

## *Electronic Supplementary Information*

### **Computational design of metal hydrides on a defective metal–organic framework HKUST-1 for ethylene dimerization**

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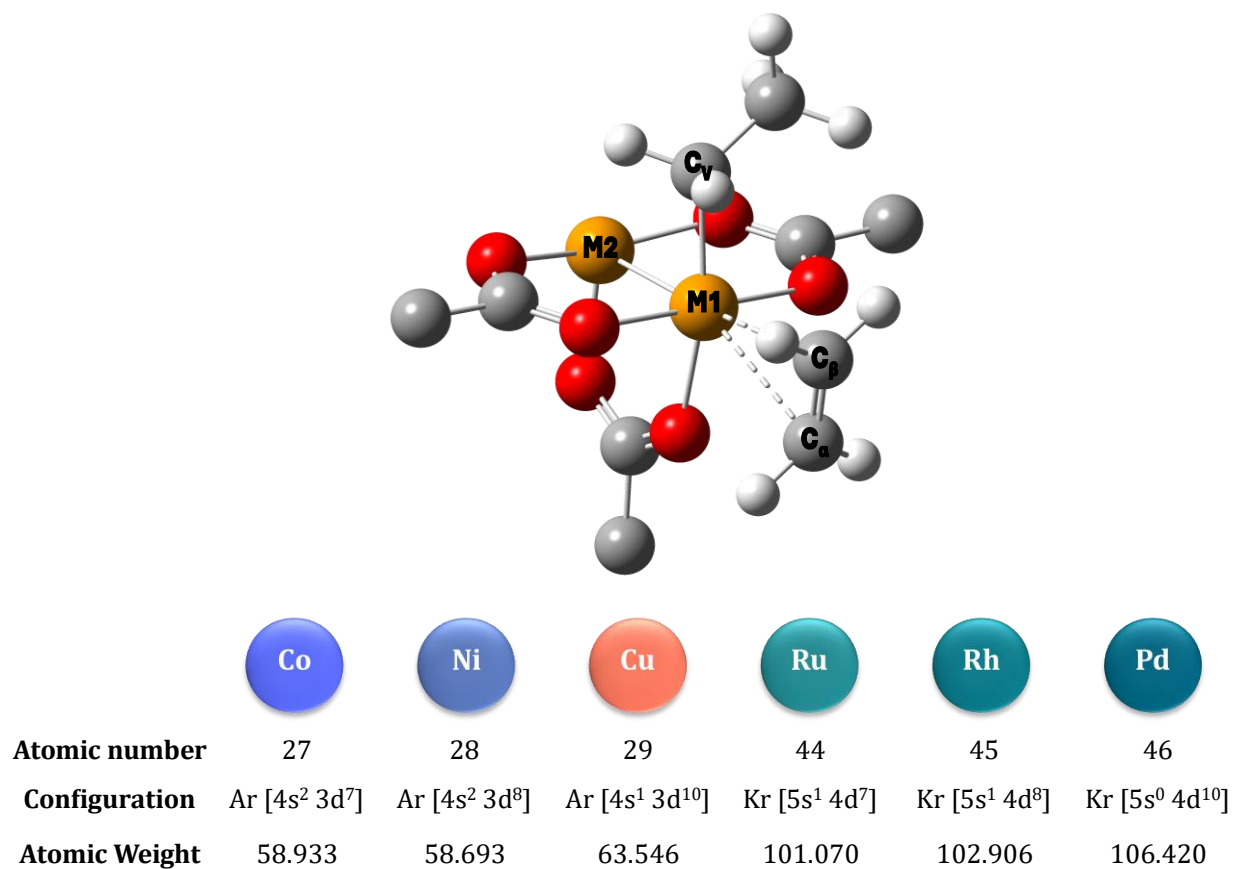
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## S1. Heterogeneous Catalysts for ethylene dimerization

**Table S1.** Heterogeneous catalysts for ethylene dimerization.

Catalyst	TOF (h <sup>-1</sup> )	Butene Selectivity (%)	Temperature (°C)	Pressure (bar)	Reference
NiSO <sub>4</sub> -Al <sub>2</sub> O <sub>3</sub>	46	100	20	0.4	1
NiSO <sub>4</sub> -Al <sub>2</sub> O <sub>3</sub> -ZrO <sub>2</sub>	223	100	20	0.4	2
Ni-SiO <sub>2</sub> -Al <sub>2</sub> O <sub>3</sub>	N.A.	83.9	275	1	3
NiO-TiO <sub>2</sub> /SO <sub>4</sub> <sup>2-</sup>	5.2	100	20	0.4	4
NiO-ZrO <sub>2</sub> /WO <sub>3</sub>	32.6	100	20	0.4	5
NiO-ZrO <sub>2</sub> /MoO <sub>3</sub>	21.5	100	20	0.4	6
NiO/Al <sub>2</sub> O <sub>3</sub> -TiO <sub>2</sub> /WO <sub>3</sub>	12.1	100	20	0.4	7
NiO-ZrO <sub>2</sub> /SO <sub>4</sub> <sup>2-</sup>	8.1	100	20	0.4	8
Ni-MCM-22	876	81	150	40	9
Ni-MCM-36	4193	81	70	40	9
Ni/sulphated alumina	752	88.8	50	0.7	10
Ni-MIL101	10455	95	25	30	11
MFU-4l(Ni)	41500	96	25	50	12
NU-1000(Ni)	16	99	45	2	13
DHKUST-1(Ru)	204	99	50 (80)	5 (55)	14-15
DHKUST-1(Rh)	1	99	50	5	15
Ni-MOF-5	352000	35	35	50	16

## S2. Transition metals



**Fig. S1.** Transition metals used in the design of H-M-DHKUST-1.

### S3. Stability and multiplicity tests

**Table S2.** Stability on H-Co-DHKUST-1.

Multiplicity state	Stability	$E^{\text{ele}}$ (Hartree)	$\Delta E$ (kcal/mol)
Closed-shell singlet	Instable	-4578.8193	10.79
Open-shell singlet		-4578.8274	5.77
Triplet	Stable	-4578.8255	6.91
Quintet		-4578.8365	0.00
Septet		-4578.8042	20.27

**Table S3.** Stability on H-Ni-DHKUST-1.

Multiplicity state	Stability	$E^{\text{ele}}$ (Hartree)	$\Delta E$ (kcal/mol)
Closed-shell singlet	Instable	-4829.9137	29.09
Open-shell singlet		-4829.9418	11.46
Triplet	Stable	-4829.9601	0.00
Quintet		-4829.8950	41.12

**Table S4.** Stability on H-Cu-DHKUST-1.

Multiplicity state	Stability	$E^{\text{ele}}$ (Hartree)	$\Delta E$ (kcal/mol)
Closed-shell singlet	Stable	-5094.2746	0.00
Triplet		-5094.2387	22.54

\*Only closed shell exists. The stability calculation of open shell leads to closed shell.

**Table S5.** Stability on H-Ru-DHKUST-1.

Multiplicity state	Stability	$E^{\text{ele}}$ (Hartree)	$\Delta E$ (kcal/mol)
Closed-shell singlet	Instable	-2003.1617	12.38
Open-shell singlet		-2003.1735	5.00
Triplet	Stable	-2003.1815	0.00
Quintet		-2003.1800	0.91
Septet		-2003.1071	46.64
Nonet		-2002.9843	123.74

**Table S6.** Stability on H-Rh-DHKUST-1.

Multiplicity state	Stability	$E^{\text{ele}}$ (Hartree)	$\Delta E$ (kcal/mol)
Closed-shell singlet*		-2034.5180	0.00
Triplet	Stable	-2034.4993	11.76
Quintet		-2034.4682	31.26
Septet		-2034.3847	83.65

\*Only closed shell exists. The stability calculation of open shell leads to closed shell.

**Table S7.** Stability on H-Pd-DHKUST-1.

Multiplicity state	Stability	$E^{\text{ele}}$ (Hartree)	$\Delta E$ (kcal/mol)
Closed-shell singlet	Instable	-2069.1608	1.56
Open-shell singlet		-2069.1633	0.00
Triplet	Stable	-2069.1596	2.36
Quintet		-2069.0488	71.89

**Table S8.** Stable configurations and electronic energies of intermediates and transition states on H-Cu-DHKUST-1 and H-Rh-DHKUST-1.

Species	H-Cu-DHKUST-1		H-Rh-DHKUST-1	
	Stable configuration	$E^{\text{ele}}$ (kcal/mol)	Stable configuration	$E^{\text{ele}}$ (kcal/mol)
<b>1</b>	Closed shell	-5094.2746		-2034.5180
<b>2</b>	Open shell	-5172.8125		-2113.1441
<b>TS2-3</b>		-5172.7796		-2113.1327
<b>3</b>	Closed shell	-5172.8374		-2113.1333
<b>4</b>		-5251.3676	Closed shell	-2191.7193
<b>TS4-5</b>	Open shell	-5251.3323		-2191.6499
<b>5</b>	Closed shell	-5251.4040		-2191.6821
<b>6</b>		-5251.4006		-2191.7234
<b>TS6-7</b>	Open shell	-5251.3481		-2191.6946
<b>7</b>		-5251.3829		-2191.7108

#### S4. Optimized M-M bond distances and NBO analysis

**Table S9.** Optimized M-M bond distances ( $\text{\AA}$ ), NBO charges ( $Q$  in terms of  $e$ ), and NBO spin density distributions ( $\rho$ ) in ground-state intermediates and transition states on H-Co-DHKUST-1.

	Multiplicity	$\ell_{\text{Co1-Co2}}$	$Q_{\text{Co1}}$	$\rho_{\text{Co1}}$	$Q_{\text{Co2}}$	$\rho_{\text{Co2}}$
<b>1</b>	5	2.45	0.537	1.514	0.985	2.351
<b>2</b>	5	2.37	0.397	1.294	1.028	2.498
<b>TS<sub>2-3</sub></b>	3	2.46	0.138	-0.300	0.977	2.219
<b>3</b>	5	2.41	0.699	1.511	1.009	2.389
<b>4</b>	5	2.44	0.619	1.521	1.006	2.367
<b>TS<sub>4-5</sub></b>	3	2.61	0.348	-0.076	0.871	2.083
<b>5</b>	7	2.8	0.931	2.553	1.094	2.580
<b>6</b>	7	2.70	0.880	2.515	1.078	2.537
<b>TS<sub>6-7</sub></b>	3	2.47	0.158	-0.257	0.961	2.189
<b>7</b>	5	2.44	0.490	1.312	1.015	2.452

**Table S10.** Optimized M-M bond distances ( $\text{\AA}$ ), NBO charges ( $Q$  in terms of  $e$ ), and NBO spin density distributions ( $\rho$ ) in ground-state intermediates and transition states on H-Ni-DHKUST-1.

	Multiplicity	$\ell_{\text{Ni1-Ni2}}$	$Q_{\text{Ni1}}$	$\rho_{\text{Ni1}}$	$Q_{\text{Ni2}}$	$\rho_{\text{Ni2}}$
<b>1</b>	3	2.33	0.507	0.427	0.986	1.432
<b>2</b>	$1_{os}$	2.58	0.689	-1.307	0.946	1.380
<b>TS<sub>2-3</sub></b>	3	2.41	0.365	0.618	0.924	1.281
<b>3</b>	3	2.35	0.653	0.505	0.974	1.403
<b>4</b>	3	2.36	0.561	0.567	0.948	1.354
<b>TS<sub>4-5</sub></b>	3	2.47	0.563	0.929	0.851	1.206
<b>5</b>	3	2.42	0.744	1.095	0.820	1.169
<b>6</b>	3	2.43	0.628	0.953	0.841	1.174
<b>TS<sub>6-7</sub></b>	3	2.42	0.393	0.636	0.910	1.262
<b>7</b>	$1_{os}$	2.60	0.717	-1.333	0.945	1.394

**Table S11.** Optimized M-M bond distances ( $\text{\AA}$ ), NBO charges ( $Q$  in terms of  $e$ ), and NBO spin density distributions ( $\rho$ ) in ground-state intermediates and transition states on H-Cu-DHKUST-1.

	Multiplicity	$\ell_{\text{Cu1-Cu2}}$	$Q_{\text{Cu1}}$	$\rho_{\text{Cu1}}$	$Q_{\text{Cu2}}$	$\rho_{\text{Cu2}}$
<b>1</b>	$1_{cs}$	2.41	0.786	0.000	0.800	0.000
<b>2</b>	$1_{os}$	2.48	0.661	-0.173	0.804	0.173
<b>TS<sub>2-3</sub></b>	$1_{os}$	2.5	0.714	-0.116	0.822	0.107
<b>3</b>	$1_{cs}$	2.53	0.834	0.000	0.770	0.000
<b>4</b>	$1_{cs}$	2.57	0.733	0.000	0.781	0.000
<b>TS<sub>4-5</sub></b>	$1_{os}$	2.91	0.675	0.069	0.840	-0.259
<b>5</b>	$1_{cs}$	2.58	0.837	0.000	0.744	0.000
<b>6</b>	$1_{cs}$	2.54	0.835	0.000	0.770	0.000
<b>TS<sub>6-7</sub></b>	$1_{os}$	2.51	0.755	-0.227	0.813	0.188
<b>7</b>	$1_{os}$	2.49	0.665	-0.147	0.796	0.148



**Table S12.** Optimized M-M bond distances ( $\text{\AA}$ ), NBO charges ( $Q$  in terms of  $e$ ), and NBO spin density distributions ( $\rho$ ) in ground-state intermediates and transition states on H-Ru-DHKUST-1.

	Multiplicity	$\ell_{\text{Ru1-Ru2}}$	$Q_{\text{Ru1}}$	$\rho_{\text{Ru1}}$	$Q_{\text{Ru2}}$	$\rho_{\text{Ru2}}$
<b>1</b>	5	2.25	0.435	1.428	0.873	2.374
<b>2</b>	5	2.32	0.041	0.952	0.921	2.776
<b>TS<sub>2-3</sub></b>	5	2.40	0.030	0.800	0.898	2.923
<b>3</b>	3	2.24	0.591	1.172	0.834	0.870
<b>4</b>	3	2.36	0.321	0.915	0.560	1.044
<b>TS<sub>4-5</sub></b>	5	2.39	0.201	0.913	0.820	2.795
<b>5</b>	5	2.42	0.353	0.844	0.815	2.913
<b>6</b>	5	2.43	0.213	0.825	0.833	2.918
<b>TS<sub>6-7</sub></b>	5	2.40	0.053	0.829	0.889	2.906
<b>7</b>	5	2.30	0.102	1.068	0.903	2.693

**Table S13.** Optimized M-M bond distances ( $\text{\AA}$ ), NBO charges ( $Q$  in terms of  $e$ ), and NBO spin density distributions ( $\rho$ ) in ground-state intermediates and transition states on H-Rh-DHKUST-1.

	Multiplicity	$\ell_{\text{Rh1-Rh2}}$	$Q_{\text{Rh1}}$	$\rho_{\text{Rh1}}$	$Q_{\text{Rh2}}$	$\rho_{\text{Rh2}}$
<b>1</b>	$1_{cs}$	2.40	0.363	0.000	0.808	0.000
<b>2</b>	$1_{cs}$	2.47	0.124	0.000	0.718	0.000
<b>TS<sub>2-3</sub></b>	3	2.64	0.189	-0.045	0.777	1.815
<b>3</b>	3	2.37	0.583	0.567	0.829	1.257
<b>4</b>	$1_{cs}$	2.42	0.369	0.000	0.529	0.000
<b>TS<sub>4-5</sub></b>	3	2.71	0.349	-0.011	0.732	1.803
<b>5</b>	3	2.73	0.418	-0.002	0.722	1.813
<b>6</b>	3	2.69	0.323	-0.026	0.740	1.813
<b>TS<sub>6-7</sub></b>	3	2.65	0.212	-0.041	0.770	1.815
<b>7</b>	$1_{cs}$	2.48	0.131	0.000	0.714	0.000

**Table S14.** Optimized M-M bond distances ( $\text{\AA}$ ), NBO charges ( $Q$  in terms of  $e$ ), and NBO spin density distributions ( $\rho$ ) in ground-state intermediates and transition states on H-Pd-DHKUST-1.

	Multiplicity	$\ell_{\text{Pd1-Pd2}}$	$Q_{\text{Pd1}}$	$\rho_{\text{Pd1}}$	$Q_{\text{Pd2}}$	$\rho_{\text{Pd2}}$
<b>1</b>	3	2.54	0.473	0.395	0.815	1.166
<b>2</b>	3	2.56	0.348	0.446	0.770	1.066
<b>TS<sub>2-3</sub></b>	3	2.59	0.355	0.526	0.713	0.928
<b>3</b>	3	2.54	0.627	0.414	0.804	1.139
<b>4</b>	3	2.58	0.530	0.457	0.773	1.070
<b>TS<sub>4-5</sub></b>	3	2.62	0.512	0.609	0.657	0.822
<b>5</b>	3	2.60	0.667	0.679	0.636	0.780
<b>6</b>	1 <sub>os</sub>	2.55	0.606	0.332	0.766	-0.182
<b>TS<sub>6-7</sub></b>	3	2.60	0.379	0.532	0.703	0.904
<b>7</b>	3	2.57	0.361	0.440	0.763	1.054

## S5. Gibbs energies at different multiplicities

**Table S15.** Gibbs energies  $G$  (Hartree) and relative Gibbs energies  $\Delta G$  (kcal/mol) at 298.15 K on H-Co-DHKUST-1. The ground-state  $\Delta G$  are bold.

H-Co-DHKUST-1	Open-shell singlet		Triplet		Quintet		Septet	
	$G$	$\Delta G$	$G$	$\Delta G$	$G$	$\Delta G$	$G$	$\Delta G$
<b>1</b>	-4578.574581	20.8	-4578.60021	4.8	-4578.607781	<b>0.0</b>	-4578.604964	1.8
<b>2</b>	-4657.101661	-6.7	-4657.101499	-6.6	-4657.102342	<b>-7.2</b>	-4657.101001	-6.3
<b>TS<sub>2-3</sub></b>	-4657.076017	9.4	-4657.100932	<b>-6.3</b>	-4657.094476	-2.2	-4657.094492	-2.2
<b>3</b>	-4657.094451	-2.2	-4657.117409	-16.6	-4657.130826	<b>-25.0</b>	-4657.127440	-22.9
<b>4</b>	-4735.597776	-14.9	-4735.604811	-19.3	-4735.611596	<b>-23.5</b>	-4735.605480	-19.7
<b>TS<sub>4-5</sub></b>	-4735.543087	19.5	-4735.580879	<b>-4.3</b>	-4735.576177	-1.3	-4735.571910	1.4
<b>5</b>	-4735.569227	3.1	-4735.613223	-24.5	-4735.630779	-35.6	-4735.636708	<b>-39.3</b>
<b>6</b>	-4735.585011	-6.8	-4735.620982	-29.4	-4735.637492	-32.7	-4735.631169	<b>-35.8</b>
<b>TS<sub>6-7</sub></b>	-4735.583972	-6.2	-4735.614655	<b>-25.4</b>	-4735.60594	-20.0	-4735.608296	-21.5
<b>7</b>	-4735.590903	-10.5	-4735.615607	-26.0	-4735.618159	<b>-27.6</b>	-4735.615375	-25.9
<b>8</b>	-4735.571554	1.6	-4735.597183	-14.5	-4735.604754	<b>-19.2</b>	-4735.601937	-17.5

**Table S16.** Gibbs energies  $G$  (Hartree) and relative Gibbs energies  $\Delta G$  (kcal/mol) at 298.15 K on H-Ni-DHKUST-1. The ground-state  $\Delta G$  are bold.

H-Ni-DHKUST-1	Open-shell singlet		Triplet		Quintet	
	$G$	$\Delta G$	$G$	$\Delta G$	$G$	$\Delta G$
<b>1</b>	-4829.701308	11.1	-4829.71897	<b>0.0</b>	-4829.698732	12.7
<b>2</b>	-4908.206225	<b>-2.6</b>	-4908.204802	-1.7	-4908.192149	6.3
<b>TS<sub>2-3</sub></b>	-4908.195303	4.3	-4908.198781	<b>2.1</b>	-4908.185044	10.7
<b>3</b>	-4908.220225	-11.4	-4908.236986	<b>-21.9</b>	-4908.209759	-4.8
<b>4</b>	-4986.702126	-10.6	-4986.717848	<b>-20.4</b>	-4986.674985	6.5
<b>TS<sub>4-5</sub></b>	-4986.676181	5.7	-4986.681963	<b>2.1</b>	-4986.653301	20.1
<b>5</b>	-4986.725624	-25.3	-4986.729564	<b>-27.8</b>	-4986.718093	-20.6
<b>6</b>	-4986.724294	-24.5	-4986.727446	<b>-26.5</b>	-4986.714461	-18.3
<b>TS<sub>6-7</sub></b>	-4986.707442	-13.9	-4986.711603	<b>-16.5</b>	-4986.700005	-9.2
<b>7</b>	-4986.721622	<b>-22.8</b>	-4986.718983	-21.1	-4986.708715	-14.7
<b>8</b>	-4986.698281	-8.2	-4986.715943	<b>-19.2</b>	-4986.695705	-6.5

**Table S17.** Gibbs energies  $G$  (Hartree) and relative Gibbs energies  $\Delta G$  (kcal/mol) at 298.15 K on H-Cu-DHKUST-1. The ground-state  $\Delta G$  are bold.

H-Cu-DHKUST-1	Closed-shell singlet		Open-shell singlet		Triplet	
	$G$	$\Delta G$	$G$	$\Delta G$	$G$	$\Delta G$
<b>1</b>	-5094.034373	<b>0.0</b>	-	-	-5094.010025	15.3
<b>2</b>	-5172.524994	-4.7	-5172.525355	<b>-4.9</b>	-5172.504878	7.9
<b>TS<sub>2-3</sub></b>	-	-	-5172.496033	<b>13.5</b>	-5172.488658	18.1
<b>3</b>	-5172.544082	<b>-16.7</b>	-	-	-5172.525756	-5.2
<b>4</b>	-5251.029195	<b>-17.9</b>	-	-	-5251.010752	-6.3
<b>TS<sub>4-5</sub></b>	-5250.990767	6.2	-5250.992953	<b>4.9</b>	-5250.989711	6.9
<b>5</b>	-5251.057863	<b>-35.9</b>	-	-	-5251.035971	-22.1
<b>6</b>	-5251.055532	<b>-34.4</b>	-	-	-5251.034244	-21.1
<b>TS<sub>6-7</sub></b>	-5251.009696	-5.6	-5251.010184	<b>-6.0</b>	-5251.004728	-2.5
<b>7</b>	-5251.042143	-26.0	-5251.042563	<b>-26.3</b>	-5251.021828	-13.3
<b>8</b>	-5251.031346	<b>-19.2</b>	-	-	-5251.006998	-4.0

**Table S18.** Gibbs energies  $G$  (Hartree) and relative Gibbs energies  $\Delta G$  (kcal/mol) at 298.15 K on H-Ru-DHKUST-1. The ground-state  $\Delta G$  are bold.

H-Ru-DHKUST-1	Open-shell singlet		Triplet		Quintet		Septet	
	$G$	$\Delta G$	$G$	$\Delta G$	$G$	$\Delta G$	$G$	$\Delta G$
<b>1</b>	-2002.991456	14.9	-2003.00190	8.3	-2003.015168	<b>0.0</b>	-2002.985543	18.6
<b>2</b>	-2081.491919	4.0	-2081.504834	-4.1	-2081.511465	<b>-8.2</b>	-2081.462688	22.4
<b>TS<sub>2-3</sub></b>	-2081.484517	8.7	-2081.492584	3.6	-2081.503961	<b>-3.5</b>	-2081.458785	24.8
<b>3</b>	-2081.504530	-3.9	-2081.515317	<b>-10.7</b>	-2081.508824	-6.6	-2081.501185	-1.8
<b>4</b>	-2160.018816	-23.4	-2160.026104	<b>-28.0</b>	-2160.014936	-21.0	-2159.969193	7.7
<b>TS<sub>4-5</sub></b>	-2159.948358	20.8	-2159.957012	15.4	-2159.966653	<b>9.3</b>	-2159.935851	28.6
<b>5</b>	-2159.987221	-3.6	-2159.992363	-6.8	-2160.003614	<b>-13.9</b>	-2159.988221	-4.2
<b>6</b>	-2159.996378	-9.3	-2160.007156	-16.1	-2160.017325	<b>-22.5</b>	-2160.008990	-17.3
<b>TS<sub>6-7</sub></b>	-2159.994615	-8.2	-2160.005869	-15.3	-2160.014799	<b>-20.9</b>	-2159.965404	10.1
<b>7</b>	-2160.003232	-13.6	-2160.016330	-21.9	-2160.024412	<b>-26.9</b>	-2159.970171	7.1
<b>8</b>	-2002.991456	-4.4	-2003.001900	-10.9	-2003.015168	<b>-19.2</b>	-2002.985543	-0.6

**Table S19.** Gibbs energies  $G$  (Hartree) and relative Gibbs energies  $\Delta G$  (kcal/mol) at 298.15 K on H-Rh-DHKUST-1. The ground-state  $\Delta G$  are bold.

H-Rh-DHKUST-1	Closed-shell singlet		Triplet		Quintet	
	$G$	$\Delta G$	$G$	$\Delta G$	$G$	$\Delta G$
<b>1</b>	-2034.339756	<b>0.0</b>	-2034.337955	1.1	-2034.328038	7.4
<b>2</b>	-2112.852553	<b>-18.6</b>	-2112.850043	-17.0	-2112.81282	6.3
<b>TS<sub>2-3</sub></b>	-2112.842169	-12.1	-2112.843745	<b>-13.1</b>	-2112.810897	7.5
<b>3</b>	-2112.840255	-10.9	-2112.852563	<b>-18.6</b>	-2112.846198	-14.6
<b>4</b>	-2191.37350	<b>-42.3</b>	-2191.352584	-29.2	-2191.327055	-13.2
<b>TS<sub>4-5</sub></b>	-2191.30394	1.3	-2191.310383	<b>-2.7</b>	-2191.279439	16.7
<b>5</b>	-2191.333929	-17.5	-2191.345271	<b>-24.6</b>	-2191.336031	-18.8
<b>6</b>	-2191.351142	-28.3	-2191.354935	<b>-30.7</b>	-2191.327019	-13.1
<b>TS<sub>6-7</sub></b>	-2191.349845	-27.5	-2191.354755	<b>-30.5</b>	-2191.321693	-9.8
<b>7</b>	-2191.365326	<b>-37.2</b>	-2191.362681	-35.5	-2191.327660	-13.5
<b>8</b>	-2191.336729	<b>-19.2</b>	-2191.334928	-18.1	-2191.325011	-11.9



**Table S20.** Gibbs energies  $G$  (Hartree) and relative Gibbs energies  $\Delta G$  (kcal/mol) at 298.15 K on H-Pd-DHKUST-1. The ground-state  $\Delta G$  are bold.

H-Pd-DHKUST-1	Open-shell singlet		Triplet	
	$G$	$\Delta G$	$G$	$\Delta G$
<b>1</b>	-2069.029769	0.5	-2069.030625	<b>0.0</b>
<b>2</b>	-2147.516961	-2.0	-2147.519436	<b>-3.5</b>
<b>TS<sub>2-3</sub></b>	-2147.508144	3.5	-2147.510833	<b>1.9</b>
<b>3</b>	-2147.530799	-10.7	-2147.532116	<b>-11.5</b>
<b>4</b>	-2226.027841	-19.4	-2226.031976	<b>-22.0</b>
<b>TS<sub>4-5</sub></b>	-2225.982212	9.2	-2225.984178	<b>8.0</b>
<b>5</b>	-2226.034709	-23.7	-2226.037496	<b>-25.4</b>
<b>6</b>	-2226.053849	<b>-35.7</b>	-2226.037418	-25.4
<b>TS<sub>6-7</sub></b>	-2226.020107	-14.5	-2226.023289	<b>-16.5</b>
<b>7</b>	-2226.030270	-20.9	-2226.032720	<b>-22.4</b>
<b>8</b>	-2226.026742	-18.7	-2226.027598	<b>-19.2</b>

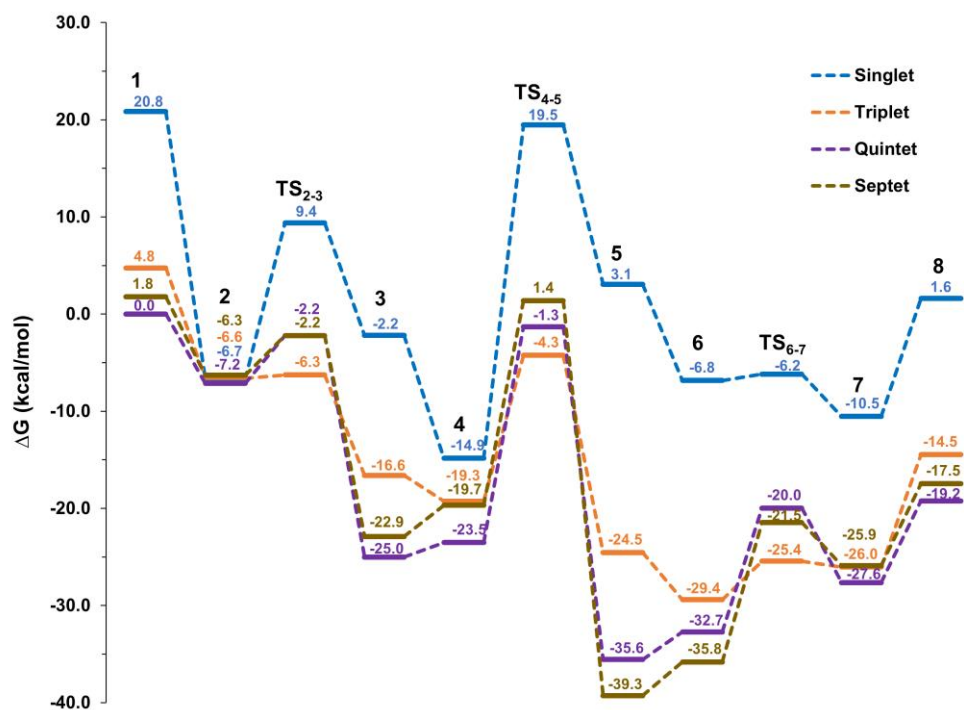


Fig. S2.  $\Delta G$  at different multiplicities on H-Co-DHKUST-1 at 298.15 K.

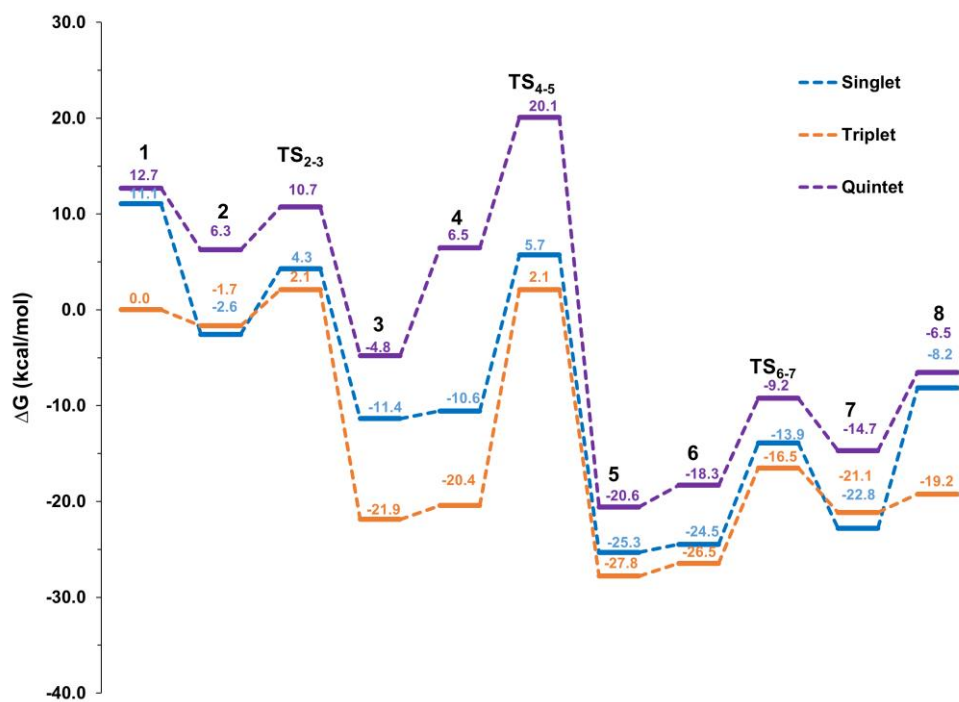


Fig. S3.  $\Delta G$  at different multiplicities on H-Ni-DHKUST-1 at 298.15 K.

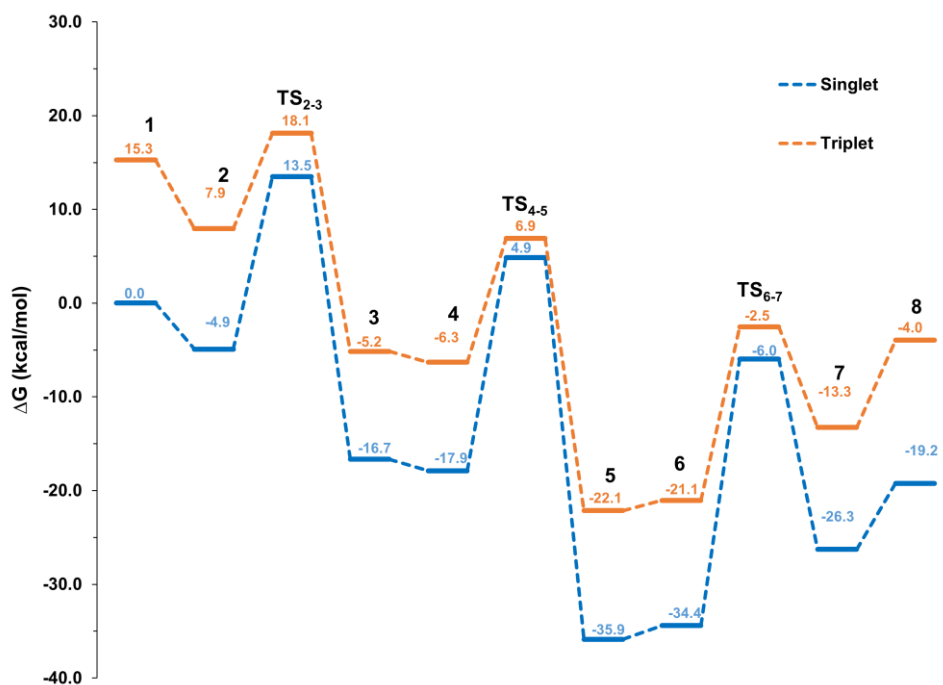


Fig. S4.  $\Delta G$  at different multiplicities on H-Cu-DHKUST-1 at 298.15 K.

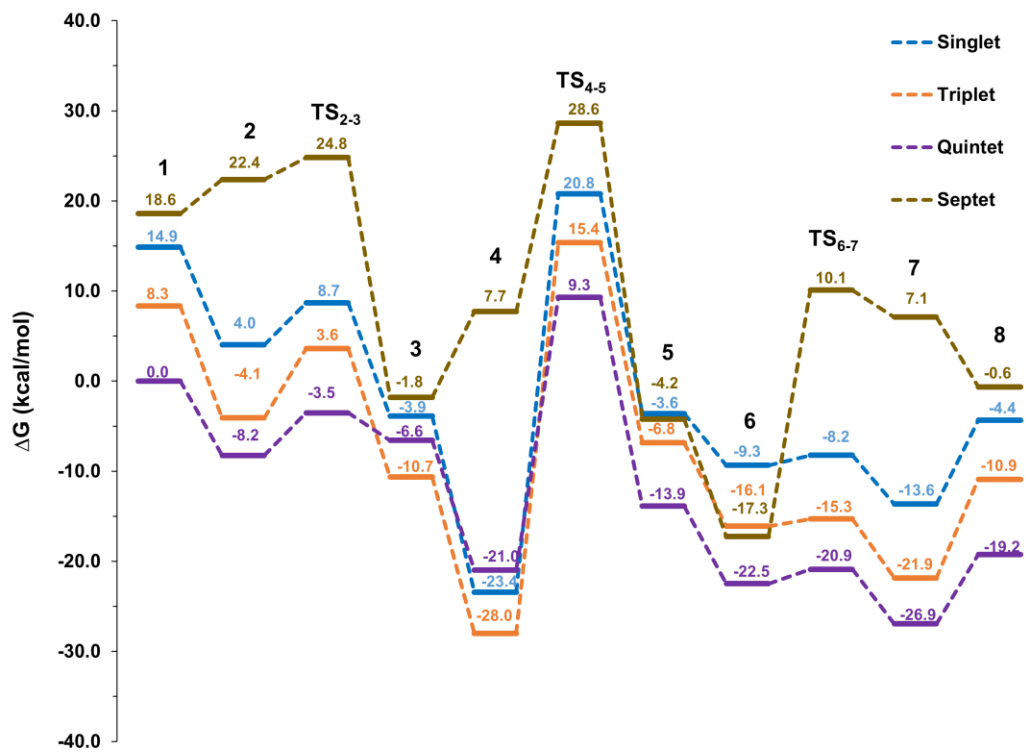


Fig. S5.  $\Delta G$  at different multiplicities on H-Ru-DHKUST-1 at 298.15 K.

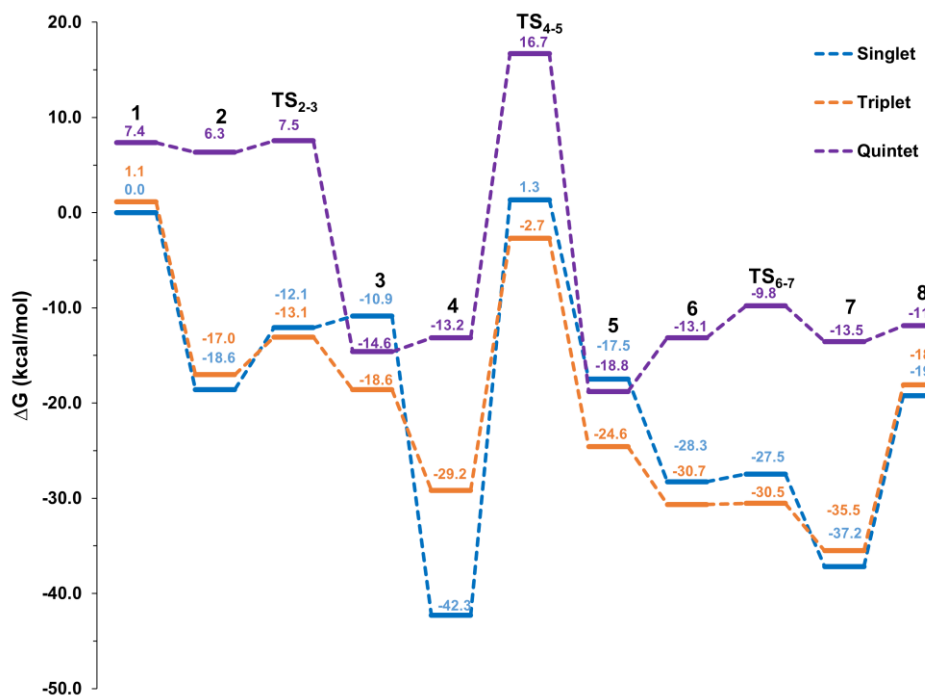


Fig. S6.  $\Delta G$  at different multiplicities on H-Rh-DHKUST-1 at 298.15 K.

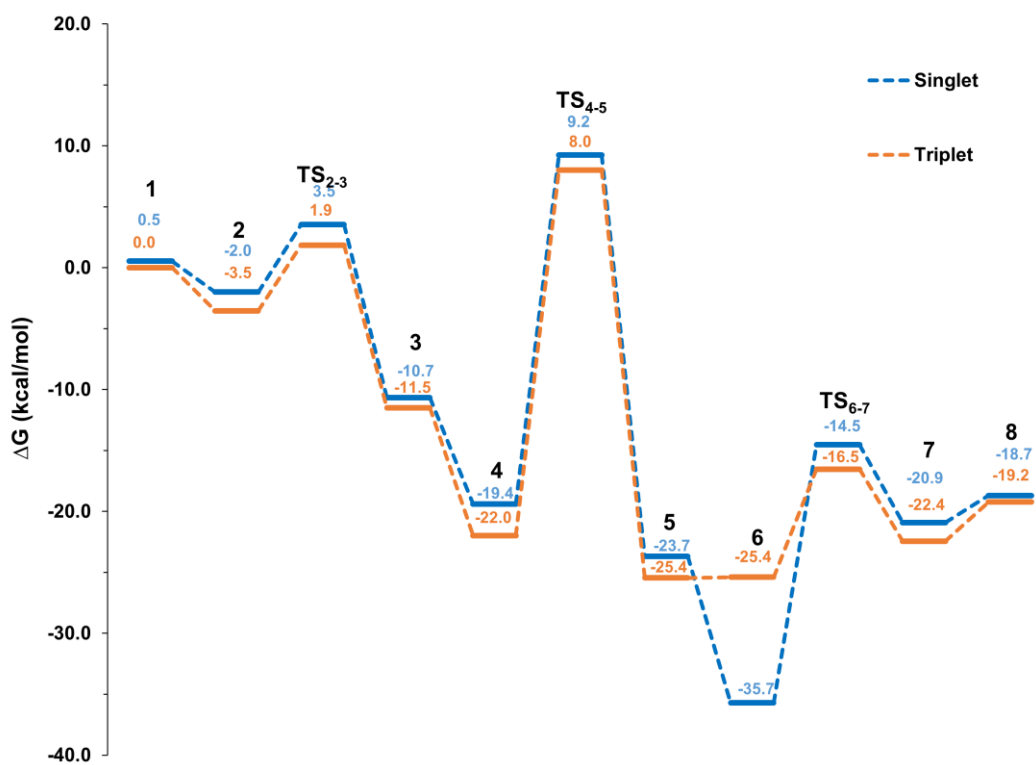
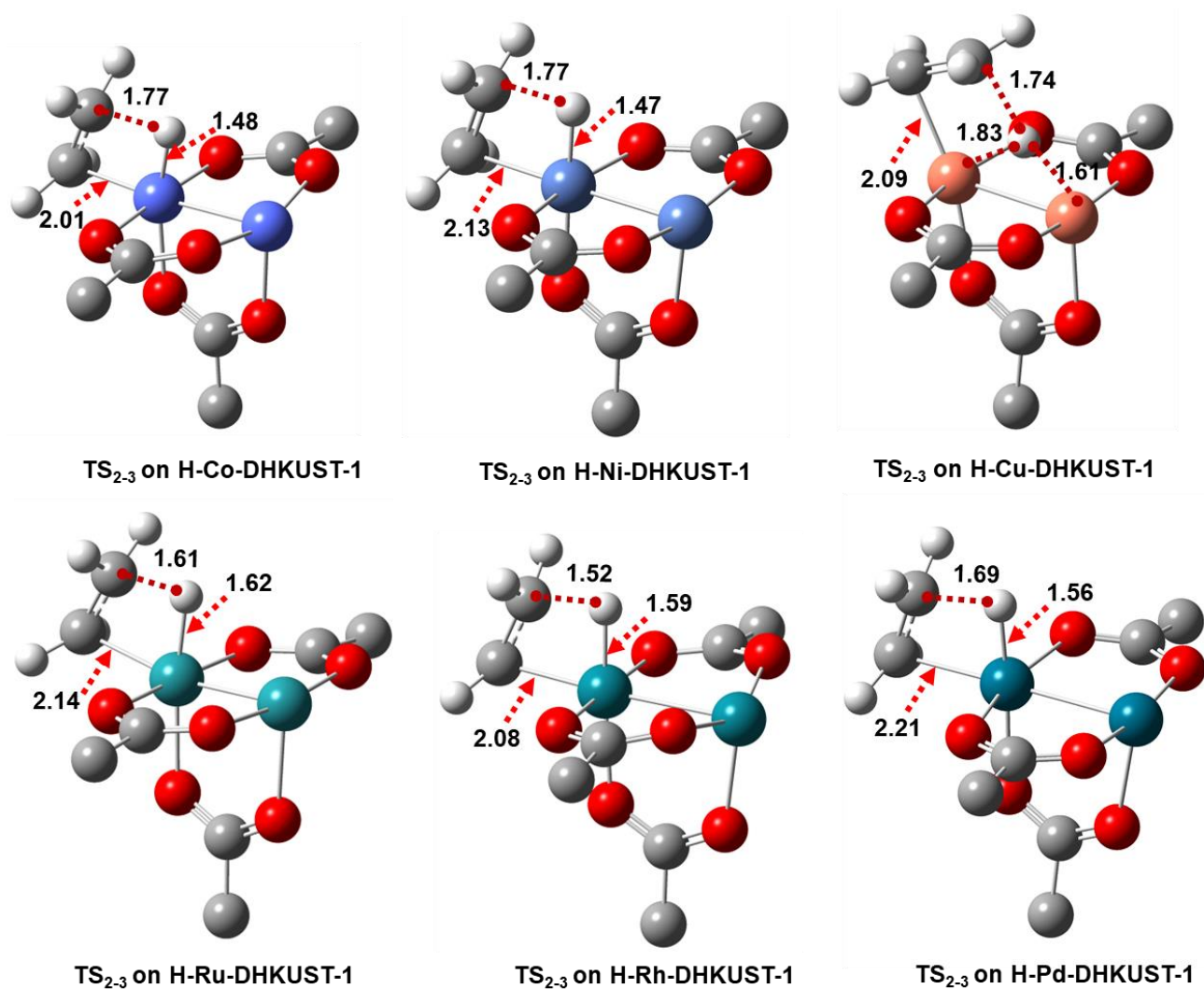


Fig. S7.  $\Delta G$  at different multiplicities on H-Pd-DHKUST-1 at 298.15 K.

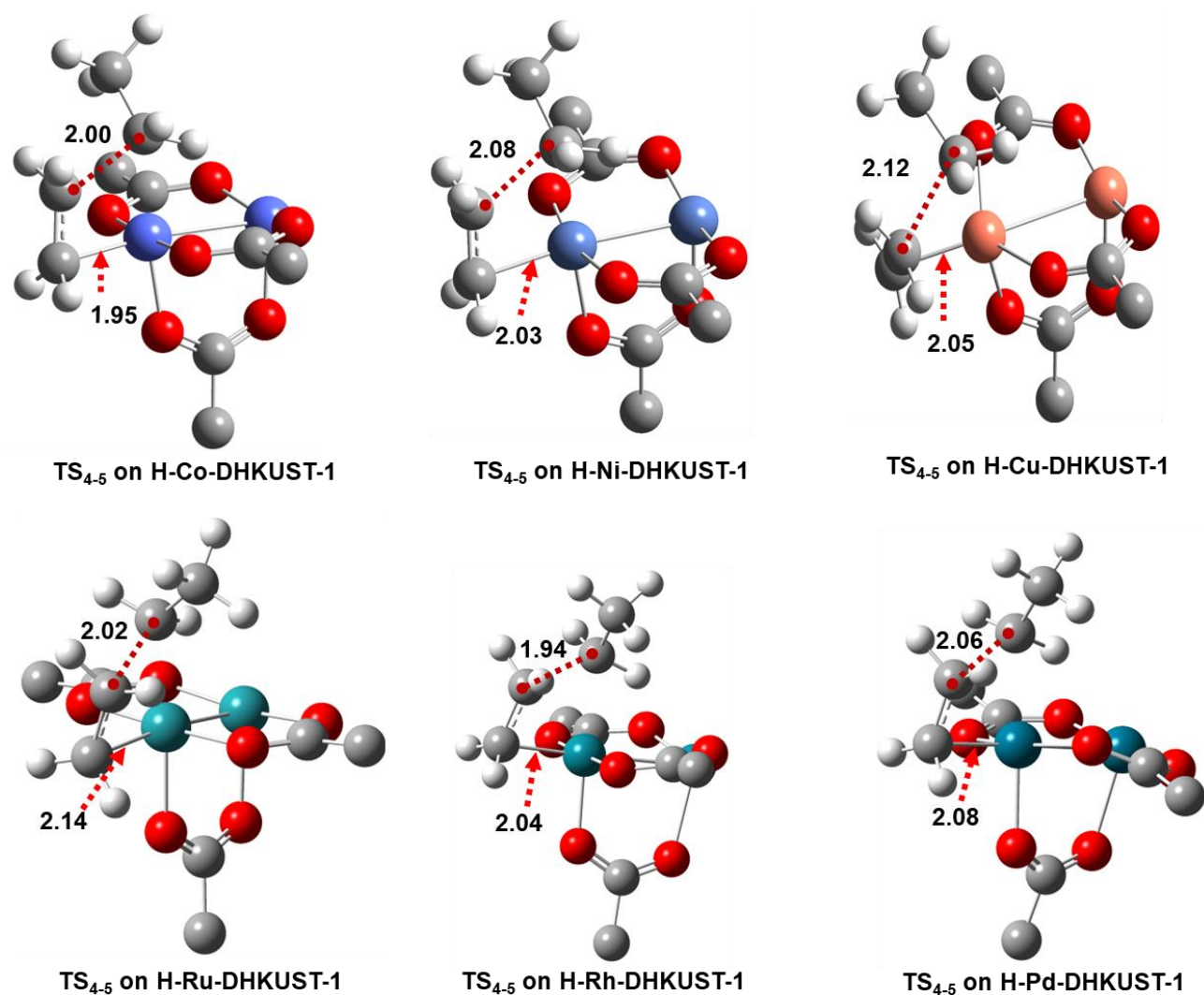
## S6. Frequencies and structures of transition states.

**Table S21.** Imaginary frequencies ( $\text{cm}^{-1}$ ) of transition states.

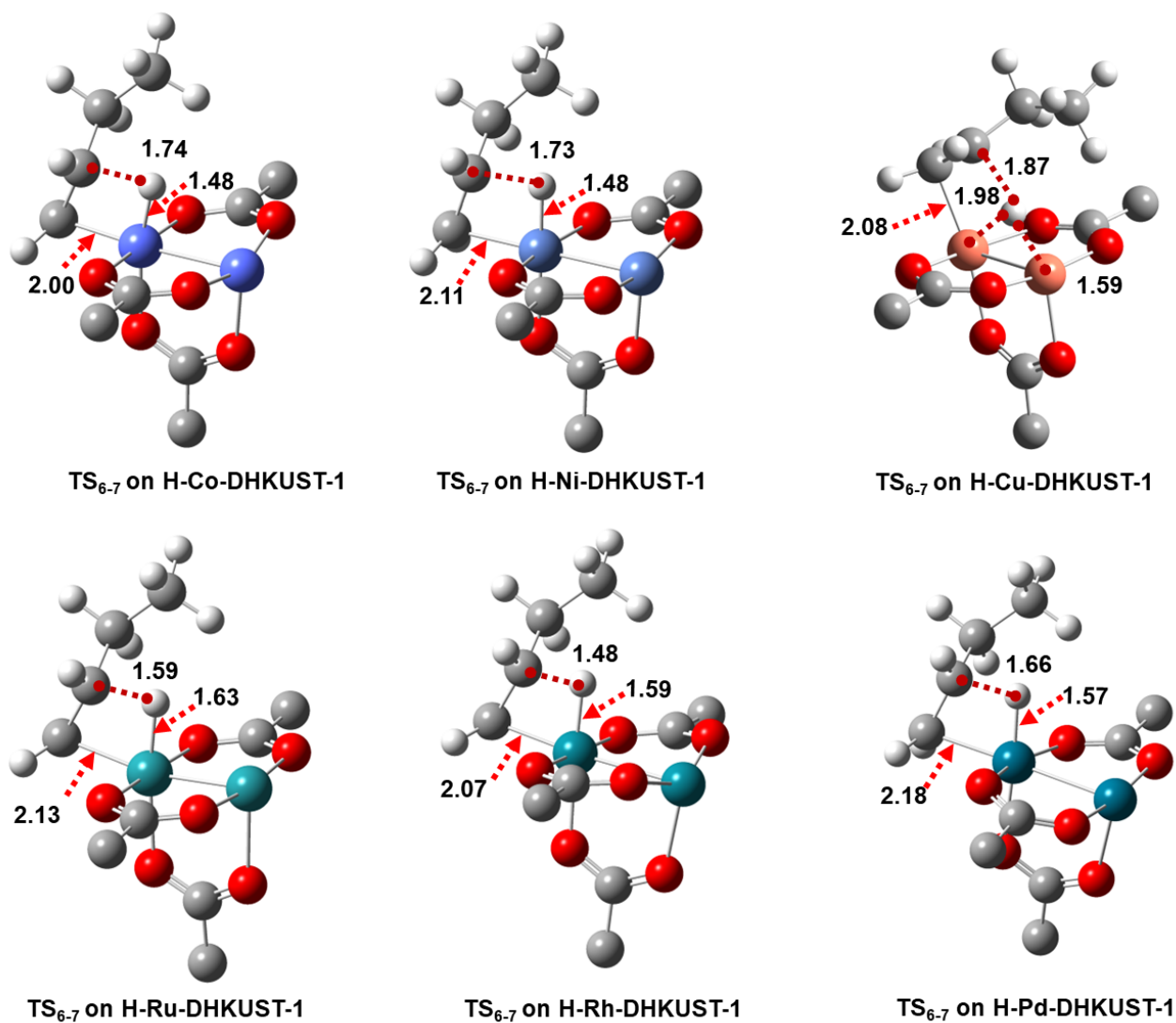
Step	H-Co- DHKUST-1	H-Ni- DHKUST-1	H-Cu- DHKUST-1	H-Ru- DHKUST-1	H-Rh- DHKUST-1	H-Pd- DHKUST-1
Hydrogenation	-631.6	-765.8	-620.9	-599.1	-507.2	-768.6
C-C coupling	-388.0	-458.9	-435.5	-504.8	-441.8	-451.2
$\beta$ -H elimination	-557.9	-673.6	-425.1	-541.5	-447.0	-693.5



**Fig. S8.** Optimized structures and key bond distances (Å) of hydrogenation transition state (TS<sub>2-3</sub>) on H-M-DHKUST-1. Carbon, oxygen, and hydrogen atoms are in grey, red, and white, respectively.

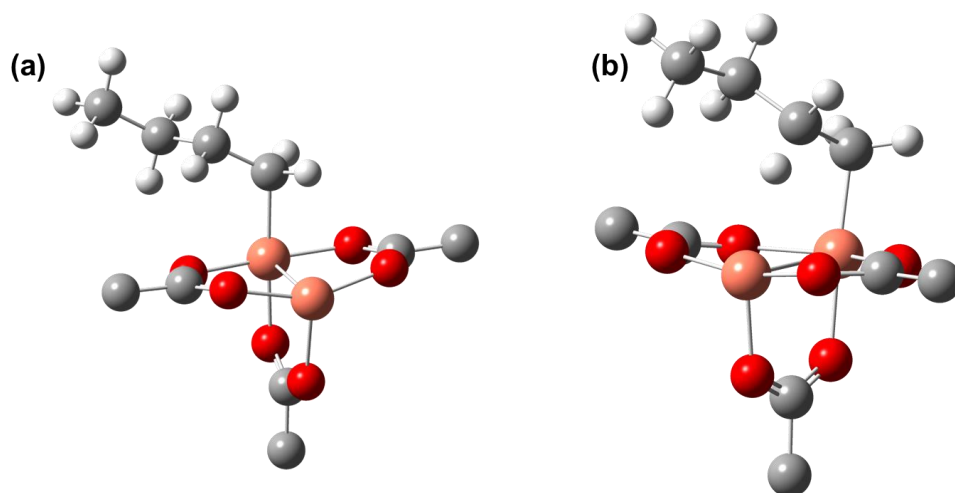


**Fig. S9.** Optimized structures and key bond distances (Å) of C-C coupling transition state (TS<sub>4-5</sub>) on H-M-DHKUST-1. Carbon, oxygen, and hydrogen atoms are in grey, red, and white, respectively.

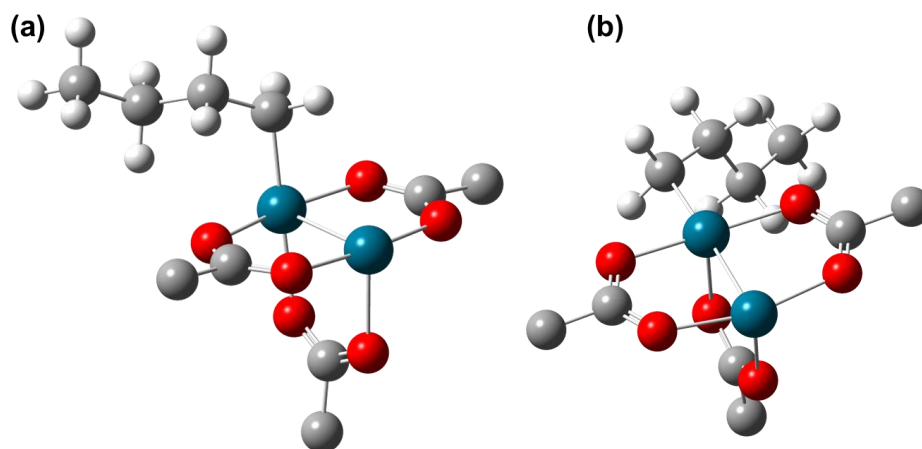


**Fig. S10.** Optimized structures and key bond distances (Å) of  $\beta$ -H elimination transition state (TS<sub>6-7</sub>) on H-M-DHKUST-1. Carbon, oxygen, and hydrogen atoms are in grey, red, and white, respectively.





**Fig. S11.** Optimized structures of intermediate **6** on H-Cu-DHKUST-1 with different multiplicities (a) closed-shell singlet and (b) triplet. Carbon, oxygen, and hydrogen atoms are in grey, red, and white, respectively.



**Fig. S12.** Optimized structures of intermediate **6** on H-Pd-DHKUST-1 with different multiplicities (a) open-shell singlet and (b) triplet. Carbon, oxygen, and hydrogen atoms are in grey, red, and white, respectively.

## S7. Coordinates of intermediates and transition states at ground state

### H-Co-DHKUST-1

INT1

0 5

O	0.00040800	0.76658300	-1.23137100
C	-0.00076500	1.30702100	-0.08867600
O	-0.00149100	0.67945600	1.00901000
O	-1.89105100	-1.39839100	1.10766400
C	-2.48593000	-1.49985900	-0.00728800
O	-1.89012400	-1.53039300	-1.12419800
O	1.89082200	-1.53059900	-1.12407600
C	2.48662000	-1.50021700	-0.00719300
O	1.89152800	-1.39908000	1.10777700
C	3.97106900	-1.54920100	0.01260200
C	4.69015800	-1.55078300	-1.18577300
C	4.64777500	-1.55411300	1.23602300
C	6.09263000	-1.55053500	-1.16261700
C	6.04929700	-1.56088400	1.26427400
C	6.77334700	-1.55761500	0.06351900
H	4.15385800	-1.54143400	-2.13542900
H	4.07672000	-1.54627000	2.16502100
H	7.86384600	-1.55531200	0.08259500
C	-3.97039700	-1.54919500	0.01241900
C	-4.64712600	-1.55485300	1.23581400
C	-4.68942300	-1.55067800	-1.18597300
C	-6.04864500	-1.56232300	1.26402600
C	-6.09189400	-1.55103900	-1.16286400
C	-6.77265100	-1.55892400	0.06324700
H	-4.07609100	-1.54710400	2.16482800
H	-4.15308700	-1.54077600	-2.13560300
H	-7.86315200	-1.55713500	0.08228900
C	-0.00111300	2.79664400	-0.02950600
C	-0.00149400	3.44614300	1.20619900
C	-0.00072800	3.54115500	-1.21060000
C	-0.00146700	4.84683600	1.26310800
C	-0.00077600	4.94209000	-1.15823200
C	-0.00111500	5.59799700	0.08022500
H	-0.00176400	2.85366100	2.12187600
H	-0.00038700	3.02193300	-2.16970000
H	-0.00110300	6.68775400	0.12318300
C	-0.00044100	5.70390600	-2.36718800
C	-6.83356000	-1.52757000	-2.38656300
C	-0.00170900	5.50898000	2.52902300
C	-6.73796200	-1.56124300	2.51806300
C	6.73857800	-1.55888200	2.51832900
C	6.83433200	-1.52725200	-2.38630300
N	0.00005300	6.32312700	-3.35318200
N	-0.00159100	6.04275100	3.56360800
N	-7.44174000	-1.49896900	-3.37974500
N	-7.29248700	-1.55618400	3.54243500
N	7.29308800	-1.55280800	3.54270700
N	7.44249900	-1.49848200	-3.37949900
Co	0.00048400	-1.30312000	1.06533000
Co	0.00041000	-1.22237200	-1.38520300
H	-0.00211400	-2.79731500	1.05622800

## INT2

0 5

O	-0.00029700	0.69353500	-1.28181800
C	-0.00088300	1.17266300	-0.11680300
O	0.00458600	0.48096200	0.94683200
O	-1.93688000	-1.66673600	1.27747700
C	-2.52136900	-1.43703000	0.17457200
O	-1.94300900	-1.29175900	-0.93682000
O	1.95493700	-1.28230500	-0.93649300
C	2.53529100	-1.42569700	0.17417500
O	1.95333700	-1.65860500	1.27767200
C	4.01777700	-1.30751800	0.19223200
C	4.72469800	-1.10975900	-0.99617800
C	4.69740100	-1.37257100	1.40882100
C	6.12028300	-0.97975800	-0.96732800
C	6.09079400	-1.23203100	1.44170200
C	6.80624100	-1.03839700	0.25366400
H	4.18241800	-1.05468100	-1.94070700
H	4.13524800	-1.52534800	2.33050900
H	7.89114600	-0.92993800	0.27797400
C	-4.00434300	-1.32516500	0.19546200
C	-4.68030500	-1.39947900	1.41348300
C	-4.71547800	-1.12396200	-0.98997300
C	-6.07408500	-1.26529700	1.45120500
C	-6.11158700	-0.99944500	-0.95624700
C	-6.79376300	-1.06786100	0.26644400
H	-4.11492100	-1.55469200	2.33274900
H	-4.17623700	-1.06161900	-1.93580600
H	-7.87902400	-0.96394800	0.29441000
C	-0.00993900	2.66049500	0.00853300
C	-0.00044300	3.29369100	1.25448500
C	-0.02969500	3.42179300	-1.15984300
C	-0.01014900	4.69676900	1.32781800
C	-0.04095500	4.81970400	-1.09219000
C	-0.03083800	5.46139500	0.15197000
H	0.01467100	2.69063400	2.16355800
H	-0.03686100	2.91479700	-2.12501600
H	-0.03911300	6.55049000	0.20913200
C	-0.06347700	5.56261100	-2.31027100
C	0.00038700	5.37899800	2.58652400
C	-6.85074500	-0.79572100	-2.16234100
C	-6.74781100	-1.32011200	2.70788200
C	6.76997800	-1.27624100	2.69597000
C	6.85350400	-0.78067700	-2.17765000
N	-0.08260700	6.11849000	-3.33231100
N	0.00862500	5.97578600	3.58740900
N	-7.46563900	-0.62933500	-3.13693500
N	-7.27168900	-1.35971100	3.74605000
N	7.30069900	-1.30664000	3.73100500
N	7.46131600	-0.61840200	-3.15731400
Co	0.00790700	-1.54735500	1.27481400
Co	0.00616500	-1.30491400	-1.08557900
C	0.01001400	-2.87126100	-2.70538700
C	0.00668200	-1.63387900	-3.26698800
H	0.93419100	-1.13669100	-3.56161400
H	-0.92351600	-1.14160700	-3.56138000
H	0.00965200	-2.62815300	-0.17152800
H	-0.91655600	-3.42622800	-2.54197700

H 0.93951300 -3.42138500 -2.54223500

TS2-3

0 3

O -0.00461200 0.59101400 -1.07117200  
C -0.00174000 1.18092700 0.04422800  
O 0.00729700 0.61365100 1.17109000  
O -1.89260600 -1.67055800 1.20056800  
C -2.50347100 -1.48371200 0.10688500  
O -1.93503600 -1.37827000 -1.01545500  
O 1.94615700 -1.36272800 -1.01337100  
C 2.51725500 -1.47050400 0.10752500  
O 1.90969200 -1.66500800 1.20155500  
C 4.00241900 -1.34503400 0.14681900  
C 4.72315200 -1.14813400 -1.03453100  
C 4.67153300 -1.39118200 1.37324800  
C 6.11749300 -0.99768100 -0.99264700  
C 6.06494300 -1.23465000 1.42351700  
C 6.78897000 -1.03969500 0.23825200  
H 4.19179100 -1.10597700 -1.98606100  
H 4.09947000 -1.54095400 2.28968700  
H 7.87209700 -0.91619400 0.27374100  
C -3.98897900 -1.36438700 0.14979100  
C -4.65396600 -1.41895500 1.37801400  
C -4.71422100 -1.16401300 -1.02832700  
C -6.04764500 -1.26797900 1.43365600  
C -6.10896000 -1.01786100 -0.98093400  
C -6.77624500 -1.06892300 0.25196700  
H -4.07846900 -1.57106900 2.29187600  
H -4.18614700 -1.11522100 -1.98138500  
H -7.85963900 -0.94911000 0.29164100  
C -0.01081400 2.67404300 0.03038100  
C -0.00089800 3.36763200 1.24067700  
C -0.03056500 3.37572200 -1.17643100  
C -0.01034800 4.76859800 1.25012800  
C -0.04115700 4.77852700 -1.17155900  
C -0.03078500 5.47815300 0.04289400  
H 0.01410700 2.80653000 2.17557300  
H -0.03818300 2.82289800 -2.11672400  
H -0.03880900 6.56871200 0.04678300  
C -0.06331100 5.50740100 -2.40047600  
C 0.00044900 5.46300800 2.49745300  
C -6.85502800 -0.80679700 -2.18527200  
C -6.72445500 -1.30385400 2.69541700  
C 6.74749100 -1.26061700 2.68259500  
C 6.85755500 -0.79206900 -2.20149400  
N -0.08209300 6.11352100 -3.39446300  
N 0.00954000 6.00787800 3.52591600  
N -7.46564200 -0.63258100 -3.16250800  
N -7.27133800 -1.32609300 3.72427900  
N 7.30105300 -1.27424600 3.70808700  
N 7.46131300 -0.62292900 -3.18382800  
Co 0.00778000 -1.39659100 1.39237000  
Co 0.00567700 -1.38957900 -1.06730200  
C 0.01240400 -2.86817500 -2.49440300  
C 0.00740300 -1.58836300 -3.06742600  
H 0.93403800 -1.13618500 -3.42750600  
H -0.92262000 -1.14383600 -3.42828600  
H 0.01163600 -2.83039800 -0.72327900

H -0.90600800 -3.46114300 -2.47565000  
H 0.93557500 -3.45368800 -2.47500500

INT3

0 5

O -0.03729500 0.67127500 -1.06359400  
C -0.06430500 1.27134200 0.04410400  
O -0.06748900 0.69974600 1.17124900  
O -1.91374700 -1.62676100 1.04434900  
C -2.52110700 -1.45186500 -0.05554300  
O -1.94807500 -1.34127900 -1.17470400  
O 1.94668300 -1.25938500 -1.16527000  
C 2.51716400 -1.33535900 -0.04151000  
O 1.91081600 -1.50889700 1.05858600  
C 3.99930500 -1.20287700 0.00410500  
C 4.71927200 -0.96986800 -1.17024800  
C 4.66570300 -1.27266000 1.23078700  
C 6.11073400 -0.80118000 -1.11874100  
C 6.05722000 -1.10719100 1.28811400  
C 6.78127700 -0.87083300 0.11092100  
H 4.18912400 -0.90886700 -2.12154700  
H 4.09288300 -1.44784800 2.14203000  
H 7.86273900 -0.73524500 0.15172600  
C -4.00658100 -1.35341400 -0.01120500  
C -4.67111000 -1.44736300 1.21464600  
C -4.73149100 -1.12731300 -1.18386200  
C -6.06582900 -1.31294700 1.27330700  
C -6.12661000 -0.99152300 -1.13131500  
C -6.79522200 -1.08488600 0.09792200  
H -4.09455500 -1.61731500 2.12450300  
H -4.20279500 -1.04809300 -2.13460200  
H -7.87951400 -0.97448600 0.13954800  
C -0.09213100 2.76337200 0.03902000  
C -0.09352900 3.43600100 1.26048700  
C -0.11432400 3.48588000 -1.15653400  
C -0.11521000 4.83529200 1.29589100  
C -0.13948100 4.88939400 -1.12574400  
C -0.13915600 5.56638400 0.10242200  
H -0.07621300 2.85886000 2.18528400  
H -0.11219300 2.95073500 -2.10729100  
H -0.15710800 6.65658100 0.12551500  
C -0.16546500 5.65600000 -2.33308300  
C -0.11076400 5.49095800 2.56304000  
C -6.87119800 -0.74395800 -2.32769100  
C -6.74122800 -1.39399800 2.53273100  
C 6.73606100 -1.16415100 2.54718500  
C 6.84744800 -0.54224300 -2.31742100  
N -0.18767400 6.31322800 -3.29454600  
N -0.10449000 5.98025000 3.61874100  
N -7.47918000 -0.53619000 -3.29928800  
N -7.28530300 -1.45415900 3.56123600  
N 7.28506700 -1.20454400 3.57408700  
N 7.44629100 -0.32377600 -3.29228600  
Co -0.01007000 -1.31082500 1.22909600  
Co 0.00494100 -1.33229300 -1.17581100  
C 1.19575700 -4.10129900 -0.81720900  
C -0.01717000 -3.27857700 -1.13971900  
H -0.25495100 -3.27608500 -2.22564600  
H -0.92381200 -3.61662100 -0.61614700

H	1.46933000	-4.05107200	0.24690000
H	1.01005000	-5.16616200	-1.03627900
H	2.07718100	-3.80816500	-1.40237100

INT4

0 5

O	0.07276500	1.12528500	-1.42257100
C	0.08105000	1.53286600	-0.23041100
O	0.07147900	0.78960500	0.78961300
O	-1.92517800	-1.17463600	0.82214200
C	-2.49684700	-1.12900400	-0.30248000
O	-1.89911500	-1.08977900	-1.41715500
O	1.93908400	-1.19286200	-1.41689300
C	2.52860100	-1.26742900	-0.29966000
O	1.94837500	-1.31070800	0.82082800
C	4.01238300	-1.31316100	-0.29730600
C	4.72422600	-1.22364000	-1.49389200
C	4.69163400	-1.44013500	0.91427600
C	6.12499900	-1.26043800	-1.47603500
C	6.09057700	-1.48142700	0.93241100
C	6.81291700	-1.39062100	-0.26298800
H	4.18366300	-1.12243900	-2.43561000
H	4.12391800	-1.50626900	1.84257800
H	7.90293900	-1.41990600	-0.25087200
C	-3.98031500	-1.14688600	-0.30857000
C	-4.66798800	-1.26843700	0.89894000
C	-4.68428700	-1.04772800	-1.50912500
C	-6.06739500	-1.29240500	0.90912900
C	-6.08544400	-1.06785700	-1.49916400
C	-6.78176900	-1.19099400	-0.29017400
H	-4.10669500	-1.34387600	1.83065200
H	-4.13710900	-0.95279200	-2.44768800
H	-7.87211000	-1.20745600	-0.28428100
C	0.09913100	3.01090500	-0.00807600
C	0.09979200	3.53833100	1.28476900
C	0.10964800	3.86752600	-1.10958500
C	0.11055800	4.92828100	1.47793700
C	0.12054200	5.25649900	-0.92301800
C	0.12108300	5.79009500	0.37239300
H	0.09052300	2.85964500	2.13914600
H	0.10794900	3.44131700	-2.11348600
H	0.12881900	6.87053900	0.52076200
C	0.12876900	6.12177400	-2.05971400
C	-6.81323400	-0.96175300	-2.72095900
C	0.10874500	5.47769100	2.79815800
C	-6.75373300	-1.42162100	2.15147000
C	6.76838100	-1.61677700	2.17890000
C	6.86096200	-1.16279300	-2.69369500
N	0.13411500	6.81142900	-2.99770500
N	0.10618200	5.93654600	3.86881600
N	-7.41414100	-0.87458200	-3.71318600
N	-7.28828400	-1.52968100	3.17865800
N	7.29611000	-1.72977700	3.20911600
N	7.46856200	-1.08171700	-3.68238300
Co	0.00841700	-1.23950100	0.82107300
Co	0.02559200	-0.88774800	-1.59273000
C	0.01819500	-3.15653300	0.32935100
C	-0.08429500	-1.76417300	3.46002100
H	0.75400000	-3.32350900	-0.47367300

H	0.51877700	-3.44405200	1.27284600
C	-1.26193800	-3.91162300	0.11359100
C	-0.12733200	-0.42977600	3.45961600
H	-0.99197200	-2.36845300	3.36388800
H	0.85681900	-2.30838900	3.58201900
H	-1.98074200	-3.77020400	0.93270000
H	-1.76712700	-3.63921700	-0.82412300
H	-1.06288900	-4.99474600	0.05071300
H	-1.06693200	0.11628400	3.34170400
H	0.77713400	0.17593300	3.55988600

TS4-5

O 3

O	0.01791500	1.19655200	-1.34448000
C	0.06212600	1.57510100	-0.14791800
O	0.08988100	0.82058400	0.86818700
O	-1.91208700	-1.08678400	0.79607100
C	-2.48019000	-1.11744800	-0.33627700
O	-1.87645800	-1.15120300	-1.44368400
O	1.90038800	-1.18323000	-1.43071100
C	2.50137800	-1.22408100	-0.32143800
O	1.93055700	-1.23103500	0.80952000
C	3.98862900	-1.27577400	-0.31889400
C	4.70292800	-1.16366200	-1.51400000
C	4.67138200	-1.42747300	0.89012100
C	6.10517800	-1.19588300	-1.49829700
C	6.07138800	-1.47581900	0.90852900
C	6.79232200	-1.35610300	-0.28664900
H	4.16172500	-1.04420600	-2.45348500
H	4.10507500	-1.50827400	1.81823300
H	7.88244100	-1.38550800	-0.27567200
C	-3.96803100	-1.13249000	-0.33432400
C	-4.65644300	-1.26563300	0.87394000
C	-4.67682300	-1.00756300	-1.53124300
C	-6.05743800	-1.28284200	0.88916000
C	-6.07924600	-1.00466900	-1.51819500
C	-6.77256200	-1.14720500	-0.30793300
H	-4.09425600	-1.35620500	1.80401200
H	-4.13092400	-0.90390200	-2.46987200
H	-7.86309700	-1.15048200	-0.29921100
C	0.08490000	3.04697200	0.11032600
C	0.09364300	3.54367200	1.41503700
C	0.09428700	3.92997200	-0.97105000
C	0.10925400	4.92827600	1.64020300
C	0.11441700	5.31426400	-0.75161300
C	0.12086500	5.81687700	0.55650300
H	0.08642300	2.84566900	2.25303800
H	0.08609800	3.52811000	-1.98490500
H	0.13437400	6.89341000	0.73066200
C	0.12819900	6.21175700	-1.86371100
C	-6.81249000	-0.84868200	-2.73514200
C	0.11100900	5.43898000	2.97520800
C	-6.74867500	-1.43942900	2.12998900
C	6.75359600	-1.64872500	2.15203700
C	6.84678000	-1.05973900	-2.71283400
N	0.14029100	6.93611300	-2.77541300
N	0.11008000	5.85737800	4.06203600
N	-7.41894300	-0.71428000	-3.72003300
N	-7.29505300	-1.57430300	3.14928300
N	7.28903200	-1.79632100	3.17530800

N	7.46344100	-0.94377400	-3.69384200
Co	0.00913400	-1.13301300	0.85172100
Co	0.01832400	-0.76990400	-1.72941500
C	-0.00190800	-3.22532600	0.59575600
C	-0.14809300	-2.51875900	2.46548800
H	-0.01910900	-2.71707600	-0.39735300
H	1.00082100	-3.65784300	0.69124400
C	-1.10304300	-4.24580900	0.63401800
C	0.02409700	-1.14154700	2.79968400
H	-1.15278900	-2.92127600	2.61923400
H	0.64141200	-3.21390800	2.76691500
H	-1.05299100	-4.88482400	1.52688500
H	-2.09988800	-3.78261500	0.61383000
H	-1.03753300	-4.91137300	-0.23981000
H	-0.83974000	-0.55512700	3.12227200
H	0.99844500	-0.77584200	3.13227100

INT5

0 7

O	0.00373600	1.32850800	-1.12321600
C	-0.01326200	1.72907900	0.08715000
O	-0.03225300	0.97739900	1.09025400
O	-1.88191100	-1.24360600	0.47653900
C	-2.47192200	-1.16469200	-0.62635600
O	-1.87133100	-1.01377700	-1.74297300
O	1.87641300	-1.02298600	-1.73945900
C	2.47615200	-1.13380400	-0.61743500
O	1.88610600	-1.16464000	0.48747200
C	3.96681800	-1.17902900	-0.61109800
C	4.69078200	-0.92950900	-1.77976900
C	4.64070000	-1.40662700	0.59391500
C	6.09370400	-0.88977200	-1.74196100
C	6.04259900	-1.38746200	0.63607700
C	6.76934300	-1.12377600	-0.53501000
H	4.15706900	-0.74612100	-2.71338400
H	4.06312200	-1.58906000	1.50127700
H	7.85923800	-1.09170700	-0.50580400
C	-3.96294600	-1.19885200	-0.62268300
C	-4.64012000	-1.42593000	0.58057700
C	-4.68361800	-0.93909600	-1.79133100
C	-6.04179200	-1.39454300	0.62141300
C	-6.08635800	-0.89133900	-1.75563200
C	-6.76515000	-1.12312000	-0.54995200
H	-4.06511900	-1.61633800	1.48790000
H	-4.14734700	-0.75538300	-2.72340700
H	-7.85482500	-1.08324500	-0.52202600
C	-0.00985200	3.19769500	0.33232500
C	-0.01115800	3.63479900	1.65603300
C	-0.00387300	4.12785800	-0.71151500
C	-0.00541900	5.00176900	1.94849200
C	-0.00011500	5.50219800	-0.42048800
C	-0.00039600	5.94099600	0.91168300
H	-0.01574800	2.89917500	2.46035400
H	-0.00245800	3.77907400	-1.74523800
H	0.00350500	7.00844600	1.13487800
C	0.00414600	6.48947400	-1.45581200
C	-6.82903000	-0.57983000	-2.94009600
C	-0.00372100	5.39453600	3.31823800
C	-6.73347400	-1.61640600	1.85759100
C	6.73186300	-1.61423800	1.87277500



C	6.83925400	-0.58317600	-2.92579200
N	0.00722500	7.33619200	-2.25578000
N	-0.00158900	5.63930000	4.45504200
N	-7.43619400	-0.30992700	-3.89753500
N	-7.29417700	-1.78957200	2.86503200
N	7.29154800	-1.79245000	2.87993000
N	7.44792000	-0.31572600	-3.88293300
Co	-0.00446100	-1.01945600	1.19064600
Co	0.00333600	-0.56413500	-1.57065500
C	0.36388300	-4.15333100	1.17381600
C	-0.39312900	-3.61886800	2.38546500
H	0.15474400	-3.50547600	0.29645200
H	1.44968400	-4.04766500	1.34772600
C	0.02527000	-5.58779700	0.82874400
C	0.01330800	-2.22762400	2.80609300
H	-1.47694200	-3.64893200	2.17299000
H	-0.25371200	-4.33018000	3.22473500
H	0.27102400	-6.26543600	1.65943000
H	-1.04835600	-5.71044500	0.62247000
H	0.57178200	-5.94387000	-0.05485400
H	-0.65424700	-1.78363800	3.56130100
H	1.05483600	-2.17164800	3.16745700

#### INT6

0 7

O	0.23694900	0.81924100	-1.21720600
C	0.23120500	1.47958500	-0.15274200
O	0.16938900	0.98242300	1.02035600
O	-1.84475400	-1.22695700	1.54629300
C	-2.47097000	-1.06794200	0.44454500
O	-1.90530100	-1.01637200	-0.67274200
O	1.96000900	-1.45231200	-0.70763100
C	2.54081900	-1.44591700	0.40226300
O	1.92556900	-1.42887500	1.52199800
C	4.03383600	-1.39527400	0.42407700
C	4.74386400	-1.37606800	-0.78202700
C	4.71934000	-1.29275500	1.63830300
C	6.14204200	-1.25012400	-0.77996200
C	6.11743300	-1.16158500	1.65064000
C	6.82762600	-1.14193400	0.44044300
H	4.19635100	-1.44530500	-1.72304900
H	4.15671000	-1.29890100	2.57291200
H	7.91302300	-1.03335100	0.44792900
C	-3.95170200	-0.87965500	0.49570200
C	-4.60145200	-0.73623000	1.72515500
C	-4.67940500	-0.77144500	-0.69541300
C	-5.97920800	-0.46826200	1.76807800
C	-6.06055700	-0.52144800	-0.66242400
C	-6.70835200	-0.36601300	0.57354200
H	-4.02426800	-0.81298000	2.64769200
H	-4.15894800	-0.86992300	-1.64934800
H	-7.77823000	-0.15561200	0.60513000
C	0.29851100	2.96198700	-0.25460400
C	0.35067600	3.76513000	0.88677700
C	0.30178400	3.54402900	-1.52113700
C	0.40964000	5.16055400	0.75555700
C	0.35264400	4.93562400	-1.65322800
C	0.40882700	5.74926500	-0.51603900
H	0.34584400	3.29997900	1.87325000
H	0.26034400	2.90468000	-2.40333500

H	0.45061400	6.83426800	-0.61721000
C	0.34050500	5.50142100	-2.96041200
C	0.46997800	6.00293000	1.90720300
C	-6.81122900	-0.40050500	-1.88033200
C	-6.63533700	-0.26970700	3.02738900
C	6.81844800	-1.02275900	2.89384900
C	6.87269800	-1.20839000	-2.01502100
N	0.32342600	5.91798500	-4.04576600
N	0.52097000	6.71414700	2.82724700
N	-7.42850700	-0.29431500	-2.86452900
N	-7.16258200	-0.09036700	4.05170100
N	7.38682000	-0.89696700	3.90414300
N	7.47234300	-1.16416900	-3.01465000
Co	0.06353900	-0.92766300	1.36975700
Co	0.02829900	-1.17552100	-1.32065400
C	-0.45392900	-3.67699300	-1.63645800
C	-0.13011400	-2.63701300	-2.68684300
H	0.84005000	-2.75429200	-3.18840700
H	-0.93161700	-2.46553700	-3.41926200
H	-0.24019800	-3.29496300	-0.59862400
H	0.23977300	-4.53596500	-1.69613400
C	-1.89844100	-4.15545900	-1.64932400
H	-2.06460900	-4.73524800	-2.57253300
C	-2.28214400	-4.97399200	-0.43507000
H	-2.18577900	-4.38884300	0.49368100
H	-3.31983100	-5.32989200	-0.48822000
H	-1.64059000	-5.86060200	-0.32160800
H	-2.56266200	-3.27925800	-1.73913400

TS6-7

0 3

O	-0.16228100	0.77198200	1.03193900
C	-0.13554100	1.54030000	0.03068400
O	-0.06088000	1.17275800	-1.17316800
O	1.86579100	-1.06674500	-1.54991700
C	2.47513400	-1.02254900	-0.44228900
O	1.91052500	-1.03555100	0.68701300
O	-1.93817600	-1.33852300	0.73844600
C	-2.51813200	-1.27037800	-0.38017000
O	-1.92084800	-1.16213700	-1.49096000
C	-4.00477600	-1.31565400	-0.38912600
C	-4.70570900	-1.54120100	0.79787300
C	-4.69889500	-1.11246600	-1.58350900
C	-6.10721200	-1.57155600	0.79091700
C	-6.10070400	-1.12503400	-1.59169500
C	-6.80757200	-1.35915700	-0.40446500
H	-4.15425000	-1.69207200	1.72651400
H	-4.14185800	-0.93520400	-2.50420700
H	-7.89806600	-1.37315300	-0.41013000
C	3.96131600	-0.96193100	-0.45902600
C	4.63912300	-0.74126500	-1.65990600
C	4.67727400	-1.11596900	0.73018200
C	6.03905500	-0.66125100	-1.67052700
C	6.07793700	-1.06442000	0.71949600
C	6.76137700	-0.83030500	-0.48121900
H	4.07060800	-0.62107900	-2.58290100
H	4.13905000	-1.27531800	1.66525400
H	7.85063100	-0.77684600	-0.49023400
C	-0.19921200	3.01028500	0.29390900
C	-0.23860600	3.90082700	-0.78034300

C	-0.21772500	3.49548700	1.60253600
C	-0.30070300	5.28228200	-0.54983000
C	-0.27218500	4.87712200	1.83888500
C	-0.31580500	5.77353800	0.76241700
H	-0.22192200	3.50775500	-1.79750400
H	-0.18698700	2.79023100	2.43407000
H	-0.36089600	6.84774700	0.94554900
C	-0.28088000	5.37655400	3.17789800
C	-0.34965100	6.18861300	-1.65389500
C	6.80591300	-1.25280300	1.93481800
C	6.73447400	-0.39514400	-2.89068000
C	-6.80984900	-0.88838100	-2.80969100
C	-6.82450000	-1.81738400	2.00275000
N	-0.28482800	5.78508100	4.26835100
N	-0.39152900	6.92103500	-2.55829000
N	7.38985800	-1.41722800	2.92866000
N	7.30287600	-0.16584300	-3.88070200
N	-7.38354400	-0.68607500	-3.80244700
N	-7.40713400	-2.02240300	2.98988400
Co	-0.04285900	-0.78241800	-1.68103400
Co	-0.01116700	-1.18709400	0.75850100
C	1.37835000	-3.71069100	1.96736900
C	0.12042700	-2.88752400	1.97637000
H	1.30987500	-4.36875600	2.85193900
H	2.24231200	-3.05755600	2.16061100
C	1.60345300	-4.54816400	0.72702800
C	0.02046200	-1.67879000	2.69546100
H	-0.80632100	-3.46223400	1.84462200
H	0.73692900	-5.18831300	0.50496900
H	1.77574000	-3.91858100	-0.16007600
H	2.47546700	-5.20611000	0.83480400
H	-0.93772300	-1.34415100	3.09720400
H	0.91673400	-1.24237400	3.14599200
H	0.07661800	-2.58138100	0.26356100

#### INT7

0 5

O	-0.18482800	0.80424300	1.05818500
C	-0.17658400	1.56907400	0.05799700
O	-0.11158000	1.19167100	-1.14669600
O	1.90427600	-0.87817400	-1.54818200
C	2.48990000	-0.93133300	-0.42706200
O	1.92067100	-1.04878100	0.69368700
O	-1.95137600	-1.37991200	0.73085300
C	-2.54108500	-1.24299100	-0.37608500
O	-1.97468000	-1.05079900	-1.49260100
C	-4.02518800	-1.30625400	-0.37472800
C	-4.71769700	-1.54653800	0.81225600
C	-4.72361700	-1.10318200	-1.56482000
C	-6.11786700	-1.58699700	0.80699200
C	-6.12335500	-1.13608400	-1.56903800
C	-6.82589900	-1.38032600	-0.38342000
H	-4.16194400	-1.69783100	1.73809600
H	-4.17169000	-0.91240800	-2.48544200
H	-7.91606700	-1.40624600	-0.38538700
C	3.97355700	-0.86838100	-0.43055700
C	4.65464900	-0.63740800	-1.62575900
C	4.68201500	-1.03514400	0.75948400
C	6.05328300	-0.56616100	-1.63027900
C	6.08139000	-0.97878300	0.75270400

C	6.77206400	-0.74072700	-0.44173300
H	4.08976700	-0.50707900	-2.54919000
H	4.13876600	-1.20570300	1.68964300
H	7.86133200	-0.68946500	-0.44556200
C	-0.24799800	3.04066700	0.30874900
C	-0.29144100	3.92699100	-0.76876500
C	-0.26805500	3.53048200	1.61573800
C	-0.35825600	5.30912300	-0.54224900
C	-0.32840400	4.91237400	1.84828200
C	-0.37533900	5.80460500	0.76844800
H	-0.27359300	3.53129700	-1.78489600
H	-0.23395300	2.82789100	2.44941200
H	-0.42434700	6.87932300	0.94760200
C	-0.33934700	5.41515800	3.18626700
C	-0.40880400	6.21306200	-1.64825200
C	6.80312000	-1.16492200	1.96773500
C	6.74382100	-0.30712000	-2.85022400
C	-6.82743600	-0.90949900	-2.78746800
C	-6.82837500	-1.83477500	2.01801800
N	-0.34512200	5.82499300	4.27629100
N	-0.45107900	6.94501800	-2.55299300
N	7.38412400	-1.32358200	2.96271900
N	7.29701300	-0.08794500	-3.84951600
N	-7.38527400	-0.71608200	-3.78943900
N	-7.40808300	-2.03751100	3.00580900
Co	-0.04835800	-0.77303700	-1.59237900
Co	-0.01387600	-1.19506400	0.81186000
C	1.61347200	-4.02231000	1.62786200
C	0.28014900	-3.42051600	1.92691800
H	1.70261600	-4.91792600	2.27038300
H	2.40887600	-3.34206300	1.97116000
C	1.83383500	-4.43585500	0.18538700
C	0.06387700	-2.39721700	2.78562100
H	-0.59203600	-3.92788000	1.49252500
H	1.04332300	-5.11536100	-0.16542300
H	1.84075500	-3.57328900	-0.49624300
H	2.79081100	-4.96017800	0.06338200
H	-0.94590500	-2.11426300	3.09198400
H	0.89873200	-1.91234100	3.30305300
H	0.04166000	-2.17205300	-0.41128000

## H-Ni-DHKUST-1

### INT1

0 3

O	-0.00006800	0.73332400	-1.19783100
C	-0.00016700	1.28964000	-0.06822700
O	-0.00025100	0.68218800	1.04502100
O	-1.91067000	-1.56141400	1.09664000
C	-2.48603800	-1.45634500	-0.02478800
O	-1.89722900	-1.30365100	-1.13684400
O	1.89742000	-1.30379000	-1.13682800
C	2.48616600	-1.45615800	-0.02471700
O	1.91074600	-1.56091800	1.09671500
C	3.97467500	-1.49692900	-0.03450100
C	4.68409800	-1.47203800	-1.23786500
C	4.65899800	-1.54447100	1.18233900
C	6.08688200	-1.49948300	-1.22283600
C	6.06012100	-1.56262700	1.20253700
C	6.77592800	-1.54258100	-0.00201600
H	4.14152500	-1.43106900	-2.18320500
H	4.09305500	-1.56078000	2.11410500
H	7.86644500	-1.55814500	0.00865100
C	-3.97455000	-1.49712500	-0.03463800
C	-4.65890600	-1.54514300	1.18216800
C	-4.68394600	-1.47173400	-1.23800700
C	-6.06003000	-1.56328700	1.20233000
C	-6.08673300	-1.49914000	-1.22301900
C	-6.77580800	-1.54272600	-0.00223200
H	-4.09298300	-1.56183000	2.11394000
H	-4.14135200	-1.43039100	-2.18331900
H	-7.86632500	-1.55826400	0.00840200
C	-0.00019200	2.78122900	-0.01816500
C	-0.00044500	3.42715800	1.21902000
C	0.00007800	3.52806500	-1.19809000
C	-0.00043600	4.82708100	1.28270300
C	0.00011300	4.92989900	-1.13948400
C	-0.00015000	5.58125400	0.10212000
H	-0.00064700	2.83171200	2.13249100
H	0.00027900	3.01187400	-2.15912600
H	-0.00012600	6.67094100	0.14764500
C	0.00043900	5.70714300	-2.33973600
C	-6.82663900	-1.48042500	-2.44736100
C	-0.00070400	5.47520300	2.55613200
C	-6.74915300	-1.59428600	2.45515200
C	6.74921600	-1.59312600	2.45538300
C	6.82680800	-1.48132000	-2.44717400
N	0.00073200	6.35321400	-3.30869500
N	-0.00093000	5.98351600	3.60358600
N	-7.44209000	-1.46683600	-3.43616400
N	-7.29292400	-1.61337400	3.48487500
N	7.29296500	-1.61180000	3.48511700
N	7.44226200	-1.46818700	-3.43598100
Ni	-0.00000900	-1.28271300	1.15016200
Ni	0.00011000	-1.25028500	-1.17525700
H	-0.00013800	-2.69811600	-1.00326100

### INT2

0 1

O	-0.00924700	0.60538800	-1.16502400
C	-0.00340800	1.20227500	-0.05909200

O	0.00832900	0.62971000	1.06695700
O	-1.92232800	-1.47984300	1.29722800
C	-2.53832700	-1.40719900	0.18677700
O	-2.02979500	-1.38904700	-0.96086700
O	2.03918600	-1.36604600	-0.95792000
C	2.55140900	-1.39067300	0.18809100
O	1.93904200	-1.47439600	1.29963300
C	4.03790300	-1.28671000	0.26188300
C	4.76851500	-1.16036900	-0.91858400
C	4.69132200	-1.27410500	1.49338000
C	6.16011100	-1.01843600	-0.87134300
C	6.08456900	-1.13193500	1.54148000
C	6.82456500	-1.00428700	0.36003100
H	4.24306800	-1.16181500	-1.87370300
H	4.11051000	-1.36486700	2.41175900
H	7.90804900	-0.88771600	0.40031500
C	-4.02489100	-1.30813400	0.26519900
C	-4.67382400	-1.30266100	1.49904400
C	-4.76008000	-1.17818200	-0.91210200
C	-6.06719500	-1.16480500	1.55299800
C	-6.15180600	-1.03878700	-0.85890900
C	-6.81178700	-1.03265400	0.37500100
H	-4.08940900	-1.39578300	2.41486800
H	-4.23811200	-1.17417800	-1.86914200
H	-7.89536100	-0.91859300	0.41978800
C	-0.01182700	2.69598100	-0.07374500
C	-0.00111200	3.41965200	1.12070100
C	-0.03172600	3.36695700	-1.29706700
C	-0.01003300	4.82266200	1.09175500
C	-0.04148800	4.76802500	-1.33201800
C	-0.03043200	5.49852900	-0.13652000
H	0.01411700	2.88484600	2.07127300
H	-0.03998600	2.78910900	-2.22194800
H	-0.03780800	6.58889200	-0.16047600
C	-0.06321400	5.44247000	-2.59156300
C	0.00112300	5.57587700	2.30790500
C	-6.88684000	-0.88551300	-2.06972400
C	-6.73112600	-1.14067900	2.81337700
C	6.75417500	-1.09883700	2.79874000
C	6.88930600	-0.87172300	-2.08640900
N	-0.08139500	5.97322600	-3.62769600
N	0.01003600	6.20272400	3.28968600
N	-7.46554400	-0.75309600	-3.06966200
N	-7.27149400	-1.11241500	3.84263100
N	7.30090200	-1.06267500	3.82441400
N	7.46141200	-0.74578200	-3.09094600
Ni	0.00803900	-1.33632900	1.29715500
Ni	0.00479200	-1.39116400	-1.28586800
C	0.01691100	-3.39928600	-2.16683200
C	0.01210300	-2.44220800	-3.13570100
H	0.94315300	-2.09375500	-3.59251000
H	-0.92231000	-2.10411500	-3.59342900
H	0.01005500	-2.33593000	0.01375900
H	-0.91076600	-3.85896600	-1.81849900
H	0.94924300	-3.84876100	-1.81760400

TS2-3

03

O	-0.00362100	0.61530900	-1.13315400
C	-0.00243100	1.17449400	-0.00085200

O	0.00471900	0.58280900	1.11263700
O	-1.90064900	-1.63384900	1.27117200
C	-2.52309500	-1.48827700	0.17834300
O	-1.98780500	-1.39861000	-0.95785000
O	1.99912800	-1.38387800	-0.95611700
C	2.53700300	-1.47430200	0.17890900
O	1.91730900	-1.62543300	1.27240900
C	4.02319300	-1.36376400	0.23871200
C	4.74980300	-1.19393600	-0.94100400
C	4.68220800	-1.38215600	1.46900700
C	6.14187900	-1.04009200	-0.89507900
C	6.07488800	-1.22531400	1.51975500
C	6.80773400	-1.05535800	0.33749100
H	4.22204100	-1.17137400	-1.89483200
H	4.10390500	-1.50699600	2.38527300
H	7.89018300	-0.92836900	0.37784100
C	-4.00953200	-1.38329700	0.24171300
C	-4.66455500	-1.41002100	1.47389000
C	-4.74043800	-1.20960400	-0.93489000
C	-6.05746200	-1.25819400	1.53002100
C	-6.13286900	-1.05965900	-0.88349900
C	-6.79466300	-1.08383900	0.35119100
H	-4.08294600	-1.53750400	2.38766200
H	-4.21584900	-1.18054800	-1.89031100
H	-7.87733600	-0.96020800	0.39570000
C	-0.01116800	2.66813900	0.01500900
C	-0.00122400	3.35908000	1.22830600
C	-0.03064400	3.37161400	-1.18940200
C	-0.01023000	4.76181200	1.23721200
C	-0.04100100	4.77292900	-1.18535700
C	-0.03047200	5.47146400	0.02865500
H	0.01355800	2.79703000	2.16302600
H	-0.03825800	2.82011500	-2.13001800
H	-0.03814400	6.56204200	0.03418000
C	-0.06296300	5.48097500	-2.42517500
C	0.00077100	5.47868400	2.47393700
C	-6.87257500	-0.86511700	-2.09034100
C	-6.72722900	-1.26166500	2.79167600
C	6.75020700	-1.21913300	2.77856900
C	6.87566900	-0.85121100	-2.10628700
N	-0.08158600	6.03983100	-3.44606400
N	0.00977900	6.07348200	3.47504300
N	-7.46542400	-0.69993500	-3.07867300
N	-7.27141200	-1.25471400	3.82068400
N	7.30098200	-1.20379900	3.80401800
N	7.46153200	-0.69132400	-3.09960300
Ni	0.00767700	-1.39593600	1.23693400
Ni	0.00568100	-1.35457100	-1.17071700
C	0.01138300	-2.68189500	-2.91806800
C	0.00636800	-1.35803900	-3.30140600
H	0.93523700	-0.83248300	-3.53271800
H	-0.92640700	-0.83970300	-3.53327200
H	0.01168100	-2.82799500	-1.15672000
H	-0.91369200	-3.26420100	-2.93358900
H	0.94091700	-3.25707200	-2.93312800

### INT3

0 3

O	0.06688500	0.82410200	-1.15485900
C	0.06550500	1.46007200	-0.07117000

O	0.04728600	0.93432100	1.08285200
O	-1.89383000	-1.27195600	1.23665900
C	-2.47894300	-1.19763500	0.11662000
O	-1.90197900	-1.11127200	-1.00640500
O	1.92272400	-1.23746000	-1.02187900
C	2.50306000	-1.31080600	0.09988900
O	1.92200800	-1.34024400	1.22436500
C	3.99123800	-1.36275300	0.10359400
C	4.70213900	-1.42230600	-1.09672900
C	4.67314500	-1.34346500	1.32219200
C	6.10367400	-1.46874600	-1.07766500
C	6.07391100	-1.38064800	1.34519600
C	6.79162800	-1.44583200	0.14362600
H	4.16032400	-1.43267800	-2.04326000
H	4.10579400	-1.29472800	2.25202100
H	7.88172900	-1.47745200	0.15745400
C	-3.96682400	-1.21938000	0.12416000
C	-4.64373900	-1.19017200	1.34528100
C	-4.68307700	-1.26512800	-1.07383500
C	-6.04466900	-1.20163800	1.37349200
C	-6.08526100	-1.28692200	-1.04939400
C	-6.76797500	-1.25266400	0.17463000
H	-4.07205000	-1.15323500	2.27299600
H	-4.14546600	-1.28281600	-2.02288000
H	-7.85840800	-1.26439500	0.19251800
C	0.08527500	2.95284000	-0.12327000
C	0.09470100	3.67828200	1.06868900
C	0.09126200	3.62176500	-1.34916300
C	0.11037200	5.07913000	1.04167000
C	0.10571400	5.02485400	-1.38180200
C	0.11563700	5.75544500	-0.18500100
H	0.08928400	3.14334000	2.01880500
H	0.08352800	3.04331900	-2.27419200
H	0.12690900	6.84574700	-0.21040000
C	0.10896500	5.72590000	-2.62853300
C	-6.82761000	-1.34373200	-2.26956300
C	0.11971100	5.80513200	2.27207800
C	-6.72810000	-1.15587100	2.62790900
C	6.76437800	-1.34762300	2.59635000
C	6.83864600	-1.54063600	-2.30139800
C	0.02350400	-3.11914200	-1.11784500
C	-1.26182400	-3.88090600	-0.99038100
H	-1.07591200	-4.95980500	-1.12634600
H	-1.72371100	-3.77481300	0.00256600
H	-2.00811200	-3.59140700	-1.74203700
H	0.77443600	-3.43102700	-0.37411000
H	0.48527800	-3.21475000	-2.11680800
N	0.11072700	6.31464800	-3.63356800
N	0.12678500	6.37319500	3.28829600
N	-7.43992600	-1.39323600	-3.25869700
N	-7.26992400	-1.11357100	3.65760500
N	7.31442200	-1.31638400	3.62215200
N	7.44284300	-1.60314300	-3.29475500
Ni	0.01955500	-1.01786300	1.26513200
Ni	0.00296300	-1.18107600	-1.07860300

INT4

0 3

O	0.02622200	1.08794200	-1.30096200
C	0.07790600	1.53182800	-0.11780800



O	0.11318500	0.83150500	0.92633400
O	-1.90449400	-1.08782300	0.73896000
C	-2.48428100	-1.10787800	-0.38499700
O	-1.90699500	-1.12341200	-1.50901200
O	1.94451700	-1.15420400	-1.49867100
C	2.51435500	-1.24547900	-0.37431400
O	1.92907000	-1.29091900	0.74598000
C	4.00212000	-1.30067200	-0.35257500
C	4.72234500	-1.19290300	-1.54278600
C	4.67387600	-1.44878900	0.86184800
C	6.12336200	-1.23170100	-1.51791200
C	6.07393100	-1.49240100	0.88925300
C	6.80254000	-1.38279500	-0.30192200
H	4.18625800	-1.07437100	-2.48511500
H	4.10012800	-1.52803400	1.78558200
H	7.89254400	-1.41292100	-0.28331500
C	-3.97166700	-1.13149100	-0.36598100
C	-4.64875600	-1.26881000	0.84707100
C	-4.68629000	-1.01974100	-1.55899800
C	-6.04947300	-1.29692100	0.86960200
C	-6.08757600	-1.03822800	-1.53829700
C	-6.77249300	-1.17877800	-0.32433300
H	-4.07871900	-1.35402900	1.77293600
H	-4.14558900	-0.91387700	-2.50020600
H	-7.86284500	-1.19546200	-0.30926700
C	0.09585000	3.01760300	0.05506900
C	0.10242000	3.55474600	1.34241700
C	0.10147400	3.86539200	-1.05459700
C	0.11196800	4.94366100	1.52789400
C	0.11602400	5.25733800	-0.87492700
C	0.12010300	5.79850200	0.41839700
H	0.09792600	2.88121400	2.20027800
H	0.09476000	3.43395900	-2.05653800
H	0.12896700	6.88001800	0.55882200
C	0.12621000	6.13831600	-2.00154400
C	-6.82011700	-0.90930800	-2.75642700
C	0.11053500	5.47478800	2.85367700
C	-6.73757900	-1.44578800	2.11187200
C	6.75342400	-1.64669600	2.13544300
C	6.86380300	-1.11189700	-2.73247600
N	0.13547200	6.87125400	-2.90681400
N	0.10652600	5.88228900	3.94420000
N	-7.41441800	-0.80008900	-3.75090800
N	-7.28953000	-1.56975600	3.12910000
N	7.29481500	-1.77362500	3.15790900
N	7.46823400	-1.01106700	-3.72183700
Ni	0.00644700	-1.20231200	0.81420600
Ni	0.02027400	-0.86881800	-1.52638900
C	-0.00466600	-3.12851700	0.40171700
C	-0.05943700	-1.96855700	3.31804500
H	0.45186600	-3.20771900	-0.60260400
H	0.74394200	-3.48833000	1.12210400
C	-1.30357500	-3.87391600	0.48667900
C	-0.02581800	-0.63310800	3.35624100
H	-1.00352300	-2.51919300	3.28618400
H	0.85526500	-2.56618200	3.35748500
H	-1.83335400	-3.71074700	1.43602500
H	-1.99710700	-3.62492200	-0.32827900
H	-1.11949700	-4.95916200	0.41254500
H	-0.93797700	-0.03194700	3.33333300

H 0.91590600 -0.08119700 3.40656200

TS4-5

0 3

O 0.01807600 1.15276600 -1.23772700  
C 0.13673300 1.57423400 -0.05889200  
O 0.23965200 0.85699800 0.97637500  
O -1.98138900 -0.97155200 0.70837200  
C -2.51004800 -1.03355200 -0.43095200  
O -1.89012600 -1.07759700 -1.53422600  
O 1.92694700 -1.12294700 -1.51308900  
C 2.53587300 -1.29288900 -0.41484800  
O 1.99775300 -1.41539000 0.71428400  
C 4.02231700 -1.34176100 -0.44924300  
C 4.72425000 -1.16617300 -1.64015600  
C 4.71101700 -1.53097200 0.74740500  
C 6.12557900 -1.17682600 -1.62536800  
C 6.10907500 -1.54519800 0.76073700  
C 6.82432400 -1.36756400 -0.42726500  
H 4.17711400 -1.01073300 -2.57087000  
H 4.14775000 -1.65773000 1.67166100  
H 7.91472400 -1.37034800 -0.42229300  
C -3.99613500 -1.07407400 -0.46797700  
C -4.69295600 -1.24559100 0.72707300  
C -4.68899100 -0.92980400 -1.66780000  
C -6.09095900 -1.28603500 0.72677400  
C -6.08995400 -0.94376900 -1.66331400  
C -6.79725900 -1.12844600 -0.46966800  
H -4.13730600 -1.34722300 1.65968800  
H -4.13520300 -0.79428700 -2.59768500  
H -7.88752300 -1.14543400 -0.47436000  
C 0.14967100 3.05434600 0.15482900  
C 0.15313400 3.55015600 1.45768400  
C 0.14100300 3.93749600 -0.92762900  
C 0.13986600 4.93128500 1.68849300  
C 0.14080500 5.32331800 -0.70160500  
C 0.13707300 5.82235600 0.60902500  
H 0.15968000 2.85019100 2.29340600  
H 0.13400600 3.53880400 -1.94317000  
H 0.12971600 6.89878500 0.78422000  
C 0.14087900 6.25114700 -1.79055000  
C -6.80958500 -0.75501400 -2.87592300  
C 0.11934200 5.40353800 3.03487100  
C -6.77675400 -1.48871200 1.95743800  
C 6.78041600 -1.72760800 2.00228100  
C 6.85945200 -0.97593700 -2.82819000  
N 0.14234700 7.03587200 -2.65152800  
N 0.09432800 5.74128300 4.14825300  
N -7.40641000 -0.58786700 -3.85888400  
N -7.30064000 -1.66471900 2.98010000  
N 7.28353700 -1.87380300 3.03987600  
N 7.47607100 -0.80415000 -3.79834400  
Ni 0.01764900 -1.11437400 0.95236800  
Ni 0.02438500 -0.80757800 -1.50296300  
C -0.16114400 -3.29394500 0.81664200  
C -0.30897100 -2.43408900 2.70562400  
H -0.16091300 -2.80767900 -0.18059200  
H 0.82534400 -3.74377900 0.96576600  
C -1.32040400 -4.22905000 0.93580800  
C 0.06522300 -1.10374900 2.97851500

H	-1.37084100	-2.67064700	2.80989400
H	0.36624500	-3.22913700	3.03304700
H	-1.31519500	-4.79694300	1.87631300
H	-2.28394900	-3.70568200	0.86075200
H	-1.29059600	-4.96498600	0.11691200
H	-0.69434100	-0.34599700	3.18315700
H	1.09516700	-0.84974500	3.23966100

INT5

0 3

O	0.03256700	1.38907900	-1.19702300
C	0.01058200	1.66910300	0.03040700
O	-0.01821900	0.82955100	0.97456000
O	-1.91541000	-1.39166200	0.45557100
C	-2.48643400	-1.11001300	-0.63998000
O	-1.90065100	-0.80277700	-1.71502800
O	1.92382100	-0.83647200	-1.70864500
C	2.50045000	-1.12019900	-0.62169100
O	1.92111600	-1.36147500	0.47842700
C	3.98975100	-1.16217400	-0.61330600
C	4.70864300	-0.86388700	-1.77211100
C	4.66545700	-1.46553600	0.57015700
C	6.11063700	-0.86578300	-1.74564500
C	6.06629100	-1.47038400	0.60019700
C	6.79236400	-1.16997700	-0.55945700
H	4.17019800	-0.62144500	-2.68917600
H	4.09304700	-1.68922600	1.47075200
H	7.88275700	-1.16690400	-0.53890600
C	-3.97598000	-1.13129500	-0.63838800
C	-4.66118600	-1.42719800	0.54159400
C	-4.68536700	-0.81999400	-1.79967000
C	-6.06207800	-1.41121500	0.56556900
C	-6.08731900	-0.80314500	-1.77974400
C	-6.77856400	-1.09927700	-0.59699900
H	-4.09622400	-1.65983900	1.44474100
H	-4.13943000	-0.58270500	-2.71366200
H	-7.86888400	-1.08079800	-0.58129800
C	0.01953300	3.11319700	0.41468400
C	0.01720500	3.46301800	1.76493400
C	0.03121100	4.10827300	-0.56490000
C	0.02716300	4.81184600	2.14375700
C	0.03942600	5.46059600	-0.19044100
C	0.03776700	5.81443200	1.16612600
H	0.00873000	2.67595700	2.51947000
H	0.03360400	3.82192500	-1.61756900
H	0.04492700	6.86538500	1.45737700
C	0.04944900	6.49179000	-1.18074300
C	-6.81941700	-0.47047900	-2.96035800
C	0.02690500	5.14890900	3.53124700
C	-6.75240500	-1.69987000	1.78254400
C	6.74686900	-1.76888500	1.82027600
C	6.85269800	-0.54390800	-2.92303200
N	0.05719900	7.34627300	-1.97201500
N	0.02698000	5.39435500	4.66909800
N	-7.42113400	-0.19374600	-3.91764500
N	-7.29956800	-1.93135800	2.78373000
N	7.28597000	-2.00868500	2.82388000
N	7.46276300	-0.27551900	-3.87741500
Ni	-0.00201600	-1.13130700	0.61965800
Ni	0.01476900	-0.51861100	-1.72274500

C	0.25312900	-4.01072300	1.68578400
C	-0.50346300	-3.07910000	2.62821500
H	0.10985800	-3.66579600	0.64102400
H	1.33676900	-3.91385400	1.86747500
C	-0.17959800	-5.45636800	1.79650300
C	-0.03750500	-1.66741800	2.60136000
H	-1.58522300	-3.12902800	2.42131500
H	-0.39397000	-3.45684800	3.66660200
H	-0.00580700	-5.84726600	2.80946900
H	-1.25193500	-5.57504500	1.58406700
H	0.36736300	-6.10322300	1.09855800
H	-0.71150300	-0.90168300	3.00173600
H	1.02009000	-1.48713600	2.83278300

INT6

0 3

O	-0.11432000	0.75562100	1.08382800
C	-0.14476500	1.56913100	0.11620300
O	-0.12290900	1.26025400	-1.10338800
O	1.86164900	-0.82643300	-1.70989200
C	2.49304600	-1.01462800	-0.63035300
O	1.97087100	-1.25137200	0.49318100
O	-1.96394900	-1.48483300	0.54942400
C	-2.53005400	-1.26500900	-0.55527000
O	-1.94200000	-0.99220000	-1.64227200
C	-4.01784000	-1.31490300	-0.57704600
C	-4.71390200	-1.64033200	0.58742700
C	-4.71465700	-1.00031600	-1.74369300
C	-6.11441800	-1.65404600	0.58840800
C	-6.11600300	-1.00488700	-1.74258400
C	-6.82032100	-1.33423300	-0.57770500
H	-4.15691900	-1.87475200	1.49490000
H	-4.15990800	-0.74076900	-2.64607600
H	-7.91082700	-1.33513600	-0.57788000
C	3.97929700	-0.93894200	-0.67808500
C	4.63467800	-0.58712800	-1.85844500
C	4.71357100	-1.18874200	0.48126400
C	6.03229400	-0.47862900	-1.87450500
C	6.11029600	-1.09258800	0.46456700
C	6.77459500	-0.73450700	-0.71430100
H	4.05031900	-0.38687200	-2.75740200
H	4.18919800	-1.45015800	1.40067300
H	7.86161400	-0.64855300	-0.72901400
C	-0.21209600	3.02201900	0.46062200
C	-0.26885800	3.98294100	-0.55096200
C	-0.21737200	3.41586500	1.79876800
C	-0.33213500	5.34548000	-0.22248400
C	-0.27817000	4.77583600	2.13198600
C	-0.33622300	5.74402600	1.12141700
H	-0.26368100	3.66113000	-1.59326600
H	-0.17325600	2.65536300	2.57897100
H	-0.38434600	6.80286400	1.37824800
C	-0.27998000	5.16602200	3.50581900
C	-0.39314700	6.33730700	-1.25055300
C	6.84329400	-1.35087900	1.66046100
C	6.70985000	-0.08952400	-3.06809000
C	-6.83057100	-0.65587600	-2.92642700
C	-6.81736100	-1.98191200	1.78576500
N	-0.27953800	5.46460500	4.63100100
N	-0.44412800	7.15445500	-2.07885200

N	7.41611600	-1.56545600	2.65009700
N	7.27087300	0.23812300	-4.03323600
N	-7.41207200	-0.36039700	-3.88966200
N	-7.37715400	-2.24779700	2.77056300
Ni	-0.05258400	-0.64757400	-1.63866800
Ni	-0.00294300	-1.18536000	0.73457200
C	1.44919100	-3.85680800	2.37532000
C	0.15786700	-3.11271700	2.06656900
H	1.44673200	-4.10882600	3.44796600
H	2.29360400	-3.16451400	2.23396400
C	1.64173400	-5.10047000	1.53614000
C	0.03204600	-1.75585800	2.64113400
H	-0.74305900	-3.71855900	2.26591700
H	0.80593100	-5.80598500	1.65120800
H	1.71606700	-4.85386200	0.46582500
H	2.55935400	-5.63618400	1.81012200
H	-0.92653600	-1.42769800	3.05224100
H	0.91805800	-1.29709100	3.09306400
H	0.09567600	-3.05543000	0.92059700

TS6-7

0 3

O	-0.19920400	0.75251400	1.10357400
C	-0.17535600	1.51472400	0.09667400
O	-0.10260300	1.14568200	-1.10618800
O	1.85649800	-0.96904700	-1.67221000
C	2.48501900	-0.98024400	-0.57481000
O	1.96101800	-1.02222400	0.56930100
O	-1.98936200	-1.42797600	0.61521000
C	-2.54427000	-1.29814400	-0.50617600
O	-1.94753700	-1.10512400	-1.60581400
C	-4.03134900	-1.35441100	-0.53350700
C	-4.72994000	-1.63624500	0.64041500
C	-4.72400200	-1.08639400	-1.71345800
C	-6.12993500	-1.65412200	0.63710400
C	-6.12522300	-1.09141000	-1.71496700
C	-6.83304400	-1.37872200	-0.54157400
H	-4.17574800	-1.83388300	1.55820800
H	-4.16736400	-0.86080700	-2.62375800
H	-7.92352100	-1.38082900	-0.54509000
C	3.97147700	-0.93862200	-0.62744800
C	4.63122100	-0.66306200	-1.82455400
C	4.70170000	-1.15537400	0.54074300
C	6.03069500	-0.58984300	-1.84645700
C	6.10051800	-1.10763500	0.51473500
C	6.77035500	-0.81838500	-0.67949300
H	4.05053800	-0.49225500	-2.73188500
H	4.17367100	-1.35647300	1.47310500
H	7.85934100	-0.76562800	-0.70121700
C	-0.23456200	2.98371300	0.36592200
C	-0.27585100	3.90054500	-0.68707300
C	-0.24099500	3.43588700	1.68503500
C	-0.32697500	5.27706500	-0.41734700
C	-0.28432700	4.80893400	1.95933100
C	-0.32940600	5.73331500	0.90844000
H	-0.26827900	3.53496700	-1.71486000
H	-0.20847200	2.70952300	2.49749900
H	-0.36514800	6.80285500	1.11886400
C	-0.27706400	5.24825000	3.31753600
C	-0.37615300	6.23181000	-1.48133400

C	6.83120500	-1.34822600	1.71491500
C	6.71102600	-0.26324100	-3.05563100
C	-6.83611100	-0.78248500	-2.91100100
C	-6.83384700	-1.93983400	1.84377600
N	-0.26539600	5.57292300	4.43515700
N	-0.41819900	7.02909300	-2.32953300
N	7.40370600	-1.55211800	2.70672200
N	7.27068200	0.01855600	-4.03540100
N	-7.41463300	-0.51658200	-3.88420200
N	-7.39224900	-2.17139300	2.83764300
Ni	-0.05574200	-0.78208200	-1.56570200
Ni	-0.01298700	-1.18791300	0.82012700
C	1.54635000	-3.50494400	2.37795400
C	0.20423400	-2.83177600	2.32780800
H	1.55361000	-4.09316300	3.31239800
H	2.32600500	-2.73951200	2.50740200
C	1.86620900	-4.40861800	1.20654600
C	-0.02899700	-1.58387800	2.88866200
H	-0.66350100	-3.49449300	2.20361300
H	1.08702900	-5.16951100	1.05332600
H	1.95383600	-3.83616700	0.27005700
H	2.81503000	-4.93999900	1.35495900
H	-1.03820700	-1.25449300	3.14165900
H	0.80191800	-0.98945000	3.27898000
H	0.12022900	-2.64651600	0.61454300

#### INT7

0 1

O	-0.25982300	0.82634200	1.11200400
C	-0.20665500	1.55379000	0.08875100
O	-0.10581300	1.12430900	-1.09414800
O	1.90424500	-0.85942600	-1.50919500
C	2.50276600	-0.86695500	-0.38857900
O	1.98160300	-0.90594300	0.75392900
O	-2.03232100	-1.38756900	0.78996600
C	-2.55455800	-1.26180300	-0.34477400
O	-1.96003700	-1.07392000	-1.45252200
C	-4.04221700	-1.31912200	-0.40126800
C	-4.75653800	-1.54502800	0.77322500
C	-4.71715400	-1.11135200	-1.60204800
C	-6.15484100	-1.56520700	0.74954500
C	-6.11734100	-1.12437500	-1.62248800
C	-6.84341900	-1.35367500	-0.44889900
H	-4.21496900	-1.69527100	1.70709000
H	-4.14931000	-0.92752100	-2.51451700
H	-7.93362200	-1.35970500	-0.46828500
C	3.99081000	-0.84301700	-0.43556600
C	4.66166000	-0.64704500	-1.64049000
C	4.70885100	-1.01426300	0.74601400
C	6.06146000	-0.61392200	-1.65719300
C	6.10741300	-1.00402800	0.72352500
C	6.79173100	-0.79845100	-0.47825200
H	4.09032900	-0.51164800	-2.55932700
H	4.17066000	-1.15289800	1.68395400
H	7.88178000	-0.77898300	-0.49717400
C	-0.25876800	3.03369100	0.28259500
C	-0.27989900	3.89697700	-0.81500800
C	-0.27354200	3.55019500	1.57811300
C	-0.32019300	5.28540200	-0.61488600
C	-0.30324000	4.93591600	1.78330100

C	-0.32939000	5.80668400	0.68658200
H	-0.26476200	3.48195200	-1.82368600
H	-0.25621800	2.86419500	2.42567900
H	-0.35496600	6.88570500	0.84329100
C	-0.29884000	5.44751900	3.11645500
C	-0.34940600	6.18301800	-1.72799500
C	6.82213000	-1.20694900	1.93637800
C	6.74960400	-0.38060400	-2.87960500
C	-6.81027700	-0.88308400	-2.84095800
C	-6.86615800	-1.78707500	1.96114600
N	-0.28793100	5.83889800	4.21264000
N	-0.37458500	6.92968000	-2.62164700
N	7.37795100	-1.38512800	2.94121000
N	7.31116900	-0.17883600	-3.87651200
N	-7.37627700	-0.67367600	-3.83392100
N	-7.42016400	-1.96483600	2.96703900
Ni	-0.03999700	-0.81017000	-1.48620000
Ni	-0.01894400	-1.16494700	1.08456600
C	1.55750200	-3.95174600	1.42288400
C	0.24825700	-3.33949500	1.79924000
H	1.63264600	-4.88209600	2.01617800
H	2.38075100	-3.31511000	1.78275900
C	1.72617800	-4.29381300	-0.04389100
C	0.07279600	-2.43297200	2.80261800
H	-0.64743300	-3.78036000	1.34159300
H	0.90354100	-4.92648100	-0.40784100
H	1.75133700	-3.39777800	-0.68006800
H	2.66012000	-4.84381400	-0.21772000
H	-0.92448800	-2.20152900	3.18654200
H	0.93008300	-2.05953300	3.37342000
H	0.04856200	-1.94416500	-0.31890700

## H-Cu-DHKUST-1

### INT1

0 1

O	0.00009300	0.89484200	-1.34812500
C	-0.00003900	1.33551800	-0.15933100
O	-0.00014100	0.63206700	0.88413700
O	-1.91355900	-1.67088900	1.07040200
C	-2.48869100	-1.49255900	-0.03943000
O	-1.91944800	-1.28977300	-1.15228900
O	1.91955800	-1.28984800	-1.15225000
C	2.48875800	-1.49250400	-0.03934600
O	1.91358300	-1.67071300	1.07048300
C	3.97960900	-1.50881300	-0.04033000
C	4.68800900	-1.44486200	-1.24305100
C	4.66298700	-1.57196200	1.17536400
C	6.09061000	-1.45431400	-1.22922600
C	6.06395300	-1.56344900	1.19312000
C	6.78009800	-1.50930800	-0.00968900
H	4.14486900	-1.38909800	-2.18698000
H	4.09971100	-1.61883900	2.10760300
H	7.87067500	-1.50738300	0.00192600
C	-3.97954200	-1.50888200	-0.04046900
C	-4.66295100	-1.57250900	1.17518100
C	-4.68791200	-1.44447500	-1.24318400
C	-6.06391700	-1.56403700	1.19290500
C	-6.09051400	-1.45392600	-1.22939600
C	-6.78003300	-1.50941800	-0.00989900
H	-4.09969900	-1.61973600	2.10741700
H	-4.14474700	-1.38834500	-2.18707700
H	-7.87061000	-1.50750800	0.00168800
C	-0.00007400	2.82610900	-0.00667200
C	-0.00035400	3.41313300	1.26062600
C	0.00018100	3.62971500	-1.14668800
C	-0.00038800	4.81150000	1.38789100
C	0.00016900	5.02559700	-1.02606500
C	-0.00012000	5.61989200	0.24194600
H	-0.00055100	2.77300100	2.14410500
H	0.00039400	3.15812400	-2.12986500
H	-0.00013700	6.70617300	0.33931000
C	0.00045800	5.82544700	-2.20879300
C	-6.82841700	-1.40569200	-2.45372100
C	-0.00069700	5.43440400	2.67626400
C	-6.75187200	-1.60243100	2.44441500
C	6.75188600	-1.60130300	2.44466000
C	6.82853600	-1.40659500	-2.45355700
N	0.00070200	6.44572200	-3.19372200
N	-0.00095600	5.96841900	3.71184500
N	-7.44207900	-1.37138300	-3.44296400
N	-7.29291200	-1.62569500	3.47483200
N	7.29291800	-1.62410900	3.47509100
N	7.44220700	-1.37271900	-3.44280900
H	0.00004600	-2.39315500	-0.30280800
Cu	0.00006000	-1.10227100	-1.23442900
Cu	0.00000200	-1.51448900	1.14369600

### INT2

0 1

O	0.00654200	0.50656100	0.88703100
C	0.00551300	1.22017900	-0.14672500



O	-0.00286200	0.79633500	-1.34146000
O	1.90744800	-1.36478500	-1.31897000
C	2.51768600	-1.52195000	-0.22228700
O	1.98971500	-1.73395500	0.90117500
O	-2.00379700	-1.71828200	0.90052900
C	-2.53322200	-1.50711200	-0.22258900
O	-1.92429600	-1.35603000	-1.32073300
C	-4.02294800	-1.37995400	-0.28035000
C	-4.75342800	-1.27532100	0.90415900
C	-4.67605200	-1.30883400	-1.51448300
C	-6.14179300	-1.08232300	0.85876600
C	-6.06820900	-1.14170500	-1.56536000
C	-6.80168500	-1.02218200	-0.37621300
H	-4.23385800	-1.32434300	1.86157300
H	-4.09494400	-1.37781500	-2.43456800
H	-7.88173400	-0.87467200	-0.41239000
C	4.00774700	-1.40087900	-0.28381100
C	4.65691300	-1.33837700	-1.52036500
C	4.74249300	-1.29229200	0.89777600
C	6.04929100	-1.17624200	-1.57693300
C	6.13132500	-1.10330000	0.84648800
C	6.78720300	-1.05220300	-0.39109400
H	4.07251700	-1.41010800	-2.43812400
H	4.22615900	-1.33454700	1.85728000
H	7.86753700	-0.90799400	-0.43171200
C	0.01479700	2.71060400	0.01482200
C	0.00473200	3.50485000	-1.13008300
C	0.03359800	3.30920800	1.27690000
C	0.01276200	4.90023000	-1.02289300
C	0.04292700	4.70967100	1.39016600
C	0.03211900	5.50798000	0.23699500
H	-0.00957400	3.02511900	-2.10889500
H	0.04139000	2.67811900	2.16701100
H	0.03895400	6.59501100	0.32466500
C	0.06396300	5.35976200	2.66487200
C	0.00085800	5.66975500	-2.22268000
C	6.87212400	-0.93739700	2.05821300
C	6.71968400	-1.11973100	-2.84083300
C	-6.74429700	-1.07579300	-2.82595000
C	-6.87665500	-0.92231400	2.07478800
N	0.08160200	5.93666200	3.67714500
N	-0.00984700	6.23806600	-3.23747900
N	7.46467500	-0.78467200	3.04915400
N	7.27051200	-1.07208900	-3.86649800
N	-7.30187500	-1.02022200	-3.84762900
N	-7.46228100	-0.77520300	3.07065300
C	-0.01091900	-2.64363900	3.20581300
C	-0.00539600	-1.30677500	3.39288500
H	-0.93230200	-0.73724400	3.50042400
H	0.92622000	-0.74490600	3.49996100
H	-0.01051100	-2.47858300	-0.34799400
H	0.91853900	-3.21874600	3.16925000
H	-0.94504800	-3.21115200	3.16970400
Cu	-0.00690400	-1.66421400	1.16353200
Cu	-0.00798000	-1.20055100	-1.26815800

TS2-3

O 1

O	-0.03281900	0.57816600	-1.00509100
C	-0.01821300	1.26402200	0.05970000

O	0.00116800	0.78713700	1.22454100
O	-1.87251800	-1.43354200	1.15575500
C	-2.56113500	-1.44521600	0.07542400
O	-2.11009900	-1.56323700	-1.07809400
O	2.11757300	-1.49331900	-1.07652100
C	2.57418200	-1.40171000	0.07734700
O	1.89042500	-1.41812600	1.16045000
C	4.04944200	-1.25096700	0.23434000
C	4.80872400	-1.13338200	-0.92768200
C	4.66823100	-1.20540200	1.48384100
C	6.19412500	-0.96484300	-0.85029400
C	6.05999200	-1.04607800	1.56128100
C	6.82721900	-0.92322200	0.39543900
H	4.30761200	-1.16541200	-1.89507900
H	4.06786500	-1.29024600	2.39057600
H	7.90778900	-0.79277800	0.46241500
C	-4.03540300	-1.29080700	0.23728800
C	-4.64890000	-1.24489900	1.48929700
C	-4.79873800	-1.16743200	-0.92153600
C	-6.03965300	-1.08097600	1.57286000
C	-6.18279000	-0.99006400	-0.83787600
C	-6.81078400	-0.94990500	0.41056000
H	-4.04522100	-1.33354200	2.39343700
H	-4.30167500	-1.20027600	-1.89102800
H	-7.89035900	-0.81382100	0.48219400
C	-0.02393100	2.75686700	-0.06610400
C	-0.00953800	3.53009900	1.09567900
C	-0.04171700	3.37831500	-1.31683300
C	-0.01259600	4.92910100	1.01473200
C	-0.04476700	4.78016700	-1.40581200
C	-0.03017600	5.55674500	-0.23779500
H	0.00442700	3.03038900	2.06502200
H	-0.05282400	2.76500000	-2.21914100
H	-0.03235300	6.64530000	-0.30597200
C	-0.06201700	5.43737800	-2.67781600
C	0.00291400	5.70101800	2.21769600
C	-6.91987800	-0.84193200	-2.04646000
C	-6.69796400	-1.03837300	2.83685100
C	6.72465600	-1.00023900	2.82192100
C	6.92626600	-0.82975600	-2.06332300
N	-0.07559300	5.99646600	-3.70029800
N	0.01611900	6.30363500	3.21406800
N	-7.46338100	-0.71914900	-3.06659000
N	-7.26936800	-1.00087200	3.84930200
N	7.30305100	-0.95925400	3.83028900
N	7.46357800	-0.72018200	-3.08819700
C	0.03828300	-3.80482500	-1.08874600
C	0.03182600	-3.27360100	-2.36051100
H	0.96699800	-3.15722700	-2.91688200
H	-0.90544400	-3.18406600	-2.91831900
H	0.01666600	-2.49973300	0.06399800
H	-0.88891200	-4.16307900	-0.63390000
H	0.97425300	-4.13685700	-0.63188100
Cu	0.00214400	-1.41295000	-1.40982800
Cu	0.00801300	-1.25481900	1.08346300

INT3

O 1

O	0.05892500	0.87582700	-1.16659900
C	0.06758500	1.48844500	-0.05751700

O	0.05940400	0.95900000	1.07898000
O	-1.88009000	-1.39934600	1.19618200
C	-2.47388600	-1.24161500	0.09973500
O	-1.92106200	-1.07149100	-1.03402600
O	1.93906900	-1.18720400	-1.04925700
C	2.49512600	-1.35538900	0.08264100
O	1.90474000	-1.48072400	1.18554000
C	3.98682400	-1.39759900	0.08919900
C	4.70290700	-1.42692800	-1.10948300
C	4.66567900	-1.38525600	1.30998300
C	6.10505800	-1.45610300	-1.08818400
C	6.06727900	-1.39289000	1.33538600
C	6.78944600	-1.43405900	0.13487800
H	4.16553500	-1.42605900	-2.05838100
H	4.09514900	-1.35951100	2.23896200
H	7.87988700	-1.44549200	0.15181800
C	-3.96504100	-1.25458300	0.11246500
C	-4.63770900	-1.23080000	1.33656200
C	-4.68740800	-1.27221700	-1.08293000
C	-6.03890400	-1.21478500	1.36886500
C	-6.08985200	-1.27728000	-1.05454700
C	-6.76763500	-1.24351400	0.17195300
H	-4.06225600	-1.21460500	2.26273300
H	-4.15529000	-1.27904500	-2.03502200
H	-7.85800600	-1.23606100	0.19424100
C	0.08698700	2.98607400	-0.11338900
C	0.09726700	3.70381900	1.08308700
C	0.09089600	3.66436500	-1.33357700
C	0.11098500	5.10481200	1.06676500
C	0.10439700	5.06791000	-1.35568600
C	0.11457200	5.79057400	-0.15459300
H	0.09350100	3.15895100	2.02765800
H	0.08236300	3.09453600	-2.26370800
H	0.12460200	6.88102900	-0.17230000
C	0.10623100	5.77547600	-2.59802800
C	-6.83346600	-1.31193300	-2.27532300
C	0.11947600	5.82257000	2.30186800
C	-6.72169400	-1.15928700	2.62385300
C	6.75834600	-1.34906100	2.58645000
C	6.84071800	-1.50528100	-2.31324600
C	0.03383900	-3.09531900	-1.17730500
C	-1.25156500	-3.83898700	-1.11550700
H	-1.03769200	-4.91004100	-1.28647600
H	-1.73512500	-3.78059500	-0.13104400
H	-1.97174200	-3.53447700	-1.88499100
H	0.75050200	-3.35453200	-0.38762800
H	0.53149200	-3.09907100	-2.16034300
N	0.10691100	6.36675900	-3.60142200
N	0.12532100	6.38600200	3.32065700
N	-7.44182400	-1.34491600	-3.26781100
N	-7.26951700	-1.10449500	3.64998700
N	7.31489300	-1.30364900	3.60841800
N	7.44102400	-1.55109100	-3.31012500
Cu	0.02006700	-1.08637400	1.39659800
Cu	0.00106400	-1.10572100	-1.12853800

INT4

O 1

O	0.02896700	1.15486100	-1.37828700
C	0.04467200	1.54538100	-0.18907300

O	0.04992900	0.81518200	0.84704100
O	-1.93372200	-1.19447200	0.68499600
C	-2.48338100	-1.24277800	-0.45998200
O	-1.88891600	-1.26295300	-1.56596300
O	1.90719800	-1.30409800	-1.53897700
C	2.49928500	-1.30487400	-0.43136500
O	1.94856400	-1.26127800	0.71311300
C	3.99066600	-1.34848400	-0.42519500
C	4.70401200	-1.21393200	-1.61787300
C	4.67289000	-1.49283200	0.78432400
C	6.10650400	-1.21360300	-1.59727900
C	6.07351600	-1.51037400	0.80643100
C	6.79438300	-1.36651900	-0.38551500
H	4.16188600	-1.09766400	-2.55721300
H	4.10702200	-1.58745500	1.71133400
H	7.88486800	-1.36798900	-0.37181000
C	-3.97502000	-1.26561300	-0.45518400
C	-4.66365900	-1.39867000	0.75221600
C	-4.68176100	-1.12174900	-1.65046300
C	-6.06473500	-1.39677800	0.76864900
C	-6.08388300	-1.10025600	-1.63534700
C	-6.77863100	-1.24298900	-0.42643500
H	-4.10320700	-1.49793200	1.68248300
H	-4.13416000	-1.01390400	-2.58762400
H	-7.86906300	-1.22836800	-0.41680100
C	0.05760700	3.02591000	0.05181700
C	0.05875400	3.52786400	1.35334300
C	0.06528500	3.90444500	-1.03294900
C	0.06586600	4.91242300	1.57520900
C	0.07482100	5.29026800	-0.81698400
C	0.07449500	5.79733600	0.48956800
H	0.05341500	2.83354500	2.19480300
H	0.06352400	3.49724700	-2.04492900
H	0.08057400	6.87459900	0.65966700
C	0.08425000	6.19327500	-1.92479500
C	-6.81461000	-0.91677300	-2.84897400
C	0.06248300	5.41500500	2.91196500
C	-6.75549400	-1.54122700	2.01056300
C	6.75381500	-1.66558500	2.05264900
C	6.84785100	-1.04306000	-2.80666700
N	0.09220100	6.93467800	-2.82274700
N	0.05791700	5.80970100	4.00722700
N	-7.41844700	-0.75534500	-3.83099000
N	-7.30002400	-1.66089100	3.03257000
N	7.28509000	-1.79371600	3.08051500
N	7.46500600	-0.89381900	-3.78245000
C	-0.07270700	-3.17698400	0.66442200
C	0.65060200	-0.77685700	3.44965700
H	-0.62436300	-3.30576700	-0.27628100
H	0.98231400	-3.44630200	0.54507500
C	-0.73742300	-3.74633700	1.86775000
C	-0.68101100	-0.67739600	3.45711400
H	1.17106200	-1.66302200	3.82564500
H	1.28183600	0.03379100	3.07631700
H	-0.17186300	-3.57654800	2.79359100
H	-1.76328000	-3.37988600	2.00531100
H	-0.80748100	-4.84342000	1.74593000
H	-1.32236000	-1.47775800	3.83727900
H	-1.18863400	0.21660600	3.08556500
Cu	0.00690200	-1.19245300	0.85258200

Cu 0.01699000 -0.88069900 -1.69886500

TS4-5

0 1

O	0.15918200	1.22668300	-1.25137000
C	0.00061800	1.58730200	-0.06761700
O	-0.18459000	0.84307500	0.94323900
O	-1.90195500	-1.64387200	0.38405200
C	-2.46859500	-1.32523200	-0.68710700
O	-1.88253400	-1.02082100	-1.76847300
O	1.90491100	-1.18380000	-1.72457200
C	2.49746200	-1.21723600	-0.61018000
O	1.94179900	-1.19852800	0.51785000
C	3.99304400	-1.27661100	-0.62049600
C	4.71089500	-1.06680500	-1.79919400
C	4.67425000	-1.51325500	0.57475400
C	6.11423100	-1.07804600	-1.77626100
C	6.07486400	-1.55123100	0.59945200
C	6.79892400	-1.32697600	-0.57847200
H	4.17145200	-0.88024500	-2.72894200
H	4.10301400	-1.66463400	1.49107800
H	7.88934900	-1.34019500	-0.56448700
C	-3.96609100	-1.28243100	-0.69165200
C	-4.65974200	-1.50523900	0.49922300
C	-4.67127600	-0.98644500	-1.85930700
C	-6.05909300	-1.42649200	0.53317800
C	-6.07243100	-0.91525000	-1.83483400
C	-6.76933300	-1.13319100	-0.63820800
H	-4.09731300	-1.72889300	1.40671200
H	-4.12121300	-0.80510100	-2.78379500
H	-7.85787200	-1.06874500	-0.61920800
C	0.02978700	3.06094400	0.22190400
C	0.02325400	3.49561700	1.54563100
C	0.07612700	3.99602800	-0.81536500
C	0.07079900	4.86272300	1.84478000
C	0.10676500	5.36922800	-0.52184100
C	0.10813900	5.80496300	0.81110700
H	-0.01295200	2.76021600	2.34898500
H	0.08630200	3.64606400	-1.84876400
H	0.13948800	6.87115300	1.03820100
C	0.13827700	6.35116800	-1.56175700
C	-6.79934800	-0.60756300	-3.02604100
C	0.08562000	5.26267900	3.21398900
C	-6.75275100	-1.62997800	1.76674300
C	6.75191000	-1.80975400	1.83161000
C	6.86108600	-0.81996500	-2.96722000
N	0.16100500	7.18344800	-2.37650400
N	0.10261300	5.53315000	4.34572800
N	-7.39832400	-0.35382600	-3.99171400
N	-7.30262700	-1.78900400	2.78129200
N	7.28111500	-2.02492500	2.84660500
N	7.48371300	-0.59746800	-3.92567600
C	0.26091500	-3.28186200	1.59319000
C	0.29940500	-1.90334500	3.20258000
H	0.31476600	-3.05263100	0.51796100
H	1.24784700	-3.62388600	1.92133600
C	-0.90267300	-4.14333500	1.93729800
C	-0.66836200	-0.88591600	3.12856700
H	0.04170000	-2.81988800	3.73694500
H	1.35162600	-1.61642300	3.30086500

H	-0.88373000	-4.50721500	2.97352100
H	-1.85772700	-3.63398100	1.75427700
H	-0.89899300	-5.03032900	1.28275100
H	-1.73032900	-1.12579100	3.22758800
H	-0.39406500	0.16865300	3.18866700
Cu	0.00054200	-1.12124900	1.20903300
Cu	0.02020300	-0.77587600	-1.68138900

#### INT5

0 1

O	0.14434700	1.25776300	-1.32639400
C	0.08257500	1.71055800	-0.16010400
O	-0.00379000	1.02788900	0.90437500
O	-1.90897900	-1.02106600	1.05107200
C	-2.47790900	-1.03575100	-0.08869700
O	-1.90521600	-1.05005400	-1.20450200
O	1.89792700	-1.26644200	-1.19422600
C	2.49056800	-1.16378100	-0.09260700
O	1.93829900	-1.00472900	1.04457500
C	3.98147000	-1.22556500	-0.08170700
C	4.69005900	-1.20961600	-1.28570600
C	4.66867100	-1.27283600	1.13304300
C	6.09265400	-1.23135500	-1.27385500
C	6.06953600	-1.31285500	1.14882700
C	6.78461700	-1.28790200	-0.05559400
H	4.14317900	-1.16846900	-2.22857100
H	4.10806700	-1.27314800	2.06807700
H	7.87501800	-1.30750100	-0.04649400
C	-3.97069700	-1.03972500	-0.06570500
C	-4.65176500	-1.07379900	1.15283300
C	-4.68506500	-0.98678800	-1.26498400
C	-6.05322400	-1.05716300	1.17661300
C	-6.08743600	-0.96234300	-1.24543300
C	-6.77385300	-0.99971700	-0.02341700
H	-4.08605700	-1.10545000	2.08430000
H	-4.14194100	-0.95536600	-2.21034700
H	-7.86417600	-0.97953500	-0.00772900
C	0.10864200	3.20042900	-0.00121600
C	0.11305600	3.79073800	1.26375900
C	0.12864800	4.00089000	-1.14384500
C	0.14156300	5.18872000	1.38601300
C	0.14927600	5.39707400	-1.02733300
C	0.15772800	5.99469200	0.23936100
H	0.09600300	3.15670600	2.15104500
H	0.12633200	3.52472900	-2.12493000
H	0.17677600	7.08100300	0.33413400
C	0.16033400	6.20051100	-2.20803500
C	-6.82706500	-0.88894500	-2.46719900
C	0.15537700	5.80563500	2.67561200
C	-6.73891400	-1.08928500	2.43020300
C	6.75896600	-1.37044700	2.39935300
C	6.82908400	-1.18424500	-2.49893800
N	0.16645900	6.83480400	-3.18415800
N	0.16931600	6.32316600	3.71891500
N	-7.43935200	-0.82283000	-3.45571100
N	-7.28102700	-1.11482800	3.46036900
N	7.30155000	-1.41948900	3.42840000
N	7.44148000	-1.13668000	-3.48845400
C	-0.29425500	-4.03292000	-0.57332800
C	0.55006700	-3.84410500	0.67764900

H	-0.24364500	-3.09827600	-1.16946500
H	0.18122200	-4.79833300	-1.20568500
C	-1.73982600	-4.40120200	-0.31506400
C	0.06584300	-2.85645100	1.68025700
H	0.58302700	-4.81239200	1.22346700
H	1.60138900	-3.65177300	0.41067500
H	-1.82428200	-5.36760300	0.20421100
H	-2.25819800	-3.65848900	0.30939500
H	-2.30765300	-4.48374200	-1.25134500
H	-0.97330100	-2.98587000	2.00800400
H	0.74795300	-2.69594700	2.52749200
Cu	0.01549800	-0.95150400	1.12008500
Cu	0.01823500	-0.77922500	-1.45027400

#### INT6

0 1

O	-0.25412400	0.91763700	-1.14517900
C	-0.31043300	1.65827300	-0.11956100
O	-0.27564100	1.27375400	1.07380200
O	-1.97631300	-1.26675900	1.41848600
C	-2.53661100	-1.33236300	0.29519600
O	-1.95686100	-1.27188100	-0.83596600
O	1.87412500	-0.80104000	-0.72128300
C	2.40192300	-0.83877100	0.43661400
O	1.78705100	-0.94604200	1.52675200
C	3.88970300	-0.74792300	0.48524200
C	4.65055300	-0.87339900	-0.67974500
C	4.51973700	-0.52648500	1.71200300
C	6.04999600	-0.79693800	-0.61517500
C	5.91564000	-0.41845000	1.77641800
C	6.68393400	-0.56182200	0.61291200
H	4.15123600	-1.03472400	-1.63626700
H	3.91452900	-0.42873800	2.61388100
H	7.77093700	-0.48781800	0.66168500
C	-4.02202200	-1.48130900	0.27204500
C	-4.73769400	-1.39969500	1.46928900
C	-4.69793600	-1.67224900	-0.93503200
C	-6.13615800	-1.50151900	1.46168400
C	-6.09548400	-1.79097100	-0.94580700
C	-6.81688100	-1.70192000	0.25264400
H	-4.19839000	-1.24632900	2.40464800
H	-4.13265200	-1.72426800	-1.86610900
H	-7.90438500	-1.78420700	0.24386600
C	-0.42770500	3.13315600	-0.35831300
C	-0.54513800	3.98705900	0.73879500
C	-0.41452500	3.65750400	-1.65200000
C	-0.65285400	5.37106800	0.54828300
C	-0.51532600	5.04370000	-1.84809900
C	-0.63665800	5.90299000	-0.74737600
H	-0.55165200	3.56191600	1.74295400
H	-0.32234200	2.98159900	-2.50318200
H	-0.71695700	6.97987600	-0.90003500
C	-0.49139800	5.59385500	-3.16729800
C	-0.77696600	6.23007700	1.68278700
C	-6.78633800	-1.99693600	-2.18075800
C	-6.87007600	-1.39023800	2.68456000
C	6.55001800	-0.15294800	3.02983900
C	6.83710600	-0.95676500	-1.79867700
C	1.43695100	-3.66559500	-0.79281300
C	0.09733700	-3.02177900	-0.68606500

H	-0.57751300	-3.22099400	-1.53318100
H	-0.42266200	-3.18905500	0.26693500
H	2.11052100	-3.33507300	0.01710500
H	1.26368000	-4.73617300	-0.54864300
C	2.11859600	-3.57577700	-2.14876600
H	2.22850300	-2.51580500	-2.43054900
H	1.45288700	-4.01243600	-2.91288400
C	3.46698600	-4.26448400	-2.18143800
H	4.15951000	-3.83394000	-1.44162000
H	3.38257200	-5.33681300	-1.95156600
H	3.94721800	-4.17951200	-3.16493200
N	-0.46949000	6.05652900	-4.23587700
N	-0.87781700	6.91101500	2.62169200
N	-7.34582400	-2.16736600	-3.18787900
N	-7.46696200	-1.29057700	3.67985200
N	7.05403500	0.07497100	4.05453900
N	7.48640900	-1.09262200	-2.75613900
Cu	-0.02902600	-1.03810800	-0.88676300
Cu	-0.13280300	-0.70680900	1.63032700

TS6-7

0 1

O	-0.25979900	0.97245100	-1.01896000
C	-0.27836000	1.66166600	0.04022900
O	-0.26447100	1.19496400	1.21142200
O	-1.90940000	-1.18366600	1.17485700
C	-2.55553700	-1.30400500	0.07965400
O	-2.06389500	-1.36874200	-1.06485200
O	2.03382900	-0.83839600	-1.10068600
C	2.50978200	-0.78544000	0.05114300
O	1.85022900	-0.74984000	1.14381100
C	3.99203900	-0.79676200	0.18665000
C	4.75175000	-0.90161400	-0.97503400
C	4.61654900	-0.72511000	1.43095500
C	6.14628700	-0.94622400	-0.89832900
C	6.01580000	-0.75863500	1.50394300
C	6.78695100	-0.87186700	0.34111400
H	4.24698600	-0.95219400	-1.94000300
H	4.01429900	-0.64183900	2.33647100
H	7.87500600	-0.90399800	0.40470500
C	-4.03788800	-1.36150000	0.20274000
C	-4.67464700	-1.32347100	1.44238700
C	-4.78629300	-1.42970000	-0.96885400
C	-6.07455600	-1.35662900	1.50113700
C	-6.18212500	-1.45832100	-0.90781700
C	-6.83459600	-1.42363800	0.32735200
H	-4.08135900	-1.26183100	2.35540600
H	-4.27197000	-1.45051200	-1.92960300
H	-7.92359700	-1.44343900	0.37873000
C	-0.30637000	3.15269900	-0.09059500
C	-0.33586600	3.92456800	1.07057100
C	-0.28134900	3.77386000	-1.34095400
C	-0.33916700	5.32264300	0.98991800
C	-0.28213100	5.17563100	-1.42785700
C	-0.31200200	5.95216100	-0.26046700
H	-0.35118500	3.42495200	2.03972700
H	-0.25543300	3.16084300	-2.24316200
H	-0.31057200	7.04069900	-0.32811300
C	-0.24327200	5.83711000	-2.69585100
C	-0.36058600	6.08488000	2.19666900



C	-6.90998800	-1.51110500	-2.12726500
C	-6.74934800	-1.31401500	2.75384800
C	6.67910600	-0.68551300	2.76098100
C	6.88315500	-1.08294300	-2.10537300
C	0.30546900	-3.55178900	-0.97360400
C	0.17405000	-2.93107700	-2.20546500
H	1.06227500	-2.79209200	-2.83250600
H	-0.80274600	-2.89612800	-2.69772200
H	0.09961100	-2.13343100	0.22983800
H	-0.61084200	-3.91169200	-0.48634200
C	1.60025700	-4.08282300	-0.45234200
H	2.43286900	-3.48548900	-0.85886900
H	1.72172700	-5.07736700	-0.92234600
C	1.69893200	-4.23112800	1.05194000
H	1.68948900	-3.25654700	1.56051400
H	0.86345700	-4.82194800	1.45419400
H	2.62649900	-4.74135000	1.34070900
N	-0.20657700	6.40591100	-3.71195300
N	-0.37369700	6.66820500	3.20371100
N	-7.44776100	-1.54840000	-3.15618200
N	-7.32676700	-1.27822500	3.76202200
N	7.24872800	-0.63069100	3.77257300
N	7.42573600	-1.20979100	-3.12444500
Cu	-0.02023300	-1.02163200	-1.40163600
Cu	-0.05047000	-0.81393100	1.09629200

#### INT7

0 1

O	0.06076100	0.75491300	0.87491900
C	0.10393300	1.64594800	-0.00786800
O	0.11921800	1.44393500	-1.26058600
O	1.95719300	-0.78835400	-1.57573600
C	2.52722900	-1.23015100	-0.53893900
O	1.96645900	-1.60837300	0.52472000
O	-1.96970700	-1.47365800	0.48349800
C	-2.48124000	-1.05881800	-0.59100300
O	-1.86121200	-0.65151900	-1.61298400
C	-3.96931100	-1.02655800	-0.67110900
C	-4.72456500	-1.32922900	0.46034600
C	-4.60197900	-0.67510900	-1.86503500
C	-6.12248300	-1.27239700	0.40279900
C	-6.00142700	-0.63398100	-1.92759900
C	-6.76588000	-0.92883800	-0.79164600
H	-4.21940900	-1.59806300	1.38842700
H	-4.00115400	-0.43293700	-2.74200700
H	-7.85464500	-0.88714100	-0.83680000
C	4.01617400	-1.28451800	-0.58485800
C	4.69413400	-1.01723600	-1.77597000
C	4.72787500	-1.57637800	0.57711200
C	6.09493900	-1.05245700	-1.80492000
C	6.12780300	-1.59118200	0.55353600
C	6.81610100	-1.33495500	-0.63779000
H	4.12771000	-0.78081500	-2.67705800
H	4.18792800	-1.77840000	1.50236100
H	7.90633500	-1.35032700	-0.65662700
C	0.14229000	3.08505000	0.41568200
C	0.20691800	4.06462300	-0.57362200
C	0.11310800	3.45798100	1.76202400
C	0.24362800	5.42034400	-0.22802400
C	0.14816000	4.81819500	2.11568300

C	0.21392600	5.80204900	1.11770800
H	0.22843600	3.75950200	-1.61996300
H	0.06248400	2.68360800	2.52937900
H	0.24138900	6.85723600	1.39210700
C	0.11800400	5.24376000	3.48274600
C	0.31052800	6.38205500	-1.27893200
C	6.84115100	-1.85472600	1.75860100
C	6.79698700	-0.79443600	-3.02082800
C	-6.65670400	-0.28680700	-3.14707000
C	-6.88066800	-1.55533400	1.57561300
C	-0.00823500	-2.77904600	2.73756000
C	-0.04689000	-1.45676600	3.02626800
H	-0.99167900	-0.94678600	3.23849400
H	0.86655200	-0.87011500	3.14721800
H	0.00034100	-1.95534500	-0.85382100
H	0.97619500	-3.24553500	2.58768800
C	-1.18274300	-3.69999000	2.69613000
H	-2.11453700	-3.11550500	2.74648700
H	-1.15628500	-4.29837400	3.62464100
C	-1.18892900	-4.63311300	1.49902000
H	-1.27359200	-4.07489400	0.55473700
H	-0.26764800	-5.23124500	1.44748800
H	-2.03241300	-5.33387200	1.54050500
N	0.09533300	5.64631500	4.57645100
N	0.36469900	7.11095900	-2.18412500
N	7.39745900	-2.06018900	2.75890600
N	7.37873400	-0.58849600	-4.00740400
N	-7.19898200	-0.00747100	-4.13796900
N	-7.47582200	-1.78085600	2.54888400
Cu	-0.00161400	-1.47498200	0.78627900
Cu	0.05441900	-0.53006100	-1.51320300

## H-Ru-DHKUST-1

INT1

0 5

O	0.10297800	0.92639800	-1.18336400
C	0.08931600	1.49911100	-0.05542100
O	0.11484000	0.90019300	1.05574600
O	-1.98124000	-1.19293000	1.07647000
C	-2.58952600	-1.23856500	-0.03328900
O	-2.00130100	-1.29742800	-1.15926800
O	2.04768200	-1.51788900	-1.15633800
C	2.63912400	-1.48705400	-0.03088500
O	2.03361900	-1.42029400	1.07971000
C	4.10149800	-1.48161300	-0.00948200
C	4.81093100	-1.43415000	-1.20516300
C	4.76564400	-1.44224400	1.21337600
C	6.20277900	-1.33182100	-1.16905400
C	6.15741100	-1.34446900	1.23467000
C	6.88854300	-1.29066500	0.04645400
H	4.27900100	-1.44657700	-2.15644100
H	4.19653900	-1.46190800	2.14254000
H	7.97407300	-1.19371100	0.06690000
C	-4.05151300	-1.25663300	-0.00948300
C	-4.71425100	-1.29687100	1.21400600
C	-4.76224600	-1.29232200	-1.20452900
C	-6.10663000	-1.38519400	1.23578400
C	-6.15506800	-1.37522000	-1.16741200
C	-6.83973800	-1.42096400	0.04825700
H	-4.14412000	-1.28211600	2.14265600
H	-4.23153100	-1.27302300	-2.15632700
H	-7.92659500	-1.50135600	0.06937900
C	0.01773500	2.99194800	-0.03141700
C	-0.02793400	3.65525100	1.19566100
C	-0.03138800	3.72201000	-1.22125400
C	-0.12693400	5.05254300	1.23919300
C	-0.12932500	5.12160700	-1.18381200
C	-0.17736100	5.78894300	0.04842600
H	0.00750800	3.07269100	2.11694600
H	0.00134900	3.19285200	-2.17470100
H	-0.25751900	6.87620800	0.07885400
C	-0.19164300	5.88089000	-2.39469200
C	-6.86634800	-1.46032300	-2.38694000
C	-0.18766700	5.71454400	2.50389200
C	-6.76438300	-1.49137000	2.48437600
C	6.81240800	-1.23580600	2.48487900
C	6.91000800	-1.19989400	-2.38736800
N	-0.24879700	6.51406700	-3.37086800
N	-0.24243200	6.23179800	3.54553900
N	-7.41802600	-1.55853500	-3.40138500
N	-7.26860300	-1.61249200	3.52111200
N	7.30865300	-1.10884000	3.52489500
N	7.45762500	-1.04753300	-3.39753600
H	-0.06731500	-2.90786900	1.11566600
Ru	0.02841400	-1.31692800	-1.17547900
Ru	0.02786800	-1.29577300	1.06970600

INT2

0 5

O	-0.00664900	0.81201100	-1.07312300
C	-0.00715100	1.40286500	0.03774000

O	-0.00156600	0.82465100	1.16548400
O	-2.02650900	-1.51338600	1.25130600
C	-2.62435800	-1.43271500	0.13103700
O	-2.03827300	-1.41537600	-0.98905400
O	2.04987800	-1.39792000	-0.98827400
C	2.63698300	-1.41236500	0.13140000
O	2.04057600	-1.49644000	1.25211500
C	4.10104000	-1.28262500	0.15796600
C	4.80867900	-1.08674400	-1.02533600
C	4.76321800	-1.28978300	1.38405100
C	6.19084900	-0.88589000	-0.97461300
C	6.14587000	-1.09384400	1.42518100
C	6.86983900	-0.89119900	0.24741900
H	4.27985200	-1.06849200	-1.97844500
H	4.19599000	-1.42976200	2.30403400
H	7.94650800	-0.72336400	0.28129500
C	-4.08887000	-1.30862500	0.16009800
C	-4.74758400	-1.32330600	1.38789000
C	-4.80012600	-1.10705800	-1.02016400
C	-6.13017400	-1.12900700	1.43436100
C	-6.18236400	-0.90735500	-0.96402000
C	-6.85780400	-0.92032200	0.26002700
H	-4.17743500	-1.46688800	2.30547600
H	-4.27410800	-1.08221300	-1.97469600
H	-7.93438700	-0.75280700	0.29797500
C	-0.01495900	2.90126100	0.03508900
C	-0.00416000	3.59743000	1.24549300
C	-0.03305900	3.60551500	-1.17199300
C	-0.01063600	5.00019600	1.25493600
C	-0.04115900	5.00943800	-1.17131400
C	-0.02954600	5.70800000	0.04510400
H	0.00964100	3.03701300	2.18121400
H	-0.04109200	3.05061300	-2.11123400
H	-0.03521900	6.79869200	0.04907900
C	-0.06138900	5.73948600	-2.40368000
C	0.00224100	5.70390700	2.50073200
C	-6.89689300	-0.64201000	-2.16060200
C	-6.77757800	-1.10350200	2.69712500
C	6.79944000	-1.06254700	2.68474100
C	6.90036500	-0.62988800	-2.17610500
N	-0.07834700	6.34551900	-3.39923800
N	0.01336000	6.26539100	3.52148300
N	-7.46505100	-0.39622000	-3.14225200
N	-7.27095000	-1.06438600	3.74704600
N	7.30146300	-1.01942500	3.73042800
N	7.46190700	-0.39364000	-3.16384800
C	0.01080800	-2.46442200	-3.08844700
C	0.00525600	-1.10726100	-3.29488800
H	0.93040100	-0.55134700	-3.46555500
H	-0.92436600	-0.55897900	-3.46589300
H	0.01338300	-3.00793300	-0.74979300
H	-0.91266500	-3.04693700	-3.11690100
H	0.93904800	-3.03931800	-3.11660700
Ru	0.00649000	-1.40377000	1.29738400
Ru	0.00595200	-1.42243600	-1.02598100

TS2-3

0 5

O	-0.00719600	0.79441100	-1.07262300
C	-0.00759200	1.41478500	0.02586000

O	-0.00230900	0.86030300	1.16291000
O	-2.03112000	-1.48000600	1.25084900
C	-2.62372100	-1.38658100	0.12786300
O	-2.04711100	-1.36094800	-0.99530400
O	2.05738400	-1.34139700	-0.99439400
C	2.63515800	-1.36398200	0.12829900
O	2.04424500	-1.46089300	1.25180700
C	4.10017600	-1.23705100	0.15669200
C	4.80874400	-1.05633800	-1.02781400
C	4.76121500	-1.23833300	1.38280000
C	6.19232200	-0.86888200	-0.97826500
C	6.14504500	-1.05164100	1.42191400
C	6.87143100	-0.86729600	0.24319200
H	4.27948500	-1.04167700	-1.98074400
H	4.19253100	-1.36686100	2.30352000
H	7.94957600	-0.70910500	0.27572200
C	-4.08914000	-1.26502900	0.15885900
C	-4.74665100	-1.27302800	1.38675500
C	-4.80119500	-1.07796800	-1.02265200
C	-6.13019900	-1.08632100	1.43124800
C	-6.18459500	-0.88995700	-0.96766200
C	-6.86009500	-0.89518100	0.25589100
H	-4.17511900	-1.40543200	2.30512600
H	-4.27478200	-1.05711300	-1.97705800
H	-7.93792300	-0.73572800	0.29251800
C	-0.01476500	2.91054100	-0.01536500
C	-0.00367400	3.62739400	1.18309300
C	-0.03242400	3.59319500	-1.23549500
C	-0.00939500	5.02969900	1.16932300
C	-0.03979300	4.99745500	-1.25767200
C	-0.02786700	5.71631600	-0.05264500
H	0.00977400	3.08264300	2.12794200
H	-0.04072200	3.02327300	-2.16582300
H	-0.03297600	6.80693200	-0.06769700
C	-0.05962200	5.71177400	-2.49998200
C	0.00386000	5.75060900	2.40547100
C	-6.89936700	-0.64778100	-2.16759700
C	-6.77721400	-1.05134700	2.69286200
C	6.79847500	-1.01274000	2.68020100
C	6.90252100	-0.63799500	-2.18303500
N	-0.07625200	6.31128000	-3.49969500
N	0.01536600	6.32070600	3.42148400
N	-7.46492100	-0.42441800	-3.15557100
N	-7.27108000	-1.00341700	3.74180100
N	7.30134600	-0.96291700	3.72479500
N	7.46203700	-0.42646300	-3.17700100
C	0.01411200	-3.06752300	-2.43346000
C	0.00820600	-1.83623300	-3.14345700
H	0.93278900	-1.47213600	-3.60060500
H	-0.91969800	-1.48128500	-3.60106600
H	0.01340000	-2.96126600	-0.82674700
H	-0.89708000	-3.67449000	-2.41380600
H	0.93122700	-3.66549500	-2.41346800
Ru	0.00593500	-1.36685600	1.34022400
Ru	0.00518200	-1.35543400	-1.05990200

INT3

0 3

O	0.17782700	1.08338900	-1.13045200
C	0.24576200	1.60632700	0.04783200

O	0.33272800	0.94924100	1.09969400
O	-1.99432100	-0.94243400	0.97453900
C	-2.58501700	-0.80827500	-0.13315400
O	-1.99926500	-0.73855700	-1.25755000
O	2.08677000	-1.14856500	-1.27364200
C	2.65805800	-1.39199300	-0.16497800
O	2.05164500	-1.59475500	0.92304900
C	4.12664700	-1.39765600	-0.13862700
C	4.84275200	-1.25308200	-1.32250000
C	4.78722200	-1.46821400	1.08494800
C	6.23686500	-1.17832800	-1.27574300
C	6.18010800	-1.37278600	1.12175200
C	6.91674300	-1.23516200	-0.05703600
H	4.31337200	-1.18029300	-2.27255500
H	4.21220300	-1.56536700	2.00575100
H	8.00324100	-1.15224300	-0.02505900
C	-4.05345000	-0.81913400	-0.12193300
C	-4.72195500	-0.97978900	1.08849400
C	-4.75732200	-0.79970300	-1.32168400
C	-6.10946400	-1.13524500	1.09417600
C	-6.14485100	-0.96252800	-1.30468800
C	-6.83322500	-1.12493300	-0.10030400
H	-4.15502200	-1.02097700	2.01860100
H	-4.22046700	-0.69905500	-2.26501400
H	-7.91296800	-1.27480400	-0.09578900
C	0.17875500	3.09124000	0.10988300
C	0.13281900	3.68726000	1.37120300
C	0.11835200	3.88129200	-1.04123200
C	0.01555100	5.07735900	1.49010400
C	0.01151800	5.27624800	-0.92567100
C	-0.04219500	5.87586100	0.34094300
H	0.17545400	3.05551000	2.25905900
H	0.14772700	3.41007200	-2.02451800
H	-0.13525600	6.95889500	0.42886500
C	-0.05940700	6.10474500	-2.08959900
C	-6.83749400	-1.05460500	-2.53662900
C	-0.06547300	5.66028100	2.79129700
C	-6.75833800	-1.39548600	2.32665100
C	6.83481600	-1.35346900	2.37868000
C	6.95412400	-0.99339400	-2.48290100
N	-0.12424400	6.80131400	-3.02092400
N	-0.14336900	6.10106800	3.86572100
N	-7.36741200	-1.18692100	-3.55968800
N	-7.24140200	-1.66099400	3.34724400
N	7.33977000	-1.29551900	3.42149900
N	7.51221000	-0.81691900	-3.48406200
Ru	0.04796100	-0.89944900	-1.25712200
Ru	0.02422900	-1.30564200	0.94686600
C	-0.26036900	-3.33630100	1.02778300
H	0.60452800	-3.85849800	0.58163400
H	-0.13762000	-3.45664500	2.12744100
C	-1.57095200	-3.92822400	0.56541000
H	-2.43316800	-3.51235100	1.10570800
H	-1.74915500	-3.75405100	-0.50921800
H	-1.60465700	-5.02077100	0.70783600

INT4

0 3

O	0.14530800	1.21494700	-1.22511800
C	0.16034700	1.68316100	-0.02728900

O	0.18690500	1.00612100	1.02140300
O	-1.99325500	-1.08055800	0.88465700
C	-2.57417900	-0.84518300	-0.21647000
O	-1.97981800	-0.68322400	-1.32798100
O	2.04061700	-0.97554400	-1.36069300
C	2.62596200	-1.21324800	-0.25729500
O	2.03429900	-1.42667200	0.84201700
C	4.09269300	-1.21377600	-0.24418100
C	4.80119200	-1.06399200	-1.43257100
C	4.76244100	-1.32459700	0.97159900
C	6.19697900	-1.03057800	-1.39686300
C	6.15726000	-1.27348100	0.99599300
C	6.88650300	-1.13211400	-0.18634300
H	4.26637200	-0.96683800	-2.37745900
H	4.19487000	-1.43165700	1.89576800
H	7.97561400	-1.09103300	-0.16483500
C	-4.04029100	-0.82800400	-0.20850400
C	-4.71372500	-0.99415800	0.99867600
C	-4.74378200	-0.74404000	-1.40652300
C	-6.10638600	-1.08489400	1.00347500
C	-6.13675800	-0.84818800	-1.38973800
C	-6.83028200	-1.01198000	-0.18822300
H	-4.14978000	-1.07817900	1.92736500
H	-4.20551800	-0.63218900	-2.34791900
H	-7.91613800	-1.10787400	-0.18484200
C	0.12225600	3.17098200	0.09417300
C	0.09325600	3.73423400	1.37100900
C	0.08910800	3.99500100	-1.03342000
C	0.02607300	5.12451700	1.52825800
C	0.02481700	5.38899500	-0.88084300
C	-0.00719600	5.95580200	0.40123300
H	0.11642600	3.07731200	2.24123100
H	0.10817200	3.54693500	-2.02777000
H	-0.06177900	7.03866500	0.51896500
C	-0.01915800	6.24677700	-2.02457400
C	-6.84216000	-0.86364600	-2.61770000
C	-0.01983100	5.68020700	2.84357600
C	-6.76369200	-1.32283800	2.23538000
C	6.82189800	-1.33475200	2.24558900
C	6.91488200	-0.87062300	-2.60681500
N	-0.06056700	6.96183800	-2.94318300
N	-0.06322300	6.10692200	3.92590800
N	-7.39754300	-0.92834300	-3.63360700
N	-7.25242700	-1.55930600	3.26010900
N	7.33203000	-1.36331800	3.28676600
N	7.48530500	-0.73129100	-3.60667500
C	-0.08868200	-2.91976400	-0.42063600
C	-0.07477200	-2.62462500	2.58925400
H	-0.02893000	-2.61936700	-1.57215100
H	0.86086800	-3.47644000	-0.33561100
C	-1.26603200	-3.86390100	-0.35884800
C	0.06489500	-1.30731600	3.06345900
H	-1.05175600	-3.11786500	2.61933300
H	0.78199900	-3.30631400	2.56950000
H	-1.30281100	-4.35975300	0.62055100
H	-2.23406400	-3.36614800	-0.50681400
H	-1.20058100	-4.65914900	-1.11821100
H	-0.80108300	-0.75768800	3.44442100
H	1.03726700	-0.93254000	3.39667500
Ru	0.03213000	-0.80724900	-1.40517700

Ru 0.01676900 -1.28797400 0.90593400

TS4-5

0 5

O	0.21749600	1.37806500	-1.30459100
C	0.21097000	1.74521700	-0.10001000
O	0.23133400	0.97172400	0.90193000
O	-1.98912000	-0.91399100	0.75256800
C	-2.57112900	-0.82054200	-0.36601100
O	-1.98340200	-0.77308000	-1.49065200
O	2.08196500	-1.23566000	-1.51266500
C	2.66001000	-1.35066400	-0.38582500
O	2.06924500	-1.40734400	0.72932900
C	4.12926200	-1.36114500	-0.36681200
C	4.84061500	-1.15019000	-1.54447700
C	4.79567500	-1.47665000	0.84971600
C	6.23235600	-1.03656300	-1.49370200
C	6.18692200	-1.37166200	0.88730500
C	6.91797600	-1.15244800	-0.28206200
H	4.30630100	-1.03781200	-2.48799300
H	4.22579900	-1.61521700	1.76815900
H	8.00214500	-1.04442100	-0.24707100
C	-4.03962800	-0.83057400	-0.35996600
C	-4.71918800	-1.04438700	0.83603400
C	-4.73734600	-0.71716200	-1.55859900
C	-6.11013300	-1.16199000	0.82650800
C	-6.12971900	-0.82672500	-1.55419700
C	-6.82849900	-1.04806800	-0.36547100
H	-4.16081500	-1.14793300	1.76656000
H	-4.19246500	-0.56886500	-2.49101200
H	-7.91332300	-1.15474500	-0.37208900
C	0.14665600	3.21125900	0.18050800
C	0.08761500	3.68094000	1.49402300
C	0.10273900	4.11251300	-0.88506400
C	-0.02119600	5.05656100	1.74474100
C	-0.00523800	5.48879000	-0.63972700
C	-0.06728200	5.96372500	0.67722200
H	0.11731600	2.96793500	2.31883300
H	0.14338000	3.73076200	-1.90604800
H	-0.15710400	7.03331000	0.87069100
C	-0.06930400	6.40690100	-1.73340900
C	-6.82626500	-0.77584200	-2.78577800
C	-0.10288200	5.53537300	3.08912100
C	-6.77412800	-1.47175200	2.03839300
C	6.83226200	-1.41750700	2.14740800
C	6.94492700	-0.72100200	-2.67680600
N	-0.12996200	7.15046600	-2.62756000
N	-0.17891500	5.92303800	4.18465800
N	-7.36964500	-0.77112400	-3.81003100
N	-7.27362400	-1.77465000	3.04024000
N	7.30690200	-1.41909500	3.20567900
N	7.50922600	-0.41122100	-3.64163600
C	-0.16743100	-3.39530900	0.97818600
C	-0.36612300	-2.43381500	2.74444000
H	-0.01891900	-3.06753600	-0.07888600
H	0.75967100	-3.92157000	1.23555900
C	-1.40051100	-4.25280400	1.03755400
C	0.13765000	-1.11637900	2.92540500
H	-1.45084300	-2.55510300	2.81904700
H	0.18322300	-3.26902800	3.18900800



H	-1.53646500	-4.72089000	2.02341200
H	-2.31120400	-3.67502100	0.82157900
H	-1.35209400	-5.06872300	0.30079500
H	-0.56292900	-0.32144800	3.19611000
H	1.16687100	-0.97626900	3.26806200
Ru	0.07277800	-0.82149800	-1.58527500
Ru	0.03962300	-1.13840300	0.78497000

#### INT5

0 5

O	0.24734900	1.34320700	-1.21719900
C	0.23783300	1.76839000	-0.04051800
O	0.24176800	1.02635200	1.00372300
O	-1.98515200	-0.74174900	0.74196700
C	-2.57359000	-0.74075500	-0.37640700
O	-2.00054500	-0.76728000	-1.51011300
O	2.08681200	-1.24201500	-1.50934800
C	2.65735900	-1.27694400	-0.37393900
O	2.06736200	-1.23562800	0.74295200
C	4.12597700	-1.31879800	-0.34367300
C	4.84684100	-1.14234700	-1.52032500
C	4.78292700	-1.43054700	0.87855300
C	6.23988900	-1.05273800	-1.46295700
C	6.17630000	-1.36127100	0.92081600
C	6.91730100	-1.17059100	-0.24746200
H	4.31995200	-1.03397700	-2.46844400
H	4.20501300	-1.54220600	1.79575200
H	8.00337400	-1.08557300	-0.20824000
C	-4.04213800	-0.76563600	-0.35546200
C	-4.71144800	-0.96476700	0.84915600
C	-4.74757000	-0.67278500	-1.55015000
C	-6.10187700	-1.09294700	0.84888800
C	-6.13931100	-0.78211900	-1.53443900
C	-6.82887900	-0.99417700	-0.33949000
H	-4.14547000	-1.04941700	1.77711600
H	-4.20978500	-0.53564000	-2.48825800
H	-7.91340700	-1.10405000	-0.33693900
C	0.18623500	3.23505500	0.20846300
C	0.12629100	3.72551400	1.51414300
C	0.14869200	4.11792000	-0.87388300
C	0.02264900	5.10414000	1.74142800
C	0.04510900	5.49866400	-0.64972800
C	-0.01761000	5.99416400	0.66018500
H	0.14892400	3.02867800	2.35248600
H	0.18911800	3.72026800	-1.88890700
H	-0.10465800	7.06699000	0.83595200
C	-0.01675300	6.41088100	-1.74944800
C	-6.83603000	-0.73166200	-2.76471600
C	-0.06221100	5.58979000	3.08174200
C	-6.76546900	-1.39684400	2.06253200
C	6.81980900	-1.41633700	2.18139100
C	6.95764700	-0.75213200	-2.64594500
N	-0.07818900	7.16523100	-2.63471500
N	-0.14122500	5.96216500	4.18173200
N	-7.36375900	-0.71723700	-3.79661600
N	-7.28052700	-1.69713500	3.05724200
N	7.30168700	-1.42781800	3.23622500
N	7.51681800	-0.44533800	-3.61438900
C	-0.25109200	-3.61035600	1.23259600
C	-0.78989400	-2.98580600	2.51793000

H	-0.22916300	-2.87272400	0.36305700
H	0.80873000	-3.88609700	1.36013600
C	-1.06510000	-4.77477300	0.71360300
C	-0.08935000	-1.67657100	2.76443200
H	-1.87434000	-2.81997100	2.40393700
H	-0.68684000	-3.71509100	3.34368700
H	-1.11518800	-5.56565300	1.47596000
H	-2.09996400	-4.47378100	0.49345400
H	-0.64068800	-5.21737300	-0.19662300
H	-0.64946000	-0.95918400	3.38177900
H	0.93788300	-1.78697200	3.14659800
Ru	0.05798000	-0.89170300	-1.61935800
Ru	.04648300	-0.95175400	0.79552600

INT6

0 5

O	-0.29338800	0.96644400	1.05828700
C	-0.31966400	1.71853600	0.03316400
O	-0.32492200	1.31053500	-1.15550200
O	1.97272300	-0.69770600	-1.45329800
C	2.55874800	-0.68609900	-0.32531100
O	1.98852900	-0.77309600	0.79828100
O	-2.06988800	-1.37377400	0.80732800
C	-2.65488400	-1.35907800	-0.31190600
O	-2.07973400	-1.28419000	-1.44380900
C	-4.12499900	-1.38205800	-0.30696300
C	-4.81369700	-1.51522000	0.89505500
C	-4.81446300	-1.17246500	-1.49764300
C	-6.20779400	-1.43605700	0.89999600
C	-6.20760800	-1.07434200	-1.47778000
C	-6.91662300	-1.21377000	-0.28307600
H	-4.26129400	-1.65407400	1.82441000
H	-4.26166900	-1.04917200	-2.42878000
H	-8.00301700	-1.12466500	-0.26935600
C	4.02693800	-0.62161700	-0.33360700
C	4.70048500	-0.46999200	-1.54182800
C	4.73303900	-0.78882400	0.85392400
C	6.09659900	-0.49019500	-1.55739500
C	6.12857600	-0.82523000	0.82325400
C	6.82275600	-0.66924900	-0.37843600
H	4.13509700	-0.35473800	-2.46643400
H	4.19413000	-0.91525400	1.79323200
H	7.91202100	-0.70702500	-0.39826700
C	-0.31539100	3.19073000	0.27445300
C	-0.31357500	4.05452800	-0.82268300
C	-0.27031600	3.70791000	1.57145100
C	-0.26127900	5.44161000	-0.62830900
C	-0.21930600	5.09589500	1.77133800
C	-0.21490700	5.96482600	0.67078000
H	-0.34275800	3.63513400	-1.82908300
H	-0.26557600	3.02489100	2.42195600
H	-0.16934600	7.04339900	0.82604000
C	-0.15473700	5.63530500	3.09457800
C	-0.23816700	6.31579200	-1.75928000
C	6.83319200	-1.08957600	2.02255000
C	6.76788700	-0.37735900	-2.79888400
C	-6.88764400	-0.75359200	-2.67840500
C	-6.89477300	-1.52265500	2.13546300
N	-0.09362800	6.08505100	4.16735800
N	-0.21048000	7.01494000	-2.69022500

N	7.37978600	-1.35651300	3.00976400
N	7.28580300	-0.31128600	-3.83418300
N	-7.40852400	-0.43768100	-3.66537200
N	-7.42741800	-1.56535800	3.16471400
C	1.68851800	-3.85172200	1.63337400
C	0.31835400	-3.19303200	1.67120700
H	1.74476000	-4.53951300	2.49266500
H	2.45353800	-3.08259700	1.82397300
C	1.98719400	-4.58615800	0.34429800
C	0.09509800	-2.11749700	2.65587600
H	-0.50316800	-3.92898500	1.63099500
H	1.24489100	-5.37156300	0.13888700
H	1.98082700	-3.90285900	-0.52084300
H	2.97255900	-5.06904100	0.36717900
H	-0.84823900	-2.12792800	3.21276000
H	0.96190200	-1.83149400	3.26469600
H	0.18071800	-2.79825000	0.53666800
Ru	-0.04107400	-1.06416400	0.86887000
Ru	-0.07065500	-0.89065600	-1.55684500

TS6-7

0 5

O	-0.29029100	0.95169100	1.07983600
C	-0.30350300	1.71450400	0.07438900
O	-0.30291600	1.32298900	-1.12755000
O	1.96415900	-0.69745800	-1.50517200
C	2.55749300	-0.73396600	-0.38092900
O	1.98692200	-0.86628000	0.73791300
O	-2.06213300	-1.45279400	0.73829200
C	-2.65792900	-1.37069500	-0.37198000
O	-2.08693600	-1.22792900	-1.50021800
C	-4.12728000	-1.38633600	-0.35955500
C	-4.81134300	-1.54541500	0.84225500
C	-4.82105900	-1.13963000	-1.54059600
C	-6.20457200	-1.45119400	0.85702200
C	-6.21325800	-1.03287400	-1.51162300
C	-6.91739400	-1.19462600	-0.31684900
H	-4.25588100	-1.71304600	1.76502100
H	-4.27211400	-0.99474600	-2.47086500
H	-8.00278000	-1.09547900	-0.29502000
C	4.02457400	-0.66745400	-0.39028700
C	4.69608100	-0.48180100	-1.59502100
C	4.73296100	-0.86081900	0.79208500
C	6.09227800	-0.49474900	-1.61234000
C	6.12869300	-0.88520200	0.76004100
C	6.82060800	-0.69697000	-0.43840200
H	4.12933800	-0.34457900	-2.51580300
H	4.19633600	-1.01204200	1.72890800
H	7.91012600	-0.72522600	-0.45969100
C	-0.29225600	3.18815900	0.32074400
C	-0.28924700	4.06870500	-0.76300400
C	-0.24556500	3.68639000	1.62463000
C	-0.23551600	5.45322600	-0.54698300
C	-0.19099500	5.07054500	1.84689600
C	-0.18649100	5.95639300	0.76017600
H	-0.32026100	3.66569300	-1.77606900
H	-0.24294600	2.98839700	2.46296200
H	-0.13954400	7.03248400	0.93161300
C	-0.12433200	5.58382700	3.18019000
C	-0.21553700	6.34996100	-1.66071800

C	6.83712900	-1.16156200	1.95454800
C	6.76274400	-0.34537600	-2.85055700
C	-6.89457800	-0.67922000	-2.70224300
C	-6.88725100	-1.55299700	2.09406600
N	-0.06173800	6.00484700	4.26445200
N	-0.19173800	7.07435500	-2.57251000
N	7.38855500	-1.43176000	2.93824400
N	7.28177200	-0.24727800	-3.88279300
N	-7.41242200	-0.33744500	-3.68213100
N	-7.41877300	-1.60377300	3.12363600
C	1.62908000	-3.72264000	1.90497100
C	0.27002500	-3.06653300	1.93119600
H	1.64442900	-4.42462800	2.75678700
H	2.39505900	-2.96709800	2.13884400
C	1.97624000	-4.45637900	0.62784400
C	0.01875400	-1.94998600	2.78210700
H	-0.56710700	-3.76506100	1.78593900
H	1.21358600	-5.20499600	0.36693500
H	2.05729700	-3.76608000	-0.22679500
H	2.93481100	-4.98461900	0.711170500
H	-0.96655800	-1.82580500	3.23958000
H	0.85801200	-1.51551800	3.33624600
H	0.17439100	-2.71607800	0.38045500
Ru	-0.03647900	-1.15935300	0.79759800
Ru	-0.07914800	-0.84650300	-1.58033200

#### INT7

0 5

O	-0.25059700	0.88495500	1.06636200
C	-0.27262300	1.68819900	0.09812900
O	-0.29070100	1.35473600	-1.12390500
O	1.93673100	-0.69056700	-1.64278800
C	2.55131400	-0.83112300	-0.53940900
O	1.98447200	-1.04603100	0.57044000
O	-2.05448100	-1.55380700	0.58527100
C	-2.67091800	-1.39118300	-0.50648900
O	-2.10509000	-1.15683400	-1.62090100
C	-4.13768200	-1.40712500	-0.48002100
C	-4.81046200	-1.62989900	0.71812700
C	-4.84203000	-1.08925100	-1.63776000
C	-6.20235000	-1.52187500	0.75418100
C	-6.23280900	-0.97582100	-1.58813800
C	-6.92561000	-1.19652800	-0.39604500
H	-4.24749700	-1.85416100	1.62413500
H	-4.30181200	-0.89346300	-2.56380400
H	-8.00952600	-1.08773500	-0.35616600
C	4.01618700	-0.77196300	-0.56127100
C	4.67597900	-0.50545000	-1.75755200
C	4.73599700	-1.03020600	0.60157200
C	6.07195700	-0.50009500	-1.78510200
C	6.13145400	-1.02570100	0.56059700
C	6.81170200	-0.75801800	-0.62926100
H	4.10077200	-0.31523100	-2.66357500
H	4.20888600	-1.24747500	1.53056600
H	7.90137800	-0.76257800	-0.65787800
C	-0.25347400	3.15359100	0.40512300
C	-0.26031400	4.08598200	-0.63424800
C	-0.19650300	3.58987800	1.73025000
C	-0.20701900	5.45899200	-0.35153400
C	-0.14205100	4.96135900	2.02016500

C	-0.14773100	5.89890700	0.97789700
H	-0.30045600	3.73282100	-1.66550300
H	-0.18780200	2.85144500	2.53307200
H	-0.10183100	6.96562700	1.20055300
C	-0.06769100	5.40726400	3.37708300
C	-0.20049400	6.41065900	-1.41908700
C	6.85268800	-1.33181600	1.73985100
C	6.73374600	-0.26087800	-3.01391000
C	-6.92160300	-0.54934400	-2.75026600
C	-6.87119500	-1.67103800	1.99407900
N	0.00001400	5.77054000	4.48181700
N	-0.18894400	7.18260700	-2.29130300
N	7.41555800	-1.60895400	2.71501700
N	7.25030700	-0.08291800	-4.03663900
N	-7.44165900	-0.14567100	-3.70508400
N	-7.38992100	-1.75239500	3.02825500
C	1.61558100	-3.20509000	2.81098800
C	0.23176700	-2.66182600	2.65931200
H	1.63283900	-3.69848200	3.80098700
H	2.32773100	-2.36941500	2.89851200
C	2.06587300	-4.20021000	1.76051300
C	-0.12747100	-1.37869100	2.96009900
H	-0.56221800	-3.39719500	2.47652100
H	1.33617700	-5.01309000	1.63416900
H	2.19340400	-3.72318700	0.77889000
H	3.02400800	-4.66037000	2.03625600
H	-1.17347700	-1.08461900	3.06657200
H	0.62068600	-0.64226200	3.26832900
H	0.14980700	-2.81956400	0.11306900
Ru	-0.03410800	-1.29845000	0.60211500
Ru	-0.10035800	-0.80230800	-1.64262000

## H-Rh-DHKUST-1

INT1

0 1

O	-0.11512000	0.84823600	-1.22513000
C	-0.07650100	1.43299300	-0.13600900
O	-0.05998600	0.86120600	1.02839400
O	-2.02973400	-1.23612900	1.12492900
C	-2.60458700	-1.37881400	-0.00212300
O	-2.04363800	-1.50014600	-1.12347900
O	2.02489600	-1.27613000	-1.13291000
C	2.58305500	-1.17177700	-0.00804200
O	2.00537800	-1.07391600	1.12175100
C	4.05430500	-1.20071400	0.01973200
C	4.76290700	-1.27861700	-1.17425500
C	4.71922000	-1.21703100	1.24165800
C	6.15526100	-1.37524500	-1.13811600
C	6.11090700	-1.32954100	1.26470000
C	6.84133100	-1.40297400	0.07764400
H	4.22834100	-1.28128900	-2.12410900
H	4.15122900	-1.16830000	2.17028600
H	7.92693800	-1.49933400	0.09910700
C	-4.07618900	-1.38795600	0.02337300
C	-4.74291500	-1.34096500	1.24356200
C	-4.78610100	-1.40607900	-1.17243100
C	-6.13880500	-1.31450800	1.26351100
C	-6.18146100	-1.36182300	-1.13966500
C	-6.86985700	-1.32180400	0.07458300
H	-4.17448000	-1.31734300	2.17286800
H	-4.25106000	-1.43589900	-2.12161700
H	-7.95919100	-1.28533300	0.09268100
C	-0.02885900	2.92169000	-0.08407700
C	0.00726100	3.59887600	1.13600200
C	0.00230100	3.63511300	-1.28475500
C	0.07625200	4.99869100	1.15756800
C	0.07428300	5.03529100	-1.26621200
C	0.11046400	5.71941800	-0.04319900
H	-0.01398800	3.03683800	2.06990000
H	-0.02368500	3.09042400	-2.22958600
H	0.16833100	6.80836600	-0.02686300
C	0.12130800	5.77348200	-2.48986900
C	-6.89748400	-1.31929700	-2.35969500
C	0.12049700	5.68346500	2.41030200
C	-6.80271500	-1.25430200	2.51258300
C	6.76762800	-1.42576500	2.51523600
C	6.86489800	-1.49334500	-2.35651100
N	0.16632100	6.38374500	-3.48064000
N	0.16012800	6.22543400	3.43970700
N	-7.46243300	-1.25529100	-3.36999000
N	-7.31247100	-1.19397100	3.55231100
N	7.26923700	-1.54317400	3.55402700
N	7.41758100	-1.61459700	-3.36821300
H	0.08098200	-2.96044600	-1.05620100
Rh	0.00847600	-1.41989000	-1.20159900
Rh	0.01496300	-1.08896400	1.17052600

INT2

0 1

O	0.01563100	0.72845800	1.12206700
C	0.01096300	1.34735000	0.04617900

O	0.00158400	0.81782600	-1.12912000
O	2.01976600	-1.21446700	-1.30140600
C	2.59584700	-1.33432900	-0.17814300
O	2.04965800	-1.50395200	0.94915900
O	-2.05974300	-1.47345800	0.94963100
C	-2.60673100	-1.30672400	-0.17780800
O	-2.03162800	-1.19559400	-1.30240000
C	-4.08141300	-1.20886300	-0.20210700
C	-4.79398700	-1.09604400	0.98770700
C	-4.74348200	-1.17831200	-1.42703400
C	-6.18183200	-0.93166400	0.94515700
C	-6.13343600	-1.03954200	-1.45988900
C	-6.86236900	-0.91012200	-0.27512000
H	-4.26509200	-1.11237900	1.94077200
H	-4.17205100	-1.25387100	-2.35184100
H	-7.94462500	-0.78141000	-0.30178200
C	4.07077000	-1.24062400	-0.20514500
C	4.72910800	-1.21481800	-1.43210500
C	4.78668700	-1.12013600	0.98198000
C	6.11844600	-1.07255800	-1.47025000
C	6.17397500	-0.95141000	0.93397500
C	6.85071200	-0.93473800	-0.28859000
H	4.15493000	-1.29491600	-2.35479600
H	4.26083000	-1.13144400	1.93682000
H	7.93232500	-0.80159400	-0.31926800
C	0.01616500	2.84171400	0.05817000
C	0.00328100	3.56936100	-1.13384000
C	0.03356300	3.51043800	1.28563000
C	0.00725100	4.97163700	-1.10071000
C	0.03853400	4.91308100	1.32494400
C	0.02511400	5.64500400	0.12879600
H	-0.01019800	3.04218700	-2.08825200
H	0.04323400	2.92856000	2.20828000
H	0.02847700	6.73536300	0.15492100
C	0.05708500	5.60428300	2.57928800
C	-0.00727700	5.71299800	-2.32395900
C	6.89274800	-0.74909900	2.13973300
C	6.77069100	-1.03895500	-2.72998500
C	-6.79247300	-1.00505200	-2.71615700
C	-6.89639400	-0.74389900	2.15562800
N	0.07235800	6.17508900	3.59524600
N	-0.01962800	6.30896900	-3.32464000
N	7.46446400	-0.54953100	3.12969100
N	7.27055800	-1.00446100	-3.77697200
N	-7.30188600	-0.97176400	-3.75860900
N	-7.46249000	-0.55963300	3.15172700
C	-0.01298100	-2.68996200	2.91157500
C	-0.00312400	-1.33679000	3.21631300
H	-0.92604500	-0.80477100	3.46184600
H	0.92749700	-0.81799500	3.46104400
H	-0.01796400	-3.03702800	0.67118100
H	0.90802000	-3.27743200	2.94271500
H	-0.94227900	-3.26415600	2.94369700
Rh	0.00561300	-1.13485400	-1.38896600
Rh	0.00539700	-1.53767200	1.05187100

TS2-3

0 3

O	-0.01012500	0.77790700	-1.00887400
C	-0.00775700	1.41848700	0.07498200

O	0.00013900	0.91464500	1.23261000
O	-2.00601200	-1.67952700	1.16509100
C	-2.59759400	-1.47615900	0.06965400
O	-2.04325100	-1.37494400	-1.06611500
O	2.05343600	-1.35205000	-1.06340600
C	2.60994900	-1.45271200	0.07145100
O	2.02134400	-1.66092900	1.16743200
C	4.08212100	-1.28809400	0.11175600
C	4.79603600	-1.07035400	-1.06476900
C	4.73893600	-1.29536300	1.34195900
C	6.17761100	-0.85667400	-1.00823600
C	6.11937800	-1.07259400	1.39579200
C	6.84639300	-0.85542200	0.22047400
H	4.27156500	-1.05319200	-2.02032400
H	4.16734800	-1.45823000	2.25586600
H	7.92109100	-0.67594800	0.26221700
C	-4.07011900	-1.31611200	0.11340200
C	-4.72288200	-1.32986400	1.34561800
C	-4.78791600	-1.09204700	-1.05966600
C	-6.10295000	-1.10714000	1.40545700
C	-6.16922600	-0.87770400	-0.99707200
C	-6.83387500	-0.88311300	0.23395500
H	-4.14813000	-1.49681200	2.25676800
H	-4.26663500	-1.06916800	-2.01686300
H	-7.90822000	-0.70266200	0.28032700
C	-0.01513900	2.91572100	0.00177500
C	-0.00382400	3.64120100	1.19385600
C	-0.03334900	3.58974000	-1.22286700
C	-0.01009100	5.04179000	1.17239000
C	-0.04087900	4.99483100	-1.25172900
C	-0.02894100	5.72194400	-0.05178500
H	0.01005100	3.10349200	2.14219000
H	-0.04195500	3.01529700	-2.15042900
H	-0.03440800	6.81237500	-0.07442100
C	-0.06094300	5.71355300	-2.49093200
C	0.00289300	5.75307100	2.41177800
C	-6.89196500	-0.62428000	-2.19534700
C	-6.75500200	-1.07693500	2.67021300
C	6.77782500	-1.03715800	2.65722300
C	6.89530900	-0.61323700	-2.21150900
N	-0.07764000	6.33377700	-3.47778500
N	0.01418900	6.29318900	3.44327900
N	-7.46494000	-0.40572400	-3.18214500
N	-7.27077000	-1.03453000	3.71085500
N	7.30164700	-0.99096600	3.69371600
N	7.46201700	-0.40460100	-3.20402600
C	0.01554000	-2.90851100	-2.58757700
C	0.00752800	-1.60188700	-3.16937400
H	0.93039600	-1.19305700	-3.59067300
H	-0.92006200	-1.20479500	-3.59151600
H	0.01563400	-2.95593400	-1.06949400
H	-0.89660900	-3.51275800	-2.64815700
H	0.93529600	-3.50119700	-2.64750000
Rh	0.00519000	-1.23724300	1.52922600
Rh	0.00517700	-1.37111500	-1.10199100

INT3

0 3

O	-0.00845700	0.77809500	-1.01528000
C	-0.00665400	1.40805000	0.08531500



O	0.00078100	0.89474400	1.23007700
O	-2.00761600	-1.68558000	1.13946200
C	-2.59560400	-1.44658900	0.05174200
O	-2.04180600	-1.30208700	-1.08148200
O	2.05138600	-1.28090800	-1.07857600
C	2.60761100	-1.42405000	0.05371200
O	2.02283300	-1.66728000	1.14208900
C	4.08081500	-1.27028900	0.09320100
C	4.79501600	-1.04583200	-1.08143700
C	4.73871200	-1.29657400	1.32217100
C	6.17856000	-0.84732100	-1.02399600
C	6.12047400	-1.08417000	1.37662000
C	6.84895300	-0.86297300	0.20331300
H	4.26952900	-1.01300000	-2.03599600
H	4.16662100	-1.46491500	2.23475500
H	7.92520900	-0.69346200	0.24567400
C	-4.06915000	-1.29769900	0.09477700
C	-4.72292000	-1.33067000	1.32570200
C	-4.78734600	-1.06708600	-1.07631700
C	-6.10436900	-1.11866500	1.38617600
C	-6.17067100	-0.86828000	-1.01281100
C	-6.83687100	-0.89078600	0.21675500
H	-4.14757400	-1.50296100	2.23546800
H	-4.26509900	-1.02839800	-2.03245000
H	-7.91282300	-0.72057100	0.26376800
C	-0.01434500	2.90402800	0.00829000
C	-0.00326100	3.62318800	1.20437700
C	-0.03269300	3.58386000	-1.21351100
C	-0.00989600	5.02365900	1.19031700
C	-0.04062300	4.98926300	-1.23445000
C	-0.02891000	5.70994000	-0.03050500
H	0.01069300	3.08005100	2.14965200
H	-0.04115900	3.01597900	-2.14497500
H	-0.03469800	6.80046700	-0.04755500
C	-0.06093100	5.71584900	-2.46940100
C	0.00285400	5.72762200	2.43406400
C	-6.89352100	-0.61437600	-2.20988400
C	-6.75616700	-1.10207700	2.65042800
C	6.77863600	-1.06223800	2.63761600
C	6.89632400	-0.60328600	-2.22609500
N	-0.07786000	6.34394100	-3.45134200
N	0.01396200	6.26053000	3.46933800
N	-7.46517500	-0.39724300	-3.19741600
N	-7.27101400	-1.06868800	3.69156200
N	7.30140300	-1.02505100	3.67470800
N	7.46178200	-0.39601800	-3.21927400
C	0.01571900	-3.06117100	-2.47585800
C	0.00832400	-1.73300400	-3.10445100
H	0.92564200	-1.39838200	-3.60033400
H	-0.91228000	-1.40903600	-3.60131000
H	0.01466400	-3.03386400	-1.26850200
H	-0.88875000	-3.66604000	-2.62381100
H	0.92742300	-3.65535800	-2.62268900
Rh	0.00530700	-1.26999700	1.56858400
Rh	0.00481700	-1.28952700	-1.11681100

INT4

O 1

O	0.12344500	1.21881700	-1.22156000
C	0.17590100	1.66874900	-0.02057300

O	0.24231600	0.99126100	1.02418600
O	-2.00742300	-1.04164200	0.89462100
C	-2.56953000	-0.80195400	-0.21323500
O	-2.00991800	-0.65112700	-1.33830700
O	2.06192500	-0.92515100	-1.35930400
C	2.61728000	-1.19588800	-0.25458900
O	2.04741500	-1.47444200	0.84047300
C	4.09278300	-1.17805000	-0.23325800
C	4.80236600	-1.02474800	-1.41981800
C	4.76166500	-1.29399900	0.98142000
C	6.19882400	-0.99722000	-1.38493400
C	6.15740300	-1.24690100	1.00705400
C	6.88738300	-1.10378900	-0.17445700
H	4.26667700	-0.92700100	-2.36407600
H	4.19331400	-1.40800600	1.90415100
H	7.97682100	-1.07096300	-0.15272800
C	-4.04492400	-0.77253400	-0.19451100
C	-4.71551800	-0.94288600	1.01275400
C	-4.75139100	-0.69358700	-1.39030900
C	-6.10812300	-1.04713300	1.02001400
C	-6.14401600	-0.80948600	-1.37294000
C	-6.83432900	-0.97987000	-0.17066000
H	-4.14898800	-1.02614000	1.93983700
H	-4.21366200	-0.58106600	-2.33185100
H	-7.91892800	-1.08961300	-0.16600000
C	0.13464500	3.15935200	0.10765200
C	0.10952900	3.71762900	1.38634700
C	0.09653900	3.98738100	-1.01639600
C	0.03939500	5.10759400	1.54911600
C	0.03316100	5.38085700	-0.85885600
C	0.00308200	5.94294100	0.42522400
H	0.13751200	3.05710200	2.25368600
H	0.11232500	3.54309300	-2.01243700
H	-0.05210500	7.02532100	0.54715200
C	-0.01053900	6.24108000	-2.00067300
C	-6.84657300	-0.84237000	-2.60273000
C	-0.00653200	5.66055300	2.86580800
C	-6.76107700	-1.30745300	2.25034000
C	6.82357400	-1.32994000	2.25485100
C	6.91798900	-0.85521100	-2.59682800
N	-0.04987100	6.95567100	-2.91973700
N	-0.05108700	6.08835200	3.94779800
N	-7.39318300	-0.92755200	-3.62215400
N	-7.24644700	-1.57107800	3.27036600
N	7.33816500	-1.38646000	3.29289300
N	7.48982100	-0.74210100	-3.59944200
C	-0.10375500	-2.86383800	-0.45333600
C	-0.12324100	-2.71325800	2.52302800
H	-0.02640400	-2.54833000	-1.60413300
H	0.84422000	-3.41959400	-0.35780300
C	-1.28679000	-3.79495600	-0.41816800
C	0.06808600	-1.43444900	3.05608700
H	-1.12232900	-3.15933500	2.51530000
H	0.70974700	-3.41933300	2.44702200
H	-1.32989100	-4.32446600	0.54269300
H	-2.24982100	-3.28912300	-0.56269900
H	-1.21214200	-4.56602900	-1.20146700
H	-0.77787600	-0.85897700	3.44260200
H	1.05945300	-1.10194800	3.37630100
Rh	0.02518300	-0.79335700	-1.44418000

Rh 0.01478700 -1.30697200 0.92184600

TS4-5

0 3

O	0.05742000	1.36778500	-1.27230700
C	0.11617000	1.77180700	-0.08421700
O	0.18137400	1.04977100	0.95368200
O	-1.99314200	-0.87209500	0.85722300
C	-2.55315700	-1.03068900	-0.26999300
O	-1.97663700	-1.20241800	-1.37491900
O	2.02383000	-1.38474000	-1.36846500
C	2.60401900	-1.31368800	-0.25329100
O	2.04694000	-1.19832100	0.88017900
C	4.08005800	-1.33872000	-0.23596400
C	4.78841500	-1.21607600	-1.42702400
C	4.75213100	-1.40650000	0.98051100
C	6.18357200	-1.13801500	-1.39111700
C	6.14713000	-1.35256200	1.00385600
C	6.87477400	-1.21449600	-0.17956200
H	4.25015400	-1.14954200	-2.37273800
H	4.18587900	-1.48094200	1.90842400
H	7.96252600	-1.14590200	-0.15786000
C	-4.02867200	-1.03812200	-0.25248800
C	-4.70421000	-1.13687900	0.96025600
C	-4.73325200	-0.95578700	-1.44864700
C	-6.10057300	-1.16538700	0.97200800
C	-6.13014400	-0.95534500	-1.42342800
C	-6.82524500	-1.06702000	-0.21728100
H	-4.14104600	-1.19665100	1.89159200
H	-4.19209100	-0.88307600	-2.39220100
H	-7.91525400	-1.07708900	-0.20532100
C	0.10091100	3.25169900	0.13597300
C	0.08467900	3.77712100	1.42915300
C	0.08348100	4.10963900	-0.96558300
C	0.04593100	5.16584300	1.62292000
C	0.05057200	5.49877400	-0.77730900
C	0.03050300	6.02963200	0.51946700
H	0.09664300	3.09847500	2.28273400
H	0.09264300	3.68554600	-1.97032800
H	0.00022100	7.10946400	0.66946700
C	0.03096900	6.37397100	-1.90767900
C	-6.84331000	-0.83049000	-2.64022500
C	0.01328600	5.70310400	2.94694600
C	-6.77305700	-1.30531700	2.21094800
C	6.80419600	-1.39151200	2.25830300
C	6.89969500	-0.91435600	-2.59304200
N	0.01313700	7.08367800	-2.83096500
N	-0.01928400	6.13906600	4.02629000
N	-7.40984400	-0.71370000	-3.64526000
N	-7.29206400	-1.43637800	3.23996800
N	7.29353300	-1.40495300	3.30987900
N	7.47413400	-0.68457400	-3.57422700
C	-0.03813400	-3.29006600	0.65481500
C	-0.33196700	-2.63257800	2.46139800
H	-0.00250400	-2.80511500	-0.34566500
H	0.95623000	-3.72892900	0.80268900
C	-1.14722100	-4.30764800	0.61816500
C	0.03484700	-1.30929000	2.90931000
H	-1.40228600	-2.85135200	2.52637600
H	0.27537100	-3.46718700	2.82972700

H	-1.18234700	-4.93133400	1.52285500
H	-2.13399300	-3.83574800	0.50360200
H	-1.01307200	-4.98230500	-0.23969800
H	-0.74312700	-0.67878200	3.35303800
H	1.03904000	-1.14618000	3.31498200
Rh	0.05302000	-0.74524900	-1.79801900
Rh	0.02771500	-1.02633900	0.89340400

INT5

0 3

O	0.04726100	1.39886800	-1.24263300
C	0.10971700	1.76412800	-0.05004800
O	0.17437300	1.00529700	0.97437100
O	-1.99464200	-0.86629400	0.75677000
C	-2.55006700	-0.99209600	-0.37735600
O	-1.97296300	-1.12296300	-1.48679300
O	2.03637300	-1.28360700	-1.46885000
C	2.60895900	-1.26115200	-0.34848300
O	2.04783100	-1.18712200	0.78674100
C	4.08407800	-1.30373200	-0.32512700
C	4.79944300	-1.14159400	-1.50686300
C	4.74902200	-1.43337000	0.89016300
C	6.19510500	-1.08558300	-1.46175900
C	6.14455100	-1.40314300	0.92078100
C	6.87979800	-1.22513800	-0.25241900
H	4.26688100	-1.02770900	-2.45123900
H	4.17698600	-1.53913800	1.81151100
H	7.96837000	-1.17481700	-0.22354900
C	-4.02543700	-1.00695100	-0.36234700
C	-4.70314600	-1.15607800	0.84393700
C	-4.72730300	-0.88030000	-1.55582400
C	-6.09933700	-1.19353400	0.85008100
C	-6.12397300	-0.88487000	-1.53391200
C	-6.82180000	-1.04954600	-0.33575900
H	-4.14215100	-1.24916800	1.77387900
H	-4.18422400	-0.76840700	-2.49439400
H	-7.91176500	-1.06508500	-0.32705200
C	0.10277500	3.23033100	0.23876100
C	0.08524900	3.70038500	1.55304800
C	0.09362800	4.13327700	-0.82668800
C	0.05365000	5.07976200	1.80411300
C	0.06799900	5.51330100	-0.58003400
C	0.04664500	5.98915800	0.73803800
H	0.09042700	2.98871600	2.37918900
H	0.10346400	3.75146900	-1.84829100
H	0.02192800	7.06190000	0.93319600
C	0.05733900	6.43784500	-1.67071400
C	-6.83184700	-0.70773200	-2.74667400
C	0.01955900	5.55771800	3.15026500
C	-6.77557400	-1.39221600	2.07855900
C	6.79668600	-1.50991300	2.17345500
C	6.91741100	-0.81937200	-2.65057300
N	0.04690700	7.19155600	-2.55851900
N	-0.01423900	5.94057500	4.24931400
N	-7.38979800	-0.54403000	-3.74971700
N	-7.30037100	-1.57490800	3.09658100
N	7.28487800	-1.58089400	3.22308000
N	7.49381900	-0.55306300	-3.62107000
C	-0.12411400	-3.42765800	1.49827800
C	-0.64206000	-2.69860300	2.74444200

H	-0.15565600	-2.82993100	0.51761700
H	0.94530600	-3.66510600	1.61120100
C	-0.93474400	-4.65709000	1.14584300
C	-0.03159100	-1.32903300	2.81569200
H	-1.73879600	-2.62030100	2.67745300
H	-0.43685900	-3.32686600	3.63144100
H	-0.94320700	-5.35049200	1.99911900
H	-1.98097900	-4.39666600	0.92955800
H	-0.53203900	-5.19588800	0.27924000
H	-0.64349400	-0.55326200	3.29403700
H	1.00763300	-1.29791100	3.17418200
Rh	0.05907100	-0.70351800	-1.90831700
Rh	0.03004500	-0.99720600	0.80016400

INT6

0 1

O	-0.15882200	1.25900400	-1.21639100
C	-0.27068200	1.74297800	-0.07741800
O	-0.34220500	1.08694700	1.02701700
O	-2.04720700	-1.24228300	1.00219500
C	-2.63714900	-1.19306600	-0.12190500
O	-2.09289100	-1.08531200	-1.25546800
O	1.97396400	-0.81640700	-1.28829000
C	2.52811300	-0.62905700	-0.16998900
O	1.95449500	-0.55312000	0.96097400
C	4.00068300	-0.56845400	-0.15634800
C	4.70027600	-0.55954100	-1.35853600
C	4.67894200	-0.63358700	1.05723500
C	6.09551500	-0.62107500	-1.34114800
C	6.07397700	-0.71211400	1.06227600
C	6.79404300	-0.69835600	-0.13406200
H	4.15583600	-0.53112600	-2.30245700
H	4.11837000	-0.65863100	1.99184500
H	7.88153700	-0.77379800	-0.12740500
C	-4.10975600	-1.25729000	-0.08627300
C	-4.76459100	-1.37676200	1.13577400
C	-4.83361000	-1.17219000	-1.27154000
C	-6.16060800	-1.41303400	1.16856500
C	-6.22960500	-1.20133400	-1.22673500
C	-6.90430700	-1.32461600	-0.00980700
H	-4.18586100	-1.43393300	2.05739600
H	-4.30845600	-1.07308300	-2.22157200
H	-7.99387200	-1.34477100	0.01941700
C	-0.31185500	3.22886500	0.07623400
C	-0.32820900	3.81600200	1.34235200
C	-0.29483900	4.03132500	-1.06643400
C	-0.32124700	5.21247300	1.46869200
C	-0.29373200	5.42821900	-0.94446800
C	-0.30599000	6.02167600	0.32514800
H	-0.33566600	3.18263500	2.22970300
H	-0.27502000	3.55763300	-2.04882500
H	-0.29801200	7.10789000	0.42235000
C	-0.26626900	6.25151600	-2.11272000
C	-0.31335800	5.80789300	2.76733000
C	-6.96309700	-1.08648400	-2.43328900
C	-6.81385400	-1.52652700	2.42079200
C	6.74571200	-0.88705500	2.29770100
C	6.79185200	-0.67599600	-2.57317700
C	0.42428300	-3.40813100	0.30795900
C	0.01514800	-3.01402400	-1.09581300

H	0.74866300	-3.40956800	-1.81828100
H	-0.98124000	-3.40491800	-1.35413500
H	0.12365600	-2.69915200	1.17815900
H	-0.20808500	-4.23885400	0.67876900
C	1.88865700	-3.76306200	0.50328400
H	2.52290800	-3.06911000	-0.07026200
H	2.04712400	-4.73895400	0.01412300
C	2.32819800	-3.82283900	1.94936900
H	2.22809900	-2.83984700	2.43617500
H	1.72640100	-4.53813900	2.52923800
H	3.37804100	-4.12923600	2.04602500
N	-0.23822900	6.92438500	-3.06272700
N	-0.29717000	6.28344200	3.82993900
N	-7.54705900	-0.97884800	-3.42963800
N	-7.31781800	-1.61451100	3.46184500
N	7.26174400	-1.08535000	3.31755500
N	7.32777800	-0.76100700	-3.59807900
Rh	0.05810000	-0.99683500	-1.34187600
Rh	0.04464800	-0.90340000	1.04518500

TS6-7

0 3

O	-0.22430800	0.94811200	1.01907700
C	-0.17332000	1.74504300	0.04488600
O	-0.09105000	1.42527600	-1.17308800
O	1.96377500	-1.07143700	-1.50163100
C	2.55140600	-0.97971000	-0.39119100
O	2.00324700	-0.97020500	0.75168500
O	-2.04662700	-1.39174800	0.79568600
C	-2.61024900	-1.35776500	-0.33853100
O	-2.03265700	-1.29271200	-1.45708900
C	-4.08654100	-1.36928500	-0.33697500
C	-4.78037700	-1.54206200	0.85676200
C	-4.77326500	-1.13564400	-1.52500100
C	-6.17613900	-1.48249500	0.85741900
C	-6.16840100	-1.05579900	-1.51098800
C	-6.88097100	-1.23598900	-0.32309300
H	-4.23162300	-1.70539400	1.78412400
H	-4.21695500	-0.98957700	-2.45089600
H	-7.96897500	-1.16776500	-0.31435000
C	4.02467100	-0.88937300	-0.40470400
C	4.68978900	-0.66635300	-1.60693200
C	4.73797600	-1.02174300	0.78258900
C	6.08316300	-0.55946700	-1.61322400
C	6.13266500	-0.94366700	0.76174700
C	6.81576400	-0.70524800	-0.43260000
H	4.11878400	-0.56433800	-2.52989100
H	4.20681700	-1.18438300	1.72043200
H	7.90328200	-0.63011700	-0.44338000
C	-0.21420600	3.21223100	0.34546600
C	-0.24230100	4.11735700	-0.71686400
C	-0.21565100	3.68242000	1.66093300
C	-0.27522300	5.49666100	-0.47199200
C	-0.23994500	5.06392500	1.91303400
C	-0.27205700	5.97295100	0.84538800
H	-0.23815100	3.73702800	-1.73873300
H	-0.19364300	2.96728700	2.48455200
H	-0.29315600	7.04562800	1.04159500
C	-0.22745800	5.56627100	3.25322100
C	-0.30985100	6.40372000	-1.57617200

C	6.84543800	-1.11290800	1.97458600
C	6.75507600	-0.28182900	-2.83023000
C	-6.85615100	-0.73520100	-2.70874600
C	-6.86857300	-1.63706900	2.08421600
N	-0.21328700	6.00076000	4.33434000
N	-0.33844800	7.11873500	-2.49495500
N	7.39618900	-1.26837400	2.98364400
N	7.29177100	-0.03508900	-3.82877500
N	-7.39800100	-0.43375100	-3.68952200
N	-7.40491800	-1.75111000	3.10655100
C	1.50192800	-3.71326100	2.07182000
C	0.18758800	-2.96878900	2.03255100
H	1.47141000	-4.33912600	2.98017500
H	2.31554000	-2.99192800	2.24037800
C	1.78905400	-4.56902300	0.85724800
C	0.01250200	-1.76325100	2.79786500
H	-0.69570100	-3.62369100	1.97131400
H	0.98680000	-5.29833500	0.67179500
H	1.88702400	-3.95580700	-0.05283200
H	2.72245000	-5.13480300	0.97094100
H	-0.95660500	-1.54840500	3.25675300
H	0.88129600	-1.34564700	3.31861300
H	0.10558700	-2.74434200	0.56742500
Rh	0.02139700	-1.17612900	0.81234500
Rh	0.07314600	-0.65344200	-1.78899100

#### INT7

0 1

O	0.35002900	0.86501500	1.15937400
C	0.28500100	1.64892800	0.19970700
O	0.20559600	1.32175300	-1.04418700
O	2.09938100	-0.82767500	-1.52632300
C	2.63175800	-1.24993200	-0.45571000
O	2.04657300	-1.59979900	0.60820500
O	-2.00514900	-0.95230800	0.65161400
C	-2.53030700	-0.68498200	-0.46723900
O	-1.93363300	-0.46575500	-1.56348900
C	-4.00546200	-0.67447900	-0.52214300
C	-4.74502300	-0.99135600	0.61274800
C	-4.64347200	-0.43142600	-1.73502200
C	-6.13748700	-1.06891200	0.52692500
C	-6.03523400	-0.52066100	-1.81254000
C	-6.79424700	-0.83414400	-0.68308100
H	-4.23413200	-1.19725300	1.55337900
H	-4.05165900	-0.20038100	-2.62039700
H	-7.87936500	-0.91526000	-0.74896800
C	4.10709300	-1.31547000	-0.45731500
C	4.80329500	-1.07064400	-1.63762200
C	4.79229800	-1.56167700	0.72781800
C	6.20016400	-1.07601000	-1.62909600
C	6.18960800	-1.54310100	0.73061400
C	6.90474100	-1.30833800	-0.44578300
H	4.25482100	-0.86422400	-2.55635500
H	4.23678600	-1.74091900	1.64830700
H	7.99473200	-1.29134300	-0.43703600
C	0.27226200	3.11969000	0.44957000
C	0.29290300	4.02600400	-0.61178900
C	0.20780900	3.58331800	1.76525300
C	0.25038600	5.40374300	-0.35749600
C	0.15363900	4.96073000	2.02263800

C	0.17792200	5.87428800	0.96014900
H	0.33816700	3.65718600	-1.63676600
H	0.18987300	2.86273200	2.58393900
H	0.13623500	6.94599800	1.15794800
C	0.05785400	5.43922000	3.36628900
N	-0.03152900	5.83394100	4.45818100
C	0.27032000	6.32525200	-1.44847900
N	0.28388700	7.06536300	-2.34683300
C	6.87738600	-1.71718700	1.95688400
N	7.41563300	-1.82600200	2.97860900
C	6.89676100	-0.80725400	-2.83410600
N	7.44078600	-0.56971000	-3.83092000
C	-6.66288300	-0.34919300	-3.07145300
N	-7.14109600	-0.24563900	-4.12321000
C	-6.87745400	-1.44544400	1.67466100
N	-7.45760000	-1.78705600	2.61916900
C	-0.24487700	-2.76126600	2.43745800
C	0.14438600	-1.50652300	2.89344800
H	-0.59558400	-0.81517600	3.30941000
H	1.19048200	-1.27742300	3.10960500
H	-0.20742100	-2.74320200	0.13040900
H	0.53850400	-3.51150900	2.27018600
C	-1.63526300	-3.29553000	2.59659700
H	-2.33135900	-2.45690400	2.75412700
H	-1.63856000	-3.85444000	3.55092000
C	-2.12801300	-4.20376300	1.48913000
H	-2.27194200	-3.65115800	0.54927000
H	-1.41684700	-5.01773100	1.28480200
H	-3.08890600	-4.66760200	1.74923100
Rh	0.09103100	-0.55460600	-1.61616100
Rh	0.01359300	-1.33585600	0.73472400



## H-Pd-DHKUST-1

INT1

0 3

O	-0.11328300	0.94717900	-1.19223800
C	-0.10868900	1.48958500	-0.04316800
O	-0.15003500	0.88891000	1.05587700
O	-2.04869500	-1.46908700	1.08769800
C	-2.63267800	-1.51079500	-0.03821400
O	-2.10317100	-1.52736100	-1.18107200
O	2.05487400	-1.21235100	-1.18483200
C	2.58140900	-1.18845800	-0.04116500
O	1.99486900	-1.17224300	1.08424600
C	4.05679600	-1.21530400	0.01247100
C	4.77692400	-1.25740500	-1.17578800
C	4.70914400	-1.27477400	1.23968100
C	6.16751400	-1.37314900	-1.13172700
C	6.10093200	-1.38860700	1.27077100
C	6.84191700	-1.43618400	0.08842200
H	4.25134000	-1.22592300	-2.12987700
H	4.13250700	-1.25714200	2.16419600
H	7.92636300	-1.54316900	0.11806000
C	-4.10862400	-1.49684400	0.01337200
C	-4.76308600	-1.45194700	1.24023200
C	-4.82708200	-1.43807300	-1.17546800
C	-6.15463900	-1.33466500	1.27101700
C	-6.21771700	-1.31937300	-1.13224200
C	-6.89359900	-1.27032600	0.08799800
H	-4.18776400	-1.47907900	2.16531800
H	-4.29961600	-1.45430300	-2.12892900
H	-7.97755400	-1.15820900	0.11735700
C	-0.02531200	2.98393000	-0.01801600
C	0.02662300	3.63990600	1.21281900
C	0.03501600	3.71626600	-1.20528800
C	0.14469500	5.03592900	1.26118900
C	0.15063000	5.11387900	-1.16196900
C	0.20598900	5.77547600	0.07263900
H	-0.01687600	3.05369400	2.13150400
H	-0.00130700	3.19418600	-2.16223000
H	0.30131400	6.86139500	0.10738200
C	0.22563600	5.87059600	-2.37303300
C	-6.92474100	-1.17773400	-2.35022900
C	0.21681900	5.69833900	2.52554900
C	-6.80631500	-1.21209300	2.52226000
C	6.75325700	-1.51787700	2.52057700
C	6.87589300	-1.48995700	-2.35094100
N	0.29358500	6.49331900	-3.35492700
N	0.28306900	6.22483800	3.56198300
N	-7.46076700	-1.01898500	-3.36593400
N	-7.31151300	-1.07053500	3.55637300
N	7.26240800	-1.66140200	3.55230800
N	7.41124700	-1.62489700	-3.37020300
H	0.07895700	-2.82464900	1.17100500
Pd	-0.03746000	-1.20291000	-1.37416100
Pd	-0.02928500	-1.29764700	1.16070600

INT2

0 3

O	0.01849500	0.81701800	1.07643300
C	0.01261700	1.38869600	-0.04143400

O	0.00436000	0.82465600	-1.17584200
O	2.06753300	-1.51635200	-1.28531200
C	2.62942100	-1.44360700	-0.16083600
O	2.08161600	-1.42327000	0.98083700
O	-2.08601300	-1.38519100	0.97670300
C	-2.63603000	-1.40663900	-0.16398000
O	-2.07679600	-1.48671600	-1.28919800
C	-4.11240100	-1.29201300	-0.18263100
C	-4.81863800	-1.10575300	1.00061100
C	-4.77555500	-1.30296400	-1.40610000
C	-6.20267500	-0.91656700	0.95191700
C	-6.15976000	-1.12041400	-1.44420800
C	-6.88471800	-0.92636500	-0.26687400
H	-4.28786400	-1.08414600	1.95228000
H	-4.20692800	-1.43365400	-2.32637800
H	-7.96266500	-0.76669000	-0.29879900
C	4.10597000	-1.33106100	-0.18324000
C	4.76453900	-1.34357500	-1.40911500
C	4.81541100	-1.13290500	0.99622100
C	6.14683300	-1.14911800	-1.45411100
C	6.19755100	-0.93125500	0.94063300
C	6.87485800	-0.94224800	-0.28091300
H	4.19309600	-1.48097300	-2.32663400
H	4.28801500	-1.10772800	1.94970200
H	7.95076900	-0.77045900	-0.31825200
C	0.01465100	2.89168500	-0.05126900
C	-0.00046400	3.58498500	-1.26349200
C	0.03020000	3.59790100	1.15434500
C	-0.00073800	4.98822100	-1.27494100
C	0.03098600	5.00201800	1.15199300
C	0.01525800	5.69787300	-0.06578900
H	-0.01252900	3.02432700	-2.19901200
H	0.04154400	3.04486400	2.09449700
H	0.01527500	6.78859000	-0.07188300
C	0.04720400	5.73212300	2.38486500
C	-0.01795800	5.69344900	-2.52064500
C	6.90525100	-0.65345900	2.13605900
C	6.78797500	-1.10933500	-2.71747700
C	-6.81009100	-1.08816400	-2.70308100
C	-6.90839500	-0.66173300	2.15347300
N	0.06032700	6.33525900	3.38242400
N	-0.03264600	6.26077100	-3.53835300
N	7.46284200	-0.38882200	3.11815200
N	7.26887200	-1.05160900	-3.77159300
N	-7.30356600	-1.04104600	-3.75189200
N	-7.46403200	-0.42148300	3.14284400
Pd	-0.00341900	-1.34339300	-1.42218600
Pd	-0.00224600	-1.39292500	1.13379000
C	-0.00728300	-2.18820600	3.58793600
C	-0.00078400	-0.84196600	3.62066300
H	-0.92684800	-0.26212100	3.65028600
H	0.93082100	-0.27106500	3.64979000
H	-0.01758700	-2.91752200	1.02746900
H	0.92049700	-2.76598200	3.60539500
H	-0.94054200	-2.75705200	3.60619700

TS2-3

0 3

O	-0.18656300	0.81303300	-1.09596600
C	-0.08810300	1.40127500	0.01391100

O	-0.02925400	0.85625900	1.14947500
O	-2.08678700	-1.53365400	1.28684500
C	-2.69235800	-1.52848000	0.17889100
O	-2.18937500	-1.57932600	-0.97496300
O	2.10946700	-1.20460400	-0.95111300
C	2.62281500	-1.26481300	0.19811200
O	2.02840800	-1.39198500	1.30417000
C	4.09949200	-1.17321700	0.26343600
C	4.82953300	-1.05684300	-0.91306400
C	4.74493000	-1.19131100	1.49550400
C	6.22118700	-0.95943100	-0.85490500
C	6.13775300	-1.09113200	1.54232500
C	6.88798000	-0.97541700	0.37039100
H	4.31098000	-1.03822100	-1.87118600
H	4.16032800	-1.27874900	2.41121800
H	7.97436100	-0.89618700	0.41314000
C	-4.16572500	-1.38934300	0.25244800
C	-4.79520800	-1.31889600	1.49105500
C	-4.89090000	-1.19778400	-0.91733500
C	-6.16331700	-1.04172100	1.55303500
C	-6.25573900	-0.90981700	-0.84454200
C	-6.90597200	-0.83649000	0.38806600
H	-4.21001000	-1.44066900	2.40240000
H	-4.38043600	-1.22630400	-1.87963300
H	-7.96596000	-0.58791100	0.44302300
C	-0.02044100	2.90324700	-0.01658000
C	0.04716100	3.62822100	1.17603400
C	-0.00174600	3.57517500	-1.24123000
C	0.13329100	5.02933000	1.14729700
C	0.08995400	4.97549300	-1.27953800
C	0.15602600	5.70338900	-0.08269500
H	0.03563700	3.09316400	2.12660700
H	-0.05303000	2.99845300	-2.16544800
H	0.22780200	6.79148100	-0.10792000
C	0.12546300	5.66064500	-2.53734500
C	0.20537400	5.77661100	2.36770400
C	-6.93937000	-0.59271700	-2.04289500
C	-6.77530700	-0.87735400	2.81992500
C	6.79451500	-1.10099000	2.79639900
C	6.94131800	-0.83987900	-2.06666800
N	0.16046000	6.21541900	-3.56203000
N	0.26683500	6.39054000	3.35672900
N	-7.43287000	-0.27712800	-3.04372500
N	-7.24262500	-0.69373000	3.86545800
N	7.32397500	-1.10635200	3.82795500
N	7.48676200	-0.74338300	-3.08508600
Pd	-0.03375500	-1.33004000	1.35978900
Pd	-0.04162700	-1.34866500	-1.23201900
C	0.06097900	-2.68522600	-3.10839100
C	-0.04616000	-1.33993000	-3.44355600
H	0.84024400	-0.75231600	-3.69475400
H	-1.01550800	-0.89924900	-3.68903900
H	0.08175300	-2.89370800	-1.42881200
H	-0.81868300	-3.33286000	-3.16363900
H	1.03064500	-3.18740200	-3.17077300

INT3

0 3

O	0.17446400	0.87869400	1.16204800
C	0.14430000	1.54733800	0.10628900

O	0.14108300	1.08157100	-1.07770800
O	2.11520900	-1.37215300	-1.29031000
C	2.66204500	-1.41801200	-0.15539000
O	2.09386500	-1.49373100	0.97552800
O	-1.99636700	-1.15553200	0.99526400
C	-2.56927700	-1.07621000	-0.13219300
O	-2.03079900	-1.06559100	-1.27217500
C	-4.04578000	-1.01005100	-0.11028900
C	-4.73910000	-1.11833900	1.09076300
C	-4.73067600	-0.85923100	-1.31161600
C	-6.13616100	-1.07901500	1.08037300
C	-6.12615600	-0.81758400	-1.31019600
C	-6.84047200	-0.92717900	-0.11621800
H	-4.19226400	-1.23641000	2.02646900
H	-4.17347700	-0.77859500	-2.24449100
H	-7.93028600	-0.89959300	-0.11664300
C	4.13852600	-1.33374800	-0.13634300
C	4.81356500	-1.08240300	-1.32669400
C	4.83170900	-1.41044400	1.06703200
C	6.19676700	-0.88956100	-1.30866900
C	6.21712100	-1.22746800	1.07280400
C	6.91057600	-0.96649900	-0.11134100
H	4.25404600	-1.00499700	-2.25852500
H	4.29006000	-1.58552100	1.99657900
H	7.98809500	-0.80149200	-0.09631500
C	0.09070100	3.04419000	0.20837200
C	0.02687900	3.81810300	-0.95170700
C	0.07879400	3.66220900	1.46133400
C	-0.05270500	5.21544400	-0.86566600
C	0.00071800	5.06127200	1.55494800
C	-0.06521200	5.83890300	0.38928200
H	0.03339200	3.32551500	-1.92452200
H	0.12516300	3.04568200	2.36030900
H	-0.12958900	6.92535100	0.46070600
C	-0.02217800	5.71032800	2.83150000
C	-0.13081900	5.99254500	-2.06395000
C	6.91047600	-1.24854700	2.30782100
C	6.85236900	-0.54560000	-2.51690300
C	-6.80152400	-0.67609900	-2.54690100
C	-6.84633600	-1.21021900	2.29850500
C	-0.02610800	-3.38488100	1.05226300
H	0.78953700	-3.67606100	0.37251100
H	0.28948000	-3.59222700	2.08930800
C	-1.34002000	-4.00343900	0.69075200
H	-2.14803000	-3.72728100	1.38083600
H	-1.66017700	-3.75136400	-0.33166300
H	-1.25245600	-5.10294800	0.72412400
N	-0.04662800	6.25763800	3.86020900
N	-0.19941600	6.60499300	-3.05244500
N	7.45381800	-1.23583600	3.33235600
N	7.34417000	-0.22161300	-3.51628300
N	-7.31120500	-0.56830800	-3.58296700
N	-7.42152100	-1.33011200	3.29833000
Pd	0.04619400	-1.35153000	1.08557300
Pd	0.05359300	-1.04647600	-1.43866000

INT4

0 3

O	-0.09128500	1.26168700	-1.25233000
C	-0.16725600	1.70211100	-0.06730000

O	-0.31228100	1.02117300	0.97562400
O	-2.08834700	-1.43818700	0.72068700
C	-2.64564700	-1.32254400	-0.40828500
O	-2.09301100	-1.21292100	-1.53501600
O	2.06748400	-0.88395200	-1.49227900
C	2.60758500	-0.87576700	-0.35500000
O	2.03744600	-0.88189600	0.77450300
C	4.08694500	-0.92419500	-0.32452200
C	4.80047500	-0.87721500	-1.51653100
C	4.74428100	-1.13378200	0.88319200
C	6.18574300	-1.05567700	-1.49540300
C	6.12884900	-1.32045700	0.89264400
C	6.86250800	-1.27616200	-0.29422000
H	4.27064000	-0.73742300	-2.45877100
H	4.17078700	-1.19077100	1.80812800
H	7.93968700	-1.44356000	-0.28750900
C	-4.12555500	-1.27382600	-0.38342600
C	-4.79617900	-1.34055600	0.83342900
C	-4.82752700	-1.05606400	-1.56380300
C	-6.18236400	-1.17194200	0.86930400
C	-6.21418600	-0.88953600	-1.51797900
C	-6.90370800	-0.94916100	-0.30500800
H	-4.23217100	-1.48839100	1.75406900
H	-4.28759300	-0.98241700	-2.50782500
H	-7.98249500	-0.79539300	-0.27309000
C	-0.03671900	3.18878500	0.09421300
C	0.03143200	3.72097400	1.38140300
C	0.06713800	4.03174400	-1.01462500
C	0.21577500	5.09735600	1.56905100
C	0.23911100	5.41336800	-0.83293000
C	0.31637700	5.94784000	0.46105800
H	-0.04677800	3.05055200	2.23786300
H	0.02157700	3.60558500	-2.01780800
H	0.46140500	7.01948100	0.60249700
C	0.35505600	6.29127000	-1.95658800
C	-6.90857500	-0.58021000	-2.71284100
C	0.32244800	5.61300500	2.89663100
C	-6.83272900	-1.15199900	2.12783500
C	6.76435100	-1.64969600	2.11516500
C	6.88316300	-1.10004200	-2.72633000
N	0.45784700	7.02484800	-2.85571600
N	0.42153400	6.00035200	3.99004100
N	-7.44672000	-0.28098900	-3.69558000
N	-7.31896500	-1.09376900	3.17941500
N	7.23987600	-1.97821600	3.12089800
N	7.40976800	-1.18646200	-3.75563600
Pd	-0.02654200	-1.18761100	0.92763600
Pd	-0.02518700	-0.87835400	-1.62921300
C	0.36859900	-3.19001500	0.82485300
C	-0.71658900	-1.26465100	3.44388400
H	1.05613400	-3.26913200	-0.03324100
H	0.94261100	-3.35522700	1.75009200
C	-0.82762200	-4.07836200	0.69556400
C	0.58068200	-0.91593400	3.45979900
H	-1.50802800	-0.51816300	3.33867100
H	-1.03862100	-2.30211300	3.57038500
H	-1.55193300	-3.94292400	1.51021400
H	-1.35934600	-3.93533300	-0.25535100
H	-0.50762000	-5.13426200	0.72394400
H	0.89486800	0.12623800	3.36230100

H 1.37781700 -1.65187900 3.59508500

TS4-5

0 3

O -0.14324200 1.32182100 -1.21059400  
C -0.32747800 1.72743400 -0.03801800  
O -0.57427400 1.01826400 0.98108400  
O -2.09488200 -1.77141400 0.61309500  
C -2.64792200 -1.45663200 -0.47448300  
O -2.08216500 -1.16920600 -1.56761900  
O 2.04606100 -0.76216100 -1.48907000  
C 2.61428400 -0.59263400 -0.37166900  
O 2.07046200 -0.40764000 0.74782200  
C 4.09524400 -0.70733600 -0.38254000  
C 4.79147700 -0.67590800 -1.58623800  
C 4.76328000 -0.97137500 0.80911700  
C 6.16934100 -0.91169600 -1.59205600  
C 6.13502600 -1.24329100 0.79150000  
C 6.85089900 -1.20265700 -0.40715400  
H 4.25360300 -0.49412100 -2.51701100  
H 4.20235600 -1.00591900 1.74354300  
H 7.91853900 -1.42277000 -0.42297300  
C -4.13140400 -1.36805400 -0.46317900  
C -4.80658700 -1.47851100 0.74851000  
C -4.82888100 -1.06926400 -1.63014700  
C -6.18774400 -1.26908000 0.79896600  
C -6.21284100 -0.87381000 -1.57604900  
C -6.90220600 -0.97133200 -0.36356800  
H -4.24463600 -1.69171500 1.65753300  
H -4.28657600 -0.96119100 -2.56978100  
H -7.97706500 -0.79311500 -0.32369000  
C -0.19997600 3.20288800 0.19734100  
C -0.12009600 3.67999200 1.50502100  
C -0.08045600 4.08746000 -0.87711600  
C 0.09778800 5.04314400 1.74672400  
C 0.11701700 5.45672300 -0.64026900  
C 0.21072300 5.93614300 0.67424900  
H -0.20516300 2.97795800 2.33478200  
H -0.12922000 3.70096400 -1.89611600  
H 0.38191900 6.99735200 0.85859600  
C 0.25157600 6.37641200 -1.72768000  
C -6.91477700 -0.51201200 -2.75500300  
C 0.23710400 5.49785100 3.09304400  
C -6.83594300 -1.29596000 2.06125200  
C 6.77143300 -1.65171100 1.99229600  
C 6.85782300 -0.92541500 -2.83128700  
N 0.37253300 7.14314900 -2.59628800  
N 0.36911300 5.83170200 4.20043100  
N -7.47656800 -0.18482700 -3.71664700  
N -7.31750700 -1.28464900 3.11764800  
N 7.24761100 -2.04774500 2.97432900  
N 7.38634800 -0.96645000 -3.86336200  
Pd -0.03559900 -1.05325400 0.99411800  
Pd -0.02989000 -0.83844200 -1.62028800  
C 0.73193400 -3.21801600 0.99011300  
C 0.04554700 -2.52968500 2.80359700  
H 0.71201500 -2.81378200 -0.04175700  
H 1.78359000 -3.25979300 1.29656200  
C -0.00364100 -4.52158600 1.01646800  
C 0.02321700 -1.13451000 3.06994000

H	-0.92007900	-3.04232600	2.80266800
H	0.85970100	-3.11990700	3.23217700
H	0.06273700	-5.03812900	1.98350300
H	-1.06534600	-4.38908000	0.76855100
H	0.42321200	-5.19462700	0.25697600
H	-0.91931100	-0.64646500	3.33595400
H	0.93329100	-0.62629800	3.40369600

INT5

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O	-0.18186500	1.54179700	-1.10787100
C	-0.25249200	1.78627800	0.12041800
O	-0.36303100	0.94341600	1.05856000
O	-2.04638300	-1.60197000	0.43743900
C	-2.63453400	-1.27915200	-0.64277200
O	-2.11110800	-0.92442600	-1.72929300
O	2.01622300	-0.49595900	-1.68319400
C	2.56228000	-0.69819700	-0.56934400
O	2.00039700	-0.92114100	0.54865700
C	4.04245600	-0.72323400	-0.54878000
C	4.74459900	-0.45925000	-1.71967600
C	4.71722900	-1.08622200	0.61254000
C	6.13721400	-0.56739200	-1.72627200
C	6.11015100	-1.19750200	0.59437000
C	6.83170400	-0.93506400	-0.57204900
H	4.20128700	-0.19259300	-2.62617400
H	4.15506300	-1.30524900	1.52024200
H	7.91708800	-1.03581000	-0.58676400
C	-4.11425200	-1.28876300	-0.58709900
C	-4.76233000	-1.56287600	0.61317600
C	-4.84263800	-0.91759200	-1.71266200
C	-6.15311500	-1.44930500	0.68892700
C	-6.23299300	-0.80824100	-1.62830900
C	-6.89985300	-1.07553300	-0.43039800
H	-4.17959600	-1.82963100	1.49444300
H	-4.32001600	-0.68303400	-2.63998700
H	-7.98258200	-0.96735900	-0.36341500
C	-0.17705600	3.22566600	0.53957500
C	-0.11523000	3.54875300	1.89542800
C	-0.12656300	4.23572300	-0.42328800
C	0.00682100	4.88664700	2.29593800
C	-0.01373300	5.57718800	-0.02705200
C	0.05488100	5.90419800	1.33459400
H	-0.15046400	2.75111200	2.63798700
H	-0.16791800	3.96956900	-1.48036200
H	0.15139000	6.94590600	1.64270600
C	0.04727900	6.62094200	-1.00296800
C	-6.95483800	-0.34950600	-2.75816400
C	0.10038100	5.19913100	3.68702200
C	-6.78964100	-1.64664700	1.94003800
C	6.78230400	-1.63848700	1.76137400
C	6.83238300	-0.35339200	-2.94144600
N	0.10381900	7.48178400	-1.78555600
N	0.18724800	5.43004600	4.82494300
N	-7.51383500	0.07026100	-3.68384500
N	-7.27454000	-1.77010400	2.98685900
N	7.30628100	-2.03821900	2.71612000
N	7.36519500	-0.20618900	-3.96090500
Pd	-0.03990100	-1.18526200	0.59840800
Pd	-0.06634400	-0.50516100	-1.91062500

C	1.04334800	-3.90968400	2.04626700
C	-0.10353700	-3.15356200	2.70726300
H	1.04548600	-3.69578200	0.95979200
H	2.00259600	-3.50545500	2.41336800
C	0.97879800	-5.40492400	2.26886300
C	-0.02320500	-1.66954200	2.60096700
H	-1.07602400	-3.51102600	2.32497300
H	-0.12771900	-3.40254700	3.78902700
H	1.02510100	-5.65283500	3.33937200
H	0.04330500	-5.83187200	1.87897000
H	1.80815100	-5.92871900	1.77653100
H	-0.89234300	-1.11415100	2.97771700
H	0.92652000	-1.22060600	2.92697800

INT6

0 1

O	0.40886400	0.97514500	1.15083800
C	0.44692000	1.75690700	0.17442200
O	0.43495900	1.44017000	-1.05445800
O	2.13568200	-1.09082900	-1.45090300
C	2.65394300	-1.37680300	-0.32857500
O	2.05763000	-1.58386100	0.76532100
O	-1.97937000	-0.74668100	0.70564400
C	-2.46922000	-0.52413500	-0.43575600
O	-1.85219800	-0.43836900	-1.54092600
C	-3.94042000	-0.41102300	-0.51516400
C	-4.70912800	-0.65553200	0.61858700
C	-4.54738700	-0.16484000	-1.74315500
C	-6.10265700	-0.67010300	0.51344400
C	-5.94125000	-0.17840400	-1.83765500
C	-6.72914900	-0.42880200	-0.711172700
H	-4.22091700	-0.86236100	1.57157100
H	-3.93346300	0.00817500	-2.62677000
H	-7.81595000	-0.45901700	-0.79222700
C	4.13061800	-1.45501600	-0.31112600
C	4.84747300	-1.25528000	-1.48838500
C	4.79349600	-1.66800600	0.89313600
C	6.24462800	-1.26793600	-1.45608700
C	6.19074700	-1.67015700	0.91753600
C	6.92609800	-1.47492000	-0.25388000
H	4.31653700	-1.07455600	-2.42276600
H	4.22108200	-1.80937400	1.80990700
H	8.01600900	-1.46959100	-0.22794200
C	0.49004300	3.23154600	0.45479600
C	0.56885900	4.13285800	-0.60673000
C	0.41412500	3.70308100	1.76708600
C	0.57045800	5.51258200	-0.36181500
C	0.40980300	5.08459200	2.01762000
C	0.48980900	5.99189500	0.95157500
H	0.62127800	3.75298900	-1.62744900
H	0.34868900	2.98743200	2.58795400
H	0.48383700	7.06521300	1.14511300
C	0.30913000	5.58651100	3.35358300
C	0.63981500	6.41685200	-1.46486700
C	6.85396100	-1.83388000	2.15950800
C	6.97075200	-1.03268400	-2.65238700
C	-6.54322700	-0.00200300	-3.10923800
C	-6.87607800	-1.00204600	1.65402300
C	-1.67535200	-3.69928100	0.90971700
C	-0.27217500	-3.21203800	0.69241600



H	0.43976800	-3.59770100	1.44194400
H	0.11834300	-3.44468500	-0.31296500
H	-2.36290800	-3.27226800	0.15799200
H	-1.67938000	-4.78583400	0.68870600
C	-2.22555400	-3.47962200	2.31093100
H	-2.18932300	-2.40329200	2.55287700
H	-1.55187000	-3.96254100	3.03991700
C	-3.63642700	-4.00183900	2.48557700
H	-4.33254800	-3.53787500	1.76974800
H	-3.69018200	-5.08778500	2.31850700
H	-4.02875000	-3.80746400	3.49247300
N	0.21877100	6.01837500	4.43180800
N	0.69026700	7.12808100	-2.38504500
N	7.36586700	-1.94427300	3.19469100
N	7.54976700	-0.82088200	-3.63575900
N	-7.00109100	0.10271900	-4.17014800
N	-7.48607400	-1.31886000	2.58865900
Pd	0.02668900	-1.20852000	0.90939900
Pd	0.15889300	-0.67311200	-1.58167300

TS6-7

0 3

O	-0.57672800	0.85480000	1.07799000
C	-0.41978600	1.64235900	0.10684400
O	-0.27401100	1.32663300	-1.10412600
O	1.95274700	-0.63130800	-1.63909200
C	2.54415800	-0.58781600	-0.52489700
O	2.02667500	-0.62988800	0.62308400
O	-2.14726600	-1.81949500	0.54449700
C	-2.70054200	-1.51423700	-0.54501600
O	-2.14036000	-1.18205600	-1.62739900
C	-4.18487500	-1.48363600	-0.54763100
C	-4.87325900	-1.71378700	0.63860500
C	-4.87180700	-1.09884000	-1.69538900
C	-6.25912600	-1.53958400	0.68197700
C	-6.25896900	-0.93026500	-1.64570900
C	-6.96374400	-1.15141100	-0.45933700
H	-4.32061200	-1.98807200	1.53679900
H	-4.31855100	-0.89454500	-2.61210500
H	-8.04155400	-0.99264400	-0.41852600
C	4.02554000	-0.54916600	-0.58351700
C	4.67076600	-0.33558000	-1.79716600
C	4.75968600	-0.84571200	0.55947100
C	6.06397900	-0.42551800	-1.86144100
C	6.14986400	-0.96465500	0.48026500
C	6.81486400	-0.74466800	-0.72728800
H	4.08419800	-0.12763800	-2.69212100
H	4.24181600	-1.02476200	1.50160900
H	7.89813600	-0.84862000	-0.79163300
C	-0.36274000	3.10778500	0.42254700
C	-0.32149400	4.04980500	-0.60739800
C	-0.28504700	3.52434800	1.75178400
C	-0.20459900	5.41536900	-0.30754600
C	-0.14955500	4.88649600	2.05688600
C	-0.11432700	5.83550700	1.02680700
H	-0.37083200	3.71150400	-1.64321100
H	-0.31203600	2.77794200	2.54632400
H	-0.00817000	6.89536400	1.26120300
C	-0.01863100	5.30024200	3.41859400
C	-0.15464500	6.38334900	-1.35916500

C	6.86051300	-1.40508300	1.62474500
C	6.70701100	-0.26377300	-3.11357600
C	-6.94242400	-0.44948600	-2.79189800
C	-6.92069800	-1.67948400	1.92812700
N	0.10692900	5.62410000	4.53017800
N	-0.10614400	7.17557500	-2.21165600
N	7.39445600	-1.83171600	2.56254200
N	7.20700700	-0.16710800	-4.15570900
N	-7.48155500	-0.00982700	-3.72083300
N	-7.40898500	-1.75297300	2.97829100
Pd	-0.11178200	-0.77680400	-1.68172100
Pd	-0.06458600	-1.24057600	0.87692200
C	1.93824500	-3.07738700	2.66121800
C	0.46437900	-2.83176300	2.51381500
H	2.06570500	-3.58172100	3.63570100
H	2.45204400	-2.10886000	2.75974700
C	2.56430700	-3.91378900	1.56625900
C	-0.15179700	-1.67401500	3.00936000
H	-0.16839300	-3.72486300	2.40820000
H	2.06499500	-4.88748800	1.45846400
H	2.50532600	-3.40244400	0.59285300
H	3.62476400	-4.11169100	1.76910600
H	-1.22425600	-1.65573100	3.21652200
H	0.45422400	-0.88799500	3.47014600
H	0.34422700	-2.75773500	0.86036200

#### INT7

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O	-0.36964800	0.82339600	1.08060100
C	-0.32679000	1.63396300	0.12271500
O	-0.29197300	1.34681100	-1.10981100
O	1.95045000	-0.61799200	-1.72364500
C	2.52540200	-0.73718000	-0.61118200
O	1.99372800	-0.93148500	0.52241300
O	-2.10022200	-1.65881800	0.52752600
C	-2.68913800	-1.43318100	-0.57047200
O	-2.17016200	-1.15710300	-1.68387400
C	-4.16999800	-1.44030500	-0.52447500
C	-4.83354800	-1.69065500	0.67204700
C	-4.88254400	-1.07518500	-1.66234400
C	-6.22392300	-1.55928000	0.72895600
C	-6.27156900	-0.94235300	-1.59524200
C	-6.95432300	-1.18753200	-0.40215700
H	-4.26410700	-1.95153100	1.56386600
H	-4.34762000	-0.85755200	-2.58646000
H	-8.03567200	-1.06108600	-0.34583300
C	4.00462600	-0.68622700	-0.62996600
C	4.66136100	-0.41299900	-1.82512800
C	4.72758900	-0.99296800	0.51775000
C	6.05662300	-0.45572200	-1.87016700
C	6.12301700	-1.04124600	0.46053500
C	6.79941300	-0.76847300	-0.73013400
H	4.08191600	-0.19182900	-2.72123900
H	4.20193700	-1.22007600	1.44492900
H	7.88741000	-0.82074800	-0.77393900
C	-0.28659300	3.09613200	0.45728000
C	-0.27909900	4.05269900	-0.55954600
C	-0.21271500	3.49724600	1.79207900
C	-0.19691100	5.41677600	-0.24240900
C	-0.12194400	4.85921400	2.11527300

C	-0.11641800	5.82200200	1.09686800
H	-0.32989100	3.72788100	-1.59950000
H	-0.21528300	2.73940800	2.57643000
H	-0.04365100	6.88152600	1.34510200
C	-0.01563700	5.26622800	3.48185700
C	-0.17913300	6.39543200	-1.28484200
C	6.84611900	-1.43455300	1.61323200
C	6.70486300	-0.23694700	-3.11011500
C	-6.96611800	-0.47071500	-2.73714800
C	-6.88055700	-1.72729100	1.97348200
N	0.08323600	5.59443300	4.59506700
N	-0.15831500	7.19093400	-2.13528500
N	7.41403900	-1.79963300	2.55645400
N	7.19743600	-0.08999800	-4.14960200
N	-7.49060500	-0.03215300	-3.67438700
N	-7.38841500	-1.82094400	3.01230700
Pd	-0.13617900	-0.70536700	-1.80869200
Pd	-0.04914700	-1.32043200	0.68147900
C	1.88644500	-2.87851600	3.11237500
C	0.42145500	-2.62869100	2.99950600
H	2.05841000	-3.30045200	4.12017000
H	2.42429100	-1.91711200	3.10493000
C	2.45102700	-3.83456900	2.07831600
C	-0.18462000	-1.43191900	3.17701800
H	-0.21136300	-3.51094900	2.83032400
H	1.92459800	-4.79993100	2.09006600
H	2.36505900	-3.42299000	1.06205400
H	3.51361000	-4.04130000	2.26382800
H	-1.27224300	-1.33661200	3.19212600
H	0.39250800	-0.52968000	3.40016000
H	0.19791700	-2.77628200	0.28347500

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