49981600	-1.49969400	1.11673100
O	-1.49965200	1.49969400	1.11686600
O	-1.50340300	1.50328400	-1.12222000
O	1.50325500	-1.50329100	-1.12235500
O	-1.50341400	-1.50329400	-1.12220200
O	1.50327300	1.50325400	-1.12237300
C	1.93336800	1.93343200	-0.00161800
C	-1.93350100	-1.93330700	-0.00137300
C	1.93344200	-1.93336800	-0.00159100
C	-1.93340600	1.93339200	-0.00139900
H	2.70701100	2.70666800	0.00133100
H	-2.70692000	2.70675700	0.00166200
H	2.70693000	-2.70675900	0.00135900
H	-2.70686500	-2.70682200	0.00169000
Nb	-0.00008200	-0.00001600	-1.25980800
Nb	0.00008600	0.00000700	1.26482100
C	-1.71221650	0.00287242	3.91970590
C	-0.72667213	-0.76202777	4.71419239
H	-2.32640622	-0.60818146	3.25680127
H	-2.30496262	0.74536929	4.45955476
H	-0.19631001	-0.22905949	5.49106807
C	-0.20235385	-2.10512969	4.28441866
H	0.71924785	-1.99605341	3.70024202
H	0.01540742	-2.70912639	5.16847768
H	-0.93731422	-2.63508422	3.67168453
N	-0.49856629	0.49286819	3.29057315
Br	-2.27164265	-1.52441794	6.74903905

C	-0.11546028	1.83933635	3.70387368
H	0.92777278	2.02935350	3.43820483
H	-0.74887022	2.57127716	3.18218471
H	-0.24466728	1.97896872	4.78774051
Nb-Int₂			
O	1.53759600	1.55265100	-0.64882400
O	-1.53567900	-1.47010500	-0.61217300
O	1.44607200	-1.49690700	-0.60914100
O	-1.63228400	1.51994000	-0.63664200
O	-1.55482100	1.63469800	-2.89932800
O	1.50198200	-1.43364200	-2.87210900
O	-1.56038200	-1.42774600	-2.87573400
O	1.50733300	1.63333500	-2.91347300
C	1.92056200	1.99881600	-1.76591200
C	-1.96355600	-1.86254800	-1.74840800
C	1.89113100	-1.87341700	-1.74272600
C	-1.99085800	1.98802100	-1.75620400
H	2.67694900	2.78409600	-1.74341200
H	-2.73698200	2.78418500	-1.74308100
H	2.67686800	-2.62933100	-1.74338400
H	-2.73692700	-2.62939400	-1.74305300
Nb	-0.02404100	0.10616200	-2.98415800
Nb	-0.04584800	0.01861800	-0.33577500
C	-0.42463700	0.02014900	2.66497100
C	0.72477900	-0.39838600	3.59450600
H	-0.89405700	-0.89186500	2.26440400
H	-1.19974000	0.55006400	3.24378300
H	1.29031800	0.47090100	3.92917600
C	1.62455200	-1.49172200	3.05656900

H	2.04805400	-1.15654900	2.10207300
H	2.44326400	-1.71625800	3.74788700
H	1.05869500	-2.41111500	2.86944800
N	0.09085600	0.84669600	1.58679600
Br	-0.08001600	-1.06635200	5.42307000
C	0.21494800	2.24507200	1.95685300
H	0.71376800	2.78831800	1.15149100
H	-0.77699900	2.70522000	2.12836400
H	0.80665900	2.39513200	2.87813000
Nb-Int₃			
O	1.75329500	1.54167500	-0.69263600
O	-1.36312200	-1.44361400	-0.67294600
O	1.61048000	-1.49255100	-0.67016200
O	-1.44407700	1.54271500	-0.70202800
O	-1.37532100	1.65459000	-2.96342800
O	1.68600300	-1.41150900	-2.93106200
O	-1.37899900	-1.40879300	-2.93622100
O	1.68001400	1.65378800	-2.95538000
C	2.11240300	2.00822200	-1.81337200
C	-1.78545700	-1.84122200	-1.80913600
C	2.06741700	-1.85882400	-1.80122700
C	-1.80863400	2.00895400	-1.81995100
H	2.85820300	2.80353500	-1.80086000
H	-2.55572800	2.80362400	-1.80052900
H	2.85812200	-2.60989200	-1.80083200
H	-2.55567300	-2.60995500	-1.80050100
Nb	0.15608000	0.12397200	-3.04068500
Nb	0.13435000	0.03341200	-0.39941300
C	-0.58946400	0.11020100	2.48570900

C	0.29093900	-0.32886600	3.66298900
H	-0.99850100	-0.79670600	2.01329500
H	-1.45178200	0.68756200	2.86032400
H	0.76415200	0.52944800	4.14120300
C	1.28471000	-1.42849400	3.34722000
H	1.93654500	-1.08408800	2.53420300
H	1.90276600	-1.67783500	4.21544800
H	0.77189900	-2.33505700	3.00754600
N	0.18856300	0.88148000	1.52761000
Br	-0.95794800	-1.00502500	5.21165300
C	3.95957300	1.47579400	1.32047000
O	3.86306600	2.63255900	1.47950600
O	4.12032600	0.32365600	1.19879800
C	0.26276100	2.29108000	1.87399000
H	0.69020400	2.46299200	2.87828100
H	0.89705100	2.80944800	1.15138900
H	-0.73790400	2.76326900	1.85842400
Nb-Ts₂			
O	1.49982900	1.49968000	1.11671300
O	-1.49966700	-1.49967800	1.11688400
O	1.49981600	-1.49969400	1.11673100
O	-1.49965200	1.49969400	1.11686600
O	-1.50340300	1.50328400	-1.12222000
O	1.50325500	-1.50329100	-1.12235500
O	-1.50341400	-1.50329400	-1.12220200
O	1.50327300	1.50325400	-1.12237300
C	1.93336800	1.93343200	-0.00161800
C	-1.93350100	-1.93330700	-0.00137300
C	1.93344200	-1.93336800	-0.00159100

C	-1.93340600	1.93339200	-0.00139900
H	2.70701100	2.70666800	0.00133100
H	-2.70692000	2.70675700	0.00166200
H	2.70693000	-2.70675900	0.00135900
H	-2.70686500	-2.70682200	0.00169000
Nb	-0.00008200	-0.00001600	-1.25980800
Nb	0.00008600	0.00000700	1.26482100
C	-1.32864452	-0.35460697	4.34138217
C	-0.86424056	-1.74512080	4.78479661
H	-2.22444550	-0.45797087	3.71050000
H	-1.62171788	0.21779206	5.23268352
H	-0.06858770	-1.67897987	5.52533315
C	-0.51474223	-2.71478110	3.67683144
H	0.36768557	-2.33236361	3.14878909
H	-0.26066515	-3.70012544	4.08020055
H	-1.33200650	-2.81390180	2.95695842
N	-0.27180775	0.36295050	3.61889278
Br	-2.41190948	-2.54898944	5.91530392
C	1.54082881	0.55580775	4.66081284
O	1.60436184	1.25349974	5.62883027
O	1.93576500	-0.32440250	3.95776574
C	-0.63559846	1.78719657	3.62780699
H	-0.76057918	2.11707479	4.63798528
H	0.14037002	2.35645118	3.16012964
H	-1.55138620	1.92475940	3.09179460
Nb-Int₄			
O	0.91778400	1.40580500	-1.20143300
O	-2.17946000	-1.69729600	-1.19294400
O	0.88408700	-1.74271100	-1.20917500

O	-2.17248800	1.39900900	-1.19263500
O	-2.15514200	1.38988200	-3.46188000
O	0.91341200	-1.69154500	-3.47630600
O	-2.16294600	-1.68610300	-3.46249100
O	0.91655000	1.38505300	-3.46997400
C	1.31831700	1.79533900	-2.33276500
C	-2.57006100	-2.09277100	-2.32734600
C	1.30468900	-2.11269000	-2.33862500
C	-2.56486300	1.79370100	-2.32613500
H	2.08339800	2.55481500	-2.34172800
H	-3.33053300	2.55490400	-2.34139700
H	2.08331700	-2.85861200	-2.34170000
H	-3.33047800	-2.85867500	-2.34136900
Nb	-0.61787700	-0.15045800	-3.41339400
Nb	-0.60982800	-0.15546900	-1.15357200
C	0.68901300	-0.83811400	4.23411500
C	1.82892700	0.10047400	4.62749900
H	1.17117600	-1.73726500	3.82709900
H	0.13025600	-1.13626800	5.12841600
H	2.13315200	0.69552800	3.77076700
C	3.00129400	-0.60152500	5.28905400
H	3.44256000	-1.28681900	4.55657800
H	3.76929500	0.11077900	5.60653300
H	2.68209500	-1.18225700	6.16310200
N	-0.23181600	-0.30138400	3.25324100
Br	1.12287000	1.54984200	5.94276700
C	0.21176800	-0.32048300	1.91233800
O	1.41858300	-0.52571800	1.70081000
O	-0.71695700	-0.10485900	1.03303200

C	-1.64437300	-0.24492000	3.59019200
H	-2.17876100	0.21874300	2.75926900
H	-2.07493800	-1.24966300	3.75970700
H	-1.79070000	0.35560500	4.49876100
Nb-Ts₃			
O	1.49982900	1.49968000	1.11671300
O	-1.49966700	-1.49967800	1.11688400
O	1.49981600	-1.49969400	1.11673100
O	-1.49965200	1.49969400	1.11686600
O	-1.50340300	1.50328400	-1.12222000
O	1.50325500	-1.50329100	-1.12235500
O	-1.50341400	-1.50329400	-1.12220200
O	1.50327300	1.50325400	-1.12237300
C	1.93336800	1.93343200	-0.00161800
C	-1.93350100	-1.93330700	-0.00137300
C	1.93344200	-1.93336800	-0.00159100
C	-1.93340600	1.93339200	-0.00139900
H	2.70701100	2.70666800	0.00133100
H	-2.70692000	2.70675700	0.00166200
H	2.70693000	-2.70675900	0.00135900
H	-2.70686500	-2.70682200	0.00169000
Nb	-0.00008200	-0.00001600	-1.25980800
Nb	0.00008600	0.00000700	1.26482100
C	-1.10408246	-0.51177732	6.89182296
C	-0.49405142	-1.87350394	6.65064524
H	-2.20361885	-0.59772840	6.80639305
H	-0.87972654	-0.09478550	7.87383061
H	0.57042399	-1.94016010	6.50019510
C	-1.35379644	-3.10172605	6.52840059

H	-1.77698470	-3.13455841	5.51823196
H	-0.76835803	-4.00657223	6.70339592
H	-2.17045674	-3.07591156	7.25623214
N	-0.56451642	0.37750210	5.87358270
Br	0.12207805	-2.27068446	9.12509187
C	-0.43429891	-0.22035237	4.61754796
O	-0.48278214	-1.50997646	4.74402473
O	-0.26644059	0.52526455	3.60736678
C	-0.83083946	1.79573731	6.00275585
H	-0.37516953	2.30993236	5.15544422
H	-1.91293582	2.01848087	6.00391754
H	-0.39927491	2.17456946	6.93788771
Nb-Int₅			
O	0.91410100	1.39682100	-1.20482900
O	-2.16742700	-1.69762200	-1.20245500
O	0.91344200	-1.70231800	-1.20400500
O	-2.16860700	1.39195200	-1.20240200
O	-2.16041800	1.38306100	-3.46802300
O	0.91045600	-1.68917500	-3.46904000
O	-2.15971800	-1.68807300	-3.46838800
O	0.91090300	1.38433100	-3.46940200
C	1.31829200	1.79481300	-2.33554400
C	-2.56694800	-2.09608500	-2.33432800
C	1.31742800	-2.09911500	-2.33522400
C	-2.56795300	1.79155400	-2.33406800
H	2.08339800	2.55481500	-2.34172800
H	-3.33053300	2.55490400	-2.34139700
H	2.08331700	-2.85861200	-2.34170000
H	-3.33047800	-2.85867500	-2.34136900

Nb	-0.62240800	-0.15140800	-3.42712100
Nb	-0.61754300	-0.15032200	-1.18089200
C	0.60125100	-0.43297700	4.29868000
C	1.80204500	-0.06589400	3.41636700
H	0.62874600	-1.48441400	4.62613900
H	0.56336600	0.21419800	5.18004500
H	2.05552000	0.98774600	3.55840300
C	3.02770000	-0.93621600	3.56689200
H	2.78385700	-1.99374600	3.40580600
H	3.80276100	-0.63899700	2.85176400
H	3.40763300	-0.79150000	4.58461400
N	-0.51012900	-0.22546600	3.36636100
Br	2.48225400	1.23962700	6.69291000
C	-0.07051900	-0.19751300	2.09351000
O	1.26232100	-0.18807400	2.03593400
O	-0.79990700	-0.18166000	1.08137600
C	-1.90109900	-0.36445200	3.73888000
H	-2.52095400	-0.17832600	2.85952100
H	-2.10516000	-1.37748500	4.11526900
H	-2.14854900	0.35718100	4.52505300

W-HKUST-1

W	-0.003164	0.001110	1.271896
W	0.001913	-0.001299	-1.269200
O	-1.046597	1.675489	1.148105
O	1.039738	-1.674051	1.154540
O	1.675432	1.047696	1.121798
O	-1.681887	-1.044762	1.116716
O	-1.679603	-1.033184	-1.155560
O	1.685622	1.028034	-1.150456

O	1.038409	-1.685585	-1.117715
O	-1.028820	1.686635	-1.124055
C	-1.330388	2.152200	0.011713
C	1.332621	-2.150381	0.020279
C	2.151721	1.330324	-0.014582
C	-2.151795	-1.331774	-0.021063
H	-1.910248	3.087124	0.012365
H	-3.086253	-1.912413	-0.025184
H	3.086663	1.910235	-0.015538
H	1.914795	-3.083882	0.025107

W-Int₁

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

C	3.00147700	-0.14596300	1.27764000
C	3.32717700	-0.75183400	-0.02386200
H	2.31565700	-0.65619800	1.94767800
H	3.76176100	0.46419700	1.75807800
H	4.31292900	-0.49415400	-0.40542100
C	2.84415500	-2.11956000	-0.42899400
H	2.70838500	-2.19120300	-1.51545500
H	3.61869800	-2.82735800	-0.11251500
H	1.89798500	-2.37853300	0.05553100
N	2.37067000	0.40791300	0.04323300
Br	6.21266500	-2.08929500	1.37367500
C	2.93024500	1.69194200	-0.40405100
H	2.76310500	1.80733300	-1.48035900
H	2.42386100	2.51125400	0.11893000
H	4.00927400	1.75599300	-0.20300900
W-Ts₁			
W	1.09601200	0.00178600	0.00084200
W	-1.09601800	-0.00170900	-0.00080900
O	1.12218400	1.46088200	-1.49881800
O	1.12460000	-1.45742200	1.50036600
O	1.12701300	-1.49789800	-1.45826800
O	1.11995800	1.50145500	1.46005800
O	-1.12690600	1.49786200	1.45820600
O	-1.11986200	-1.50151000	-1.45988900
O	-1.12227100	-1.46098600	1.49879800
O	-1.12468300	1.45727400	-1.50060400
C	-0.00160400	1.88371200	-1.93672200
C	0.00150800	-1.88398700	1.93643500
C	0.00461000	-1.93667900	-1.88371900

C	-0.00448500	1.93659500	1.88385200
H	-0.00218800	2.64495800	-2.72024700
H	-0.00638500	2.71998600	2.64523300
H	0.00640400	-2.72018100	-2.64499300
H	0.00217700	-2.64552500	2.71967900
C	3.89391770	-0.38790678	1.36380058
C	4.36606896	-1.44258847	0.44101231
H	3.17577900	-0.73176182	2.10982938
H	4.65677752	0.26353897	1.79717829
H	5.17724046	-1.18941365	-0.22686214
C	3.58638308	-2.70386285	0.18418801
H	2.79569596	-2.53417432	-0.55633068
H	4.25765292	-3.47929016	-0.19263407
H	3.12232807	-3.06660498	1.10594202
N	3.27001869	0.08644740	0.14104026
Br	6.34736255	-2.49962267	1.88381324
C	3.94942776	1.22430042	-0.47135379
H	3.62677026	1.33732805	-1.50971546
H	3.68797522	2.13953990	0.07884361
H	5.04264867	1.10221022	-0.44298906
W-Int₂			
W	-0.04563300	0.34255300	-0.18499400
W	-2.30744500	0.34041300	-0.18795300
O	-0.07914000	1.82285400	-1.70468900
O	-0.07897200	-1.13846200	1.32805500
O	-0.08245600	-1.17683300	-1.66482600
O	-0.09112000	1.86740700	1.29288100
O	-2.35207200	1.84451900	1.27630000
O	-2.34340200	-1.16120100	-1.65238100

O	-2.33774000	-1.12039200	1.30929600
O	-2.33878300	1.80045800	-1.68511000
C	-1.21194800	2.22645600	-2.12188300
C	-1.21039600	-1.54454700	1.74614400
C	-1.21312600	-1.59440200	-2.07110600
C	-1.22252400	2.28005400	1.69583100
H	-1.23073000	2.98714700	-2.90715300
H	-1.23492700	3.06217500	2.45832700
H	-1.22213800	-2.37799200	-2.83189900
H	-1.22636500	-2.30333600	2.53277300
C	2.98539400	-0.45480100	0.74817100
C	3.78934300	-1.41659300	-0.13311900
H	2.35662000	-1.04556900	1.42657000
H	3.68101900	0.13581600	1.37417100
H	4.36653000	-0.88156000	-0.88645700
C	3.01480500	-2.58001600	-0.71465600
H	2.18400500	-2.17589900	-1.30472400
H	3.64386000	-3.20426400	-1.35850900
H	2.59555400	-3.20544400	0.08211700
N	2.17767300	0.38407200	-0.10778100
Br	5.40249400	-2.26130000	1.01371500
C	2.91342200	1.54682900	-0.56761400
H	2.27733800	2.16682100	-1.20838900
H	3.26400000	2.18260400	0.27571400
H	3.81830300	1.30055300	-1.16076300
W-Int₃			
W	2.41982500	0.05708700	-0.36823600
W	0.15989000	0.05139600	-0.36442300
O	2.44436400	1.51543600	-1.87044700

O	2.45359300	-1.40406800	1.13071100
O	2.46032100	-1.44337400	-1.83621600
O	2.45135500	1.55704200	1.09523800
O	0.19186600	1.55570500	1.12294900
O	0.20018100	-1.45788800	-1.85889600
O	0.19464500	-1.42523500	1.14831900
O	0.18378600	1.54213300	-1.87918500
C	1.31746700	1.94137300	-2.30296700
C	1.32652500	-1.82860100	1.56725200
C	1.33103400	-1.87547000	-2.25944600
C	1.32122500	1.98419200	1.52207400
H	1.33507400	2.70002200	-3.08996200
H	1.33087700	2.77505000	2.27551800
H	1.34366600	-2.66511700	-3.01470800
H	1.33943900	-2.59046100	2.34996400
C	-2.86234600	-0.69501000	0.58336600
C	-3.79345400	0.33622600	1.22744100
H	-2.22399600	-1.12625300	1.36604300
H	-3.46587000	-1.52162200	0.16307500
H	-4.38003100	0.86772500	0.47890300
C	-3.14715600	1.26646600	2.23299500
H	-2.30828700	1.77516600	1.74448800
H	-3.85463400	2.01427900	2.60939500
H	-2.74641700	0.70216800	3.08329200
N	-2.06648500	-0.03247600	-0.42701300
Br	-5.37600600	-0.68192000	2.26506400
C	-1.95392900	3.83994700	-1.08868400
O	-2.74723800	3.50782300	-1.88156700
O	-1.18182600	4.23046200	-0.30165500

C	-2.74825400	-0.00595200	-1.70941600
H	-3.71918900	0.52749000	-1.68673300
H	-2.12913500	0.50407300	-2.45677500
H	-2.96158000	-1.02828300	-2.09202600
W-Ts₂			
W	1.09601200	0.00178600	0.00084200
W	-1.09601800	-0.00170900	-0.00080900
O	1.12218400	1.46088200	-1.49881800
O	1.12460000	-1.45742200	1.50036600
O	1.12701300	-1.49789800	-1.45826800
O	1.11995800	1.50145500	1.46005800
O	-1.12690600	1.49786200	1.45820600
O	-1.11986200	-1.50151000	-1.45988900
O	-1.12227100	-1.46098600	1.49879800
O	-1.12468300	1.45727400	-1.50060400
C	-0.00160400	1.88371200	-1.93672200
C	0.00150800	-1.88398700	1.93643500
C	0.00461000	-1.93667900	-1.88371900
C	-0.00448500	1.93659500	1.88385200
H	-0.00218800	2.64495800	-2.72024700
H	-0.00638500	2.71998600	2.64523300
H	0.00640400	-2.72018100	-2.64499300
H	0.00217700	-2.64552500	2.71967900
C	-3.97826841	-1.16794857	0.62276232
C	-4.35523510	-0.51954058	1.95815713
H	-3.35804926	-2.05632542	0.81581815
H	-4.89746728	-1.51298863	0.12882756
H	-5.08503705	0.27665735	1.81926707
C	-3.20196097	-0.07218401	2.82982673

H	-2.67639634	0.74238605	2.31600952
H	-3.55935699	0.31482181	3.78933693
H	-2.49175977	-0.88513530	3.00500499
N	-3.26976618	-0.22762106	-0.25336118
Br	-5.47558290	-1.92674222	2.99937516
C	-4.27325516	1.57337401	-0.56260504
O	-4.82620668	1.35422582	-1.59898672
O	-4.01918392	2.25728829	0.38223831
C	-3.34447454	-0.77095036	-1.61722039
H	-4.36952138	-0.91565967	-1.88784593
H	-2.88878837	-0.08462965	-2.30001905
H	-2.82949337	-1.70804620	-1.65653680

W-Int₄

W	-0.65120500	0.43649900	0.10216400
W	-2.88870800	0.44056700	0.09775600
O	-0.66633600	1.91818100	-1.41549700
O	-0.67670600	-1.01743800	1.62285400
O	-0.66973100	-1.06615000	-1.37591400
O	-0.67004600	1.95739000	1.57702700
O	-2.92855300	1.94325400	1.55990900
O	-2.92688700	-1.05868100	-1.36535500
O	-2.93302300	-1.02065600	1.59816000
O	-2.92463700	1.90307700	-1.40367600
C	-1.79414900	2.32644200	-1.83687100
C	-1.80010100	-1.43518000	2.03805400
C	-1.79393500	-1.49001500	-1.78608600
C	-1.79903600	2.37822400	1.98330800
H	-1.80891900	3.08953300	-2.62144200
H	-1.81311600	3.16456100	2.74403800

H	-1.80032700	-2.27560600	-2.54618800
H	-1.80455400	-2.20095000	2.81848400
C	4.87953600	-0.65576300	0.88852000
C	5.35064200	-1.78755700	-0.02163700
H	4.49580600	-1.15125900	1.79447900
H	5.73343000	-0.03507600	1.18188000
H	4.51914000	-2.16102900	-0.61450400
C	6.08311600	-2.89830900	0.70706000
H	5.37881700	-3.37602400	1.40125600
H	6.45738100	-3.65841900	0.01141100
H	6.93378600	-2.50887700	1.28294500
N	3.84659800	0.18727300	0.32532000
Br	6.62573200	-1.02988700	-1.48229700
C	2.53065700	-0.34149600	0.33156400
O	2.40505000	-1.55813200	0.56692600
O	1.59910900	0.51295200	0.07347600
C	4.08841100	1.61738100	0.24775100
H	3.23028300	2.08364400	-0.23699600
H	4.21123800	2.07755700	1.24562600
H	4.99260800	1.81818300	-0.34129900
W-Ts₃			
W	1.09601200	0.00178600	0.00084200
W	-1.09601800	-0.00170900	-0.00080900
O	1.12218400	1.46088200	-1.49881800
O	1.12460000	-1.45742200	1.50036600
O	1.12701300	-1.49789800	-1.45826800
O	1.11995800	1.50145500	1.46005800
O	-1.12690600	1.49786200	1.45820600
O	-1.11986200	-1.50151000	-1.45988900

O	-1.12227100	-1.46098600	1.49879800
O	-1.12468300	1.45727400	-1.50060400
C	-0.00160400	1.88371200	-1.93672200
C	0.00150800	-1.88398700	1.93643500
C	0.00461000	-1.93667900	-1.88371900
C	-0.00448500	1.93659500	1.88385200
H	-0.00218800	2.64495800	-2.72024700
H	-0.00638500	2.71998600	2.64523300
H	0.00640400	-2.72018100	-2.64499300
H	0.00217700	-2.64552500	2.71967900
C	6.61511915	-0.93449286	-1.05746696
C	6.12988830	-2.10024224	-1.89733047
H	6.92041448	-1.31452748	-0.06444629
H	7.48869923	-0.47318055	-1.51863551
H	5.59595609	-1.87798120	-2.80580613
C	6.21087972	-3.51472460	-1.39274354
H	5.43419444	-3.66073856	-0.63368234
H	6.05955101	-4.22841889	-2.20509312
H	7.18952211	-3.70936762	-0.94334037
N	5.56633964	0.06722782	-0.93948165
Br	8.15128411	-2.30491518	-3.49189043
C	4.29370209	-0.47200020	-0.73950631
O	4.20482053	-1.71014589	-1.01176774
O	3.36864714	0.29382330	-0.33658563
C	5.92205811	1.36798251	-0.41057629
H	5.02161143	1.98289463	-0.37684025
H	6.33815798	1.30371886	0.61085287
H	6.66871403	1.84515251	-1.05796642

W-Int₅

W	-0.67447000	0.44302700	0.09866800
W	-2.89455000	0.44146700	0.09759600
O	-0.67550100	1.91595600	-1.40869200
O	-0.67442500	-1.02098900	1.60925600
O	-0.67340900	-1.05854600	-1.37124100
O	-0.67719800	1.95452100	1.57004900
O	-2.93175000	1.94244600	1.55986300
O	-2.92634600	-1.05701200	-1.36306200
O	-2.92798400	-1.01879200	1.59777600
O	-2.92966800	1.90382500	-1.40221200
C	-1.80156300	2.32827600	-1.83652900
C	-1.79895000	-1.43894900	2.03471700
C	-1.79646700	-1.48981700	-1.78638900
C	-1.80428100	2.37921100	1.98308000
H	-1.80891900	3.08953300	-2.62144200
H	-1.81311600	3.16456100	2.74403800
H	-1.80032700	-2.27560600	-2.54618800
H	-1.80455400	-2.20095000	2.81848400
C	4.95597700	-0.79152400	0.16083100
C	4.06647100	-1.99012500	-0.19597200
H	5.33103900	-0.84362900	1.19533000
H	5.80726300	-0.72986700	-0.52361300
H	4.15724000	-2.20993800	-1.26315400
C	4.27887600	-3.24081700	0.62513100
H	4.17586000	-3.03128600	1.69774000
H	3.55628200	-4.01529800	0.34474400
H	5.29038900	-3.60355600	0.41190200
N	4.00612000	0.31434600	0.02293300
Br	7.31484300	-2.62973700	-1.64045500

C	2.73176600	-0.13384900	0.05405300
O	2.69231600	-1.47230600	0.01404200
O	1.71345300	0.57592000	0.11207700
C	4.37254100	1.70261500	0.19223400
H	3.48214600	2.31949800	0.05482900
H	4.78259100	1.88167700	1.19758500
H	5.13126500	1.97994200	-0.54825700

Sc-HKUST-1

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

Sc-Int₀

Sc	-0.00000500	0.00021800	1.44377700
Sc	-0.00000500	-0.00017300	-1.44390400

O	-1.49911500	-1.49387200	1.12624000
O	1.49892700	1.49449900	1.12589000
O	-1.49413400	1.49931000	1.12595100
O	1.49422800	-1.49875700	1.12635600
O	1.49367300	-1.49966100	-1.12579200
O	-1.49386100	1.49907900	-1.12620200
O	1.49955800	1.49339700	-1.12626100
O	-1.49922600	-1.49410900	-1.12591000
C	-1.90820300	-1.90109100	0.00022300
C	1.90813300	1.90119000	-0.00025800
C	-1.90125400	1.90806900	-0.00020800
C	1.90122400	-1.90806900	0.00032900
H	-2.68735300	-2.67771600	0.00034300
H	2.67745500	-2.68761300	0.00046300
H	-2.67760600	2.68749200	-0.00038800
H	2.68790900	2.67718700	-0.00043200
C	-1.12323911	0.19212315	-4.35364342
C	0.09476997	1.01303475	-4.63076959
H	-1.94460731	0.60668923	-3.77116027
H	-1.41986310	-0.54627983	-5.10130033
H	0.60465072	0.77902774	-5.57031988
C	0.24239592	2.44379974	-4.16558698
H	1.29719508	2.69390487	-3.99429829
H	-0.15497638	3.13993135	-4.91536233
H	-0.29801159	2.59959291	-3.22590247
N	0.12147414	-0.04129886	-3.61888298
C	0.85188979	-1.25930141	-3.94942114
H	1.90848047	-1.12764519	-3.68983936
H	0.45285982	-2.09074052	-3.35729596

H	0.78735136	-1.53256707	-5.01915537
Sc-Int₁			
Sc	0.06546300	0.27526300	-0.65854200
Sc	0.00211400	0.27348700	-3.63836500
O	-1.49648200	-1.20673600	-1.04602300
O	1.60695500	1.70135300	-1.04133100
O	-1.38061000	1.87017400	-1.05008100
O	1.50830300	-1.24599200	-1.04825300
O	1.57777700	-1.18813400	-3.30486800
O	-1.53577200	1.73070800	-3.30286600
O	1.48349000	1.82050000	-3.29416000
O	-1.43743500	-1.28793500	-3.30562200
C	-1.87191300	-1.63913700	-2.17236400
C	1.94164600	2.16522700	-2.17161500
C	-1.86235400	2.19266500	-2.17138100
C	1.93756100	-1.62439500	-2.17816500
H	-2.66235400	-2.40572700	-2.16696500
H	2.70245400	-2.41562400	-2.16684500
H	-2.65260700	2.95948100	-2.16769600
H	2.71290800	2.94917600	-2.16774000
C	-1.87093600	-0.16989800	2.09220600
C	-0.57799100	-0.73617600	2.54181900
H	-2.45825900	-0.67780300	1.33136300
H	-2.43083800	0.43262200	2.80495400
H	-0.28997200	-0.47389700	3.56561800
C	-0.04909800	-2.06183200	2.05111500
H	1.04709400	-2.05458300	2.00652700
H	-0.34235800	-2.83786500	2.76662000
H	-0.43898700	-2.33577700	1.06443700

N	-0.60434900	0.42415500	1.59227400
Br	-0.24090600	-0.09029000	6.04521500
C	-0.24347400	1.72589500	2.19636000
H	0.83114300	1.89744400	2.06295100
H	-0.79770000	2.52068600	1.68472500
H	-0.45935800	1.74272300	3.27163700
Sc-Ts₁			
Sc	-0.00000500	0.00021800	1.44377700
Sc	-0.00000500	-0.00017300	-1.44390400
O	-1.49911500	-1.49387200	1.12624000
O	1.49892700	1.49449900	1.12589000
O	-1.49413400	1.49931000	1.12595100
O	1.49422800	-1.49875700	1.12635600
O	1.49367300	-1.49966100	-1.12579200
O	-1.49386100	1.49907900	-1.12620200
O	1.49955800	1.49339700	-1.12626100
O	-1.49922600	-1.49410900	-1.12591000
C	-1.90820300	-1.90109100	0.00022300
C	1.90813300	1.90119000	-0.00025800
C	-1.90125400	1.90806900	-0.00020800
C	1.90122400	-1.90806900	0.00032900
H	-2.68735300	-2.67771600	0.00034300
H	2.67745500	-2.68761300	0.00046300
H	-2.67760600	2.68749200	-0.00038800
H	2.68790900	2.67718700	-0.00043200
C	-0.88455211	-0.16376472	4.45573466
C	0.32114590	-0.80109841	5.02750081
H	-1.53965393	-0.84691036	3.91289757
H	-1.44377468	0.50751455	5.11209369

H	0.93173303	-0.20217811	5.68828127
C	0.88213754	-2.09418778	4.50034798
H	1.50286636	-1.92150331	3.61309150
H	1.49639068	-2.56786323	5.26989996
H	0.07715600	-2.78304563	4.22824699
N	0.12102381	0.45956318	3.61330717
Br	-0.66078813	-1.71729395	7.33421089
C	0.42240476	1.84274999	3.97009340
H	1.36870329	2.14797841	3.51574465
H	-0.37611710	2.49574554	3.58970206
H	0.48625279	1.97141530	5.06106141
Sc-Int₂			
Sc	-0.00033900	0.25365600	-0.60166100
Sc	0.03971300	0.28931300	-3.68638300
O	-1.45888900	-1.28078800	-1.00916400
O	1.48550000	1.81577800	-1.05093800
O	-1.57759100	1.69143100	-1.04204600
O	1.51717900	-1.26270400	-1.02893200
O	1.49056900	-1.27151800	-3.29410900
O	-1.41752100	1.84116900	-3.29671100
O	1.58904300	1.74116800	-3.31384200
O	-1.51726000	-1.17458200	-3.26886700
C	-1.88387700	-1.62516600	-2.15194500
C	1.93101700	2.17158800	-2.17729500
C	-1.88532400	2.16762500	-2.17026900
C	1.90610800	-1.65315600	-2.16573400
H	-2.66235400	-2.40572700	-2.16696500
H	2.70245400	-2.41562400	-2.16684500
H	-2.65260700	2.95948100	-2.16769600

H	2.71290800	2.94917600	-2.16774000
C	-0.56259600	-0.25590300	2.37014500
C	0.27654000	-1.32866900	3.08528400
H	-1.37181800	-0.76740800	1.82555100
H	-1.04574700	0.38960700	3.12563500
H	1.12885400	-0.88266500	3.59663300
C	0.68111700	-2.51279600	2.23149400
H	1.26656900	-2.14535200	1.37976200
H	1.28914300	-3.22760700	2.79563700
H	-0.20049800	-3.03265400	1.83819200
N	0.25737700	0.51646400	1.45746900
Br	-0.81323000	-2.06508100	4.73190200
C	1.02958900	1.54602700	2.13215500
H	1.55088700	2.15861300	1.38967700
H	0.38142200	2.21647900	2.73340300
H	1.80062500	1.15165400	2.82366500

Sc-Int₃

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

C	1.06382800	-2.65559300	0.44465500
C	3.43338700	2.17147100	0.71989400
H	2.68535500	-0.23743500	-3.19592700
H	3.92606300	3.15539100	0.77026000
H	0.57646200	-3.64111900	0.37521500
H	1.81734800	-0.24751500	4.34163800
C	-1.94489100	0.33279800	-1.00577300
C	-3.28957700	0.03695400	-0.32888700
H	-1.48187800	-0.62373100	-1.27936300
H	-2.12911400	0.88917800	-1.94282200
H	-3.80222200	0.95323900	-0.03268500
C	-3.24057700	-0.97456100	0.79616100
H	-2.55937700	-0.59147300	1.56487600
H	-4.22759100	-1.13199800	1.24262700
H	-2.84522300	-1.93328300	0.44471100
N	-1.06411200	1.07031000	-0.12003500
Br	-4.62787000	-0.68930200	-1.79248400
C	-1.89498300	2.48223600	3.45880100
O	-2.77638500	1.71188600	3.46405200
O	-1.03560000	3.27605700	3.47706300
C	-1.35504700	2.49375400	-0.08837300
H	-2.31497300	2.75047900	0.40040800
H	-0.57253500	3.03249300	0.46504000
H	-1.39603500	2.93703200	-1.10390800
Sc-Ts₂			
Sc	3.49012100	-1.00487100	0.16335900
Sc	0.78963800	0.38807300	-0.10789100
O	3.42935400	-0.84366700	-1.98679500
O	2.93404300	-0.83600800	2.25663800

O	2.23612900	-2.74873300	0.01612700
O	4.09800300	1.07637100	0.24833700
O	2.09227700	2.09660400	0.01211600
O	0.22230900	-1.73189400	-0.17621300
O	0.92259000	0.17160600	2.02636600
O	1.43024400	0.19821700	-2.19958100
C	2.48665800	-0.32454600	-2.64888600
C	1.86582700	-0.33412900	2.69930400
C	0.97992300	-2.73993900	-0.11358200
C	3.34900100	2.08626200	0.16141000
H	2.59927100	-0.32247400	-3.74572600
H	3.83997900	3.07035200	0.22046100
H	0.49037800	-3.72615800	-0.17458400
H	1.73126400	-0.33255400	3.79183900
C	-2.36403300	0.15651300	-0.95116700
C	-3.14072800	-0.04354300	0.35384500
H	-2.06951000	-0.83032800	-1.34765300
H	-3.06759600	0.59464400	-1.67599700
H	-3.61234200	0.88844900	0.66776600
C	-2.41919500	-0.72786400	1.49413000
H	-1.58509300	-0.09450200	1.81912900
H	-3.08470300	-0.87404100	2.35129500
H	-2.01114400	-1.69261700	1.18113400
N	-1.21155800	1.04492700	-0.76909100
Br	-4.82985600	-1.19065500	-0.11294600
C	-1.78583700	2.88755400	0.66441000
O	-2.58658800	3.41704300	-0.02918900
O	-1.08592800	2.67182400	1.59384300
C	-1.01443000	1.82562000	-1.99761800

H	-1.90110900	2.43776900	-2.22765400
H	-0.16658100	2.51505200	-1.88064400
H	-0.79448800	1.19113700	-2.87172800
Sc-Int₄			
Sc	1.60442200	-0.23904200	0.14959900
Sc	4.60674900	0.27933000	0.30113600
O	2.37615100	-2.24201900	0.32660800
O	1.66059600	1.93663900	0.03797100
O	2.16316500	-0.26679600	-1.95500200
O	1.86437700	-0.03333300	2.28196600
O	4.09466400	0.33178300	2.41300800
O	4.39427000	0.10793500	-1.84297300
O	3.88757300	2.31971000	0.15421700
O	4.60738800	-1.88626700	0.42422600
C	3.57875700	-2.61704800	0.40824600
C	2.68249100	2.67888100	0.05653200
C	3.31165200	-0.11338200	-2.45545700
C	2.94385900	0.17927400	2.90586900
H	3.74322400	-3.70474500	0.47303500
H	2.86810000	0.23790200	4.00445900
H	3.37275200	-0.17963000	-3.55460300
H	2.49770200	3.76329700	-0.02239900
C	-3.63327200	-0.46722100	-1.68618000
C	-4.72095500	-1.00841300	-0.76004800
H	-3.35930900	-1.30658400	-2.34221000
H	-4.04252300	0.33215500	-2.31409500
H	-4.26941500	-1.56199000	0.06091900
C	-5.78479100	-1.81735100	-1.47929700
H	-5.30833400	-2.70727000	-1.91435300

H	-6.56969800	-2.14942100	-0.79371300
H	-6.25069800	-1.24232900	-2.28859800
N	-2.44241500	0.01755200	-1.01805900
Br	-5.65255200	0.56136700	0.22322800
C	-1.53147000	-0.95019200	-0.57561500
O	-1.86365300	-2.14407000	-0.60854200
O	-0.38981300	-0.49087700	-0.14415700
C	-2.10330700	1.42806200	-1.13614400
H	-1.21736800	1.63326100	-0.53689200
H	-1.88537200	1.70827500	-2.18020200
H	-2.93268400	2.04682400	-0.77308500
Sc-Ts₃			
Sc	1.58302100	-0.26505800	0.00272000
Sc	4.54320900	0.26153800	0.16265700
O	2.32576600	-2.27361900	0.12030900
O	1.62196400	1.91425700	-0.11076800
O	2.10731800	-0.29072300	-2.09646400
O	1.84531400	-0.10180500	2.13730100
O	4.05970600	0.34421000	2.27430700
O	4.33985000	0.05584400	-1.97962800
O	3.85066000	2.30093200	-0.01891400
O	4.54876100	-1.90265400	0.31020500
C	3.52857400	-2.64159400	0.25531800
C	2.64251000	2.65900600	-0.09725400
C	3.25901000	-0.14560600	-2.59716500
C	2.91154200	0.15369400	2.76663000
H	3.69768200	-3.72568400	0.33417100
H	2.82255800	0.21696300	3.86559500
H	3.32721000	-0.20056900	-3.69346700

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

Sc-Int₅

Sc	1.64721800	-0.24620800	0.15190600
Sc	4.57660200	0.28544700	0.30125600
O	2.36992700	-2.24733800	0.31451200
O	1.66628700	1.93562700	0.04128400
O	2.16782900	-0.29846600	-1.94916200
O	1.87872700	-0.06719500	2.27741500
O	4.09928400	0.33388600	2.41490700
O	4.39084900	0.10611900	-1.84066200
O	3.89111600	2.32370200	0.15252600

O	4.59553600	-1.88085600	0.42949200
C	3.57544000	-2.62050800	0.40651700
C	2.68501400	2.68240400	0.05687000
C	3.31211200	-0.12427200	-2.45652600
C	2.95022700	0.16920100	2.90884400
H	3.74322400	-3.70474500	0.47303500
H	2.86810000	0.23790200	4.00445900
H	3.37275200	-0.17963000	-3.55460300
H	2.49770200	3.76329700	-0.02239900
C	-3.78353300	0.65602900	-1.02842300
C	-3.87805800	-0.85184900	-0.74915200
H	-3.88873700	0.89508600	-2.09761700
H	-4.55237400	1.19440800	-0.46629900
H	-4.36144600	-1.01923900	0.21628400
C	-4.53248700	-1.68649200	-1.82511700
H	-4.04959800	-1.53083200	-2.79798300
H	-4.48547200	-2.75108000	-1.57082500
H	-5.58373800	-1.38243900	-1.87583700
N	-2.41708500	0.95218900	-0.58341400
Br	-7.05095800	0.41964500	0.10267100
C	-1.70576700	-0.17317600	-0.42737300
O	-2.45577200	-1.26217700	-0.59026100
O	-0.48599500	-0.25558900	-0.15930600
C	-1.86522900	2.29232200	-0.55835100
H	-0.81917200	2.25157900	-0.24926200
H	-1.92694300	2.74539400	-1.55737100
H	-2.43538700	2.91300300	0.14214900
Mo-HKUST-1			
Mo	-0.00007300	-0.00042400	-1.06100000
Mo	-0.00001200	-0.00043700	1.06101200

O	-1.49453300	1.50653800	-1.12012000
O	1.49551300	-1.50618600	-1.12032200
O	-1.50731100	-1.49470700	-1.12030000
O	1.50582300	1.49541400	-1.12045800
O	1.50580600	1.49520300	1.12013900
O	-1.50662100	-1.49517100	1.12028300
O	1.49613600	-1.50585200	1.12026200
O	-1.49462000	1.50667200	1.12047400
C	-1.91758100	1.93340800	0.00015600
C	1.91973600	-1.93195900	-0.00006000
C	-1.93386200	-1.91789400	0.00001400
C	1.93195300	1.91897500	-0.00013400
H	-2.68835700	2.71157900	0.00000200
H	2.70853700	2.69135000	0.00001800
H	-2.71187400	-2.68882000	0.00011700
H	2.69223300	-2.70841200	-0.00018100
Mo-Int₀			
Mo	-0.00007800	-0.00019600	-1.06075600
Mo	0.00003800	-0.00021700	1.06075700
O	-1.50030900	1.50289300	-1.11967700
O	1.50072200	-1.50262700	-1.11986500
O	-1.50314200	-1.50039600	-1.11966700
O	1.50252200	1.50058600	-1.11980600
O	1.50262700	1.50052600	1.11970700
O	-1.50300000	-1.50040300	1.11983300
O	1.50086300	-1.50267200	1.11963600
O	-1.50020500	1.50290900	1.11983500
C	-1.92653700	1.93020300	0.00009900
C	1.92759000	-1.92946500	-0.00014300

C	-1.93045100	-1.92663600	0.00010400
C	1.92952100	1.92718700	-0.00006000
H	-2.69975500	2.70568500	0.00012200
H	2.70404300	2.70136900	-0.00006900
H	-2.70579300	-2.69998900	0.00015700
H	2.70179300	-2.70395900	-0.00021700
C	-0.38467898	1.16158057	3.77443978
C	-1.05710643	-0.15091895	4.01821682
H	-0.84501711	1.90222156	3.12226103
H	0.22662789	1.57692157	4.57818810
H	-0.85329969	-0.59900181	4.99554837
C	-2.39973919	-0.50745426	3.42198147
H	-2.48597323	-1.59080981	3.26901712
H	-3.21606542	-0.19121507	4.08400208
H	-2.53058221	-0.01830888	2.45093272
N	0.08879962	-0.05729723	3.11578606
C	1.35433656	-0.60300302	3.59214116
H	1.39408604	-1.67398876	3.36299177
H	2.18012872	-0.10796961	3.06855987
H	1.50579994	-0.47360388	4.68002230
Mo-Int₁			
Mo	0.21016000	0.44413600	-2.67868900
Mo	0.21598000	0.43883900	-0.52647700
O	-1.29107300	1.94814900	-2.75439500
O	1.71205000	-1.05631100	-2.75615800
O	-1.29347800	-1.05518900	-2.76423300
O	1.71275500	1.94671900	-2.74821500
O	1.73251600	1.95485700	-0.50297500
O	-1.30024000	-1.06601000	-0.52131300

O	1.73280300	-1.06161800	-0.51210400
O	-1.29683900	1.96335100	-0.50935800
C	-1.71371200	2.37703400	-1.63136400
C	2.14351200	-1.48104600	-1.63420200
C	-1.71915800	-1.48176000	-1.64153900
C	2.14333400	2.37189800	-1.62750000
H	-2.48739200	3.15175000	-1.64140100
H	2.91640600	3.14743400	-1.64159200
H	-2.49343000	-2.25392400	-1.64136600
H	2.91415600	-2.25789400	-1.64174000
C	-1.31566200	-0.03887600	2.56755600
C	-0.03060400	-0.67054300	2.92532400
H	-1.97874200	-0.52647600	1.85794100
H	-1.80189400	0.57505100	3.32240500
H	0.31766000	-0.43602700	3.92973500
C	0.37049900	-2.03876200	2.43785900
H	1.45820800	-2.11336200	2.31379700
H	0.05484600	-2.75486900	3.20512900
H	-0.10431700	-2.29165900	1.48476400
N	-0.05673000	0.48995400	1.97664300
Br	-1.00514300	-1.69997600	6.12370800
C	0.40189000	1.76332100	2.54879300
H	1.48369600	1.85821600	2.40354100
H	-0.09426600	2.59337900	2.03214900
H	0.18251600	1.83056500	3.62416600
Mo-Ts₁			
Mo	-0.00007800	-0.00019600	-1.06075600
Mo	0.00003800	-0.00021700	1.06075700

O	-1.50030900	1.50289300	-1.11967700
O	1.50072200	-1.50262700	-1.11986500
O	-1.50314200	-1.50039600	-1.11966700
O	1.50252200	1.50058600	-1.11980600
O	1.50262700	1.50052600	1.11970700
O	-1.50300000	-1.50040300	1.11983300
O	1.50086300	-1.50267200	1.11963600
O	-1.50020500	1.50290900	1.11983500
C	-1.92653700	1.93020300	0.00009900
C	1.92759000	-1.92946500	-0.00014300
C	-1.93045100	-1.92663600	0.00010400
C	1.92952100	1.92718700	-0.00006000
H	-2.69975500	2.70568500	0.00012200
H	2.70404300	2.70136900	-0.00006900
H	-2.70579300	-2.69998900	0.00015700
H	2.70179300	-2.70395900	-0.00021700
C	-0.84963673	-0.28796589	4.15708716
C	0.43207202	-0.90792477	4.55670212
H	-1.54450625	-0.96977618	3.66433009
H	-1.34661602	0.33751643	4.90269857
H	1.09892256	-0.31645255	5.16795000
C	0.96330598	-2.15953522	3.91176520
H	1.47072763	-1.93085037	2.96700346
H	1.67648388	-2.64347746	4.58337728
H	0.15153178	-2.86291077	3.70477523
N	0.03250262	0.40158269	3.23201549
Br	-0.24684061	-1.94832068	6.91915298
C	0.33488360	1.77838051	3.61191829
H	1.21253140	2.13263632	3.06482118

H	-0.52062619	2.41962502	3.35570275
H	0.52251209	1.86489618	4.69272962
Mo-Int₂			
Mo	0.20801100	0.44731800	-2.66023600
Mo	0.21620600	0.44283800	-0.47035200
O	-1.29496800	1.95119600	-2.75367600
O	1.71424100	-1.05735500	-2.74712200
O	-1.29370600	-1.05199600	-2.74318200
O	1.70999800	1.94851600	-2.73927000
O	1.74337400	1.96784000	-0.48904800
O	-1.30460900	-1.08651900	-0.49367700
O	1.73873600	-1.08300700	-0.49616200
O	-1.30411800	1.98316000	-0.50198500
C	-1.71226600	2.38106900	-1.62775100
C	2.14099200	-1.48518900	-1.62549100
C	-1.71611000	-1.48454000	-1.62103600
C	2.14252500	2.37404100	-1.61851600
H	-2.48742700	3.15177100	-1.64151000
H	2.91637100	3.14745500	-1.64170100
H	-2.49346500	-2.25390300	-1.64147500
H	2.91412100	-2.25787300	-1.64184900
C	-0.74183600	-0.36743100	2.57393800
C	0.18098300	-1.26764800	3.40156700
H	-1.37887900	-1.00243900	1.94475100
H	-1.40722900	0.19909000	3.25309600
H	0.89822500	-0.68424500	3.97776800
C	0.83061100	-2.41062600	2.65132400
H	1.40248500	-1.98968600	1.81632400
H	1.50363900	-2.98722600	3.29506200

H	0.07201100	-3.08637800	2.23942500
N	0.08247200	0.49952300	1.76561500
Br	-0.93495200	-2.15026200	5.02192900
C	0.46017900	1.70220700	2.48096200
H	1.07535600	2.34436700	1.84124900
H	-0.42453100	2.29527800	2.80334400
H	1.05156900	1.51210500	3.40123600
Mo-Int₃			
Mo	0.09859400	0.45623100	-2.76554100
Mo	0.10657400	0.44243500	-0.57734400
O	-1.40344000	1.96166400	-2.85615900
O	1.60433600	-1.04681600	-2.84642500
O	-1.40579000	-1.04218400	-2.84861200
O	1.59911800	1.96221900	-2.83863500
O	1.64920800	1.96154100	-0.58781700
O	-1.41616400	-1.07608300	-0.59905500
O	1.60894300	-1.09138900	-0.59686200
O	-1.40636700	1.99391500	-0.60524200
C	-1.81873000	2.39156900	-1.72962500
C	2.02508700	-1.48326800	-1.72519800
C	-1.82687100	-1.47513500	-1.72638400
C	2.03774400	2.37883000	-1.71863400
H	-2.59641900	3.16047300	-1.74214200
H	2.80737900	3.15615700	-1.74233300
H	-2.60245700	-2.24520100	-1.74210700
H	2.80512900	-2.24917100	-1.74248100
C	-0.71045700	-0.46100800	2.45393800
C	0.30872900	-1.07023800	3.42053400
H	-1.10997700	-1.26290700	1.81722300

H	-1.56032800	-0.04631100	3.02913000
H	0.80779600	-0.30401800	4.01189700
C	1.27624900	-2.06409700	2.81161600
H	1.79403000	-1.57692200	1.97773900
H	2.01293100	-2.41428600	3.54155700
H	0.74038000	-2.93148300	2.40971400
N	-0.04310200	0.54500200	1.65932700
Br	-0.72978800	-2.11220200	4.99148700
C	3.78518200	1.28485900	1.58296400
O	3.43520500	2.12017500	2.32365800
O	4.19605100	0.45667100	0.86606900
C	-0.06154400	1.84119000	2.31127600
H	0.45500400	1.85606800	3.29206400
H	0.43988300	2.58663700	1.68353900
H	-1.09665800	2.20198500	2.49701100
Mo-Ts₂			
Mo	-0.00007800	-0.00019600	-1.06075600
Mo	0.00003800	-0.00021700	1.06075700
O	-1.50030900	1.50289300	-1.11967700
O	1.50072200	-1.50262700	-1.11986500
O	-1.50314200	-1.50039600	-1.11966700
O	1.50252200	1.50058600	-1.11980600
O	1.50262700	1.50052600	1.11970700
O	-1.50300000	-1.50040300	1.11983300
O	1.50086300	-1.50267200	1.11963600
O	-1.50020500	1.50290900	1.11983500
C	-1.92653700	1.93020300	0.00009900
C	1.92759000	-1.92946500	-0.00014300
C	-1.93045100	-1.92663600	0.00010400

C	1.92952100	1.92718700	-0.00006000
H	-2.69975500	2.70568500	0.00012200
H	2.70404300	2.70136900	-0.00006900
H	-2.70579300	-2.69998900	0.00015700
H	2.70179300	-2.70395900	-0.00021700
C	-0.91114639	-0.15764817	4.16004421
C	-0.32510851	-1.48456618	4.65163787
H	-1.83696953	-0.35806621	3.59983004
H	-1.18394344	0.45025147	5.03410973
H	0.51068852	-1.32067148	5.33017624
C	0.01685591	-2.49825350	3.58136905
H	0.83490123	-2.09439158	2.97190364
H	0.36326217	-3.43767587	4.02369651
H	-0.83686191	-2.69506575	2.92685107
N	0.04501639	0.57881155	3.32508109
Br	-1.73747355	-2.31252000	5.93196912
C	1.72711926	0.91354781	3.48626135
O	1.89102031	2.04156141	3.84485589
O	2.04775609	-0.23365865	3.40797180
C	-0.41371640	1.97450323	3.27499133
H	-0.49489071	2.35919352	4.27014162
H	0.28952928	2.56145274	2.72196711
H	-1.36969522	2.01877459	2.79640536

Mo-Int₄

Mo	-0.12954600	0.53087900	-3.39959000
Mo	-0.13148300	0.52917900	-1.23806600
O	-1.63149500	2.03836900	-3.48647000
O	1.37123400	-0.96876600	-3.49574700

O	-1.63089100	-0.96796800	-3.49929600
O	1.37503100	2.03444600	-3.48445800
O	1.39312100	2.05658000	-1.23590100
O	-1.66571300	-0.96405000	-1.25237000
O	1.39383000	-0.97832100	-1.24812000
O	-1.64861700	2.06149000	-1.23769200
C	-2.05618700	2.46773200	-2.36285200
C	1.79991000	-1.39110000	-2.36892900
C	-2.06549400	-1.38429300	-2.37171200
C	1.80087500	2.46335500	-2.36079900
H	-2.82930500	3.24353100	-2.38061300
H	2.57449300	3.23921500	-2.38080400
H	-2.83534300	-2.16214300	-2.38057800
H	2.57224300	-2.16611300	-2.38095200
C	-1.02844000	-0.67358300	4.28147400
C	-0.08725000	-1.76292300	4.79359500
H	-1.89509300	-1.20875100	3.86084600
H	-1.38575800	-0.06820400	5.12274500
H	0.56341300	-2.10004200	3.99032600
C	-0.79490900	-2.91304500	5.48495900
H	-1.42824800	-3.41873100	4.74331400
H	-0.08453700	-3.64205300	5.88628000
H	-1.43229400	-2.56066700	6.30525500
N	-0.45669600	0.19465600	3.27485600
Br	1.26931800	-0.93953100	6.14281200
C	-0.37787500	-0.33617800	1.95768800
O	-0.53743000	-1.56657900	1.83316100
O	-0.13173300	0.52620000	1.03573800
C	-0.49425600	1.62802000	3.50412400

H	0.02923300	2.11980300	2.68422200
H	-1.52609600	2.02447100	3.53735000
H	0.00217400	1.87222400	4.45215800
Mo-Ts₃			
Mo	-0.00007800	-0.00019600	-1.06075600
Mo	0.00003800	-0.00021700	1.06075700
O	-1.50030900	1.50289300	-1.11967700
O	1.50072200	-1.50262700	-1.11986500
O	-1.50314200	-1.50039600	-1.11966700
O	1.50252200	1.50058600	-1.11980600
O	1.50262700	1.50052600	1.11970700
O	-1.50300000	-1.50040300	1.11983300
O	1.50086300	-1.50267200	1.11963600
O	-1.50020500	1.50290900	1.11983500
C	-1.92653700	1.93020300	0.00009900
C	1.92759000	-1.92946500	-0.00014300
C	-1.93045100	-1.92663600	0.00010400
C	1.92952100	1.92718700	-0.00006000
H	-2.69975500	2.70568500	0.00012200
H	2.70404300	2.70136900	-0.00006900
H	-2.70579300	-2.69998900	0.00015700
H	2.70179300	-2.70395900	-0.00021700
C	-0.20656710	-0.04019050	6.78344667
C	0.39927830	-1.42474326	6.65792264
H	-1.29921489	-0.14160555	6.92329448
H	0.19368120	0.47033050	7.65968708
H	1.41279823	-1.50001622	6.30166016
C	-0.43675741	-2.66280487	6.83163418
H	-1.06248758	-2.79057506	5.94120139

H	0.19372712	-3.54514660	6.95865411
H	-1.08210467	-2.57320805	7.71088918
N	0.10303143	0.74987782	5.60139586
Br	1.52335304	-1.57441358	8.97839853
C	0.00256257	0.03561521	4.40552870
O	-0.01970063	-1.22634922	4.55378888
O	-0.03810921	0.68155076	3.31664376
C	-0.15094451	2.17520539	5.64805197
H	0.12046033	2.60413816	4.68243540
H	-1.21397615	2.40359993	5.84397575
H	0.45294020	2.63850970	6.43860408

Mo-Int₅

Mo	-0.12901300	0.53546200	-3.41280400
Mo	-0.12900700	0.53361400	-1.26888100
O	-1.63043300	2.04055700	-3.49330600
O	1.37078600	-0.96482500	-3.49528600
O	-1.63224600	-0.96308500	-3.49493300
O	1.37357600	2.03804000	-3.49408000
O	1.38500800	2.05108400	-1.24918500
O	-1.64662600	-0.97142700	-1.25073700
O	1.38395800	-0.97407700	-1.25152200
O	-1.64304600	2.05280400	-1.24811200
C	-2.05649400	2.46773000	-2.37035800
C	1.79903000	-1.39148700	-2.37187300
C	-2.06113000	-1.38830300	-2.37148300
C	1.80015800	2.46503500	-2.37102200
H	-2.82930500	3.24353100	-2.38061300
H	2.57449300	3.23921500	-2.38080400
H	-2.83534300	-2.16214300	-2.38057800

H	2.57224300	-2.16611300	-2.38095200
C	-0.20638200	-0.46291700	4.48131600
C	-0.00858600	-1.74935700	3.66987500
H	-1.23143200	-0.37316800	4.87741600
H	0.50016500	-0.42313000	5.31552600
H	1.03136500	-2.07703700	3.74994700
C	-0.94927300	-2.88714100	3.99306300
H	-1.99688400	-2.57150200	3.90443700
H	-0.77626600	-3.73420200	3.32060100
H	-0.74031000	-3.20073200	5.02234300
N	0.03064500	0.55374800	3.45560300
Br	1.43964000	-2.32468700	6.94702300
C	-0.09526000	0.03119100	2.21390500
O	-0.20799800	-1.30547500	2.26970400
O	-0.10968900	0.66941000	1.15176900
C	0.02348300	1.97352200	3.72977400
H	0.20069700	2.51116000	2.79579700
H	-0.94455200	2.28888800	4.14617800
H	0.80945900	2.21838800	4.45237200

Zn-HKUST-1

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

O	0.55572000	0.84791900	1.74197600
C	-0.55639800	1.09866400	2.27139800
C	-0.61036900	-1.10027100	-2.25679600
C	0.59752100	-2.26452500	1.09153600
C	0.56853400	2.26479200	-1.10649300
H	-0.55439200	1.57952400	3.26079000
H	0.57206200	3.25380900	-1.58812600
H	0.61324100	-3.25401900	1.57194500
H	-0.63103200	-1.58252700	-3.24529500

Zn-Int₀

Zn	-2.29759400	-0.17387400	0.11065900
Zn	0.66747100	0.15574400	-0.14098100
O	-2.44671000	-0.67858900	2.02236000
O	-2.87588400	0.25258700	-1.73537600
O	-1.41059900	-2.00150500	-0.43878000
O	-1.76051200	1.81700000	0.54695500
O	0.48882600	2.08867100	0.35256400
O	0.84481400	-1.76310300	-0.63093100
O	-0.64189800	0.50512300	-1.93978600
O	-0.20768500	-0.43685900	1.85728500
C	-1.26311100	-0.69409800	2.49132800
C	-1.81459900	0.51711800	-2.38928700
C	-0.24523700	-2.41832200	-0.67149500
C	-0.69689900	2.48729100	0.59281900
H	-1.20229400	-0.96407000	3.56076200
H	-0.76531200	3.53930300	0.86559000
H	-0.12271100	-3.46502600	-0.94551400
H	-1.98568500	0.77616300	-3.44715100
C	3.51346700	0.17669400	1.23556500

C	4.02595100	-0.41110900	-0.03352300
H	2.91263500	-0.43077100	1.90727000
H	4.07909200	0.97225300	1.71422500
H	4.93603500	0.05752300	-0.40634800
C	3.88312200	-1.86270500	-0.41781100
H	3.87416700	-1.97410900	-1.50837600
H	4.74335600	-2.41812300	-0.02330900
H	2.96496800	-2.30003000	-0.03000000
N	2.87419800	0.53212700	-0.06262900
C	3.20198500	1.89182100	-0.56335600
H	3.09275200	1.89699300	-1.65317000
H	2.47505700	2.57032900	-0.11860400
H	4.23135300	2.17182400	-0.30707700

Zn-Int₁

Zn	-3.13175300	0.34496900	1.02359400
Zn	0.00124700	0.46787100	0.35546500
O	-3.85705400	0.06133800	2.92646900
O	-3.60970500	0.65706100	-0.93970100
O	-2.64981500	-1.63203000	0.57321200
O	-2.60379100	2.35577700	1.17863200
O	-0.33238000	2.32523200	1.12321700
O	-0.38397300	-1.52094800	0.59025100
O	-1.35831500	0.71148300	-1.16188900
O	-1.62822500	0.09145000	2.75996000
C	-2.68368300	-0.01890900	3.42687400
C	-2.53936700	0.77153000	-1.59744000
C	-1.49606100	-2.12294500	0.50817200
C	-1.46692300	2.87977200	1.26462500
H	-2.60194600	-0.19872900	4.50288900

H	-1.46658000	3.96264900	1.48104300
H	-1.44089000	-3.21025200	0.34214600
H	-2.62744800	0.94016000	-2.67013400
C	2.65967100	-1.02007300	-0.14602000
C	2.36786000	-0.47212000	-1.48539900
H	2.02681600	-1.79554900	0.27528000
H	3.70426000	-0.99994600	0.15784900
H	3.25876000	-0.07999000	-1.97946900
C	1.29583500	-1.00810800	-2.40055800
H	1.75478600	-1.75429700	-3.06127800
H	0.47930500	-1.48963100	-1.85590700
H	0.87502500	-0.21385000	-3.02869600
N	1.99133800	0.31758300	-0.26014200
Br	5.88861600	-0.41334200	-1.82364200
C	2.86658500	1.48157600	0.01821200
H	2.46012400	2.36011000	-0.49338400
H	2.87164800	1.67544700	1.09662400
H	3.88864000	1.29107100	-0.33113200
Zn-Ts₁			
Zn	-1.42789900	-0.00545000	0.00413200
Zn	1.42804500	0.00560700	-0.00390900
O	-1.70521900	-0.31489500	1.94294100
O	-1.71954700	0.30064100	-1.93309100
O	-0.53922300	-1.93329500	-0.30506000
O	-0.55348800	1.92923300	0.30841100
O	1.70515000	1.94489700	0.30247500
O	1.71942500	-1.93112600	-0.31307800
O	0.53908100	0.30888400	-1.93257700
O	0.55339900	-0.30450800	1.92972400

C	-0.56253100	-0.39968400	2.50231500
C	-0.58075400	0.39448300	-2.49898300
C	0.58064000	-2.49830000	-0.39904300
C	0.56247800	2.50307500	0.39514500
H	-0.56784000	-0.57234600	3.58833800
H	0.56786900	3.58919300	0.56720600
H	0.59356300	-3.58424900	-0.57177800
H	-0.59361700	0.56659700	-3.58503000
C	4.34020215	-1.20370801	0.50244489
C	4.87659999	-0.89468338	-0.84081977
H	3.67651825	-2.06894848	0.53312056
H	5.05785357	-1.20775348	1.32648763
H	5.65088480	-0.14275550	-0.90376802
C	4.18451601	-1.31439838	-2.10904568
H	3.51042841	-0.52631226	-2.46546655
H	4.93147801	-1.50942555	-2.88222387
H	3.59777681	-2.22422339	-1.95278552
N	3.64240213	0.04893787	0.27265339
Br	6.95327338	-2.56581572	-0.90013162
C	4.20258660	1.18449760	0.99878115
H	3.83735750	2.12057161	0.56820615
H	3.88344005	1.13415969	2.04983608
H	5.30260887	1.17698795	0.96956531
Zn-Int₂			
Zn	-3.06084600	0.35483300	1.01712000
Zn	0.13608800	0.47423000	0.32616300
O	-3.84992400	0.04842700	2.91774600
O	-3.60139700	0.66666800	-0.93880700
O	-2.61669700	-1.61807700	0.56775100

O	-2.64241800	2.37681100	1.20543300
O	-0.37238900	2.31501700	1.12514700
O	-0.34664300	-1.52964400	0.50324000
O	-1.34918900	0.69695500	-1.16139100
O	-1.61902200	0.08118100	2.77004400
C	-2.68094600	-0.02772900	3.42564400
C	-2.52720400	0.76887400	-1.59677700
C	-1.46430600	-2.11609700	0.47417900
C	-1.49081100	2.88059700	1.27250400
H	-2.60194600	-0.19872900	4.50288900
H	-1.46658000	3.96264900	1.48104300
H	-1.44089000	-3.21025200	0.34214600
H	-2.62744800	0.94016000	-2.67013400
C	2.87557400	-0.54209100	-0.44117100
C	3.12354100	-0.50053900	-1.95763600
H	2.37845400	-1.49019700	-0.19566900
H	3.84863700	-0.53621700	0.08353500
H	3.52595000	0.46476900	-2.26409200
C	1.95672300	-0.93472200	-2.82293100
H	2.19468300	-0.86545400	-3.88955500
H	1.66182900	-1.96492800	-2.59338500
H	1.10288200	-0.27921400	-2.61248100
N	2.05829400	0.58207300	-0.05684800
Br	4.76355300	-1.76005100	-2.44090000
C	2.82062900	1.79250400	0.17974100
H	2.15881600	2.58758800	0.53999800
H	3.61187000	1.64358000	0.94553800
H	3.33553800	2.18712400	-0.72044100

Zn-Int₃

Zn	-3.46222100	0.32124400	0.60411700
Zn	-0.26886300	0.41716000	-0.08133100
O	-4.25792000	0.00672100	2.49558500
O	-3.93776300	0.62477500	-1.35330000
O	-3.01575800	-1.65539400	0.14796800
O	-3.06168500	2.34984500	0.78454700
O	-0.79497000	2.27479700	0.66425200
O	-0.74548100	-1.57541500	0.13233800
O	-1.68608400	0.62993000	-1.64783400
O	-2.02798500	0.06169200	2.33853500
C	-3.08653100	-0.06018400	2.99824800
C	-2.88081300	0.71941300	-2.03721100
C	-1.86442200	-2.15704400	0.06730500
C	-1.90551600	2.84679400	0.83466000
H	-3.00048800	-0.23547700	4.07142400
H	-1.86500700	3.92594100	1.04983800
H	-1.83931100	-3.24710600	-0.08903700
H	-3.02608600	0.90346500	-3.10164000
C	2.54104800	-0.44470500	0.32373700
C	3.54388100	-1.07316600	-0.65699500
H	1.94855700	-1.25677500	0.76531600
H	3.09762200	0.03815600	1.14863800
H	4.06166300	-0.30740700	-1.23431300
C	2.98144800	-2.17357200	-1.53306800
H	2.13105600	-1.76383300	-2.09021800
H	3.72363600	-2.55090800	-2.24450700
H	2.61748500	-3.00905900	-0.92485900
N	1.68834200	0.49671500	-0.37803100
Br	5.16086600	-1.88974200	0.43210800

C	0.63447800	0.62210400	-3.71357800
O	0.72276300	1.78542600	-3.62840800
O	0.55773000	-0.53553300	-3.86718400
C	2.30404000	1.81278400	-0.47402900
H	3.23696000	1.81303200	-1.07025400
H	1.62111600	2.51792500	-0.95985300
H	2.56550100	2.23809600	0.51771100
Zn-Ts₂			
Zn	-1.42789900	-0.00545000	0.00413200
Zn	1.42804500	0.00560700	-0.00390900
O	-1.70521900	-0.31489500	1.94294100
O	-1.71954700	0.30064100	-1.93309100
O	-0.53922300	-1.93329500	-0.30506000
O	-0.55348800	1.92923300	0.30841100
O	1.70515000	1.94489700	0.30247500
O	1.71942500	-1.93112600	-0.31307800
O	0.53908100	0.30888400	-1.93257700
O	0.55339900	-0.30450800	1.92972400
C	-0.56253100	-0.39968400	2.50231500
C	-0.58075400	0.39448300	-2.49898300
C	0.58064000	-2.49830000	-0.39904300
C	0.56247800	2.50307500	0.39514500
H	-0.56784000	-0.57234600	3.58833800
H	0.56786900	3.58919300	0.56720600
H	0.59356300	-3.58424900	-0.57177800
H	-0.59361700	0.56659700	-3.58503000
C	4.65585607	0.29662174	1.40754691
C	5.16130764	-1.07541440	1.86345442
H	3.97083034	0.69956228	2.16881854

H	5.51244708	0.98229974	1.34392088
H	5.95011314	-1.44379324	1.20930201
C	4.10165046	-2.12821457	2.10576718
H	3.62303358	-2.36358824	1.14697847
H	4.54390242	-3.05159395	2.49299967
H	3.33283954	-1.77275766	2.79753529
N	3.98662082	0.21982937	0.10370233
Br	6.20779854	-0.75877140	3.63097377
C	4.31039930	-0.55789810	-1.64773668
O	5.12057649	-0.09280071	-2.39283108
O	3.85725915	-1.53182891	-1.12702308
C	3.93814378	1.58634763	-0.43590663
H	4.92998145	1.98427793	-0.48891142
H	3.50841223	1.56789998	-1.41564664
H	3.34075165	2.20154114	0.20406179
Zn-Int₄			
Zn	3.82679400	-0.53913100	0.00856100
Zn	0.84126300	0.74166300	0.00458600
O	4.82903900	1.25824700	-0.18558300
O	4.15368600	-2.59131200	0.16792100
O	3.33790400	-0.50514800	-2.00854500
O	3.49074700	-0.16036100	2.01856100
O	1.29501200	0.43243300	1.97760400
O	1.14314900	0.08662100	-1.91487400
O	2.00737900	-1.96383500	0.19566600
O	2.66239700	1.88509600	-0.16474400
C	3.89544600	2.11430500	-0.22504500
C	2.90184600	-2.83900700	0.23492400
C	2.20132400	-0.27625400	-2.49907900

C	2.38955900	0.15723600	2.54068200
H	4.19125700	3.16650400	-0.32148200
H	2.39074100	0.20230300	3.64174100
H	2.13029400	-0.40967600	-3.59109200
H	2.59457700	-3.88879800	0.33303300
C	-3.90031000	0.96779600	0.35252000
C	-4.21692000	0.06022700	-0.84159000
H	-4.79553700	1.53434400	0.63241400
H	-3.60560500	0.34419500	1.20164100
H	-3.39177600	-0.63025500	-1.00975400
C	-4.64248100	0.76986600	-2.11216300
H	-3.81659600	1.41145300	-2.44505100
H	-4.86216400	0.05540400	-2.91114800
H	-5.52907500	1.39383900	-1.94882300
N	-2.84158900	1.92025500	0.04197600
Br	-5.74700900	-1.19901100	-0.24399500
C	-1.52484300	1.48770500	0.03592000
O	-1.29027300	0.24310800	0.16127100
O	-0.57929000	2.33595700	-0.10772900
C	-3.16306900	3.33455700	-0.03960600
H	-2.24713200	3.87815600	-0.27176000
H	-3.90520300	3.52563700	-0.82714000
H	-3.56834000	3.71024400	0.91315500
Zn-Ts₃			
Zn	4.04702200	-0.47669900	-0.01690100
Zn	1.17655500	0.29928800	0.10224100
O	4.88399000	1.12254000	-0.88642600
O	4.04019800	-2.29786500	0.81596300
O	3.07205000	-1.10643600	-1.77054100

O	3.68001100	0.52015400	1.79652200
O	1.47985800	1.10618400	1.90025900
O	0.87452500	-0.50422100	-1.68822800
O	1.86931200	-1.70166700	0.90095800
O	2.70944400	1.71333000	-0.79502100
C	3.90953000	1.92326300	-1.08791400
C	2.81272100	-2.49667100	1.10832100
C	1.89467100	-1.03194300	-2.22621700
C	2.66541400	1.03984500	2.34387100
H	4.17564600	2.88331700	-1.56996900
H	2.81233700	1.49977600	3.32520100
H	1.71378000	-1.47275100	-3.21035400
H	2.59007800	-3.46451700	1.58376500
C	-4.09164400	0.88950300	-0.68999200
C	-4.20093600	-0.53816600	-0.19163000
H	-4.03646300	0.88065500	-1.79387200
H	-4.97555200	1.45864700	-0.40224800
H	-4.11102500	-0.71111100	0.86770600
C	-4.34867200	-1.69445900	-1.14219600
H	-3.37366300	-1.90706000	-1.59560400
H	-4.70603000	-2.58384500	-0.61979200
H	-5.06373800	-1.45375200	-1.93441100
N	-2.91121500	1.52368500	-0.11440300
Br	-6.75912900	-0.47887600	0.43553700
C	-1.81431600	0.68200900	-0.03229400
O	-2.08007800	-0.55543000	-0.15764300
O	-0.67132600	1.19565200	0.18731700
C	-2.74958200	2.95461900	-0.27360900
H	-1.81829200	3.25262400	0.21046500

H	-2.70289500	3.25085900	-1.33600000
H	-3.59045400	3.47841200	0.19661700
Zn-Int₅			
Zn	3.91818100	-0.58217400	0.00732400
Zn	1.02675900	0.58515100	0.01336100
O	4.78007400	1.25398500	-0.18124500
O	4.16158400	-2.60753600	0.16968400
O	3.34517900	-0.49974900	-2.00342900
O	3.48960400	-0.15998100	2.00925000
O	1.27265300	0.33182000	1.98481200
O	1.13530800	0.01385100	-1.90561500
O	2.02392700	-1.95135500	0.18634700
O	2.62117100	1.93698100	-0.15362900
C	3.86530100	2.12630800	-0.21940900
C	2.90596100	-2.84169700	0.23253100
C	2.20819400	-0.30424600	-2.50008500
C	2.38866300	0.11907100	2.54606700
H	4.19125700	3.16650400	-0.32148200
H	2.39074100	0.20230300	3.64174100
H	2.13029400	-0.40967600	-3.59109200
H	2.59457700	-3.88879800	0.33303300
C	-4.20858700	0.94579200	-0.17083300
C	-3.58032500	-0.45822800	-0.29528500
H	-4.89797500	1.16068100	-0.99057200
H	-4.75792500	1.06915100	0.76698500
H	-3.90343600	-1.10860700	0.51452400
C	-3.76405700	-1.12396900	-1.64368400
H	-3.44407100	-0.46243000	-2.45915700
H	-3.18336900	-2.05161000	-1.69630800

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

Zr-HKUST-1

O	-1.39165300	-1.40021500	1.12088400
O	1.39197100	1.39703900	1.12273600
O	-1.42441500	1.36363600	1.10375400
O	1.42458800	-1.36680100	1.10163000
O	1.41429000	-1.37568500	-1.12337400
O	-1.41426100	1.37839700	-1.12123500
O	1.40145600	1.38907200	-1.10170100
O	-1.40224100	-1.38568900	-1.10350400
C	-1.82733100	-1.83146100	0.00802700
C	1.82664700	1.83197200	0.01087800
C	-1.86068300	1.79802700	-0.00804300
C	1.86179900	-1.79725800	-0.01126700
H	-2.60371100	-2.60233600	0.00630700
H	2.64637200	-2.55980100	-0.01154600
H	-2.64739700	2.55837200	-0.00618600
H	2.59944500	2.60644400	0.01109800
Zr	0.00018594	-0.00197611	1.52070415
Zr	0.00003061	0.00144382	-1.37929383

Zr-Int₀

O	-1.12153100	1.44627200	-1.49767400
O	-1.12192400	-1.44617100	1.49752300
O	-1.12291800	1.49850200	1.44620900
O	-1.12278300	-1.49841600	-1.44641900
O	1.12155800	-1.49799100	-1.44569100
O	1.12142400	1.49788600	1.44585600
O	1.12243100	-1.44656300	1.49813400
O	1.12282200	1.44649900	-1.49791400
C	0.00062900	1.87415000	-1.94001800
C	0.00013600	-1.87407500	1.94010600
C	-0.00054000	1.94128000	1.87286300
C	-0.00037200	-1.94125100	-1.87292700
H	0.00034700	2.63356300	-2.72548400
H	0.00002100	-2.72780300	-2.63122400
H	-0.00020600	2.72785300	2.63113900
H	-0.00033600	-2.63343000	2.72562700
Zr	-1.54114400	0.00004800	-0.00013400
Zr	1.54135500	-0.00007200	0.00012400
C	-3.95084143	-1.03123340	0.44377488
C	-4.20406718	0.28437744	1.10656122
H	-3.31219470	-1.77308952	0.92082544
H	-4.74248398	-1.44519812	-0.18403950
H	-5.17472792	0.73582745	0.87961852
C	-3.63644215	0.64270344	2.46106521
H	-3.48091163	1.72568834	2.54736489
H	-4.31782239	0.33177201	3.26338039
H	-2.67060679	0.14998652	2.61504858

N	-3.27670089	0.18342273	-0.01862627
C	-3.72242430	0.72707670	-1.29614875
H	-3.48797003	1.79698029	-1.33406237
H	-3.18262814	0.22728563	-2.10852620
H	-4.80718787	0.60167251	-1.47145552
Zr-Int₁			
O	-2.79283800	2.09813900	-1.78078700
O	-2.84525900	-0.81358600	1.22320700
O	-2.80089000	2.14826700	1.15626700
O	-2.81910200	-0.85132200	-1.75049400
O	-0.56409900	-0.82230000	-1.77735600
O	-0.54554000	2.16371300	1.14850800
O	-0.58976300	-0.78835400	1.23385200
O	-0.53641700	2.11280600	-1.79196400
C	-1.66934200	2.52639700	-2.22448400
C	-1.71046400	-1.21668100	1.65749700
C	-1.67444800	2.59259700	1.57566700
C	-1.68782200	-1.27361900	-2.17933700
H	-1.68474700	3.28298200	-3.01593400
H	-1.68507300	-2.07838400	-2.92167400
H	-1.68530000	3.37727200	2.34068900
H	-1.68543000	-1.98401100	2.43517700
Zr	-3.23983500	0.64383100	-0.28860000
Zr	-0.08300200	0.65554000	-0.29437300
C	2.45688500	-1.00719600	1.33106900
C	2.56902500	-1.70093400	0.03248600
H	1.60182700	-1.19851100	1.97192100
H	3.39763700	-0.72138600	1.79913000
H	3.60195300	-1.79527900	-0.30541100

C	1.62927400	-2.78762200	-0.42714500
H	1.54023600	-2.79934900	-1.51940200
H	2.04201700	-3.75380000	-0.10833200
H	0.62919700	-2.67671600	-0.00184700
N	2.10749600	-0.26993300	0.07218400
Br	6.05729000	-1.36812700	0.99317200
C	3.12805500	0.71546900	-0.36516700
H	3.04861800	0.85682200	-1.45060100
H	2.94478800	1.67540200	0.13705800
H	4.14412900	0.37614700	-0.11674300
Zr-Ts₁			
O	-1.12153100	1.44627200	-1.49767400
O	-1.12192400	-1.44617100	1.49752300
O	-1.12291800	1.49850200	1.44620900
O	-1.12278300	-1.49841600	-1.44641900
O	1.12155800	-1.49799100	-1.44569100
O	1.12142400	1.49788600	1.44585600
O	1.12243100	-1.44656300	1.49813400
O	1.12282200	1.44649900	-1.49791400
C	0.00062900	1.87415000	-1.94001800
C	0.00013600	-1.87407500	1.94010600
C	-0.00054000	1.94128000	1.87286300
C	-0.00037200	-1.94125100	-1.87292700
H	0.00034700	2.63356300	-2.72548400
H	0.00002100	-2.72780300	-2.63122400
H	-0.00020600	2.72785300	2.63113900
H	-0.00033600	-2.63343000	2.72562700
Zr	-1.54114400	0.00004800	-0.00013400
Zr	1.54135500	-0.00007200	0.00012400

C	4.27434828	-0.36798777	1.51869370
C	4.86752928	-1.22378996	0.46830438
H	3.55737765	-0.87897024	2.16282756
H	4.96626272	0.25628981	2.08932341
H	5.68870281	-0.81123095	-0.10120775
C	4.18751123	-2.46040962	-0.05312171
H	3.57446461	-2.22796613	-0.93212884
H	4.94286084	-3.19580892	-0.34022304
H	3.54089709	-2.90344893	0.70981209
N	3.66296758	0.25625208	0.35878468
Br	6.83676425	-2.35981335	1.86126456
C	4.27169862	1.52650099	-0.02394009
H	3.97815166	1.78957850	-1.04356849
H	3.91982630	2.31525805	0.65661340
H	5.36949443	1.48038120	0.03669221
Zr-Int₂			
O	-2.80156500	2.09701500	-1.78553400
O	-2.81154800	-0.80853000	1.21125600
O	-2.80360200	2.15180600	1.15682300
O	-2.80142400	-0.84384200	-1.74768300
O	-0.53614900	-0.85819100	-1.77171600
O	-0.53941500	2.18651800	1.15813200
O	-0.54782600	-0.80868200	1.22158100
O	-0.53766400	2.11152100	-1.79693000
C	-1.67567900	2.52297400	-2.22518700
C	-1.67946700	-1.22257400	1.64507100
C	-1.67551000	2.59606800	1.57210200
C	-1.67349100	-1.28095200	-2.16981300
H	-1.68474700	3.28298200	-3.01593400

H	-1.68507300	-2.07838400	-2.92167400
H	-1.68530000	3.37727200	2.34068900
H	-1.68543000	-1.98401100	2.43517700
Zr	-3.27652200	0.64561100	-0.28792200
Zr	-0.05096700	0.66195800	-0.29650100
C	2.79484400	-0.54682800	0.79723700
C	3.39475000	-1.70973100	-0.00757100
H	2.11051600	-0.95916100	1.54879500
H	3.60395200	-0.02261800	1.33438300
H	4.04126400	-1.34745200	-0.80746100
C	2.39642100	-2.73483400	-0.50417800
H	1.66364700	-2.22807100	-1.14418900
H	2.88547900	-3.52562200	-1.08266900
H	1.85371200	-3.19049500	0.33115600
N	2.07316500	0.36444700	-0.07171100
Br	4.79829200	-2.70378500	1.20179000
C	2.93907600	1.30720400	-0.76804200
H	2.33676300	2.02118100	-1.34895500
H	3.55749700	1.89710600	-0.06395400
H	3.63132800	0.82975100	-1.48571900
Zr-Int₃			
O	-2.82896900	2.13749800	-1.85372800
O	-2.85525700	-0.76919000	1.14318000
O	-2.84199800	2.19732200	1.08665300
O	-2.82583100	-0.79610500	-1.81654000
O	-0.56040800	-0.81359800	-1.84798100
O	-0.57805700	2.23463000	1.08363900
O	-0.59199400	-0.76634600	1.15168200
O	-0.56517000	2.15622500	-1.87043400

C	-1.70484500	2.56589400	-2.29635700
C	-1.72165400	-1.18075500	1.57499500
C	-1.71329200	2.64202400	1.49984000
C	-1.70035500	-1.23596100	-2.24273200
H	-1.72010100	3.32592300	-3.08629100
H	-1.72042700	-2.03544300	-2.99203100
H	-1.72065400	3.42021300	2.27033200
H	-1.72078400	-1.94107000	2.36482000
Zr	-3.30545500	0.68857000	-0.35738900
Zr	-0.08830500	0.70674100	-0.36681200
C	2.62500300	-0.46330600	1.02919700
C	3.25617400	-1.71087300	0.39441200
H	1.86303800	-0.78808400	1.74698900
H	3.39891600	0.08867500	1.58941800
H	4.01003700	-1.44939300	-0.34855300
C	2.27285100	-2.73678600	-0.13013000
H	1.64548800	-2.26091600	-0.89355700
H	2.78631700	-3.59280600	-0.57895800
H	1.61389700	-3.09193500	0.66901200
N	2.01319800	0.38378100	0.01877400
Br	4.44924600	-2.64952900	1.85038800
C	3.31432000	-0.23436800	-3.97943400
O	3.76425700	-1.20714200	-3.51141700
O	2.88395100	0.73668200	-4.46678700
C	2.95701200	1.28481100	-0.62561800
H	3.73670500	0.76544800	-1.21536700
H	2.43221400	1.95554600	-1.32271000
H	3.48675100	1.92449200	0.10515600

Zr-Ts₂

O	-1.12153100	1.44627200	-1.49767400
O	-1.12192400	-1.44617100	1.49752300
O	-1.12291800	1.49850200	1.44620900
O	-1.12278300	-1.49841600	-1.44641900
O	1.12155800	-1.49799100	-1.44569100
O	1.12142400	1.49788600	1.44585600
O	1.12243100	-1.44656300	1.49813400
O	1.12282200	1.44649900	-1.49791400
C	0.00062900	1.87415000	-1.94001800
C	0.00013600	-1.87407500	1.94010600
C	-0.00054000	1.94128000	1.87286300
C	-0.00037200	-1.94125100	-1.87292700
H	0.00034700	2.63356300	-2.72548400
H	0.00002100	-2.72780300	-2.63122400
H	-0.00020600	2.72785300	2.63113900
H	-0.00033600	-2.63343000	2.72562700
Zr	-1.54114400	0.00004800	-0.00013400
Zr	1.54135500	-0.00007200	0.00012400
C	4.55048544	-0.48629908	1.48888067
C	4.93430574	-1.91317523	1.08573981
H	3.87754280	-0.52621210	2.35877201
H	5.45936301	0.04543789	1.80375858
H	5.71031354	-1.91322115	0.32177360
C	3.78936843	-2.83129463	0.71675158
H	3.32135999	-2.44890773	-0.19894435
H	4.14712138	-3.84489687	0.50989753
H	3.03120842	-2.86460408	1.50418212
N	3.91469678	0.23563828	0.38056537
Br	5.95153685	-2.72793022	2.70467337

C	4.46695335	0.30624093	-1.58337537
O	5.27262046	1.18845677	-1.56183450
O	3.98210932	-0.67861968	-2.05241241
C	3.98822903	1.66815561	0.70210404
H	5.00916351	1.94596668	0.86152109
H	3.58643670	2.23709658	-0.11015768
H	3.42261030	1.86411982	1.58899382

Zr-Int₄

O	1.58424600	-1.05786800	-1.68630900
O	1.53561600	0.70052500	2.11730200
O	1.22289700	1.70945500	-0.67070500
O	1.88978300	-2.04724300	1.07947200
O	4.12093500	-1.71065900	0.97004800
O	3.45836500	2.03209600	-0.77487700
O	3.76724900	1.04234600	1.99519200
O	3.81664200	-0.71546400	-1.80205000
C	2.70838200	-1.13394600	-2.29094900
C	2.64023400	1.11978100	2.60120500
C	2.24983700	2.40824700	-0.96906700
C	3.09621800	-2.41813900	1.27247600
H	2.72853200	-1.58121300	-3.29213000
H	3.26121400	-3.40311200	1.72285400
H	2.08714800	3.39584200	-1.41600400
H	2.61998900	1.57421200	3.59897600
Zr	1.08041700	-0.24937300	0.24029200
Zr	4.23637000	0.22960800	0.07229900
C	-4.47171400	0.76211100	0.11060100
C	-5.24814400	-0.24933500	-0.74004200
H	-4.81115900	1.77768300	-0.12262300

H	-4.67069100	0.56122800	1.16734600
H	-5.03300700	-1.26020200	-0.39659800
C	-5.09549100	-0.10450500	-2.24212300
H	-4.03987300	-0.25337200	-2.50220300
H	-5.68765400	-0.85500500	-2.77481700
H	-5.40312500	0.89018000	-2.58485800
N	-3.03894000	0.69016300	-0.14579600
Br	-7.25157300	-0.03396300	-0.26248900
C	-2.32172000	-0.34478200	0.46071800
O	-2.92113700	-1.21253100	1.10142100
O	-1.02353900	-0.30855200	0.27271200
C	-2.41318800	1.80030700	-0.85014900
H	-1.34234600	1.62867500	-0.93367100
H	-2.83149200	1.90845500	-1.86017700
H	-2.57063100	2.74710100	-0.31225200
Zr-Ts₃			
O	1.62174100	-1.06742000	-1.81346900
O	1.57492800	0.68065100	1.98900300
O	1.25908500	1.70363600	-0.78235100
O	1.92115500	-2.06047700	0.95419200
O	4.15137000	-1.73434500	0.81743500
O	3.49424800	2.01591500	-0.91136700
O	3.80485800	1.01230500	1.85795400
O	3.85070700	-0.73260200	-1.94602400
C	2.74271900	-1.14821000	-2.42486300
C	2.67918600	1.09939400	2.47257300
C	2.28563100	2.39660800	-1.09490500
C	3.12869100	-2.43720900	1.13670200
H	2.76267700	-1.59439100	-3.41887000

H	3.29535900	-3.41629000	1.59611400
H	2.12129300	3.38266400	-1.54274400
H	2.65413400	1.56103400	3.47223600
Zr	1.12947900	-0.26129300	0.11648300
Zr	4.26386200	0.20557300	-0.07516900
C	-4.43862900	0.79534200	-0.00196700
C	-4.90215800	-0.64938700	0.02400100
H	-4.96901900	1.34513300	-0.78370100
H	-4.66332100	1.27915800	0.95757800
H	-5.15737600	-1.10334500	0.96504500
C	-5.08976700	-1.41237000	-1.26196200
H	-4.11933500	-1.76155800	-1.63346600
H	-5.73514400	-2.27768900	-1.10521300
H	-5.55001800	-0.77541000	-2.02265100
N	-2.99960000	0.84622200	-0.27505100
Br	-7.42818000	0.08348700	0.26084100
C	-2.31191800	-0.27155500	0.10985300
O	-3.01627500	-1.27635200	0.42255400
O	-1.02435900	-0.26771600	0.11233400
C	-2.39099800	2.14491500	-0.50116500
H	-1.32080900	2.02389500	-0.67414300
H	-2.84627200	2.61672700	-1.38173800
H	-2.53852000	2.80932100	0.36319700
Zr-Int₅			
O	-1.36694800	0.52630800	-1.85253200
O	-1.87721400	-0.04274300	2.26078000
O	-1.09878400	-1.79375100	-0.00718800
O	-2.13687200	2.24377100	0.43100100
O	-4.30556400	1.72833600	0.08824000

O	-3.27331400	-2.30145900	-0.34153600
O	-4.04483700	-0.56721400	1.92630900
O	-3.53581900	0.00063500	-2.18608200
C	-2.37748000	0.34305300	-2.61143800
C	-3.03216000	-0.38744300	2.68927300
C	-2.03988800	-2.62616400	-0.23695700
C	-3.36886300	2.57005900	0.32088600
H	-2.24608900	0.48396500	-3.68923100
H	-3.63167700	3.62592700	0.42918500
H	-1.77413200	-3.68122200	-0.35295000
H	-3.15986900	-0.53953000	3.76551900
Zr	-1.18022100	0.34750500	0.28247100
Zr	-4.20822900	-0.38702300	-0.19647100
C	4.30354800	-0.22597500	-0.80183900
C	4.45714000	1.10691300	-0.05413800
H	4.40786400	-0.11520000	-1.89126800
H	5.04300700	-0.94786900	-0.44165100
H	4.93184700	0.93510000	0.91483500
C	5.15570200	2.21601900	-0.80439400
H	4.68034400	2.40157800	-1.77559100
H	5.14696600	3.14312300	-0.22068800
H	6.19510900	1.90252900	-0.95095800
N	2.92055400	-0.59309200	-0.47001000
Br	7.52268600	-0.53594500	0.39115900
C	2.25993700	0.44988600	0.03998400
O	3.04657900	1.50332200	0.23033200
O	1.03638200	0.49569400	0.33278900
C	2.32775300	-1.86257100	-0.84851500
H	1.29804300	-1.91282700	-0.49053100

H	2.33459700	-1.97164700	-1.94107100
H	2.91111600	-2.67934300	-0.41016800
Tc-HKUST-1			
O	2.17330300	-0.00236300	-1.13289500
O	-2.17330400	0.00237600	-1.13289200
O	0.00239000	2.06325700	-1.10384300
O	-0.00239300	-2.06326000	-1.10384500
O	-0.00238800	-2.06315400	1.10351100
O	0.00238900	2.06314700	1.10351400
O	-2.17328100	0.00237000	1.13303700
O	2.17328300	-0.00236100	1.13303300
C	2.75974500	-0.00297200	0.00007000
C	-2.75974500	0.00299300	0.00007400
C	0.00317600	2.70373800	-0.00014300
C	-0.00317400	-2.70374300	-0.00014600
H	3.85636300	-0.00408100	0.00008500
H	-0.00450000	-3.79415000	-0.00007600
H	0.00453300	3.79414400	-0.00007000
H	-3.85636300	0.00413200	0.00009000
Tc	-0.00000200	-0.00000200	-1.27358600
Tc	0.00000100	-0.00000400	1.27368000
Tc-Int₁			
O	-1.65211600	0.10727400	-2.74355300
O	2.57408400	0.09933900	-2.72251500
O	0.45766300	-1.99627800	-2.73256000
O	0.46302600	2.20337800	-2.74164100
O	0.47612900	2.21583400	-0.48668900
O	0.46688200	-2.02709200	-0.47981700
O	2.60565100	0.07902200	-0.46491700

O	-1.67130000	0.08528600	-0.48806200
C	-2.23924300	0.09988300	-1.61447300
C	3.16607500	0.08785200	-1.59675300
C	0.46057100	-2.59480200	-1.60799400
C	0.47073100	2.78916200	-1.61020800
H	-3.33428700	0.10700400	-1.62045300
H	0.47364400	3.88326500	-1.62039600
H	0.45463500	-3.68800900	-1.62045600
H	4.26257100	0.08824500	-1.62039400
Tc	0.45946800	0.10498000	-2.70416400
Tc	0.46285100	0.07895400	-0.44287000
C	-0.93069200	0.92828400	2.46879400
C	-0.43121500	-0.40308100	2.85416100
H	-1.75798100	1.00711600	1.77026400
H	-0.84673800	1.73247500	3.19532300
H	0.02028100	-0.44658700	3.84349400
C	-1.09195600	-1.68415300	2.41782200
H	-0.36051800	-2.49577700	2.31942200
H	-1.80975400	-1.94628800	3.20338100
H	-1.61649400	-1.57198600	1.46519900
N	0.34155900	0.43860300	1.86760400
Br	-2.05199600	-0.33559400	5.90632800
C	1.55893100	1.05963200	2.41142600
H	2.40560100	0.38119600	2.26756700
H	1.75861300	1.99155800	1.87235300
H	1.45214800	1.27885600	3.48291800
Tc-Ts₁			
O	-2.11527600	0.00510200	-1.12533500
O	2.11528200	-0.00514300	-1.12529800

O	-0.00520300	-2.09582900	-1.12284400
O	0.00507700	2.09585800	-1.12285900
O	0.00520200	2.09583000	1.12284100
O	-0.00507800	-2.09585800	1.12285600
O	2.11527800	-0.00510300	1.12533600
O	-2.11528400	0.00514200	1.12529800
C	-2.70209800	0.00659800	-0.00000700
C	2.70209800	-0.00660100	0.00000800
C	-0.00666900	-2.69074300	0.00000800
C	0.00666700	2.69074300	-0.00001000
H	-3.79842900	0.00937600	-0.00003100
H	0.00950200	3.78563700	0.00002600
H	-0.00950700	-3.78563700	-0.00003400
H	3.79842900	-0.00938300	0.00002800
Tc	-0.00001500	0.00000200	-1.10236400
Tc	0.00001500	-0.00000100	1.10236500
C	-0.95685980	0.65038332	4.10128561
C	-0.54356407	-0.67835488	4.60250436
H	-1.92203584	0.65857434	3.59292892
H	-0.85089287	1.48890029	4.79392307
H	0.32903930	-0.71769878	5.23959964
C	-1.05683870	-1.96474869	4.01490075
H	-0.38906970	-2.32685120	3.22403034
H	-1.11250474	-2.72438461	4.79825692
H	-2.05467112	-1.82988277	3.58757964
N	0.16304345	0.41914287	3.20619050
Br	-1.83927594	-0.71211674	6.93247527
C	1.36691210	1.16819703	3.55286349
H	2.23366443	0.73981438	3.04271609

H	1.24919423	2.21190881	3.22742053
H	1.54556185	1.16149402	4.63868037
Tc-Int₂			
O	-1.65439000	0.10918200	-2.72319600
O	2.57921100	0.09881100	-2.71760300
O	0.46016100	-2.00943500	-2.73375000
O	0.46244200	2.21579100	-2.74738700
O	0.48943300	2.23603800	-0.48170200
O	0.45407200	-2.04573800	-0.46973700
O	2.62457400	0.08589900	-0.45156600
O	-1.69324500	0.07966600	-0.45755000
C	-2.23937100	0.09779700	-1.59285600
C	3.16724600	0.09112600	-1.58893500
C	0.45566800	-2.59591800	-1.60473300
C	0.47635200	2.79093400	-1.61012400
H	-3.33428700	0.10700400	-1.62045300
H	0.47364400	3.88326500	-1.62039600
H	0.45463500	-3.68800900	-1.62045600
H	4.26257100	0.08824500	-1.62039400
Tc	0.46102500	0.10688500	-2.71111800
Tc	0.46581500	0.08481100	-0.38149300
C	-0.76474100	0.20953700	2.51421000
C	-0.71039100	-1.06452700	3.36643400
H	-1.65535000	0.17325100	1.87807100
H	-0.85699300	1.08832500	3.17596600
H	0.21246800	-1.11981200	3.94375300
C	-1.00441900	-2.35171800	2.62684100
H	-0.29168500	-2.44338200	1.79894900
H	-0.91238500	-3.22439900	3.28228900

H	-2.01332400	-2.33378500	2.19980300
N	0.43113400	0.28751600	1.69552800
Br	-2.12400100	-0.90056100	4.94344400
C	1.52940900	0.93020500	2.39503500
H	2.42293500	0.93050400	1.76500500
H	1.28839500	1.98146900	2.65265500
H	1.79047400	0.42429500	3.34450100
Tc-Int₃			
O	-1.63657700	0.20734200	-2.80345800
O	2.59594200	0.20029300	-2.78709200
O	0.47848600	-1.90952100	-2.80264500
O	0.48029100	2.31467300	-2.82763700
O	0.51021700	2.33240300	-0.56212800
O	0.46442700	-1.95023100	-0.53882300
O	2.64477700	0.16715500	-0.52113500
O	-1.67477900	0.17683500	-0.53837600
C	-2.22135800	0.19517100	-1.67340100
C	3.18584200	0.18365800	-1.66028900
C	0.47133000	-2.49934900	-1.67576500
C	0.49548500	2.88826000	-1.68962900
H	-3.31583500	0.20400400	-1.69733200
H	0.49209600	3.98026500	-1.69727500
H	0.47308700	-3.59100900	-1.69733500
H	4.28102300	0.18524500	-1.69727300
Tc	0.47905900	0.20606000	-2.78538400
Tc	0.48097400	0.17834800	-0.45643200
C	-0.80829900	0.48058000	2.39229200
C	-0.86191500	-0.75099300	3.30380200
H	-1.67949200	0.46677100	1.72965300

H	-0.86544000	1.39451100	3.00771800
H	0.03169700	-0.83282800	3.92263800
C	-1.20467000	-2.05155100	2.60812200
H	-0.46984300	-2.22245800	1.81205500
H	-1.19227600	-2.89783400	3.30199200
H	-2.19424200	-1.99298800	2.13997600
N	0.41732800	0.44421000	1.61312300
Br	-2.33428900	-0.42964300	4.79726100
C	3.00059800	-2.76791500	2.14022300
O	2.82208100	-2.11207500	3.09123100
O	3.20581800	-3.45357100	1.21444900
C	1.51266900	1.10453700	2.30297700
H	1.71438700	0.66923600	3.29805000
H	2.42933200	1.02337200	1.71224200
H	1.30196600	2.18086300	2.46075700
Tc-Ts₂			
O	-2.11527600	0.00510200	-1.12533500
O	2.11528200	-0.00514300	-1.12529800
O	-0.00520300	-2.09582900	-1.12284400
O	0.00507700	2.09585800	-1.12285900
O	0.00520200	2.09583000	1.12284100
O	-0.00507800	-2.09585800	1.12285600
O	2.11527800	-0.00510300	1.12533600
O	-2.11528400	0.00514200	1.12529800
C	-2.70209800	0.00659800	-0.00000700
C	2.70209800	-0.00660100	0.00000800
C	-0.00666900	-2.69074300	0.00000800
C	0.00666700	2.69074300	-0.00001000
H	-3.79842900	0.00937600	-0.00003100

H	0.00950200	3.78563700	0.00002600
H	-0.00950700	-3.78563700	-0.00003400
H	3.79842900	-0.00938300	0.00002800
Tc	-0.00001500	0.00000200	-1.10236400
Tc	0.00001500	-0.00000100	1.10236500
C	-1.11624117	0.72333640	4.36767259
C	-1.69260862	-0.61192649	4.84797427
H	-1.86004694	1.22997700	3.73425008
H	-0.94194306	1.36493515	5.24284226
H	-1.04690944	-1.07701711	5.59134210
C	-2.09250705	-1.59178554	3.76633917
H	-1.18647094	-1.90758671	3.23425002
H	-2.55572803	-2.48594404	4.19537550
H	-2.77605586	-1.13637004	3.04431374
N	0.14093738	0.53636132	3.63396556
Br	-3.36804993	-0.15263220	5.98879671
C	1.66179924	-0.60110898	4.37697090
O	2.38164145	0.13872669	4.97891663
O	1.25504684	-1.68523462	4.08672277
C	0.82020269	1.83970110	3.60560973
H	0.95935069	2.19123244	4.60659103
H	1.77231028	1.73538506	3.12863038
H	0.22337806	2.54117494	3.06096782
Tc-Int₄			
O	-1.68223300	0.49338100	-3.41519000
O	2.54926300	0.48683500	-3.40374900
O	0.42839400	-1.61050100	-3.42362600
O	0.43582900	2.59818200	-3.41071200
O	0.44198500	2.62333000	-1.15221400

O	0.43091700	-1.62987500	-1.16647600
O	2.57715400	0.49239200	-1.14287000
O	-1.70778800	0.51430400	-1.15584500
C	-2.26774400	0.50511800	-2.28135500
C	3.13508200	0.48812400	-2.27150300
C	0.42856800	-2.19655500	-2.28821900
C	0.44033300	3.18610400	-2.27915400
H	-3.36414000	0.50483700	-2.29578600
H	0.44379100	4.28109800	-2.29572900
H	0.42478200	-3.29017600	-2.29578900
H	4.23271800	0.48607800	-2.29572700
Tc	0.43233300	0.49027900	-3.37369500
Tc	0.42493100	0.48680500	-1.10806300
C	-1.40866700	0.12918500	4.09392700
C	-1.32019900	-1.28079900	4.67539900
H	-2.35778800	0.15443100	3.53276800
H	-1.47864800	0.86154700	4.90546100
H	-0.87738900	-1.95721600	3.94713900
C	-2.63558200	-1.80356100	5.22103600
H	-3.34253800	-1.89146700	4.38440000
H	-2.51813000	-2.79046700	5.67785000
H	-3.06321500	-1.12389600	5.96720200
N	-0.31952700	0.49491200	3.21375100
Br	0.07390400	-1.31752800	6.21835500
C	-0.37244000	-0.03260500	1.90058700
O	-1.17740400	-0.95430900	1.68242400
O	0.46103200	0.50604500	1.06807500
C	0.45625500	1.68198600	3.52845200
H	1.25486200	1.77444700	2.79217400

H	-0.15348900	2.60300000	3.49179200
H	0.89287300	1.59264300	4.53160900
Tc-Ts₃			
O	-2.11527600	0.00510200	-1.12533500
O	2.11528200	-0.00514300	-1.12529800
O	-0.00520300	-2.09582900	-1.12284400
O	0.00507700	2.09585800	-1.12285900
O	0.00520200	2.09583000	1.12284100
O	-0.00507800	-2.09585800	1.12285600
O	2.11527800	-0.00510300	1.12533600
O	-2.11528400	0.00514200	1.12529800
C	-2.70209800	0.00659800	-0.00000700
C	2.70209800	-0.00660100	0.00000800
C	-0.00666900	-2.69074300	0.00000800
C	0.00666700	2.69074300	-0.00001000
H	-3.79842900	0.00937600	-0.00003100
H	0.00950200	3.78563700	0.00002600
H	-0.00950700	-3.78563700	-0.00003400
H	3.79842900	-0.00938300	0.00002800
Tc	-0.00001500	0.00000200	-1.10236400
Tc	0.00001500	-0.00000100	1.10236500
C	-0.23087506	-0.69506604	6.75262269
C	-0.75604741	-2.07798365	6.41928075
H	-1.08881658	-0.03106332	6.96873109
H	0.39189359	-0.73320759	7.64663679
H	-0.06974699	-2.78357914	5.98188742
C	-2.22249915	-2.40196431	6.50407852
H	-2.73235775	-1.94698680	5.64754680
H	-2.38494082	-3.48153409	6.48827003

H	-2.65347250	-2.00412046	7.42783251
N	0.56811580	-0.18133183	5.64969323
Br	-0.13007049	-3.27251372	8.61962273
C	0.02542013	-0.44934372	4.39046296
O	-0.86367714	-1.35689730	4.38953552
O	0.46364400	0.19698455	3.39306302
C	1.36138651	1.00805415	5.88440009
H	1.87826289	1.26505154	4.95878689
H	0.74064226	1.87033644	6.18721092
H	2.09747554	0.81761350	6.67568934
Tc-Int₅			
O	-1.67890600	0.49871700	-3.41130300
O	2.54694300	0.49007700	-3.41013100
O	0.42891200	-1.60440500	-3.41772000
O	0.43806100	2.59650200	-3.41470100
O	0.44582000	2.61433800	-1.16079500
O	0.43002600	-1.62090800	-1.16547200
O	2.56746700	0.49507200	-1.15445000
O	-1.69825800	0.49588300	-1.15605100
C	-2.26760000	0.50006400	-2.28218100
C	3.13581800	0.48977400	-2.28099500
C	0.42866900	-2.19624300	-2.28787900
C	0.44227500	3.18665900	-2.28553600
H	-3.36414000	0.50483700	-2.29578600
H	0.44379100	4.28109800	-2.29572900
H	0.42478200	-3.29017600	-2.29578900
H	4.23271800	0.48607800	-2.29572700
Tc	0.43373500	0.49352900	-3.37697900
Tc	0.43452800	0.48983900	-1.13842500

C	-1.24870400	-0.24213500	4.12433500
C	-1.21648500	-1.55660000	3.33317200
H	-2.25336800	0.20969100	4.14378300
H	-0.91208900	-0.40713100	5.15195400
H	-0.45252000	-2.21782700	3.75124400
C	-2.53349800	-2.28557000	3.19809000
H	-3.30407300	-1.63512600	2.76519700
H	-2.41955800	-3.17040400	2.56179100
H	-2.83401000	-2.60610700	4.20178500
N	-0.33860000	0.58696600	3.33018200
Br	-1.29499100	-2.47172100	6.81478700
C	-0.17055600	0.07176200	2.09308400
O	-0.72853800	-1.14008900	1.99500100
O	0.43408500	0.62364700	1.15585800
C	0.02221100	1.93945300	3.69145400
H	0.68056600	2.34389500	2.92045200
H	-0.87214900	2.57492800	3.77097400
H	0.53837300	1.94281100	4.65808600

Ag-HKUST-1

O	-1.51903400	-1.51528500	1.24615200
O	1.51929700	1.51759900	1.24275900
O	-1.51625800	1.52030300	1.24323100
O	1.51661700	-1.51801200	1.24581100
O	1.61209900	-1.61657900	-1.05107800
O	-1.61244500	1.61425900	-1.05366100
O	1.61529200	1.61109400	-1.05413200
O	-1.61553900	-1.61342700	-1.05073900
C	-1.93305100	-1.92921000	0.11011900
C	1.93287000	1.92938900	0.10590900

C	-1.92932200	1.93292700	0.10648300
C	1.92935800	-1.93291400	0.10968300
H	-2.71552900	-2.71084400	0.21903500
H	2.71059800	-2.71578600	0.21840100
H	-2.71064700	2.71571300	0.21386900
H	2.71585700	2.71051400	0.21307300
Ag	0.00019400	0.00135900	1.31276900
Ag	-0.00018700	-0.00136600	-1.48086000
Ag-Int₀			
O	-1.27675600	-2.11527500	-0.09318300
O	-1.28645000	2.10910500	0.10193000
O	-1.28911400	0.09443100	-2.10776600
O	-1.27386600	-0.10060800	2.11659200
O	1.01114000	-0.10243500	2.29109100
O	0.99462400	0.10669600	-2.29774800
O	0.99749200	2.29716200	0.10104800
O	1.00803500	-2.29204100	-0.10807900
C	-0.15182900	-2.72922500	-0.12469100
C	-0.16438300	2.72861600	0.12560500
C	-0.16772600	0.12452000	-2.72823500
C	-0.14818000	-0.12574400	2.72942300
H	-0.29125600	-3.82521800	-0.17458700
H	-0.28623600	-0.17655400	3.82554900
H	-0.31342800	0.17433000	-3.82341800
H	-0.30886900	3.82391500	0.17633400
Ag	-1.28000800	-0.00305800	0.00437900
Ag	1.57600100	0.00387200	-0.00539200
C	4.01542739	0.61015189	1.29633390
C	4.39402953	-0.79039163	0.93664076

H	3.27248592	0.79715076	2.07019874
H	4.77909319	1.38444793	1.19888749
H	5.42063822	-0.91297161	0.57811443
C	3.81380724	-2.00079425	1.63201430
H	3.78474175	-2.86515104	0.95633968
H	4.41714818	-2.27333149	2.50744003
H	2.79029434	-1.79835197	1.96481641
N	3.51190257	-0.01129011	0.06998061
C	4.07526389	0.47622203	-1.18351396
H	3.97184795	-0.29933373	-1.95092411
H	3.51621992	1.36049782	-1.51009363
H	5.14404472	0.75003706	-1.10667951
Ag-Int₁			
O	-2.81585500	-2.58170200	-0.77641400
O	-2.91887300	1.70212600	-0.13168700
O	-2.82304900	-0.15412200	-2.59604200
O	-2.81844500	-0.77380400	1.67860700
O	-0.58931400	-0.27223800	1.80752000
O	-0.61249900	-0.75079100	-2.76133900
O	-0.81703600	1.77501200	-0.99352100
O	-0.60170000	-2.77163200	-0.23232200
C	-1.72772100	-3.19668900	-0.54423300
C	-1.82523200	2.27575300	-0.48652400
C	-1.72476700	-0.40575400	-3.19333800
C	-1.70840000	-0.55383400	2.26810200
H	-1.80806300	-4.28732000	-0.63608900
H	-1.80304300	-0.63865600	3.36404700
H	-1.83023500	-0.28777200	-4.28492000
H	-1.82567600	3.36181300	-0.28516800

Ag	-2.81541400	-0.43205900	-0.45786800
Ag	0.23177900	-0.66603000	-0.46567100
C	2.28454000	1.51747900	0.72040600
C	3.31144400	0.47720900	0.43999600
H	1.59831900	1.34863900	1.54518600
H	2.51318500	2.55867700	0.50640000
H	4.21855200	0.82633900	-0.04751100
C	3.47574200	-0.75361100	1.31177600
H	3.09198100	-1.64968000	0.80525000
H	4.53498400	-0.89891600	1.54074500
H	2.94795000	-0.64039000	2.26320700
N	2.10676700	0.62737000	-0.43538600
Br	5.06737400	2.01475300	2.34941000
C	2.31988800	1.25834700	-1.74393700
H	2.52365500	0.48554100	-2.49280400
H	1.40743400	1.79468600	-2.01749500
H	3.16543900	1.96376800	-1.71754800
Ag-Ts₁			
O	-1.27675600	-2.11527500	-0.09318300
O	-1.28645000	2.10910500	0.10193000
O	-1.28911400	0.09443100	-2.10776600
O	-1.27386600	-0.10060800	2.11659200
O	1.01114000	-0.10243500	2.29109100
O	0.99462400	0.10669600	-2.29774800
O	0.99749200	2.29716200	0.10104800
O	1.00803500	-2.29204100	-0.10807900
C	-0.15182900	-2.72922500	-0.12469100
C	-0.16438300	2.72861600	0.12560500
C	-0.16772600	0.12452000	-2.72823500

C	-0.14818000	-0.12574400	2.72942300
H	-0.29125600	-3.82521800	-0.17458700
H	-0.28623600	-0.17655400	3.82554900
H	-0.31342800	0.17433000	-3.82341800
H	-0.30886900	3.82391500	0.17633400
Ag	-1.28000800	-0.00305800	0.00437900
Ag	1.57600100	0.00387200	-0.00539200
C	4.67954068	0.64920025	0.72249707
C	5.17206577	-0.67210285	0.27622812
H	4.20507961	0.64354737	1.70479699
H	5.36426605	1.49231238	0.60249931
H	5.77855142	-0.69805195	-0.61840967
C	4.60852307	-1.96732002	0.79427250
H	3.79651920	-2.32545528	0.15014633
H	5.39677160	-2.72368139	0.81361344
H	4.21561197	-1.84629177	1.80789704
N	3.74703563	0.42671138	-0.36827501
Br	7.54588391	-0.70957681	1.48963518
C	4.04817266	1.19155289	-1.57446653
H	3.51008745	0.77086515	-2.42799322
H	3.72230886	2.23219126	-1.43308247
H	5.12712713	1.19230784	-1.79083576
Ag-Int₂			
O	-2.89900900	-2.63638000	-0.80533400
O	-3.02266800	1.77201100	-0.15711500
O	-2.88081600	-0.18224000	-2.64104400
O	-2.84092800	-0.79771200	1.70700400
O	-0.60695600	-0.28352500	1.79499200
O	-0.65191400	-0.74758400	-2.74035500

O	-0.92334700	1.73988500	-1.02487700
O	-0.69255000	-2.72393700	-0.20453300
C	-1.80284200	-3.19648900	-0.54790200
C	-1.90585900	2.28682700	-0.50054600
C	-1.76837900	-0.41197600	-3.19494300
C	-1.73214300	-0.56795800	2.26851000
H	-1.80806300	-4.28732000	-0.63608900
H	-1.80304300	-0.63865600	3.36404700
H	-1.83023500	-0.28777200	-4.28492000
H	-1.82567600	3.36181300	-0.28516800
Ag	-2.92867300	-0.42281500	-0.45971200
Ag	0.11951500	-0.67491100	-0.45984800
C	2.34474500	1.26565600	0.51093600
C	3.72807600	0.70997200	0.90478800
H	1.65155800	1.11590400	1.34860800
H	2.41669500	2.34459900	0.30878900
H	4.42283600	0.78328700	0.06735900
C	3.70826700	-0.67829200	1.51267700
H	3.26566700	-1.36665500	0.78322400
H	4.71800500	-1.02241100	1.75815300
H	3.09428600	-0.70128200	2.41912900
N	1.91564400	0.50492000	-0.64261300
Br	4.61178200	2.01067100	2.28139600
C	2.03045100	1.23924100	-1.87893200
H	1.87076300	0.57391200	-2.73189800
H	1.27278300	2.04308600	-1.92464400
H	3.02570200	1.71486800	-1.96878600
Ag-Int₃			
O	-3.58407900	0.29875000	-1.56089100

O	-0.53166600	-2.08423100	0.68684500
O	-3.12443400	-0.37406000	1.58041000
O	-1.19545800	-1.57993300	-2.35490700
O	0.60793900	-0.30035500	-1.72898900
O	-1.41591100	1.14218400	1.84945800
O	-0.62047200	-4.08236200	1.79730400
O	-1.76549800	1.63007600	-1.16072000
C	-2.90380200	1.33464700	-1.65215300
C	-0.12238500	-2.99014000	1.49319300
C	-2.52056900	0.55969500	2.12848000
C	-0.04579800	-1.12847900	-2.45350600
H	-3.31068300	2.16986000	-2.25087500
H	0.53812300	-1.48907100	-3.30561400
H	-3.00120500	0.97660700	3.02083700
H	0.84757600	-2.68307100	1.96689000
Ag	-2.47087800	-1.47258200	-0.38650600
Ag	-0.28776700	0.56108900	0.05915900
C	2.62249600	-0.29178100	0.51117600
C	3.75276500	0.70944000	0.19231500
H	2.27456100	-0.73252200	-0.42900100
H	2.99000600	-1.09500800	1.16365500
H	4.08782200	1.21577400	1.09898300
C	3.43315700	1.68760300	-0.92020000
H	2.53559300	2.24639700	-0.63024100
H	4.25644600	2.39041500	-1.08243000
H	3.21474200	1.16258400	-1.85500300
N	1.55893100	0.48527300	1.12454100
Br	5.43666000	-0.37882400	-0.32558400
C	-1.41528300	4.08160200	0.38576600

O	-2.56662700	4.24822000	0.51145000
O	-0.25499500	3.98372500	0.27126100
C	1.42817000	0.21185000	2.53728300
H	2.38291000	0.48347900	3.02465600
H	0.62492800	0.81064600	2.96736900
H	1.25698500	-0.85673400	2.75589700
Ag-Ts₂			
O	-1.27675600	-2.11527500	-0.09318300
O	-1.28645000	2.10910500	0.10193000
O	-1.28911400	0.09443100	-2.10776600
O	-1.27386600	-0.10060800	2.11659200
O	1.01114000	-0.10243500	2.29109100
O	0.99462400	0.10669600	-2.29774800
O	0.99749200	2.29716200	0.10104800
O	1.00803500	-2.29204100	-0.10807900
C	-0.15182900	-2.72922500	-0.12469100
C	-0.16438300	2.72861600	0.12560500
C	-0.16772600	0.12452000	-2.72823500
C	-0.14818000	-0.12574400	2.72942300
H	-0.29125600	-3.82521800	-0.17458700
H	-0.28623600	-0.17655400	3.82554900
H	-0.31342800	0.17433000	-3.82341800
H	-0.30886900	3.82391500	0.17633400
Ag	-1.28000800	-0.00305800	0.00437900
Ag	1.57600100	0.00387200	-0.00539200
C	4.63439410	0.45318444	1.62092752
C	4.89574936	-0.93404449	2.21515428
H	3.96877772	1.01415628	2.29429312
H	5.58687134	0.99958543	1.57419623

H	5.66180287	-1.46691784	1.65386960
C	3.67574179	-1.79779505	2.45072485
H	3.23203870	-2.04163537	1.47736975
H	3.94696664	-2.73938777	2.93858295
H	2.92495658	-1.27737350	3.05192859
N	4.04956290	0.36408882	0.27786459
Br	5.85795536	-0.62392439	4.03106061
C	4.95052551	-0.76422895	-1.04496819
O	5.74174626	-0.05753370	-1.59489532
O	4.47350828	-1.82846580	-0.79026366
C	4.24367647	1.67255422	-0.36333603
H	5.28546805	1.91658638	-0.36764982
H	3.88228557	1.63370204	-1.36970928
H	3.70456927	2.41979425	0.18062698
Ag-Int₄			
O	-3.77811600	-1.83636500	0.75684000
O	-3.73423000	2.35805900	0.47581500
O	-3.73099700	0.11837400	-1.48234900
O	-3.76226900	0.37828100	2.70696100
O	-1.55388800	-0.15564000	2.86778900
O	-1.60657500	0.93094800	-1.69675100
O	-1.54961900	2.60456600	1.09348900
O	-1.68066600	-1.96920700	-0.11810300
C	-2.71122200	-2.44760800	0.33401100
C	-2.67669900	3.01042200	0.79115000
C	-2.68317900	0.51606000	-2.12208000
C	-2.66380500	0.09665600	3.32997800
H	-2.83006300	-3.54638100	0.43032900
H	-2.82504300	0.10228300	4.43046500

H	-2.85223500	0.45316700	-3.21850200
H	-2.84767600	4.10275200	0.78125000
Ag	-3.61398100	0.24995800	0.61173200
Ag	-0.32631600	0.67585700	0.57370800
C	4.05023300	-1.45793600	-0.06668300
C	4.07232200	-1.41774400	-1.59373600
H	3.26152900	-2.17727000	0.19601400
H	5.00364900	-1.84837100	0.30952000
H	3.28358100	-0.76393800	-1.96123400
C	4.03040400	-2.78821100	-2.24284200
H	3.07264400	-3.26136800	-1.98705200
H	4.09882700	-2.71931800	-3.33226300
H	4.84349100	-3.42993300	-1.88274000
N	3.76504000	-0.19221300	0.57532300
Br	5.78822900	-0.44292300	-2.24674300
C	2.43008600	0.22434000	0.66693400
O	1.57784000	-0.48516500	0.01890100
O	2.13693500	1.24407200	1.34450000
C	4.79806500	0.45686200	1.36270600
H	4.39835200	1.40442100	1.72480400
H	5.09195900	-0.15271500	2.23471000
H	5.68950300	0.64635700	0.75310600
Ag-Ts₃			
O	-1.27675600	-2.11527500	-0.09318300
O	-1.28645000	2.10910500	0.10193000
O	-1.28911400	0.09443100	-2.10776600
O	-1.27386600	-0.10060800	2.11659200
O	1.01114000	-0.10243500	2.29109100
O	0.99462400	0.10669600	-2.29774800

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

H	7.06968631	0.71258424	-2.58013210
Ag-Int₅			
O	3.91017800	-0.88468200	-1.93898800
O	3.61600700	-0.43995900	2.34923800
O	2.82806000	-2.57853700	0.36843500
O	4.62093800	1.22283300	0.09873200
O	2.71751400	2.22936000	-0.66213600
O	0.74376000	-1.70463300	0.60716100
O	1.78095900	0.91598900	2.18151300
O	1.70963200	-0.41851300	-2.27731800
C	2.84730900	-0.75749100	-2.62392400
C	2.66803700	0.30674500	2.79133000
C	1.55390000	-2.61212100	0.51255400
C	3.90689800	2.19080900	-0.36201200
H	3.02223700	-0.96930200	-3.66005700
H	4.52678000	3.13407900	-0.46432900
H	1.20891500	-3.67374800	0.66518800
H	2.71360900	0.42916200	3.86200800
Ag	3.66143500	-0.65918300	0.19391700
Ag	0.99034500	0.57409900	-0.13456700
C	-4.57327100	0.88906500	-0.51043200
C	-3.89287300	-0.49098300	-0.46790900
H	-4.91512200	1.15999400	-1.52343400
H	-5.43160800	0.92077300	0.15868900
H	-4.02829200	-0.94977300	0.51484200
C	-4.32352300	-1.44741900	-1.55613900
H	-4.17349000	-1.00562000	-2.54862100
H	-3.75317700	-2.37756700	-1.50323100
H	-5.38706900	-1.67014900	-1.41618300

N	-3.47538900	1.74533300	-0.08549700
Br	-7.64043900	-0.76739000	0.52422200
C	-2.27628800	1.13713600	-0.27270100
O	-2.46051800	-0.16271700	-0.57460900
O	-1.16299000	1.65687200	-0.19330800
C	-3.60778700	3.17216200	0.05833300
H	-2.64191300	3.58213200	0.35646600
H	-3.91876200	3.64112300	-0.88825800
H	-4.35541600	3.40361900	0.82382600

Mn-HKUST-1

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

Mn-Int₀

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

H	3.06962377	1.37529277	4.33146679
H	1.63105538	2.31609375	3.88159601
H	1.90802050	1.88014908	5.58994652
Mn-Int₁			
Mn	-3.39184700	-0.46149300	0.11985100
Mn	-0.32887000	0.24391500	-0.27499000
O	-2.42030800	-1.56481700	1.65163400
O	-3.30685900	0.82943500	-1.56068400
O	-3.45620600	-2.16484200	-1.14226800
O	-4.26255400	0.95953000	1.42147500
O	-2.08960000	1.42394800	1.12885400
O	-1.31629900	-1.48678300	-1.27379000
O	-1.13767900	1.47915200	-1.70717100
O	-0.26707100	-0.88909600	1.44345200
C	-1.20602900	-1.54188800	1.97815600
C	-2.35404100	1.48324500	-2.05608700
C	-2.26934900	-2.26147800	-1.57070300
C	-3.21811000	1.65451900	1.64089800
H	-0.90342900	-2.16407900	2.82358900
H	-3.32872500	2.51065700	2.33027300
H	-2.05147900	-3.09488800	-2.25994800
H	-2.60281400	2.13552100	-2.89910400
C	2.67767300	-0.15214000	0.63561500
C	2.74693700	-0.59618300	-0.77193100
H	2.11153800	-0.72519800	1.36334400
H	3.53684900	0.41352100	0.99251000
H	3.65298000	-0.26025200	-1.27819500
C	2.14325100	-1.88587600	-1.27079400
H	1.82277400	-1.79881400	-2.31682800

H	2.90152000	-2.67762800	-1.21576800
H	1.28056700	-2.20222500	-0.67504000
N	1.83037900	0.52967200	-0.39513300
Br	6.03548100	0.85160600	-0.30916200
C	2.29270100	1.88009000	-0.79578600
H	1.91325900	2.09956000	-1.79944900
H	1.88293100	2.61813600	-0.09553500
H	3.38853900	1.94015700	-0.78653100
Mn-Ts₁			
Mn	-3.29831400	-0.53199300	0.07862800
Mn	-0.30031600	0.56373400	0.02366500
O	-2.34715500	-1.52901000	1.68761200
O	-3.29772600	0.86659800	-1.50418600
O	-3.50571100	-2.25335200	-1.15634800
O	-4.08755000	0.92222400	1.40434300
O	-1.92974300	1.53854800	1.21348800
O	-1.41125600	-1.46055100	-1.18093200
O	-1.11824400	1.48237500	-1.65273400
O	-0.17707800	-0.88917700	1.49245900
C	-1.13101200	-1.53273800	2.01133300
C	-2.32787200	1.49010300	-2.00925300
C	-2.29130400	-2.28780400	-1.53921200
C	-3.09889200	1.66763300	1.66924400
H	-0.85844200	-2.17015400	2.85540000
H	-3.28373800	2.50458200	2.36208400
H	-2.00649200	-3.10096300	-2.22813700
H	-2.55782700	2.12944600	-2.86729300
C	2.73934000	0.83396300	0.78437900
C	3.14056400	0.19444000	-0.47176900

H	2.43708800	0.14209400	1.57401300
H	3.42337800	1.59422500	1.17290400
H	3.61243400	0.82398600	-1.21269900
C	2.62504700	-1.14975000	-0.90773900
H	1.77328000	-1.04971400	-1.59278500
H	3.41991400	-1.68471200	-1.43287600
H	2.31390700	-1.75161400	-0.04842900
N	1.61866400	1.34902800	-0.00497600
Br	5.68290900	-0.51396900	0.10996100
C	1.81911500	2.71934400	-0.47082500
H	1.08582400	2.95871300	-1.24803100
H	1.69468400	3.43939700	0.35785300
H	2.82505100	2.88452900	-0.88971400

Mn-Int₂

Mn	-3.27844600	-0.51594600	0.03677200
Mn	-0.25271200	0.71074400	0.06926200
O	-2.39127300	-1.52641400	1.65963400
O	-3.34886700	0.88012600	-1.54110800
O	-3.56694500	-2.26220700	-1.19083900
O	-4.12475900	0.92472000	1.37049100
O	-1.96537300	1.54243100	1.21081500
O	-1.47887600	-1.45773400	-1.21418900
O	-1.17536600	1.53306900	-1.63956100
O	-0.22779700	-0.86188800	1.46778800
C	-1.17294800	-1.51763800	1.98114800
C	-2.37359700	1.51414900	-2.02599100
C	-2.35181800	-2.28910000	-1.57257200
C	-3.14094600	1.67068300	1.64645100
H	-0.90342900	-2.16407900	2.82358900

H	-3.32872500	2.51065700	2.33027300
H	-2.05147900	-3.09488800	-2.25994800
H	-2.60281400	2.13552100	-2.89910400
C	2.73774900	0.79192900	0.74078800
C	3.57772900	-0.15000300	-0.13621400
H	2.35425500	0.21603500	1.59347100
H	3.39192300	1.58614600	1.14611500
H	3.92370400	0.35394200	-1.03892900
C	2.95030900	-1.49625900	-0.43792200
H	2.00113300	-1.32918900	-0.96131900
H	3.59626300	-2.10986000	-1.07450800
H	2.73425900	-2.04484100	0.48539900
N	1.64756700	1.33932900	-0.03390000
Br	5.43184300	-0.52377500	0.82284000
C	2.03683700	2.49665500	-0.81802200
H	1.17085700	2.88672400	-1.36549100
H	2.43301600	3.31754900	-0.18264300
H	2.81919600	2.28680600	-1.57543500

Mn-Int₃

Mn	-3.20823200	-0.81869100	-0.37337600
Mn	-0.11906300	-0.18183800	0.60630900
O	-2.06436800	-1.97675300	-1.70286400
O	-3.51411900	0.46886800	1.26540400
O	-4.07867500	0.45093700	-1.88846300
O	-3.48624300	-2.53339900	0.91504000
O	-1.41787600	-1.76138300	1.31910000
O	-2.00507900	1.03720800	-1.28833100
O	-1.39324200	1.19653300	1.63161200
O	0.03382400	-1.25337000	-1.22080200

C	-0.81534300	-1.92656200	-1.86508800
C	-2.64028100	1.17519100	1.83285900
C	-3.04874700	1.19338700	-1.97329800
C	-2.37085100	-2.56696000	1.50489500
H	-0.42723700	-2.56098800	-2.67433300
H	-2.19919400	-3.35848700	2.24529200
H	-3.06938500	2.02654600	-2.69108300
H	-3.02315800	1.85747600	2.60409400
C	2.90642100	-0.57598600	0.78080200
C	3.76082000	0.38645200	-0.06022000
H	2.61425600	-1.41920700	0.14031100
H	3.53115600	-0.98502800	1.59729500
H	4.05450400	1.26446800	0.51546800
C	3.18944800	0.75900900	-1.41273100
H	2.23171000	1.26842900	-1.25519900
H	3.85615300	1.43242800	-1.96059300
H	3.00307700	-0.13293600	-2.02059700
N	1.73637900	0.09821600	1.29335100
Br	5.65310600	-0.49984500	-0.39174200
C	-0.83375900	3.52620300	-0.27805600
O	-1.88589300	4.01441800	-0.11506300
O	0.24484900	3.10869500	-0.44533000
C	2.00422300	0.88064400	2.48470500
H	2.67019900	1.75096900	2.31684200
H	1.06655500	1.28044900	2.88840400
H	2.48335300	0.27387900	3.28264100
Mn-Ts₂			
Mn	-0.03184900	-0.00136700	-1.48968400
Mn	0.03218100	0.00204400	1.48971200

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

O	1.59546244	-2.04200421	3.76064086
C	-0.03928567	1.41465500	4.51226147
H	0.12580325	1.45564174	5.60514720
H	0.92319473	1.64491321	4.03920146
H	-0.73800634	2.23921046	4.26462193
Mn-Int₄			
Mn	0.63218200	0.39569400	-3.72466900
Mn	0.55420300	0.28519700	-0.49868800
O	1.88201800	-1.25126100	-3.28721000
O	-0.66210900	1.99135900	-3.23192300
O	2.24345600	1.67418000	-4.38356000
O	-1.01180600	-0.89025700	-4.24296700
O	-0.87791800	-0.81460300	-2.00402400
O	2.11881100	1.54550300	-2.15223800
O	-0.62032200	1.94447900	-0.95909500
O	1.88956800	-1.22450600	-1.01438400
C	2.23089700	-1.65712500	-2.14577700
C	-0.97422600	2.39617900	-2.07991700
C	2.64110700	1.97576700	-3.21230300
C	-1.39728400	-1.21672000	-3.07825000
H	2.92526700	-2.50329500	-2.13308500
H	-2.25715200	-1.90974000	-3.00991800
H	3.50424000	2.66360000	-3.13040700
H	-1.64767500	3.25902600	-2.04743700
C	-0.17847400	-0.77811900	4.13430000
C	-1.61534200	-0.25400900	4.23815500
H	0.22689600	-0.94223700	5.13888700
H	-0.18722600	-1.73412100	3.60318300
H	-2.07351100	-0.23309600	3.25014300

C	-1.78469600	1.05870200	4.97898200
H	-1.22874600	1.83772400	4.44148400
H	-2.83632500	1.35723300	5.01982700
H	-1.39968200	0.99547500	6.00322300
N	0.68593200	0.16836500	3.44212100
Br	-2.71733900	-1.70673700	5.21691200
C	0.64781100	0.23239500	2.05562900
O	-0.24925000	-0.44307500	1.44528200
O	1.48464400	0.95813600	1.42960700
C	1.73328100	0.84658700	4.18649600
H	2.27787200	1.48996200	3.49456500
H	1.31129000	1.46060200	4.99511100
H	2.43833700	0.12689400	4.63312400

Mn-Ts₃

Mn	-0.03184900	-0.00136700	-1.48968400
Mn	0.03218100	0.00204400	1.48971200
O	1.20841700	-1.53726600	-0.59975100
O	-1.23044100	1.53918100	-0.55670400
O	1.56414500	1.26501500	-1.70518900
O	-1.63223900	-1.27088600	-1.64201700
O	-1.52574100	-1.21727100	0.60826200
O	1.55000600	1.22211000	0.54810200
O	-1.23499300	1.59858300	1.69618300
O	1.30069200	-1.59826400	1.65104100
C	1.61190000	-2.02054100	0.49359500
C	-1.59295300	2.01985300	0.55214600
C	2.00987700	1.60151500	-0.56394000
C	-2.02971100	-1.60385000	-0.48182000
H	2.29366300	-2.88279600	0.44712900

H	-2.88875400	-2.28924300	-0.42970400
H	2.87263900	2.28409900	-0.55019300
H	-2.27927900	2.87952600	0.53277700
C	0.06708766	-0.79568672	7.41743033
C	0.77043288	-2.10258487	7.10645336
H	-1.01347915	-0.99473169	7.54558098
H	0.44051440	-0.37948342	8.35331710
H	1.78482748	-2.05367646	6.74756933
C	0.02886031	-3.41128311	7.10272952
H	-0.58188502	-3.46580567	6.19464123
H	0.72368017	-4.25330957	7.12075494
H	-0.62479280	-3.48766770	7.97693899
N	0.30252549	0.16788164	6.35212865
Br	1.90357738	-2.48804186	9.39286112
C	0.23798345	-0.38476890	5.07055870
O	0.32049257	-1.65233670	5.04581130
O	0.12678268	0.39674197	4.07987097
C	-0.07111382	1.54705216	6.59147591
H	0.15356187	2.12507306	5.69404551
H	-1.14782960	1.65481345	6.81422953
H	0.49874767	1.94813007	7.43919506
Mn-Int₅			
Mn	0.59766900	0.36994800	-3.82632800
Mn	0.66354900	0.37673100	-0.70686700
O	1.88410300	-1.22675800	-3.27578800
O	-0.64150300	1.98728500	-3.22655400
O	2.20579500	1.64594000	-4.29471700
O	-1.02608900	-0.90500600	-4.26372800
O	-0.85847500	-0.79878800	-2.02881400

O	2.16542600	1.57568400	-2.04719800
O	-0.59861900	1.97137600	-0.95816500
O	1.90625100	-1.22260200	-1.00710800
C	2.23971700	-1.65370300	-2.14576900
C	-0.96492600	2.40790900	-2.08470800
C	2.63979500	1.97301700	-3.14634500
C	-1.39818200	-1.21854500	-3.08970400
H	2.92526700	-2.50329500	-2.13308500
H	-2.25715200	-1.90974000	-3.00991800
H	3.50424000	2.66360000	-3.13040700
H	-1.64767500	3.25902600	-2.04743700
C	-0.60847000	-0.26433800	4.45950100
C	-1.62448100	-0.77307600	3.41381200
H	-1.06566700	0.42538300	5.17359600
H	-0.16089500	-1.08364400	5.02910400
H	-1.77468900	-1.84725800	3.50102000
C	-2.94784800	-0.03570600	3.39586800
H	-2.79636500	1.04895900	3.31593700
H	-3.56217700	-0.36779800	2.55136000
H	-3.46462000	-0.27146500	4.33241300
N	0.38039700	0.42150200	3.61470600
Br	-2.52136700	-2.22262900	6.39331100
C	0.17648600	0.16937700	2.31409400
O	-0.92836200	-0.54381600	2.11202000
O	0.91050900	0.54199600	1.37142900
C	1.55408100	1.08443200	4.14053300
H	2.13077000	1.49234600	3.30792900
H	1.25711400	1.89777300	4.81320100
H	2.17799200	0.37649200	4.70252500

Cd-HKUST-1

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

Cd-Int₀

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

O	0.46755300	1.28747600	1.62542600
O	0.47385500	-1.28617500	-1.62626900
C	-0.62660900	-1.66099800	-2.09787700
C	-0.63393500	1.65843800	2.09784900
C	0.62601100	2.10094400	-1.65762900
C	0.63299000	-2.09835700	1.65846700
H	-0.60576800	-2.34573900	-2.96134000
H	0.61455900	-2.96264300	2.34223700
H	0.60583400	2.96566500	-2.34081800
H	-0.61495300	2.34281200	2.96163700
C	4.25892782	-0.12967710	0.20678179
C	4.85656270	-0.60163618	-1.07942506
H	3.51917693	-0.73797445	0.72499056
H	4.87809083	0.49070351	0.85791977
H	5.87768851	-0.25614840	-1.26766073
C	4.50982988	-1.93367678	-1.70450183
H	4.60591328	-1.89139604	-2.79696418
H	5.17695449	-2.72280036	-1.33450756
H	3.47753007	-2.21189350	-1.46728605
N	3.82980225	0.43853807	-1.07253543
C	4.26444408	1.80123854	-1.35613132
H	4.26952188	1.95963326	-2.44055986
H	3.55485850	2.50637359	-0.90846964
H	5.27376836	2.02964816	-0.96592086
Cd-Int₁			
Cd	-3.00806400	0.81333000	0.42162400
Cd	0.31309200	0.46654700	-0.05631400
O	-3.56975400	-0.52978600	-1.30084900
O	-3.70512000	2.16067500	2.09392900

O	-2.35211100	2.42514000	-1.04024200
O	-2.42082800	-0.97889600	1.68267600
O	-0.14836400	-0.84219600	1.65389600
O	-0.07345700	2.39044400	-1.03074700
O	-1.47357900	2.02733300	1.91140700
O	-1.31970500	-0.52236900	-1.27824300
C	-2.43846800	-0.87896000	-1.73814100
C	-2.51988500	2.45400300	2.46084700
C	-1.21537000	2.85355500	-1.34414500
C	-1.26240500	-1.32665400	2.01551200
H	-2.41097400	-1.55953100	-2.59779500
H	-1.19064700	-2.17643500	2.70578200
H	-1.19937200	3.75187300	-1.97727300
H	-2.42015900	3.12902000	3.32518200
C	2.98921300	-1.27628400	0.60560200
C	2.66958800	-1.76573900	-0.75232200
H	2.31553800	-1.48457000	1.43274400
H	4.04814500	-1.16371600	0.83118800
H	3.55937400	-1.91547900	-1.36734900
C	1.48937700	-2.65187600	-1.06369600
H	1.10692200	-2.46712500	-2.07507800
H	1.81395900	-3.69880100	-1.01357500
H	0.66736200	-2.52022700	-0.35258300
N	2.43746000	-0.32438300	-0.40990900
Br	6.24311700	-1.96184400	-0.96745000
C	3.41624100	0.62969500	-0.98566800
H	3.05525900	0.95635700	-1.96734700
H	3.48901400	1.50397100	-0.32810300
H	4.40477800	0.16410700	-1.09127700

Cd-Ts₁

Cd	-1.50986600	-0.00198100	-0.00036500
Cd	1.51071900	0.00200200	0.00018400
O	-1.78629100	-1.33462300	-1.68608400
O	-1.79260900	1.32826600	1.68637600
O	-0.47476200	1.62690200	-1.28702100
O	-0.46878800	-1.62811400	1.28574600
O	1.79157900	-1.68398400	1.33139500
O	1.78554200	1.69009500	-1.32930500
O	0.46755300	1.28747600	1.62542600
O	0.47385500	-1.28617500	-1.62626900
C	-0.62660900	-1.66099800	-2.09787700
C	-0.63393500	1.65843800	2.09784900
C	0.62601100	2.10094400	-1.65762900
C	0.63299000	-2.09835700	1.65846700
H	-0.60576800	-2.34573900	-2.96134000
H	0.61455900	-2.96264300	2.34223700
H	0.60583400	2.96566500	-2.34081800
H	-0.61495300	2.34281200	2.96163700
C	4.66685784	-0.40118769	0.96583737
C	5.16174991	-1.15067761	-0.20929050
H	4.06244868	-0.99325863	1.65445916
H	5.39527500	0.22163459	1.49080137
H	5.88353251	-0.65576846	-0.84408953
C	4.48035156	-2.38612377	-0.73169547
H	3.75037661	-2.13055687	-1.50908327
H	5.22710577	-3.05728064	-1.16262345
H	3.95751393	-2.91445440	0.07078147
N	3.88433067	0.26344785	-0.06117847

Br	7.34342174	-2.26445464	0.84360187
C	4.37873878	1.58846770	-0.42235301
H	3.94601807	1.90182206	-1.37607388
H	4.07915925	2.30927778	0.35210799
H	5.47629338	1.60008986	-0.50107901
Cd-Int₂			
Cd	-2.91058300	0.81910300	0.40377800
Cd	0.46879700	0.40126800	-0.12417200
O	-3.57399000	-0.53002500	-1.30869000
O	-3.69777300	2.14573800	2.09445100
O	-2.42236100	2.48216900	-1.04867000
O	-2.40630200	-0.98781500	1.66760200
O	-0.13048800	-0.92345300	1.56488200
O	-0.14731400	2.36140000	-1.00188600
O	-1.46309400	2.02076400	1.93643700
O	-1.32568500	-0.50600600	-1.27818500
C	-2.43937800	-0.87494500	-1.74054700
C	-2.51818100	2.44495000	2.46923200
C	-1.25841900	2.86005700	-1.33678400
C	-1.24487600	-1.35592600	1.97582900
H	-2.41097400	-1.55953100	-2.59779500
H	-1.19064700	-2.17643500	2.70578200
H	-1.19937200	3.75187300	-1.97727300
H	-2.42015900	3.12902000	3.32518200
C	3.41127200	-0.88095400	-0.08944400
C	3.65918000	-1.95964800	-1.15800100
H	2.95725600	-1.36438700	0.78696600
H	4.38623000	-0.47178700	0.23634000
H	4.04739800	-1.51898300	-2.07626400

C	2.49593000	-2.89562300	-1.42178600
H	1.64057800	-2.29905400	-1.76141700
H	2.73426400	-3.63259300	-2.19547000
H	2.20419300	-3.42597400	-0.50796700
N	2.55204800	0.14848100	-0.61978400
Br	5.30547600	-3.15511200	-0.57643200
C	3.26751100	1.16139300	-1.37291700
H	2.58533000	1.96678400	-1.66869700
H	4.08692000	1.62295900	-0.78068100
H	3.73609200	0.78588400	-2.30618600

Cd-Int₃

Cd	-0.14758800	-0.00655700	-0.45725200
Cd	3.19153300	-0.67069900	0.13352200
O	1.01978500	1.91079400	-0.61672500
O	-0.01830400	-1.88640000	0.73001800
O	2.00871000	0.34277700	1.99030200
O	1.45301700	-0.91635600	-1.84873500
O	3.60234900	-1.56422600	-1.93045000
O	4.18302400	-0.18599700	2.14147200
O	2.15270700	-2.57563400	0.77362100
O	3.24030600	1.41700800	-0.74269300
C	2.23954700	2.16889600	-0.84057400
C	0.91803400	-2.70160100	0.96857700
C	3.09664800	0.28086400	2.61436300
C	2.45137400	-1.42571700	-2.42790400
H	2.45160700	3.19723000	-1.16622900
H	2.29392500	-1.77538500	-3.45657400
H	3.11606700	0.65850200	3.64806500
H	0.60650100	-3.66188000	1.40519100

C	-3.29186900	-0.44876700	-0.76084200
C	-4.25153300	0.08436600	0.31885300
H	-2.93056300	-1.43427500	-0.43634300
H	-3.86321700	-0.60660900	-1.69618800
H	-4.60870700	1.08444500	0.06997700
C	-3.74263900	0.00032100	1.74546400
H	-2.82290200	0.59330400	1.82237200
H	-4.47218700	0.39466500	2.46011900
H	-3.50537500	-1.03451600	2.01711200
N	-2.19397100	0.46920500	-0.94991100
Br	-6.05793600	-1.00442400	0.22529000
C	-0.34558300	4.15540600	0.59386200
O	0.08131500	4.89332500	-0.21058100
O	-0.78847700	3.47193800	1.43163000
C	-2.51666900	1.56432600	-1.84370200
H	-3.30092800	2.24708600	-1.45688700
H	-1.62906700	2.18316200	-2.02609500
H	-2.87828000	1.20657800	-2.83271200
Cd-Ts₂			
Cd	-1.50986600	-0.00198100	-0.00036500
Cd	1.51071900	0.00200200	0.00018400
O	-1.78629100	-1.33462300	-1.68608400
O	-1.79260900	1.32826600	1.68637600
O	-0.47476200	1.62690200	-1.28702100
O	-0.46878800	-1.62811400	1.28574600
O	1.79157900	-1.68398400	1.33139500
O	1.78554200	1.69009500	-1.32930500
O	0.46755300	1.28747600	1.62542600
O	0.47385500	-1.28617500	-1.62626900

C	-0.62660900	-1.66099800	-2.09787700
C	-0.63393500	1.65843800	2.09784900
C	0.62601100	2.10094400	-1.65762900
C	0.63299000	-2.09835700	1.65846700
H	-0.60576800	-2.34573900	-2.96134000
H	0.61455900	-2.96264300	2.34223700
H	0.60583400	2.96566500	-2.34081800
H	-0.61495300	2.34281200	2.96163700
C	-4.49780773	-0.18079731	1.89326597
C	-5.76939850	0.68086755	2.07080028
H	-3.73326665	0.20247139	2.57881260
H	-4.71753967	-1.21659522	2.20117744
H	-6.34942264	0.71566911	1.14937456
C	-5.53352801	2.06153839	2.65394539
H	-4.81209260	2.59170209	2.02162429
H	-6.45723770	2.64715734	2.70555640
H	-5.10720215	1.98931409	3.66080343
N	-3.98800537	-0.14900828	0.51860644
Br	-7.12812135	-0.34722543	3.29848303
C	-4.08892401	1.96743828	-0.59460487
O	-4.81894968	1.67477966	-1.47902158
O	-3.37650742	2.61635367	0.09272058
C	-4.77017674	-1.03816982	-0.34184180
H	-5.81895006	-0.71150967	-0.44203216
H	-4.34488179	-1.05723536	-1.34901048
H	-4.78385482	-2.07698616	0.03666078
Cd-Int₄			
Cd	-3.42938200	0.23465700	0.19514100
Cd	-0.05907000	0.57705400	0.62913200

O	-4.19659600	-1.10541700	-1.49687200
O	-4.08852700	1.57764600	1.91035200
O	-2.92571400	2.03337600	-1.08286200
O	-2.90677800	-1.43394100	1.63356500
O	-0.62952500	-1.30348700	1.63538200
O	-0.64935100	1.99486500	-0.95347400
O	-1.84013700	1.54100600	1.86689700
O	-1.96337200	-0.96685700	-1.33364400
C	-3.01416800	-1.39819900	-1.86922400
C	-2.94688300	1.91746200	2.33676100
C	-1.76311800	2.41193800	-1.37577900
C	-1.74691100	-1.80580200	1.94264400
H	-2.91190200	-2.08317300	-2.72687900
H	-1.69157500	-2.70007700	2.57669800
H	-1.70030000	3.22823100	-2.10635700
H	-2.92108700	2.60537800	3.19609800
C	4.74510500	0.28770800	-0.36932600
C	4.88942700	-1.23411600	-0.26275200
H	5.73776100	0.75226100	-0.36431300
H	4.25285400	0.53192700	-1.31589200
H	3.91928400	-1.70690100	-0.40836900
C	5.59806000	-1.73784000	0.97897600
H	5.66927800	-2.82995300	0.98123300
H	6.60881400	-1.32311300	1.06165900
H	5.01872300	-1.43089800	1.85932600
N	3.98142800	0.83371900	0.74757100
Br	5.95155900	-1.85636200	-1.92380600
C	2.59569800	0.74265900	0.72210800
O	2.06241400	0.02713100	-0.18773700

O	1.90949600	1.35914500	1.60484500
C	4.65124700	1.71423100	1.69116700
H	3.93233900	2.00229700	2.45942200
H	5.50271200	1.20417800	2.16457500
H	5.02600600	2.62704100	1.19746700
Cd-Ts₃			
Cd	-1.50986600	-0.00198100	-0.00036500
Cd	1.51071900	0.00200200	0.00018400
O	-1.78629100	-1.33462300	-1.68608400
O	-1.79260900	1.32826600	1.68637600
O	-0.47476200	1.62690200	-1.28702100
O	-0.46878800	-1.62811400	1.28574600
O	1.79157900	-1.68398400	1.33139500
O	1.78554200	1.69009500	-1.32930500
O	0.46755300	1.28747600	1.62542600
O	0.47385500	-1.28617500	-1.62626900
C	-0.62660900	-1.66099800	-2.09787700
C	-0.63393500	1.65843800	2.09784900
C	0.62601100	2.10094400	-1.65762900
C	0.63299000	-2.09835700	1.65846700
H	-0.60576800	-2.34573900	-2.96134000
H	0.61455900	-2.96264300	2.34223700
H	0.60583400	2.96566500	-2.34081800
H	-0.61495300	2.34281200	2.96163700
C	6.94434212	-0.62517487	0.99971155
C	6.45812666	-2.06238455	0.90169556
H	7.63559063	-0.52558277	1.84043222
H	7.48772545	-0.35069912	0.08577619
H	6.48126191	-2.55963979	-0.05121005

C	6.03854159	-2.81978832	2.13413538
H	5.00174928	-2.57195862	2.38776047
H	6.10896820	-3.89602943	1.96331985
H	6.68225582	-2.56442597	2.98083554
N	5.80215186	0.26629518	1.21775276
Br	8.95234676	-2.95711380	0.87592993
C	4.61810035	-0.19095934	0.70647225
O	4.61170585	-1.41378616	0.34221848
O	3.60056635	0.57860393	0.64442756
C	6.04719742	1.66936306	1.48073024
H	5.08738748	2.17084536	1.61298315
H	6.64672229	1.78083004	2.39282994
H	6.58784092	2.14968773	0.64931790
Cd-Int₅			
Cd	-3.57475500	0.22625700	0.19386100
Cd	-0.32679300	0.40418500	0.40576900
O	-4.18567000	-1.10842500	-1.49645300
O	-4.05975400	1.57351500	1.89893700
O	-2.87765600	1.98916900	-1.06870800
O	-2.87867800	-1.41317400	1.61094500
O	-0.60120500	-1.40350500	1.55139200
O	-0.59985200	1.93730100	-1.08410600
O	-1.80290500	1.55545300	1.87469500
O	-1.95247200	-0.96340800	-1.32230900
C	-3.00041200	-1.39832800	-1.86576600
C	-2.91855100	1.91877600	2.33237900
C	-1.73903200	2.38033200	-1.41935700
C	-1.73672300	-1.83744100	1.90866200
H	-2.91190200	-2.08317300	-2.72687900

H	-1.69157500	-2.70007700	2.57669800
H	-1.70030000	3.22823100	-2.10635700
H	-2.92108700	2.60537800	3.19609800
C	4.90513800	-0.52129900	-0.21555300
C	3.85575200	-1.30670300	-1.03224400
H	5.58942200	-1.18497600	0.31854600
H	5.50792600	0.13566600	-0.84850100
H	3.97491300	-1.13135600	-2.09918000
C	3.78018500	-2.78797200	-0.72409300
H	2.92989800	-3.24636000	-1.24144600
H	4.70941900	-3.24260900	-1.08371300
H	3.67249900	-2.96309700	0.35442300
N	4.06035300	0.23904900	0.71806600
Br	6.89167800	-1.81687900	-2.56402100
C	2.76448000	0.16329300	0.38527100
O	2.56217800	-0.66726300	-0.63807400
O	1.82164200	0.77277000	0.93735200
C	4.59021700	1.13608100	1.72251800
H	3.75746600	1.58464500	2.26830100
H	5.22987900	0.58338000	2.42090000
H	5.18851600	1.92968700	1.25500400

Rh-HKUST-1

O	-1.12153100	1.44627200	-1.49767400
O	-1.12192400	-1.44617100	1.49752300
O	-1.12291800	1.49850200	1.44620900
O	-1.12278300	-1.49841600	-1.44641900
O	1.12155800	-1.49799100	-1.44569100
O	1.12142400	1.49788600	1.44585600
O	1.12243100	-1.44656300	1.49813400

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

Rh-Int₀

O	1.46229400	-1.46182500	-1.13833900
O	-1.46229300	1.46183000	-1.13833600
O	1.46190800	1.46220400	-1.13839000
O	-1.46190900	-1.46220500	-1.13839000
O	-1.46192100	-1.46220400	1.13832900
O	1.46192000	1.46220100	1.13832900
O	-1.46227300	1.46184100	1.13838300
O	1.46227600	-1.46183800	1.13838000
C	1.85720400	-1.85650600	0.00001800
C	-1.85719300	1.85651800	0.00002200
C	1.85675000	1.85695900	-0.00002600
C	-1.85674600	-1.85696700	-0.00002600
H	2.63381900	-2.63267900	0.00002200
H	-2.63318100	-2.63332000	-0.00003600
H	2.63319200	2.63330500	-0.00003400
H	-2.63379500	2.63270400	0.00002700
Rh	-0.00000100	-0.00000100	1.20306600

Rh	-0.00000200	0.00000000	-1.20305800
C	-0.46852954	1.33715229	3.63963147
C	-0.95892610	0.01120905	4.12504535
H	-1.05500551	1.91178141	2.92433803
H	0.13503371	1.93758380	4.32330465
H	-0.64263815	-0.25468153	5.13833530
C	-2.28151420	-0.58128435	3.69494182
H	-2.24346228	-1.67802264	3.70946219
H	-3.08863229	-0.25987924	4.36570718
H	-2.53017541	-0.26594629	2.67609527
N	0.10980498	0.09184770	3.13128568
C	1.45931199	-0.22847475	3.58130465
H	1.61600967	-1.31074744	3.50897484
H	2.18479670	0.26893909	2.92756194
H	1.65969649	0.08373038	4.62319940
Rh-Int₁			
O	-2.62557100	-1.21354900	-1.76458300
O	-2.69554900	0.23171200	2.13515100
O	-3.45025800	1.31004000	-0.49440600
O	-1.88279700	-2.29718700	0.86457000
O	0.22841400	-1.46990200	0.60421600
O	-1.33582700	2.14256600	-0.73934100
O	-0.57250700	1.03780000	1.88799000
O	-0.52260600	-0.36050000	-2.03238500
C	-1.56553000	-0.97136500	-2.41080200
C	-1.64610100	0.81844000	2.52534800
C	-2.60149800	2.19907900	-0.78967400
C	-0.62170100	-2.36009200	0.90795900
H	-1.54298700	-1.34324300	-3.44394800

H	-0.18777600	-3.30691800	1.25165400
H	-3.01694600	3.15534500	-1.13727500
H	-1.66164100	1.19175200	3.55831900
Rh	-0.44774500	0.36506800	-0.08058000
Rh	-2.74696400	-0.52337000	0.19510700
C	2.65172800	0.48443100	0.64401700
C	2.79206000	0.45523800	-0.82495500
H	2.31954600	-0.41220600	1.15654600
H	3.31514900	1.13713200	1.20388800
H	3.52893100	1.15478300	-1.21514400
C	2.63612100	-0.79850300	-1.64417100
H	2.28687400	-0.57058900	-2.65812800
H	3.62935300	-1.25827900	-1.70159000
H	1.93914700	-1.50387400	-1.18683000
N	1.60951200	1.13611000	-0.19503800
Br	6.11617600	0.27545600	0.02727600
C	1.64365300	2.60531600	-0.21875200
H	1.18135800	2.96309700	-1.14314300
H	1.07721700	2.99209600	0.63393600
H	2.67802900	2.96867800	-0.16177600
Rh-Ts₁			
O	-2.64622600	-1.20531500	-1.79329600
O	-2.70807900	0.22079400	2.13011600
O	-3.48189700	1.30578700	-0.50960200
O	-1.88824700	-2.31097000	0.84397700
O	0.22851700	-1.47960700	0.59211000
O	-1.36257000	2.13582900	-0.74705600
O	-0.58348100	1.04003700	1.87605900
O	-0.51497700	-0.40427300	-2.04088200

C	-1.57293500	-0.98206200	-2.42590800
C	-1.65799600	0.81160800	2.50912000
C	-2.62684500	2.18821900	-0.80047600
C	-0.62812500	-2.36537600	0.88909600
H	-1.55575000	-1.35161200	-3.46012500
H	-0.20053900	-3.31528700	1.23547700
H	-3.02970900	3.14697600	-1.15345200
H	-1.67440400	1.18338300	3.54214200
Rh	-0.44931200	0.37095700	-0.09296600
Rh	-2.78119200	-0.53877500	0.18106300
C	2.73856004	1.00925234	0.64589787
C	3.31888519	0.94900653	-0.71320918
H	2.51625300	0.03176860	1.07620419
H	3.24587100	1.66504610	1.35769594
H	3.70202912	1.87042256	-1.12922385
C	3.09993156	-0.21580193	-1.63993374
H	2.22963623	-0.04394365	-2.28457351
H	3.98118008	-0.34648012	-2.27248145
H	2.93407238	-1.13884807	-1.07696107
N	1.60406940	1.59458704	-0.04631955
Br	5.88193383	0.54584807	-0.09919087
C	1.49601944	3.04226362	0.10573889
H	0.82471400	3.44903961	-0.65511849
H	1.08097535	3.27128216	1.09790510
H	2.47885284	3.52974398	0.01994623
Rh-Int₂			
O	-2.62476900	-1.20492100	-1.77286100
O	-2.69538400	0.22798200	2.14443200
O	-3.46565200	1.31422300	-0.49082800

O	-1.87556500	-2.30234800	0.86114600
O	0.24068200	-1.46969400	0.60772900
O	-1.34686400	2.14469800	-0.74083300
O	-0.57425400	1.05437300	1.89153200
O	-0.50232900	-0.38155700	-2.03448000
C	-1.55591000	-0.97368100	-2.40911800
C	-1.64707100	0.82065400	2.52479000
C	-2.61159300	2.19633700	-0.78723200
C	-0.61506700	-2.35634300	0.90550500
H	-1.54298700	-1.34324300	-3.44394800
H	-0.18777600	-3.30691800	1.25165400
H	-3.01694600	3.15534500	-1.13727500
H	-1.66164100	1.19175200	3.55831900
Rh	-0.43051700	0.38673100	-0.07755000
Rh	-2.76450600	-0.53163400	0.19707800
C	2.59180200	0.47161100	0.29735600
C	3.67649700	0.23695500	-0.75885500
H	2.25916000	-0.49867500	0.67910400
H	3.00361300	1.04127700	1.14950300
H	3.98942100	1.17287300	-1.22112400
C	3.35489100	-0.83548200	-1.77968000
H	2.40794600	-0.56235800	-2.26006900
H	4.13895700	-0.92047900	-2.53998600
H	3.22498500	-1.80896700	-1.29375100
N	1.52252900	1.16516200	-0.39930200
Br	5.48698900	-0.32783400	0.20895900
C	1.59379300	2.59545600	-0.15795400
H	0.81718300	3.11425300	-0.72632600
H	1.48208900	2.87020800	0.91224100

H	2.57084300	2.99632200	-0.48750000
Rh-Int₃			
O	-2.40176800	-0.31849600	-2.29670600
O	-3.07313200	-0.93264400	1.77582900
O	-3.52230800	1.29709100	-0.09971300
O	-1.94958800	-2.55469300	-0.42519600
O	0.12328300	-1.73988500	0.10012400
O	-1.42862300	2.12849200	0.31094000
O	-1.00168300	-0.07513700	2.24374900
O	-0.28743600	0.43305000	-1.83607900
C	-1.25732300	0.13442100	-2.59241200
C	-2.12784400	-0.57860000	2.53561100
C	-2.68278500	2.20904700	0.14121300
C	-0.71062000	-2.64626700	-0.19963500
H	-1.07661800	0.29513800	-3.66450000
H	-0.28144700	-3.65418900	-0.27159300
H	-3.09834300	3.22315900	0.21749800
H	-2.30308200	-0.72609300	3.61045000
Rh	-0.54103300	0.23360200	0.22993000
Rh	-2.83308200	-0.66762000	-0.28484300
C	2.46729600	0.12322100	0.57565200
C	3.64917400	0.79233900	-0.13615200
H	2.18684300	-0.77224800	0.01255700
H	2.77006800	-0.20810100	1.58484500
H	3.88723100	1.75906600	0.30645600
C	3.52897000	0.85661200	-1.64594700
H	2.58163800	1.35118800	-1.89066800
H	4.35816900	1.41093700	-2.09711800
H	3.50051000	-0.15005600	-2.07685000

N	1.37906600	1.08984900	0.59649800
Br	5.42295000	-0.27713000	0.30922000
C	1.06083700	3.91904800	-1.13742000
O	1.41070400	4.44173500	-0.15032500
O	0.72486000	3.47478200	-2.16429400
C	1.38050800	1.82261500	1.85518000
H	2.31869700	2.39391000	1.97556200
H	0.55934200	2.54486600	1.86906800
H	1.28070200	1.16648700	2.74163400
Rh-Ts₂			
O	-2.39692600	-0.38668000	-2.28793100
O	-3.09564100	-0.92515700	1.78672700
O	-3.52338000	1.27435000	-0.13681600
O	-1.95724600	-2.58062400	-0.36726300
O	0.12858900	-1.75394300	0.07453100
O	-1.44663700	2.09514700	0.36349500
O	-0.99900900	-0.13958800	2.24697500
O	-0.33023500	0.47314500	-1.81803700
C	-1.27459900	0.11779300	-2.58158700
C	-2.13718100	-0.60912200	2.54595800
C	-2.69253000	2.18353700	0.14950100
C	-0.71116600	-2.66782400	-0.18355600
H	-1.08413500	0.27009700	-3.65298500
H	-0.28896400	-3.67923000	-0.26007800
H	-3.10586000	3.19811800	0.22901300
H	-2.31059900	-0.75113400	3.62196500
Rh	-0.54624900	0.22098700	0.23875400
Rh	-2.82902800	-0.68761300	-0.27196400
C	2.39580175	0.28216232	0.97176849

C	3.41674979	-0.15406753	-0.08680023
H	1.94084463	-0.61543778	1.41517316
H	2.95560157	0.78154070	1.77417790
H	3.92731250	0.69938390	-0.52692097
C	2.96557084	-1.14387248	-1.13427500
H	2.12959236	-0.69646399	-1.68088263
H	3.77291584	-1.35965521	-1.84234991
H	2.62360113	-2.07617666	-0.67669931
N	1.36254558	1.21296106	0.46855564
Br	5.00634038	-1.04128672	0.97510202
C	1.97490362	2.50948728	-1.11915120
O	2.61944314	3.31641704	-0.52729990
O	1.42769438	2.07197491	-2.08173969
C	1.04381268	2.16286645	1.54094317
H	1.91939386	2.79324289	1.76325936
H	0.23502848	2.82129623	1.22002810
H	0.73936350	1.65678695	2.46935596

Rh-Int₄

O	2.24000700	-1.28274000	-3.27545000
O	-0.73172500	1.62845300	-3.29570300
O	2.21842000	1.65830800	-3.27557600
O	-0.70681600	-1.29835100	-3.28813200
O	-0.71075300	-1.29340600	-1.00222200
O	2.24493700	1.63972100	-0.98943600
O	-0.66975800	1.68555800	-1.01161400
O	2.21603300	-1.31557200	-0.98992000
C	2.61407800	-1.68212300	-2.13197600
C	-1.08735300	2.03839100	-2.14798300
C	2.61623700	2.03285400	-2.13190000

C	-1.09319700	-1.67991800	-2.14156900
H	3.39643700	-2.45635900	-2.13575500
H	-1.87056300	-2.45700000	-2.13581300
H	3.39581000	2.80962500	-2.13581100
H	-1.87117700	2.80902400	-2.13575000
Rh	0.75031300	0.17739700	-0.89120800
Rh	0.75626100	0.17732000	-3.36093700
C	-0.91522700	0.62149200	4.28098200
C	-2.17968100	-0.25519900	4.28488800
H	-1.22556600	1.63455700	3.97655400
H	-0.50262200	0.69615500	5.28993400
H	-2.09801300	-1.05197400	3.55245000
C	-3.48375800	0.50433300	4.16550100
H	-3.47069800	1.00190200	3.18782000
H	-4.34747200	-0.16554000	4.21297100
H	-3.58463300	1.26174000	4.95224400
N	0.12587300	0.12253600	3.39756500
Br	-2.26113000	-1.37433000	6.07221400
C	-0.15622400	0.25834100	2.01176500
O	-1.33922900	0.46061900	1.68847300
O	0.87628000	0.13798300	1.24485700
C	1.49816100	0.17607400	3.87627800
H	2.14344100	-0.29958700	3.13744500
H	1.85796300	1.21040700	4.02630800
H	1.57898300	-0.36212800	4.82920300
Rh-Ts₃			
O	1.46229400	-1.46182500	-1.13833900
O	-1.46229300	1.46183000	-1.13833600
O	1.46190800	1.46220400	-1.13839000

O	-1.46190900	-1.46220500	-1.13839000
O	-1.46192100	-1.46220400	1.13832900
O	1.46192000	1.46220100	1.13832900
O	-1.46227300	1.46184100	1.13838300
O	1.46227600	-1.46183800	1.13838000
C	1.85720400	-1.85650600	0.00001800
C	-1.85719300	1.85651800	0.00002200
C	1.85675000	1.85695900	-0.00002600
C	-1.85674600	-1.85696700	-0.00002600
H	2.63381900	-2.63267900	0.00002200
H	-2.63318100	-2.63332000	-0.00003600
H	2.63319200	2.63330500	-0.00003400
H	-2.63379500	2.63270400	0.00002700
Rh	-0.00000100	-0.00000100	1.20306600
Rh	-0.00000200	0.00000000	-1.20305800
C	0.64525777	-0.88824324	6.91905485
C	1.34430146	-2.16797540	6.50311320
H	-0.41494471	-1.11648533	7.13709696
H	1.09323657	-0.49267298	7.83086402
H	2.32081771	-2.08413914	6.05637650
C	0.63252161	-3.49297311	6.52274375
H	-0.05667581	-3.53357181	5.67188207
H	1.34329736	-4.31861036	6.45043141
H	0.06240796	-3.61181056	7.44912772
N	0.76340822	0.11322583	5.86935833
Br	2.68747761	-2.59759158	8.66449280
C	0.59449181	-0.40069490	4.58119585
O	0.70048478	-1.66459514	4.50723650
O	0.37800173	0.40839896	3.63088737

C	0.38467455	1.47514116	6.18677322
H	0.51523998	2.08588592	5.29239515
H	-0.66944152	1.55062312	6.50878308
H	1.02056882	1.86294857	6.99267474
Rh-Int₅			
O	2.22787400	-1.29180900	-3.27883400
O	-0.70946800	1.64035000	-3.28163000
O	2.22807000	1.64447200	-3.27833700
O	-0.70904900	-1.28763700	-3.28182200
O	-0.69722800	-1.29963500	-0.99968800
O	2.23140400	1.64692300	-0.99570900
O	-0.69824400	1.65182700	-0.99924100
O	2.23141100	-1.29385700	-0.99637700
C	2.61780200	-1.68051400	-2.13706500
C	-1.09276400	2.03338900	-2.13844300
C	2.61762000	2.03321400	-2.13655500
C	-1.09230800	-1.68156900	-2.13873200
H	3.39643700	-2.45635900	-2.13575500
H	-1.87056300	-2.45700000	-2.13581300
H	3.39581000	2.80962500	-2.13581100
H	-1.87117700	2.80902400	-2.13575000
Rh	0.75974500	0.17514900	-0.90752600
Rh	0.75864200	0.17597700	-3.35143600
C	-0.93565400	0.21580800	4.26851700
C	-1.99661300	-0.04070600	3.19118300
H	-0.97771900	1.24632300	4.65709200
H	-1.05724400	-0.48118000	5.10316000
H	-2.28947000	-1.09441600	3.20231300
C	-3.21423100	0.85282800	3.23297000

H	-2.92792400	1.91134100	3.18649900
H	-3.88575500	0.63049700	2.39587900
H	-3.73516600	0.64837900	4.17584300
N	0.29637800	0.01271900	3.50200100
Br	-3.24616100	-1.34401400	6.36036700
C	0.05588000	0.12288600	2.17666200
O	-1.25373900	0.17239500	1.92307700
O	0.93642000	0.17556600	1.29722300
C	1.61694900	0.10505000	4.08522000
H	2.35910100	-0.07761600	3.30536300
H	1.78875800	1.10269300	4.51759000
H	1.72359800	-0.64275000	4.87904600

Y-HKUST-1

O	-1.49911500	-1.49387200	1.12624000
O	1.49892700	1.49449900	1.12589000
O	-1.49413400	1.49931000	1.12595100
O	1.49422800	-1.49875700	1.12635600
O	1.49367300	-1.49966100	-1.12579200
O	-1.49386100	1.49907900	-1.12620200
O	1.49955800	1.49339700	-1.12626100
O	-1.49922600	-1.49410900	-1.12591000
C	-1.90820300	-1.90109100	0.00022300
C	1.90813300	1.90119000	-0.00025800
C	-1.90125400	1.90806900	-0.00020800
C	1.90122400	-1.90806900	0.00032900
H	-2.68735300	-2.67771600	0.00034300
H	2.67745500	-2.68761300	0.00046300
H	-2.67760600	2.68749200	-0.00038800
H	2.68790900	2.67718700	-0.00043200

Y	-0.00000500	-0.00017300	-1.44390400
Y	-0.00000500	0.00021800	1.44377700
Y-Int₀			
O	-1.59210600	1.59187700	-1.12926100
O	1.59202800	-1.59321000	-1.12756900
O	-1.59257200	-1.59272100	-1.12751700
O	1.59254400	1.59141500	-1.12936700
O	1.59245900	1.59283600	1.12746300
O	-1.59239800	-1.59147500	1.12931900
O	1.59222300	-1.59174400	1.12926500
O	-1.59212200	1.59311000	1.12757100
C	-1.99761900	1.99745600	-0.00106800
C	1.99726900	-1.99780000	0.00107500
C	-1.99772600	-1.99732200	0.00115400
C	1.99780600	1.99728900	-0.00119000
H	-2.77547300	2.77650000	-0.00150600
H	2.77607800	2.77591600	-0.00165700
H	-2.77616200	-2.77578400	0.00165200
H	2.77606300	-2.77590300	0.00151900
Y	0.00004700	0.00091600	1.60465300
Y	-0.00003000	-0.00089400	-1.60463000
C	0.58219324	-1.62524108	4.12346050
C	1.14237446	-0.34423224	4.65209481
H	1.12125968	-2.18859742	3.36330631
H	-0.02368783	-2.23253857	4.79897030
H	0.86980554	-0.11382791	5.68655719
C	2.47403947	0.21449224	4.20513619
H	2.48199699	1.30997998	4.27099161
H	3.28807365	-0.17007716	4.83292737

H	2.67684608	-0.06230177	3.16514901
N	0.04012546	-0.33530729	3.69229564
C	-1.27992203	0.01718540	4.20172302
H	-1.39381277	1.10705791	4.18420882
H	-2.04585905	-0.41956688	3.55078827
H	-1.45981617	-0.33538098	5.23444065
Y-Int₀			
O	-1.59210600	1.59187700	-1.12926100
O	1.59202800	-1.59321000	-1.12756900
O	-1.59257200	-1.59272100	-1.12751700
O	1.59254400	1.59141500	-1.12936700
O	1.59245900	1.59283600	1.12746300
O	-1.59239800	-1.59147500	1.12931900
O	1.59222300	-1.59174400	1.12926500
O	-1.59212200	1.59311000	1.12757100
C	-1.99761900	1.99745600	-0.00106800
C	1.99726900	-1.99780000	0.00107500
C	-1.99772600	-1.99732200	0.00115400
C	1.99780600	1.99728900	-0.00119000
H	-2.77547300	2.77650000	-0.00150600
H	2.77607800	2.77591600	-0.00165700
H	-2.77616200	-2.77578400	0.00165200
H	2.77606300	-2.77590300	0.00151900
Y	0.00004700	0.00091600	1.60465300
Y	-0.00003000	-0.00089400	-1.60463000
C	0.58219324	-1.62524108	4.12346050
C	1.14237446	-0.34423224	4.65209481
H	1.12125968	-2.18859742	3.36330631
H	-0.02368783	-2.23253857	4.79897030

H	0.86980554	-0.11382791	5.68655719
C	2.47403947	0.21449224	4.20513619
H	2.48199699	1.30997998	4.27099161
H	3.28807365	-0.17007716	4.83292737
H	2.67684608	-0.06230177	3.16514901
N	0.04012546	-0.33530729	3.69229564
C	-1.27992203	0.01718540	4.20172302
H	-1.39381277	1.10705791	4.18420882
H	-2.04585905	-0.41956688	3.55078827
H	-1.45981617	-0.33538098	5.23444065
Y-Int₁			
O	-2.65159700	1.83253100	1.61362800
O	-3.33575800	-1.01455100	-1.83878300
O	-3.61149900	-1.21290600	1.31370100
O	-2.36420500	2.03526500	-1.58110100
O	-0.23630600	1.26160300	-1.49846200
O	-1.47326900	-1.94351500	1.44410200
O	-1.20288800	-1.75534000	-1.68480100
O	-0.52620400	1.06765900	1.79363300
C	-1.49277900	1.80931700	2.12136400
C	-2.36064900	-1.72789700	-2.19994800
C	-2.70413100	-1.97347900	1.74680800
C	-1.13757000	2.05697700	-1.88940100
H	-1.30646300	2.51446600	2.94556600
H	-0.81543000	2.85573700	-2.57368600
H	-3.01797200	-2.74582800	2.46814300
H	-2.52671800	-2.40407900	-3.05173700
Y	-0.36007400	-0.47896800	0.03598400
Y	-3.45913400	0.58996600	-0.15259300

C	2.59229300	-0.80192900	1.69424800
C	3.14096700	-1.01903300	0.33144000
H	1.89620700	-1.52402200	2.13245200
H	3.19504100	-0.26132600	2.42227300
H	4.12772600	-0.57998400	0.13147600
C	2.81499700	-2.24251700	-0.49213000
H	2.70705200	-1.96973800	-1.55374100
H	3.64211000	-2.95348800	-0.43630700
H	1.89773400	-2.75437500	-0.16728800
N	2.06203400	-0.01115200	0.55882900
Br	6.27912300	0.37725700	-0.30450000
C	2.52473000	1.39382500	0.51961500
H	2.41297400	1.76407800	-0.50286500
H	1.89765100	1.98747500	1.19298100
H	3.58232000	1.47866400	0.79886600
Y-Ts₁			
O	-1.59210600	1.59187700	-1.12926100
O	1.59202800	-1.59321000	-1.12756900
O	-1.59257200	-1.59272100	-1.12751700
O	1.59254400	1.59141500	-1.12936700
O	1.59245900	1.59283600	1.12746300
O	-1.59239800	-1.59147500	1.12931900
O	1.59222300	-1.59174400	1.12926500
O	-1.59212200	1.59311000	1.12757100
C	-1.99761900	1.99745600	-0.00106800
C	1.99726900	-1.99780000	0.00107500
C	-1.99772600	-1.99732200	0.00115400
C	1.99780600	1.99728900	-0.00119000
H	-2.77547300	2.77650000	-0.00150600

H	2.77607800	2.77591600	-0.00165700
H	-2.77616200	-2.77578400	0.00165200
H	2.77606300	-2.77590300	0.00151900
Y	0.00004700	0.00091600	1.60465300
Y	-0.00003000	-0.00089400	-1.60463000
C	-1.17431222	-0.23228312	4.85067767
C	-0.01817136	-1.02388428	5.32426476
H	-1.90763837	-0.80466068	4.28087501
H	-1.64738159	0.42781421	5.58181600
H	0.66089870	-0.54380670	6.01510797
C	0.42672483	-2.29481945	4.65319915
H	1.19069628	-2.08896487	3.89393557
H	0.85138595	-2.96974188	5.40014961
H	-0.41482832	-2.79680004	4.16712770
N	-0.14466512	0.36988480	4.02238343
Br	-1.04837795	-2.04577018	7.56104753
C	0.29062036	1.68686555	4.47697368
H	1.24281661	1.94840078	4.00799257
H	-0.46042047	2.43568142	4.18659919
H	0.40517845	1.71667852	5.5710242

Y-Int₂

O	-1.71520500	1.66933300	-2.99719000
O	1.56753900	-1.40258500	-2.98774000
O	-1.71698000	-1.40570500	-2.99461400
O	1.57054200	1.67210500	-2.99995800
O	1.52145200	1.72710400	-0.73737300
O	-1.66323100	-1.46429800	-0.73258800
O	1.53334400	-1.46268200	-0.72474100
O	-1.67043700	1.73103900	-0.73460100

C	-2.08908100	2.10410300	-1.87143500
C	1.94593300	-1.83737400	-1.86386500
C	-2.08826200	-1.83947300	-1.86852800
C	1.94341200	2.10352200	-1.87335200
H	-2.84808600	2.90872800	-1.87353900
H	2.70346500	2.90814400	-1.87369000
H	-2.84877500	-2.64355600	-1.87038100
H	2.70345000	-2.64367500	-1.87051400
Y	-0.07691200	0.13444100	-0.16404700
Y	-0.07299100	0.13232800	-3.59076300
C	-0.46058700	-0.82341900	3.03870400
C	0.75392500	-1.47382900	3.72215600
H	-1.02615800	-1.61510900	2.52396000
H	-1.12906000	-0.40416900	3.81209200
H	1.40162100	-0.71974600	4.16930700
C	1.52861800	-2.45666400	2.86775300
H	1.87189600	-1.94388000	1.96128300
H	2.40069300	-2.85377700	3.39737100
H	0.89311000	-3.29558600	2.56153000
N	-0.03798500	0.19131700	2.09585700
Br	0.10810300	-2.49829400	5.44500200
C	0.26138000	1.46299900	2.73818800
H	0.49955700	2.22441900	1.98140600
H	-0.59641500	1.84503200	3.32756400
H	1.13047700	1.43143000	3.42357500
Y-Int₃			
O	-1.36212700	1.90248100	-3.02957700
O	2.32871500	-0.68217400	-2.97585700
O	-0.78622100	-1.26765800	-3.07764000

O	1.77067000	2.45467100	-2.94931200
O	1.82929400	2.43740800	-0.68526100
O	-0.82509600	-1.25037000	-0.80964100
O	2.36670600	-0.72655900	-0.70948100
O	-1.28843200	2.00231800	-0.76570300
C	-1.78989200	2.25983800	-1.89659300
C	2.80128500	-1.02931000	-1.85937200
C	-1.12884200	-1.71179200	-1.94556600
C	2.12253500	2.90392000	-1.82586300
H	-2.71088300	2.86481200	-1.88925800
H	2.76050900	3.80311600	-1.83294600
H	-1.77197500	-2.60719600	-1.94799600
H	3.70000300	-1.66832000	-1.89165500
Y	0.49402700	0.60459800	-0.19210700
Y	0.48644000	0.60371100	-3.57053700
C	-1.19913800	-0.60502500	2.45344200
C	-0.70362100	-1.73531200	3.36610100
H	-1.72178200	-1.06055800	1.60229800
H	-1.93729800	0.00374100	3.00587800
H	-0.11481900	-1.35093600	4.19668700
C	-0.01472100	-2.88184700	2.65685000
H	0.87797100	-2.49038600	2.15320900
H	0.29404100	-3.66812000	3.35484800
H	-0.67213400	-3.31656100	1.89352500
N	-0.09373900	0.21213700	1.98015300
Br	-2.35565300	-2.53499300	4.41022300
C	3.46568800	-0.35505800	2.59564800
O	3.39591400	-1.37778500	3.16116100
O	3.56408400	0.67449200	2.05177700

C	0.29136000	1.22339500	2.94955400
H	0.77788700	0.82344000	3.86074900
H	1.01403700	1.92767600	2.51131300
H	-0.57091300	1.82306500	3.29782200
Y-Ts₂			
O	-1.82928617	1.31390621	-1.12758345
O	1.84781305	-1.28656118	-1.12900616
O	-1.29083032	-1.82465928	-1.16134178
O	1.30940235	1.85204007	-1.09530101
O	1.29070904	1.82474899	1.16128700
O	-1.30923882	-1.85207909	1.09525291
O	1.82938804	-1.31376060	1.12758920
O	-1.84787969	1.28644151	1.12900517
C	-2.30675550	1.63069375	0.00087712
C	2.30647782	-1.63109724	-0.00087844
C	-1.63084303	-2.30626048	-0.04143036
C	1.63093685	2.30623675	0.04139388
H	-3.20519806	2.26690712	0.00121069
H	2.26619416	3.20521147	0.05752239
H	-2.26629015	-3.20510072	-0.05752769
H	3.20568749	-2.26622435	-0.00118596
Y	-0.01316493	-0.01948194	1.60448052
Y	0.01318688	0.01950101	-1.60445802
C	-1.29980536	-0.31584378	4.79691211
C	-0.81748945	-1.68081825	5.29694428
H	-2.19120147	-0.45710260	4.16713856
H	-1.60504220	0.28709548	5.66365629
H	-0.02618652	-1.57385935	6.03737112
C	-0.44916645	-2.68842798	4.22968714

H	0.43003704	-2.31446049	3.69033547
H	-0.18278683	-3.65323178	4.67281330
H	-1.26169766	-2.82783246	3.51113138
N	-0.25015076	0.38779464	4.05065358
Br	-2.35850709	-2.46165281	6.45240637
C	1.67816525	0.80565905	4.76967146
O	1.68161180	1.37285119	5.82140788
O	2.14117696	0.05340724	3.96670367
C	-0.63437123	1.80584710	4.00164483
H	-0.76858697	2.17362907	4.99744729
H	0.13543482	2.36733149	3.51478356
H	-1.54963217	1.90876811	3.45703058

Y-Int₄

O	3.51494600	2.21765600	0.06133700
O	4.15675000	-2.24531800	0.46709800
O	3.93676500	-0.24239700	-1.99289100
O	3.72978000	0.21766900	2.50958600
O	1.49658600	-0.16340500	2.44064400
O	1.69570900	-0.57682500	-2.05624700
O	1.91701600	-2.57224300	0.39736400
O	1.27351700	1.88627600	-0.01990800
C	2.31685500	2.60207400	-0.03046600
C	3.11941400	-2.96184500	0.48259300
C	2.84019600	-0.44946300	-2.58227000
C	2.59179800	0.07400700	3.03248300
H	2.15846600	3.68897100	-0.13731800
H	2.54582500	0.16121100	4.13170800
H	2.87693500	-0.52280900	-3.68310100
H	3.26426200	-4.05064700	0.58674000

Y	1.05657800	-0.43908400	0.18095700
Y	4.38096800	0.07200800	0.26943700
C	-4.57407600	0.80941300	0.28031400
C	-5.30413500	0.40655900	-1.00501800
H	-4.90452200	1.80599200	0.59545100
H	-4.82395100	0.09334000	1.06868600
H	-5.07781200	-0.63164000	-1.24394300
C	-5.10787400	1.33181000	-2.19054600
H	-4.04021900	1.35210600	-2.44367800
H	-5.66097500	0.97953600	-3.06646100
H	-5.43240400	2.35336800	-1.96103500
N	-3.13153700	0.84406900	0.07863000
Br	-7.32783000	0.33212400	-0.56177500
C	-2.43595400	-0.37354200	0.13070000
O	-3.07556900	-1.43094800	0.19561000
O	-1.13586200	-0.27501400	0.08919900
C	-2.46619300	2.13787900	0.12115200
H	-1.40527500	2.01031100	-0.08905700
H	-2.89511300	2.81757900	-0.62814300
H	-2.57047300	2.61257500	1.11090200
Y-Ts₃			
O	3.58164900	2.37304500	-0.12739300
O	4.21863400	-2.09348700	0.28360100
O	3.99216400	-0.06012800	-2.17874500
O	3.81808000	0.33661400	2.33545900
O	1.57845500	-0.02498000	2.26960100
O	1.75662700	-0.41061600	-2.22551900
O	1.97947800	-2.41494400	0.20393700
O	1.33656200	2.04561100	-0.20900000

C	2.38215600	2.75960700	-0.21549800
C	3.18150200	-2.80705600	0.30184400
C	2.89934600	-0.27810100	-2.76281500
C	2.67322900	0.21138100	2.85744200
H	2.22369400	3.84392700	-0.32197900
H	2.61105300	0.31616700	3.94704700
H	2.94216300	-0.36785300	-3.86776200
H	3.32949000	-3.89569100	0.40207900
Y	1.14670300	-0.27362400	0.01131800
Y	4.43976100	0.22451600	0.09101600
C	-4.55087900	0.72394200	-0.54486500
C	-5.00623700	-0.65086800	-0.07158200
H	-4.80474700	0.84638600	-1.61063800
H	-5.08295700	1.49893600	0.00948100
H	-5.00334900	-0.85270200	0.98660500
C	-5.45667600	-1.70914200	-1.04671700
H	-4.58069300	-2.14572900	-1.54001700
H	-6.00636500	-2.50107200	-0.53284200
H	-6.11371700	-1.27626100	-1.80585500
N	-3.11390900	0.90833700	-0.33946400
Br	-7.45013600	0.13094000	0.47280900
C	-2.37171000	-0.22600700	-0.14767300
O	-3.02851700	-1.30049700	-0.01028200
O	-1.09299400	-0.14143000	-0.10286400
C	-2.54475900	2.20773500	-0.63710800
H	-1.48091700	2.20074800	-0.39723200
H	-2.66681800	2.46339100	-1.70175000
H	-3.04373800	2.98126800	-0.03877500

Y-Int₅

O	3.51051300	2.21695600	0.05368500
O	4.15326600	-2.24369000	0.48542200
O	3.94554200	-0.22469600	-2.00220500
O	3.72747700	0.18506000	2.50640800
O	1.49466800	-0.18081800	2.44379900
O	1.71149200	-0.60693900	-2.04894600
O	1.91523500	-2.56957100	0.43629300
O	1.26725300	1.89385500	0.04344300
C	2.31128500	2.60562300	-0.01318000
C	3.11814600	-2.96263200	0.50361100
C	2.84563600	-0.45230900	-2.58403400
C	2.59164600	0.05652000	3.03598700
H	2.15846600	3.68897100	-0.13731800
H	2.54582500	0.16121100	4.13170800
H	2.87693500	-0.52280900	-3.68310100
H	3.26426200	-4.05064700	0.58674000
Y	1.08384800	-0.44221500	0.19737000
Y	4.34241100	0.06968200	0.25268900
C	-4.24954800	1.26326000	-1.36207900
C	-4.50603900	-0.24984800	-1.29475100
H	-4.26254100	1.64689000	-2.39433900
H	-4.99627700	1.80083900	-0.76954300
H	-5.05060900	-0.49082700	-0.38016400
C	-5.18992700	-0.86352400	-2.49603500
H	-4.65377400	-0.63076900	-3.42364300
H	-5.25608500	-1.95242100	-2.38439900
H	-6.20563200	-0.45314500	-2.53543000
N	-2.89067700	1.35424700	-0.81336000

Br	-7.57348300	1.14918000	-0.34565700
C	-2.30083600	0.14980700	-0.78684400
O	-3.14043600	-0.82337900	-1.14098900
O	-1.11640300	-0.09585700	-0.46662500
C	-2.21163300	2.61500700	-0.58741900
H	-1.18144500	2.42739700	-0.27987600
H	-2.20597500	3.20929100	-1.51070800
H	-2.73465300	3.18528000	0.18899800

V-HKUST-1

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

V-Int₀

V	0.00009800	0.00002700	-1.29549400
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V	-0.00010200	-0.00002600	1.29549600
O	-0.00128100	2.03527700	-1.12227000
O	0.00145900	-2.03523100	-1.12235200
O	-2.06617000	-0.00134500	-1.12908700
O	2.06634000	0.00139000	-1.12878100
O	2.06616600	0.00131400	1.12908100
O	-2.06634000	-0.00136000	1.12877500
O	0.00125800	-2.03527400	1.12227400
O	-0.00142300	2.03523000	1.12235700
C	-0.00161000	2.62186400	0.00005600
C	0.00161500	-2.62186400	-0.00005100
C	-2.64047100	-0.00154900	-0.00020000
C	2.64046900	0.00154500	0.00019400
H	-0.00245100	3.71941100	0.00007900
H	3.73974200	0.00252300	0.00027900
H	-3.73974400	-0.00251700	-0.00028200
H	0.00246100	-3.71941000	-0.00007200
C	-0.48118066	1.09948201	-3.80741641
C	0.86442733	0.69485959	-4.31718176
H	-0.56927712	1.85437008	-3.02755718
H	-1.32149358	1.06090763	-4.50354989
H	0.88268764	0.36718650	-5.36111150
C	2.14981048	1.31859043	-3.82319111
H	2.98247960	0.60678266	-3.89016503
H	2.40856169	2.20217237	-4.42068404
H	2.05064770	1.62402162	-2.77619670
N	0.12569344	-0.16842588	-3.39780294
C	-0.46362641	-1.38025020	-3.95500726
H	0.28291808	-2.18251476	-3.94305627

H	-1.31056586	-1.68869788	-3.33156384
H	-0.82409563	-1.25518041	-4.99307766
V-Int₁			
V	0.62119000	0.42404100	-3.21747000
V	0.63757400	0.45776000	-0.35797900
O	0.61630300	2.56318300	-3.17962200
O	0.61477000	-1.68482600	-3.17982200
O	-1.45595200	0.43220700	-3.06415600
O	2.68888000	0.43752400	-2.97995800
O	2.75774100	0.46749300	-0.70757900
O	-1.43315300	0.51489400	-0.79706700
O	0.69346500	-1.53496000	-0.93092500
O	0.69339500	2.40035800	-0.94256200
C	0.64685700	3.06114200	-2.02511700
C	0.64990300	-2.17836400	-2.01772100
C	-2.00368900	0.46353100	-1.92409100
C	3.27816100	0.44950000	-1.85894200
H	0.63563600	4.16058200	-1.91684400
H	4.37782900	0.44369400	-1.91664400
H	-3.10165700	0.43865400	-1.91720500
H	0.64054800	-3.27823900	-1.91699500
C	-0.62545900	0.34557300	2.47325500
C	-0.52526300	-1.11416700	2.32454500
H	-1.35557500	0.88835200	1.87762700
H	-0.38985400	0.77139500	3.44435200
H	-0.16314700	-1.61414100	3.22044000
C	-1.47838400	-1.93648600	1.49962700
H	-0.99735300	-2.85334800	1.13824800
H	-2.30847400	-2.20619200	2.16261800

H	-1.86256400	-1.37990900	0.64229100
N	0.51357000	-0.23531900	1.67916900
Br	-2.22812800	-1.15736600	5.29014900
C	1.82239100	-0.24468600	2.35596600
H	2.42346900	-1.06542100	1.95209400
H	2.34914000	0.69750800	2.16546900
H	1.70950800	-0.37657500	3.43988200
V-Ts₁			
V	0.00009800	0.00002700	-1.29549400
V	-0.00010200	-0.00002600	1.29549600
O	-0.00128100	2.03527700	-1.12227000
O	0.00145900	-2.03523100	-1.12235200
O	-2.06617000	-0.00134500	-1.12908700
O	2.06634000	0.00139000	-1.12878100
O	2.06616600	0.00131400	1.12908100
O	-2.06634000	-0.00136000	1.12877500
O	0.00125800	-2.03527400	1.12227400
O	-0.00142300	2.03523000	1.12235700
C	-0.00161000	2.62186400	0.00005600
C	0.00161500	-2.62186400	-0.00005100
C	-2.64047100	-0.00154900	-0.00020000
C	2.64046900	0.00154500	0.00019400
H	-0.00245100	3.71941100	0.00007900
H	3.73974200	0.00252300	0.00027900
H	-3.73974400	-0.00251700	-0.00028200
H	0.00246100	-3.71941000	-0.00007200
C	-0.60160803	0.39446040	4.32476084
C	-0.62580655	-1.01709907	4.76577458
H	-1.47513923	0.69974234	3.74700261

H	-0.32775074	1.13739955	5.07784115
H	0.13881135	-1.33125196	5.46258332
C	-1.42422514	-2.07693807	4.05668579
H	-0.81604525	-2.58063352	3.29581932
H	-1.76219212	-2.82171566	4.78116974
H	-2.30072957	-1.64450971	3.56555712
N	0.48479094	-0.10867684	3.50290872
Br	-2.08523694	-0.77867061	6.98433005
C	1.81389507	0.24971104	3.98829966
H	2.56800072	-0.38626717	3.51726032
H	2.02437752	1.29644849	3.72534957
H	1.88386444	0.14591856	5.08159302
V-Int₂			
V	0.63922700	0.44405600	-3.23640500
V	0.63125000	0.44145400	-0.42657200
O	0.64510400	2.57304400	-3.16693700
O	0.63377300	-1.68862700	-3.16538700
O	-1.45478700	0.44695200	-3.04405600
O	2.73170200	0.43637200	-3.04250200
O	2.73574600	0.46444000	-0.76394400
O	-1.46030300	0.41174100	-0.76604700
O	0.66325000	-1.55632100	-0.90671900
O	0.61524200	2.43720600	-0.90780700
C	0.63243300	3.06349000	-2.00870000
C	0.64559600	-2.18155400	-2.00970500
C	-2.00485800	0.43240700	-1.90902700
C	3.28034700	0.44856300	-1.90636300
H	0.63563600	4.16058200	-1.91684400
H	4.37782900	0.44369400	-1.91664400

H	-3.10165700	0.43865400	-1.91720500
H	0.64054800	-3.27823900	-1.91699500
C	-0.60005300	0.38142400	2.33057600
C	-0.70287700	-0.99940600	2.99616700
H	-1.48021700	0.53286800	1.69647800
H	-0.60626800	1.16141900	3.11015700
H	0.18628900	-1.22498300	3.58397000
C	-1.07526700	-2.13783900	2.07014200
H	-0.32690800	-2.19331400	1.27054600
H	-1.10266100	-3.09592900	2.60146400
H	-2.04980700	-1.96014400	1.60278300
N	0.60720300	0.46607000	1.52449200
Br	-2.15102300	-0.90718200	4.52354500
C	1.79593900	0.75926400	2.30912400
H	2.65864400	0.86621300	1.64490100
H	1.68032000	1.70193600	2.87803700
H	2.04331900	-0.02837200	3.04482200
V-Int₃			
V	3.20789700	-1.74440200	0.71516800
V	0.60780400	0.04677200	0.51342400
O	3.84134100	0.07904900	1.20173500
O	1.77485300	-3.02524300	0.20078200
O	3.47339100	-1.25435000	-1.33774900
O	2.77209600	-2.12001700	2.78047800
O	0.95533600	-0.82831000	2.47327500
O	1.58278700	-0.00811300	-1.37486300
O	-0.21560300	-1.97554500	-0.00047200
O	2.13364100	1.55800000	1.14077000
C	3.33039400	1.24302000	1.31523900

C	0.52373100	-2.98155800	-0.04796500
C	2.60844500	-0.50818500	-1.89844900
C	1.70823900	-1.54701600	3.17635000
H	4.06754800	2.02157400	1.59876100
H	1.40240300	-1.68435100	4.24118100
H	2.75896200	-0.25726200	-2.97449000
H	0.09380400	-3.96318800	-0.33206000
C	-1.72798500	0.68880700	-1.26747400
C	-3.18599400	1.11231500	-1.03483300
H	-1.67709700	-0.40544900	-1.20236900
H	-1.42193100	0.96488400	-2.29153600
H	-3.26559500	2.18380700	-0.85766100
C	-3.93712100	0.29163300	-0.00334600
H	-3.37433500	0.30372300	0.93738400
H	-4.94223800	0.68461400	0.18196800
H	-4.01907600	-0.75265800	-0.32445900
N	-0.85904300	1.30059200	-0.26761700
Br	-4.28453800	0.94184300	-2.83999700
C	-1.81500100	2.17527700	2.06365300
O	-1.44732400	1.24869600	2.68720400
O	-2.26506000	3.18735900	1.66650200
C	-0.39804900	2.60290900	-0.73784200
H	-1.21988700	3.33159900	-0.86714500
H	0.30376300	3.03782500	-0.01685900
H	0.12710500	2.52791700	-1.71119600
V-Ts₂			
V	3.23995600	-1.18983100	0.08411700
V	0.67178800	0.53789500	-0.09056100
O	3.92241600	0.60220800	0.57958200

O	1.83566500	-2.52006900	-0.42457200
O	3.41959600	-0.67081400	-1.94802400
O	2.72201900	-1.50552000	2.09871200
O	0.87374800	-0.20798700	1.91395900
O	1.54469700	0.60796500	-2.06035200
O	-0.10772900	-1.41305800	-0.66539300
O	2.19166600	2.03651500	0.46541200
C	3.38782100	1.76458900	0.67158600
C	0.59214900	-2.45017800	-0.69267900
C	2.57979200	0.07832500	-2.53966400
C	1.67063000	-0.94776800	2.54575700
H	4.08712300	2.57335900	0.96531400
H	1.42197800	-1.13256600	3.60773400
H	2.77853700	0.29452300	-3.60793700
H	0.11337900	-3.41140300	-0.96550700
C	-2.50705200	0.64162400	-0.69602600
C	-3.21059600	0.09274500	0.55064700
H	-2.18271800	-0.19751200	-1.31682500
H	-3.26001200	1.20739300	-1.26139700
H	-3.86185200	0.82725400	1.00397300
C	-2.40532500	-0.67550800	1.56904400
H	-1.68712900	0.01098000	2.02971800
H	-3.05743100	-1.06497800	2.35782400
H	-1.85385700	-1.50082000	1.11404000
N	-1.30501200	1.52057300	-0.51313600
Br	-4.65973000	-1.24843900	-0.24469800
C	-1.45533585	3.14599261	0.96179242
O	-0.86522916	2.73451356	1.96831455
O	-2.25696552	3.96607440	0.48043219

C	-1.05018800	2.15886100	-1.83385600
H	-1.91663100	2.76709300	-2.13721700
H	-0.17857800	2.80661500	-1.75119100
H	-0.86537800	1.38994400	-2.58971900
V-Int₄			
V	-0.82190600	-0.65992400	-3.97320300
V	-0.86806200	-0.66621900	-1.11619100
O	-0.83485300	1.40842600	-3.83950100
O	-0.82591300	-2.72444300	-3.77810500
O	-2.97503000	-0.66592800	-3.92932100
O	1.30216300	-0.63902200	-3.98732600
O	1.11762200	-0.74264900	-1.74394100
O	-2.85236800	-0.69815800	-1.68456000
O	-0.91501500	-2.78139200	-1.50233000
O	-0.93617300	1.39544500	-1.56699800
C	-0.87710900	1.95148500	-2.69429700
C	-0.86563100	-3.29963700	-2.64883800
C	-3.48930100	-0.67963800	-2.77938800
C	1.77836200	-0.68348500	-2.81509600
H	-0.86016200	3.04480500	-2.69842200
H	2.88203100	-0.67208300	-2.69822200
H	-4.59745500	-0.67712300	-2.69878300
H	-0.85525000	-4.39401600	-2.69857300
C	1.96702900	0.04459600	3.49199000
C	1.82911300	1.47960400	3.99369000
H	2.82835800	0.05125400	2.80732300
H	2.20956700	-0.61801000	4.32997300
H	1.26236600	2.07180600	3.27994500
C	3.14971400	2.13141500	4.36091900

H	3.75835600	2.21388400	3.44943800
H	2.99980000	3.13705300	4.77244300
H	3.70421100	1.53654200	5.09635600
N	0.80542500	-0.46968100	2.79587300
Br	0.60048900	1.51682900	5.67063800
C	0.64506100	-0.04792000	1.45929100
O	1.34017200	0.89622600	1.05572300
O	-0.24757000	-0.71155500	0.78738100
C	0.18224100	-1.68375200	3.29628900
H	-0.73320300	-1.86504200	2.73088500
H	0.83502200	-2.56958200	3.18362600
H	-0.06646000	-1.56329300	4.35930000
V-Ts₃			
V	0.00009800	0.00002700	-1.29549400
V	-0.00010200	-0.00002600	1.29549600
O	-0.00128100	2.03527700	-1.12227000
O	0.00145900	-2.03523100	-1.12235200
O	-2.06617000	-0.00134500	-1.12908700
O	2.06634000	0.00139000	-1.12878100
O	2.06616600	0.00131400	1.12908100
O	-2.06634000	-0.00136000	1.12877500
O	0.00125800	-2.03527400	1.12227400
O	-0.00142300	2.03523000	1.12235700
C	-0.00161000	2.62186400	0.00005600
C	0.00161500	-2.62186400	-0.00005100
C	-2.64047100	-0.00154900	-0.00020000
C	2.64046900	0.00154500	0.00019400
H	-0.00245100	3.71941100	0.00007900
H	3.73974200	0.00252300	0.00027900

H	-3.73974400	-0.00251700	-0.00028200
H	0.00246100	-3.71941000	-0.00007200
C	-0.62833276	-0.16929951	7.04091101
C	-0.89945887	-1.62108076	6.71964204
H	-1.59521248	0.36495759	7.09904082
H	-0.10270414	-0.00628512	7.98202611
H	-0.07209039	-2.24858171	6.43347749
C	-2.30013432	-2.16948097	6.72021539
H	-2.78225436	-1.90123928	5.77352982
H	-2.29344715	-3.25616548	6.82595178
H	-2.87980348	-1.74832441	7.54722808
N	0.19246866	0.34373411	5.95378445
Br	-0.32910852	-2.44736860	9.09707824
C	-0.17003994	-0.14651298	4.69670245
O	-0.90499546	-1.20855458	4.85473145
O	0.26504345	0.44905247	3.66685233
C	0.76645848	1.66547195	6.10394948
H	1.33083928	1.90014365	5.20041634
H	-0.00648786	2.44249626	6.24300249
H	1.43731068	1.68642733	6.97213815

V-Int₅

V	-0.84422500	-0.66941000	-4.00443500
V	-0.87426700	-0.66948000	-1.14679400
O	-0.85310800	1.39056800	-3.81320100
O	-0.85692700	-2.73149500	-3.79734000
O	-3.00225000	-0.66959900	-3.97722100
O	1.27856300	-0.66997800	-3.95961700
O	1.12337900	-0.68182200	-1.71354600
O	-2.81652300	-0.68403100	-1.74365100

O	-0.88797100	-2.76274200	-1.52277700
O	-0.90457200	1.40196200	-1.54026800
C	-0.87270400	1.95023200	-2.67653300
C	-0.86699500	-3.29894800	-2.66499400
C	-3.49263100	-0.67640700	-2.81944400
C	1.77481500	-0.67402600	-2.79817500
H	-0.86016200	3.04480500	-2.69842200
H	2.88203100	-0.67208300	-2.69822200
H	-4.59745500	-0.67712300	-2.69878300
H	-0.85525000	-4.39401600	-2.69857300
C	1.60839700	0.16120000	3.65044100
C	1.63654900	1.40358900	2.75021900
H	2.57766800	-0.36081400	3.67657200
H	1.32285900	0.43837700	4.67013900
H	0.94394500	2.15502300	3.13803300
C	2.99598000	2.01021200	2.49522100
H	3.69268800	1.26603200	2.08989400
H	2.92076700	2.84631400	1.79130800
H	3.36906100	2.38614000	3.45451700
N	0.61258700	-0.66546800	2.96179800
Br	1.82569500	2.54903800	6.14736600
C	0.41755300	-0.23281600	1.70391700
O	1.05165300	0.91410600	1.47174400
O	-0.27764700	-0.81747400	0.84419100
C	0.14857100	-1.94041300	3.46527000
H	-0.56397800	-2.36225400	2.75390100
H	0.98946300	-2.63759500	3.58833000
H	-0.33667400	-1.80147100	4.43744100

Fe-HKUST-1

Fe	0.00000400	0.00000500	-1.21633500
Fe	0.00000500	0.00001900	1.21676100
O	-0.00099300	2.02372700	-1.12416800
O	0.00099600	-2.02370800	-1.12418000
O	-2.04877200	-0.00085600	-1.13025500
O	2.04878000	0.00087300	-1.13024900
O	2.04741900	0.00020400	1.12977300
O	-2.04741300	-0.00030000	1.12976700
O	0.00011300	-2.02465000	1.12409800
O	-0.00014600	2.02466600	1.12411100
C	-0.00094300	2.60182200	-0.00020800
C	0.00091900	-2.60180300	-0.00021700
C	-2.61849000	-0.00089100	0.00001100
C	2.61849700	0.00083600	0.00001700
H	-0.00133000	3.70067700	-0.00073300
H	3.71843500	0.00149900	0.00081400
H	-3.71842800	-0.00158200	0.00080600
H	0.00130500	-3.70065900	-0.00074700

Fe-Int₀

Fe	2.08189600	0.17900800	0.11497100
Fe	-0.40849200	-0.12431200	-0.10423600
O	1.73140400	1.11307400	1.86571500
O	2.24637200	-0.77047500	-1.65419200
O	1.92777000	1.94485100	-0.89810600
O	2.20048900	-1.58366900	1.12762600
O	-0.06113300	-1.61255300	1.24936300
O	-0.21272800	1.40876000	-1.40789400
O	0.06908400	-1.40250800	-1.64065300

O	-0.50018500	1.20651300	1.47498200
C	0.55432400	1.49109200	2.11093300
C	1.25172400	-1.41638100	-2.08385000
C	0.82722200	2.12770000	-1.47967100
C	1.09628800	-2.04739500	1.51643600
H	0.43969900	2.13664100	2.96787800
H	1.13018700	-2.91871500	2.15490900
H	0.74774400	2.99628900	-2.11763800
H	1.44155100	-2.05839400	-2.93001700
C	-3.12515900	-0.20517610	1.15939467
C	-3.47263100	0.43634790	-0.13884933
H	-2.56658200	0.35962490	1.90013567
H	-3.77127800	-0.98817010	1.55213867
H	-4.35743100	0.03875390	-0.63824033
C	-3.16856700	1.88324590	-0.44572933
H	-2.96656200	2.02506590	-1.51316233
H	-4.03275600	2.50192090	-0.17317733
H	-2.30063900	2.23661290	0.11658967
N	-2.36336500	-0.54468910	-0.06234733
C	-2.63905200	-1.87464310	-0.63369933
H	-2.38692700	-1.86654810	-1.69721933
H	-2.01042600	-2.61263310	-0.12817033
H	-3.69526800	-2.15521910	-0.51097833

Fe-Int₁

Fe	0.41363200	0.38750400	-3.40221400
Fe	0.43476100	0.37554500	-0.32656900
O	0.43027400	2.38701500	-3.16538700
O	0.38077600	-1.62675500	-3.21714400
O	-1.61384400	0.40640000	-3.25390200

O	2.41333600	0.35951800	-3.14917200
O	2.44529600	0.73484900	-0.91078500
O	-1.53858400	0.07693700	-1.01468000
O	0.86089500	-1.58140900	-1.00232800
O	0.16586100	2.41016000	-0.91206800
C	0.25229100	2.94980500	-2.03766100
C	0.64506700	-2.15709100	-2.09189200
C	-2.12942100	0.20658000	-2.11134300
C	2.97995500	0.58483400	-2.03290000
H	0.16676800	4.04024100	-2.08194300
H	4.07038600	0.65494100	-2.08214700
H	-3.21841300	0.13651000	-2.07931300
H	0.68529200	-3.24854700	-2.08292200
C	-1.29493900	0.45761500	2.22708500
C	-0.69086900	-0.88366300	2.37621300
H	-2.01877200	0.64304200	1.43809100
H	-1.37627200	1.05344800	3.13383900
H	-0.36304000	-1.08418200	3.39812800
C	-1.11107400	-2.08819600	1.57201000
H	-0.27036300	-2.77563800	1.42216200
H	-1.88808000	-2.61891400	2.13722400
H	-1.51613800	-1.81674200	0.59399400
N	0.09683200	0.22192500	1.73141900
Br	-0.68888000	-0.16600800	5.86520000
C	1.17652900	0.79984500	2.56718400
H	2.10104000	0.24325200	2.37959900
H	1.32541900	1.84639500	2.27831700
H	0.91939200	0.73848000	3.63277500

Fe-Ts₁

Fe	-0.00054000	0.00014700	-1.19374800
Fe	0.00043500	-0.00007400	1.38086100
O	-0.13713400	1.95079900	-1.17840300
O	0.13623600	-1.95043800	-1.17885200
O	-1.95153200	-0.13651000	-1.17669200
O	1.95024600	0.13690000	-1.17787000
O	2.01767200	0.14682800	1.08565800
O	-2.01670200	-0.14757100	1.08688500
O	0.14807200	-2.01741900	1.08457700
O	-0.14636900	2.01725700	1.08504600
C	-0.18192700	2.54923900	-0.06284000
C	0.18197500	-2.54915300	-0.06344900
C	-2.54928000	-0.18205000	-0.06084300
C	2.54909600	0.18186500	-0.06253000
H	-0.25933300	3.64443700	-0.10280800
H	3.64428500	0.25913700	-0.10301200
H	-3.64451400	-0.25929400	-0.10017800
H	0.25919100	-3.64435100	-0.10378700
C	-0.84370735	-0.04461675	4.50088603
C	-0.71590529	-1.48361221	4.77568157
H	-1.77685350	0.23249229	4.00647297
H	-0.64401658	0.61849042	5.35003678
H	0.13306269	-1.78896987	5.37035130
C	-1.43218598	-2.52786627	3.96746680
H	-0.94633046	-2.66217146	2.99442120
H	-1.42452809	-3.48024623	4.50373850
H	-2.47370171	-2.23617832	3.79854518
N	0.26951819	-0.21705300	3.57222128

Br	-2.08602279	-1.79161606	7.05185281
C	1.54863978	0.16454665	4.15971108
H	2.37025304	-0.18506969	3.52841449
H	1.62838323	1.26401735	4.24854339
H	1.69020987	-0.25066436	5.17146290
Fe-Int₂			
Fe	0.42636200	0.39872400	-3.36359500
Fe	0.42044300	0.40231400	-0.21084300
O	0.46876600	2.41873400	-3.21177500
O	0.38776900	-1.62174900	-3.20331800
O	-1.57911000	0.43789600	-3.16728700
O	2.43415300	0.35312700	-3.17523100
O	2.43234500	0.74688700	-0.93766800
O	-1.58296100	0.03632800	-0.93111300
O	0.77459300	-1.59979300	-0.96482100
O	0.06809400	2.38567200	-0.97606000
C	0.23243400	2.94886400	-2.07627100
C	0.61796700	-2.15726200	-2.07025200
C	-2.12774800	0.20134400	-2.04203900
C	2.97948300	0.58743400	-2.04807300
H	0.16676800	4.04024100	-2.08194300
H	4.07038600	0.65494100	-2.08214700
H	-3.21841300	0.13651000	-2.07931300
H	0.68529200	-3.24854700	-2.08292200
C	-0.67412500	0.05055500	2.56764000
C	-0.41544700	-1.33018100	3.18844100
H	-1.59807000	-0.00092600	1.97557700
H	-0.83954300	0.78864500	3.37349100
H	0.54099500	-1.35423100	3.71045500

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

Fe-Int₃

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

C	-1.08623800	0.27930100	2.24378700
C	-0.89928900	-0.91254800	3.18664100
H	-1.87689700	0.03378300	1.52470900
H	-1.42969300	1.15384400	2.82434600
H	-0.07583500	-0.74534000	3.88233900
C	-0.82807700	-2.26691600	2.51008400
H	0.00006600	-2.25288400	1.79193800
H	-0.65956200	-3.07419700	3.23132500
H	-1.75177800	-2.47394300	1.95697200
N	0.16679300	0.53889400	1.56411100
Br	-2.53397100	-0.98370100	4.55302100
C	3.16840700	-1.43822700	2.35109000
O	3.51699400	-0.53989600	3.01579500
O	2.85995900	-2.36761500	1.71241200
C	0.98824600	1.49772600	2.28104500
H	1.24358400	1.18543000	3.31178400
H	1.93487300	1.65115500	1.75137800
H	0.49017900	2.48667900	2.36969500
Fe-Ts₂			
Fe	-0.00054000	0.00014700	-1.19374800
Fe	0.00043500	-0.00007400	1.38086100
O	-0.13713400	1.95079900	-1.17840300
O	0.13623600	-1.95043800	-1.17885200
O	-1.95153200	-0.13651000	-1.17669200
O	1.95024600	0.13690000	-1.17787000
O	2.01767200	0.14682800	1.08565800
O	-2.01670200	-0.14757100	1.08688500
O	0.14807200	-2.01741900	1.08457700
O	-0.14636900	2.01725700	1.08504600

C	-0.18192700	2.54923900	-0.06284000
C	0.18197500	-2.54915300	-0.06344900
C	-2.54928000	-0.18205000	-0.06084300
C	2.54909600	0.18186500	-0.06253000
H	-0.25933300	3.64443700	-0.10280800
H	3.64428500	0.25913700	-0.10301200
H	-3.64451400	-0.25929400	-0.10017800
H	0.25919100	-3.64435100	-0.10378700
C	-1.12298391	0.36312497	4.39020238
C	-1.37220752	-1.07755720	4.84549566
H	-2.03342770	0.73713938	3.88899411
H	-0.99203983	0.97439312	5.29642969
H	-0.56553959	-1.43891035	5.48133987
C	-1.74440312	-2.08355568	3.78160191
H	-0.88645389	-2.22392821	3.11404872
H	-1.98816934	-3.05437762	4.22558416
H	-2.59035999	-1.73628275	3.18122847
N	0.06582503	0.51622176	3.53688521
Br	-2.94389774	-0.98453252	6.22571264
C	1.82267617	-0.62138833	4.46716708
O	2.33759068	0.24139375	5.10187846
O	1.66778366	-1.71846019	4.04101553
C	0.51019323	1.91520285	3.61531058
H	0.83212448	2.16544583	4.63875418
H	1.36467210	2.07494967	2.94984571
H	-0.28368178	2.62103855	3.31835858
Fe-Int₄			
Fe	1.12086800	-0.00840000	-0.18289700
Fe	4.21467100	0.03957200	0.33342600

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

O	-0.73989200	0.26315600	-0.61464700
C	-2.93405800	1.42736700	-1.70073300
H	-2.00122800	1.92826100	-1.44333300
H	-2.97194900	1.30937300	-2.79876500
H	-3.77983900	2.05067300	-1.38821700
Fe-Ts₃			
Fe	-0.00054000	0.00014700	-1.19374800
Fe	0.00043500	-0.00007400	1.38086100
O	-0.13713400	1.95079900	-1.17840300
O	0.13623600	-1.95043800	-1.17885200
O	-1.95153200	-0.13651000	-1.17669200
O	1.95024600	0.13690000	-1.17787000
O	2.01767200	0.14682800	1.08565800
O	-2.01670200	-0.14757100	1.08688500
O	0.14807200	-2.01741900	1.08457700
O	-0.14636900	2.01725700	1.08504600
C	-0.18192700	2.54923900	-0.06284000
C	0.18197500	-2.54915300	-0.06344900
C	-2.54928000	-0.18205000	-0.06084300
C	2.54909600	0.18186500	-0.06253000
H	-0.25933300	3.64443700	-0.10280800
H	3.64428500	0.25913700	-0.10301200
H	-3.64451400	-0.25929400	-0.10017800
H	0.25919100	-3.64435100	-0.10378700
C	-1.00708114	-1.02417704	-6.83827108
C	-2.25004568	-1.62145767	-6.22783997
H	-0.25888142	-1.83323119	-6.94572319
H	-1.11228683	-0.54202685	-7.81088504
H	-2.99323866	-0.96522000	-5.80682000

C	-2.41538269	-3.11251134	-6.11612085
H	-1.88581791	-3.45397789	-5.21983720
H	-3.47021503	-3.38427577	-6.03793778
H	-1.99543778	-3.61581496	-6.99271913
N	-0.57556742	-0.02760888	-5.87134793
Br	-3.56939848	-1.37466074	-8.38975472
C	-0.70980957	-0.44723469	-4.53299711
O	-1.57179699	-1.45381809	-4.56896212
O	-0.07752461	0.18271053	-3.64240963
C	0.51157584	0.84809724	-6.25804862
H	0.73447347	1.50804569	-5.41838421
H	1.43156608	0.28959491	-6.51245234
H	0.22024190	1.44738510	-7.13051056

Fe-Int₅

Fe	0.47524900	0.43435600	1.22564400
Fe	0.48181900	0.44958100	4.15248500
O	0.52230600	2.55906100	1.61324500
O	0.47066400	-1.67341900	1.59877900
O	-1.50486700	0.46858200	1.79144500
O	2.48098800	0.39856400	1.78202500
O	2.49231000	0.79861600	4.01441100
O	-1.52612300	0.08807600	4.02565500
O	0.83244800	-1.47828100	3.83628400
O	0.12892600	2.37488200	3.84670300
C	0.29700100	3.01111000	2.75345200
C	0.67872600	-2.12035300	2.74645100
C	-2.06967800	0.24725300	2.89164600
C	3.03870500	0.63413500	2.88247800
H	0.22571900	4.09020300	2.86410000

H	4.12933700	0.70490300	2.86389600
H	-3.15946200	0.18647200	2.86673000
H	0.74424300	-3.19858500	2.86312100
C	0.31524200	-0.61851200	-4.00751300
C	-0.89349500	-1.20249100	-3.25919100
H	1.11068300	-1.36404400	-4.16903500
H	0.00749500	-0.20890900	-4.96749200
H	-1.80058200	-0.68017800	-3.56657800
C	-1.07624600	-2.70249400	-3.33142000
H	-0.23784000	-3.21584900	-2.84869500
H	-2.00658100	-2.99827700	-2.81352800
H	-1.15494400	-2.98554800	-4.38556700
N	0.76597500	0.40440500	-3.06064900
Br	-2.01620000	-1.14852500	-6.32107200
C	0.27668900	0.15830800	-1.83171700
O	-0.63311300	-0.81168300	-1.84620600
O	0.61296900	0.76513100	-0.79449700
C	1.85052600	1.32418300	-3.32516100
H	1.97086800	1.98296100	-2.46287200
H	2.79245600	0.78327200	-3.49794800
H	1.62021600	1.91992300	-4.21508900