

Supporting Information

Origins of Enantioselectivity in Asymmetric Ketone Hydrogenation Catalyzed by RuH₂(binap)(cydn) Complex: Insights from a Computational Study

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Table S1. B3LYP/BSI and B3LYP/BSII^a (in Parenthesis) energies (unit: kcal/mol) relative to reactants for four possible TSs of HT step in hydrogenation of **1** and **1'** catalyzed by matched A and mismatched B.

Ketone	Catalyst	TS _{ax-out}	TS _{ax-in}	TS _{eq-out}	TS _{eq-in}
1	A	7.9 (3.9)	9.9 (5.8)	11.6 (7.9)	14.0 (9.4)
1	B	10.3 (6.3)	12.3 (8.2)	9.4 (5.7)	13.9 (9.7)
1'	A	2.1	5.5	6.1	9.8

^a See ref. [37]

1 means acetophenone.

1' means α -(dimethylamino) acetone.

Table S2. Bond lengths (Å) of six-member-ring for stationary points in HT step in hydrogenations of **1-15** catalyzed by matched A.

Species	Ru ¹ -H ²	C ⁵ -H ²	C ⁵ -O ⁶	O ⁶ -H ⁴	N ³ -H ⁴	Ru ¹ -N ³	H ² -H _α
ABS₁	1.72	4.02	1.23	2.31	1.02	2.23	2.24
ABS₂	1.72	3.98	1.23	2.29	1.02	2.23	2.24
ABS₃	1.72	4.01	1.23	2.28	1.02	2.23	2.26
ABS₄	1.72	4.02	1.23	2.31	1.02	2.22	2.22
ABS₅	1.72	4.05	1.23	2.27	1.02	2.22	2.25
ABS₆	1.72	4.02	1.23	2.30	1.02	2.22	2.21
ABS₇	1.72	4.01	1.23	2.34	1.02	2.22	2.20
ABS₈	1.73	3.72	1.23	2.31	1.02	2.22	2.17
ABS₉	1.73	3.98	1.23	2.35	1.02	2.23	2.18
ABS₁₀	1.72	3.96	1.22	2.30	1.02	2.23	2.21
ABS₁₁	1.72	4.02	1.22	2.30	1.02	2.23	2.24
ABS₁₂	1.72	4.02	1.23	2.27	1.02	2.22	2.26
ABS₁₃	1.72	3.99	1.23	2.29	1.02	2.22	2.33
ABS₁₄	<i>na</i>	<i>na</i>	<i>na</i>	<i>na</i>	<i>na</i>	<i>na</i>	<i>na</i>
ABS₁₅	<i>na</i>	<i>na</i>	<i>na</i>	<i>na</i>	<i>na</i>	<i>na</i>	<i>na</i>
INTf₁/INTu₁	1.73/1.73	3.68/3.87	1.23/1.23	2.46/3.34	1.02/1.02	2.23/2.22	2.28/2.23
INTf₂/INTu₂	1.72/1.73	3.45/3.97	1.23/1.23	2.75/2.37	1.02/1.02	2.22/2.23	3.10/2.25
INTf₃/INTu₃	1.72/1.72	3.40/3.98	1.23/1.23	2.65/2.36	1.02/1.02	2.22/2.22	3.04/2.22
INTf₄/INTu₄	1.73/1.73	3.74/3.90	1.23/1.23	2.43/3.25	1.02/1.02	2.23/2.23	2.24/2.32
INTf₅/INTu₅	1.73/1.73	3.68/3.93	1.23/1.23	2.47/3.58	1.02/1.02	2.22/2.22	2.27/2.34
INTf₆/INTu₆	1.73/1.74	3.64/3.90	1.23/1.23	2.65/3.62	1.02/1.02	2.22/2.22	2.27/2.26
INTf₇/INTu₇	1.73/1.73	3.58/3.93	1.23/1.23	2.52/3.55	1.02/1.02	2.22/2.22	2.31/2.30
INTf₈/INTu₈	1.73/ <i>na</i>	3.66/ <i>na</i>	1.23/ <i>na</i>	2.29/ <i>na</i>	1.02/ <i>na</i>	2.22/ <i>na</i>	2.24/ <i>na</i>
INTf₉/INTu₉	1.73/1.73	3.39/3.86	1.22/1.23	2.70/3.69	1.02/1.02	2.22/2.22	2.44/2.20
INTf₁₀/INTu₁₀	1.72/1.72	3.58/3.26	1.22/1.22	2.50/2.45	1.02/1.02	2.22/2.22	3.10/2.73
INTf₁₁/INTu₁₁	1.73/1.73	3.44/3.32	1.22/1.22	2.37/2.46	1.02/1.02	2.22/2.22	2.60/2.66

INTf₁₂/INTu₁₂	1.73/ <i>na</i>	3.83/ <i>na</i>	1.23/ <i>na</i>	2.26/ <i>na</i>	1.02/ <i>na</i>	2.22/ <i>na</i>	2.22/ <i>na</i>
INTf₁₃/INTu₁₃	1.72/ <i>na</i>	3.66/ <i>na</i>	1.23/ <i>na</i>	2.64/ <i>na</i>	1.02/ <i>na</i>	2.22/ <i>na</i>	2.28/ <i>na</i>
INTf₁₄/INTu₁₄	<i>na/na</i>	<i>na/na</i>	<i>na/na</i>	<i>na/na</i>	<i>na/na</i>	<i>na/na</i>	<i>na/na</i>
INTf₁₅/INTu₁₅	<i>na/na</i>	<i>na/na</i>	<i>na/na</i>	<i>na/na</i>	<i>na/na</i>	<i>na/na</i>	<i>na/na</i>
TSf₁/TSu₁	1.83/1.88	1.81/1.77	1.26/1.26	1.88/1.84	1.03/1.03	2.18/2.18	2.60/2.60
TSf₂/TSu₂	1.83/1.88	1.82/1.78	1.26/1.26	1.89/1.84	1.03/1.03	2.19/2.18	2.59/2.58
TSf₃/TSu₃	1.83/1.89	1.82/1.78	1.26/1.26	1.89/1.84	1.03/1.03	2.19/2.18	2.52/2.57
TSf₄/TSu₄	1.84/1.89	1.80/1.77	1.26/1.26	1.87/1.84	1.03/1.03	2.19/2.19	2.59/2.60
TSf₅/TSu₅	1.84/1.89	1.77/1.74	1.26/1.26	1.86/1.83	1.03/1.03	2.19/2.18	2.59/2.59
TSf₆/TSu₆	1.84/1.88	1.83/1.80	1.25/1.26	1.89/1.86	1.03/1.03	2.19/2.18	2.62/2.60
TSf₇/TSu₇	1.84/1.89	1.81/1.78	1.26/1.26	1.88/1.85	1.03/1.03	2.19/2.19	2.60/2.61
TSf₈/TSu₈	1.84/1.86	1.77/1.72	1.26/1.26	1.84/1.84	1.03/1.03	2.19/2.19	2.51/2.49
TSf₉/TSu₉	1.82/1.87	1.87/1.83	1.25/1.25	1.93/1.88	1.03/1.03	2.25/2.19	2.62/2.59
TSf₁₀/TSu₁₀	1.85/1.88	1.77/1.75	1.26/1.26	1.82/1.79	1.04/1.04	2.19/2.19	2.57/2.53
TSf₁₁/TSu₁₁	1.86/1.77	1.77/3.32	1.26/1.22	1.82/2.46	1.04/1.02	2.19/2.22	2.56/2.55
TSf₁₂/TSu₁₂	1.82/1.84	1.76/1.74	1.26/1.26	1.88/1.87	1.03/1.03	2.19/2.19	2.55/2.53
TSf₁₃/TSu₁₃	1.82/1.86	1.74/1.70	1.26/1.27	1.87/1.83	1.03/1.04	2.19/2.19	2.41/2.49
TSf₁₄/TSu₁₄	1.94/1.98	1.83/1.81	1.26/1.26	1.83/1.83	1.04/1.04	2.19/2.18	<i>na/na</i>
TSf₁₅/TSu₁₅	1.89/1.86	1.73/1.75	1.26/1.26	1.87/1.86	1.03/1.03	2.19/2.19	<i>na/na</i>
Pf₁/Pu₁	3.50/4.16	1.10/1.10	1.41/1.42	1.01/1.00	1.82/1.89	2.07/2.06	<i>na/na</i>
Pf₂/Pu₂	3.34/3.33	1.10/1.11	1.41/1.41	1.01/1.01	1.80/1.77	2.07/2.07	<i>na/na</i>
Pf₃/Pu₃	3.30/4.09	1.11/1.10	1.41/1.41	1.01/1.00	1.78/1.89	2.07/2.06	<i>na/na</i>
Pf₄/Pu₄	3.55/4.12	1.10/1.10	1.41/1.42	1.01/1.00	1.83/1.92	2.07/2.06	<i>na/na</i>
Pf₅/Pu₅	3.60/4.16	1.10/1.10	1.41/1.42	1.00/1.00	1.83/1.91	2.07/2.06	<i>na/na</i>
Pf₆/Pu₆	3.42/4.29	1.10/1.10	1.41/1.42	1.01/1.02	1.80/1.78	2.07/2.09	<i>na/na</i>
Pf₇/Pu₇	3.27/3.81	1.11/1.10	1.41/1.41	1.01/1.00	1.79/1.86	2.07/2.06	<i>na/na</i>
Pf₈/Pu₈	3.52/4.03	1.10/1.10	1.42/1.42	1.01/1.01	1.82/1.84	2.07/2.08	<i>na/na</i>
Pf₉/Pu₉	3.44/3.57	1.10/1.10	1.41/1.41	1.01/1.01	1.80/1.80	2.07/2.06	<i>na/na</i>
Pf₁₀/Pu₁₀	3.66/3.66	1.10/1.10	1.42/1.42	1.00/1.00	1.84/1.87	2.07/2.06	<i>na/na</i>
Pf₁₁/Pu₁₁	3.71/3.68	1.10/1.10	1.42/1.42	1.00/1.00	1.85/1.86	2.06/2.06	<i>na/na</i>

Pf₁₂/Pu₁₂	3.68/3.89	1.11/1.11	1.42/1.42	1.00/1.00	1.85/1.90	2.06/2.06	<i>na/na</i>
Pf₁₃/Pu₁₃	3.29/3.29	1.11/1.11	1.41/1.41	1.01/1.01	1.79/1.80	2.07/2.07	<i>na/na</i>
Pf₁₄/Pu₁₄	3.71/3.94	1.10/1.10	1.42/1.42	1.01/1.00	1.87/1.90	2.07/2.07	<i>na/na</i>
Pf₁₅/Pu₁₅	3.22/3.52	1.11/1.11	1.40/1.41	1.02/1.01	1.74/1.79	2.08/2.07	<i>na/na</i>

Table S3. Relative free energy^a, potential energies^b and solvation energy (benzene)^c (unit: kcal/mol) for **1-15d** in HT step of hydrogenation.

Ketone	A+	ABS	INTf	INTu	TSf	TSu	Pf	Pu
1	0.0	15.5	15.6	16.2	28.6	30.0	16.4	17.5
	0.0	-0.9	0.4	0.7	7.9	9.9	-2.9	-2.2
	<i>0.0</i>	<i>1.3</i>	<i>2.3</i>	<i>1.9</i>	<i>11.7</i>	<i>13.8</i>	<i>1.6</i>	<i>2.2</i>
2	0.0	14.3	18.3	16.7	27.9	31.1	19.5	20.0
	0.0	1.1	3.0	1.1	9.0	11.1	-1.0	0.2
	<i>0.0</i>	<i>3.2</i>	<i>4.1</i>	<i>3.1</i>	<i>12.8</i>	<i>15.0</i>	<i>3.3</i>	<i>4.3</i>
3	0.0	15.3	16.7	16.6	27.5	30.6	20.0	19.9
	0.0	1.0	2.8	1.0	8.6	10.7	-1.6	-0.9
	<i>0.0</i>	<i>2.9</i>	<i>4.0</i>	<i>3.0</i>	<i>12.4</i>	<i>14.6</i>	<i>2.8</i>	<i>3.6</i>
4	0.0	16.2	16.2	17.3	28.5	30.3	18.3	18.2
	0.0	-0.7	0.8	0.3	8.7	10.8	1.7	-1.2
	<i>0.0</i>	<i>1.5</i>	<i>2.9</i>	<i>2.1</i>	<i>12.6</i>	<i>14.8</i>	<i>2.8</i>	<i>3.4</i>
5	0.0	15.9	19.4	13.7	30.3	32.2	20.3	19.9
	0.0	0.0	1.1	0.4	9.9	12.0	0.0	0.4
	<i>0.0</i>	<i>2.2</i>	<i>3.0</i>	<i>2.3</i>	<i>13.8</i>	<i>16.0</i>	<i>4.5</i>	<i>5.0</i>
6	0.0	16.6	18.3	16.7	27.9	30.8	18.5	18.6
	0.0	1.5	2.6	2.0	9.2	11.1	-1.3	-1.5
	<i>0.0</i>	<i>3.5</i>	<i>4.3</i>	<i>3.8</i>	<i>13.0</i>	<i>14.9</i>	<i>3.1</i>	<i>2.8</i>
7	0.0	15.6	17.6	18.8	29.5	30.3	22.8	20.7
	0.0	1.1	2.4	1.8	9.3	11.6	0.9	-0.3
	<i>0.0</i>	<i>3.2</i>	<i>4.2</i>	<i>3.6</i>	<i>13.1</i>	<i>15.5</i>	<i>3.5</i>	<i>4.3</i>
8	0.0	14.2	14.1	na	27.1	28.5	17.2	15.8
	0.0	-1.7	-2.0	na	6.0	7.4	-3.6	-3.7
	<i>0.0</i>	<i>0.7</i>	<i>0.3</i>	<i>na</i>	<i>10.3</i>	<i>11.4</i>	<i>1.2</i>	<i>1.2</i>
9	0.0	15.2	16.2	16.9	24.8	27.6	14.1	14.8
	0.0	-0.3	0.9	0.3	6.0	7.7	-5.3	-4.3
	<i>0.0</i>	<i>1.7</i>	<i>2.4</i>	<i>0.9</i>	<i>9.7</i>	<i>11.3</i>	<i>-1.2</i>	<i>-0.1</i>
10	0.0	15.7	16.8	15.2	31.2	30.4	17.3	19.8
	0.0	-1.3	1.5	0.8	10.5	10.3	-3.3	-3.0
	<i>0.0</i>	<i>0.8</i>	<i>2.8</i>	<i>2.8</i>	<i>13.8</i>	<i>14.0</i>	<i>1.2</i>	<i>1.3</i>
11	0.0	11.6	16.1	15.9	28.5	29.2	17.0	17.3
	0.0	-2.7	-0.9	-0.9	8.9	8.6	-5.2	-4.9
	<i>0.0</i>	<i>-0.7</i>	<i>0.7</i>	<i>0.9</i>	<i>12.1</i>	<i>12.1</i>	<i>-0.8</i>	<i>-0.6</i>
12	0.0	13.3	13.7	na	28.6	27.1	17.6	18.1
	0.0	-2.7	-0.1	na	8.0	7.9	-2.0	-1.5
	<i>0.0</i>	<i>-0.5</i>	<i>1.8</i>	<i>na</i>	<i>11.4</i>	<i>11.4</i>	<i>2.3</i>	<i>2.9</i>
13	0.0	14.7	14.2	na	27.8	28.2	23.1	22.7

	0.0	-0.1	1.3	na	7.6	8.9	1.3	2.3
	<i>0.0</i>	<i>2.0</i>	<i>2.9</i>	<i>na</i>	<i>11.2</i>	<i>12.4</i>	<i>5.7</i>	<i>6.5</i>
14	0.0	na	na	na	34.6	36.7	16.0	17.1
	0.0	na	na	na	14.7	16.9	-4.6	-3.5
	<i>0.0</i>	<i>na</i>	<i>na</i>	<i>na</i>	<i>18.7</i>	<i>21.2</i>	<i>-0.1</i>	<i>1.1</i>
15	0.0	na	na	na	29.5	30.9	24.7	24.4
	0.0	na	na	na	11.2	11.8	4.7	4.4
	<i>0.0</i>	<i>na</i>	<i>na</i>	<i>na</i>	<i>16.3</i>	<i>15.3</i>	<i>8.9</i>	<i>9.0</i>

^a The free energies with solvent effect (benzene) at B3LYP/BSI level are written in normal font.

^b The potential energies in the gas phase at B3LYP/BSI level are written in bold.

^c The potential energies with solvent effect (benzene) for TSs at B3LYP/BSI level are written in italic.

Table S4. Calculated imaginary frequencies of HT-TSs in hydrogenations of selected fifteen ketones at B3LYP/BSI level (LANL2DZ basis set for Ru, 6-31G* for other atoms).

	TSf	TSu
1	-402.5625 <i>i</i>	-493.4609 <i>i</i>
2	-347.0193 <i>i</i>	-561.3540 <i>i</i>
3	-377.4592 <i>i</i>	-458.4013 <i>i</i>
4	-403.5030 <i>i</i>	-487.5842 <i>i</i>
5	-425.3780 <i>i</i>	-517.5309 <i>i</i>
6	-476.0543 <i>i</i>	-350.3519 <i>i</i>
7	-385.4378 <i>i</i>	-526.3057 <i>i</i>
8	-400.3399 <i>i</i>	-474.1496 <i>i</i>
9	-302.3883 <i>i</i>	-404.0510 <i>i</i>
10	-430.5844 <i>i</i>	-538.2646 <i>i</i>
11	-464.6191 <i>i</i>	-498.2676 <i>i</i>
12	-370.6081 <i>i</i>	-411.9189 <i>i</i>
13	-334.4218 <i>i</i>	-455.9493 <i>i</i>
14	-631.4508 <i>i</i>	-648.0425 <i>i</i>
15	-542.9993 <i>i</i>	-418.5006 <i>i</i>

Table S5. Energies (E, E+ZPEC, H and G, unit: a.u.) for all reported structures.

Path 1				
Complex	E	E+ZPEC	H	G
K1	-384.754901	-384.762700	-384.753956	-384.795455
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
ABS1	-3204.214779	-3204.270594	-3204.213835	-3204.364395
INTf1	-3204.213494	-3204.269491	-3204.21255	-3204.364259
INTu1	-3204.214279	-3204.269276	-3204.213334	-3204.360148
TSf1	-3204.194121	-3204.250165	-3204.193177	-3204.341297
TSu1	-3204.198792	-3204.254063	-3204.197848	-3204.343456
Pf1	-3204.209366	-3204.266552	-3204.208422	-3204.362976
Pu1	-3204.209612	-3204.266086	-3204.208668	-3204.361178
Path 2				
Complex	E	E+ZPEC	H	G
K2	-463.320374	-463.330947	-463.319430	-463.368380
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
ABS2	-3282.778493	-3282.838032	-3282.777549	-3282.939887
INTf2	-3282.777656	-3282.836245	-3282.776711	-3282.933432
INTu2	-3282.778045	-3282.837321	-3282.777101	-3282.936066
TSf2	-3282.763718	-3282.822683	-3282.762774	-3282.918205
TSu2	-3282.761448	-3282.819683	-3282.760504	-3282.913090
Pf2	-3282.775495	-3282.834435	-3282.774551	-3282.931603
Pu2	-3282.775223	-3282.833533	-3282.774279	-3282.930728
Path 3				
Complex	E	E+ZPEC	H	G
K3	-424.036579	-424.045781	-424.035635	-424.080881
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
ABS3	-3243.493423	-3243.552129	-3243.492479	-3243.652107
INTf3	-3243.493324	-3243.551502	-3243.49238	-3243.649964
INTu3	-3243.494205	-3243.552037	-3243.493261	-3243.650112
TSf3	-3243.480497	-3243.538108	-3243.479553	-3243.632699
TSu3	-3243.477073	-3243.534627	-3243.476129	-3243.627774
Pf3	-3243.492478	-3243.549944	-3243.491533	-3243.644726
Pu3	-3243.491034	-3243.548705	-3243.49009	-3243.644811
Path 4				
Complex	E	E+ZPEC	H	G
K4	-3243.654194	-3243.654194	-3243.654194	-3243.654194
A	-3243.654194	-3243.654194	-3243.654194	-3243.654194
ABS4	-3243.654194	-3243.654194	-3243.654194	-3243.654194
INTf4	-3243.654194	-3243.654194	-3243.654194	-3243.654194

INTu4	-3243.654194	-3243.654194	-3243.654194	-3243.654194
TSf4	-3243.654194	-3243.654194	-3243.654194	-3243.654194
TSu4	-3243.654194	-3243.654194	-3243.654194	-3243.654194
Pf4	-3243.654194	-3243.654194	-3243.654194	-3243.654194
Pu4	-3243.654194	-3243.654194	-3243.654194	-3243.654194

Path 5

Complex	E	E+ZPEC	H	G
K5	-499.242760	-499.253153	-499.241816	-499.289418
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
ABS5	-3318.703338	-3318.762587	-3318.702394	-3318.861956
INTf5	-3318.703051	-3318.761374	-3318.702107	-3318.856403
INTu5	-3318.702304	-3318.762522	-3318.701359	-3318.865506
TSf5	-3318.684806	-3318.743416	-3318.683862	-3318.839104
TSu5	-3318.681976	-3318.740808	-3318.681032	-3318.836060
Pf5	-3318.696824	-3318.755817	-3318.695880	-3318.854995
Pu5	-3318.696191	-3318.755319	-3318.695247	-3318.855570

Path 6

Complex	E	E+ZPEC	H	G
K6	-844.356891	-844.365923	-844.355946	-844.400894
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
ABS6	-3663.814579	-3663.872363	-3663.813635	-3663.970970
INTf6	-3663.813810	-3663.871667	-3663.812866	-3663.968272
INTu6	-3663.814577	-3663.872485	-3663.813632	-3663.970792
TSf6	-3663.799815	-3663.857153	-3663.798871	-3663.952961
TSu6	-3663.797282	-3663.854738	-3663.796338	-3663.948318
Pf6	-3663.812779	-3663.870400	-3663.811835	-3663.967913
Pu6	-3663.813136	-3663.870689	-3663.812192	-3663.967766

Path 7

Complex	E	E+ZPEC	H	G
K7	-538.347426	-538.357790	-538.346482	-538.394132
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
ABS7	-3357.805456	-3357.864714	-3357.804512	-3357.966378
INTf7	-3357.804361	-3357.863668	-3357.803417	-3357.963132
INTu7	-3357.806268	-3357.864659	-3357.805324	-3357.961152
TSf7	-3357.790067	-3357.848786	-3357.789122	-3357.944173
TSu7	-3357.787306	-3357.846340	-3357.786362	-3357.942934
Pf7	-3357.804487	-3357.861664	-3357.803543	-3357.954871
Pu7	-3357.801368	-3357.860366	-3357.800424	-3357.958257

Path 8

Complex	E	E+ZPEC	H	G
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K8	-382.559136	-382.56637	-382.558192	-382.598481
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
ABS8	-3202.022136	-3202.078060	-3202.021192	-3202.172086
INTf8	-3202.022340	-3202.078133	-3202.021396	-3202.172234
TSf8	-3202.008132	-3202.062714	-3202.007188	-3202.151514
TSu8	-3202.006510	-3202.061001	-3202.005566	-3202.149277
Pf8	-3202.017928	-3202.073529	-3202.016983	-3202.167313
Pu8	-3202.017266	-3202.073708	-3202.016321	-3202.169426

Path 9

Complex	E	E+ZPEC	H	G
K9	-400.798899	-400.806605	-400.797954	-400.839376
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
ABS9	-3220.260245	-3220.316706	-3220.259300	-3220.412365
INTf9	-3220.259231	-3220.315849	-3220.258287	-3220.410719
INTu9	-3220.261221	-3220.316883	-3220.260277	-3220.409663
TSf9	-3220.248275	-3220.304379	-3220.247331	-3220.396968
TSu9	-3220.245078	-3220.301036	-3220.244134	-3220.392643
Pf9	-3220.260776	-3220.317801	-3220.259831	-3220.414092
Pu9	-3220.260528	-3220.316825	-3220.259583	-3220.412966

Path 10

Complex	E	E+ZPEC	H	G
K10	-388.304926	-388.314245	-388.303982	-388.349047
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
ABS10	-3207.766469	-3207.824299	-3207.765525	-3207.920066
INTf10	-3207.763290	-3207.821255	-3207.762346	-3207.918270
INTu10	-3207.763952	-3207.822296	-3207.763008	-3207.920762
TSf10	-3207.746403	-3207.803697	-3207.745459	-3207.895349
TSu10	-3207.746223	-3207.803680	-3207.745279	-3207.896647
Pf10	-3207.763232	-3207.820840	-3207.762288	-3207.917491
Pu10	-3207.763835	-3207.820562	-3207.762891	-3207.913479

Path 11

Complex	E	E+ZPEC	H	G
K11	-271.635877	-271.643711	-271.634933	-271.675775
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
ABS11	-3091.098866	-3091.156312	-3091.097922	-3091.253773
INTf11	-3091.098934	-3091.154701	-3091.097990	-3091.246613
INTu11	-3091.097604	-3091.154035	-3091.096660	-3091.246934
TSf11	-3091.080088	-3091.135893	-3091.079144	-3091.226871
TSu11	-3091.079851	-3091.135521	-3091.078907	-3091.225742
Pf11	-3091.096924	-3091.152766	-3091.095979	-3091.245262
Pu11	-3091.096634	-3091.152480	-3091.095690	-3091.244658

Path 12

Complex	E	E+ZPEC	H	G
K12	-270.42039	-270.426926	-270.419446	-270.457307
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
ABS12	-3089.883987	-3089.939147	-3089.883043	-3090.032277
INTf12	-3089.880194	-3089.936402	-3089.879250	-3090.031596
TSf12	-3089.866331	-3089.920135	-3089.865386	-3090.007846
TSu12	-3089.865530	-3089.920079	-3089.864585	-3090.010267
Pf12	-3089.875892	-3089.931496	-3089.874948	-3090.025316
Pu12	-3089.875969	-3089.930882	-3089.875025	-3090.024601

Path 13

Complex	E	E+ZPEC	H	G
K13	-388.287153	-388.298308	-388.286208	-388.335401
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
ABS13	-3207.745827	-3207.806724	-3207.744883	-3207.908106
INTf13	-3207.744475	-3207.805499	-3207.743531	-3207.908894
TSf13	-3207.732471	-3207.791824	-3207.731527	-3207.887299
TSu13	-3207.730866	-3207.790358	-3207.729921	-3207.886572
Pf13	-3207.739484	-3207.798172	-3207.738540	-3207.894724
Pu13	-3207.737358	-3207.796975	-3207.736413	-3207.895355

Path 14

Complex	E	E+ZPEC	H	G
K14	-502.596893	-502.607867	-502.595949	-502.643761
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
TSf14	-3322.030104	-3322.089976	-3322.029160	-3322.184384
TSu14	-3322.026371	-3322.086347	-3322.025427	-3322.181106
Pf14	-3322.057272	-3322.117475	-3322.056328	-3322.214094
Pu14	-3322.055170	-3322.115348	-3322.054226	-3322.212276

Path 15

Complex	E	E+ZPEC	H	G
K15	-653.802948	-653.816047	-653.802003	-653.858619
A	-2819.463755	-2819.511466	-2819.462811	-2819.593646
TSf15	-3473.242267	-3473.304116	-3473.241322	-3473.406282
TSu15	-3473.243162	-3473.304657	-3473.242217	-3473.404080
Pf15	-3473.251661	-3473.312529	-3473.250717	-3473.413985
Pu15	-3473.251404	-3473.312365	-3473.250460	-3473.414458

Figure S1. The linear relationship between experimental ee values and predicted ones of 13 ketone substrates

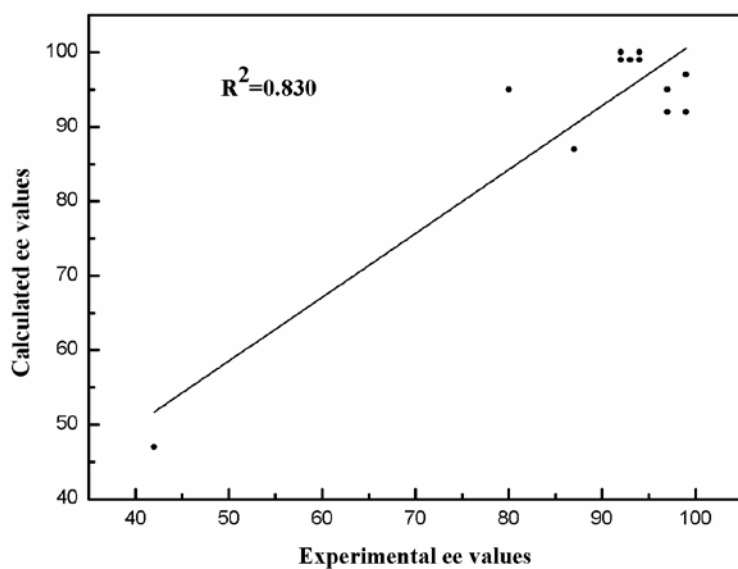
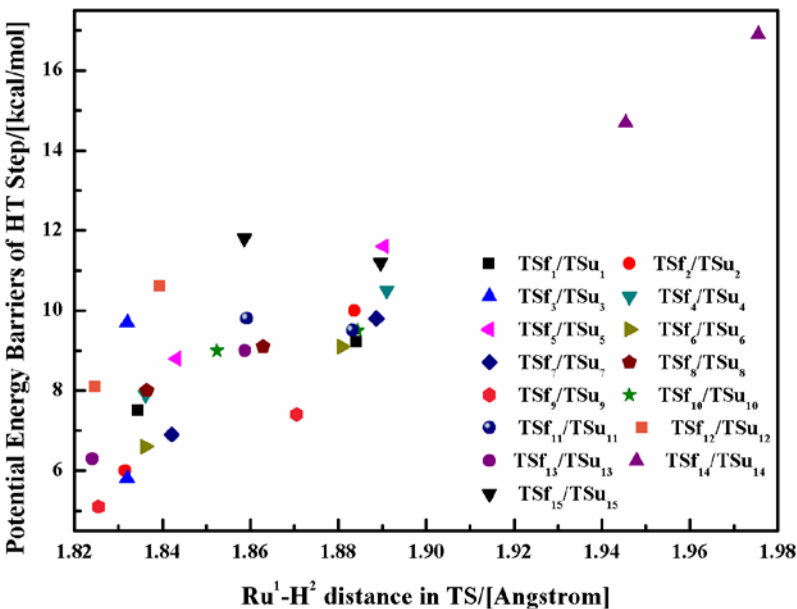
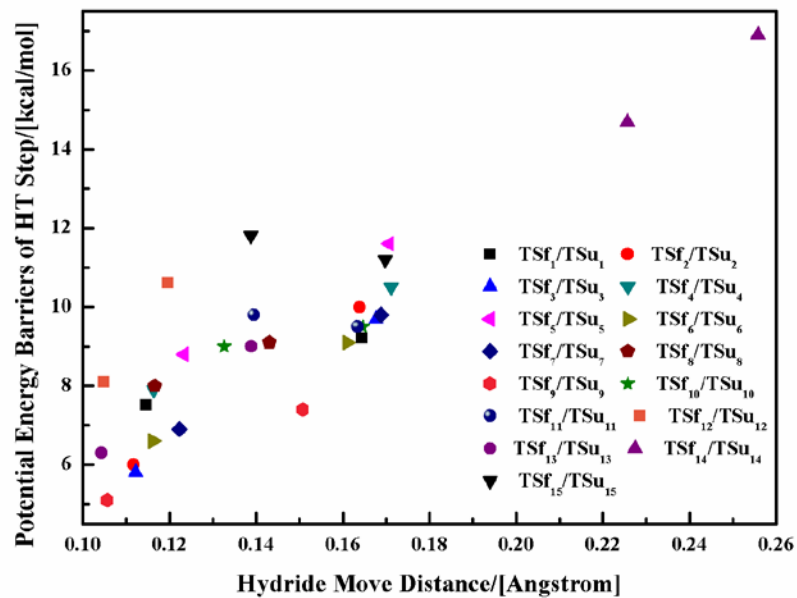


Figure S2. A) Relationship between Ru¹-H² distance of TS and energy barrier of HT step. B) Relationship between hydride move distance (HMD) and HT energy barrier.

(A)



(B)



The Cartesian coordinates of stationary points optimized at B3LYP/BSI level for all systems.

A catalyst

Coordinates (Angstroms)			
	X	Y	Z
Ru	1.714736	0.002247	-0.001835
H	1.844080	-0.073207	1.711449
H	1.843110	0.077869	-1.715174
N	3.446837	1.401400	0.036344
H	3.282999	2.181341	-0.596639
H	3.521108	1.794362	0.974194
N	3.448326	-1.395000	-0.039562
H	3.285167	-2.175222	0.593244
H	3.523211	-1.787668	-0.977501
P	0.148725	1.647275	0.172114
P	0.152120	-1.646092	-0.173234
C	4.692232	-0.686929	0.335108
H	4.633636	-0.531611	1.421099
C	4.691606	0.694632	-0.337965
H	4.633535	0.539250	-1.423975
C	-3.482196	-0.378502	-2.894307
C	-2.544626	-1.352927	-3.311292
C	-1.524807	-1.744334	-2.480910
C	-1.371392	-1.207443	-1.171901
C	-2.298813	-0.268771	-0.705746
C	-3.360903	0.173830	-1.578072
H	-2.642101	-1.790584	-4.302449
H	-0.823909	-2.491026	-2.832246
C	-3.480929	0.370564	2.894674
C	-2.544844	1.346519	3.311436
C	-1.526460	1.740252	2.480407
C	-1.373169	1.204323	1.171023
C	-2.298971	0.263936	0.705146
C	-3.359589	-0.180989	1.578098
H	-2.642321	1.783474	4.302902
H	-0.826456	2.487978	2.831499
C	2.193703	5.232474	2.426446
C	1.542556	5.467409	1.216563
C	0.888392	4.425968	0.549033
C	0.879518	3.123713	1.073028

C	1.560948	2.897995	2.286604
C	2.198541	3.940439	2.960509
H	2.696094	6.043989	2.946794
H	1.536507	6.465300	0.784818
H	0.384614	4.638849	-0.386726
H	1.598486	1.885355	2.679682
H	2.704029	3.741352	3.902670
C	-1.641223	3.810136	-3.564918
C	-2.195064	4.041743	-2.302866
C	-1.684611	3.382242	-1.184717
C	-0.608703	2.487177	-1.309162
C	-0.065208	2.257774	-2.578979
C	-0.579286	2.915186	-3.700044
H	-2.042923	4.319426	-4.437436
H	-3.029845	4.729070	-2.191125
H	-2.123545	3.567044	-0.207617
H	0.749641	1.542832	-2.668686
H	-0.151672	2.721703	-4.681017
C	-1.630333	-3.811455	3.565862
C	-2.182600	-4.047021	2.303849
C	-1.674522	-3.386707	1.185108
C	-0.602635	-2.486767	1.308940
C	-0.060533	-2.253620	2.578672
C	-0.572262	-2.911840	3.700336
H	-2.030211	-4.321405	4.438831
H	-3.014299	-4.738149	2.192588
H	-2.112009	-3.574839	0.207999
H	0.751106	-1.534980	2.667862
H	-0.145887	-2.715329	4.681247
C	2.209850	-5.227824	-2.420861
C	1.569310	-5.460613	-1.204911
C	0.911229	-4.420479	-0.539197
C	0.887291	-3.121798	-1.071461
C	1.558796	-2.897805	-2.290891
C	2.200360	-3.939089	-2.962798
H	2.715395	-6.038343	-2.939698
H	1.574720	-6.455785	-0.766925
H	0.415870	-4.631619	0.401479
H	2.697956	-3.741573	-3.909475
C	-5.324421	-1.561538	2.037422
C	-4.315212	-1.164234	1.188702
H	-6.036330	-2.314739	1.709911
H	-4.242299	-1.610295	0.204409
C	-5.442684	-1.001586	3.331378

C	-4.534214	-0.057009	3.747642
H	-6.245521	-1.321097	3.990577
H	-4.605243	0.380655	4.740889
C	-5.328644	1.550521	-2.036510
C	-4.318059	1.155467	-1.188374
H	-6.041699	2.302546	-1.708791
H	-4.245221	1.602129	-0.204347
C	-5.446854	0.989764	-3.330122
C	-4.536939	0.046697	-3.746658
H	-6.250792	1.307476	-3.988848
H	-4.607909	-0.391546	-4.739653
H	1.586281	-1.887225	-2.689952
C	5.968049	1.482536	0.001089
H	5.956380	2.445067	-0.526635
H	5.964545	1.713342	1.077564
C	5.969596	-1.473508	-0.003543
H	5.958767	-2.436055	0.524175
H	5.966666	-1.704314	-1.080019
C	7.240701	-0.681799	0.342143
H	7.299598	-0.544837	1.431688
H	8.129462	-1.254972	0.051353
C	7.240090	0.692146	-0.344191
H	7.299471	0.555238	-1.433717
H	8.128162	1.266249	-0.053128

B catalyst

Coordinates (Angstroms)			
	X	Y	Z
Ru	1.732865	0.000143	-0.000130
H	1.862348	-0.023688	1.714769
H	1.862294	0.023952	-1.715042
N	3.463040	1.396444	-0.019816
H	3.527769	1.769984	-0.965395
H	3.305929	2.182624	0.609745
N	3.463014	-1.396195	0.019632
H	3.527725	-1.769791	0.965190
H	3.305890	-2.182330	-0.609976
P	0.159336	1.648589	0.137236
P	0.159527	-1.648526	-0.137325
C	4.710343	-0.687829	-0.342097

H	4.656893	-0.524383	-1.427378
C	4.710333	0.688056	0.341986
H	4.656809	0.524606	1.427262
C	-3.461304	-0.416635	-2.895362
C	-2.512410	-1.386347	-3.297802
C	-1.497398	-1.765214	-2.455932
C	-1.358779	-1.218099	-1.149429
C	-2.292969	-0.277734	-0.700718
C	-3.353123	0.148474	-1.583528
H	-2.597725	-1.830873	-4.287029
H	-0.787920	-2.508808	-2.796647
C	-3.461186	0.416305	2.895479
C	-2.512325	1.386073	3.297876
C	-1.497390	1.765015	2.455945
C	-1.358836	1.217924	1.149419
C	-2.292960	0.277474	0.700777
C	-3.353033	-0.148799	1.583642
H	-2.597607	1.830588	4.287112
H	-0.787922	2.508634	2.796627
C	2.114144	5.329675	2.323775
C	1.417535	5.533133	1.133307
C	0.797350	4.461749	0.482087
C	0.863175	3.160550	1.005366
C	1.588595	2.967652	2.199202
C	2.197497	4.039540	2.854682
H	2.592097	6.164340	2.830371
H	1.351876	6.529579	0.703214
H	0.262328	4.649495	-0.441381
H	1.682373	1.957670	2.590382
H	2.740912	3.864122	3.780267
C	-1.627357	3.705681	-3.660557
C	-2.203018	3.948637	-2.410609
C	-1.695990	3.318506	-1.274012
C	-0.601291	2.442760	-1.367174
C	-0.036868	2.200815	-2.625567
C	-0.547540	2.828141	-3.765133
H	-2.026213	4.191961	-4.547398
H	-3.052664	4.620991	-2.322438
H	-2.153051	3.511306	-0.306848
H	0.790039	1.497350	-2.691979
H	-0.103249	2.624749	-4.736662
C	-1.626846	-3.705564	3.660615
C	-2.202529	-3.948610	2.410690
C	-1.695588	-3.318475	1.274058

C	-0.600928	-2.442671	1.367171
C	-0.036447	-2.200677	2.625520
C	-0.547071	-2.827966	3.765127
H	-2.025648	-4.191829	4.547487
H	-3.052128	-4.621030	2.322570
H	-2.152689	-3.511292	0.306915
H	0.790495	-1.497244	2.691873
H	-0.102767	-2.624505	4.736635
C	2.114497	-5.329599	-2.323716
C	1.418105	-5.533014	-1.133113
C	0.797882	-4.461638	-0.481915
C	0.863446	-3.160496	-1.005355
C	1.588680	-2.967623	-2.199311
C	2.197615	-4.039508	-2.854772
H	2.592467	-6.164262	-2.830297
H	1.352646	-6.529420	-0.702896
H	0.263027	-4.649343	0.441662
H	2.740875	-3.864116	-3.780451
C	-5.329366	-1.504781	2.066877
C	-4.320630	-1.126092	1.209100
H	-6.051084	-2.253266	1.750105
H	-4.257869	-1.581996	0.228609
C	-5.434169	-0.931920	3.356309
C	-4.513554	0.007025	3.758518
H	-6.236309	-1.237046	4.023148
H	-4.574247	0.454380	4.748143
C	-5.329543	1.504364	-2.066699
C	-4.320752	1.125731	-1.208962
H	-6.051277	2.252825	-1.749908
H	-4.257967	1.581662	-0.228486
C	-5.434380	0.931479	-3.356118
C	-4.513733	-0.007420	-3.758358
H	-6.236563	1.236559	-4.022927
H	-4.574447	-0.454785	-4.747977
H	1.682314	-1.957664	-2.590588
C	5.985575	1.478468	0.005134
H	5.980453	1.714492	-1.070366
H	5.974367	2.438152	0.537838
C	5.985549	-1.478265	-0.005165
H	5.980357	-1.714288	1.070336
H	5.974358	-2.437949	-0.537869
C	7.257975	-0.685911	-0.345189
H	7.318851	0.545861	1.434276
H	8.145906	-1.260618	-0.054880

C	7.257966	0.686088	0.345239
H	7.318933	-0.545687	-1.434222
H	8.145925	1.260778	0.054989

TS_{1Aax-out}

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.146063	0.499344	0.338412
H	-1.797861	-0.072982	-1.278034
H	-0.846144	1.028338	1.879845
N	-2.591157	2.136326	0.132033
H	-2.164981	3.061460	0.149486
H	-3.029062	2.013374	-0.796189
N	-3.015787	-0.372480	1.193186
H	-3.272202	-1.234157	0.711644
H	-2.812425	-0.622691	2.160160
P	0.673993	1.726288	-0.384642
P	0.176156	-1.319177	0.853385
C	-4.154400	0.582606	1.131888
H	-4.607584	0.448196	0.145292
C	-3.623350	2.019276	1.185583
H	-3.115147	2.176505	2.145392
C	4.441424	-0.280212	2.602173
C	3.428039	-0.852029	3.406609
C	2.206624	-1.174586	2.870972
C	1.902888	-0.954759	1.498148
C	2.889700	-0.424235	0.659173
C	4.176599	-0.069244	1.210705
H	3.630018	-1.038812	4.459058
H	1.462747	-1.623820	3.515713
C	3.412705	-0.955261	-3.113308
C	2.601803	0.079080	-3.640252
C	1.863621	0.882742	-2.809034
C	1.897646	0.733049	-1.392989
C	2.707836	-0.258474	-0.828392
C	3.461068	-1.136879	-1.692794
H	2.569271	0.228664	-4.717246
H	1.245237	1.660201	-3.241478
C	-0.566159	5.218002	-3.275690
C	0.524174	5.400123	-2.423020

C	0.922673	4.381767	-1.553949
C	0.239663	3.153677	-1.521521
C	-0.863049	2.991483	-2.377061
C	-1.261336	4.008578	-3.247013
H	-0.874735	6.014804	-3.947873
H	1.068960	6.341108	-2.427682
H	1.765983	4.557836	-0.897129
H	-1.434482	2.071996	-2.354375
H	-2.124330	3.845768	-3.886994
C	3.295215	4.151508	2.639155
C	3.819550	3.797517	1.394637
C	3.056901	3.041024	0.503800
C	1.759201	2.621206	0.839044
C	1.247672	2.978871	2.093836
C	2.007992	3.738648	2.985718
H	3.888967	4.738723	3.335138
H	4.826253	4.100108	1.118993
H	3.478560	2.773223	-0.460432
H	0.255776	2.634115	2.369126
H	1.593693	4.002634	3.955837
C	1.183243	-4.746223	-2.163459
C	1.620082	-4.843317	-0.839039
C	1.335383	-3.823023	0.068115
C	0.590440	-2.699040	-0.328722
C	0.172993	-2.606013	-1.660063
C	0.467364	-3.621935	-2.574067
H	1.412155	-5.538178	-2.871829
H	2.190851	-5.710253	-0.515572
H	1.690693	-3.904181	1.092280
H	-0.367895	-1.716974	-1.968358
H	0.142591	-3.529557	-3.607457
C	-2.127941	-3.514114	4.310501
C	-1.859748	-4.191339	3.122357
C	-1.125188	-3.574707	2.103575
C	-0.645211	-2.263465	2.246853
C	-0.950742	-1.582383	3.443738
C	-1.669583	-2.202719	4.466460
H	-2.693213	-3.996486	5.103526
H	-2.219011	-5.207618	2.980734
H	-0.929990	-4.128005	1.192134
H	-1.876758	-1.657149	5.383898
C	4.986150	-3.014941	-2.042141
C	4.265622	-2.202700	-1.194762
H	5.587439	-3.821268	-1.630363

H	4.303292	-2.381720	-0.127268
C	4.948348	-2.813927	-3.441848
C	4.171876	-1.804965	-3.962058
H	5.525807	-3.458541	-4.099223
H	4.122275	-1.641111	-5.036187
C	6.439191	0.830117	0.977772
C	5.221882	0.499259	0.425032
H	7.214313	1.261912	0.349984
H	5.053868	0.676590	-0.630216
C	6.690987	0.613847	2.353324
C	5.707246	0.070140	3.145184
H	7.656192	0.877538	2.777403
H	5.880583	-0.101986	4.205034
H	-0.636065	-0.549184	3.557739
C	-4.778189	3.026151	1.048550
H	-4.385887	4.050056	1.109821
H	-5.228336	2.917497	0.051429
C	-5.221094	0.331986	2.206226
H	-5.606265	-0.691251	2.110401
H	-4.754846	0.407081	3.200985
C	-6.369526	1.350118	2.099524
H	-6.911753	1.181204	1.158225
H	-7.091251	1.187741	2.909672
C	-5.846133	2.794381	2.130527
H	-5.411978	3.002791	3.119509
H	-6.674355	3.501427	1.998702
C	-3.126588	0.047801	-2.495041
O	-3.563705	1.223637	-2.421379
C	-2.224332	-0.327621	-3.671995
H	-1.777581	-1.318471	-3.570858
H	-2.853186	-0.331507	-4.574450
H	-1.435122	0.413366	-3.808830
C	-5.832132	-3.095841	-1.216807
C	-6.300989	-1.827554	-1.564266
C	-5.402304	-0.829064	-1.946164
C	-4.022087	-1.078651	-1.992061
C	-3.562942	-2.360665	-1.652808
C	-4.459169	-3.357406	-1.261921
H	-6.527983	-3.875515	-0.917768
H	-7.367294	-1.615661	-1.542673
H	-5.751532	0.161455	-2.220859
H	-2.499428	-2.574436	-1.672013
H	-4.083695	-4.342018	-0.994181

TS_{1Aax-in}

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.310167	-0.670540	0.194225
H	-1.981476	0.680928	-0.934131
H	-1.032614	-1.928730	1.218145
N	-3.129064	-0.249524	1.328382
H	-2.958809	0.061414	2.283431
H	-3.604800	0.514083	0.818642
N	-2.808332	-2.055245	-0.731529
H	-2.858745	-1.962345	-1.744585
H	-2.453508	-2.993402	-0.548752
P	0.075531	0.617870	1.505886
P	0.465737	-1.489686	-1.049598
C	-4.164093	-1.886829	-0.139533
H	-4.629776	-1.053322	-0.675822
C	-4.014684	-1.436463	1.319849
H	-3.495991	-2.223082	1.883580
C	4.563510	-1.969942	1.244820
C	3.834511	-3.090714	0.782766
C	2.659746	-2.925923	0.093224
C	2.126649	-1.637089	-0.190833
C	2.833137	-0.500689	0.218389
C	4.064702	-0.658490	0.956874
H	4.218544	-4.089436	0.978616
H	2.133662	-3.806517	-0.252246
C	2.963728	3.018769	-1.320778
C	1.905981	3.649682	-0.623326
C	1.121843	2.941212	0.252000
C	1.351187	1.562212	0.516972
C	2.416188	0.909937	-0.116136
C	3.222074	1.631333	-1.071239
H	1.713563	4.706286	-0.794705
H	0.310799	3.450617	0.757195
C	-2.396831	3.833077	3.870892
C	-1.457592	3.060531	4.553800
C	-0.685798	2.116786	3.870460
C	-0.842223	1.922569	2.487468
C	-1.812430	2.690268	1.819388
C	-2.571117	3.644346	2.498522

H	-2.992452	4.570201	4.403485
H	-1.318516	3.189220	5.624411
H	0.036441	1.532042	4.426761
H	-1.975361	2.533935	0.759516
H	-3.299319	4.232315	1.947680
C	2.514164	-1.199135	5.059812
C	2.847779	0.058022	4.550772
C	2.143449	0.582602	3.467091
C	1.094449	-0.137560	2.870658
C	0.770126	-1.396765	3.391104
C	1.474593	-1.924003	4.476370
H	3.064341	-1.610522	5.902276
H	3.662035	0.627610	4.990716
H	2.411975	1.562494	3.082329
H	-0.032386	-1.961643	2.927113
H	1.210233	-2.905199	4.863353
C	1.744472	0.276430	-5.178810
C	2.490553	-0.765470	-4.619570
C	2.136393	-1.292247	-3.377628
C	1.023482	-0.790749	-2.681750
C	0.290037	0.255014	-3.247387
C	0.645787	0.789194	-4.488862
H	2.024701	0.688854	-6.144662
H	3.351937	-1.163690	-5.149976
H	2.724008	-2.100906	-2.950576
H	-0.554015	0.640012	-2.684236
H	0.067423	1.606020	-4.914063
C	-0.818222	-5.855775	-2.226203
C	-0.520284	-4.930403	-3.224862
C	-0.082930	-3.643446	-2.892258
C	0.059097	-3.249741	-1.552340
C	-0.267527	-4.191204	-0.554496
C	-0.687981	-5.479797	-0.885946
H	-1.152602	-6.856806	-2.485568
H	-0.623521	-5.204911	-4.271700
H	0.146973	-2.946748	-3.690177
H	-0.919238	-6.189088	-0.094959
C	5.047961	1.736825	-2.692703
C	4.287640	1.021147	-1.794983
H	5.849888	1.240541	-3.232943
H	4.496229	-0.030406	-1.640428
C	4.794405	3.110011	-2.921590
C	3.769813	3.732791	-2.248248
H	5.405100	3.664514	-3.629160

H	3.556118	4.786109	-2.415465
C	5.993212	0.270202	2.139466
C	4.823424	0.449899	1.435176
H	6.547221	1.137034	2.490196
H	4.469668	1.455491	1.243639
C	6.480462	-1.029973	2.412071
C	5.774280	-2.124753	1.972610
H	7.406001	-1.158373	2.966963
H	6.130401	-3.132220	2.175375
H	-0.204168	-3.897539	0.488954
C	-5.395167	-1.184664	1.948389
H	-5.274060	-0.881406	2.997056
H	-5.874207	-0.345958	1.424787
C	-5.043634	-3.140181	-0.250374
H	-5.159856	-3.420964	-1.305693
H	-4.538131	-3.982678	0.247472
C	-6.420550	-2.913149	0.398362
H	-6.969831	-2.157155	-0.180275
H	-7.012715	-3.835544	0.352551
C	-6.283852	-2.435782	1.852178
H	-5.845835	-3.241322	2.460096
H	-7.273387	-2.227567	2.277364
C	-3.444250	1.488707	-1.521417
O	-4.364137	1.204521	-0.707389
C	-3.457067	0.795507	-2.887002
H	-2.534285	0.921296	-3.454712
H	-3.667062	-0.270288	-2.771375
H	-4.278795	1.235670	-3.470141
C	-2.329943	5.675549	-1.705499
C	-1.483781	4.723391	-2.280228
C	-1.798547	3.366183	-2.208873
C	-2.960604	2.933650	-1.555041
C	-3.801459	3.898346	-0.978597
C	-3.491328	5.257224	-1.053122
H	-2.085551	6.733042	-1.766791
H	-0.573065	5.036712	-2.784430
H	-1.117163	2.641880	-2.640084
H	-4.703875	3.554602	-0.483667
H	-4.160558	5.990180	-0.608509

TS_{1Aeq-out}

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.150051	0.230009	-0.518116
H	-1.781436	-0.163843	1.171816
H	-0.871014	0.568195	-2.110829
N	-2.965157	-0.782463	-1.278997
H	-2.744537	-1.546740	-1.915092
H	-3.485174	-1.190356	-0.500635
N	-2.666464	1.829180	-0.417428
H	-2.798138	2.017442	0.588756
H	-2.322265	2.673358	-0.873299
P	0.259057	-1.580638	-0.669822
P	0.598373	1.710558	-0.076910
C	-3.974572	1.414960	-0.990622
H	-4.567940	1.041647	-0.148559
C	-3.789100	0.242308	-1.963139
H	-3.188591	0.584319	-2.813967
C	4.826418	0.485116	-1.798848
C	4.115674	1.614627	-2.267048
C	2.899446	1.948762	-1.728194
C	2.302292	1.193100	-0.678558
C	2.979951	0.075296	-0.174961
C	4.255578	-0.297910	-0.744242
H	4.545285	2.217600	-3.063918
H	2.383459	2.819859	-2.110770
C	2.785841	-1.608831	3.286041
C	1.728859	-2.524528	3.066676
C	1.064491	-2.551615	1.866836
C	1.407157	-1.674346	0.800046
C	2.469508	-0.777765	0.960110
C	3.171659	-0.730934	2.220414
H	1.451141	-3.211167	3.863356
H	0.260615	-3.264532	1.727217
C	-2.227900	-5.568960	-0.637323
C	-1.147266	-5.452263	-1.511053
C	-0.369144	-4.291085	-1.525561
C	-0.655362	-3.219050	-0.664117
C	-1.757985	-3.347819	0.198993
C	-2.531649	-4.509009	0.219676
H	-2.832450	-6.472341	-0.629164
H	-0.904351	-6.265675	-2.190294
H	0.459393	-4.227736	-2.220284
H	-2.006199	-2.515377	0.849667

H	-3.379008	-4.574873	0.896360
C	2.942250	-2.415623	-4.403986
C	3.221556	-3.052489	-3.192513
C	2.447351	-2.778909	-2.064710
C	1.382996	-1.864036	-2.125781
C	1.115163	-1.230005	-3.345779
C	1.888697	-1.503717	-4.476653
H	3.546537	-2.626038	-5.282784
H	4.047491	-3.755198	-3.121786
H	2.674311	-3.280948	-1.128280
H	0.301463	-0.512211	-3.391723
H	1.668484	-0.998943	-5.414207
C	1.477664	3.810575	4.006633
C	2.537042	3.520452	3.145123
C	2.299798	2.853561	1.941593
C	1.003692	2.451199	1.584549
C	-0.054896	2.754061	2.453966
C	0.182282	3.428527	3.654518
H	1.661278	4.331430	4.943063
H	3.550513	3.815017	3.405874
H	3.129853	2.661624	1.270657
H	-1.072984	2.460108	2.214079
H	-0.653764	3.646972	4.313976
C	-0.187765	5.715607	-2.454322
C	0.321581	5.767505	-1.157308
C	0.571483	4.590491	-0.446103
C	0.312040	3.330154	-1.012060
C	-0.203505	3.296996	-2.321568
C	-0.446137	4.472376	-3.035252
H	-0.381565	6.631897	-3.006177
H	0.527767	6.726959	-0.689540
H	0.971889	4.665500	0.557313
H	-0.838619	4.413595	-4.047805
C	4.914350	0.175179	3.677599
C	4.261964	0.154047	2.465069
H	5.741126	0.863795	3.830788
H	4.587088	0.820706	1.676264
C	4.519779	-0.689689	4.725478
C	3.476239	-1.562818	4.527346
H	5.041595	-0.662515	5.678261
H	3.160560	-2.237897	5.319501
C	6.201856	-1.774848	-0.869986
C	4.987929	-1.442298	-0.310722
H	6.733688	-2.653556	-0.514492

H	4.579363	-2.065445	0.474984
C	6.762849	-0.985338	-1.901468
C	6.082195	0.119741	-2.355092
H	7.723132	-1.255964	-2.332324
H	6.492593	0.735073	-3.152479
H	-0.419117	2.332138	-2.769363
C	-5.149794	-0.263374	-2.466951
H	-5.003481	-1.099331	-3.164099
H	-5.728654	-0.654743	-1.617065
C	-4.743391	2.562416	-1.660115
H	-4.892579	3.375085	-0.938059
H	-4.130512	2.971463	-2.477960
C	-6.095827	2.082901	-2.215438
H	-6.750212	1.806294	-1.376309
H	-6.596705	2.904057	-2.742795
C	-5.932093	0.872811	-3.148879
H	-5.395320	1.183317	-4.057127
H	-6.914088	0.509901	-3.476061
C	-2.762442	0.332070	2.562438
O	-3.037197	1.548755	2.380935
C	-1.684991	-0.052280	3.575565
H	-2.124785	0.022272	4.581663
H	-1.302835	-1.064951	3.436882
H	-0.847156	0.639053	3.512962
C	-6.174006	-2.357465	2.333003
C	-4.920376	-2.869608	2.675122
C	-3.803414	-2.031824	2.722608
C	-3.913416	-0.663577	2.427380
C	-5.187094	-0.158551	2.119936
C	-6.303257	-0.993513	2.060320
H	-7.042544	-3.010040	2.299646
H	-4.812632	-3.923124	2.922284
H	-2.843471	-2.451652	3.003712
H	-5.281029	0.911362	1.967104
H	-7.279217	-0.575694	1.824499

TS_{1Aeq-in}

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.388489	-0.604078	0.080514

H	2.053782	0.954056	-0.810259
H	1.128055	-1.993510	0.917453
N	2.933936	-1.804739	-0.963283
H	2.520068	-2.621272	-1.410418
H	3.376685	-1.264549	-1.706694
N	3.159040	-0.248695	1.326053
H	3.376000	0.756751	1.227788
H	2.962978	-0.461572	2.302620
P	-0.310774	-1.181565	-1.369511
P	-0.089474	0.288329	1.628083
C	4.354933	-0.988902	0.850349
H	4.870073	-0.295982	0.175365
C	3.938176	-2.226846	0.046636
H	3.405651	-2.911820	0.717339
C	-4.192053	-2.041509	1.905783
C	-3.231148	-2.097697	2.942321
C	-2.056221	-1.395143	2.846792
C	-1.752193	-0.581675	1.719484
C	-2.688083	-0.474987	0.684086
C	-3.922930	-1.220894	0.763260
H	-3.436361	-2.703607	3.822147
H	-1.349839	-1.452065	3.664662
C	-3.325159	2.396798	-1.796636
C	-2.447055	2.033406	-2.845856
C	-1.624132	0.942232	-2.724471
C	-1.632524	0.124730	-1.559821
C	-2.512107	0.424306	-0.514025
C	-3.359152	1.588135	-0.613797
H	-2.432023	2.632782	-3.753476
H	-0.959737	0.690601	-3.542405
C	1.454310	-1.793477	-5.682410
C	1.829551	-0.712153	-4.881226
C	1.273921	-0.558303	-3.610618
C	0.316236	-1.461391	-3.116052
C	-0.044379	-2.546663	-3.930551
C	0.521664	-2.710680	-5.198735
H	1.889282	-1.921965	-6.670179
H	2.559885	0.008280	-5.241982
H	1.584301	0.259889	-2.969118
H	-0.766005	-3.275668	-3.581618
H	0.227874	-3.561644	-5.808287
C	-2.695782	-5.178071	-0.900861
C	-3.195357	-4.161000	-1.717359
C	-2.503820	-2.954993	-1.834305

C	-1.302360	-2.741903	-1.137768
C	-0.814802	-3.768837	-0.318908
C	-1.504859	-4.977922	-0.201907
H	-3.236075	-6.116491	-0.805860
H	-4.129033	-4.301144	-2.255529
H	-2.904392	-2.171152	-2.471158
H	0.099217	-3.598889	0.242338
H	-1.113369	-5.760831	0.443149
C	-1.470178	4.729823	1.942044
C	-2.021510	3.772892	2.800278
C	-1.629292	2.439829	2.700094
C	-0.669274	2.047077	1.749790
C	-0.125025	3.010290	0.897766
C	-0.526241	4.347308	0.990393
H	-1.781203	5.769006	2.015765
H	-2.760785	4.065072	3.542146
H	-2.064757	1.701624	3.368593
H	0.607648	2.706771	0.159168
H	-0.094880	5.080464	0.316494
C	1.984476	-0.323165	5.805919
C	1.603578	0.953849	5.397818
C	0.941922	1.141667	4.179819
C	0.650778	0.056617	3.337500
C	1.068566	-1.224358	3.752384
C	1.713645	-1.414044	4.975288
H	2.493723	-0.468722	6.754998
H	1.819044	1.814817	6.025409
H	0.657941	2.145913	3.888620
H	2.010737	-2.416064	5.275486
C	-5.057245	3.090082	0.297876
C	-4.249479	1.982403	0.426478
H	-5.722068	3.367278	1.111671
H	-4.282778	1.401999	1.340139
C	-5.026853	3.874119	-0.879474
C	-4.173538	3.531776	-1.901980
H	-5.671461	4.744442	-0.969213
H	-4.130580	4.127124	-2.811192
C	-6.081502	-1.904537	-0.161579
C	-4.910461	-1.187046	-0.264627
H	-6.813702	-1.855198	-0.963368
H	-4.734659	-0.584034	-1.146767
C	-6.341170	-2.704475	0.976244
C	-5.409886	-2.769903	1.985694
H	-7.270446	-3.263442	1.047281

H	-5.589039	-3.382486	2.866393
H	0.901044	-2.072857	3.096492
C	5.167497	-2.941551	-0.535803
H	4.853302	-3.830949	-1.098524
H	5.670315	-2.273504	-1.251692
C	5.325704	-1.371963	1.976263
H	5.632586	-0.467190	2.514962
H	4.801363	-2.014063	2.700887
C	6.555945	-2.112335	1.425374
H	7.143048	-1.420199	0.804856
H	7.209491	-2.422501	2.249986
C	6.151861	-3.331428	0.581473
H	5.678148	-4.082412	1.230441
H	7.039971	-3.808368	0.149181
C	3.376384	2.070953	-0.945175
O	4.002610	2.053774	0.148780
C	1.510016	5.819441	-2.054957
H	2.391549	5.736767	-0.974861
H	2.933404	4.504370	-0.604950
H	2.613459	3.337945	-1.313119
C	1.721294	3.430611	-2.390966
C	1.169604	4.658223	-2.755970
C	1.088522	6.777900	-2.347753
C	2.661092	6.633433	-0.421628
C	3.623989	4.418887	0.227449
C	1.435856	2.535089	-2.934282
H	0.472440	4.709948	-3.588599
H	4.063913	1.423373	-2.158964
H	4.889089	2.087335	-2.452316
H	4.504614	0.460957	-1.887861
H	3.414170	1.298500	-3.026817

TS_{1Bax-out}

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.205593	0.615544	0.346161
H	0.690932	1.669239	1.495917
H	-0.206162	-0.973757	1.267677
N	-0.491005	1.490433	-0.943437
H	2.119788	-0.356859	-1.021179

H	2.755915	2.104060	-0.112048
N	3.343793	1.698766	-0.863954
H	2.390636	3.003692	-0.421221
H	2.842102	0.076996	1.759407
P	2.484337	0.233199	2.701143
P	3.065913	-0.915576	1.693787
C	4.064759	0.895498	1.537279
H	4.590307	0.426481	0.698838
C	3.636561	2.290176	1.065720
H	3.033225	2.762383	1.853257
C	-3.382318	-2.734640	-1.725418
C	-2.303208	-3.510895	-1.238188
C	-1.415895	-2.986632	-0.332061
C	-1.553555	-1.661752	0.170490
C	-2.617000	-0.865596	-0.268319
C	-3.537468	-1.392361	-1.248336
H	-2.186127	-4.533394	-1.590566
H	-0.596275	-3.602479	0.018795
C	-4.470378	1.960686	1.561492
C	-3.687969	3.077519	1.185481
C	-2.560138	2.917066	0.421123
C	-2.130715	1.639273	-0.034115
C	-2.900779	0.511774	0.278309
C	-4.078154	0.661852	1.102529
H	-3.993823	4.070663	1.507157
H	-1.995335	3.797358	0.144392
C	0.839755	5.837946	-2.114473
C	0.514081	4.924960	-3.115972
C	0.064047	3.641879	-2.788270
C	-0.068511	3.240271	-1.449681
C	0.297681	4.164855	-0.449341
C	0.731356	5.450519	-0.776042
H	1.184193	6.836242	-2.370840
H	0.608792	5.205578	-4.161850
H	-0.179256	2.953557	-3.589017
H	0.259723	3.859249	0.592550
H	0.992831	6.146606	0.017184
C	-1.972643	-0.432836	-4.932428
C	-2.534318	0.771328	-4.499294
C	-2.104481	1.354346	-3.307459
C	-1.089307	0.755036	-2.542408
C	-0.546648	-0.457982	-2.978081
C	-0.986124	-1.051130	-4.164066
H	-2.313764	-0.891614	-5.856750

H	-3.315431	1.250236	-5.084186
H	-2.560934	2.281986	-2.971873
H	0.212823	-0.931906	-2.363984
H	-0.560068	-1.998417	-4.485128
C	-2.464772	-0.092153	5.273403
C	-2.838961	-1.182861	4.485325
C	-2.191134	-1.425877	3.273778
C	-1.156078	-0.586779	2.827358
C	-0.794732	0.506135	3.625730
C	-1.443002	0.752317	4.838571
H	-2.972174	0.100541	6.215189
H	-3.641614	-1.840446	4.808801
H	-2.493352	-2.277167	2.670110
H	-0.019525	1.177799	3.269190
H	-1.152036	1.610494	5.439530
C	2.339694	-4.698272	2.564514
C	1.368843	-4.208105	3.437959
C	0.574578	-3.117156	3.073377
C	0.739105	-2.492149	1.826522
C	1.734331	-2.987244	0.963480
C	2.520272	-4.084395	1.322869
H	2.955295	-5.547406	2.850617
H	1.224769	-4.672282	4.410589
H	-0.170012	-2.755225	3.772245
H	3.274146	-4.447007	0.630558
C	-6.014836	-0.268673	2.270934
C	-4.891952	-0.441817	1.492591
H	-6.612576	-1.132373	2.550392
H	-4.619534	-1.439277	1.170720
C	-6.397444	1.020201	2.711502
C	-5.634680	2.109639	2.362649
H	-7.287090	1.143854	3.323235
H	-5.909397	3.108286	2.694557
C	-5.495132	-1.164402	-2.693942
C	-4.616944	-0.627853	-1.778756
H	-6.308223	-0.554811	-3.079285
H	-4.743944	0.398620	-1.457679
C	-5.346881	-2.498271	-3.141474
C	-4.305958	-3.262061	-2.667720
H	-6.049682	-2.911412	-3.860157
H	-4.170082	-4.286151	-3.008068
H	1.898671	-2.496808	0.008557
C	4.868637	3.163362	0.773864
H	5.414209	2.725466	-0.072876

H	4.544878	4.165762	0.462904
C	4.982364	0.971527	2.764739
H	4.416256	1.386705	3.614068
H	5.296935	-0.038915	3.057911
C	6.209264	1.858184	2.489088
H	5.271565	3.782674	2.812333
H	6.824521	1.937740	3.393965
C	5.792482	3.253931	2.000070
H	6.835410	1.378101	1.723962
H	6.680178	3.851630	1.758774
C	3.486054	-0.371155	-2.040016
O	4.357892	0.393452	-1.529839
C	4.472826	-4.595826	-2.015235
H	5.328794	-3.647783	-1.449394
H	4.973393	-2.298100	-1.441015
H	3.758537	-1.868081	-1.993304
C	2.905503	-2.829940	-2.556391
C	3.256803	-4.180064	-2.566368
C	4.750894	-5.646693	-2.033253
C	6.281194	-3.958577	-1.026045
C	5.639595	-1.544837	-1.034017
C	1.954452	-2.526652	-2.983314
H	2.582257	-4.909308	-3.008415
H	2.804887	0.146526	-3.309384
H	3.574537	0.179785	-4.093383
H	1.977817	-0.464364	-3.668058
H	2.442576	1.164391	-3.146380

TS_{1Bax-in}

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.292144	-0.681769	0.198104
H	0.881475	-1.848684	1.273547
H	-0.445374	-1.372337	-1.167798
N	-0.123419	0.611774	1.496576
H	2.155098	0.592817	-0.975730
H	3.058887	-0.304587	1.418651
N	3.595646	0.433292	0.925805
H	2.840737	0.016755	2.360278
H	2.733336	-2.195219	-0.574784

P	2.336610	-3.102341	-0.333200
P	2.812260	-2.175469	-1.590977
C	4.075496	-2.046233	0.055311
H	4.590061	-1.254410	-0.497957
C	3.895938	-1.523728	1.486543
H	3.332528	-2.266894	2.067048
C	-3.256374	2.236722	-2.267744
C	-2.383875	1.654241	-3.218193
C	-1.618004	0.563905	-2.890789
C	-1.677907	-0.034745	-1.601064
C	-2.548212	0.491211	-0.639912
C	-3.338783	1.655212	-0.960829
H	-2.330598	2.080432	-4.217638
H	-0.963623	0.139382	-3.642230
C	-4.344046	-1.405928	2.177841
C	-3.381818	-1.321263	3.211143
C	-2.174491	-0.705422	2.996318
C	-1.834756	-0.125648	1.741744
C	-2.770145	-0.162372	0.700760
C	-4.040799	-0.818461	0.907412
H	-3.612508	-1.747134	4.185194
H	-1.469964	-0.649394	3.815772
C	1.835122	0.806695	5.769692
C	1.514830	1.985525	5.098614
C	0.891273	1.942937	3.847219
C	0.578112	0.718794	3.234423
C	0.936604	-0.463534	3.913811
C	1.543404	-0.421199	5.169756
H	2.314505	0.841529	6.744494
H	1.748242	2.948695	5.545202
H	0.653651	2.875497	3.349436
H	0.751546	-1.421450	3.437843
H	1.795651	-1.350059	5.675531
C	-1.207921	5.088293	0.786907
C	-1.844959	4.377561	1.808627
C	-1.541504	3.033354	2.014039
C	-0.587840	2.384348	1.209166
C	0.043060	3.102956	0.190357
C	-0.269663	4.449618	-0.022404
H	-1.448276	6.135697	0.621908
H	-2.582090	4.868628	2.439168
H	-2.043998	2.486472	2.807764
H	0.774692	2.601507	-0.434933
H	0.228654	4.991856	-0.818987

C	-3.108315	-5.045168	-0.026726
C	-3.518790	-4.173505	-1.038196
C	-2.744679	-3.057511	-1.356345
C	-1.546976	-2.791984	-0.671642
C	-1.148723	-3.672367	0.342312
C	-1.922768	-4.790385	0.663184
H	-3.713206	-5.912687	0.224485
H	-4.446913	-4.356300	-1.573212
H	-3.074855	-2.385923	-2.143977
H	-0.237557	-3.456011	0.892073
H	-1.599968	-5.458695	1.457816
C	1.268899	-2.894734	-5.268570
C	0.331095	-3.677853	-4.596085
C	-0.225291	-3.241168	-3.389794
C	0.149183	-2.009941	-2.827688
C	1.111114	-1.242756	-3.508285
C	1.658248	-1.671146	-4.718559
H	1.697754	-3.236127	-6.207138
H	0.025839	-4.636498	-5.008171
H	-0.951298	-3.872029	-2.891285
H	2.395280	-1.053250	-5.225557
C	-6.237423	-1.545069	0.114438
C	-5.031699	-0.919379	-0.112652
H	-6.971342	-1.602330	-0.685234
H	-4.831019	-0.495546	-1.088748
C	-6.529727	-2.114667	1.376140
C	-5.596209	-2.046201	2.383266
H	-7.485708	-2.603600	1.543735
H	-5.800486	-2.481049	3.359059
C	-4.984749	3.360848	-0.366307
C	-4.223584	2.265202	-0.025140
H	-5.649165	3.803885	0.370885
H	-4.292316	1.859763	0.976767
C	-4.906740	3.919296	-1.663887
C	-4.054252	3.367189	-2.590985
H	-5.514636	4.782654	-1.921036
H	-3.975621	3.787153	-3.591209
H	1.434324	-0.308925	-3.061494
C	5.265301	-1.297078	2.149165
H	5.789191	-0.499189	1.605968
H	5.120596	-0.944502	3.178953
C	4.912229	-3.332631	0.025726
H	4.360975	-4.133746	0.543481
H	5.050385	-3.663890	-1.012290

C	6.275295	-3.126781	0.709327
H	5.621959	-3.345470	2.761688
H	6.833863	-4.070886	0.721348
C	6.108865	-2.582394	2.136168
H	6.869740	-2.416179	0.118064
H	7.091305	-2.391980	2.585447
C	3.683825	1.345476	-1.382224
O	4.472401	1.122238	-0.419537
C	2.696393	5.499671	-2.102138
H	3.538719	5.125953	-1.052872
H	3.796838	3.776989	-0.807597
H	3.215155	2.776864	-1.599227
C	2.349934	3.162492	-2.634552
C	2.095648	4.510730	-2.887449
C	2.506401	6.550540	-2.306245
C	4.007067	5.887187	-0.433590
C	4.473693	3.467894	-0.018167
C	1.859193	2.408013	-3.242143
H	1.428440	4.790095	-3.699292
H	3.959558	0.580221	-2.682758
H	4.927434	0.938494	-3.059918
H	4.051851	-0.491300	-2.496103
H	3.216598	0.744387	-3.464116

TS_{1Beq-out}

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.168029	0.432309	0.327904
H	-0.894007	0.948552	1.874286
H	0.637172	1.721821	-0.353938
N	0.204559	-1.357166	0.816318
H	-1.815110	-0.098652	-1.319727
H	-2.999969	-0.471458	1.180040
N	-3.515256	-0.974483	0.455106
H	-2.769895	-1.145402	1.908926
H	-2.665770	2.038425	0.081552
P	-2.320589	2.918928	0.459239
P	-2.803455	2.147052	-0.930648
C	-3.990338	1.690039	0.662612
H	-4.556763	1.244775	-0.162261

C	-3.830036	0.618537	1.745426
H	-3.243541	1.040310	2.570580
C	3.430405	-0.826847	-3.155943
C	2.601568	0.205657	-3.657670
C	1.847805	0.974759	-2.807699
C	1.878367	0.786159	-1.396648
C	2.708951	-0.201967	-0.855866
C	3.483256	-1.040833	-1.740104
H	2.570057	0.384136	-4.730283
H	1.222212	1.756128	-3.222092
C	4.441626	-0.227717	2.574786
C	3.440706	-0.829335	3.373058
C	2.228540	-1.177268	2.832472
C	1.923026	-0.956254	1.460289
C	2.896427	-0.391525	0.628094
C	4.173405	-0.009762	1.185034
H	3.644783	-1.018029	4.424763
H	1.493035	-1.646651	3.472502
C	-1.939454	-3.738038	4.258705
C	-1.610790	-4.391471	3.072136
C	-0.929845	-3.715348	2.054290
C	-0.564185	-2.367357	2.197335
C	-0.930113	-1.713430	3.392460
C	-1.596643	-2.392020	4.414035
H	-2.463844	-4.266211	5.050674
H	-1.881814	-5.434762	2.930871
H	-0.686840	-4.250445	1.143760
H	-0.703672	-0.657200	3.505535
H	-1.853384	-1.865108	5.329803
C	1.233529	-4.696926	-2.286500
C	1.761873	-4.771727	-0.994423
C	1.477389	-3.773407	-0.062957
C	0.643533	-2.694342	-0.402916
C	0.133552	-2.622954	-1.702554
C	0.426454	-3.616144	-2.641359
H	1.462061	-5.471669	-3.013808
H	2.403670	-5.603723	-0.715578
H	1.903827	-3.836488	0.934949
H	-0.478338	-1.766111	-1.964662
H	0.028913	-3.540415	-3.650500
C	3.264464	4.042850	2.744419
C	3.746954	3.809842	1.454758
C	2.980717	3.084278	0.542233
C	1.720024	2.577134	0.899567

C	1.249363	2.816112	2.197070
C	2.014844	3.543050	3.112185
H	3.861775	4.605451	3.457471
H	4.724165	4.183366	1.160672
H	3.368106	2.910352	-0.457631
H	0.284413	2.409641	2.483678
H	1.633114	3.714475	4.115851
C	-0.722055	5.326101	-3.043117
C	0.251285	5.540072	-2.066108
C	0.692192	4.487075	-1.259988
C	0.170088	3.191943	-1.418376
C	-0.821321	2.998457	-2.394861
C	-1.261369	4.048643	-3.201664
H	-1.064518	6.149404	-3.665036
H	0.671256	6.532725	-1.922724
H	1.442206	4.687857	-0.504828
H	-2.039090	3.857994	-3.935994
C	6.411994	0.950408	0.964899
C	5.203812	0.595270	0.407180
H	7.175957	1.409749	0.343014
H	5.031433	0.782587	-0.645559
C	6.668259	0.724992	2.338054
C	5.697650	0.148587	3.123023
H	7.626183	1.008212	2.766057
H	5.874081	-0.029969	4.181301
C	5.054865	-2.871384	-2.132605
C	4.315682	-2.096352	-1.266724
H	5.677713	-3.670623	-1.739428
H	4.360708	-2.296515	-0.203226
C	5.008456	-2.641417	-3.527654
C	4.207443	-1.639830	-4.024347
H	5.599795	-3.257437	-4.199920
H	4.152691	-1.452921	-5.094440
H	-1.281789	2.025679	-2.511461
C	-5.200335	0.166982	2.274361
H	-5.760123	-0.316952	1.460514
H	-5.065533	-0.587412	3.060988
C	-4.772111	2.899290	1.192799
H	-4.186479	3.388244	1.987236
H	-4.900317	3.636427	0.390107
C	-6.139826	2.470476	1.751764
H	-5.484610	1.776635	3.694885
H	-6.662510	3.338295	2.172610
C	-5.998478	1.367570	2.812547

H	-6.763273	2.099621	0.925724
H	-6.988239	1.039221	3.153027
C	-3.067920	0.066370	-2.567092
O	-3.442835	1.265978	-2.549196
C	-2.167762	-0.393151	-3.718106
H	-1.807044	-1.417239	-3.606124
H	-2.770391	-0.346635	-4.636623
H	-1.314256	0.276845	-3.835996
C	-5.980112	-2.866077	-1.230194
C	-6.357501	-1.562241	-1.557523
C	-5.394423	-0.635217	-1.963242
C	-4.039987	-0.990880	-2.050105
C	-3.674100	-2.307859	-1.729796
C	-4.633972	-3.234448	-1.318286
H	-6.725980	-3.590771	-0.914059
H	-7.403146	-1.268225	-1.505846
H	-5.672533	0.378739	-2.232924
H	-2.631273	-2.604875	-1.774617
H	-4.329401	-4.247205	-1.066195

TS_{1Beq-in}

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.476217	-0.488141	0.033745
H	-1.404675	-2.011443	0.641401
H	0.031407	0.143776	1.673884
N	0.234185	-1.132123	-1.387755
H	-1.907073	1.235592	-0.628125
H	-3.075940	-1.320222	-1.263974
N	-3.461867	-0.605943	-1.880137
H	-2.706924	-2.062004	-1.857351
H	-3.300420	-0.165325	1.232076
P	-3.173262	-0.477510	2.192963
P	-3.451504	0.854578	1.229819
C	-4.517183	-0.773517	0.628849
H	-5.000447	0.041127	0.074571
C	-4.129336	-1.865091	-0.374853
H	-3.650391	-2.684798	0.173471
C	3.212628	2.909013	-0.394138
C	2.187977	3.425954	0.435132

C	1.322818	2.584485	1.086072
C	1.426930	1.169506	0.973328
C	2.436378	0.614056	0.178498
C	3.335702	1.488406	-0.536189
H	2.083497	4.502971	0.540633
H	0.538405	3.011421	1.698977
C	4.190703	-2.782328	0.595988
C	3.325805	-3.621244	-0.144755
C	2.191197	-3.116228	-0.728218
C	1.835274	-1.742659	-0.619883
C	2.678331	-0.871240	0.079381
C	3.870925	-1.390702	0.707043
H	3.572766	-4.675348	-0.250337
H	1.560004	-3.786280	-1.297325
C	-1.552607	-4.750995	-3.801998
C	-1.130038	-3.608696	-4.480024
C	-0.545671	-2.545711	-3.782524
C	-0.374100	-2.598212	-2.389490
C	-0.834297	-3.748845	-1.716383
C	-1.402506	-4.815853	-2.413629
H	-2.001113	-5.578733	-4.345004
H	-1.250829	-3.537360	-5.558027
H	-0.224258	-1.670553	-4.335229
H	-0.762453	-3.792074	-0.634261
H	-1.734750	-5.696307	-1.869094
C	1.992159	1.582902	-4.755461
C	2.461361	0.274041	-4.609441
C	1.953479	-0.539790	-3.598162
C	0.952100	-0.065368	-2.732379
C	0.497509	1.247716	-2.880189
C	1.018714	2.069708	-3.884059
H	2.395326	2.221630	-5.537203
H	3.229460	-0.108296	-5.277160
H	2.334163	-1.551555	-3.484783
H	-0.247933	1.620157	-2.184136
H	0.671588	3.095011	-3.974659
C	2.094258	-3.022393	4.431732
C	2.657140	-1.753162	4.282609
C	2.066317	-0.822114	3.427819
C	0.905378	-1.140210	2.703556
C	0.352244	-2.417449	2.862161
C	0.940963	-3.351023	3.718613
H	2.554838	-3.749593	5.095614
H	3.561924	-1.488623	4.823185

H	2.514285	0.161789	3.323730
H	-0.537133	-2.674541	2.295390
H	0.497062	-4.338009	3.824710
C	-1.961736	2.764150	5.024395
C	-1.014043	1.806560	5.387079
C	-0.385926	1.027177	4.412880
C	-0.688975	1.192210	3.050218
C	-1.652695	2.153246	2.702818
C	-2.279530	2.933307	3.676340
H	-2.453128	3.365555	5.785062
H	-0.761380	1.657338	6.433992
H	0.336088	0.284483	4.728280
H	-3.027445	3.662030	3.375213
C	5.891265	-1.094374	2.053027
C	4.762794	-0.572372	1.460554
H	6.550441	-0.442369	2.620230
H	4.546025	0.482971	1.571012
C	6.201111	-2.469778	1.930925
C	5.362711	-3.292979	1.216948
H	7.095816	-2.869157	2.401068
H	5.581857	-4.353403	1.114844
C	5.215676	1.858483	-2.053717
C	4.360400	1.000681	-1.398384
H	5.985270	1.454518	-2.706295
H	4.461989	-0.067450	-1.546275
C	5.099664	3.258966	-1.890601
C	4.112363	3.768587	-1.080020
H	5.783865	3.924924	-2.409817
H	4.000581	4.842637	-0.950347
H	-1.927358	2.286419	1.663731
C	-5.370922	-2.400525	-1.102829
H	-5.830225	-1.588764	-1.687425
H	-5.077853	-3.181335	-1.817125
C	-5.517027	-1.317890	1.657957
H	-5.025597	-2.101230	2.255746
H	-5.803913	-0.517740	2.351597
C	-6.763071	-1.898944	0.966326
H	-5.964987	-3.833269	0.404572
H	-7.437488	-2.334882	1.713541
C	-6.392940	-2.950715	-0.092693
H	-7.317477	-1.080483	0.485287
H	-7.293295	-3.294323	-0.616520
C	-3.103722	2.458910	-0.772410
O	-3.835653	2.373574	0.255047

C	-0.690847	6.060486	-1.049542
H	-1.403921	5.753716	0.111488
H	-2.155227	4.581057	0.183501
H	-2.194638	3.677190	-0.887941
C	-1.497589	4.012258	-2.058810
C	-0.750404	5.188265	-2.138452
C	-0.111738	6.978291	-1.113409
C	-1.389710	6.438123	0.956469
C	-2.753791	4.359182	1.058896
C	-1.542272	3.359143	-2.923606
H	-0.220738	5.429195	-3.057098
H	-3.689560	1.976634	-2.108583
H	-4.271624	2.797652	-2.550164
H	-2.936785	1.659639	-2.834938
H	-4.387006	1.157075	-1.918824

ABS₁

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.561286	0.834332	-0.616176
H	-1.365292	0.062681	0.700490
H	0.016568	1.677455	-1.991740
N	-2.380640	0.432402	-1.834533
H	-2.147273	-0.027819	-2.711878
H	-3.001556	-0.192923	-1.316870
N	-1.830666	2.624535	-0.205736
H	-1.884755	2.817550	0.792022
H	-1.362393	3.423107	-0.633060
P	0.515774	-1.106803	-1.137765
P	1.192354	1.610203	0.622116
C	-3.192773	2.461579	-0.768902
H	-3.738963	1.812985	-0.072178
C	-3.081625	1.707678	-2.101747
H	-2.423994	2.284772	-2.765502
C	5.426501	0.489681	-1.125947
C	4.941929	1.819066	-1.140671
C	3.725226	2.126927	-0.586242
C	2.907556	1.139314	0.031315
C	3.360635	-0.183560	0.091480
C	4.630162	-0.526756	-0.505472

H	5.548736	2.598052	-1.597240
H	3.385030	3.154494	-0.613299
C	2.590595	-2.911908	2.689552
C	1.434457	-3.496925	2.119904
C	0.883543	-2.985614	0.972207
C	1.450530	-1.868307	0.297251
C	2.615327	-1.282512	0.806352
C	3.188753	-1.789072	2.030590
H	0.986015	-4.361758	2.604380
H	-0.002918	-3.455983	0.564762
C	-2.700155	-4.289948	-2.407500
C	-1.569264	-4.111859	-3.203380
C	-0.577556	-3.198020	-2.832551
C	-0.697526	-2.439857	-1.656685
C	-1.856329	-2.616471	-0.875555
C	-2.840547	-3.535482	-1.240147
H	-3.469383	-5.001284	-2.697707
H	-1.451701	-4.684517	-4.120211
H	0.289087	-3.078975	-3.472012
H	-1.979774	-2.002432	0.011962
H	-3.726186	-3.648459	-0.620278
C	3.541521	-1.426945	-4.687638
C	3.447214	-2.471236	-3.764146
C	2.567213	-2.372916	-2.686257
C	1.763736	-1.232863	-2.516200
C	1.869458	-0.190807	-3.445599
C	2.753083	-0.287375	-4.523902
H	4.231042	-1.501118	-5.524998
H	4.065857	-3.357871	-3.877353
H	2.504582	-3.189932	-1.972080
H	1.259267	0.696728	-3.295108
H	2.827082	0.532751	-5.234253
C	1.490609	0.929609	5.240351
C	2.571926	1.490529	4.555389
C	2.504982	1.673271	3.174034
C	1.354187	1.305841	2.456043
C	0.279856	0.738828	3.151536
C	0.348060	0.550978	4.534854
H	1.544938	0.781963	6.316156
H	3.470174	1.778371	5.096023
H	3.353022	2.108988	2.651765
H	-0.593508	0.431214	2.580556
H	-0.491676	0.101946	5.060355
C	1.016144	6.309496	0.406696

C	1.101206	5.685348	1.650007
C	1.198846	4.292228	1.739601
C	1.205385	3.490768	0.587067
C	1.097025	4.136408	-0.661862
C	1.015422	5.526726	-0.751528
H	0.945711	7.392153	0.338385
H	1.094487	6.279628	2.560584
H	1.267909	3.836490	2.720365
H	0.945480	5.998293	-1.729052
C	4.885560	-1.733355	3.790160
C	4.348971	-1.218762	2.630741
H	5.770703	-1.273889	4.222474
H	4.816213	-0.359484	2.165223
C	4.295118	-2.851086	4.425528
C	3.167862	-3.422553	3.883369
H	4.730117	-3.250070	5.338147
H	2.696257	-4.278570	4.360957
C	6.363801	-2.153230	-1.079448
C	5.144217	-1.856413	-0.512573
H	6.726428	-3.177865	-1.067411
H	4.560425	-2.650907	-0.064301
C	7.147373	-1.139643	-1.679837
C	6.681079	0.153707	-1.702915
H	8.109111	-1.386165	-2.122029
H	7.266041	0.945688	-2.165236
H	1.051872	3.524905	-1.559163
C	-4.457910	1.529672	-2.767336
H	-4.329060	1.041572	-3.742745
H	-5.065393	0.854145	-2.150747
C	-3.943856	3.793157	-0.927409
H	-4.049866	4.276091	0.053210
H	-3.335439	4.469883	-1.547246
C	-5.318149	3.601057	-1.588370
H	-5.964455	3.013461	-0.920540
H	-5.807459	4.573664	-1.723100
C	-5.185154	2.873798	-2.934275
H	-4.626089	3.509939	-3.636297
H	-6.174578	2.712292	-3.379838
C	-5.240439	-0.970082	1.008087
O	-4.919423	-0.724575	-0.151976
C	-4.229518	-0.853054	2.130730
H	-4.100728	-1.817021	2.638751
H	-3.268248	-0.525464	1.722136
H	-4.570691	-0.135310	2.887343

C	-9.291706	-2.165954	1.819927
C	-8.874440	-1.897207	0.512005
C	-7.560433	-1.511828	0.265987
C	-6.643462	-1.389844	1.323188
C	-7.070454	-1.663284	2.632452
C	-8.387856	-2.048620	2.878401
H	-9.576176	-1.989754	-0.312518
H	-7.216519	-1.300313	-0.741105
H	-6.377542	-1.576580	3.463252
H	-8.709506	-2.257587	3.894960
H	-10.317338	-2.466692	2.012774

INTf₁

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.757874	0.241660	-0.787309
H	1.425123	-0.081163	0.774377
H	0.332496	0.593123	-2.407302
N	2.368240	1.756821	-1.061256
H	1.980650	2.647956	-1.364778
H	2.839194	1.928733	-0.171485
N	2.423320	-0.968438	-1.646030
H	2.569799	-1.822507	-1.112207
H	2.128352	-1.255150	-2.578930
P	-0.785185	1.684775	0.086627
P	-0.705844	-1.510549	-0.759862
C	3.683100	-0.190795	-1.713800
H	4.106105	-0.201678	-0.701214
C	3.346787	1.267206	-2.057658
H	2.826659	1.278048	-3.024901
C	-5.161014	-0.337119	-1.774969
C	-4.366175	-1.091903	-2.669686
C	-3.086568	-1.455565	-2.333692
C	-2.507298	-1.104191	-1.082087
C	-3.267379	-0.378229	-0.157785
C	-4.609775	0.026441	-0.503832
H	-4.783566	-1.383372	-3.631115
H	-2.507917	-2.035239	-3.041799
C	-3.040731	-0.356695	3.681883
C	-2.078956	0.662839	3.881625

C	-1.481238	1.281127	2.812866
C	-1.808896	0.944725	1.469293
C	-2.776721	-0.036417	1.226504
C	-3.392987	-0.717381	2.340729
H	-1.818632	0.951760	4.897728
H	-0.744565	2.053398	2.998249
C	1.479776	5.339137	1.986071
C	0.326225	5.571945	1.237388
C	-0.388636	4.504488	0.685318
C	0.033607	3.178770	0.875521
C	1.203964	2.962487	1.626834
C	1.919071	4.026914	2.176562
H	2.037749	6.171767	2.407205
H	-0.021565	6.589039	1.073222
H	-1.274381	4.716281	0.098174
H	1.555261	1.942494	1.750199
H	2.833400	3.826712	2.728482
C	-3.925232	3.890536	-2.584421
C	-4.086890	3.878689	-1.196802
C	-3.172135	3.198245	-0.392553
C	-2.079192	2.522399	-0.960593
C	-1.930931	2.535849	-2.353303
C	-2.847736	3.215546	-3.159378
H	-4.640521	4.416818	-3.211706
H	-4.930725	4.390243	-0.740970
H	-3.311091	3.192210	0.685393
H	-1.098201	1.988190	-2.788115
H	-2.721047	3.211782	-4.239482
C	-0.991295	-4.472122	2.850541
C	-1.921472	-4.559840	1.811204
C	-1.861812	-3.665191	0.742620
C	-0.865952	-2.674721	0.690278
C	0.056573	-2.592862	1.739418
C	-0.006556	-3.484618	2.813683
H	-1.042210	-5.164953	3.686870
H	-2.698771	-5.319470	1.837664
H	-2.593219	-3.740298	-0.058126
H	0.803834	-1.803445	1.701379
H	0.711733	-3.402571	3.626304
C	0.582423	-4.421638	-4.226749
C	0.404224	-4.926961	-2.940038
C	-0.019793	-4.090405	-1.901557
C	-0.268342	-2.726951	-2.125152
C	-0.061609	-2.226828	-3.427432

C	0.346271	-3.064736	-4.466356
H	0.906768	-5.073826	-5.033698
H	0.592363	-5.978255	-2.735774
H	-0.154023	-4.511832	-0.912243
H	0.484673	-2.654539	-5.464031
C	-4.941097	-2.375213	3.253554
C	-4.356925	-1.753650	2.172253
H	-5.672171	-3.162782	3.090001
H	-4.631558	-2.060502	1.170457
C	-4.596918	-2.001787	4.573995
C	-3.661871	-1.014073	4.777913
H	-5.067203	-2.497490	5.419198
H	-3.379515	-0.717839	5.785791
C	-6.715044	1.155301	0.020240
C	-5.434552	0.790513	0.372597
H	-7.317341	1.737361	0.713023
H	-5.043861	1.091701	1.336808
C	-7.253253	0.782328	-1.233946
C	-6.485440	0.053419	-2.111341
H	-8.265649	1.074730	-1.499915
H	-6.879245	-0.237871	-3.082534
H	-0.204118	-1.164107	-3.604924
C	4.620741	2.125688	-2.140495
H	4.352433	3.150182	-2.430964
H	5.066597	2.186204	-1.137903
C	4.707895	-0.779106	-2.696807
H	4.955816	-1.806669	-2.399723
H	4.245023	-0.841655	-3.693914
C	5.979079	0.081170	-2.778276
H	6.498652	0.050147	-1.810128
H	6.669332	-0.341261	-3.519136
C	5.639598	1.537351	-3.129995
H	5.225982	1.577745	-4.148457
H	6.549675	2.149988	-3.139359
C	4.736609	0.702396	2.189093
O	4.613374	1.721490	1.513656
C	3.640092	0.296381	3.150061
H	2.838783	-0.181830	2.566099
H	3.969483	-0.376912	3.944089
H	3.213020	1.199379	3.593902
C	8.281192	-1.679840	1.651062
C	8.208383	-0.378013	1.144094
C	7.052802	0.375756	1.327201
C	5.958113	-0.152948	2.033122

C	6.044348	-1.457771	2.544015
C	7.196875	-2.219158	2.345561
H	9.181860	-2.270469	1.506359
H	9.053758	0.045587	0.608711
H	6.976303	1.386817	0.941001
H	5.208551	-1.891747	3.083183
H	7.248786	-3.231499	2.736455

Tsf₁

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.146063	0.499344	0.338412
H	-1.797861	-0.072982	-1.278034
H	-0.846144	1.028338	1.879845
N	-2.591157	2.136326	0.132033
H	-2.164981	3.061460	0.149486
H	-3.029062	2.013374	-0.796189
N	-3.015787	-0.372480	1.193186
H	-3.272202	-1.234157	0.711644
H	-2.812425	-0.622691	2.160160
P	0.673993	1.726288	-0.384642
P	0.176156	-1.319177	0.853385
C	-4.154400	0.582606	1.131888
H	-4.607584	0.448196	0.145292
C	-3.623350	2.019276	1.185583
H	-3.115147	2.176505	2.145392
C	4.441424	-0.280212	2.602173
C	3.428039	-0.852029	3.406609
C	2.206624	-1.174586	2.870972
C	1.902888	-0.954759	1.498148
C	2.889700	-0.424235	0.659173
C	4.176599	-0.069244	1.210705
H	3.630018	-1.038812	4.459058
H	1.462747	-1.623820	3.515713
C	3.412705	-0.955261	-3.113308
C	2.601803	0.079080	-3.640252
C	1.863621	0.882742	-2.809034
C	1.897646	0.733049	-1.392989
C	2.707836	-0.258474	-0.828392
C	3.461068	-1.136879	-1.692794

H	2.569271	0.228664	-4.717246
H	1.245237	1.660201	-3.241478
C	-0.566159	5.218002	-3.275690
C	0.524174	5.400123	-2.423020
C	0.922673	4.381767	-1.553949
C	0.239663	3.153677	-1.521521
C	-0.863049	2.991483	-2.377061
C	-1.261336	4.008578	-3.247013
H	-0.874735	6.014804	-3.947873
H	1.068960	6.341108	-2.427682
H	1.765983	4.557836	-0.897129
H	-1.434482	2.071996	-2.354375
H	-2.124330	3.845768	-3.886994
C	3.295215	4.151508	2.639155
C	3.819550	3.797517	1.394637
C	3.056901	3.041024	0.503800
C	1.759201	2.621206	0.839044
C	1.247672	2.978871	2.093836
C	2.007992	3.738648	2.985718
H	3.888967	4.738723	3.335138
H	4.826253	4.100108	1.118993
H	3.478560	2.773223	-0.460432
H	0.255776	2.634115	2.369126
H	1.593693	4.002634	3.955837
C	1.183243	-4.746223	-2.163459
C	1.620082	-4.843317	-0.839039
C	1.335383	-3.823023	0.068115
C	0.590440	-2.699040	-0.328722
C	0.172993	-2.606013	-1.660063
C	0.467364	-3.621935	-2.574067
H	1.412155	-5.538178	-2.871829
H	2.190851	-5.710253	-0.515572
H	1.690693	-3.904181	1.092280
H	-0.367895	-1.716974	-1.968358
H	0.142591	-3.529557	-3.607457
C	-2.127941	-3.514114	4.310501
C	-1.859748	-4.191339	3.122357
C	-1.125188	-3.574707	2.103575
C	-0.645211	-2.263465	2.246853
C	-0.950742	-1.582383	3.443738
C	-1.669583	-2.202719	4.466460
H	-2.693213	-3.996486	5.103526
H	-2.219011	-5.207618	2.980734
H	-0.929990	-4.128005	1.192134

H	-1.876758	-1.657149	5.383898
C	4.986150	-3.014941	-2.042141
C	4.265622	-2.202700	-1.194762
H	5.587439	-3.821268	-1.630363
H	4.303292	-2.381720	-0.127268
C	4.948348	-2.813927	-3.441848
C	4.171876	-1.804965	-3.962058
H	5.525807	-3.458541	-4.099223
H	4.122275	-1.641111	-5.036187
C	6.439191	0.830117	0.977772
C	5.221882	0.499259	0.425032
H	7.214313	1.261912	0.349984
H	5.053868	0.676590	-0.630216
C	6.690987	0.613847	2.353324
C	5.707246	0.070140	3.145184
H	7.656192	0.877538	2.777403
H	5.880583	-0.101986	4.205034
H	-0.636065	-0.549184	3.557739
C	-4.778189	3.026151	1.048550
H	-4.385887	4.050056	1.109821
H	-5.228336	2.917497	0.051429
C	-5.221094	0.331986	2.206226
H	-5.606265	-0.691251	2.110401
H	-4.754846	0.407081	3.200985
C	-6.369526	1.350118	2.099524
H	-6.911753	1.181204	1.158225
H	-7.091251	1.187741	2.909672
C	-5.846133	2.794381	2.130527
H	-5.411978	3.002791	3.119509
H	-6.674355	3.501427	1.998702
C	-3.126588	0.047801	-2.495041
O	-3.563705	1.223637	-2.421379
C	-2.224332	-0.327621	-3.671995
H	-1.777581	-1.318471	-3.570858
H	-2.853186	-0.331507	-4.574450
H	-1.435122	0.413366	-3.808830
C	-5.832132	-3.095841	-1.216807
C	-6.300989	-1.827554	-1.564266
C	-5.402304	-0.829064	-1.946164
C	-4.022087	-1.078651	-1.992061
C	-3.562942	-2.360665	-1.652808
C	-4.459169	-3.357406	-1.261921
H	-6.527983	-3.875515	-0.917768
H	-7.367294	-1.615661	-1.542673

H	-5.751532	0.161455	-2.220859
H	-2.499428	-2.574436	-1.672013
H	-4.083695	-4.342018	-0.994181

TSu₁

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.310167	-0.670540	0.194225
H	-1.981476	0.680928	-0.934131
H	-1.032614	-1.928730	1.218145
N	-3.129064	-0.249524	1.328382
H	-2.958809	0.061414	2.283431
H	-3.604800	0.514083	0.818642
N	-2.808332	-2.055245	-0.731529
H	-2.858745	-1.962345	-1.744585
H	-2.453508	-2.993402	-0.548752
P	0.075531	0.617870	1.505886
P	0.465737	-1.489686	-1.049598
C	-4.164093	-1.886829	-0.139533
H	-4.629776	-1.053322	-0.675822
C	-4.014684	-1.436463	1.319849
H	-3.495991	-2.223082	1.883580
C	4.563510	-1.969942	1.244820
C	3.834511	-3.090714	0.782766
C	2.659746	-2.925923	0.093224
C	2.126649	-1.637089	-0.190833
C	2.833137	-0.500689	0.218389
C	4.064702	-0.658490	0.956874
H	4.218544	-4.089436	0.978616
H	2.133662	-3.806517	-0.252246
C	2.963728	3.018769	-1.320778
C	1.905981	3.649682	-0.623326
C	1.121843	2.941212	0.252000
C	1.351187	1.562212	0.516972
C	2.416188	0.909937	-0.116136
C	3.222074	1.631333	-1.071239
H	1.713563	4.706286	-0.794705
H	0.310799	3.450617	0.757195
C	-2.396831	3.833077	3.870892
C	-1.457592	3.060531	4.553800

C	-0.685798	2.116786	3.870460
C	-0.842223	1.922569	2.487468
C	-1.812430	2.690268	1.819388
C	-2.571117	3.644346	2.498522
H	-2.992452	4.570201	4.403485
H	-1.318516	3.189220	5.624411
H	0.036441	1.532042	4.426761
H	-1.975361	2.533935	0.759516
H	-3.299319	4.232315	1.947680
C	2.514164	-1.199135	5.059812
C	2.847779	0.058022	4.550772
C	2.143449	0.582602	3.467091
C	1.094449	-0.137560	2.870658
C	0.770126	-1.396765	3.391104
C	1.474593	-1.924003	4.476370
H	3.064341	-1.610522	5.902276
H	3.662035	0.627610	4.990716
H	2.411975	1.562494	3.082329
H	-0.032386	-1.961643	2.927113
H	1.210233	-2.905199	4.863353
C	1.744472	0.276430	-5.178810
C	2.490553	-0.765470	-4.619570
C	2.136393	-1.292247	-3.377628
C	1.023482	-0.790749	-2.681750
C	0.290037	0.255014	-3.247387
C	0.645787	0.789194	-4.488862
H	2.024701	0.688854	-6.144662
H	3.351937	-1.163690	-5.149976
H	2.724008	-2.100906	-2.950576
H	-0.554015	0.640012	-2.684236
H	0.067423	1.606020	-4.914063
C	-0.818222	-5.855775	-2.226203
C	-0.520284	-4.930403	-3.224862
C	-0.082930	-3.643446	-2.892258
C	0.059097	-3.249741	-1.552340
C	-0.267527	-4.191204	-0.554496
C	-0.687981	-5.479797	-0.885946
H	-1.152602	-6.856806	-2.485568
H	-0.623521	-5.204911	-4.271700
H	0.146973	-2.946748	-3.690177
H	-0.919238	-6.189088	-0.094959
C	5.047961	1.736825	-2.692703
C	4.287640	1.021147	-1.794983
H	5.849888	1.240541	-3.232943

H	4.496229	-0.030406	-1.640428
C	4.794405	3.110011	-2.921590
C	3.769813	3.732791	-2.248248
H	5.405100	3.664514	-3.629160
H	3.556118	4.786109	-2.415465
C	5.993212	0.270202	2.139466
C	4.823424	0.449899	1.435176
H	6.547221	1.137034	2.490196
H	4.469668	1.455491	1.243639
C	6.480462	-1.029973	2.412071
C	5.774280	-2.124753	1.972610
H	7.406001	-1.158373	2.966963
H	6.130401	-3.132220	2.175375
H	-0.204168	-3.897539	0.488954
C	-5.395167	-1.184664	1.948389
H	-5.274060	-0.881406	2.997056
H	-5.874207	-0.345958	1.424787
C	-5.043634	-3.140181	-0.250374
H	-5.159856	-3.420964	-1.305693
H	-4.538131	-3.982678	0.247472
C	-6.420550	-2.913149	0.398362
H	-6.969831	-2.157155	-0.180275
H	-7.012715	-3.835544	0.352551
C	-6.283852	-2.435782	1.852178
H	-5.845835	-3.241322	2.460096
H	-7.273387	-2.227567	2.277364
C	-3.444250	1.488707	-1.521417
O	-4.364137	1.204521	-0.707389
C	-3.457067	0.795507	-2.887002
H	-2.534285	0.921296	-3.454712
H	-3.667062	-0.270288	-2.771375
H	-4.278795	1.235670	-3.470141
C	-2.329943	5.675549	-1.705499
C	-1.483781	4.723391	-2.280228
C	-1.798547	3.366183	-2.208873
C	-2.960604	2.933650	-1.555041
C	-3.801459	3.898346	-0.978597
C	-3.491328	5.257224	-1.053122
H	-2.085551	6.733042	-1.766791
H	-0.573065	5.036712	-2.784430
H	-1.117163	2.641880	-2.640084
H	-4.703875	3.554602	-0.483667
H	-4.160558	5.990180	-0.608509

Pf ₁			

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.86274700	0.44357500	-0.84415400
H	0.24415000	0.74325900	-2.26531500
N	2.43579100	1.77387300	-0.63504900
H	2.20665900	2.76517000	-0.55328200
N	2.52570300	-0.61554100	-1.88651800
H	2.63405200	-1.60406900	-1.65974800
H	2.25218500	-0.59022600	-2.86959400
P	-0.79480700	1.79251300	0.05177300
P	-0.53013900	-1.42992400	-0.91316900
C	3.81116900	0.11163500	-1.70053600
H	4.18183000	-0.17901000	-0.71044500
C	3.48090800	1.60524600	-1.64876700
H	3.11322400	1.89363300	-2.65422700
C	-5.12795900	-0.67736000	-1.63081500
C	-4.33336500	-1.36429500	-2.57885300
C	-3.00564500	-1.60992800	-2.33361300
C	-2.37415400	-1.19393000	-1.12745800
C	-3.13023800	-0.53683500	-0.15115700
C	-4.52590900	-0.26314100	-0.39877700
H	-4.78980500	-1.70102300	-3.50700700
H	-2.43003600	-2.14694300	-3.07692100
C	-2.68472200	-0.57725700	3.66260600
C	-1.84727200	0.54798900	3.84658200
C	-1.38290900	1.25952600	2.76949600
C	-1.72664600	0.91729700	1.42956300
C	-2.58713000	-0.16627200	1.20610900
C	-3.06001300	-0.94227600	2.32910700
H	-1.57447600	0.84605100	4.85647800
H	-0.74398400	2.11486200	2.94835300
C	0.82378800	5.71836300	2.05582300
C	-0.31285400	5.78132500	1.24901000
C	-0.82528100	4.62537600	0.65476600
C	-0.21082600	3.37810700	0.85645200
C	0.94307400	3.33439600	1.65943900
C	1.45158600	4.48840900	2.25750000
H	1.22107300	6.62039300	2.51434100
H	-0.80719300	6.73401900	1.07549600
H	-1.70542300	4.70746800	0.02851500

H	1.47405400	2.40282900	1.81479800
H	2.34961600	4.41347000	2.86444100
C	-4.05765000	3.63657600	-2.73205500
C	-4.31564000	3.47781100	-1.36905000
C	-3.35665000	2.89632100	-0.53901200
C	-2.12802400	2.45561600	-1.05577900
C	-1.87964900	2.62472000	-2.42533400
C	-2.83655900	3.21079700	-3.25683700
H	-4.80440100	4.08823900	-3.38003800
H	-5.26577100	3.79889300	-0.95090700
H	-3.56573700	2.78582500	0.52064800
H	-0.93220700	2.29139000	-2.83555300
H	-2.62578600	3.33286000	-4.31633600
C	-0.26383300	-4.52880200	2.57271400
C	-1.22186100	-4.70861200	1.57114300
C	-1.33026200	-3.78441900	0.53170400
C	-0.47654400	-2.67071000	0.47208000
C	0.47470500	-2.50020500	1.48502200
C	0.58224800	-3.42004000	2.53092300
H	-0.18471000	-5.24588900	3.38558900
H	-1.88958100	-5.56570100	1.60408200
H	-2.08215400	-3.93028700	-0.23961500
H	1.12476100	-1.62969000	1.45449300
H	1.31977700	-3.26523800	3.31436600
C	0.90981000	-3.91232200	-4.62894500
C	0.91343000	-4.50404100	-3.36724900
C	0.43764200	-3.80279700	-2.25334300
C	-0.04461100	-2.49039300	-2.37628500
C	-0.02116700	-1.89949100	-3.65628800
C	0.43680500	-2.60399000	-4.76950100
H	1.27502700	-4.45940800	-5.49397600
H	1.28400300	-5.51825000	-3.24114600
H	0.44635400	-4.29006600	-1.28483800
H	0.42984500	-2.12801400	-5.74693300
C	-4.34589600	-2.80022300	3.26355900
C	-3.90135400	-2.08306700	2.17525100
H	-4.98371800	-3.66692700	3.11104700
H	-4.19140900	-2.39563000	1.17973300
C	-3.97952700	-2.42293700	4.57711200
C	-3.16204400	-1.33375800	4.76683100
H	-4.34080700	-2.99493100	5.42755100
H	-2.86455800	-1.03106700	5.76819200
C	-6.68458000	0.66596100	0.27712000
C	-5.35608500	0.41616600	0.54060000

H	-7.28977000	1.18635300	1.01482200
H	-4.93165800	0.74368200	1.48200800
C	-7.26992000	0.25028200	-0.94250100
C	-6.50186400	-0.40703900	-1.87444500
H	-8.31997300	0.45100300	-1.13738300
H	-6.93368900	-0.73300900	-2.81790500
H	-0.36167200	-0.87489600	-3.77517900
C	4.76347500	2.41695400	-1.38423900
H	4.52276200	3.48861200	-1.38873200
H	5.12971000	2.17975800	-0.37725000
C	4.87624700	-0.21868500	-2.75285300
H	5.10323900	-1.29352600	-2.73948700
H	4.47996600	0.01198600	-3.75414400
C	6.15369200	0.60298000	-2.50210200
H	6.60478400	0.27739000	-1.55460800
H	6.89026900	0.39812800	-3.28941600
C	5.84934100	2.10854700	-2.42975100
H	5.51478200	2.45776500	-3.41804700
H	6.76612700	2.66559800	-2.19800700
C	4.88800700	-1.94213400	1.81197200
C	6.05286400	-2.64750500	1.50035900
C	4.91662800	-0.55422100	2.00212800
H	3.94410200	-2.47745900	1.90588300
C	7.26764000	-1.97032900	1.37467000
H	6.01057000	-3.72400500	1.35289700
C	6.13988900	0.11590400	1.87215500
C	7.30652200	-0.58579400	1.56191700
H	8.17560200	-2.51576100	1.13054000
H	6.15817200	1.19307400	2.00612300
H	8.24865600	-0.05117200	1.46646000
C	3.65045700	0.21032600	2.38661400
H	2.78871400	-0.33830000	1.96837400
O	3.65273900	1.53919400	1.90568600
H	3.25416200	1.55607500	0.98041300
C	3.48633500	0.26222600	3.91146200
H	3.49963400	-0.74226900	4.34948300
H	4.30554200	0.84059300	4.35297000
H	2.54035700	0.75010300	4.16964900

Pu1

Coordinates (Angstroms)		
X	Y	Z

Ru	-0.73783700	1.09799700	-0.73527000
H	-2.63827000	-1.26204000	2.11249500
H	0.00104000	1.73907400	-1.97669700
N	-2.69159700	0.70467900	-1.25674100
H	-2.88362900	-0.03461700	-1.93190200
H	-3.34046300	0.26647700	0.46814300
N	-1.71802900	3.07359200	-0.40633200
H	-1.47200200	3.55605600	0.45801700
H	-1.34893400	3.65263000	-1.16161800
P	0.16214700	-0.93309300	-1.36206500
P	1.15179100	1.71766200	0.47088400
C	-3.19592100	2.95083000	-0.53436400
H	-3.54775500	2.54736000	0.42197200
C	-3.46913800	1.89431500	-1.60936500
H	-3.13261200	2.31747600	-2.57812900
C	5.29862000	-0.03797100	-0.91214800
C	5.02968300	1.35079500	-0.94497100
C	3.83267800	1.84288600	-0.48931100
C	2.81879800	0.99118500	0.03456100
C	3.05373900	-0.38607600	0.10912000
C	4.30599900	-0.91932300	-0.37346100
H	5.78736000	2.02738000	-1.33399800
H	3.66025400	2.91140400	-0.52347000
C	1.68401400	-2.95550200	2.61456900
C	0.53712800	-3.41420400	1.92510300
C	0.17216700	-2.85877100	0.72457600
C	0.92311700	-1.81378500	0.11315900
C	2.09397500	-1.36488400	0.73981000
C	2.47751900	-1.92406800	2.01520700
H	-0.05195900	-4.22096800	2.35591700
H	-0.70562100	-3.24240100	0.22107200
C	-3.02347100	-3.90953400	-3.11643400
C	-1.83286000	-3.68889600	-3.80809500
C	-0.85996600	-2.83097700	-3.28907400
C	-1.05587400	-2.17131100	-2.06416100
C	-2.27421900	-2.38772400	-1.39319500
C	-3.24248800	-3.25400100	-1.90363500
H	-3.77768200	-4.57944300	-3.52131100
H	-1.65294300	-4.18525700	-4.75853400
H	0.05280600	-2.67921400	-3.85187200
H	-2.47990400	-1.86491600	-0.46634500
H	-4.16633400	-3.40403500	-1.35283200
C	3.38454000	-1.20391400	-4.73034400
C	3.23834100	-2.25109900	-3.81792600

C	2.29838500	-2.15782600	-2.79178300
C	1.49199100	-1.01608400	-2.65467500
C	1.64441700	0.02520800	-3.58033200
C	2.58411000	-0.06742000	-4.60975100
H	4.11829000	-1.27464900	-5.52917600
H	3.86113200	-3.13784400	-3.89857300
H	2.19017500	-2.98146000	-2.09215000
H	1.02174000	0.90886000	-3.48760500
H	2.68910600	0.75148400	-5.31701600
C	0.86546500	1.26997900	5.10833500
C	2.11162200	1.49985400	4.52067600
C	2.21968500	1.61316000	3.13441600
C	1.08527800	1.49929600	2.31431500
C	-0.16037700	1.26408600	2.91473700
C	-0.26823800	1.15207800	4.30345100
H	0.78051200	1.17889600	6.18812800
H	3.00014000	1.58551900	5.14092500
H	3.19330800	1.79232700	2.68612300
H	-1.04924200	1.16400100	2.29459100
H	-1.23911800	0.96823200	4.75534100
C	1.67199900	6.36234300	0.00227700
C	1.62090100	5.80741700	1.27993600
C	1.50891700	4.42274300	1.44741500
C	1.43572500	3.56501400	0.33903500
C	1.47046200	4.14378400	-0.94549800
C	1.59963700	5.52239200	-1.11303800
H	1.76269300	7.43771900	-0.12627000
H	1.67102300	6.44933700	2.15590900
H	1.47857800	4.01566900	2.45181800
H	1.63722500	5.94155200	-2.11552400
C	3.98329800	-2.04748700	3.93785700
C	3.63654000	-1.49425000	2.72546900
H	4.87219700	-1.69488800	4.45435400
H	4.25418900	-0.71187400	2.30219800
C	3.19457000	-3.06864400	4.51863800
C	2.06735000	-3.50896900	3.86605500
H	3.48045700	-3.49876900	5.47474100
H	1.44756200	-4.29212900	4.29667800
C	5.81195000	-2.79384400	-0.81942100
C	4.61073800	-2.31194200	-0.34861200
H	6.01258400	-3.86151300	-0.78554500
H	3.87971700	-3.00620700	0.04741300
C	6.78689700	-1.91389800	-1.34643900
C	6.52911300	-0.56402200	-1.39070600

H	7.73159000	-2.30625200	-1.71325400
H	7.26514800	0.12782600	-1.79377800
H	1.39218500	3.50165900	-1.81808200
C	-4.98656200	1.65584300	-1.72383100
H	-5.18343500	0.91430700	-2.50958700
H	-5.34315100	1.22357100	-0.77976400
C	-3.91318200	4.27481300	-0.82592200
H	-3.71211500	5.00198600	-0.02694200
H	-3.51454500	4.70666300	-1.75718300
C	-5.42839700	4.04577800	-0.97363900
H	-5.83834500	3.73487800	-0.00201100
H	-5.92573600	4.98813800	-1.23603800
C	-5.73796500	2.96477500	-2.02249500
H	-5.44632300	3.33290300	-3.01728700
H	-6.81935800	2.78175900	-2.06395200
C	-3.65703700	-0.83888500	2.13173000
O	-3.70231900	0.37086000	1.39670900
C	-3.99891100	-0.48379300	3.58437500
H	-3.95173500	-1.36725500	4.22986100
H	-3.29860700	0.26941900	3.95988400
H	-5.01123600	-0.06844300	3.63767800
C	-6.43789900	-3.88209000	0.77066800
C	-5.23493900	-4.24806300	1.37962400
C	-4.33331800	-3.26461000	1.79189300
C	-4.61852100	-1.90485600	1.61024700
C	-5.82646100	-1.54884600	0.99807200
C	-6.72860400	-2.52861700	0.57958000
H	-7.14086300	-4.64474900	0.44548000
H	-4.99556600	-5.29827900	1.52741400
H	-3.39401000	-3.55535400	2.25935700
H	-6.04676200	-0.49620800	0.85112900
H	-7.66116400	-2.23533400	0.10354200

ABS₂

Coordinates (Angstroms)			
	X	Y	Z
Ru	0.442026	1.059012	0.412377
H	1.277788	-0.129395	-0.511439
H	-0.168494	2.338849	1.373391
N	2.213413	1.097191	1.768114
H	1.941173	0.964610	2.740083

H	2.844938	0.331583	1.523498
N	1.752365	2.600326	-0.530699
H	1.842384	2.440548	-1.531862
H	1.279774	3.496864	-0.419158
P	-0.710011	-0.547477	1.546730
P	-1.231962	1.348882	-1.113051
C	3.090896	2.637970	0.104633
H	3.651899	1.789647	-0.307901
C	2.922666	2.385806	1.609655
H	2.251128	3.156518	2.011110
C	-5.588647	0.909453	0.640559
C	-5.082028	2.158054	0.208616
C	-3.827395	2.253450	-0.338785
C	-2.989632	1.114879	-0.504704
C	-3.462719	-0.143560	-0.116054
C	-4.773906	-0.257487	0.477696
H	-5.701876	3.045682	0.315094
H	-3.471238	3.224294	-0.659714
C	-2.560777	-3.607793	-1.520739
C	-1.453643	-3.941724	-0.703993
C	-0.976135	-3.053039	0.225839
C	-1.573732	-1.776447	0.425016
C	-2.691627	-1.420083	-0.337522
C	-3.187227	-2.331981	-1.341509
H	-0.984484	-4.916204	-0.822200
H	-0.125191	-3.337125	0.832689
C	2.310508	-3.076997	4.114270
C	1.109119	-2.664423	4.689298
C	0.176499	-1.939560	3.940750
C	0.425220	-1.611490	2.598158
C	1.650011	-2.022702	2.037761
C	2.578699	-2.750061	2.782883
H	3.035344	-3.637734	4.699152
H	0.890995	-2.902616	5.727582
H	-0.745705	-1.627713	4.416369
H	1.870660	-1.742255	1.011970
H	3.521069	-3.042008	2.326701
C	-3.922600	0.487113	4.781254
C	-3.843378	-0.814536	4.279825
C	-2.908708	-1.126712	3.292231
C	-2.036314	-0.145545	2.792342
C	-2.128804	1.157190	3.298063
C	-3.065621	1.470917	4.286210
H	-4.653632	0.731930	5.547927

H	-4.515631	-1.584334	4.650037
H	-2.858194	-2.141900	2.907410
H	-1.465986	1.915909	2.888740
H	-3.127978	2.488325	4.665295
C	-1.287036	-0.921270	-5.204752
C	-2.393352	-0.156928	-4.824419
C	-2.397653	0.502730	-3.595165
C	-1.294283	0.415492	-2.729130
C	-0.194080	-0.357810	-3.118174
C	-0.190639	-1.022186	-4.347816
H	-1.286055	-1.440253	-6.160127
H	-3.255855	-0.080728	-5.481891
H	-3.264690	1.092836	-3.309099
H	0.643081	-0.441005	-2.428471
H	0.668582	-1.625416	-4.631979
C	-0.992085	5.820486	-2.563273
C	-1.018401	4.796354	-3.508402
C	-1.130217	3.461070	-3.104989
C	-1.210374	3.119340	-1.745809
C	-1.160656	4.165617	-0.801584
C	-1.064665	5.498170	-1.204894
H	-0.910804	6.857690	-2.878492
H	-0.954667	5.030241	-4.568396
H	-1.153425	2.686725	-3.862809
H	-1.041427	6.285524	-0.455025
C	-4.756779	-2.916746	-3.122725
C	-4.294597	-2.021723	-2.183399
H	-5.602963	-2.648156	-3.749871
H	-4.779087	-1.058134	-2.083907
C	-4.139861	-4.179787	-3.281969
C	-3.061101	-4.511824	-2.496099
H	-4.516017	-4.878786	-4.024386
H	-2.569351	-5.475615	-2.608328
C	-6.567699	-1.580421	1.483659
C	-5.311310	-1.499692	0.925370
H	-6.947417	-2.543460	1.815141
H	-4.715326	-2.398765	0.827150
C	-7.367778	-0.422855	1.631957
C	-6.881585	0.795437	1.219461
H	-8.358545	-0.499605	2.072110
H	-7.479856	1.697072	1.330235
H	-1.174435	3.913038	0.255347
C	4.274897	2.442197	2.343240
H	4.109315	2.313131	3.421286

H	4.891000	1.595019	2.012808
C	3.853456	3.942635	-0.173614
H	3.998427	4.061580	-1.255686
H	3.232738	4.790546	0.155303
C	5.202349	3.987379	0.562164
H	5.864513	3.208759	0.156752
H	5.698032	4.948301	0.376183
C	5.015705	3.760664	2.069389
H	4.444625	4.599092	2.494737
H	5.988121	3.756794	2.577338
C	5.117071	-1.178507	-0.361639
O	4.740779	-0.642257	0.679903
C	4.102806	-1.639602	-1.392645
H	3.178070	-1.079191	-1.208311
H	4.448034	-1.404893	-2.407695
C	9.344970	-1.785996	-0.907238
C	8.843399	-1.268435	0.291499
C	7.473963	-1.079668	0.448374
C	6.582400	-1.406304	-0.587896
C	7.096799	-1.927269	-1.786355
C	8.470216	-2.114339	-1.944572
H	9.522556	-1.014332	1.100780
H	7.065169	-0.680969	1.370805
H	6.430452	-2.186847	-2.602202
H	8.856562	-2.515791	-2.877294
C	3.812709	-3.155659	-1.290278
H	4.734264	-3.727095	-1.461773
H	3.489988	-3.385182	-0.267076
C	2.729491	-3.600366	-2.278333
H	3.026755	-3.390500	-3.313744
H	2.545521	-4.677860	-2.197387
H	1.783730	-3.081706	-2.086464
H	10.414602	-1.932955	-1.031415

INTf₂

Coordinates (Angstroms)			
	X	Y	Z
Ru	-0.642856	-1.104636	0.055845
H	-1.442102	0.416534	0.175635
H	-0.083774	-2.723746	-0.048445

N	-2.143665	-1.873106	1.503514
H	-1.692405	-2.365268	2.271973
H	-2.636753	-1.077977	1.910649
N	-2.316143	-1.753160	-1.274457
H	-2.532057	-1.035598	-1.963152
H	-1.988859	-2.567945	-1.792384
P	0.891097	-0.490566	1.631415
P	0.721265	-0.494206	-1.667766
C	-3.529887	-2.084826	-0.491902
H	-3.996043	-1.126136	-0.231222
C	-3.103857	-2.763774	0.817038
H	-2.545838	-3.675292	0.564537
C	5.284854	-1.435002	-0.924905
C	4.520457	-2.152951	-1.874961
C	3.206878	-1.830253	-2.105678
C	2.560461	-0.764928	-1.418152
C	3.289135	-0.010276	-0.491405
C	4.666426	-0.349952	-0.223657
H	4.988439	-2.966996	-2.424355
H	2.652535	-2.399978	-2.840535
C	2.812127	3.667290	0.524326
C	1.878623	3.529010	1.579628
C	1.379432	2.296433	1.916194
C	1.783536	1.110153	1.241047
C	2.724559	1.198563	0.209612
C	3.238244	2.491941	-0.175310
H	1.561626	4.416125	2.123970
H	0.663957	2.224167	2.726162
C	-1.353600	0.270567	5.692451
C	-0.138087	-0.413597	5.708145
C	0.571506	-0.628863	4.522388
C	0.082537	-0.157521	3.293272
C	-1.148298	0.526126	3.296306
C	-1.859701	0.739021	4.477652
H	-1.906587	0.427278	6.615340
H	0.262889	-0.791718	6.645548
H	1.505579	-1.176260	4.564842
H	-1.551367	0.868436	2.347450
H	-2.819871	1.245177	4.431376
C	4.289262	-3.373421	3.046189
C	4.359172	-2.015930	3.368933
C	3.367358	-1.140483	2.925332
C	2.288203	-1.606998	2.156701
C	2.232590	-2.968523	1.832927

C	3.226169	-3.845612	2.275421
H	5.064174	-4.055263	3.387824
H	5.190806	-1.636542	3.957165
H	3.434282	-0.085901	3.179256
H	1.409510	-3.316263	1.213222
H	3.170760	-4.899132	2.011252
C	0.591976	3.793919	-3.535701
C	1.584425	2.896231	-3.938139
C	1.647234	1.623698	-3.369921
C	0.713940	1.223966	-2.398067
C	-0.273226	2.133138	-1.999021
C	-0.331974	3.410373	-2.563254
H	0.547422	4.788503	-3.972639
H	2.315041	3.190698	-4.687344
H	2.427293	0.936024	-3.687062
H	-0.973643	1.820660	-1.226416
H	-1.097364	4.111258	-2.236560
C	-0.477684	-3.157364	-5.357263
C	-0.425417	-1.772184	-5.502512
C	-0.029826	-0.960833	-4.433301
C	0.315765	-1.516283	-3.191297
C	0.236115	-2.917821	-3.054180
C	-0.143464	-3.727664	-4.125402
H	-0.779856	-3.786759	-6.190498
H	-0.690157	-1.312704	-6.451827
H	0.005762	0.112643	-4.578257
H	-0.182836	-4.806642	-3.994895
C	4.657351	3.908254	-1.574635
C	4.170037	2.664315	-1.239811
H	5.366776	4.004881	-2.392462
H	4.497511	1.796600	-1.799331
C	4.242301	5.060911	-0.867085
C	3.333839	4.937267	0.158063
H	4.637223	6.036601	-1.137891
H	2.997380	5.812830	0.708972
C	6.776378	0.012761	0.958025
C	5.462104	0.353449	0.727267
H	7.354868	0.569664	1.690638
H	5.021194	1.172043	1.282899
C	7.380101	-1.055550	0.253638
C	6.643287	-1.763342	-0.666716
H	8.418640	-1.313748	0.443286
H	7.088287	-2.590562	-1.215206
H	0.454921	-3.359050	-2.085285

C	-4.326795	-3.120987	1.677923
H	-3.995925	-3.635284	2.589836
H	-4.813871	-2.188515	1.999107
C	-4.540417	-2.946091	-1.267610
H	-4.856988	-2.413850	-2.174012
H	-4.038005	-3.867564	-1.600633
C	-5.759432	-3.312238	-0.405285
H	-6.324050	-2.397647	-0.176318
H	-6.434991	-3.965395	-0.971635
C	-5.331168	-3.990340	0.904452
H	-4.870932	-4.962935	0.676443
H	-6.207451	-4.199211	1.530455
C	-4.434791	1.788923	1.219436
O	-4.451640	0.978925	2.140751
C	-3.530982	3.009625	1.269557
H	-2.976188	3.111993	0.329270
H	-2.794350	2.834949	2.058125
C	-7.174577	1.199976	-2.053761
C	-7.380056	0.568356	-0.822850
C	-6.480587	0.769138	0.221104
C	-5.370496	1.614699	0.056760
C	-5.179344	2.252215	-1.179339
C	-6.072031	2.038123	-2.230776
H	-7.873557	1.041049	-2.870576
H	-8.242924	-0.076542	-0.679536
H	-6.621475	0.285809	1.182513
H	-4.324572	2.902533	-1.332954
H	-5.906581	2.527285	-3.186679
C	-4.313727	4.308950	1.560489
H	-5.067277	4.472483	0.779830
H	-4.864777	4.188665	2.502461
C	-3.392125	5.529246	1.653895
H	-3.963722	6.439089	1.869305
H	-2.648042	5.403714	2.449213
H	-2.848668	5.688558	0.714584

TSf₂

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.020570	0.624570	-0.487970

H	1.805477	-0.241009	0.922398
H	0.593001	1.445452	-1.862211
N	2.471953	2.214714	-0.068953
H	2.044260	3.117119	0.132326
H	2.981171	1.916706	0.779661
N	2.820982	-0.024112	-1.639348
H	3.115820	-0.957791	-1.353442
H	2.545325	-0.086985	-2.618548
P	-0.742589	1.645251	0.600229
P	-0.330628	-1.081423	-1.251966
C	3.957567	0.922220	-1.478681
H	4.491756	0.601465	-0.579438
C	3.418226	2.329420	-1.200837
H	2.834815	2.664322	-2.067856
C	-4.733247	0.188766	-2.403627
C	-3.785626	-0.182479	-3.386119
C	-2.521705	-0.577194	-3.026433
C	-2.107674	-0.634419	-1.666166
C	-3.024618	-0.307243	-0.660267
C	-4.355451	0.120527	-1.023884
H	-4.072442	-0.155172	-4.435062
H	-1.828407	-0.865633	-3.805729
C	-3.222729	-1.578956	2.964324
C	-2.371258	-0.653280	3.615046
C	-1.711377	0.313705	2.900178
C	-1.868308	0.445185	1.490603
C	-2.718367	-0.433948	0.810643
C	-3.392492	-1.479311	1.545015
H	-2.245452	-0.718564	4.693585
H	-1.061721	1.004169	3.424840
C	0.698108	4.564000	3.992457
C	-0.458373	4.876548	3.275598
C	-0.917106	4.028432	2.265020
C	-0.230048	2.842955	1.951589
C	0.938565	2.549909	2.673852
C	1.397900	3.396839	3.684623
H	1.053819	5.229227	4.775332
H	-1.007853	5.788227	3.497340
H	-1.810537	4.304485	1.718089
H	1.512984	1.663706	2.435778
H	2.310933	3.137894	4.213996
C	-3.629245	4.535799	-1.682855
C	-4.043111	3.941193	-0.489337
C	-3.201707	3.048249	0.175628

C	-1.934398	2.729229	-0.339315
C	-1.534508	3.328739	-1.541253
C	-2.373626	4.225453	-2.206612
H	-4.284408	5.230044	-2.203000
H	-5.024716	4.162901	-0.079104
H	-3.537078	2.592906	1.102784
H	-0.567363	3.065398	-1.958347
H	-2.045554	4.677483	-3.139625
C	-1.069125	-5.057737	1.094367
C	-1.617995	-4.898817	-0.181512
C	-1.413231	-3.714223	-0.888618
C	-0.637842	-2.677723	-0.340449
C	-0.109185	-2.841726	0.943758
C	-0.323088	-4.023505	1.659099
H	-1.235337	-5.978221	1.647994
H	-2.213598	-5.694745	-0.621636
H	-1.856464	-3.596986	-1.874228
H	0.452525	-2.020774	1.378005
H	0.087729	-4.130321	2.659957
C	1.674853	-2.484842	-5.263840
C	1.498076	-3.397834	-4.225768
C	0.854116	-3.013589	-3.044485
C	0.376203	-1.705248	-2.871720
C	0.589311	-0.786231	-3.920165
C	1.217141	-1.173495	-5.104847
H	2.169236	-2.786217	-6.183564
H	1.858679	-4.418202	-4.329468
H	0.727569	-3.746398	-2.255898
H	1.353828	-0.446973	-5.902191
C	-4.883859	-3.413573	1.645085
C	-4.236356	-2.440551	0.916391
H	-5.519675	-4.132326	1.134803
H	-4.365140	-2.407316	-0.158465
C	-4.726410	-3.490215	3.048777
C	-3.906556	-2.591087	3.689920
H	-5.246523	-4.259871	3.612891
H	-3.765296	-2.640041	4.767300
C	-6.597461	0.900149	-0.433627
C	-5.335966	0.494431	-0.058561
H	-7.320873	1.177803	0.328602
H	-5.082179	0.459998	0.993811
C	-6.961198	0.959398	-1.799843
C	-6.042344	0.610917	-2.761433
H	-7.960296	1.279746	-2.083002

H	-6.301577	0.652296	-3.816898
H	0.275313	0.245118	-3.788196
C	4.573577	3.312023	-0.952409
H	4.171317	4.318392	-0.775017
H	5.102233	3.015372	-0.035097
C	4.934929	0.916427	-2.662364
H	5.332056	-0.096588	-2.806126
H	4.388233	1.179320	-3.581486
C	6.083091	1.916437	-2.442866
H	6.702397	1.572248	-1.602240
H	6.736018	1.936177	-3.324282
C	5.553600	3.326496	-2.137908
H	5.041453	3.722744	-3.027188
H	6.387229	4.008206	-1.929138
C	3.222368	-0.335424	2.054590
O	3.639830	0.842800	2.189946
C	2.407877	-0.960397	3.196138
H	2.001939	-1.932808	2.899080
H	1.561830	-0.308134	3.431305
C	5.856686	-3.069379	-0.051630
C	6.337650	-1.889267	0.518552
C	5.461431	-1.018052	1.169594
C	4.091835	-1.309909	1.266706
C	3.621879	-2.505433	0.701493
C	4.494911	-3.373255	0.042433
H	6.534913	-3.749260	-0.560832
H	7.396322	-1.647902	0.460688
H	5.819932	-0.096646	1.617897
H	2.565648	-2.747124	0.755131
C	4.110166	-4.290146	-0.397333
H	3.289632	-1.130549	4.449229
H	4.156511	-1.760034	4.206015
C	3.687724	-0.147407	4.727457
H	2.526642	-1.743698	5.627379
H	3.170862	-1.845420	6.508871
H	1.668015	-1.122497	5.911484
H	2.143933	-2.741653	5.378556

TSu₂

Coordinates (Angstroms)

X	Y	Z
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Ru	-1.070444	-0.808760	0.387293
H	-1.962609	0.642509	-0.416428
H	-0.582982	-2.176884	1.161989
N	-2.701930	-0.669717	1.832880
H	-2.391691	-0.496512	2.787683
H	-3.277905	0.133350	1.529507
N	-2.632030	-2.142360	-0.501631
H	-2.839302	-1.919265	-1.473778
H	-2.214445	-3.072390	-0.505604
P	0.449901	0.362828	1.658317
P	0.524245	-1.330881	-1.211211
C	-3.887243	-2.135207	0.296856
H	-4.454436	-1.259208	-0.035259
C	-3.536955	-1.891938	1.771564
H	-2.911540	-2.720426	2.130206
C	4.939097	-1.889559	0.367335
C	4.187960	-2.973401	-0.144434
C	2.916453	-2.779927	-0.622399
C	2.301614	-1.496281	-0.633101
C	3.021494	-0.390733	-0.166436
C	4.355914	-0.581475	0.354515
H	4.631949	-3.966379	-0.156281
H	2.373975	-3.631614	-1.011836
C	2.795714	3.319788	-1.145600
C	1.831509	3.777489	-0.216127
C	1.211103	2.902283	0.639324
C	1.526040	1.514939	0.651276
C	2.508338	1.026754	-0.219214
C	3.138285	1.928131	-1.153700
H	1.579060	4.835027	-0.191074
H	0.467131	3.283565	1.327361
C	-1.770576	3.036464	4.815615
C	-0.717136	2.223306	5.233004
C	-0.016801	1.441976	4.309657
C	-0.360465	1.453903	2.947082
C	-1.442241	2.258760	2.547470
C	-2.130372	3.051646	3.466629
H	-2.310848	3.646887	5.534814
H	-0.432330	2.193187	6.281869
H	0.797171	0.821261	4.663282
H	-1.749122	2.260590	1.508034
H	-2.950415	3.673491	3.119939
C	3.469514	-1.781897	4.514690

C	3.671481	-0.447917	4.153377
C	2.790130	0.178385	3.272153
C	1.692511	-0.514526	2.734252
C	1.500669	-1.851296	3.105874
C	2.382697	-2.480526	3.988248
H	4.157388	-2.272332	5.198799
H	4.519694	0.103682	4.549931
H	2.957330	1.217040	3.001059
H	0.659546	-2.393980	2.685431
H	2.219458	-3.520359	4.261180
C	1.050939	1.064369	-5.184330
C	1.962767	0.051751	-4.871219
C	1.836626	-0.660476	-3.678465
C	0.790813	-0.374625	-2.784928
C	-0.111964	0.641635	-3.107173
C	0.014047	1.360250	-4.299102
H	1.154039	1.621639	-6.111872
H	2.775735	-0.179052	-5.555067
H	2.551016	-1.445456	-3.444296
H	-0.904394	0.854937	-2.397200
H	-0.694631	2.151144	-4.533067
C	-0.696834	-5.568625	-2.846520
C	-0.568420	-4.498408	-3.730086
C	-0.158460	-3.242451	-3.268874
C	0.124293	-3.026410	-1.911118
C	-0.031309	-4.114148	-1.027363
C	-0.424225	-5.370846	-1.489635
H	-1.009473	-6.545097	-3.206980
H	-0.783520	-4.634644	-4.786999
H	-0.060310	-2.430028	-3.979771
H	-0.521651	-6.195174	-0.787300
C	4.701966	2.381303	-2.977233
C	4.108369	1.496526	-2.104896
H	5.434765	2.019261	-3.693607
H	4.377711	0.448149	-2.145678
C	4.366155	3.755702	-2.952899
C	3.429338	4.209817	-2.054522
H	4.845099	4.444227	-3.643987
H	3.154533	5.261808	-2.024239
C	6.407171	0.277731	1.372489
C	5.138154	0.488379	0.880453
H	6.976138	1.115940	1.766183
H	4.723670	1.488767	0.896868
C	6.976642	-1.017494	1.372010

C	6.251291	-2.076815	0.880064
H	7.979845	-1.170465	1.760865
H	6.669860	-3.080674	0.875498
H	0.147714	-3.961040	0.032897
C	-4.814897	-1.809734	2.621398
H	-4.547672	-1.657144	3.675684
H	-5.391913	-0.929618	2.305999
C	-4.734565	-3.404265	0.125283
H	-4.996611	-3.536043	-0.933081
H	-4.134865	-4.281983	0.413867
C	-6.006293	-3.344820	0.988299
H	-6.657142	-2.542022	0.614096
H	-6.571180	-4.279874	0.887690
C	-5.670845	-3.077852	2.463765
H	-5.124081	-3.939976	2.873835
H	-6.592277	-2.984755	3.051601
C	-3.536202	1.449615	-0.634948
O	-4.299121	1.005952	0.266285
C	-3.768240	0.953597	-2.071886
H	-3.774877	-0.141485	-2.070306
H	-2.966371	1.275733	-2.742722
C	-2.554903	5.666128	-0.373881
C	-3.609358	5.116574	0.357962
C	-3.876294	3.748457	0.281393
C	-3.098584	2.906009	-0.528605
C	-2.042823	3.469539	-1.258658
C	-1.771166	4.835585	-1.179551
H	-2.344571	6.731197	-0.317651
H	-4.229458	5.754579	0.983412
H	-4.695359	3.305051	0.838342
H	-1.406858	2.835889	-1.866363
C	-0.941461	5.250436	-1.746275
H	-5.123478	1.458712	-2.603844
H	-5.909080	1.137365	-1.909524
C	-5.131353	2.556552	-2.595972
H	-5.429058	0.953149	-4.017398
H	-6.399736	1.320975	-4.370702
H	-4.666961	1.284447	-4.733941
H	-5.457694	-0.143647	-4.050958

Pf2

	Coordinates (Angstroms)		
	X	Y	Z

Ru	-0.64349500	0.37528800	-1.08732000
H	0.11837300	1.00816100	-2.31619600
N	-2.23220900	-0.67200500	-1.90519900
H	-2.01604500	-1.50228300	-2.45817300
N	-2.19169100	1.96229900	-1.32139800
H	-2.32482900	2.57360600	-0.51570800
H	-1.82121200	2.56113600	-2.06039800
P	0.90013800	-1.35163600	-1.14943100
P	0.76708100	1.75608900	0.16336300
C	-3.48947300	1.37205000	-1.75201000
H	-3.96127900	0.98236400	-0.84224100
C	-3.16589000	0.17653500	-2.65138300
H	-2.69613500	0.57714600	-3.57239300
C	5.39287700	1.31963900	-0.63794600
C	4.69352900	2.50475300	-0.96742300
C	3.35604400	2.63052300	-0.68635500
C	2.61885200	1.58853700	-0.05602600
C	3.27834800	0.41107600	0.31173300
C	4.68345400	0.26129100	0.01650100
H	5.23141800	3.32109000	-1.44435300
H	2.85500900	3.55529000	-0.94332900
C	2.50530900	-1.94427900	3.24478600
C	1.62802100	-2.86473000	2.62460000
C	1.24799200	-2.69909800	1.31676300
C	1.71853800	-1.61361600	0.52244900
C	2.61633700	-0.69881400	1.08892400
C	3.00659400	-0.84729900	2.47188400
H	1.25762600	-3.71202400	3.19732500
H	0.57761500	-3.42520100	0.87490900
C	-0.96512000	-5.53293200	-2.19401900
C	0.24002900	-5.15376000	-2.78603400
C	0.82405600	-3.92228200	-2.47888500
C	0.21435800	-3.04196400	-1.56935400
C	-1.00788300	-3.43267400	-0.99277800
C	-1.58837700	-4.66513000	-1.29607500
H	-1.41807200	-6.49067400	-2.43742500
H	0.73259500	-5.81566000	-3.49408000
H	1.75700600	-3.65327100	-2.95936600
H	-1.53439800	-2.77172100	-0.31451600
H	-2.53689600	-4.92797500	-0.83591100
C	4.33990400	-1.27337300	-4.30349400

C	4.49677700	-2.00583000	-3.12518500
C	3.48810800	-2.00458600	-2.16099400
C	2.31021200	-1.26532100	-2.35194900
C	2.16345500	-0.53668100	-3.54128100
C	3.16973500	-0.54119700	-4.50957700
H	5.12530700	-1.27325100	-5.05492200
H	5.40674100	-2.57351100	-2.95077700
H	3.61905500	-2.58540000	-1.25314900
H	1.25565700	0.03540200	-3.70182100
H	3.03744600	0.03003000	-5.42501800
C	0.27213700	1.89091400	4.80529000
C	1.30432900	2.61921300	4.20714000
C	1.48094800	2.57723500	2.82405700
C	0.62125800	1.81516800	2.01578200
C	-0.40568900	1.08740600	2.62860500
C	-0.58055900	1.12041000	4.01420000
H	0.14038100	1.91865800	5.88375800
H	1.97717800	3.21353100	4.82001400
H	2.29051500	3.14218800	2.36916000
H	-1.06062300	0.47989400	2.00993000
H	-1.37645600	0.53924400	4.47294800
C	-0.30771400	6.13680300	-1.14046000
C	-0.41804200	5.77500100	0.20084700
C	-0.05245000	4.49136700	0.62204300
C	0.42352600	3.53836500	-0.29188600
C	0.50759700	3.91407000	-1.64824300
C	0.16038700	5.19885200	-2.06570000
H	-0.58701700	7.13551700	-1.46530700
H	-0.78659000	6.49150900	0.93065700
H	-0.14149400	4.23948900	1.67279100
H	0.24957000	5.46528500	-3.11594900
C	4.25345700	-0.10749700	4.44071600
C	3.88788300	0.06413100	3.12418400
H	4.92595200	0.60682200	4.90844400
H	4.27414400	0.91251200	2.57286100
C	3.76148200	-1.20121600	5.19138000
C	2.90158900	-2.09710400	4.60088700
H	4.06071900	-1.32707800	6.22846100
H	2.50824800	-2.94136200	5.16244800
C	6.75850400	-1.03213300	0.04955400
C	5.41889400	-0.91481400	0.34681900
H	7.28986100	-1.94230900	0.31511500
H	4.91183100	-1.73459600	0.84133300
C	7.45025100	0.02038200	-0.59591300

C	6.77567900	1.17063400	-0.93114300
H	8.50774300	-0.08366700	-0.82340100
H	7.29005200	1.98974900	-1.42847100
H	0.84585000	3.18689200	-2.38078400
C	-4.46712800	-0.52923600	-3.07824800
H	-4.22517200	-1.35840700	-3.75675300
H	-4.93535400	-0.97364100	-2.19061700
C	-4.44280000	2.36999100	-2.41995500
H	-4.67126800	3.19556700	-1.73219700
H	-3.94755900	2.81329100	-3.29813400
C	-5.73767200	1.66331900	-2.86039100
H	-6.28175400	1.32915900	-1.96606400
H	-6.39225900	2.37363600	-3.38120300
C	-5.44003500	0.45039800	-3.75710000
H	-5.00403200	0.79975500	-4.70506200
H	-6.37478300	-0.06310100	-4.01590600
C	-4.96733100	0.82872500	2.26953300
C	-6.12295500	1.59549800	2.43019600
C	-4.96615900	-0.31269600	1.45466500
H	-4.05205000	1.12331000	2.78125900
C	-7.30126000	1.23085900	1.77416200
H	-6.10220000	2.47939800	3.06320000
C	-6.15198200	-0.66740900	0.79952100
C	-7.31086100	0.09677700	0.95891900
H	-8.20216700	1.82679500	1.89553600
H	-6.14772900	-1.54387200	0.15980300
H	-8.22385500	-0.19555000	0.44554200
C	-3.69836600	-1.15653100	1.30900200
H	-2.84502400	-0.45566100	1.28940000
O	-3.69827800	-1.93179500	0.12842500
H	-3.19386900	-1.43271100	-0.59158500
C	-3.48244000	-2.08942100	2.52237700
H	-3.47042200	-1.48209100	3.43937800
H	-2.48196800	-2.53250000	2.42132800
C	-4.52090900	-3.20859000	2.65749900
H	-5.51947900	-2.77042300	2.78347400
H	-4.54624400	-3.77677600	1.72040600
C	-4.22442600	-4.14931000	3.83060400
H	-4.21971900	-3.60825300	4.78568400
H	-4.97531300	-4.94498400	3.90433800
H	-3.24316500	-4.62805500	3.71870700

Pu2

Coordinates (Angstroms)			
	X	Y	Z

Ru		0.63462000	1.27991300 0.62109100
H		2.60735900	-1.00072500 -0.78347900
H		-0.21417300	2.34294000 1.41964700
N		2.37270200	1.09767500 1.72845000
H		2.30308200	0.68293600 2.65791100
H		3.47846700	-0.00056500 0.88750200
N		1.88102400	2.96185800 -0.16332700
H		1.90133200	3.07111100 -1.17736300
H		1.40998900	3.79456900 0.19286100
P		-0.55974100	-0.37348600 1.71273200
P		-0.98260300	1.53221700 -1.04496300
C		3.26244200	2.88687000 0.38939400
H		3.78654800	2.12620000 -0.20269600
C		3.14604700	2.33970700 1.81407100
H		2.61247000	3.10292500 2.41570500
C		-5.44815800	0.56315500 0.10595700
C		-5.04247700	1.86659200 -0.26607000
C		-3.74572100	2.11673600 -0.63905300
C		-2.76095500	1.08877900 -0.67291200
C		-3.12580700	-0.21941700 -0.33674100
C		-4.48453600	-0.49593800 0.06547100
H		-5.77399800	2.67152900 -0.25582100
H		-3.46987300	3.12474300 -0.92285500
C		-1.65789700	-3.53804900 -1.59855300
C		-0.66785800	-3.78198400 -0.61823600
C		-0.43594000	-2.87380300 0.38368600
C		-1.17444300	-1.66094800 0.49205800
C		-2.18938300	-1.39773700 -0.43865100
C		-2.43153500	-2.33504400 -1.51004400
H		-0.08269200	-4.69708500 -0.66743300
H		0.32956700	-3.09745400 1.11490300
C		1.99825400	-2.78805400 4.82531800
C		0.73469600	-2.32236500 5.18908200
C		-0.05205100	-1.61930900 4.27334200
C		0.40964000	-1.36369100 2.97123900
C		1.69746500	-1.81695300 2.63049000
C		2.47797800	-2.53112000 3.54029700
H		2.60637100	-3.33864600 5.53844800
H		0.35237400	-2.50553300 6.19020300
H		-1.02837000	-1.26969700 4.58560600

H	2.10964500	-1.60206100	1.65236900
H	3.46132600	-2.87704200	3.23531000
C	-4.22734800	0.68699600	4.39791800
C	-4.08621100	-0.60641000	3.89050800
C	-3.01011500	-0.91788800	3.05931100
C	-2.06044700	0.05758600	2.71494500
C	-2.21152100	1.35104500	3.23365700
C	-3.28694500	1.66372200	4.06837800
H	-5.06612300	0.93073200	5.04485500
H	-4.81671900	-1.37266300	4.13515100
H	-2.90708700	-1.92918700	2.67733100
H	-1.48085900	2.11117400	2.97760000
H	-3.38797300	2.67278300	4.46005200
C	-0.17347500	-0.43594100	-5.20357400
C	-1.44656300	0.06682400	-4.92305900
C	-1.71667600	0.63720000	-3.67867500
C	-0.71815400	0.71477300	-2.69411100
C	0.55242300	0.20265500	-2.98757200
C	0.82656900	-0.36815000	-4.23266000
H	0.03491300	-0.88198200	-6.17250500
H	-2.23149000	0.01089700	-5.67289400
H	-2.71037200	1.02563300	-3.47224900
H	1.32885200	0.24771400	-2.22829100
H	1.81929500	-0.75887400	-4.44079600
C	-1.04570400	6.09198600	-2.17552900
C	-0.86600000	5.14201400	-3.17950800
C	-0.88688100	3.77629800	-2.87552100
C	-1.07882000	3.33213100	-1.55808500
C	-1.24263200	4.30611600	-0.55259700
C	-1.23834600	5.66725200	-0.85752600
H	-1.03333400	7.15227600	-2.41370900
H	-0.71160600	5.45800800	-4.20817600
H	-0.75238600	3.05847900	-3.67684500
H	-1.38039200	6.39670500	-0.06395800
C	-3.64111300	-3.03617500	-3.51633400
C	-3.42647500	-2.12196500	-2.50918900
H	-4.40649400	-2.84210900	-4.26322900
H	-4.02384600	-1.21906200	-2.47645200
C	-2.87610500	-4.22436200	-3.59010800
C	-1.90324300	-4.46385600	-2.64861000
H	-3.05800200	-4.93904800	-4.38825200
H	-1.30290300	-5.36977500	-2.68913400
C	-6.22736100	-2.03414600	0.82428800
C	-4.92577300	-1.79870300	0.44081000

H	-6.53128600	-3.03936200	1.10433100
H	-4.22037200	-2.62056500	0.42555300
C	-7.17254700	-0.98135300	0.85671200
C	-6.78480700	0.28995200	0.50459400
H	-8.19718500	-1.18034100	1.15906600
H	-7.49658800	1.11200500	0.52535100
H	-1.37208900	3.98771700	0.47757900
C	4.54858300	2.17048800	2.42922100
H	4.45010200	1.81201200	3.46267600
H	5.08773800	1.39334000	1.87249700
C	4.03882600	4.20828200	0.32872200
H	4.12787400	4.55109900	-0.71153600
H	3.47494100	4.98288300	0.87122600
C	5.43185100	4.04927300	0.96510500
H	6.03191400	3.36563800	0.34762500
H	5.95474600	5.01395900	0.96243000
C	5.33893700	3.48943600	2.39381700
H	4.84676300	4.23066400	3.04114200
H	6.34599700	3.33916500	2.80296000
C	3.69121800	-1.19995300	-0.69635800
O	4.19676000	-0.57200800	0.46311800
C	4.36472200	-0.61313800	-1.96205500
H	4.06425400	0.44240800	-2.04081000
H	3.96542100	-1.12172500	-2.85206700
C	4.20593100	-5.51003000	-0.52174800
C	4.89891200	-4.68338000	0.36413300
C	4.72731500	-3.29735400	0.31693200
C	3.86368600	-2.71648700	-0.61900000
C	3.16788500	-3.55525000	-1.50148900
C	3.33668000	-4.93998000	-1.45567300
H	4.33808100	-6.58833800	-0.48386500
H	5.57632000	-5.11787800	1.09559700
H	5.25357500	-2.64524500	1.00582800
H	2.47834200	-3.12241100	-2.22376700
H	2.78768500	-5.57445100	-2.14763300
C	5.89475900	-0.70128100	-1.95898600
H	6.26744400	-0.22013500	-1.04752300
H	6.19883600	-1.75431400	-1.90085100
C	6.52929900	-0.05192600	-3.19347700
H	7.62295000	-0.12469700	-3.16518700
H	6.18899000	-0.53389700	-4.11901600
H	6.26979100	1.01245500	-3.26279000

ABS₃

	Coordinates (Angstroms)		
	X	Y	Z

Ru	-0.505574	0.826121	-0.641043
H	-1.310260	-0.005454	0.636146
H	0.070218	1.734821	-1.974940
N	-2.293819	0.412761	-1.906585
H	-2.034696	-0.017443	-2.792061
H	-2.906744	-0.243160	-1.417515
N	-1.829829	2.568707	-0.205706
H	-1.909263	2.728252	0.796268
H	-1.373204	3.391640	-0.597594
P	0.643543	-1.058188	-1.214919
P	1.199629	1.605345	0.660107
C	-3.175132	2.391430	-0.801984
H	-3.722408	1.712715	-0.135170
C	-3.022700	1.676749	-2.152158
H	-2.369606	2.287256	-2.789799
C	5.507547	0.683381	-1.028146
C	4.979434	1.996019	-1.010410
C	3.740856	2.245609	-0.475191
C	2.941577	1.211663	0.088371
C	3.436584	-0.097189	0.113729
C	4.730931	-0.378458	-0.461259
H	5.570491	2.809516	-1.425526
H	3.368953	3.262468	-0.474783
C	2.679795	-2.932271	2.599126
C	1.552382	-3.526440	1.982906
C	1.017253	-2.992660	0.838119
C	1.573046	-1.841559	0.212129
C	2.708448	-1.242739	0.769694
C	3.265302	-1.774627	1.991192
H	1.113229	-4.415915	2.429806
H	0.151776	-3.469199	0.394132
C	-2.395914	-4.338385	-2.673495
C	-1.222843	-4.128200	-3.397077
C	-0.286793	-3.180759	-2.970859
C	-0.503062	-2.421451	-1.809392
C	-1.700728	-2.634882	-1.099557
C	-2.632369	-3.583987	-1.521888
H	-3.123437	-5.073822	-3.007800
H	-1.029458	-4.700209	-4.301380

H	0.612233	-3.036215	-3.557852
H	-1.897246	-2.028991	-0.219690
H	-3.552879	-3.718751	-0.959797
C	3.742337	-1.117280	-4.716069
C	3.698654	-2.184656	-3.815658
C	2.796775	-2.164112	-2.751421
C	1.921804	-1.079610	-2.571328
C	1.978020	-0.013216	-3.477203
C	2.882014	-0.032461	-4.542627
H	4.448539	-1.130611	-5.542638
H	4.373871	-3.028091	-3.935204
H	2.774961	-2.997997	-2.054639
H	1.314168	0.833077	-3.317240
H	2.916448	0.805890	-5.234506
C	1.438775	0.763322	5.254533
C	2.512375	1.384083	4.610258
C	2.463303	1.614405	3.235354
C	1.338072	1.235544	2.483666
C	0.271846	0.607495	3.137823
C	0.322394	0.372294	4.514658
H	1.479066	0.578959	6.325271
H	3.390650	1.682113	5.177511
H	3.304881	2.096196	2.743934
H	-0.581182	0.293131	2.540331
H	-0.510698	-0.122858	5.008437
C	0.872412	6.300573	0.619379
C	0.937203	5.630622	1.839884
C	1.080019	4.239042	1.879067
C	1.152516	3.484697	0.697372
C	1.063407	4.175523	-0.528761
C	0.937225	5.564839	-0.567575
H	0.767200	7.382169	0.590526
H	0.879686	6.187784	2.771875
H	1.132553	3.746593	2.843087
H	0.883839	6.072308	-1.528009
C	4.915688	-1.732696	3.794906
C	4.394764	-1.194754	2.638926
H	5.777574	-1.265175	4.264018
H	4.850802	-0.309402	2.212907
C	4.338510	-2.884453	4.379530
C	3.240080	-3.466096	3.790905
H	4.760513	-3.301394	5.290231
H	2.778824	-4.348330	4.229306
C	6.531065	-1.928078	-1.042711

C	5.288880	-1.689764	-0.497814
H	6.927650	-2.940065	-1.053724
H	4.721111	-2.516778	-0.089412
C	7.294527	-0.870199	-1.590446
C	6.786114	0.407400	-1.583971
H	8.274562	-1.070514	-2.015486
H	7.355682	1.232682	-2.005441
H	1.069859	3.599735	-1.450416
C	-4.385652	1.484537	-2.841240
H	-4.233788	1.019844	-3.824686
H	-4.985999	0.782868	-2.246815
C	-3.950553	3.711025	-0.939392
H	-4.083268	4.166130	0.051258
H	-3.345199	4.415454	-1.530629
C	-5.309207	3.509242	-1.628746
H	-5.955823	2.894581	-0.986032
H	-5.814506	4.475449	-1.749852
C	-5.139271	2.816459	-2.988696
H	-4.583001	3.480456	-3.666691
H	-6.117692	2.644157	-3.454054
C	-5.174137	-1.061211	0.853541
O	-4.790740	-0.901451	-0.304159
C	-4.170755	-1.093415	1.994262
H	-3.251985	-0.620969	1.627673
H	-4.542155	-0.507487	2.844124
C	-9.389201	-1.619082	1.528769
C	-8.875957	-1.533726	0.230352
C	-7.510915	-1.352959	0.033048
C	-6.635342	-1.256760	1.128551
C	-7.161567	-1.344976	2.427653
C	-8.530837	-1.523870	2.625526
H	-9.542587	-1.609351	-0.624453
H	-7.093187	-1.285930	-0.965948
H	-6.508066	-1.271955	3.290603
H	-8.926357	-1.588217	3.635437
C	-3.860258	-2.532795	2.454584
H	-4.749956	-3.046595	2.834463
H	-3.452658	-3.124563	1.628470
H	-3.109294	-2.513733	3.250819
H	-10.456076	-1.759467	1.684099

INTf₃

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.736438	0.454783	-0.873455
H	1.467459	0.004406	0.620238
H	0.253413	0.960206	-2.440550
N	2.252919	2.078158	-0.981699
H	1.810352	2.973155	-1.180832
H	2.713044	2.172431	-0.075481
N	2.448992	-0.548799	-1.892270
H	2.642359	-1.455014	-1.471527
H	2.162278	-0.727953	-2.853956
P	-0.851370	1.695916	0.202478
P	-0.624024	-1.372389	-1.000625
C	3.667101	0.293867	-1.859462
H	4.092312	0.177749	-0.854683
C	3.257152	1.764238	-2.021643
H	2.740716	1.871684	-2.984749
C	-5.155907	-0.341842	-1.812789
C	-4.343203	-0.957176	-2.794151
C	-3.040415	-1.287334	-2.517859
C	-2.453486	-1.040090	-1.245022
C	-3.231023	-0.458322	-0.236740
C	-4.597712	-0.087337	-0.518529
H	-4.765329	-1.167940	-3.774400
H	-2.447924	-1.758380	-3.291932
C	-2.934142	-0.849573	3.577504
C	-2.015350	0.185188	3.876356
C	-1.467666	0.946392	2.875236
C	-1.806184	0.747787	1.506845
C	-2.731299	-0.246279	1.169719
C	-3.294541	-1.075431	2.209446
H	-1.748576	0.371251	4.914626
H	-0.763773	1.727231	3.136219
C	1.283709	5.192575	2.507613
C	0.098428	5.458269	1.821740
C	-0.579231	4.434898	1.151304
C	-0.086731	3.119919	1.157565
C	1.114821	2.871808	1.847836
C	1.793021	3.891766	2.516086
H	1.811326	5.992831	3.020735
H	-0.303744	6.468318	1.799036
H	-1.490958	4.673964	0.616548

H	1.520896	1.864324	1.831591
H	2.730817	3.664224	3.015291
C	-4.151147	4.057711	-2.119361
C	-4.285936	3.859468	-0.743036
C	-3.322997	3.130324	-0.044602
C	-2.208790	2.590384	-0.708335
C	-2.087306	2.790591	-2.089199
C	-3.051711	3.519863	-2.789534
H	-4.903753	4.621800	-2.664799
H	-5.145580	4.263619	-0.214621
H	-3.440714	2.979373	1.025206
H	-1.236433	2.346539	-2.600243
H	-2.944923	3.661817	-3.862474
C	-0.645017	-4.686792	2.301982
C	-1.598111	-4.725257	1.280794
C	-1.616480	-3.729095	0.304195
C	-0.678149	-2.683155	0.327067
C	0.268120	-2.651407	1.358178
C	0.283766	-3.646311	2.339551
H	-0.635156	-5.458937	3.067331
H	-2.332791	-5.525969	1.250313
H	-2.365653	-3.767354	-0.482618
H	0.968922	-1.818963	1.380383
H	1.017902	-3.603595	3.141381
C	0.730100	-3.826293	-4.781167
C	0.607592	-4.475584	-3.553936
C	0.166647	-3.778978	-2.423175
C	-0.155555	-2.414562	-2.492900
C	-0.004890	-1.767273	-3.736917
C	0.420389	-2.465813	-4.867690
H	1.067865	-4.370141	-5.659731
H	0.852987	-5.531454	-3.468359
H	0.077882	-4.312062	-1.483706
H	0.514479	-1.943849	-5.817150
C	-4.749671	-2.894560	2.952448
C	-4.213503	-2.130822	1.939397
H	-5.448003	-3.692020	2.711933
H	-4.493263	-2.336763	0.913473
C	-4.398819	-2.653538	4.301605
C	-3.504971	-1.652287	4.601702
H	-4.831431	-3.260420	5.092689
H	-3.217926	-1.456311	5.632501
C	-6.744579	0.870998	0.154358
C	-5.441004	0.536620	0.446776

H	-7.360532	1.345809	0.913764
H	-5.045076	0.754525	1.431055
C	-7.289265	0.605517	-1.124262
C	-6.504665	0.013430	-2.085813
H	-8.320045	0.872413	-1.342126
H	-6.903155	-0.193862	-3.076430
H	-0.204603	-0.700229	-3.795141
C	4.486593	2.686491	-1.979442
H	4.170215	3.727402	-2.127876
H	4.930489	2.630009	-0.974698
C	4.717054	-0.111868	-2.907092
H	5.019629	-1.153892	-2.740122
H	4.253365	-0.072913	-3.905002
C	5.943045	0.815154	-2.877865
H	6.471414	0.680931	-1.923647
H	6.646684	0.528554	-3.669396
C	5.533221	2.287266	-3.032452
H	5.116897	2.445544	-4.038083
H	6.412510	2.938483	-2.953353
C	4.376454	0.441989	2.335680
O	4.393712	1.586506	1.893648
C	3.422741	0.048100	3.452699
H	2.874540	-0.859245	3.174997
H	2.686324	0.849415	3.545176
C	7.253709	-2.378754	0.808611
C	7.452946	-1.001790	0.664872
C	6.508788	-0.106487	1.161089
C	5.359401	-0.571807	1.821978
C	5.174130	-1.955483	1.970162
C	6.112008	-2.853068	1.457550
H	7.987606	-3.078807	0.418346
H	8.345271	-0.629791	0.168593
H	6.645209	0.965154	1.057201
H	4.290103	-2.338813	2.469205
C	5.951341	-3.921969	1.567239
H	4.153131	-0.160716	4.793665
H	3.431883	-0.404355	5.580690
H	4.882980	-0.975077	4.738309
H	4.684778	0.748808	5.094585

TSf₃

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.079792	0.511984	-0.455144
H	1.794532	-0.097677	1.117609
H	0.720269	1.073186	-1.973319
N	2.535492	2.143696	-0.272133
H	2.109755	3.068974	-0.251540
H	3.011053	2.001499	0.634289
N	2.912318	-0.342956	-1.400842
H	3.190950	-1.211493	-0.944595
H	2.666565	-0.578478	-2.361637
P	-0.710421	1.725027	0.361542
P	-0.263651	-1.296326	-0.949787
C	4.052676	0.611911	-1.373885
H	4.553086	0.456202	-0.413523
C	3.521328	2.049460	-1.371147
H	2.972178	2.228463	-2.304156
C	-4.605463	-0.246788	-2.491095
C	-3.625118	-0.796916	-3.349709
C	-2.379073	-1.119669	-2.874389
C	-2.016889	-0.922906	-1.512441
C	-2.967727	-0.412100	-0.621439
C	-4.279705	-0.055514	-1.109654
H	-3.872455	-0.966818	-4.395306
H	-1.661231	-1.551896	-3.558984
C	-3.326326	-1.004656	3.161354
C	-2.496705	0.024173	3.669553
C	-1.796308	0.842744	2.820348
C	-1.889849	0.714513	1.404883
C	-2.721211	-0.270323	0.859467
C	-3.434401	-1.164542	1.741520
H	-2.419447	0.157723	4.746376
H	-1.162571	1.615909	3.238244
C	0.641761	5.180516	3.245183
C	-0.481922	5.372533	2.439217
C	-0.914438	4.364972	1.573870
C	-0.232423	3.138178	1.498747
C	0.903445	2.965753	2.307545
C	1.335669	3.972139	3.173727
H	0.976577	5.969055	3.914556
H	-1.026394	6.312920	2.477715
H	-1.783434	4.548313	0.953531
H	1.472798	2.046355	2.250343

H	2.223173	3.802237	3.777289
C	-3.455307	4.189264	-2.518560
C	-3.929469	3.814394	-1.260075
C	-3.130840	3.046273	-0.411579
C	-1.846512	2.634868	-0.803800
C	-1.385656	3.013810	-2.071830
C	-2.181738	3.785414	-2.921357
H	-4.077167	4.785582	-3.181463
H	-4.925183	4.109833	-0.940248
H	-3.514380	2.763424	0.564230
H	-0.404153	2.676851	-2.390723
H	-1.805856	4.065707	-3.902497
C	-1.136969	-4.785319	2.038268
C	-1.638017	-4.851975	0.734832
C	-1.394132	-3.812474	-0.162418
C	-0.626468	-2.699471	0.222131
C	-0.143787	-2.637534	1.533077
C	-0.397595	-3.672443	2.437920
H	-1.334061	-5.592164	2.739391
H	-2.226962	-5.710086	0.420529
H	-1.799389	-3.870194	-1.169485
H	0.416193	-1.758037	1.834420
H	-0.021876	-3.603811	3.455763
C	1.890870	-3.428476	-4.540477
C	1.671657	-4.127178	-3.354753
C	0.981233	-3.528841	-2.295045
C	0.497393	-2.214877	-2.393920
C	0.754268	-1.511893	-3.589579
C	1.428601	-2.113954	-4.652793
H	2.421723	-3.896549	-5.365228
H	2.035144	-5.146085	-3.246752
H	0.824251	-4.098876	-1.386612
H	1.598319	-1.551628	-5.567804
C	-4.939577	-3.051822	2.125938
C	-4.256993	-2.224823	1.261603
H	-5.555983	-3.853419	1.727500
H	-4.339009	-2.387586	0.194038
C	-4.843020	-2.872208	3.525734
C	-4.047141	-1.869400	4.028185
H	-5.390975	-3.528261	4.196903
H	-3.952609	-1.721832	5.101659
C	-6.535363	0.824192	-0.761635
C	-5.291996	0.494517	-0.269515
H	-7.284037	1.241194	-0.093086

H	-5.077862	0.657772	0.779639
C	-6.847953	0.625602	-2.127357
C	-5.897054	0.101785	-2.970994
H	-7.833291	0.887728	-2.503380
H	-6.116764	-0.055572	-4.024524
H	0.437263	-0.476362	-3.671156
C	4.682926	3.052282	-1.262634
H	4.290015	4.077566	-1.282569
H	5.177487	2.920552	-0.289599
C	5.067307	0.385945	-2.502751
H	5.454422	-0.639645	-2.449706
H	4.555465	0.485606	-3.472578
C	6.221624	1.399989	-2.424240
H	6.805154	1.207603	-1.512632
H	6.905570	1.256267	-3.269868
C	5.700579	2.845159	-2.396838
H	5.222850	3.077805	-3.359945
H	6.535495	3.547825	-2.285490
C	3.170867	0.007725	2.298262
O	3.598573	1.188173	2.235729
C	2.308863	-0.395050	3.504573
H	1.895702	-1.398745	3.370105
H	1.469607	0.299736	3.587536
C	5.843466	-3.081864	0.830848
C	6.318664	-1.819924	1.192641
C	5.430579	-0.838280	1.637754
C	4.054654	-1.098577	1.733044
C	3.589660	-2.374306	1.377920
C	4.475055	-3.354302	0.924773
H	6.531182	-3.848416	0.483062
H	7.381991	-1.600282	1.133581
H	5.784747	0.147246	1.923826
H	2.528723	-2.594668	1.433082
C	4.094739	-4.333928	0.645863
H	3.152052	-0.347223	4.791511
H	2.540351	-0.603193	5.664288
H	3.989606	-1.053324	4.748524
H	3.562853	0.656631	4.938403

TSu₃

Coordinates (Angstroms)

	X	Y	Z

Ru	-1.197779	-0.750590	0.290494
H	-1.979496	0.643924	-0.712931
H	-0.808626	-2.054321	1.219293
N	-2.942220	-0.460413	1.570366
H	-2.713843	-0.206344	2.530125
H	-3.469353	0.321394	1.146511
N	-2.712410	-2.131747	-0.611652
H	-2.831086	-1.990991	-1.613523
H	-2.319433	-3.065872	-0.500652
P	0.233735	0.506196	1.582812
P	0.512382	-1.424140	-1.119251
C	-4.030777	-2.034261	0.071976
H	-4.548216	-1.182745	-0.382519
C	-3.800551	-1.666838	1.543884
H	-3.232266	-2.472258	2.027667
C	4.763146	-1.916980	0.876206
C	4.034274	-3.028412	0.392066
C	2.812931	-2.856447	-0.209153
C	2.230032	-1.568992	-0.378953
C	2.931767	-0.439456	0.056952
C	4.212058	-0.606033	0.705532
H	4.455501	-4.025530	0.499874
H	2.287396	-3.729507	-0.573745
C	2.868549	3.172700	-1.256347
C	1.831436	3.721336	-0.464726
C	1.122272	2.933853	0.407084
C	1.411521	1.550757	0.572925
C	2.456206	0.975456	-0.160700
C	3.184827	1.782585	-1.109856
H	1.595112	4.778656	-0.559261
H	0.325489	3.382566	0.987181
C	-2.162692	3.487314	4.305707
C	-1.153108	2.709874	4.872704
C	-0.403128	1.835555	4.081256
C	-0.651869	1.716616	2.703223
C	-1.691247	2.487823	2.152622
C	-2.428545	3.373255	2.939891
H	-2.741155	4.170301	4.922675
H	-0.941499	2.780412	5.936844
H	0.374794	1.245551	4.549930
H	-1.926967	2.390603	1.099008
H	-3.211740	3.966555	2.477345

C	2.962303	-1.437072	4.848464
C	3.225403	-0.142743	4.394289
C	2.433805	0.421498	3.393977
C	1.366669	-0.295524	2.826931
C	1.112666	-1.591812	3.292772
C	1.904708	-2.158832	4.294418
H	3.580317	-1.879066	5.625886
H	4.052375	0.425581	4.811511
H	2.648253	1.429975	3.051385
H	0.294667	-2.153281	2.852119
H	1.694107	-3.168402	4.639098
C	1.430133	0.587470	-5.233606
C	2.303135	-0.384776	-4.736569
C	2.059444	-0.978890	-3.498252
C	0.934673	-0.612619	-2.740518
C	0.071828	0.362796	-3.246264
C	0.314065	0.962277	-4.485097
H	1.624209	1.051926	-6.196996
H	3.177204	-0.677095	-5.313122
H	2.744621	-1.733932	-3.122016
H	-0.784265	0.641682	-2.641582
H	-0.366278	1.722275	-4.861886
C	-0.675013	-5.758463	-2.507669
C	-0.447804	-4.765904	-3.459314
C	-0.043377	-3.485220	-3.066436
C	0.133807	-3.165167	-1.711223
C	-0.119290	-4.175195	-0.760494
C	-0.506144	-5.457307	-1.152956
H	-0.983679	-6.754387	-2.814330
H	-0.580368	-4.982799	-4.516339
H	0.133750	-2.735594	-3.829037
H	-0.680495	-6.220298	-0.398136
C	4.919896	2.054972	-2.810150
C	4.230313	1.257825	-1.924040
H	5.709849	1.622791	-3.418769
H	4.482616	0.207497	-1.845752
C	4.608785	3.429352	-2.938557
C	3.600254	3.971147	-2.176840
H	5.163019	4.048773	-3.638684
H	3.343712	5.024464	-2.265468
C	6.188567	0.304752	1.821290
C	4.970528	0.492457	1.206573
H	6.740876	1.164367	2.191906
H	4.578052	1.496797	1.105054

C	6.727589	-0.994317	1.976481
C	6.023023	-2.080297	1.513286
H	7.690942	-1.128890	2.461091
H	6.417967	-3.087270	1.627082
H	-0.022514	-3.940397	0.295324
C	-5.144550	-1.484865	2.268122
H	-4.965162	-1.240292	3.323695
H	-5.670248	-0.628299	1.824526
C	-4.889592	-3.300255	-0.059840
H	-5.064029	-3.523023	-1.120956
H	-4.337646	-4.157191	0.357315
C	-6.228591	-3.143522	0.681999
H	-6.827011	-2.368362	0.182928
H	-6.803926	-4.075326	0.616859
C	-6.013191	-2.748380	2.150961
H	-5.523689	-3.577645	2.682894
H	-6.978929	-2.587759	2.645774
C	-3.510548	1.453528	-1.131125
O	-4.356628	1.101757	-0.264170
C	-3.632225	0.839019	-2.536335
H	-3.663303	-0.250428	-2.440228
H	-2.768931	1.089689	-3.157711
C	-2.454479	5.659671	-1.142642
C	-3.575072	5.191675	-0.453825
C	-3.868075	3.826940	-0.439486
C	-3.049286	2.906168	-1.111743
C	-1.926381	3.387805	-1.799054
C	-1.630395	4.751074	-1.812583
H	-2.223929	6.721939	-1.157844
H	-4.226397	5.890452	0.066015
H	-4.739763	3.445956	0.082771
H	-1.258894	2.694238	-2.298139
C	-0.749906	5.102829	-2.344256
H	-4.923754	1.324565	-3.217639
H	-4.917840	2.412428	-3.349462
H	-5.037760	0.865747	-4.206738
H	-5.795797	1.062930	-2.609975

Pf3

Coordinates (Angstroms)

X Y Z

Ru	0.76021300	0.40446100	-0.93137800
H	0.07846900	0.69814900	-2.32388700
N	2.34077100	1.74156700	-0.81473500
H	2.11077100	2.73189700	-0.72598300
N	2.37434600	-0.66314700	-2.04260600
H	2.50557800	-1.64425800	-1.79672500
H	2.04375400	-0.66624800	-3.00821600
P	-0.84084100	1.77796800	0.02365300
P	-0.65234500	-1.45500500	-0.93096200
C	3.66187400	0.07920800	-1.94864400
H	4.10211700	-0.19860500	-0.98372600
C	3.32233900	1.57077800	-1.88912000
H	2.89019100	1.84704200	-2.87191300
C	-5.25216400	-0.61903000	-1.53558300
C	-4.49471600	-1.32494500	-2.49985500
C	-3.16623900	-1.59478200	-2.28649200
C	-2.49672600	-1.18515400	-1.09896200
C	-3.21544200	-0.50960600	-0.10731800
C	-4.61173300	-0.21107000	-0.32088200
H	-4.98055500	-1.65722800	-3.41458600
H	-2.61967100	-2.14580700	-3.04125800
C	-2.67377200	-0.54534800	3.69400400
C	-1.81279000	0.56600400	3.85246300
C	-1.36414400	1.26628300	2.76118200
C	-1.74791800	0.92505600	1.43196500
C	-2.63160700	-0.14453400	1.23443200
C	-3.08861500	-0.90877400	2.37186800
H	-1.50950700	0.86287200	4.85394300
H	-0.70743600	2.11192600	2.92048700
C	0.92716900	5.67441500	1.95907600
C	-0.22255100	5.76040100	1.17369300
C	-0.77738500	4.61251700	0.60238700
C	-0.19372500	3.35079200	0.80545600
C	0.97506300	3.28317300	1.58612200
C	1.52497500	4.42967500	2.16167700
H	1.35779200	6.56950600	2.40073300
H	-0.69434400	6.72431000	0.99952000
H	-1.66766300	4.71188700	-0.00672900
H	1.48426100	2.33915700	1.74336700
H	2.43152700	4.33915000	2.75371400
C	-4.15663200	3.69258500	-2.64855100
C	-4.37078000	3.53926700	-1.27734400
C	-3.39638900	2.93753800	-0.48034100

C	-2.19589400	2.47077100	-1.03879000
C	-1.99145300	2.63450700	-2.41628600
C	-2.96368600	3.24092400	-3.21476100
H	-4.91555900	4.15998400	-3.27069200
H	-5.29888100	3.88057500	-0.82697300
H	-3.57136400	2.83148700	0.58592100
H	-1.06628900	2.28113800	-2.85922900
H	-2.78696100	3.35832900	-4.28097700
C	-0.36095400	-4.51296200	2.58745500
C	-1.33020100	-4.70052500	1.59794500
C	-1.44533000	-3.78811700	0.54910600
C	-0.58617100	-2.67982400	0.46714000
C	0.37575300	-2.50077400	1.46829600
C	0.48946600	-3.40873600	2.52398100
H	-0.27642000	-5.22097700	3.40772100
H	-2.00141100	-5.55406700	1.64804800
H	-2.20602200	-3.93932900	-0.21255300
H	1.02835800	-1.63309100	1.42233100
H	1.23592500	-3.24757000	3.29752000
C	0.64188700	-4.00063100	-4.65787600
C	0.67846000	-4.57600400	-3.38915300
C	0.24550700	-3.85530700	-2.27027700
C	-0.22642400	-2.53933300	-2.39534000
C	-0.23558500	-1.96499200	-3.68315700
C	0.17963200	-2.68874600	-4.80082100
H	0.97367800	-4.56297200	-5.52656900
H	1.04161700	-5.59265600	-3.26127900
H	0.27913400	-4.33008500	-1.29616700
H	0.14754700	-2.22515300	-5.78369100
C	-4.38076000	-2.74204100	3.34491200
C	-3.95166400	-2.03624700	2.24307500
H	-5.03579900	-3.59902700	3.21174300
H	-4.27015100	-2.34788500	1.25600400
C	-3.97605100	-2.36581900	4.64749300
C	-3.13597700	-1.28989600	4.81271200
H	-4.32555200	-2.92867600	5.50888200
H	-2.80857900	-0.98888900	5.80519600
C	-6.73549000	0.75991300	0.40491700
C	-5.40549800	0.48704100	0.63603500
H	-7.31236400	1.29410600	1.15533700
H	-4.95150600	0.81078900	1.56484500
C	-7.35878600	0.35046400	-0.79788500
C	-6.62650200	-0.32425000	-1.74600500
H	-8.40958900	0.56961400	-0.96716900

H	-7.08770200	-0.64593500	-2.67694400
H	-0.56859700	-0.93825600	-3.80510900
C	4.61139200	2.39490500	-1.71115900
H	4.36143100	3.46443900	-1.70678500
H	5.04172900	2.16686600	-0.72756100
C	4.66067700	-0.24985100	-3.06453600
H	4.89784300	-1.32253000	-3.05820400
H	4.19886100	-0.03076600	-4.04001800
C	5.94394700	0.58495800	-2.90212700
H	6.45935200	0.27135500	-1.98356600
H	6.62988400	0.38013200	-3.73386200
C	5.63145600	2.08845900	-2.82145200
H	5.22993200	2.42649400	-3.78848000
H	6.55589900	2.65550100	-2.65351800
C	5.14244500	-2.02544800	1.59752900
C	6.37366900	-2.62946700	1.33784100
C	5.02627400	-0.62986000	1.67720100
H	4.25818600	-2.64606100	1.73603900
C	7.51409400	-1.84323000	1.15397300
H	6.44248200	-3.71287800	1.27527800
C	6.17480400	0.14844500	1.48956200
C	7.40967400	-0.45285800	1.23175700
H	8.47392800	-2.31084000	0.94996100
H	6.08070300	1.22785200	1.54465700
H	8.29224700	0.16699600	1.09224400
C	3.67321100	0.01817100	1.97914600
H	2.91368700	-0.53045900	1.39326400
O	3.64326200	1.38404600	1.62612300
H	3.19113900	1.47989700	0.72530200
C	3.28471200	-0.12843000	3.46829200
H	3.30766400	-1.19382100	3.73673100
H	2.24333400	0.20457700	3.56928500
C	4.17464800	0.67033600	4.42506100
H	3.81896900	0.57518900	5.45762800
H	5.21247400	0.31998200	4.39356000
H	4.16771000	1.73082300	4.15556500

Pu3

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.61214600	1.13680700	-0.82065800

H	-2.69414500	-1.13523600	1.86552500
H	0.22435000	1.79835300	-1.98793400
N	-2.53551100	0.76649300	-1.45720100
H	-2.69764000	0.03854900	-2.15246000
H	-3.36489200	0.29269600	0.17440100
N	-1.59510300	3.11379200	-0.52030500
H	-1.38788100	3.58821900	0.35854900
H	-1.18536100	3.69533900	-1.25242100
P	0.31762700	-0.88868400	-1.42939500
P	1.20445900	1.71276500	0.51473200
C	-3.06522900	3.00184200	-0.72194600
H	-3.46430800	2.58062300	0.20784000
C	-3.29047500	1.96637800	-1.82790000
H	-2.90410200	2.40326000	-2.77147700
C	5.42527300	-0.00732500	-0.67864300
C	5.15532000	1.38149400	-0.69685600
C	3.93366000	1.86247000	-0.29817400
C	2.89438600	0.99867900	0.15077900
C	3.12802300	-0.37956200	0.20860000
C	4.40629600	-0.90095200	-0.21510600
H	5.93190800	2.06710000	-1.02857500
H	3.76195400	2.93137900	-0.31851800
C	1.61914900	-2.99429000	2.58387700
C	0.50332400	-3.42664000	1.82950200
C	0.20423500	-2.84470300	0.62354400
C	0.99547800	-1.79682000	0.07011300
C	2.13552600	-1.36976600	0.76532800
C	2.44968100	-1.95776200	2.04685900
H	-0.11518900	-4.23458700	2.21434200
H	-0.65263500	-3.20914000	0.07207000
C	-2.75270700	-3.85821200	-3.38685400
C	-1.51998400	-3.63972000	-4.00135800
C	-0.58228600	-2.78030600	-3.42351000
C	-0.85712400	-2.11697000	-2.21598300
C	-2.11609300	-2.33055000	-1.62444800
C	-3.04972600	-3.19864700	-2.19306100
H	-3.47900900	-4.53006800	-3.83704200
H	-1.27939100	-4.13927300	-4.93658800
H	0.36535900	-2.63012400	-3.92569800
H	-2.37936200	-1.80623500	-0.71319900
H	-4.00722500	-3.34629000	-1.70253000
C	3.69656800	-1.10381000	-4.64396800
C	3.52522800	-2.15503800	-3.74067300
C	2.53934700	-2.07744000	-2.75703400

C	1.71246300	-0.94722000	-2.65311700
C	1.89105500	0.09874500	-3.56894800
C	2.87596200	0.02137900	-4.55651700
H	4.46531600	-1.16254000	-5.41020300
H	4.16313400	-3.03295700	-3.79543200
H	2.41093100	-2.90449200	-2.06505300
H	1.25281300	0.97361700	-3.50207900
H	3.00033400	0.84320500	-5.25721600
C	0.66155900	1.09302800	5.10917600
C	1.93277800	1.37730200	4.60430000
C	2.11816500	1.54313200	3.23166800
C	1.03658200	1.43002000	2.34312000
C	-0.23387400	1.14135800	2.86096900
C	-0.42004600	0.97414000	4.23561400
H	0.51707300	0.96004000	6.17821500
H	2.78076000	1.46419000	5.27872000
H	3.11052200	1.76361200	2.84756300
H	-1.07924100	1.04491100	2.18277400
H	-1.40976200	0.74594400	4.62155500
C	1.73472300	6.37063500	0.22426400
C	1.59967900	5.77661200	1.47789600
C	1.48435500	4.38694400	1.59509000
C	1.49247400	3.56311600	0.45885300
C	1.61108700	4.18148100	-0.80213900
C	1.74363600	5.56503100	-0.91830400
H	1.82778000	7.44975700	0.13485100
H	1.58599600	6.39138100	2.37440600
H	1.38741900	3.94956900	2.58242900
H	1.84714100	6.01492200	-1.90266700
C	3.85504400	-2.13418700	4.04030800
C	3.57377500	-1.55196000	2.82445700
H	4.71917100	-1.79978300	4.60841200
H	4.21835800	-0.76581000	2.45113100
C	3.03100600	-3.16112100	4.55836700
C	1.93464100	-3.57745900	3.84069100
H	3.26539600	-3.61404200	5.51795000
H	1.28796100	-4.36408200	4.22262900
C	5.93828000	-2.76426300	-0.61753000
C	4.71185900	-2.29357200	-0.20376800
H	6.13879300	-3.83226600	-0.59598700
H	3.96103800	-2.99662300	0.13573500
C	6.93937500	-1.87210300	-1.06972700
C	6.68172700	-0.52180700	-1.09894100
H	7.90379100	-2.25557600	-1.39186900

H	7.43766500	0.17920700	-1.44535700
H	1.59567200	3.56669700	-1.69742400
C	-4.80200700	1.73880200	-2.02147400
H	-4.96298600	1.01300500	-2.82987500
H	-5.20749100	1.29392500	-1.10349900
C	-3.76225600	4.33455200	-1.02210100
H	-3.59796000	5.04494400	-0.19994000
H	-3.31674300	4.78280100	-1.92391500
C	-5.26918300	4.11575500	-1.24883900
H	-5.72787000	3.78696700	-0.30535500
H	-5.74920700	5.06566000	-1.51621700
C	-5.53018600	3.05763800	-2.33346900
H	-5.18642600	3.44355600	-3.30471300
H	-6.60890800	2.88176700	-2.43327300
C	-3.74887400	-0.81374100	1.81915100
O	-3.86807100	0.35987200	1.03822900
C	-4.16997600	-0.44894400	3.26018200
H	-3.46771400	0.31543100	3.61700500
H	-4.03615000	-1.33211100	3.89845600
C	-6.09223400	-4.18078900	0.38668000
C	-6.42943300	-2.88097600	0.00256100
C	-5.66890000	-1.79488300	0.44425400
C	-4.56242600	-1.99011200	1.27926100
C	-4.22761200	-3.30024400	1.65129200
C	-4.98419700	-4.38762200	1.21297700
H	-6.68369500	-5.02538600	0.04262600
H	-7.28762400	-2.71040400	-0.64310500
H	-5.92387100	-0.78415100	0.14357400
H	-3.36109100	-3.46836500	2.28880100
H	-4.70666800	-5.39581400	1.51060700
C	-5.60056500	0.08264500	3.38736800
H	-6.33738700	-0.67132100	3.08956400
H	-5.81458500	0.37017200	4.42336200
H	-5.74007900	0.96219800	2.75187500

ABS₄

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.347349	0.904966	-0.583710
H	-1.227290	0.085681	0.649065
H	0.308573	1.826814	-1.871287

N	-2.116933	0.611399	-1.894213
H	-1.854944	0.172512	-2.774385
H	-2.783813	-0.008981	-1.430415
N	-1.587153	2.710062	-0.141904
H	-1.695406	2.848538	0.860480
H	-1.068137	3.513685	-0.493713
P	0.699696	-1.024950	-1.204298
P	1.374523	1.534772	0.774245
C	-2.917386	2.624735	-0.792173
H	-3.530206	1.971661	-0.157952
C	-2.757430	1.920700	-2.147544
H	-2.043158	2.497971	-2.749616
C	5.629425	0.517658	-0.993110
C	5.162013	1.849795	-0.896878
C	3.940430	2.125067	-0.335766
C	3.099138	1.099060	0.179210
C	3.536547	-0.229496	0.130947
C	4.810566	-0.537230	-0.475080
H	5.786267	2.657647	-1.272616
H	3.616006	3.156210	-0.275904
C	2.701944	-3.135360	2.505376
C	1.540466	-3.655965	1.885886
C	1.009999	-3.053676	0.773032
C	1.603248	-1.901137	0.185482
C	2.771005	-1.372860	0.747064
C	3.325082	-1.978475	1.934891
H	1.071597	-4.544409	2.303604
H	0.119428	-3.475071	0.323257
C	-2.558587	-4.055234	-2.724951
C	-1.410624	-3.849522	-3.488791
C	-0.408412	-2.981773	-3.042979
C	-0.534380	-2.297596	-1.823079
C	-1.709823	-2.501206	-1.073813
C	-2.704391	-3.375143	-1.513345
H	-3.336469	-4.730217	-3.073090
H	-1.287748	-4.363757	-4.438962
H	0.471334	-2.839935	-3.659277
H	-1.839593	-1.943586	-0.150851
H	-3.602458	-3.510245	-0.916127
C	3.752348	-1.176893	-4.743178
C	3.636032	-2.272707	-3.884064
C	2.748977	-2.225984	-2.808390
C	1.960245	-1.086512	-2.576547
C	2.089519	0.007998	-3.440287

C	2.980249	-0.037036	-4.516114
H	4.447206	-1.211262	-5.578710
H	4.242433	-3.160234	-4.046199
H	2.669163	-3.083130	-2.144694
H	1.493652	0.895266	-3.238889
H	3.072959	0.823614	-5.174436
C	1.553870	0.386710	5.304797
C	2.656696	0.999680	4.703972
C	2.622908	1.322379	3.347341
C	1.485117	1.044348	2.571180
C	0.388148	0.425244	3.181942
C	0.423059	0.097822	4.540262
H	1.582179	0.129346	6.360774
H	3.545839	1.218460	5.290036
H	3.486861	1.796240	2.888167
H	-0.477700	0.191709	2.566160
H	-0.433751	-0.389917	4.999549
C	1.255078	6.230962	1.035124
C	1.272361	5.480606	2.209614
C	1.353455	4.084502	2.159056
C	1.410914	3.406455	0.931349
C	1.369698	4.179024	-0.247858
C	1.304903	5.572165	-0.196896
H	1.198110	7.315752	1.076374
H	1.225707	5.977991	3.175436
H	1.370304	3.527401	3.088577
H	1.288561	6.143241	-1.122315
C	5.007124	-2.080395	3.706471
C	4.489183	-1.473555	2.583942
H	5.896358	-1.669479	4.177511
H	4.974244	-0.590909	2.185562
C	4.391956	-3.230617	4.254263
C	3.259817	-3.741293	3.663538
H	4.811890	-3.702670	5.138646
H	2.769408	-4.621308	4.073912
C	6.532190	-2.132800	-1.160282
C	5.307589	-1.868371	-0.588351
H	6.881594	-3.159653	-1.230935
H	4.705867	-2.689186	-0.217920
C	7.338104	-1.082323	-1.659202
C	6.888729	0.214752	-1.578115
H	8.303754	-1.303333	-2.106351
H	7.491501	1.035087	-1.961402
H	1.367207	3.666157	-1.206246

C	-4.101037	1.817796	-2.890360
H	-3.937755	1.358961	-3.874773
H	-4.763145	1.144543	-2.330182
C	-3.607721	3.990105	-0.940540
H	-3.750400	4.442075	0.050171
H	-2.940468	4.663447	-1.500719
C	-4.949558	3.875908	-1.681468
H	-5.652921	3.290807	-1.071634
H	-5.393952	4.871356	-1.804959
C	-4.771156	3.192514	-3.045167
H	-4.154497	3.832222	-3.693623
H	-5.740996	3.083096	-3.546225
C	-5.148044	-0.784867	0.753877
O	-4.778300	-0.503408	-0.384261
C	-4.163528	-0.787940	1.906270
H	-4.096966	-1.786641	2.355998
H	-3.176035	-0.485776	1.543244
H	-4.489096	-0.101502	2.697877
C	-9.309847	-1.755194	1.413178
C	-8.822099	-1.434023	0.134570
C	-7.482809	-1.126681	-0.063855
C	-6.579551	-1.127544	1.013507
C	-7.061332	-1.447818	2.290986
C	-8.407473	-1.755684	2.484007
H	-9.506648	-1.426161	-0.710827
H	-7.106912	-0.879697	-1.051343
H	-6.390088	-1.457587	3.143942
H	-8.763228	-1.999535	3.482067
C	-10.765863	-2.099043	1.616413
H	-11.019202	-3.049315	1.128866
H	-11.012210	-2.194084	2.678338
H	-11.420237	-1.332897	1.183754

INTf₄

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.531575	0.296592	-0.854401
H	1.277662	-0.058589	0.662863
H	0.028544	0.687073	-2.443091
N	2.104033	1.850838	-1.145242

H	1.693166	2.743643	-1.410764
H	2.602428	2.003957	-0.266814
N	2.185303	-0.855733	-1.810762
H	2.360395	-1.725504	-1.312026
H	1.867993	-1.114367	-2.744598
P	-0.997872	1.677918	0.132221
P	-0.890319	-1.488445	-0.818600
C	3.429566	-0.054721	-1.886877
H	3.873728	-0.081625	-0.883832
C	3.057343	1.404423	-2.185564
H	2.505634	1.427907	-3.135050
C	-5.413366	-0.394514	-1.590311
C	-4.644615	-1.103247	-2.543582
C	-3.342550	-1.445122	-2.278496
C	-2.713094	-1.116018	-1.045193
C	-3.444946	-0.436233	-0.064877
C	-4.810879	-0.054218	-0.336045
H	-5.100323	-1.377141	-3.492688
H	-2.784291	-1.990012	-3.029229
C	-3.048184	-0.519997	3.759492
C	-2.105703	0.519409	3.948045
C	-1.568605	1.181223	2.873167
C	-1.944052	0.873483	1.535213
C	-2.898194	-0.124105	1.305319
C	-3.447261	-0.852957	2.424362
H	-1.810463	0.787817	4.960215
H	-0.844394	1.967161	3.049756
C	1.274632	5.320604	2.045480
C	0.091730	5.552021	1.343742
C	-0.624689	4.486249	0.790350
C	-0.174130	3.163675	0.931395
C	1.026397	2.948995	1.634395
C	1.742068	4.011843	2.186342
H	1.833157	6.151902	2.468505
H	-0.278441	6.566675	1.217911
H	-1.534494	4.696920	0.240799
H	1.400739	1.933307	1.719644
H	2.677804	3.814472	2.702349
C	-4.312850	3.885204	-2.316792
C	-4.404481	3.830862	-0.923756
C	-3.434739	3.151193	-0.186156
C	-2.356490	2.518365	-0.826999
C	-2.278092	2.574492	-2.224134
C	-3.249705	3.253889	-2.963634

H	-5.070925	4.410466	-2.892566
H	-5.236167	4.308272	-0.412002
H	-3.518423	3.110976	0.896732
H	-1.455601	2.059650	-2.714782
H	-3.177136	3.283730	-4.048326
C	-0.925399	-4.578314	2.693791
C	-1.903535	-4.655285	1.698521
C	-1.919959	-3.722647	0.661152
C	-0.953281	-2.704444	0.596159
C	0.017369	-2.633375	1.601802
C	0.030709	-3.563541	2.644810
H	-0.916852	-5.301211	3.505838
H	-2.658828	-5.436395	1.735224
H	-2.687239	-3.790587	-0.105999
H	0.740690	-1.822262	1.556243
H	0.786220	-3.490292	3.423800
C	0.304978	-4.245687	-4.441439
C	0.201492	-4.798947	-3.166282
C	-0.194290	-4.010092	-2.080324
C	-0.488385	-2.647185	-2.243904
C	-0.356618	-2.097902	-3.536098
C	0.022690	-2.888481	-4.621753
H	0.607349	-4.861046	-5.285026
H	0.426472	-5.850935	-3.007992
H	-0.270317	-4.468627	-1.101349
H	0.102935	-2.440842	-5.609652
C	-4.909656	-2.578771	3.352276
C	-4.388925	-1.911083	2.266079
H	-5.624716	-3.382458	3.196568
H	-4.696413	-2.198128	1.267974
C	-4.520712	-2.231931	4.667590
C	-3.604943	-1.224235	4.861004
H	-4.941409	-2.763840	5.516910
H	-3.288162	-0.948296	5.864392
C	-6.915025	1.005079	0.320319
C	-5.610759	0.663023	0.600789
H	-7.497330	1.551418	1.057844
H	-5.181551	0.945819	1.554065
C	-7.503645	0.654916	-0.917762
C	-6.761388	-0.028271	-1.852095
H	-8.534446	0.928880	-1.126547
H	-7.193827	-0.301413	-2.812039
H	-0.533255	-1.033923	-3.669470
C	4.311676	2.289744	-2.288717

H	4.014543	3.313512	-2.552622
H	4.784198	2.340847	-1.298243
C	4.441962	-0.601258	-2.905823
H	4.716932	-1.629680	-2.636464
H	3.957141	-0.652880	-3.893130
C	5.693197	0.286436	-2.999151
H	6.235093	0.250190	-2.043330
H	6.375290	-0.107867	-3.762769
C	5.314619	1.740810	-3.316164
H	4.873924	1.790142	-4.322887
H	6.211394	2.372526	-3.338085
C	4.683169	0.791324	1.962348
O	4.461044	1.789290	1.278208
C	3.615342	0.285202	2.909321
H	2.799864	-0.141981	2.306011
H	3.963980	-0.450162	3.636464
H	3.194195	1.142071	3.443618
C	5.992145	0.078100	1.835751
C	7.029941	0.709777	1.126512
C	6.233160	-1.193831	2.376280
C	8.264875	0.092920	0.973204
C	6.846559	1.697372	0.716146
C	7.470332	-1.814520	2.205779
H	5.455126	-1.716798	2.922522
H	8.507145	-1.184487	1.506627
H	9.059051	0.606098	0.435414
H	7.634382	-2.803195	2.627561
C	9.843457	-1.859943	1.313684
H	9.978877	-2.690951	2.012920
H	9.937110	-2.265182	0.297354
H	10.671215	-1.156190	1.456367

TSf₄

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.981618	0.669140	0.343834
H	-1.697777	0.107071	-1.250704
H	-0.625497	1.233229	1.859734
N	-2.289431	2.409989	0.088767
H	-1.792187	3.298811	0.068279

H	-2.744580	2.286380	-0.831446
N	-2.912777	-0.017180	1.235180
H	-3.243663	-0.865009	0.774525
H	-2.724356	-0.260556	2.206895
P	0.929427	1.708355	-0.428610
P	0.187296	-1.235925	0.917715
C	-3.968303	1.027888	1.154540
H	-4.445802	0.897639	0.178988
C	-3.318802	2.415849	1.151494
H	-2.792174	2.565384	2.102386
C	4.569155	-0.535121	2.540346
C	3.525102	-0.975633	3.387146
C	2.266334	-1.199841	2.889065
C	1.953789	-1.006241	1.514277
C	2.965580	-0.602536	0.635260
C	4.292696	-0.350628	1.147268
H	3.733031	-1.139141	4.442295
H	1.496492	-1.547239	3.565834
C	3.359780	-1.277718	-3.130839
C	2.637159	-0.186390	-3.671249
C	1.991651	0.701541	-2.848803
C	2.039049	0.583508	-1.430190
C	2.765266	-0.464180	-0.853056
C	3.417248	-1.429073	-1.707092
H	2.598999	-0.060085	-4.751024
H	1.440715	1.523427	-3.290472
C	-0.042286	5.247714	-3.365916
C	1.064476	5.352428	-2.521603
C	1.385535	4.316352	-1.641378
C	0.606980	3.147324	-1.588936
C	-0.511027	3.063757	-2.436093
C	-0.831971	4.098372	-3.317257
H	-0.290652	6.058164	-4.046671
H	1.682725	6.246670	-2.541077
H	2.243934	4.432779	-0.991009
H	-1.155584	2.194639	-2.397463
H	-1.709579	3.997309	-3.950074
C	3.813154	3.941143	2.504372
C	4.277996	3.526807	1.254657
C	3.434266	2.826522	0.391364
C	2.112708	2.524533	0.759292
C	1.661134	2.942354	2.018302
C	2.503063	3.645567	2.883011
H	4.470103	4.484375	3.178959

H	5.300525	3.738398	0.953497
H	3.810822	2.510544	-0.577133
H	0.648405	2.690655	2.318338
H	2.133606	3.957600	3.856988
C	0.837440	-4.842450	-1.985003
C	1.281080	-4.935697	-0.662524
C	1.101128	-3.865042	0.213057
C	0.453777	-2.692607	-0.213616
C	0.030252	-2.604855	-1.543231
C	0.221024	-3.671710	-2.426188
H	0.984960	-5.674412	-2.668743
H	1.776119	-5.839571	-0.316198
H	1.463217	-3.943845	1.234976
H	-0.430826	-1.679266	-1.873671
H	-0.106459	-3.583435	-3.459068
C	-2.227066	-3.070116	4.507817
C	-2.038317	-3.821246	3.349177
C	-1.275978	-3.314483	2.291017
C	-0.687936	-2.042126	2.365188
C	-0.913166	-1.283482	3.532575
C	-1.660684	-1.794838	4.594330
H	-2.814048	-3.467311	5.331731
H	-2.481901	-4.809965	3.261652
H	-1.144947	-3.922553	1.403465
H	-1.805307	-1.192522	5.487937
C	4.762632	-3.443625	-2.032458
C	4.130998	-2.551161	-1.194841
H	5.297122	-4.290421	-1.609966
H	4.169801	-2.707778	-0.123846
C	4.719153	-3.272579	-3.436040
C	4.025295	-2.211648	-3.969548
H	5.226572	-3.980761	-4.085770
H	3.972014	-2.069157	-5.046548
C	6.623074	0.323612	0.835406
C	5.367352	0.090205	0.320275
H	7.419818	0.658798	0.176431
H	5.191616	0.246309	-0.736928
C	6.886410	0.131968	2.212439
C	5.874941	-0.287445	3.043947
H	7.882040	0.317555	2.606514
H	6.056409	-0.437271	4.105814
H	-0.513290	-0.275480	3.590817
C	-4.386724	3.508093	0.979841
H	-3.910683	4.497566	0.998391

H	-4.851007	3.397612	-0.010529
C	-5.037856	0.908638	2.248833
H	-5.506899	-0.082354	2.198025
H	-4.554477	0.983749	3.235430
C	-6.100736	2.012167	2.109954
H	-6.665937	1.848542	1.181366
H	-6.823305	1.942783	2.932573
C	-5.462332	3.409757	2.075186
H	-5.005800	3.625320	3.052533
H	-6.232350	4.174706	1.916113
C	-3.011131	0.299472	-2.459973
O	-3.350235	1.510021	-2.422236
C	-2.149698	-0.181402	-3.629930
H	-1.787170	-1.203669	-3.505748
H	-2.781340	-0.154207	-4.529973
H	-1.301286	0.486308	-3.787527
C	-5.976391	-2.583586	-1.069520
C	-6.320408	-1.282564	-1.454001
C	-5.347351	-0.372364	-1.872210
C	-3.993583	-0.732110	-1.921917
C	-3.646299	-2.038744	-1.544992
C	-4.619522	-2.941989	-1.119885
H	-7.364773	-0.977302	-1.430138
H	-5.621023	0.634877	-2.170931
H	-2.605794	-2.345309	-1.558453
H	-4.320578	-3.945266	-0.821917
C	-7.026077	-3.580074	-0.634937
H	-7.207845	-4.333592	-1.412945
H	-6.718797	-4.120841	0.268122
H	-7.981877	-3.088906	-0.424937

TSu₄

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.198557	-0.927494	0.165894
H	-2.016984	0.466701	-0.815024
H	-0.773327	-2.243463	1.058400
N	-3.032461	-0.807590	1.355090
H	-2.880733	-0.584747	2.337422
H	-3.584269	-0.043501	0.929118

N	-2.565589	-2.348484	-0.884541
H	-2.634009	-2.157330	-1.882741
H	-2.126343	-3.264714	-0.799500
P	0.086598	0.363675	1.574212
P	0.619298	-1.448455	-1.169646
C	-3.924450	-2.367542	-0.279355
H	-4.468497	-1.526397	-0.721492
C	-3.803708	-2.066047	1.220224
H	-3.208026	-2.856505	1.696232
C	4.786376	-1.750316	1.028503
C	4.150769	-2.888972	0.480413
C	2.951946	-2.773101	-0.177002
C	2.300737	-1.518429	-0.341930
C	2.911142	-0.361820	0.155910
C	4.166444	-0.469746	0.862635
H	4.626305	-3.861824	0.583888
H	2.499981	-3.664760	-0.591660
C	2.675203	3.279702	-1.053966
C	1.566236	3.734440	-0.301199
C	0.869539	2.875294	0.510655
C	1.242558	1.509666	0.653153
C	2.356376	1.026351	-0.044345
C	3.074149	1.908633	-0.932657
H	1.265036	4.776615	-0.377968
H	0.016789	3.252354	1.061081
C	-2.613597	3.094487	4.275585
C	-1.584700	2.359399	4.864209
C	-0.746000	1.561928	4.080808
C	-0.923159	1.478962	2.689113
C	-1.981618	2.205475	2.115347
C	-2.808543	3.014906	2.895398
H	-3.261664	3.717628	4.886738
H	-1.427535	2.403303	5.939173
H	0.044443	1.002782	4.566160
H	-2.160034	2.133473	1.048988
H	-3.605236	3.575874	2.415621
C	2.764399	-1.534677	4.906699
C	2.973006	-0.211880	4.509718
C	2.199702	0.341954	3.489424
C	1.205296	-0.413794	2.845673
C	1.005749	-1.738559	3.254317
C	1.779614	-2.295266	4.275670
H	3.368602	-1.968475	5.699444
H	3.743699	0.387273	4.987222

H	2.370649	1.372887	3.192385
H	0.245494	-2.329616	2.753187
H	1.612254	-3.327062	4.575303
C	1.659545	0.817050	-5.120318
C	2.519885	-0.183458	-4.658017
C	2.237541	-0.856566	-3.469505
C	1.083808	-0.545193	-2.730601
C	0.234892	0.459744	-3.200127
C	0.517709	1.140802	-4.387205
H	1.884182	1.343826	-6.044192
H	3.414525	-0.435156	-5.222101
H	2.914781	-1.630639	-3.117992
H	-0.641445	0.696154	-2.606113
H	-0.151454	1.923735	-4.735985
C	-0.250035	-5.779336	-2.782493
C	-0.050712	-4.733066	-3.681318
C	0.262072	-3.450014	-3.218735
C	0.374783	-3.181749	-1.845368
C	0.148129	-4.246621	-0.949080
C	-0.147362	-5.530025	-1.410768
H	-0.487443	-6.776752	-3.142959
H	-0.134307	-4.908942	-4.750888
H	0.417970	-2.657318	-3.941350
H	-0.303121	-6.334801	-0.696406
C	4.866788	2.346413	-2.535726
C	4.188267	1.477845	-1.710231
H	5.710737	1.985517	-3.117751
H	4.501777	0.442646	-1.653713
C	4.474778	3.702223	-2.636892
C	3.397469	4.153429	-1.911059
H	5.021261	4.378559	-3.288816
H	3.077599	5.190734	-1.980497
C	6.028659	0.525162	2.096879
C	4.833168	0.657643	1.426143
H	6.510113	1.405495	2.514693
H	4.387444	1.639781	1.327785
C	6.635752	-0.743923	2.248421
C	6.021279	-1.856396	1.723882
H	7.580524	-0.834884	2.777707
H	6.470262	-2.841027	1.832770
H	0.189889	-4.055467	0.118959
C	-5.196597	-2.014436	1.870305
H	-5.095302	-1.820910	2.946714
H	-5.753825	-1.169265	1.443568

C	-4.684998	-3.676391	-0.529338
H	-4.781157	-3.850111	-1.609524
H	-4.100576	-4.517797	-0.124572
C	-6.072301	-3.648669	0.134458
H	-6.691923	-2.887522	-0.360342
H	-6.578534	-4.610715	-0.013581
C	-5.970011	-3.322781	1.632744
H	-5.457987	-4.147887	2.149815
H	-6.971522	-3.252382	2.074747
C	-3.559866	1.178253	-1.296530
O	-4.432545	0.729637	-0.503455
C	-3.541775	0.623267	-2.724479
H	-2.652659	0.896572	-3.294541
H	-3.642619	-0.464591	-2.712836
H	-4.419176	1.033030	-3.245312
C	-2.844639	5.472850	-1.085882
C	-3.957759	4.867343	-0.489127
C	-4.139500	3.485382	-0.539455
C	-3.215504	2.657294	-1.193856
C	-2.103287	3.261400	-1.794861
C	-1.922305	4.642290	-1.738381
H	-4.697789	5.487418	0.013822
H	-5.008654	3.020558	-0.085295
H	-1.353146	2.652298	-2.286826
H	-1.045873	5.083017	-2.209278
C	-2.630119	6.966742	-1.007790
H	-2.029457	7.239616	-0.129131
H	-2.101157	7.343537	-1.890302
H	-3.581102	7.504693	-0.928393

Pf4

Coordinates (Angstroms)			
	X	Y	Z

Ru		0.68961400	0.53407900 -0.84358000
H		0.05310500	0.84293600 -2.25443300
N		2.19646900	1.93700900 -0.62043100
H		1.91698000	2.91258500 -0.51064400
N		2.39367200	-0.41881100 -1.92260000
H		2.56008900	-1.40242100 -1.70996800
H		2.10644200	-0.39631000 -2.90178800

P	-1.02268100	1.77792500	0.09837800
P	-0.61218700	-1.40234500	-0.93857100
C	3.64027100	0.37573700	-1.74326000
H	4.04335000	0.08754700	-0.76515600
C	3.22889000	1.84744600	-1.65667200
H	2.82575500	2.13369600	-2.64909700
C	-5.24258600	-0.84537400	-1.62504000
C	-4.42208800	-1.47876800	-2.58824100
C	-3.08414600	-1.67141100	-2.35121600
C	-2.46721700	-1.25197900	-1.13870700
C	-3.24846200	-0.64931500	-0.14715400
C	-4.65538100	-0.43140000	-0.38578700
H	-4.86662600	-1.81681400	-3.52168400
H	-2.48812100	-2.16811500	-3.10640900
C	-2.78355600	-0.75734000	3.66295400
C	-1.99419800	0.39831900	3.86950400
C	-1.56816200	1.15509100	2.80746700
C	-1.90410000	0.82922300	1.46144800
C	-2.71755400	-0.28524300	1.21663700
C	-3.15125400	-1.10647000	2.32308400
H	-1.72814600	0.68374000	4.88483700
H	-0.96664600	2.03349000	3.00353500
C	0.45337400	5.71445700	2.18727500
C	-0.69217000	5.75266300	1.39144300
C	-1.16446500	4.59261400	0.77231400
C	-0.50011400	3.36592700	0.93850700
C	0.66145400	3.34777600	1.73102200
C	1.13067400	4.50555300	2.35314500
H	0.81949000	6.61997100	2.66450800
H	-1.22457000	6.68935600	1.24555400
H	-2.05233700	4.65564400	0.15470400
H	1.23058100	2.43444300	1.85651100
H	2.03742600	4.45049100	2.94906500
C	-4.39280200	3.54113000	-2.60913100
C	-4.62526600	3.34950500	-1.24570300
C	-3.63316700	2.79133200	-0.43894100
C	-2.39569400	2.40761900	-0.97976300
C	-2.17319000	2.60996300	-2.34916700
C	-3.16367500	3.17224700	-3.15751900
H	-5.16549600	3.97444600	-3.23897500
H	-5.58104700	3.62653000	-0.80929900
H	-3.82301900	2.65510100	0.62139200
H	-1.21886100	2.32176800	-2.77736100
H	-2.97254100	3.32071500	-4.21737100

C	-0.17547100	-4.54474100	2.49030500
C	-1.13538500	-4.74819400	1.49515000
C	-1.29379600	-3.81166700	0.47341000
C	-0.48958300	-2.66130600	0.42541100
C	0.46367600	-2.46690800	1.43249800
C	0.62132800	-3.39963200	2.46048200
H	-0.05692800	-5.27183600	3.28938500
H	-1.76542500	-5.63363600	1.51935000
H	-2.04696600	-3.97529300	-0.29304900
H	1.07490900	-1.56820800	1.41300900
H	1.35962200	-3.22683600	3.23939200
C	0.91225800	-3.74985000	-4.70772800
C	0.94528500	-4.36658400	-3.45841800
C	0.44719400	-3.70758900	-2.32856900
C	-0.08677600	-2.41307100	-2.42324300
C	-0.09344000	-1.79580800	-3.69085700
C	0.38686900	-2.45885500	-4.82001900
H	1.29478600	-4.26437600	-5.58518600
H	1.35616300	-5.36773800	-3.35482300
H	0.47840900	-4.21338500	-1.37004400
H	0.35626000	-1.96415100	-5.78765900
C	-4.35312200	-3.03782800	3.21974200
C	-3.94574600	-2.27713900	2.14656300
H	-4.95594400	-3.92612400	3.05000900
H	-4.23000600	-2.57727500	1.14551900
C	-3.99382100	-2.67716600	4.53989200
C	-3.22148800	-1.55942200	4.75126200
H	-4.32532300	-3.28389900	5.37831400
H	-2.93061900	-1.26833900	5.75799600
C	-6.84996500	0.38926900	0.31402000
C	-5.51129200	0.19110200	0.56964200
H	-7.47491700	0.86719900	1.06388000
H	-5.09879800	0.51569900	1.51730600
C	-7.42023500	-0.02479100	-0.91325100
C	-6.62744500	-0.62904100	-1.86032200
H	-8.47843400	0.13492600	-1.10190900
H	-7.04767000	-0.95342200	-2.80955700
H	-0.47585800	-0.78356100	-3.78650500
C	4.46915300	2.72555300	-1.40130500
H	4.16877100	3.78187600	-1.38144700
H	4.86897000	2.49214600	-0.40624000
C	4.70207200	0.12355700	-2.81997800
H	4.98994900	-0.93668400	-2.82902300
H	4.27424000	0.34708000	-3.80992500

C	5.93538800	1.01286200	-2.57931500
H	6.42326100	0.69868500	-1.64627700
H	6.66642000	0.86380900	-3.38427100
C	5.54765300	2.49707500	-2.47429800
H	5.17192600	2.84257100	-3.44908200
H	6.43624500	3.10184800	-2.25243300
C	4.89078800	-1.68017800	1.66870300
C	6.07978200	-2.31133500	1.29649200
C	4.84992400	-0.30128600	1.90578000
H	3.98299600	-2.27207200	1.77835300
C	7.26712100	-1.58415900	1.14665200
H	6.08433100	-3.38511200	1.11889400
C	6.03580100	0.42934400	1.75849300
C	7.22236200	-0.20281300	1.38728600
H	6.01170700	1.50106800	1.93101700
H	8.13264000	0.38536300	1.28519900
C	3.56289800	0.38509400	2.36036400
H	2.71443100	-0.20991500	1.97922700
O	3.46595000	1.71735100	1.89801700
H	3.05362700	1.72328900	0.97894600
C	3.47058200	0.41539100	3.89164000
H	3.55236100	-0.59171000	4.31588700
H	4.28200500	1.02778100	4.30046400
H	2.51643200	0.85569500	4.20044700
C	8.54930700	-2.25855400	0.71450300
H	8.54785000	-3.32387700	0.96961100
H	8.69676700	-2.18419600	-0.37166600
H	9.42365800	-1.79934400	1.18952400

Pu4

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.44943500	1.32256300	-0.75570800
H	-2.61782100	-0.68504000	2.11396100
H	0.42239300	1.88614900	-1.94953900
N	-2.43548000	1.23895300	-1.28465900
H	-2.74417600	0.56467000	-1.98424200
H	-3.20515400	0.81908200	0.42158600
N	-1.11854700	3.40727100	-0.37296200
H	-0.77797200	3.82253500	0.49376600
H	-0.68775400	3.94411500	-1.12672700

P	0.15325800	-0.80554000	-1.42729100
P	1.48196200	1.60927600	0.50783900
C	-2.60061800	3.50169000	-0.46153700
H	-2.98314800	3.11006400	0.48795700
C	-3.04535200	2.54053500	-1.56817900
H	-2.67416800	2.95217700	-2.52940100
C	5.36303500	-0.71838200	-0.80282400
C	5.30705400	0.69547200	-0.80464100
C	4.18212300	1.35227000	-0.37367200
C	3.03426900	0.65147700	0.09460300
C	3.05643600	-0.74679200	0.13601900
C	4.23029800	-1.45207600	-0.32240400
H	6.17097600	1.25868300	-1.15048600
H	4.17426600	2.43510600	-0.38407200
C	1.23487300	-3.14034200	2.52355200
C	0.05425300	-3.40157000	1.78932000
C	-0.18557800	-2.76526700	0.59740200
C	0.73403100	-1.83167600	0.03764900
C	1.93911700	-1.58273600	0.70929500
C	2.19234800	-2.22483900	1.97815900
H	-0.66374400	-4.12018100	2.17878700
H	-1.09851700	-2.99459300	0.06332200
C	-3.37110800	-3.24638400	-3.34683100
C	-2.13672100	-3.19710800	-3.99428900
C	-1.06622000	-2.50094100	-3.42766600
C	-1.20720300	-1.83494400	-2.19860500
C	-2.46608400	-1.87749800	-1.57137300
C	-3.53352500	-2.58270400	-2.12965000
H	-4.20116200	-3.79104900	-3.78958800
H	-1.99907700	-3.70279300	-4.94688200
H	-0.12101100	-2.47950800	-3.95594900
H	-2.62159600	-1.34651700	-0.63978900
H	-4.48764600	-2.60040000	-1.61112500
C	3.36709600	-1.42133000	-4.75696700
C	3.09236100	-2.45224300	-3.85589400
C	2.15716200	-2.26056600	-2.83868200
C	1.48756100	-1.03449000	-2.69753000
C	1.76934200	-0.00904600	-3.61070600
C	2.70177600	-0.20096900	-4.63277700
H	4.09598700	-1.56922500	-5.54971400
H	3.61023400	-3.40390600	-3.93865200
H	1.94623000	-3.07256500	-2.14924000
H	1.25229900	0.93978300	-3.51339400
H	2.90770700	0.60614600	-5.33138500

C	1.00568900	1.06604900	5.12019300
C	2.28725700	1.14109100	4.56935300
C	2.44767900	1.28193100	3.19070200
C	1.33126300	1.35123800	2.34202200
C	0.04950400	1.27396000	2.90579300
C	-0.11142000	1.13235200	4.28654800
H	0.87979600	0.95237400	6.19381300
H	3.16166800	1.08459200	5.21259100
H	3.44762400	1.33957000	2.76935500
H	-0.82642500	1.32176700	2.26178000
H	-1.11065300	1.06907200	4.70856600
C	2.70582700	6.13300800	0.19680200
C	2.53491800	5.55887600	1.45537300
C	2.21284000	4.20255800	1.57807500
C	2.04514200	3.39490900	0.44242300
C	2.20393600	3.99539400	-0.82248400
C	2.54223700	5.34280800	-0.94494100
H	2.95981800	7.18559300	0.10327200
H	2.65440800	6.16290500	2.35133800
H	2.09260000	3.77851100	2.56872200
H	2.67127900	5.77771800	-1.93300700
C	3.59728500	-2.61968400	3.94037900
C	3.37739800	-1.98999100	2.73557900
H	4.51011100	-2.41575100	4.49395200
H	4.11864200	-1.29705300	2.35686900
C	2.64760500	-3.52727500	4.46615300
C	1.48982100	-3.77741800	3.76794100
H	2.83469800	-4.01971700	5.41663000
H	0.74636300	-4.46959300	4.15658300
C	5.45114200	-3.52168800	-0.77824500
C	4.32056000	-2.87510200	-0.33030700
H	5.48677600	-4.60795100	-0.77095700
H	3.48023000	-3.46106900	0.02161500
C	6.56635700	-2.78686600	-1.24612600
C	6.51680800	-1.41284600	-1.25717500
H	7.45372900	-3.30858700	-1.59437000
H	7.36284700	-0.83077600	-1.61534600
H	2.05533200	3.39512700	-1.71533700
C	-4.58427300	2.52341300	-1.64881800
H	-4.90089600	1.85308300	-2.45923200
H	-4.97661400	2.10436000	-0.71310500
C	-3.12925100	4.92418100	-0.67958700
H	-2.80901900	5.58032400	0.14174700
H	-2.69533300	5.33650200	-1.60394200

C	-4.66486100	4.91656700	-0.79129500
H	-5.09117400	4.62295400	0.17853300
H	-5.03004300	5.93003500	-1.00051400
C	-5.14889300	3.93685300	-1.87303200
H	-4.83264300	4.30416000	-2.86071700
H	-6.24597400	3.90922200	-1.88907600
C	-3.62963300	-0.24639500	2.08352900
O	-3.62733800	0.94648500	1.31870900
C	-4.02114000	0.15275100	3.51216300
H	-4.00986300	-0.71320100	4.18258700
H	-3.32659200	0.90919500	3.89303100
H	-5.02945800	0.58119100	3.51589400
C	-6.42924600	-3.29262900	0.69317200
C	-6.67110300	-1.93066600	0.46533400
C	-5.76658700	-0.95376400	0.88442000
C	-4.58719400	-1.30840600	1.54902200
C	-4.33934400	-2.66845600	1.77388800
C	-5.24544400	-3.64354300	1.35658300
H	-7.58428400	-1.63003000	-0.04499600
H	-5.96839400	0.09681100	0.69943700
H	-3.42586100	-2.96770000	2.28528300
H	-5.02930000	-4.69332800	1.54527000
C	-7.39836100	-4.34999800	0.21463800
H	-7.13445600	-4.71440500	-0.78765700
H	-7.40532200	-5.21937400	0.88151000
H	-8.42048900	-3.96005100	0.15819200

ABS₅

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.128648	0.999336	-0.492180
H	-1.051821	0.084672	0.638035
H	0.584852	2.019194	-1.670077
N	-1.871004	0.915228	-1.868442
H	-1.599693	0.554620	-2.780953
H	-2.582008	0.284700	-1.490716
N	-1.335034	2.783553	0.122074
H	-1.485520	2.784184	1.128332
H	-0.779997	3.611623	-0.091475
P	0.860736	-0.892810	-1.291544
P	1.591531	1.434817	0.941908

C	-2.636911	2.832686	-0.589440
H	-3.306219	2.145396	-0.056936
C	-2.443158	2.271668	-2.005212
H	-1.678292	2.876158	-2.510055
C	5.833970	0.425377	-0.859422
C	5.414083	1.759242	-0.642920
C	4.194672	2.026380	-0.073266
C	3.308782	0.988794	0.332296
C	3.698158	-0.344926	0.164057
C	4.969860	-0.642155	-0.452487
H	6.072694	2.574717	-0.933996
H	3.905387	3.058800	0.077941
C	2.712071	-3.448196	2.209440
C	1.546721	-3.858455	1.518734
C	1.060589	-3.123685	0.467287
C	1.705452	-1.938128	0.014371
C	2.878256	-1.514142	0.649250
C	3.385980	-2.260270	1.776618
H	1.039697	-4.768621	1.832225
H	0.165702	-3.464336	-0.038558
C	-2.471092	-3.645743	-3.144533
C	-1.299704	-3.415865	-3.864652
C	-0.277441	-2.629707	-3.323313
C	-0.406346	-2.052754	-2.049590
C	-1.604005	-2.279175	-1.343687
C	-2.619079	-3.072307	-1.879216
H	-3.264806	-4.256805	-3.567039
H	-1.173979	-3.847072	-4.854934
H	0.620934	-2.467793	-3.907051
H	-1.732013	-1.804359	-0.375166
H	-3.534151	-3.227273	-1.313522
C	3.952931	-0.805524	-4.797863
C	3.798953	-1.970609	-4.042153
C	2.901047	-1.997244	-2.974691
C	2.139059	-0.863005	-2.648090
C	2.304810	0.300524	-3.409704
C	3.206289	0.328824	-4.477100
H	4.656336	-0.782807	-5.626636
H	4.384407	-2.855685	-4.277937
H	2.790795	-2.908881	-2.393195
H	1.729262	1.181741	-3.135725
H	3.327608	1.242043	-5.055063
C	1.645016	-0.127280	5.350078
C	2.788574	0.474577	4.818282

C	2.792692	0.920430	3.496465
C	1.652713	0.778950	2.687021
C	0.515209	0.168136	3.228174
C	0.511676	-0.282350	4.551236
H	1.643566	-0.480485	6.378377
H	3.679894	0.588498	5.430235
H	3.689115	1.383662	3.091815
H	-0.351596	0.037185	2.584370
H	-0.377170	-0.761618	4.955243
C	1.668737	6.090639	1.625024
C	1.677885	5.238395	2.728039
C	1.697023	3.850368	2.552209
C	1.700339	3.282903	1.268297
C	1.670654	4.158261	0.163279
C	1.665994	5.542832	0.338875
H	1.658730	7.168866	1.763211
H	1.672219	5.648907	3.734935
H	1.707244	3.212942	3.428593
H	1.655582	6.194458	-0.531838
C	5.026747	-2.611810	3.555111
C	4.552840	-1.869836	2.496002
H	5.919541	-2.285820	4.082488
H	5.074781	-0.967291	2.202509
C	4.362060	-3.791535	3.965279
C	3.225264	-4.194344	3.304527
H	4.747864	-4.370496	4.800297
H	2.696702	-5.094958	3.609262
C	6.640698	-2.229373	-1.270340
C	5.419294	-1.974391	-0.687378
H	6.952853	-3.257386	-1.435520
H	4.783304	-2.803760	-0.403277
C	7.491106	-1.167583	-1.659341
C	7.089153	0.131954	-1.458054
H	8.453565	-1.381525	-2.116692
H	7.726657	0.961683	-1.755244
H	1.627625	3.730310	-0.835136
C	-3.752250	2.310612	-2.812217
H	-3.559422	1.952790	-3.832635
H	-4.468605	1.612237	-2.360025
C	-3.262122	4.236837	-0.616611
H	-3.434289	4.584681	0.410736
H	-2.541099	4.935625	-1.068436
C	-4.569707	4.266182	-1.424937
H	-5.326930	3.654078	-0.914109

H	-4.964358	5.289327	-1.459023
C	-4.354083	3.724343	-2.845695
H	-3.679262	4.399174	-3.392759
H	-5.302142	3.716550	-3.397774
C	-5.044685	-0.608135	0.484007
O	-4.606630	-0.229010	-0.601918
C	-4.120532	-0.748480	1.678824
H	-4.107799	-1.783981	2.041263
H	-3.106481	-0.452999	1.391663
H	-4.462674	-0.121086	2.511503
C	-9.236762	-1.515452	0.832241
C	-8.687913	-1.087849	-0.391422
C	-7.338048	-0.802819	-0.482764
C	-6.489828	-0.931884	0.635808
C	-7.049802	-1.360469	1.847054
C	-8.409221	-1.652144	1.955907
H	-9.348476	-0.991513	-1.247329
H	-6.904354	-0.474729	-1.421547
H	-6.425167	-1.472176	2.727796
H	-8.809439	-1.981050	2.907788
O	-10.569857	-1.769016	0.820471
C	-11.192694	-2.204490	2.021607
H	-12.246726	-2.343574	1.776339
H	-10.771447	-3.156193	2.369674
H	-11.100191	-1.453492	2.816531

INTf₅

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.395890	0.511003	0.779665
H	-1.164368	0.035627	-0.692216
H	0.134878	1.048890	2.316243
N	-1.821809	2.215067	0.848155
H	-1.329184	3.095352	0.985313
H	-2.315619	2.288926	-0.042997
N	-2.140820	-0.361452	1.862134
H	-2.406186	-1.264669	1.475169
H	-1.833902	-0.533749	2.818841
P	1.239084	1.637587	-0.350404
P	0.885110	-1.369368	0.977512

C	-3.304566	0.557790	1.848114
H	-3.779616	0.439251	0.866205
C	-2.794835	2.002837	1.942317
H	-2.226986	2.103845	2.876848
C	5.460164	-0.500943	1.736754
C	4.626609	-1.042748	2.743635
C	3.309746	-1.327384	2.484140
C	2.728299	-1.105103	1.204312
C	3.524861	-0.596252	0.171787
C	4.907423	-0.273110	0.435069
H	5.043870	-1.233044	3.730149
H	2.700738	-1.741696	3.277615
C	3.193867	-1.131251	-3.622365
C	2.317758	-0.072093	-3.961284
C	1.808059	0.752933	-2.991148
C	2.145524	0.597267	-1.617074
C	3.028878	-0.420643	-1.241282
C	3.551598	-1.315291	-2.247276
H	2.052915	0.080956	-5.005365
H	1.136303	1.551340	-3.282133
C	-0.751680	5.144670	-2.766571
C	0.441687	5.383238	-2.085208
C	1.076680	4.353287	-1.384217
C	0.532498	3.059026	-1.353977
C	-0.676819	2.837939	-2.039938
C	-1.311360	3.865208	-2.738985
H	-1.246995	5.949529	-3.303983
H	0.883530	6.376793	-2.090182
H	1.996167	4.571348	-0.854048
H	-1.122478	1.848596	-1.995163
H	-2.257212	3.667484	-3.236083
C	4.649599	3.948695	1.860836
C	4.764222	3.694421	0.491876
C	3.767917	2.977480	-0.171467
C	2.639188	2.506738	0.520148
C	2.538190	2.762528	1.893466
C	3.536565	3.478664	2.558926
H	5.428027	4.503315	2.379050
H	5.633778	4.045567	-0.057796
H	3.870153	2.783245	-1.235926
H	1.674997	2.372539	2.427431
H	3.445009	3.664229	3.626586
C	0.763800	-4.828888	-2.168052
C	1.715370	-4.860222	-1.145010

C	1.776157	-3.821848	-0.215468
C	0.882805	-2.739462	-0.288516
C	-0.062367	-2.716010	-1.320625
C	-0.120880	-3.753597	-2.255055
H	0.721084	-5.634585	-2.896834
H	2.415661	-5.688964	-1.076538
H	2.523523	-3.854273	0.573307
H	-0.729554	-1.859124	-1.382836
H	-0.854556	-3.716717	-3.057164
C	-0.567966	-3.593192	4.863192
C	-0.486401	-4.296900	3.662850
C	-0.017075	-3.670086	2.503082
C	0.374848	-2.322293	2.516398
C	0.265971	-1.618564	3.733721
C	-0.188013	-2.248145	4.893580
H	-0.927764	-4.083097	5.764452
H	-0.785894	-5.341408	3.621414
H	0.039544	-4.243898	1.585401
H	-0.249094	-1.684495	5.821651
C	4.924841	-3.223584	-2.919246
C	4.426877	-2.396454	-1.936985
H	5.590040	-4.039333	-2.648097
H	4.703264	-2.571561	-0.904485
C	4.577252	-3.024159	-4.275978
C	3.725047	-1.999110	-4.614297
H	4.979482	-3.681259	-5.042595
H	3.440866	-1.834047	-5.651257
C	7.089315	0.568825	-0.279645
C	5.771665	0.278377	-0.555546
H	7.721089	0.988736	-1.058145
H	5.380621	0.475975	-1.546061
C	7.628122	0.329349	1.006577
C	6.823708	-0.192304	1.992252
H	8.670039	0.561087	1.211303
H	7.217410	-0.377779	2.989091
H	0.522060	-0.562203	3.747595
C	-3.961289	3.005146	1.927507
H	-3.568247	4.024629	2.037757
H	-4.450014	2.956753	0.944549
C	-4.333549	0.252653	2.949010
H	-4.708930	-0.772276	2.829180
H	-3.826998	0.291308	3.925895
C	-5.496764	1.257920	2.938218
H	-6.071115	1.135282	2.009272

H	-6.185498	1.039687	3.763928
C	-4.982843	2.701991	3.035654
H	-4.512099	2.854136	4.018083
H	-5.819672	3.409088	2.978335
C	-4.457652	0.888247	-2.093276
O	-4.220602	1.982561	-1.581722
C	-3.440189	0.261391	-3.024798
H	-2.641125	-0.176994	-2.408179
H	-3.850759	-0.500528	-3.690590
H	-2.983062	1.053590	-3.623645
C	-5.723684	0.170383	-1.770779
C	-6.732235	0.865150	-1.071135
C	-5.957875	-1.169819	-2.107955
C	-7.922751	0.248617	-0.730923
C	-6.555970	1.904326	-0.814076
C	-7.146716	-1.810965	-1.758032
H	-5.202466	-1.741594	-2.637057
H	-8.139365	-1.100475	-1.069478
H	-8.708630	0.781164	-0.204483
H	-7.288786	-2.851348	-2.026172
O	-9.335159	-1.616783	-0.687927
C	-9.623223	-2.973191	-1.000194
H	-10.621691	-3.164023	-0.603787
H	-9.623288	-3.143842	-2.084271
H	-8.906624	-3.655130	-0.525000

TSf₅

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.815676	0.817593	0.354024
H	-1.606102	0.302246	-1.229334
H	-0.399166	1.361624	1.859998
N	-1.963203	2.663333	0.087667
H	-1.388565	3.503723	0.056522
H	-2.432295	2.569474	-0.829919
N	-2.788507	0.312062	1.264506
H	-3.192438	-0.508970	0.814071
H	-2.615907	0.064496	2.237912
P	1.172638	1.680802	-0.450141
P	0.193916	-1.174345	0.934958

C	-3.750325	1.443669	1.172160
H	-4.235593	1.344362	0.197020
C	-2.984745	2.770970	1.152478
H	-2.445634	2.887682	2.101068
C	4.622149	-0.818641	2.544411
C	3.545955	-1.158403	3.397264
C	2.272255	-1.282825	2.902371
C	1.975310	-1.083698	1.524870
C	3.016013	-0.775505	0.640569
C	4.360083	-0.628784	1.149236
H	3.740771	-1.324471	4.454515
H	1.476577	-1.554287	3.584020
C	3.334054	-1.534870	-3.117701
C	2.690421	-0.401342	-3.670862
C	2.125253	0.548510	-2.858671
C	2.177982	0.451294	-1.438604
C	2.823831	-0.641330	-0.849287
C	3.394068	-1.666510	-1.692060
H	2.649838	-0.291586	-4.752346
H	1.635413	1.403162	-3.310032
C	0.492458	5.242835	-3.441923
C	1.618358	5.255932	-2.616495
C	1.852459	4.210777	-1.719936
C	0.965634	3.123816	-1.632255
C	-0.168256	3.132024	-2.461532
C	-0.403222	4.176345	-3.358345
H	0.312068	6.060671	-4.135137
H	2.319489	6.085683	-2.663468
H	2.728563	4.255432	-1.084318
H	-0.892015	2.329469	-2.397487
H	-1.296618	4.148164	-3.976343
C	4.244078	3.722227	2.429640
C	4.672268	3.228969	1.195655
C	3.769691	2.584404	0.348594
C	2.425343	2.416561	0.718752
C	2.010515	2.911350	1.962559
C	2.911224	3.560313	2.810209
H	4.946626	4.222643	3.091282
H	5.711085	3.335154	0.894641
H	4.117220	2.203961	-0.607436
H	0.978695	2.761314	2.264976
H	2.569852	3.934327	3.772514
C	0.522664	-4.811884	-1.981837
C	0.982595	-4.942788	-0.668181

C	0.900963	-3.864568	0.212982
C	0.337159	-2.645058	-0.199483
C	-0.101811	-2.520485	-1.521117
C	-0.009678	-3.595652	-2.409671
H	0.594292	-5.650328	-2.669830
H	1.414185	-5.882741	-0.333191
H	1.275967	-3.974051	1.227379
H	-0.495127	-1.559981	-1.839680
H	-0.347214	-3.478709	-3.436501
C	-2.324742	-2.818288	4.546435
C	-2.184532	-3.593104	3.396432
C	-1.396676	-3.145655	2.330330
C	-0.733462	-1.909884	2.388159
C	-0.909675	-1.125260	3.546830
C	-1.683073	-1.578302	4.616524
H	-2.931796	-3.170108	5.376419
H	-2.686300	-4.554826	3.322539
H	-1.303988	-3.771068	1.449961
H	-1.788654	-0.958177	5.503368
C	4.583889	-3.780391	-1.994991
C	4.028170	-2.829939	-1.167362
H	5.059494	-4.656743	-1.562485
H	4.068355	-2.970701	-0.094293
C	4.538017	-3.630480	-3.400856
C	3.919330	-2.529818	-3.946146
H	4.984768	-4.385066	-4.042850
H	3.865794	-2.401410	-5.024907
C	6.738404	-0.155289	0.828650
C	5.466775	-0.288485	0.316925
H	7.559403	0.104548	0.165429
H	5.303196	-0.129482	-0.741788
C	6.986916	-0.352746	2.207696
C	5.944908	-0.675737	3.044443
H	7.995203	-0.246872	2.599011
H	6.114574	-0.827814	4.107931
H	-0.447268	-0.143488	3.592688
C	-3.954152	3.949721	0.967377
H	-3.394001	4.894305	0.976244
H	-4.425647	3.868813	-0.022384
C	-4.828930	1.429632	2.264535
H	-5.382304	0.482726	2.223665
H	-4.343815	1.475501	3.252106
C	-5.791507	2.619165	2.107420
H	-6.364202	2.494299	1.177579

H	-6.521187	2.621008	2.926580
C	-5.035280	3.955840	2.061599
H	-4.562787	4.140078	3.037775
H	-5.736050	4.782878	1.893738
C	-2.892427	0.590430	-2.415476
O	-3.133929	1.826743	-2.383575
C	-2.085535	0.039272	-3.594227
H	-1.810484	-1.010491	-3.473878
H	-2.721174	0.120944	-4.488034
H	-1.184177	0.631572	-3.760185
C	-6.075021	-2.017420	-1.015306
C	-6.322816	-0.686507	-1.382186
C	-5.276931	0.126739	-1.802204
C	-3.956580	-0.352633	-1.873512
C	-3.728209	-1.685602	-1.514422
C	-4.766712	-2.515898	-1.081124
H	-7.343350	-0.317747	-1.336616
H	-5.462163	1.156333	-2.092048
H	-2.721331	-2.088191	-1.548445
H	-4.543959	-3.540187	-0.803399
O	-7.163089	-2.737938	-0.612051
C	-6.973858	-4.096644	-0.255777
H	-7.960683	-4.476017	0.016728
H	-6.579114	-4.684207	-1.095430
H	-6.296997	-4.200237	0.603221

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Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.032707	-1.186214	0.111633
H	-2.044912	0.158661	-0.748969
H	-0.435529	-2.503807	0.897706
N	-2.836224	-1.377459	1.324613
H	-2.686161	-1.211942	2.318598
H	-3.486469	-0.655383	0.968655
N	-2.235859	-2.686814	-1.027846
H	-2.346650	-2.439562	-2.009805
H	-1.680765	-3.541665	-1.010248
P	0.111114	0.136032	1.611655
P	0.811474	-1.369166	-1.278666

C	-3.569571	-2.916303	-0.409481
H	-4.220589	-2.119752	-0.784752
C	-3.457432	-2.704769	1.106920
H	-2.766723	-3.451082	1.521220
C	5.016303	-1.354187	0.868580
C	4.515147	-2.509176	0.223468
C	3.303245	-2.482049	-0.419640
C	2.504161	-1.305473	-0.472313
C	2.976879	-0.131955	0.125036
C	4.244821	-0.148455	0.817322
H	5.105279	-3.422801	0.240311
H	2.955672	-3.382143	-0.910065
C	2.312070	3.547062	-0.765427
C	1.175825	3.809084	0.036786
C	0.591776	2.810522	0.774785
C	1.112471	1.486511	0.789564
C	2.261929	1.193770	0.045724
C	2.861521	2.223565	-0.768257
H	0.763488	4.815386	0.059107
H	-0.283684	3.042703	1.368067
C	-2.871984	2.279115	4.535553
C	-1.781750	1.586073	5.060966
C	-0.860301	0.966994	4.211714
C	-1.014847	1.023189	2.815919
C	-2.136439	1.699700	2.303638
C	-3.045721	2.333842	3.151253
H	-3.583766	2.765697	5.197619
H	-1.639806	1.525152	6.137203
H	-0.021801	0.438640	4.648553
H	-2.300953	1.727577	1.232655
H	-3.889743	2.864059	2.720311
C	3.043166	-1.669285	4.777422
C	3.072068	-0.301923	4.493622
C	2.223622	0.227988	3.521666
C	1.332322	-0.596005	2.813994
C	1.312227	-1.964912	3.109330
C	2.161684	-2.497787	4.082388
H	3.705653	-2.084384	5.532730
H	3.760446	0.351916	5.022397
H	2.253260	1.293774	3.313341
H	0.630801	-2.606933	2.559871
H	2.134104	-3.563951	4.294352
C	1.477122	1.329407	-5.031746
C	2.470126	0.417894	-4.660402

C	2.300310	-0.381506	-3.530065
C	1.129602	-0.286790	-2.758938
C	0.147735	0.632399	-3.136209
C	0.316506	1.438277	-4.265397
H	1.613211	1.954284	-5.910672
H	3.379489	0.333469	-5.250162
H	3.079777	-1.085284	-3.249680
H	-0.740630	0.702414	-2.517187
H	-0.456510	2.150703	-4.543653
C	0.446552	-5.624856	-3.244111
C	0.501586	-4.491920	-4.053977
C	0.662997	-3.222229	-3.488450
C	0.764980	-3.055988	-2.098311
C	0.685359	-4.210268	-1.292270
C	0.540737	-5.478148	-1.857058
H	0.326897	-6.610973	-3.685020
H	0.422613	-4.588869	-5.133918
H	0.708547	-2.359483	-4.143059
H	0.496487	-6.351800	-1.211292
C	4.563661	2.992471	-2.344920
C	4.001219	1.987102	-1.590601
H	5.430347	2.778483	-2.964794
H	4.427102	0.991878	-1.626407
C	4.022979	4.299966	-2.324044
C	2.917589	4.565471	-1.550283
H	4.479172	5.085946	-2.920055
H	2.485536	5.563479	-1.525340
C	5.989274	0.953948	2.129365
C	4.777414	0.997999	1.476620
H	6.366484	1.846364	2.621955
H	4.214279	1.923036	1.467134
C	6.747036	-0.240452	2.166872
C	6.263841	-1.369823	1.549203
H	7.702927	-0.261796	2.683435
H	6.829500	-2.298526	1.570623
H	0.723454	-4.103119	-0.212277
C	-4.834869	-2.858706	1.771960
H	-4.738098	-2.724564	2.857749
H	-5.492918	-2.058686	1.406541
C	-4.174922	-4.288350	-0.738506
H	-4.269806	-4.402140	-1.826750
H	-3.489444	-5.079646	-0.396139
C	-5.544027	-4.466660	-0.060452
H	-6.256026	-3.752037	-0.496694

H	-5.937473	-5.469444	-0.268409
C	-5.454712	-4.230230	1.455172
H	-4.841217	-5.021598	1.911034
H	-6.449940	-4.306678	1.910171
C	-3.646774	0.707948	-1.156194
O	-4.448154	0.097163	-0.393439
C	-3.592604	0.271025	-2.624546
H	-2.759052	0.700616	-3.182247
H	-3.552859	-0.818297	-2.700117
H	-4.526798	0.604057	-3.098967
C	-3.491490	5.014716	-0.631751
C	-4.501045	4.237152	-0.046085
C	-4.495791	2.856871	-0.203149
C	-3.494348	2.206947	-0.946516
C	-2.496285	2.997511	-1.523959
C	-2.481223	4.386293	-1.370957
H	-5.281978	4.740261	0.516825
H	-5.276745	2.246901	0.238874
H	-1.690613	2.532850	-2.081416
H	-1.681135	4.959478	-1.825921
O	-3.581611	6.362855	-0.425545
C	-2.597562	7.197283	-1.009639
H	-2.865949	8.218869	-0.732905
H	-1.593371	6.971501	-0.624958
H	-2.588408	7.109041	-2.104490

Pf5

Coordinates (Angstroms)			
	X	Y	Z

Ru		0.51343900	0.61189600 -0.85744300
H		-0.14786800	0.90004300 -2.26069600
N		1.95102600	2.08610300 -0.64507800
H		1.62628800	3.04678800 -0.52822900
N		2.25235000	-0.25487100 -1.95260400
H		2.46952300	-1.22881900 -1.74160100
H		1.95592500	-0.24645800 -2.92924200
P		-1.24695300	1.76175300 0.11536000
P		-0.69295900	-1.38691300 -0.95356800
C		3.45998200	0.60084600 -1.78396600
H		3.88660000	0.33279300 -0.80993800

C	2.97528400	2.04942000	-1.69272100
H	2.54747400	2.31353600	-2.68103300
C	-5.35228100	-1.03863000	-1.57478800
C	-4.51544500	-1.62436900	-2.55396100
C	-3.16759200	-1.75916400	-2.33399600
C	-2.55588400	-1.32447800	-1.12413500
C	-3.35177500	-0.76712700	-0.11766900
C	-4.76994200	-0.61170600	-0.33763400
H	-4.95515900	-1.97218300	-3.48609800
H	-2.55836700	-2.21975800	-3.10147500
C	-2.82329500	-0.88612900	3.68417300
C	-2.07904600	0.29956800	3.88829700
C	-1.70558600	1.08434400	2.82677100
C	-2.05251800	0.75722100	1.48386800
C	-2.81943500	-0.39019100	1.24195900
C	-3.19949600	-1.23867900	2.34755400
H	-1.80647800	0.58606900	4.90158300
H	-1.13901100	1.98616900	3.02091900
C	0.05343300	5.75981000	2.20435100
C	-1.10651900	5.74145600	1.42879000
C	-1.52755500	4.56156100	0.81021300
C	-0.79654900	3.37077900	0.95740700
C	0.37771400	3.41005700	1.72989000
C	0.79641200	4.58761900	2.35086300
H	0.37960200	6.68098700	2.68058600
H	-1.69002700	6.64948300	1.29782300
H	-2.42744900	4.58137500	0.20732100
H	0.99629100	2.52756900	1.83946800
H	1.71535300	4.57681100	2.93027700
C	-4.74364300	3.36045300	-2.53322200
C	-4.94406700	3.15801000	-1.16622700
C	-3.91332500	2.64777700	-0.37636100
C	-2.66790200	2.32388500	-0.93789600
C	-2.47841800	2.53565700	-2.31089000
C	-3.50787800	3.05000300	-3.10233000
H	-5.54646900	3.75654300	-3.14975400
H	-5.90470600	3.38882200	-0.71390500
H	-4.07985000	2.50140600	0.68660400
H	-1.51868600	2.29254600	-2.75502500
H	-3.34179500	3.20692300	-4.16518700
C	-0.01470800	-4.54452800	2.42098200
C	-1.02375100	-4.75916100	1.47826500
C	-1.25626100	-3.81840800	0.47465600
C	-0.47891800	-2.65183300	0.39298700

C	0.52717900	-2.44809500	1.34578600
C	0.75893100	-3.38498000	2.35566300
H	0.16086900	-5.27470800	3.20664800
H	-1.63505300	-5.65644900	1.53008700
H	-2.04695900	-3.99104000	-0.25081900
H	1.12296600	-1.53988800	1.29660300
H	1.53707900	-3.20451100	3.09301900
C	0.85980300	-3.64013200	-4.77008200
C	0.92163700	-4.27352700	-3.53012800
C	0.41958000	-3.64325400	-2.38582300
C	-0.14646700	-2.36099000	-2.45652500
C	-0.18409100	-1.72696700	-3.71513600
C	0.30035500	-2.36172900	-4.85871800
H	1.24563100	-4.13252500	-5.65874700
H	1.35788100	-5.26572700	-3.44554700
H	0.47209300	-4.16170300	-1.43504200
H	0.24614600	-1.85492000	-5.81903000
C	-4.30916000	-3.22342600	3.24683600
C	-3.94980500	-2.43853200	2.17389700
H	-4.88053400	-4.13268900	3.07926200
H	-4.24088300	-2.74009900	1.17524100
C	-3.94129400	-2.86011500	4.56391000
C	-3.20997000	-1.71454700	4.77224300
H	-4.23425900	-3.48633100	5.40234900
H	-2.91378100	-1.42055300	5.77657800
C	-6.99063600	0.10291900	0.39527700
C	-5.64159200	-0.03779600	0.63384600
H	-7.62761600	0.54474100	1.15706400
H	-5.23262100	0.29594500	1.57982000
C	-7.55588300	-0.32318100	-0.83021500
C	-6.74793400	-0.88156200	-1.79251600
H	-8.62218900	-0.20867800	-1.00562100
H	-7.16419700	-1.21430600	-2.74060600
H	-0.59526800	-0.72443400	-3.79160100
C	4.17109000	2.99107700	-1.45225400
H	3.81638600	4.03039400	-1.43026600
H	4.59418000	2.78110500	-0.46161300
C	4.52188100	0.40273300	-2.87142700
H	4.86424800	-0.64122500	-2.88297900
H	4.07217000	0.60236800	-3.85679800
C	5.71037800	1.35513800	-2.64581200
H	6.22647500	1.06840800	-1.71913400
H	6.43814000	1.24293300	-3.45958100
C	5.24754700	2.81738100	-2.53753800

H	4.84290300	3.14188700	-3.50805000
H	6.10627400	3.46732200	-2.32637600
C	4.90243500	-1.34973900	1.61102700
C	6.12101300	-1.91699300	1.21804600
C	4.77280600	0.01884300	1.85553500
H	4.03700300	-2.00081300	1.72671400
C	7.24327700	-1.09614600	1.06383600
H	6.17812100	-2.98439800	1.03529200
C	5.90973200	0.82623100	1.69126900
C	7.12779000	0.28272900	1.30129100
H	5.81848500	1.89426400	1.86324800
H	8.00948400	0.90422000	1.17506000
C	3.45381300	0.62264300	2.33354200
H	2.63697000	-0.03095300	1.97993800
O	3.26049100	1.94142300	1.86067700
H	2.84117800	1.91550100	0.94550300
C	3.39198000	0.66820400	3.86591900
H	3.54584200	-0.32615900	4.30006100
H	4.17175900	1.33552900	4.24976000
H	2.41876900	1.05190300	4.19060000
O	8.48350800	-1.53244200	0.68503900
C	8.65890000	-2.91607600	0.44106500
H	9.70758000	-3.04293500	0.16449900
H	8.44606900	-3.51660600	1.33612700
H	8.02322500	-3.26703400	-0.38365300

Pu5

Coordinates (Angstroms)			
	X	Y	Z
Ru	-0.19176800	1.39470800	-0.72980700
H	-2.63593800	-0.40769700	2.11679600
H	0.71540600	1.87351100	-1.93348300
N	-2.17045900	1.50078700	-1.28437400
H	-2.52706700	0.84952500	-1.98275500
H	-2.96733500	1.19806800	0.42912900
N	-0.66867900	3.53828300	-0.35761100
H	-0.31672800	3.92300800	0.51891500
H	-0.16492400	4.02843400	-1.09771000
P	0.21551000	-0.77996500	-1.40624200
P	1.75510400	1.50263100	0.53429900
C	-2.13083100	3.77975300	-0.49233600

H	-2.57911800	3.44330200	0.44924100
C	-2.63662100	2.85266900	-1.60176400
H	-2.19580500	3.21117200	-2.55483700
C	5.42553300	-1.10621200	-0.85505800
C	5.48053100	0.30749400	-0.83636700
C	4.41603500	1.04337200	-0.38062500
C	3.22274700	0.42813300	0.09429300
C	3.13592700	-0.96829900	0.11569100
C	4.24510500	-1.75606400	-0.36890200
H	6.38135700	0.80664600	-1.18641000
H	4.49284800	2.12341900	-0.37615000
C	1.15898500	-3.23158000	2.50842100
C	-0.05482900	-3.37720300	1.79668300
C	-0.25819900	-2.71143600	0.61434700
C	0.73121400	-1.85902200	0.04396900
C	1.96438800	-1.72138400	0.69563800
C	2.18365800	-2.39866400	1.95286100
H	-0.82776700	-4.03013600	2.19640200
H	-1.19766300	-2.85149400	0.09540100
C	-3.55049600	-2.90207600	-3.24549200
C	-2.32198100	-2.99710400	-3.89908400
C	-1.18261300	-2.39704500	-3.35723100
C	-1.24649100	-1.68634100	-2.14713500
C	-2.49813900	-1.58581900	-1.51170800
C	-3.63575100	-2.19285500	-2.04632000
H	-4.43553300	-3.36905300	-3.67011700
H	-2.24316800	-3.53970700	-4.83795900
H	-0.24402700	-2.48503300	-3.89043100
H	-2.59286400	-1.01530500	-0.59499500
H	-4.58373300	-2.09827800	-1.52513200
C	3.28947400	-1.66519500	-4.80677600
C	2.95625700	-2.66678300	-3.89255500
C	2.06529500	-2.39650000	-2.85349100
C	1.49842700	-1.12074100	-2.70419900
C	1.83835600	-0.12507400	-3.63048100
C	2.72677400	-0.39509500	-4.67385100
H	3.98417600	-1.87423300	-5.61625700
H	3.39400600	-3.65726300	-3.98231900
H	1.80716800	-3.18583600	-2.15396600
H	1.40164400	0.86257500	-3.52679700
H	2.97861800	0.39005200	-5.38237300
C	1.23155100	0.90117500	5.13395700
C	2.51595100	0.88230100	4.58485100
C	2.69024900	1.04053700	3.20981600

C	1.58490000	1.22057900	2.36278200
C	0.29994000	1.23807200	2.92480500
C	0.12537400	1.07939000	4.30208900
H	1.09479800	0.77372000	6.20471500
H	3.38145600	0.73873400	5.22657500
H	3.69280400	1.02461700	2.79095200
H	-0.56807600	1.37599400	2.28273000
H	-0.87647500	1.09047500	4.72250300
C	3.34165400	5.91720000	0.31338700
C	3.11805900	5.33460900	1.55978800
C	2.68691400	4.00680300	1.65483000
C	2.46160100	3.23685000	0.50322200
C	2.67391300	3.84714000	-0.74921700
C	3.12049100	5.16506800	-0.84421000
H	3.68026500	6.94741700	0.24158200
H	3.28092900	5.90980700	2.46782600
H	2.52675500	3.57523400	2.63648400
H	3.28899800	5.60706200	-1.82313600
C	3.58552900	-2.93987200	3.88222900
C	3.39900600	-2.27895300	2.68854100
H	4.52372000	-2.82472400	4.41870100
H	4.19142000	-1.65090100	2.30058600
C	2.56901300	-3.76530600	4.41819100
C	1.38014600	-3.90284900	3.74129700
H	2.72971200	-4.28381700	5.35959000
H	0.58553100	-4.53052000	4.13822000
C	5.29549700	-3.90788700	-0.86740700
C	4.22448600	-3.18165300	-0.39576300
H	5.24696800	-4.99367600	-0.87375500
H	3.34607900	-3.70508600	-0.03822800
C	6.45811800	-3.25548200	-1.34208700
C	6.51572300	-1.88176400	-1.33452100
H	7.29747000	-3.83973700	-1.70958000
H	7.39975600	-1.36217100	-1.69697000
H	2.48151900	3.27821700	-1.65428900
C	-4.16548300	2.98873000	-1.73052800
H	-4.52449800	2.34173400	-2.54207400
H	-4.62646300	2.62477000	-0.80286300
C	-2.50610400	5.24536300	-0.74319300
H	-2.14516400	5.87760200	0.07997500
H	-2.00587900	5.59835800	-1.65849700
C	-4.03066800	5.39007800	-0.90208900
H	-4.51239300	5.15350900	0.05733500
H	-4.28640300	6.43193500	-1.13311500

C	-4.57789800	4.44856300	-1.98767000
H	-4.19611800	4.76812600	-2.96872200
H	-5.67117300	4.53107800	-2.03830300
C	-3.55923400	0.19577500	2.08207200
O	-3.34301900	1.38254900	1.33726400
C	-3.89496400	0.63672300	3.51230800
H	-4.03743000	-0.22842900	4.16861800
H	-3.08814500	1.26027000	3.91241200
H	-4.81725800	1.22806400	3.51322300
C	-6.79877200	-2.29949500	0.60300100
C	-6.82701700	-0.90995000	0.40705200
C	-5.77962600	-0.11720400	0.86156100
C	-4.67359900	-0.68040800	1.51666300
C	-4.65521800	-2.06545600	1.69499900
C	-5.70240100	-2.88037100	1.25055000
H	-7.68300000	-0.47697500	-0.10207600
H	-5.80594800	0.95695300	0.70724200
H	-3.80496700	-2.52948800	2.19199400
H	-5.64725600	-3.95193300	1.40676100
O	-7.87837000	-2.99079400	0.12485700
C	-7.89762300	-4.39710000	0.29181600
H	-8.83407600	-4.74050000	-0.15246800
H	-7.05504700	-4.87849200	-0.22348500
H	-7.87588900	-4.68037900	1.35303500

ABS₆

Coordinates (Angstroms)			
	X	Y	Z
Ru	-0.141810	0.978852	-0.525646
H	-1.064432	0.107878	0.641059
H	0.562950	1.961346	-1.738772
N	-1.885293	0.825393	-1.888900
H	-1.611396	0.429134	-2.785574
H	-2.585775	0.201923	-1.482415
N	-1.349183	2.786935	0.011715
H	-1.492075	2.843129	1.017608
H	-0.795694	3.601813	-0.250440
P	0.858361	-0.935038	-1.261264
P	1.576943	1.466113	0.895671
C	-2.656009	2.796261	-0.691383
H	-3.317712	2.132893	-0.120065

C	-2.472031	2.168834	-2.080872
H	-1.718497	2.755736	-2.622116
C	5.819919	0.455354	-0.902989
C	5.387304	1.789893	-0.717839
C	4.168634	2.058912	-0.147442
C	3.296217	1.022931	0.289793
C	3.699094	-0.310406	0.154072
C	4.969677	-0.610252	-0.463331
H	6.035573	2.604519	-1.033421
H	3.869951	3.091874	-0.020163
C	2.768515	-3.363957	2.297596
C	1.600761	-3.806880	1.631280
C	1.096145	-3.108638	0.563654
C	1.722898	-1.929655	0.070501
C	2.897236	-1.474432	0.680065
C	3.424781	-2.182228	1.822954
H	1.107507	-4.713348	1.975842
H	0.201124	-3.473683	0.075083
C	-2.473381	-3.766001	-2.996175
C	-1.315570	-3.540754	-3.739048
C	-0.292926	-2.733168	-3.230682
C	-0.407971	-2.128519	-1.968461
C	-1.593108	-2.350197	-1.239910
C	-2.607611	-3.165743	-1.741718
H	-3.266821	-4.394812	-3.392255
H	-1.200401	-3.993007	-4.721140
H	0.595216	-2.576716	-3.831137
H	-1.712920	-1.853870	-0.281284
H	-3.511822	-3.318883	-1.158108
C	3.918746	-0.947327	-4.796152
C	3.770994	-2.090544	-4.006488
C	2.882574	-2.086655	-2.930856
C	2.123888	-0.943046	-2.629802
C	2.283905	0.198655	-3.424902
C	3.175949	0.196306	-4.500561
H	4.614715	-0.948499	-5.631446
H	4.353682	-2.982384	-4.222762
H	2.777375	-2.981446	-2.322777
H	1.711309	1.087628	-3.170594
H	3.292950	1.092976	-5.104688
C	1.658948	0.009508	5.339135
C	2.799623	0.595567	4.784141
C	2.794587	1.009174	3.451903
C	1.648315	0.850294	2.654672

C	0.512964	0.257546	3.219844
C	0.518674	-0.160825	4.553388
H	1.664772	-0.319051	6.375522
H	3.695902	0.721929	5.386266
H	3.688247	1.461601	3.029499
H	-0.359493	0.113898	2.586601
H	-0.368399	-0.626984	4.976200
C	1.612727	6.135090	1.478698
C	1.634155	5.306623	2.599449
C	1.665831	3.915335	2.453019
C	1.667949	3.321075	1.181204
C	1.627719	4.172590	0.058071
C	1.611241	5.560411	0.204362
H	1.593729	7.215845	1.594026
H	1.629267	5.738479	3.597346
H	1.687327	3.296602	3.342240
H	1.593184	6.193636	-0.679671
C	5.089509	-2.465046	3.591071
C	4.595685	-1.759199	2.516576
H	5.985133	-2.115132	4.097865
H	5.104863	-0.860889	2.189936
C	4.441751	-3.638753	4.043414
C	3.301732	-4.072441	3.408125
H	4.843254	-4.189214	4.890189
H	2.786352	-4.969312	3.744797
C	6.651843	-2.200626	-1.250879
C	5.431490	-1.943336	-0.666779
H	6.973684	-3.229244	-1.391788
H	4.805803	-2.771473	-0.357432
C	7.488788	-1.140441	-1.672130
C	7.074457	0.159636	-1.501858
H	8.450582	-1.356155	-2.129999
H	7.701462	0.987927	-1.824285
H	1.588673	3.723816	-0.931415
C	-3.790488	2.157475	-2.873263
H	-3.607276	1.749217	-3.876255
H	-4.495974	1.477693	-2.377006
C	-3.289754	4.193955	-0.783398
H	-3.452824	4.593468	0.226446
H	-2.577808	4.872146	-1.278761
C	-4.606607	4.174634	-1.576824
H	-5.353822	3.585011	-1.026259
H	-5.008209	5.192347	-1.657532
C	-4.405045	3.562639	-2.970976

H	-3.743144	4.213516	-3.560924
H	-5.360052	3.519364	-3.509175
C	-5.018074	-0.631941	0.588783
O	-4.621036	-0.294139	-0.523064
C	-4.062181	-0.730349	1.759394
H	-4.033625	-1.755295	2.150453
H	-3.057903	-0.436792	1.436653
H	-4.387350	-0.081874	2.582682
C	-9.183919	-1.517595	1.084461
C	-8.692038	-1.138109	-0.167536
C	-7.337596	-0.858038	-0.302839
C	-6.466922	-0.950857	0.795334
C	-6.986256	-1.336174	2.040766
C	-8.341822	-1.620401	2.192238
H	-9.364331	-1.066163	-1.015929
H	-6.928268	-0.563008	-1.263257
H	-6.336153	-1.417877	2.905689
H	-8.743193	-1.917767	3.155026
Cl	-10.891470	-1.871780	1.266571

INTf₆

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.422417	0.518336	0.789702
H	-1.186731	0.086117	-0.700407
H	0.098170	1.011650	2.342038
N	-1.828498	2.237321	0.892594
H	-1.324815	3.099903	1.089082
H	-2.282933	2.363772	-0.012493
N	-2.183947	-0.366783	1.830269
H	-2.437920	-1.267844	1.430727
H	-1.898411	-0.545851	2.792418
P	1.235706	1.658617	-0.293982
P	0.838651	-1.380691	0.951685
C	-3.347795	0.550275	1.795187
H	-3.787181	0.450688	0.794320
C	-2.845272	1.993874	1.939621
H	-2.316797	2.074922	2.898977
C	5.416854	-0.582625	1.762491
C	4.570745	-1.141395	2.749390

C	3.252558	-1.404414	2.474231
C	2.682338	-1.141979	1.196877
C	3.491167	-0.614870	0.183207
C	4.875491	-0.314186	0.463794
H	4.979312	-1.362046	3.733191
H	2.633912	-1.832430	3.252902
C	3.183630	-1.039753	-3.626885
C	2.327521	0.042393	-3.943406
C	1.820632	0.846806	-2.954666
C	2.141503	0.645822	-1.582576
C	3.007564	-0.394451	-1.228077
C	3.526303	-1.267810	-2.254491
H	2.076002	0.229883	-4.985165
H	1.164667	1.663986	-3.228943
C	-0.707833	5.257130	-2.612644
C	0.478394	5.465334	-1.909368
C	1.100824	4.408028	-1.238139
C	0.550977	3.116137	-1.260864
C	-0.650859	2.925794	-1.969071
C	-1.273457	3.980031	-2.638088
H	-1.193274	6.083179	-3.126334
H	0.924478	6.456330	-1.873650
H	2.014848	4.602491	-0.689632
H	-1.099785	1.937005	-1.965378
H	-2.214851	3.804051	-3.151487
C	4.651991	3.865506	2.011998
C	4.773889	3.652337	0.636669
C	3.774905	2.967211	-0.055540
C	2.636191	2.487616	0.613372
C	2.527862	2.702174	1.993180
C	3.528838	3.386589	2.687420
H	5.432491	4.395334	2.552499
H	5.651152	4.010694	0.104206
H	3.883187	2.804633	-1.124678
H	1.656988	2.305331	2.509078
H	3.431425	3.540133	3.759615
C	0.694935	-4.765163	-2.273399
C	1.643657	-4.828588	-1.249226
C	1.711462	-3.812728	-0.295546
C	0.828193	-2.720784	-0.345854
C	-0.114105	-2.665307	-1.379091
C	-0.179990	-3.680324	-2.337381
H	0.646687	-5.553481	-3.020533
H	2.336092	-5.665101	-1.198217

H	2.456070	-3.870527	0.494368
H	-0.773008	-1.800979	-1.421801
H	-0.911197	-3.618767	-3.140282
C	-0.667156	-3.675897	4.774910
C	-0.582230	-4.353583	3.559943
C	-0.098030	-3.705563	2.418034
C	0.305828	-2.362000	2.464271
C	0.193505	-1.684496	3.696077
C	-0.275350	-2.335381	4.838034
H	-1.038607	-4.182279	5.662174
H	-0.890824	-5.394045	3.492850
H	-0.039544	-4.259878	1.488537
H	-0.338542	-1.791891	5.777904
C	4.876206	-3.177446	-2.968307
C	4.382859	-2.370241	-1.967365
H	5.526617	-4.010587	-2.714802
H	4.647891	-2.578334	-0.937957
C	4.543139	-2.935109	-4.321730
C	3.709929	-1.887804	-4.638331
H	4.941765	-3.576899	-5.103018
H	3.437453	-1.689505	-5.672587
C	7.071270	0.521734	-0.214386
C	5.752392	0.253366	-0.506400
H	7.712927	0.954760	-0.977440
H	5.370474	0.481024	-1.494004
C	7.598622	0.242441	1.068520
C	6.781951	-0.296022	2.034856
H	8.641623	0.456958	1.286012
H	7.167052	-0.512016	3.028895
H	0.459504	-0.631342	3.736316
C	-4.014048	2.992737	1.900535
H	-3.629947	4.011742	2.040967
H	-4.468508	2.959296	0.899866
C	-4.414852	0.220654	2.852295
H	-4.783191	-0.802072	2.698015
H	-3.943123	0.239632	3.846928
C	-5.579652	1.223751	2.822206
H	-6.121932	1.118841	1.871879
H	-6.295678	0.987449	3.619000
C	-5.073892	2.666750	2.965257
H	-4.638617	2.801658	3.966247
H	-5.909850	3.373190	2.891243
C	-4.373478	0.939864	-2.240233
O	-4.242845	2.068913	-1.776584

C	-3.314007	0.355416	-3.148008
H	-2.542324	-0.107919	-2.513756
H	-3.698857	-0.385609	-3.853035
H	-2.834948	1.168511	-3.698288
C	-7.849686	-1.318787	-1.131530
C	-7.794782	0.055232	-0.881144
C	-6.654763	0.761957	-1.248253
C	-5.575370	0.119480	-1.877211
C	-5.659721	-1.259475	-2.122792
C	-6.788831	-1.985213	-1.745039
H	-8.633571	0.554870	-0.408366
H	-6.583890	1.828680	-1.063208
H	-4.836869	-1.784401	-2.596712
H	-6.848706	-3.052929	-1.926066
Cl	-9.279956	-2.220647	-0.667402

TSf₆

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.809625	0.798151	0.360550
H	-1.589477	0.254002	-1.210068
H	-0.394575	1.362800	1.861378
N	-1.982505	2.629201	0.082215
H	-1.415261	3.474387	0.046377
H	-2.451441	2.530479	-0.832397
N	-2.768841	0.280836	1.297556
H	-3.165392	-0.560704	0.880696
H	-2.577912	0.063784	2.274908
P	1.165462	1.676422	-0.457397
P	0.223008	-1.179345	0.949880
C	-3.748706	1.394756	1.189164
H	-4.234245	1.274108	0.216173
C	-3.002916	2.733238	1.148780
H	-2.461475	2.868626	2.093493
C	4.656656	-0.768247	2.528995
C	3.590380	-1.119213	3.389784
C	2.315073	-1.261038	2.903686
C	2.006838	-1.069107	1.527648
C	3.038170	-0.752678	0.635345
C	4.383483	-0.587256	1.134765

H	3.794148	-1.279929	4.446149
H	1.527281	-1.540892	3.591065
C	3.347242	-1.528523	-3.120003
C	2.692457	-0.402959	-3.676417
C	2.120846	0.545367	-2.866839
C	2.178177	0.454478	-1.446607
C	2.836634	-0.628801	-0.854217
C	3.413064	-1.652861	-1.693948
H	2.648805	-0.297989	-4.758267
H	1.623063	1.394204	-3.320579
C	0.403231	5.215943	-3.455865
C	1.526737	5.259187	-2.628422
C	1.787107	4.221046	-1.730653
C	0.929313	3.111246	-1.643880
C	-0.203117	3.089763	-2.475033
C	-0.464467	4.126224	-3.373298
H	0.202542	6.028259	-4.149918
H	2.205661	6.107191	-2.674767
H	2.660816	4.289036	-1.093872
H	-0.902531	2.266434	-2.407951
H	-1.355799	4.074814	-3.992783
C	4.242025	3.762678	2.383647
C	4.659709	3.279949	1.141842
C	3.755461	2.622051	0.307020
C	2.419678	2.431305	0.697009
C	2.015429	2.915663	1.948246
C	2.918150	3.577179	2.784072
H	4.946028	4.273177	3.035931
H	5.691834	3.404702	0.825387
H	4.094730	2.249168	-0.654992
H	0.990766	2.747986	2.265501
H	2.585416	3.942600	3.752657
C	0.571740	-4.832839	-1.944805
C	1.029185	-4.952935	-0.629345
C	0.940553	-3.869412	0.244609
C	0.371884	-2.655281	-0.176799
C	-0.064557	-2.541391	-1.500355
C	0.034836	-3.621829	-2.381750
H	0.648225	-5.675511	-2.626973
H	1.463597	-5.888851	-0.286971
H	1.313195	-3.970933	1.260662
H	-0.461182	-1.584336	-1.825662
H	-0.300255	-3.513542	-3.410363
C	-2.278605	-2.811351	4.576381

C	-2.147219	-3.587551	3.426282
C	-1.361589	-3.144243	2.356750
C	-0.693126	-1.911080	2.410958
C	-0.860728	-1.124725	3.569786
C	-1.630971	-1.574227	4.643222
H	-2.884255	-3.159793	5.408715
H	-2.655107	-4.546004	3.354301
H	-1.275438	-3.770863	1.476513
H	-1.729863	-0.953362	5.530320
C	4.619925	-3.757771	-1.990519
C	4.059002	-2.808081	-1.165565
H	5.104430	-4.627940	-1.555488
H	4.103981	-2.943200	-0.091947
C	4.568174	-3.615009	-3.396950
C	3.938385	-2.522352	-3.945606
H	5.019290	-4.368859	-4.036708
H	3.880447	-2.399647	-5.024792
C	6.753282	-0.084727	0.797004
C	5.480309	-0.236427	0.293902
H	7.566714	0.182882	0.127596
H	5.307889	-0.083958	-0.764367
C	7.012918	-0.273111	2.175253
C	5.980562	-0.606131	3.020017
H	8.022184	-0.152602	2.559712
H	6.159007	-0.751679	4.082961
H	-0.394870	-0.144507	3.613211
C	-3.989392	3.895914	0.953081
H	-3.442175	4.847987	0.948115
H	-4.462979	3.796517	-0.034119
C	-4.824541	1.381320	2.284820
H	-5.363961	0.425813	2.261075
H	-4.336477	1.448265	3.269567
C	-5.804537	2.554746	2.115230
H	-6.378569	2.410552	1.188839
H	-6.531764	2.556284	2.936407
C	-5.067328	3.901091	2.050330
H	-4.594840	4.104277	3.022647
H	-5.779850	4.716142	1.873933
C	-2.922223	0.529589	-2.439079
O	-3.181297	1.756602	-2.399705
C	-2.098248	-0.015442	-3.605807
H	-1.793845	-1.054905	-3.470663
H	-2.732864	0.036842	-4.502768
H	-1.214023	0.599979	-3.777038

C	-6.011425	-2.121705	-0.986895
C	-6.312812	-0.811703	-1.354739
C	-5.282652	0.020881	-1.794869
C	-3.958208	-0.434286	-1.875819
C	-3.688295	-1.761243	-1.510236
C	-4.703781	-2.605459	-1.060077
H	-7.335533	-0.452525	-1.302288
H	-5.491504	1.044403	-2.089533
H	-2.672593	-2.138703	-1.552670
H	-4.484792	-3.627922	-0.770046
Cl	-7.297174	-3.183537	-0.422228

TSu₆

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.968315	-1.230415	0.137371
H	-2.007338	0.051460	-0.765355
H	-0.330392	-2.502598	0.968112
N	-2.774142	-1.467361	1.343207
H	-2.634236	-1.276305	2.334074
H	-3.451190	-0.779842	0.975705
N	-2.100606	-2.809502	-0.973400
H	-2.210732	-2.594475	-1.962928
H	-1.511286	-3.640149	-0.926273
P	0.110203	0.182748	1.605640
P	0.893808	-1.377899	-1.231714
C	-3.429766	-3.074907	-0.360365
H	-4.107985	-2.313931	-0.760270
C	-3.339266	-2.823660	1.151315
H	-2.620994	-3.530649	1.587030
C	5.092154	-1.069495	0.906061
C	4.647721	-2.273131	0.310387
C	3.433595	-2.333018	-0.326329
C	2.576633	-1.200788	-0.422202
C	2.989923	0.017562	0.128105
C	4.259370	0.092175	0.814099
H	5.283206	-3.154519	0.360633
H	3.130080	-3.268790	-0.777654
C	2.129681	3.628183	-0.874378
C	0.985942	3.856779	-0.072200

C	0.457101	2.851134	0.697458
C	1.045016	1.556354	0.746531
C	2.206497	1.301084	0.007557
C	2.747769	2.335566	-0.840740
H	0.524409	4.841570	-0.074962
H	-0.425874	3.055155	1.290317
C	-2.980774	2.286797	4.444378
C	-1.834102	1.713759	4.993792
C	-0.881955	1.106117	4.170664
C	-1.060538	1.054968	2.777874
C	-2.234491	1.614146	2.242776
C	-3.177295	2.234900	3.063041
H	-3.717383	2.763645	5.085941
H	-1.672657	1.737826	6.068668
H	-0.000875	0.670530	4.625605
H	-2.407692	1.557742	1.174330
H	-4.064821	2.672692	2.615743
C	3.105000	-1.397142	4.830164
C	3.092337	-0.042666	4.489428
C	2.225514	0.420799	3.499680
C	1.357396	-0.458492	2.831108
C	1.379386	-1.814109	3.182829
C	2.247044	-2.280249	4.173873
H	3.781928	-1.760231	5.599318
H	3.762895	0.652781	4.987042
H	2.223829	1.476998	3.245691
H	0.717088	-2.498759	2.662072
H	2.252429	-3.336950	4.430191
C	1.463881	1.218040	-5.072401
C	2.489510	0.357424	-4.669848
C	2.346619	-0.411370	-3.514799
C	1.170480	-0.337235	-2.749604
C	0.155663	0.530938	-3.158798
C	0.297267	1.306593	-4.312583
H	1.579248	1.820099	-5.969931
H	3.403602	0.289425	-5.254334
H	3.151726	-1.075109	-3.210341
H	-0.735498	0.586608	-2.542270
H	-0.500546	1.980702	-4.615434
C	0.752222	-5.720293	-3.030470
C	0.761420	-4.618750	-3.884256
C	0.855198	-3.321457	-3.368121
C	0.933450	-3.095664	-1.984787
C	0.900493	-4.219840	-1.134217

C	0.823844	-5.514487	-1.649553
H	0.685853	-6.727726	-3.432692
H	0.699564	-4.761668	-4.960184
H	0.867487	-2.484375	-4.056781
H	0.815401	-6.363148	-0.969891
C	4.397721	3.143030	-2.452766
C	3.894391	2.133807	-1.662655
H	5.271054	2.955717	-3.071948
H	4.373032	1.162211	-1.669327
C	3.788571	4.420169	-2.469002
C	2.675608	4.651969	-1.695263
H	4.198655	5.209630	-3.093172
H	2.191407	5.625935	-1.698225
C	5.949730	1.331581	2.074125
C	4.734238	1.288234	1.427984
H	6.282102	2.260199	2.530700
H	4.124461	2.182311	1.387195
C	6.768841	0.180344	2.150494
C	6.342011	-0.994892	1.578610
H	7.727063	0.227898	2.660925
H	6.955367	-1.891522	1.631374
H	0.921904	-4.069077	-0.059047
C	-4.713403	-3.017618	1.811854
H	-4.628665	-2.854768	2.894670
H	-5.401031	-2.253264	1.424772
C	-3.980801	-4.476409	-0.661025
H	-4.063248	-4.618743	-1.746866
H	-3.267668	-5.232323	-0.296216
C	-5.346633	-4.692505	0.012667
H	-6.083471	-4.016615	-0.443760
H	-5.699039	-5.714299	-0.175056
C	-5.276965	-4.419259	1.523148
H	-4.635970	-5.175324	2.000420
H	-6.271406	-4.524538	1.973951
C	-3.682139	0.532241	-1.212367
O	-4.453190	-0.077746	-0.426841
C	-3.589922	0.044723	-2.660361
H	-2.755173	0.471702	-3.217639
H	-3.525700	-1.045137	-2.692992
H	-4.521961	0.338365	-3.164627
C	-3.626810	4.831225	-0.812817
C	-4.624688	4.071759	-0.204957
C	-4.584801	2.682655	-0.327167
C	-3.566207	2.041472	-1.047518

C	-2.578506	2.833181	-1.648239
C	-2.598802	4.222255	-1.533200
H	-5.421693	4.560316	0.346353
H	-5.352255	2.066447	0.129524
H	-1.761502	2.368237	-2.187266
H	-1.823673	4.825763	-1.993467
Cl	-3.661507	6.586542	-0.670040

Pf6

Coordinates (Angstroms)			
	X	Y	Z
Ru	-0.51083900	0.68546200	0.83543500
H	0.18767400	1.06680400	2.19842600
N	-1.95011100	2.14773100	0.53655500
H	-1.62308700	3.09547400	0.34465500
N	-2.22690000	-0.08280900	2.03362100
H	-2.44723300	-1.07163000	1.91491400
H	-1.90786700	0.01174200	2.99846400
P	1.23749500	1.75397500	-0.24873000
P	0.69346800	-1.30506800	1.06736300
C	-3.43779500	0.75649200	1.81630200
H	-3.87852900	0.41216800	0.87283200
C	-2.95759100	2.19344300	1.60097200
H	-2.51407000	2.53625900	2.55726500
C	5.36232700	-0.93783500	1.59990000
C	4.53563800	-1.43690900	2.63398800
C	3.18385400	-1.57714100	2.44417600
C	2.55796800	-1.23351200	1.21260100
C	3.34241400	-0.76291600	0.15415400
C	4.76528000	-0.60372600	0.34134400
H	4.98630900	-1.71382600	3.58444300
H	2.58277400	-1.97029200	3.25431200
C	2.77181000	-1.15692200	-3.62346300
C	2.03349400	0.01603300	-3.90701000
C	1.67238600	0.87665900	-2.90162600
C	2.03071800	0.64657500	-1.54151300
C	2.79335100	-0.48526800	-1.22306700
C	3.15459800	-1.41591200	-2.26747500
H	1.75479100	0.23092500	-4.93621500
H	1.10771600	1.76478300	-3.15545200

C	-0.05735600	5.58200600	-2.64010300
C	1.11998600	5.60894000	-1.89170200
C	1.53623500	4.47839300	-1.18432100
C	0.78295900	3.29282800	-1.21233300
C	-0.40737600	3.28634000	-1.96095700
C	-0.82144500	4.41454600	-2.67066100
H	-0.38015100	6.46484200	-3.18605500
H	1.72109800	6.51399900	-1.85199200
H	2.45114300	4.53243100	-0.60662000
H	-1.03989400	2.40710700	-1.98324100
H	-1.75210800	4.37191800	-3.22969500
C	4.73744400	3.57307700	2.24695200
C	4.94997100	3.21308400	0.91486900
C	3.91800700	2.63701700	0.17302500
C	2.66041100	2.40218500	0.75047200
C	2.45854900	2.77129200	2.08838600
C	3.48866900	3.35314100	2.83039100
H	5.54081800	4.02099500	2.82614900
H	5.92058700	3.37208000	0.45304300
H	4.09350700	2.36793400	-0.86403000
H	1.48952400	2.59693400	2.54440700
H	3.31358700	3.63281800	3.86622400
C	0.01556800	-4.69911600	-2.06937300
C	0.98706800	-4.86849900	-1.07910900
C	1.21774700	-3.85900900	-0.14426100
C	0.47215100	-2.66916900	-0.17704700
C	-0.49557500	-2.51167100	-1.17633000
C	-0.72254600	-3.51607200	-2.12022100
H	-0.15748300	-5.48275100	-2.80224500
H	1.57140400	-5.78421500	-1.04083900
H	1.98128000	-3.99664500	0.61700500
H	-1.06026600	-1.58390300	-1.21801700
H	-1.46842800	-3.37053600	-2.89763800
C	-0.84620100	-3.23409400	5.06176500
C	-0.95354400	-3.94968300	3.87065000
C	-0.45361100	-3.41845200	2.67617700
C	0.15638400	-2.15487300	2.64642200
C	0.23695000	-1.43520100	3.85620600
C	-0.24454200	-1.97200600	5.05003100
H	-1.23017900	-3.65003000	5.98936900
H	-1.42431500	-4.92952100	3.86338700
H	-0.54367100	-3.99983100	1.76545500
H	-0.15541500	-1.40100000	5.97086500
C	4.23770600	-3.47165100	-3.02868400

C	3.89239600	-2.60891200	-2.01238600
H	4.79925400	-4.37354600	-2.79960000
H	4.18322700	-2.84324600	-0.99580600
C	3.86750200	-3.19810900	-4.36664100
C	3.14520200	-2.06349800	-4.65215200
H	4.15044000	-3.88477700	-5.15994900
H	2.84556600	-1.83882300	-5.67319600
C	6.98132300	0.03114500	-0.47553900
C	5.62781600	-0.11546400	-0.68368600
H	7.61066900	0.40593700	-1.27845500
H	5.20838400	0.14642500	-1.64742000
C	7.56089000	-0.30329600	0.77152900
C	6.76222300	-0.77702900	1.78546100
H	8.63048400	-0.18534300	0.92277500
H	7.18916500	-1.03828000	2.75100800
H	0.67976700	-0.44334800	3.85591000
C	-4.15848200	3.11131800	1.30125300
H	-3.80668000	4.14599000	1.19162700
H	-4.59080600	2.82160900	0.33488500
C	-4.48623200	0.64663900	2.92935900
H	-4.82479100	-0.39343200	3.03167700
H	-4.02624200	0.92842600	3.88933500
C	-5.68038700	1.57387100	2.63846700
H	-6.20351500	1.21025600	1.74294400
H	-6.40084500	1.52502400	3.46456000
C	-5.22453500	3.02385700	2.40710800
H	-4.81294300	3.42755800	3.34420300
H	-6.08734200	3.65205900	2.15158300
C	-4.81899900	-1.59755700	-1.55056600
C	-6.03372900	-2.18673400	-1.19514100
C	-4.72212500	-0.22303400	-1.80247100
H	-3.93229000	-2.22426600	-1.62847700
C	-7.16817300	-1.38320700	-1.09110000
H	-6.09981300	-3.25166100	-0.99766400
C	-5.87764600	0.55879800	-1.68635900
C	-7.10171200	-0.01113600	-1.33280000
H	-5.80336100	1.62616800	-1.86771400
H	-7.99470600	0.59944000	-1.24635400
C	-3.39831900	0.40604700	-2.23744600
H	-2.58482200	-0.16053600	-1.75164300
O	-3.30977300	1.76924500	-1.88530200
H	-2.85394200	1.85162400	-0.98602800
C	-3.21722300	0.29132600	-3.75782300
H	-3.29919700	-0.74829400	-4.09494200

H	-3.98757300	0.88016900	-4.26793900
H	-2.23572700	0.68188000	-4.04635400
Cl	-8.70783600	-2.11229700	-0.63924500

Pu6

Coordinates (Angstroms)			
	X	Y	Z
Ru	-0.36967200	1.01191900	-0.75802200
H	-2.79097900	-1.79735400	1.40251500
H	0.29788700	1.61489600	-2.05201100
N	-2.32307900	0.67650800	-1.41254100
H	-2.45775000	-0.02373300	-2.14095600
H	-2.80574900	0.26136100	0.24680400
N	-1.32620200	3.00300400	-0.44279900
H	-1.13532700	3.44844800	0.45484000
H	-0.88678400	3.59758300	-1.14656500
P	0.54332600	-1.02718300	-1.34581500
P	1.52445100	1.65278600	0.43934900
C	-2.79340800	2.92563900	-0.68418700
H	-3.22209400	2.50626000	0.23366100
C	-3.01373400	1.90522000	-1.80537000
H	-2.57719700	2.33800900	-2.72911700
C	5.69211000	-0.22713300	-0.69647200
C	5.45045800	1.16316100	-0.80096700
C	4.24191700	1.69344100	-0.42559100
C	3.18964800	0.88083300	0.08435600
C	3.39530600	-0.49508500	0.22811700
C	4.65904600	-1.06890900	-0.17055200
H	6.23762100	1.80979800	-1.18217400
H	4.08947100	2.76187200	-0.51408600
C	1.85256900	-2.95170300	2.74624300
C	0.73224600	-3.41285000	2.01573100
C	0.43636100	-2.88879200	0.78277500
C	1.23764800	-1.87903300	0.17602900
C	2.38546400	-1.43111700	0.84484200
C	2.69242100	-1.95179700	2.15633200
H	0.10642200	-4.19323400	2.44299600
H	-0.42631400	-3.26847800	0.25001600
C	-2.54066100	-4.09919300	-3.12725200
C	-1.27660600	-3.98475300	-3.70538800
C	-0.33578400	-3.09296100	-3.18391700

C	-0.63671200	-2.29473400	-2.06797500
C	-1.92267200	-2.41060200	-1.50955900
C	-2.86175600	-3.30530200	-2.02514900
H	-3.27146000	-4.79173500	-3.53667400
H	-1.01563500	-4.58948800	-4.57029800
H	0.63450700	-3.02337100	-3.66009500
H	-2.19786100	-1.78042900	-0.67325600
H	-3.84719700	-3.36586000	-1.57060300
C	3.86095200	-1.31196400	-4.61783900
C	3.74204100	-2.31996600	-3.65884800
C	2.77323200	-2.22310600	-2.65966400
C	1.91234700	-1.11587100	-2.59521400
C	2.03947900	-0.11267900	-3.56630000
C	3.00590500	-0.21008900	-4.56989200
H	4.61607200	-1.38538200	-5.39623200
H	4.40782000	-3.17838800	-3.68127200
H	2.68685400	-3.01678800	-1.92370900
H	1.37617300	0.74521300	-3.52907000
H	3.08956300	0.57819000	-5.31384200
C	1.15394000	1.49504700	5.09035700
C	2.40917400	1.70064300	4.51239100
C	2.54325600	1.72561000	3.12389500
C	1.42557700	1.54642700	2.29176100
C	0.17126900	1.33068400	2.88192700
C	0.03818800	1.30866100	4.27340900
H	1.04918500	1.47429900	6.17209900
H	3.28424600	1.83806600	5.14252100
H	3.52374600	1.88864000	2.68407200
H	-0.70394100	1.16215200	2.25767600
H	-0.94026600	1.14093800	4.71562600
C	2.11911600	6.24943700	-0.31427600
C	2.03836700	5.77879100	0.99522100
C	1.90466500	4.40927900	1.24940800
C	1.83974200	3.48275400	0.19736500
C	1.90635400	3.97653400	-1.12091200
C	2.05584200	5.33996300	-1.37433900
H	2.22611600	7.31308200	-0.51010400
H	2.08169800	6.47521500	1.82889800
H	1.85140400	4.06836800	2.27727700
H	2.11671700	5.69291900	-2.40086400
C	4.09322600	-2.03087800	4.15852000
C	3.81822000	-1.51256500	2.91283400
H	4.95755300	-1.67151000	4.71074500
H	4.46709100	-0.75046600	2.49927300

C	3.26184000	-3.02421200	4.72815300
C	2.16339000	-3.47064400	4.03211700
H	3.49191400	-3.42729900	5.71071700
H	1.51080300	-4.23133200	4.45439800
C	6.14694000	-2.98612600	-0.47323100
C	4.93529200	-2.46465200	-0.07695600
H	6.32489200	-4.05501400	-0.38906700
H	4.17374300	-3.12987700	0.31156100
C	7.16231400	-2.14476500	-0.98704600
C	6.93336300	-0.79325700	-1.09499000
H	8.11506900	-2.56793800	-1.29375700
H	7.70056900	-0.13109700	-1.48965900
H	1.83528700	3.28068800	-1.95170100
C	-4.52229600	1.72561800	-2.06037800
H	-4.67001300	1.02202600	-2.89055300
H	-4.97896500	1.26450000	-1.17409700
C	-3.45116300	4.27800100	-0.98478400
H	-3.29272600	4.97370900	-0.14899100
H	-2.97040200	4.72716500	-1.86764300
C	-4.95540700	4.09891600	-1.25784200
H	-5.44905400	3.76378900	-0.33385100
H	-5.40623000	5.06453900	-1.51939900
C	-5.20786300	3.06758400	-2.36963300
H	-4.82329600	3.46347000	-3.32131000
H	-6.28657900	2.92049500	-2.50767800
C	-3.37273200	-0.94173500	1.78293700
O	-2.86613800	0.27341300	1.26016700
C	-3.19154200	-0.90012300	3.30470500
H	-3.57223500	-1.81524500	3.77137500
H	-2.13003700	-0.79489200	3.55029200
H	-3.73637900	-0.04683500	3.72446000
C	-7.53818200	-1.61894000	0.83770400
C	-7.09507900	-0.32347900	1.10596300
C	-5.74680200	-0.11258400	1.39305400
C	-4.83525300	-1.17595900	1.41583100
C	-5.30915000	-2.46373300	1.14119100
C	-6.65557600	-2.69677200	0.85188100
H	-7.79642900	0.50435000	1.08870900
H	-5.38756000	0.89180300	1.59493000
H	-4.61803600	-3.30435500	1.15316700
H	-7.01406200	-3.69801900	0.63683600
Cl	-9.23882300	-1.89477300	0.46917700

ABS₇

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.069057	0.947142	-0.608605
H	-0.847123	0.212832	0.652758
H	0.768770	1.790461	-1.926922
N	-1.718358	0.688692	-1.902842
H	-1.477968	0.209772	-2.768154
H	-2.409167	0.112428	-1.417724
N	-1.087984	2.820414	-0.225768
H	-1.183336	2.996122	0.772094
H	-0.539126	3.590240	-0.606981
P	1.017299	-1.052893	-1.165310
P	1.823738	1.540719	0.723953
C	-2.425305	2.770131	-0.865306
H	-3.060704	2.165840	-0.205520
C	-2.303342	2.015170	-2.196824
H	-1.567955	2.540897	-2.820261
C	6.012522	0.275034	-1.039007
C	5.609929	1.630044	-0.974656
C	4.407135	1.977593	-0.413099
C	3.522712	1.006870	0.135572
C	3.897406	-0.341642	0.122248
C	5.149361	-0.725558	-0.486343
H	6.268465	2.397118	-1.376494
H	4.131452	3.024068	-0.380178
C	2.960429	-3.135805	2.590493
C	1.770823	-3.623100	1.997943
C	1.254838	-3.030768	0.872976
C	1.891996	-1.923528	0.245589
C	3.087350	-1.430258	0.780052
C	3.626722	-2.023811	1.980737
H	1.268526	-4.477655	2.446344
H	0.341501	-3.425202	0.444910
C	-2.408488	-3.968892	-2.528483
C	-1.261670	-3.853836	-3.313185
C	-0.210803	-3.021096	-2.915039
C	-0.286716	-2.282675	-1.723046
C	-1.460496	-2.394671	-0.952838
C	-2.504091	-3.233296	-1.344641
H	-3.223977	-4.616985	-2.839738
H	-1.177923	-4.412182	-4.242484

H	0.667484	-2.948842	-3.545572
H	-1.546760	-1.792650	-0.052837
H	-3.400013	-3.297555	-0.732704
C	4.020819	-1.484827	-4.723106
C	3.854027	-2.544463	-3.827660
C	2.981842	-2.414832	-2.746634
C	2.257973	-1.227418	-2.546059
C	2.437761	-0.169769	-3.446096
C	3.314066	-0.297822	-4.527043
H	4.704258	-1.583862	-5.562880
H	4.409597	-3.468556	-3.966010
H	2.862644	-3.244517	-2.054589
H	1.892944	0.754666	-3.268681
H	3.446854	0.534890	-5.213813
C	1.972424	0.515453	5.284974
C	3.100192	1.056892	4.662199
C	3.073998	1.342988	3.297188
C	1.919302	1.099729	2.534308
C	0.797081	0.552385	3.167398
C	0.824261	0.261311	4.534115
H	1.994480	0.286209	6.347557
H	4.002586	1.247749	5.237643
H	3.957607	1.760580	2.821274
H	-0.082341	0.343259	2.562150
H	-0.052417	-0.171221	5.010878
C	1.933472	6.242600	0.834387
C	1.933958	5.530448	2.032588
C	1.945550	4.131196	2.026723
C	1.948758	3.412386	0.821067
C	1.926641	4.147467	-0.382228
C	1.930888	5.543082	-0.375991
H	1.930138	7.329642	0.840828
H	1.928273	6.060368	2.982074
H	1.950987	3.603977	2.973756
H	1.927562	6.084479	-1.319232
C	5.320666	-2.146640	3.739481
C	4.817728	-1.550648	2.604360
H	6.231314	-1.760869	4.190451
H	5.335566	-0.701134	2.176265
C	4.662790	-3.253369	4.325942
C	3.503815	-3.731639	3.760731
H	5.071422	-3.717547	5.219734
H	2.980449	-4.577510	4.201084
C	6.785758	-2.418932	-1.145208

C	5.581239	-2.081463	-0.569108
H	7.084707	-3.462911	-1.192680
H	4.944718	-2.862642	-0.172136
C	7.635961	-1.421598	-1.678422
C	7.250159	-0.102760	-1.626722
H	8.585118	-1.700267	-2.128644
H	7.887267	0.677656	-2.036876
H	1.884143	3.603396	-1.322426
C	-3.653557	1.944246	-2.930825
H	-3.514786	1.446232	-3.899820
H	-4.340395	1.318444	-2.345681
C	-3.059679	4.157454	-1.055999
H	-3.178361	4.647244	-0.080227
H	-2.368452	4.784053	-1.640708
C	-4.409026	4.074291	-1.787545
H	-5.132807	3.539223	-1.156026
H	-4.812802	5.082615	-1.941956
C	-4.266529	3.339886	-3.128618
H	-3.627372	3.931519	-3.800518
H	-5.242867	3.254819	-3.621693
C	-7.141593	-0.782649	0.090312
C	-8.517166	-1.033822	0.305458
C	-6.244825	-0.707072	1.143919
C	-9.447669	-1.113574	-0.767941
C	-8.988004	-1.212468	1.648848
C	-6.720566	-0.888085	2.474408
C	-10.780168	-1.357530	-0.525985
H	-9.085392	-0.978031	-1.783972
C	-10.369221	-1.462638	1.863754
C	-8.051790	-1.132515	2.715492
H	-6.029158	-0.833077	3.308737
C	-11.244229	-1.533250	0.802274
H	-11.483208	-1.416699	-1.352088
H	-10.725925	-1.598019	2.881937
H	-8.406562	-1.268799	3.734210
H	-12.298916	-1.725159	0.979802
H	-6.767475	-0.645158	-0.920017
C	-4.804413	-0.434987	0.837771
O	-4.440162	-0.269745	-0.324438
C	-3.808590	-0.365263	1.977332
H	-3.785811	-1.312078	2.531580
H	-2.811117	-0.151789	1.580028
H	-4.093497	0.416571	2.693011

INTf₇

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.261074	0.499056	0.770761
H	-0.987328	0.059666	-0.733228
H	0.219948	1.000081	2.335227
N	-1.706956	2.186293	0.846494
H	-1.225920	3.065402	1.026359
H	-2.169087	2.284613	-0.058603
N	-2.021991	-0.419246	1.786651
H	-2.263234	-1.318030	1.374383
H	-1.737318	-0.606898	2.747269
P	1.398666	1.668151	-0.277609
P	1.022367	-1.383387	0.941138
C	-3.198086	0.483056	1.758719
H	-3.642638	0.378261	0.760992
C	-2.714204	1.933114	1.900064
H	-2.181452	2.023007	2.856144
C	5.588531	-0.549845	1.790317
C	4.740105	-1.121206	2.767927
C	3.426089	-1.393459	2.481875
C	2.862231	-1.127953	1.202237
C	3.673946	-0.587966	0.197647
C	5.053929	-0.278152	0.489588
H	5.143555	-1.344325	3.753297
H	2.805900	-1.831433	3.253744
C	3.397842	-0.984255	-3.617953
C	2.536437	0.094454	-3.931859
C	2.015832	0.886395	-2.940267
C	2.327272	0.676162	-1.567306
C	3.198575	-0.360475	-1.215197
C	3.731467	-1.221439	-2.244898
H	2.291548	0.289083	-4.973904
H	1.355553	1.700630	-3.212785
C	-0.535292	5.275258	-2.590271
C	0.640827	5.484382	-1.870343
C	1.260175	4.425356	-1.199131
C	0.717019	3.131001	-1.238205
C	-0.474996	2.939824	-1.962309
C	-1.094207	3.995674	-2.631840

H	-1.018231	6.102577	-3.104332
H	1.081276	6.477377	-1.821832
H	2.166370	4.620171	-0.637865
H	-0.919334	1.949182	-1.971165
H	-2.027624	3.818524	-3.159359
C	4.768851	3.873911	2.096569
C	4.912607	3.672288	0.721655
C	3.927413	2.988096	0.009002
C	2.781365	2.497278	0.656704
C	2.650923	2.700584	2.036323
C	3.637741	3.384544	2.750954
H	5.538511	4.403106	2.653053
H	5.796159	4.038753	0.205350
H	4.052333	2.834706	-1.059644
H	1.774009	2.295751	2.535569
H	3.523115	3.529478	3.822670
C	0.947930	-4.765424	-2.289923
C	1.887142	-4.819271	-1.256458
C	1.933855	-3.803900	-0.300993
C	1.038811	-2.721945	-0.358637
C	0.106480	-2.675828	-1.401348
C	0.061492	-3.690471	-2.361326
H	0.916026	-5.553295	-3.038443
H	2.588577	-5.647906	-1.199499
H	2.671164	-3.854486	0.496233
H	-0.561356	-1.818628	-1.450005
H	-0.662518	-3.636045	-3.171231
C	-0.483565	-3.705196	4.748766
C	-0.384352	-4.378626	3.532510
C	0.099847	-3.722481	2.395253
C	0.489482	-2.374957	2.447362
C	0.361989	-1.701853	3.680117
C	-0.106625	-2.360722	4.817587
H	-0.854871	-4.217863	5.632508
H	-0.681711	-5.422076	3.460741
H	0.169511	-4.273737	1.464697
H	-0.181671	-1.820173	5.758287
C	5.100750	-3.115188	-2.964205
C	4.593766	-2.320024	-1.960406
H	5.755107	-3.945822	-2.712590
H	4.852129	-2.534922	-0.930702
C	4.776434	-2.863844	-4.318096
C	3.938073	-1.819907	-4.632332
H	5.185665	-3.496148	-5.101660

H	3.672084	-1.614831	-5.666979
C	7.247604	0.579093	-0.168806
C	5.932914	0.301926	-0.471309
H	7.890965	1.021500	-0.925036
H	5.555870	0.532077	-1.460196
C	7.768368	0.296628	1.116099
C	6.949413	-0.253909	2.073665
H	8.808130	0.518156	1.342004
H	7.329526	-0.472678	3.069036
H	0.615004	-0.645671	3.724269
C	-3.896759	2.915540	1.864628
H	-3.526022	3.940062	2.001523
H	-4.355217	2.873222	0.866462
C	-4.253989	0.139438	2.822462
H	-4.609647	-0.888107	2.670583
H	-3.776317	0.165399	3.814187
C	-5.432538	1.126541	2.798986
H	-5.980710	1.011750	1.853425
H	-6.139300	0.881767	3.601575
C	-4.945816	2.576750	2.936145
H	-4.506668	2.719711	3.934412
H	-5.792122	3.271353	2.865937
C	-4.460473	-1.877505	-2.666574
C	-5.317732	-1.407983	-2.195454
C	-6.405306	-2.175723	-1.850315
C	-5.297620	-0.011416	-1.916137
C	-7.544818	-1.597021	-1.228219
C	-6.406662	-3.243556	-2.055127
C	-6.393625	0.569849	-1.299032
H	-8.689705	-2.359208	-0.874150
C	-7.536902	-0.189347	-0.951284
C	-6.369647	1.636104	-1.093006
H	-9.776255	-1.759855	-0.276361
C	-8.695082	-3.426016	-1.084226
H	-8.676714	0.398448	-0.334632
H	-9.770706	-0.368361	-0.004191
H	-10.646528	-2.353808	-0.010802
H	-8.667560	1.466272	-0.130250
H	-10.636089	0.089712	0.466511
C	-4.128296	0.860322	-2.261246
O	-4.014561	1.973423	-1.754227
C	-3.076889	0.344092	-3.219809
H	-2.297659	-0.160625	-2.629171
H	-3.471896	-0.349916	-3.966446

H	-2.606449	1.193654	-3.719860
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Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.637578	0.767707	0.402708
H	-1.445996	0.227372	-1.161820
H	-0.205541	1.331549	1.897286
N	-1.839470	2.580361	0.149588
H	-1.284187	3.433128	0.106035
H	-2.319089	2.475375	-0.760194
N	-2.570454	0.219539	1.376698
H	-2.963178	-0.626393	0.964425
H	-2.357066	0.002990	2.349460
P	1.311589	1.680549	-0.438898
P	0.431690	-1.202172	0.956165
C	-3.567838	1.320034	1.291226
H	-4.075169	1.189463	0.330952
C	-2.843499	2.669509	1.232946
H	-2.288497	2.817633	2.167922
C	4.903280	-0.767097	2.419143
C	3.864454	-1.139037	3.304413
C	2.577308	-1.285848	2.851963
C	2.229437	-1.079223	1.487655
C	3.232901	-0.742723	0.571094
C	4.589819	-0.570512	1.035545
H	4.098931	-1.311651	4.352514
H	1.810952	-1.581649	3.556722
C	3.455163	-1.465519	-3.200866
C	2.779063	-0.337402	-3.725750
C	2.218589	0.594400	-2.889561
C	2.309307	0.483583	-1.472589
C	2.990933	-0.601879	-0.911127
C	3.555281	-1.609416	-1.778643
H	2.709950	-0.217128	-4.804677
H	1.704511	1.445874	-3.319528
C	0.446374	5.281040	-3.334853
C	1.561463	5.338426	-2.497210
C	1.853860	4.281421	-1.631692
C	1.037293	3.138371	-1.587814

C	-0.089534	3.103729	-2.426726
C	-0.381630	4.158551	-3.293440
H	0.220597	6.107569	-4.004020
H	2.209043	6.211771	-2.510074
H	2.720120	4.360862	-0.986317
H	-0.765378	2.258827	-2.390136
H	-1.267687	4.095286	-3.919287
C	4.458390	3.709203	2.367448
C	4.834190	3.285348	1.091080
C	3.908611	2.645063	0.266272
C	2.592189	2.415378	0.699557
C	2.229802	2.842395	1.983837
C	3.154698	3.484253	2.810886
H	5.179409	4.205123	3.012373
H	5.850511	3.442277	0.739695
H	4.215136	2.317530	-0.722971
H	1.220227	2.647111	2.332246
H	2.854641	3.804281	3.805868
C	0.760711	-4.839488	-1.961435
C	1.240689	-4.962101	-0.654173
C	1.156776	-3.883736	0.226492
C	0.570354	-2.672599	-0.179416
C	0.111598	-2.556091	-1.495004
C	0.206059	-3.631288	-2.383301
H	0.833444	-5.678052	-2.649116
H	1.689165	-5.895723	-0.323738
H	1.547142	-3.986770	1.235714
H	-0.299598	-1.601960	-1.809857
H	-0.147413	-3.520690	-3.405434
C	-1.960654	-2.871173	4.638547
C	-1.854802	-3.640184	3.480971
C	-1.101123	-3.185707	2.393290
C	-0.439338	-1.948633	2.437051
C	-0.580853	-1.169895	3.604312
C	-1.319648	-1.630059	4.695097
H	-2.541388	-3.228240	5.484922
H	-2.357607	-4.601990	3.417376
H	-1.034645	-3.806128	1.506941
H	-1.399214	-1.014586	5.587879
C	4.772096	-3.699577	-2.133407
C	4.222944	-2.766391	-1.282089
H	5.273753	-4.571633	-1.722228
H	4.294384	-2.916146	-0.211828
C	4.686383	-3.537413	-3.536061

C	4.034937	-2.442519	-4.054140
H	5.128546	-4.278264	-4.196934
H	3.950765	-2.305017	-5.129826
C	6.944357	-0.040532	0.638626
C	5.659203	-0.197562	0.169369
H	7.736134	0.244215	-0.049412
H	5.455371	-0.032065	-0.881275
C	7.244174	-0.245222	2.006316
C	6.238992	-0.599280	2.875030
H	8.262699	-0.120491	2.364159
H	6.448635	-0.757338	3.930487
H	-0.120553	-0.186822	3.640618
C	-3.853039	3.814320	1.050382
H	-3.322521	4.775653	1.030943
H	-4.342409	3.701832	0.072395
C	-4.617503	1.293057	2.411694
H	-5.140769	0.328461	2.404228
H	-4.108636	1.374004	3.384971
C	-5.621918	2.447800	2.257099
H	-6.214383	2.284930	1.345645
H	-6.330182	2.442243	3.094808
C	-4.910627	3.806850	2.167513
H	-4.423707	4.026093	3.129247
H	-5.641279	4.607578	1.999157
C	-2.498645	-2.142380	-1.436024
C	-3.518026	-1.776857	-1.382729
C	-4.512918	-2.597871	-0.902743
C	-3.801765	-0.439671	-1.781511
C	-5.859148	-2.146783	-0.805511
C	-4.277957	-3.613496	-0.591321
C	-5.105334	0.015114	-1.700392
H	-6.909775	-2.968336	-0.318392
C	-6.158896	-0.808437	-1.220404
C	-5.318326	1.032981	-2.015374
H	-8.201150	-2.492539	-0.245078
C	-6.678438	-3.984048	-0.005204
H	-7.501559	-0.348955	-1.133592
H	-8.499814	-1.170403	-0.657006
H	-8.997021	-3.131898	0.127620
H	-7.727815	0.665429	-1.454197
H	-9.522283	-0.807120	-0.596649
C	-2.762721	0.504482	-2.368339
O	-3.005142	1.737108	-2.347733
C	-1.963237	-0.065312	-3.541914

H	-1.690985	-1.114281	-3.409623
H	-2.602769	0.007447	-4.433640
H	-1.060850	0.521809	-3.719902

TSu₇

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.369922	1.517467	0.172490
H	1.747685	0.687191	-0.817097
H	-0.624834	2.477056	1.064989
N	2.038191	2.282179	1.361692
H	2.002154	2.018891	2.345132
H	2.890639	1.870399	0.946952
N	0.897526	3.416453	-0.883960
H	1.046298	3.283467	-1.882904
H	0.076215	4.014282	-0.796233
P	-0.151407	-0.232167	1.574972
P	-1.482646	1.117290	-1.162745
C	2.085643	4.076411	-0.278433
H	2.963073	3.591495	-0.718589
C	2.119773	3.756025	1.221985
H	1.218640	4.168487	1.694966
C	-5.294413	-0.595071	1.031715
C	-5.270934	0.713107	0.493894
C	-4.160585	1.180162	-0.163102
C	-2.996095	0.380591	-0.336635
C	-2.986615	-0.929130	0.155369
C	-4.144159	-1.430972	0.859390
H	-6.148304	1.346526	0.604596
H	-4.181565	2.182938	-0.569604
C	-1.058052	-4.026350	-1.054935
C	0.132052	-3.905160	-0.298621
C	0.341214	-2.817159	0.510939
C	-0.629560	-1.786520	0.648633
C	-1.840277	-1.887795	-0.047910
C	-2.055891	-3.004587	-0.936178
H	0.887411	-4.684324	-0.369208
H	1.268767	-2.748020	1.064812
C	3.524228	-1.383245	4.261145
C	2.271396	-1.225328	4.853381

C	1.154121	-0.911879	4.074583
C	1.268596	-0.743218	2.684074
C	2.544332	-0.876875	2.107281
C	3.656570	-1.207884	2.882438
H	4.390373	-1.634236	4.868160
H	2.155360	-1.347827	5.927481
H	0.194245	-0.796990	4.562727
H	2.667828	-0.718031	1.042408
H	4.623420	-1.325571	2.401976
C	-3.403989	0.152418	4.912251
C	-2.964379	-1.109253	4.504965
C	-2.021228	-1.224703	3.483735
C	-1.502242	-0.084097	2.848596
C	-1.950908	1.174970	3.266985
C	-2.894837	1.292856	4.290292
H	-4.140779	0.243559	5.706323
H	-3.361236	-2.004770	4.975583
H	-1.685655	-2.211529	3.177679
H	-1.558716	2.058154	2.772406
H	-3.233692	2.279057	4.598445
C	-1.297349	-1.320490	-5.141121
C	-2.538458	-0.897237	-4.656245
C	-2.617903	-0.188808	-3.457137
C	-1.455051	0.113519	-2.729522
C	-0.221106	-0.318000	-3.222324
C	-0.137950	-1.032055	-4.420712
H	-1.238033	-1.876890	-6.072981
H	-3.445540	-1.124146	-5.210790
H	-3.587973	0.134840	-3.088999
H	0.663175	-0.086441	-2.637566
H	0.829915	-1.364853	-4.788116
C	-2.798627	5.344415	-2.752675
C	-2.492781	4.329533	-3.657507
C	-2.148553	3.052172	-3.201452
C	-2.094781	2.762209	-1.829054
C	-2.386001	3.806393	-0.926830
C	-2.744873	5.075975	-1.381789
H	-3.071297	6.334657	-3.107960
H	-2.522675	4.524215	-4.726659
H	-1.921399	2.281333	-3.928704
H	-2.977884	5.857760	-0.662925
C	-3.428056	-4.236313	-2.541150
C	-3.240587	-3.150457	-1.715389
H	-4.341517	-4.316010	-3.124673

H	-4.006493	-2.386534	-1.659780
C	-2.443237	-5.247607	-2.640202
C	-1.281970	-5.137898	-1.911907
H	-2.605429	-6.101917	-3.292045
H	-0.511194	-5.902463	-1.978890
C	-5.316849	-3.194954	2.081805
C	-4.199827	-2.742993	1.414852
H	-5.326300	-4.201253	2.492382
H	-3.343697	-3.398055	1.311674
C	-6.450912	-2.363386	2.238748
C	-6.433299	-1.088619	1.723979
H	-7.327125	-2.732578	2.765011
H	-7.293463	-0.432786	1.837749
H	-2.314128	3.617712	0.140324
C	3.367992	4.372140	1.875702
H	3.364990	4.156567	2.952631
H	4.260829	3.889998	1.454535
C	2.140859	5.589281	-0.531523
H	2.147788	5.785227	-1.612167
H	1.228077	6.058042	-0.131079
C	3.375551	6.219658	0.134614
H	4.282344	5.837221	-0.354743
H	3.370334	7.306058	-0.018022
C	3.432037	5.890070	1.633825
H	2.588344	6.376995	2.145159
H	4.345917	6.302487	2.078834
C	2.159563	-1.514070	-2.279071
C	3.113794	-1.727360	-1.811773
C	3.577872	-3.021360	-1.782233
C	3.845573	-0.673157	-1.197974
C	4.805175	-3.350051	-1.143158
C	2.999983	-3.816655	-2.247704
C	5.037584	-0.972936	-0.563772
H	5.317905	-4.673513	-1.100347
C	5.548469	-2.296949	-0.517506
C	5.595106	-0.162222	-0.103708
H	6.512582	-4.947946	-0.470555
C	4.750996	-5.470628	-1.576458
H	6.778768	-2.613207	0.121631
H	7.250457	-3.907388	0.145976
H	6.894617	-5.965124	-0.445815
H	7.345084	-1.810997	0.589603
H	8.192622	-4.135287	0.637488
C	3.462521	0.795620	-1.295042

O	4.014239	1.598599	-0.496416
C	3.190702	1.278649	-2.723473
H	2.547571	0.613183	-3.301103
H	2.757604	2.281433	-2.714169
H	4.161633	1.340796	-3.235589

Pf7

Coordinates (Angstroms)			
	X	Y	Z

Ru		-0.34062300	0.65117500 0.83825900
H		-2.43434800	-0.31794200 -1.48603300
H		0.35927600	1.07649500 2.18705600
N		-1.81805200	2.08199200 0.56716600
H		-1.51302300	3.03594800 0.36994300
H		-2.73367100	1.73477900 -0.92952700
N		-2.01597400	-0.15667400 2.06624100
H		-2.22248700	-1.14792000 1.94305000
H		-1.67744500	-0.06541500 3.02478300
P		1.36019700	1.75766800 -0.28178100
P		0.92864600	-1.29813500 1.07964100
C		-3.24683700	0.66183400 1.88269100
H		-3.70857800	0.31077600 0.95212100
C		-2.79981700	2.10781200 1.65590100
H		-2.34068400	2.46083200 2.60106800
C		5.58989400	-0.77578000 1.55151900
C		4.79168400	-1.28258100 2.60413900
C		3.44240100	-1.46616400 2.43411500
C		2.79130800	-1.16159300 1.20550300
C		3.54771600	-0.68493800 0.12976100
C		4.96724800	-0.47991800 0.29578200
H		5.26246200	-1.53036100 3.55290100
H		2.86331400	-1.86430600 3.25770400
C		2.93855000	-1.15662700 -3.63288100
C		2.16182700	-0.01065300 -3.92433200
C		1.78770100	0.85419700 -2.92727600
C		2.17063000	0.65627800 -1.56882300
C		2.97232800	-0.44635600 -1.24393600
C		3.34681700	-1.38264400 -2.27842200
H		1.86336900	0.17980300 -4.95280500
H		1.19317800	1.72083700 -3.18698600

C	-0.08524800	5.50404100	-2.71533100
C	1.10032200	5.58035000	-1.98356300
C	1.56099200	4.47525700	-1.26358800
C	0.84428200	3.26686800	-1.26160100
C	-0.35568400	3.21070600	-1.99279000
C	-0.81327300	4.31331100	-2.71590200
H	-0.44224800	6.36683200	-3.27198700
H	1.67337300	6.50415900	-1.96725500
H	2.48154400	4.56721700	-0.69984300
H	-0.96086200	2.31209600	-1.99080200
H	-1.74881700	4.23282500	-3.26250500
C	4.83521200	3.72394600	2.13626500
C	5.03932300	3.35375300	0.80562500
C	4.01605300	2.73410700	0.08729600
C	2.77566100	2.46561000	0.68710400
C	2.58212200	2.84532300	2.02318800
C	3.60348600	3.47042400	2.74176100
H	5.63194600	4.20580100	2.69712500
H	5.99703500	3.53871800	0.32679300
H	4.18483000	2.45727400	-0.94886900
H	1.62644400	2.64520600	2.49649900
H	3.43488800	3.75742200	3.77667500
C	0.36611200	-4.77314900	-1.99074000
C	1.32238700	-4.90231200	-0.97967800
C	1.51799900	-3.86769600	-0.06472600
C	0.75028300	-2.69334000	-0.13695100
C	-0.20093500	-2.57577600	-1.15716300
C	-0.39169300	-3.60530800	-2.08211100
H	0.22047300	-5.57636200	-2.70825400
H	1.92218100	-5.80616600	-0.90975100
H	2.27000300	-3.97420800	0.71294800
H	-0.78060200	-1.65975100	-1.23285500
H	-1.12565100	-3.49064500	-2.87574200
C	-0.52575900	-3.19410000	5.12181200
C	-0.63433300	-3.92888900	3.94259600
C	-0.15650600	-3.40747600	2.73481000
C	0.43275800	-2.13489600	2.67922900
C	0.51391600	-1.39591300	3.87738600
C	0.05455200	-1.92256200	5.08443600
H	-0.89256000	-3.60230200	6.05976100
H	-1.08902700	-4.91626600	3.95495900
H	-0.24769900	-4.00380500	1.83390500
H	0.14389400	-1.33598000	5.99542000
C	4.47819100	-3.41856200	-3.02194300

C	4.12231900	-2.54954600	-2.01471400
H	5.06781300	-4.30065300	-2.78633400
H	4.43274500	-2.75934000	-0.99858800
C	4.08257400	-3.17730300	-4.35879700
C	3.32449300	-2.06833800	-4.65229500
H	4.37435500	-3.86853800	-5.14492500
H	3.00474100	-1.86886400	-5.67246800
C	7.15258700	0.20791200	-0.55983200
C	5.80152100	0.01778600	-0.74783600
H	7.76009000	0.58878200	-1.37660400
H	5.36209100	0.25191600	-1.70982500
C	7.75777600	-0.08941600	0.68444100
C	6.98662300	-0.57053900	1.71607300
H	8.82519600	0.06278800	0.81972600
H	7.43334700	-0.80349200	2.67992400
H	0.93779600	-0.39610800	3.85764400
C	-4.02746900	2.99914000	1.38523100
H	-3.70137200	4.04082200	1.26276200
H	-4.47900700	2.69539600	0.43189700
C	-4.26127400	0.53106900	3.02432100
H	-4.57666700	-0.51549800	3.13448200
H	-3.78032600	0.82089100	3.97164600
C	-5.48125900	1.43470000	2.76797300
H	-6.02566400	1.05935400	1.89038200
H	-6.17484200	1.37489000	3.61619700
C	-5.06064300	2.89269600	2.52024600
H	-4.63093600	3.30750800	3.44434500
H	-5.94281000	3.50266500	2.28754700
H	-3.74086200	-2.45403900	-1.54399400
C	-4.64118200	-1.84974400	-1.44474400
C	-5.83247800	-2.45189100	-1.11061000
C	-4.55968700	-0.44512600	-1.65914900
C	-7.02207200	-1.68630200	-0.97013300
H	-5.87799900	-3.52646100	-0.94621000
C	-5.70155800	0.31651700	-1.52442700
C	-8.27103200	-2.26998700	-0.62711800
C	-6.95006400	-0.27005400	-1.18090200
H	-5.63655000	1.38932500	-1.68130800
C	-9.40166400	-1.49368100	-0.49832300
H	-8.32014700	-3.34515900	-0.46858000
C	-8.13578000	0.50198600	-1.03833600
C	-9.33261900	-0.09366300	-0.70615600
H	-10.35170200	-1.95239100	-0.23722300
H	-8.08080400	1.57602200	-1.20046500

H	-10.23082500	0.50946800	-0.60251700
C	-3.22870400	0.18636500	-2.06613900
O	-3.18703400	1.57395900	-1.81965700
C	-2.94903400	-0.04918600	-3.55825400
H	-3.00448000	-1.11299000	-3.81709200
H	-3.68986500	0.48889700	-4.15969300
H	-1.95288800	0.32574100	-3.81617700

Pu7

Coordinates (Angstroms)			
	X	Y	Z
Ru	0.05804500	1.52104100	-0.64550400
H	-2.35486500	0.05270100	1.91861000
H	1.03362600	2.00507700	-1.79035100
N	-1.88701400	1.85631800	-1.23732400
H	-2.28225700	1.29601700	-1.99214400
H	-2.87581200	1.53073300	0.30362700
N	-0.23245300	3.66230000	-0.10918200
H	0.11660400	3.94256200	0.80714500
H	0.34596100	4.15971700	-0.78737900
P	0.27966300	-0.61858500	-1.48553400
P	1.99986300	1.36139400	0.63440800
C	-1.65951600	4.05416100	-0.27225800
H	-2.17775000	3.68950600	0.62238200
C	-2.20791400	3.26853700	-1.46741400
H	-1.69623200	3.64840700	-2.37511300
C	5.43425200	-1.49242700	-0.86721500
C	5.62688800	-0.09574600	-0.74784900
C	4.62606700	0.71031700	-0.26706000
C	3.36510900	0.18564600	0.13601200
C	3.14219400	-1.19335000	0.06095600
C	4.18219200	-2.05283200	-0.45425400
H	6.58241400	0.33373200	-1.04054300
H	4.80806100	1.77456100	-0.18478800
C	0.90952200	-3.41371100	2.25866000
C	-0.29426500	-3.40113300	1.51576800
C	-0.40960900	-2.63955000	0.38026000
C	0.66501200	-1.84353400	-0.11165200
C	1.89063100	-1.86539100	0.56889200
C	2.01730900	-2.64060100	1.78145300
H	-1.13227700	-4.00750300	1.85235700

H	-1.34643000	-2.65864600	-0.16125000
C	-3.60075600	-2.27829300	-3.55041000
C	-2.37010000	-2.40525400	-4.19398400
C	-1.20171100	-1.93907700	-3.58634100
C	-1.23746100	-1.33285900	-2.31947400
C	-2.49129500	-1.19240600	-1.69547600
C	-3.65783600	-1.66865700	-2.29609300
H	-4.50841700	-2.64520700	-4.02245700
H	-2.31156600	-2.87043200	-5.17491600
H	-0.26121300	-2.05053900	-4.11154900
H	-2.56511600	-0.70300400	-0.73094500
H	-4.60683700	-1.55533500	-1.78058700
C	3.35241100	-1.51560100	-4.88398400
C	2.91056100	-2.54868000	-4.05485400
C	2.01845700	-2.27897100	-3.01666900
C	1.55886700	-0.97306800	-2.78275700
C	2.00655200	0.05429700	-3.62501000
C	2.89596400	-0.21472400	-4.66778500
H	4.04826700	-1.72443200	-5.69250200
H	3.26484500	-3.56417100	-4.20958500
H	1.67579600	-3.09250000	-2.38430700
H	1.65284200	1.06620400	-3.45726700
H	3.23191000	0.59518300	-5.31047400
C	1.41874200	0.55466500	5.19590500
C	2.70064000	0.46925500	4.64658000
C	2.89358200	0.68638000	3.28196000
C	1.80828200	0.99322300	2.44560800
C	0.52738800	1.07406400	3.00860700
C	0.33165800	0.85703000	4.37474300
H	1.26887600	0.38157700	6.25840300
H	3.55000900	0.22861900	5.28075900
H	3.89440000	0.61801400	2.86408300
H	-0.31911500	1.30533800	2.36599600
H	-0.66918000	0.91984200	4.79324800
C	3.95389000	5.63180800	0.65031600
C	3.65266000	5.01440500	1.86296800
C	3.11395100	3.72303200	1.88638500
C	2.85654400	3.02607600	0.69564000
C	3.15177500	3.67129500	-0.52233300
C	3.70438000	4.95156300	-0.54547000
H	4.37490000	6.63359800	0.63352700
H	3.83770100	5.53329000	2.80018200
H	2.89514100	3.26266600	2.84335600
H	3.93442500	5.42101500	-1.49872700

C	3.31647700	-3.43088600	3.69657400
C	3.21925900	-2.67800900	2.54767000
H	4.24668900	-3.43498400	4.25865900
H	4.07246200	-2.09675200	2.22055500
C	2.21863900	-4.19750200	4.15387800
C	1.03990100	-4.18328900	3.44613500
H	2.30945100	-4.78993300	5.06034100
H	0.18381900	-4.76341800	3.78298300
C	5.02977900	-4.25960700	-1.08120400
C	4.02217100	-3.46382000	-0.58287200
H	4.87472700	-5.33200100	-1.16602600
H	3.08606200	-3.91985200	-0.28413600
C	6.26458700	-3.69603200	-1.48168800
C	6.45661000	-2.33866400	-1.37577700
H	7.05300700	-4.33490900	-1.87038200
H	7.39767900	-1.88664900	-1.68061600
H	2.94058900	3.16163600	-1.45788000
C	-3.71063300	3.56527000	-1.63871300
H	-4.09204100	3.02172300	-2.51375500
H	-4.24818300	3.18146200	-0.76204900
C	-1.88306300	5.56403200	-0.41688800
H	-1.49974300	6.09303500	0.46678300
H	-1.31160700	5.93474000	-1.28213700
C	-3.37818900	5.87132900	-0.61917600
H	-3.92306000	5.61253000	0.29973900
H	-3.52070900	6.94808800	-0.77580500
C	-3.96551400	5.07453600	-1.79601000
H	-3.50977100	5.42634700	-2.73361600
H	-5.04192900	5.27093200	-1.88088300
H	-3.32457300	-2.13553800	2.65432900
C	-4.20654600	-1.89461200	2.06373800
C	-5.13008800	-2.87433500	1.78198900
C	-4.37617300	-0.56411700	1.58790900
C	-6.28398400	-2.58683200	1.00277800
H	-4.98601800	-3.88820300	2.14948600
C	-5.48445300	-0.26468400	0.82422900
C	-7.25996400	-3.57058100	0.69020200
C	-6.46002200	-1.25125500	0.51235100
H	-5.60728200	0.74870500	0.45310600
C	-8.36282200	-3.25406300	-0.07222400
H	-7.12133300	-4.58250600	1.06464100
C	-7.60881500	-0.95881000	-0.27322100
C	-8.53827200	-1.93483000	-0.55862900
H	-9.10283800	-4.01557000	-0.30384400

H	-7.74222700	0.05477000	-0.64435100
H	-9.41199500	-1.69574900	-1.15926900
C	-3.35848200	0.50971400	1.96840600
O	-3.42095700	1.65092400	1.13817800
C	-3.59498400	0.98574600	3.40920100
H	-3.56821600	0.15146500	4.11885700
H	-2.83112800	1.71915600	3.68982500
H	-4.57611300	1.46771800	3.47967100

ABS₈

Coordinates (Angstroms)			
	X	Y	Z
Ru	-0.773440	1.009234	-0.459965
H	-0.203735	2.004866	-1.731194
H	-1.569292	0.106408	0.777225
N	-1.965099	2.785700	0.190156
H	-1.990069	2.857903	1.205037
H	-1.473950	3.611946	-0.149354
N	-2.632563	0.818100	-1.662067
H	-2.432422	0.451365	-2.590485
H	-3.265079	0.158168	-1.206056
P	1.044277	1.544240	0.812327
P	0.214063	-0.877596	-1.281061
C	-3.295910	2.136115	-1.764005
H	-2.640642	2.763795	-2.382724
C	-3.344565	2.738329	-0.352815
H	-3.899843	2.033343	0.278418
C	2.343778	-3.246946	2.189978
C	1.145343	-3.708016	1.593605
C	0.578733	-3.029342	0.544568
C	1.170344	-1.854747	0.000437
C	2.371959	-1.382147	0.539459
C	2.964432	-2.068023	1.663423
H	0.677207	-4.611672	1.978273
H	-0.340663	-3.404046	0.111529
C	5.183687	0.555788	-1.224879
C	4.746960	1.888199	-1.034418
C	3.558865	2.152388	-0.400623
C	2.724199	1.113406	0.098688
C	3.132561	-0.217689	-0.043234
C	4.370781	-0.512534	-0.725306

H	5.367464	2.704939	-1.396876
H	3.256761	3.183844	-0.269857
C	1.008363	6.223521	1.303741
C	1.084988	5.417039	2.437964
C	1.143630	4.024253	2.315769
C	1.118124	3.405647	1.055833
C	1.018167	4.234858	-0.080392
C	0.976130	5.624443	0.040958
H	0.968873	7.305608	1.399887
H	1.102912	5.867309	3.427562
H	1.208367	3.422988	3.215085
H	0.950272	3.769709	-1.060082
H	0.913115	6.239728	-0.853584
C	1.504113	0.156368	5.256672
C	2.565027	0.809102	4.622976
C	2.445169	1.206093	3.291239
C	1.261119	0.965084	2.573900
C	0.207197	0.305661	3.216754
C	0.328349	-0.096936	4.549706
H	1.599900	-0.159328	6.292648
H	3.488313	1.001347	5.163871
H	3.277030	1.710604	2.806312
H	-0.693859	0.099606	2.643425
H	-0.495986	-0.615925	5.033546
C	3.079556	-0.791181	-4.974811
C	3.017263	-1.935492	-4.175630
C	2.188378	-1.959332	-3.053725
C	1.405275	-0.843274	-2.714523
C	1.480516	0.300406	-3.519262
C	2.312387	0.325804	-4.641790
H	3.728853	-0.770313	-5.846657
H	3.620735	-2.805891	-4.420269
H	2.149452	-2.854064	-2.437832
H	0.891046	1.169417	-3.236600
H	2.363530	1.223532	-5.253492
C	-3.146024	-3.753861	-2.874034
C	-2.006991	-3.542856	-3.649844
C	-0.974942	-2.721815	-3.185000
C	-1.059011	-2.095584	-1.930726
C	-2.221362	-2.311910	-1.164927
C	-3.250890	-3.132850	-1.627080
H	-3.950302	-4.386637	-3.241182
H	-1.916473	-4.012736	-4.626303
H	-0.106365	-2.569078	-3.814134

H	-4.146081	-3.261776	-1.025098
C	6.025424	-2.096060	-1.582159
C	4.835946	-1.843455	-0.935656
H	6.350912	-3.123086	-1.726326
H	4.237385	-2.673582	-0.581117
C	6.826070	-1.033016	-2.062644
C	6.406909	0.264849	-1.887467
H	7.763851	-1.244846	-2.569534
H	7.005944	1.095019	-2.255100
C	4.718750	-2.306283	3.349503
C	4.164640	-1.623026	2.289924
H	5.634608	-1.939328	3.805575
H	4.646854	-0.724388	1.925328
C	4.106275	-3.478193	3.852501
C	2.939788	-3.932541	3.282755
H	4.555048	-4.010833	4.686900
H	2.450607	-4.827971	3.659979
H	-2.314404	-1.803055	-0.209647
C	-4.050997	4.103900	-0.344693
H	-4.110355	4.483234	0.684288
H	-3.437123	4.822661	-0.909428
C	-4.698292	2.067292	-2.391831
H	-4.620131	1.675949	-3.414959
H	-5.303836	1.349758	-1.821944
C	-5.388079	3.440760	-2.393664
H	-4.834484	4.130042	-3.048300
H	-6.397356	3.353606	-2.814582
C	-5.450913	4.028086	-0.976017
H	-6.098951	3.397243	-0.350573
H	-5.907066	5.025755	-0.992865
H	-7.413282	-4.655840	3.099137
C	-6.999774	-3.918883	2.425359
C	-6.159154	-2.818117	2.752967
C	-7.178438	-3.857259	1.071033
C	-5.885883	-2.159727	1.575243
H	-5.803620	-2.546551	3.736456
O	-6.517840	-2.805683	0.541369
H	-7.726773	-4.468844	0.369750
C	-5.101957	-0.967547	1.238233
O	-5.047587	-0.558755	0.080732
C	-4.366382	-0.262002	2.357972
H	-4.844710	0.707956	2.542157
H	-4.346855	-0.823191	3.295247
H	-3.339810	-0.072176	2.014538

INTf₈

	Coordinates (Angstroms)		
	X	Y	Z

Ru	0.861241	0.092631	-0.777016
H	0.463478	0.292630	-2.428078
H	1.504640	-0.092784	0.818308
N	2.490501	-1.247503	-1.500385
H	2.593430	-2.063400	-0.900663
H	2.200379	-1.593125	-2.414524
N	2.525305	1.518244	-1.160871
H	2.173533	2.390167	-1.551128
H	2.984758	1.748992	-0.277862
P	-0.660924	-1.599135	-0.590887
P	-0.637665	1.668225	-0.076428
C	3.507579	0.907502	-2.084552
H	3.012548	0.848831	-3.063372
C	3.780135	-0.524409	-1.602036
H	4.174554	-0.455750	-0.581034
C	-3.015405	0.082380	3.670079
C	-2.023695	1.086491	3.781549
C	-1.390301	1.572142	2.665918
C	-1.708023	1.109187	1.357997
C	-2.704124	0.139298	1.199931
C	-3.359446	-0.402987	2.366688
H	-1.769321	1.470868	4.767098
H	-0.632528	2.336860	2.785031
C	-5.056762	-0.380868	-1.795363
C	-4.282577	-1.258321	-2.590841
C	-3.023573	-1.635068	-2.196301
C	-2.445213	-1.173575	-0.980514
C	-3.188393	-0.326692	-0.149898
C	-4.508749	0.091124	-0.558891
H	-4.699557	-1.634298	-3.522647
H	-2.461078	-2.310504	-2.828528
C	0.601854	-4.865439	-3.734197
C	0.420616	-5.231893	-2.401767
C	0.000948	-4.288726	-1.456873
C	-0.238849	-2.954691	-1.821897
C	-0.028541	-2.595136	-3.169154

C	0.374079	-3.539462	-4.114486
H	0.922118	-5.600509	-4.468219
H	0.601883	-6.257193	-2.088241
H	-0.136476	-4.604671	-0.429196
H	-0.163322	-1.556058	-3.457296
H	0.514947	-3.236422	-5.149409
C	-1.086534	-4.179754	3.287466
C	-2.002753	-4.344406	2.244943
C	-1.899359	-3.562905	1.094161
C	-0.875012	-2.609751	0.963228
C	0.032400	-2.448341	2.016524
C	-0.073076	-3.228025	3.171706
H	-1.170751	-4.784654	4.186974
H	-2.802171	-5.076084	2.331763
H	-2.619624	-3.697009	0.290983
H	0.804491	-1.688770	1.914454
H	0.634598	-3.085660	3.985306
C	-3.670462	3.712010	-2.988904
C	-3.839479	3.847118	-1.608636
C	-2.957126	3.215363	-0.731859
C	-1.889621	2.442834	-1.218940
C	-1.732966	2.310412	-2.604284
C	-2.617829	2.940783	-3.483120
H	-4.360656	4.200189	-3.672602
H	-4.663803	4.435927	-1.214488
H	-3.099611	3.324963	0.340010
H	-0.919161	1.691106	-2.973647
H	-2.485461	2.823637	-4.556172
C	1.719868	5.417972	1.498144
C	0.613006	5.610844	0.671987
C	-0.128522	4.517792	0.212884
C	0.221605	3.206142	0.571998
C	1.349928	3.028734	1.394792
C	2.087661	4.119012	1.856636
H	2.297278	6.269339	1.849824
H	0.321552	6.615776	0.376136
H	-0.979116	4.697891	-0.433636
H	2.964115	3.948334	2.476215
C	-6.571711	1.351948	-0.192256
C	-5.312826	0.974427	0.219352
H	-7.158684	2.027197	0.425020
H	-4.921871	1.359603	1.153178
C	-7.106923	0.873068	-1.411367
C	-6.358426	0.026374	-2.194707

H	-8.102119	1.177245	-1.724874
H	-6.750766	-0.347780	-3.137702
C	-4.976291	-1.907177	3.415954
C	-4.355321	-1.419479	2.287475
H	-5.731246	-2.683337	3.320633
H	-4.624688	-1.818832	1.317313
C	-4.639578	-1.410908	4.697332
C	-3.674669	-0.438097	4.816170
H	-5.139286	-1.801284	5.580044
H	-3.397850	-0.048341	5.793301
H	1.651541	2.016360	1.645419
C	4.808562	-1.234560	-2.496863
H	5.009543	-2.239527	-2.101959
H	4.372345	-1.371046	-3.498652
C	4.815254	1.708909	-2.207217
H	4.592734	2.711982	-2.595076
H	5.240710	1.838304	-1.203311
C	5.834282	0.998102	-3.112502
H	5.448577	0.955262	-4.141976
H	6.766109	1.575757	-3.152158
C	6.111886	-0.427995	-2.614368
H	6.595244	-0.377560	-1.628527
H	6.810713	-0.942033	-3.286296
H	8.502277	-2.141210	3.037864
C	7.832167	-1.409095	2.610001
C	6.533178	-1.049432	3.067489
C	8.064416	-0.632607	1.508834
C	6.063443	-0.077076	2.213689
H	6.013421	-1.457118	3.922495
O	7.012384	0.175083	1.253395
H	8.899413	-0.545239	0.829417
C	4.819956	0.697578	2.143855
O	4.659746	1.550065	1.273359
C	3.732961	0.392282	3.150010
H	2.867379	0.010272	2.588781
H	4.024600	-0.328235	3.917416
H	3.420893	1.324743	3.631479

TSf₈

Coordinates (Angstroms)

X Y Z

Ru	-1.281360	0.488492	0.310157
H	-1.775111	-0.218343	-1.311258
H	-1.095290	1.156904	1.810967
N	-2.829638	1.998539	-0.034803
H	-2.479659	2.954524	-0.068579
H	-3.225693	1.768183	-0.962109
N	-3.128010	-0.467946	1.133810
H	-3.308532	-1.360608	0.679077
H	-2.948217	-0.658290	2.118921
P	0.499234	1.757098	-0.425041
P	0.108329	-1.227094	1.001047
C	-4.327721	0.398840	0.977061
H	-4.719119	0.186977	-0.022369
C	-3.892522	1.866823	0.985646
H	-3.435364	2.101446	1.955319
C	4.438106	-0.049670	2.472855
C	3.458098	-0.545113	3.364639
C	2.210956	-0.893634	2.910745
C	1.850050	-0.781966	1.538682
C	2.796073	-0.316760	0.618688
C	4.109152	0.066583	1.083708
H	3.705628	-0.648416	4.418802
H	1.488465	-1.276886	3.619789
C	3.137855	-1.015727	-3.149919
C	2.321663	0.011968	-3.681142
C	1.627169	0.853542	-2.850110
C	1.710926	0.749291	-1.432592
C	2.538579	-0.226729	-0.864667
C	3.246987	-1.143142	-1.726612
H	2.249463	0.125342	-4.760614
H	1.002404	1.624622	-3.284727
C	-0.731812	5.253018	-3.329556
C	0.395923	5.401381	-2.520784
C	0.785501	4.378983	-1.652859
C	0.058075	3.178727	-1.574374
C	-1.080751	3.051156	-2.388251
C	-1.470820	4.071948	-3.258704
H	-1.033757	6.051836	-4.002136
H	0.977768	6.319029	-2.559304
H	1.658834	4.530849	-1.030429
H	-1.676240	2.148707	-2.341378
H	-2.357171	3.936434	-3.873102
C	3.089313	4.252450	2.567289

C	3.636862	3.850253	1.347710
C	2.884376	3.073463	0.465560
C	1.575203	2.679151	0.785615
C	1.040214	3.085234	2.015885
C	1.789552	3.866672	2.898148
H	3.674472	4.856167	3.256419
H	4.653569	4.129886	1.084888
H	3.325018	2.767357	-0.478347
H	0.037520	2.763829	2.280063
H	1.356582	4.169151	3.848674
C	0.961076	-5.072493	-1.513223
C	1.640921	-4.868805	-0.308825
C	1.408349	-3.714119	0.436853
C	0.485221	-2.749489	-0.003763
C	-0.189656	-2.963636	-1.209369
C	0.048664	-4.118048	-1.961094
H	1.146772	-5.969521	-2.098587
H	2.356481	-5.606659	0.045503
H	1.944541	-3.563671	1.370129
H	-0.898787	-2.215320	-1.548331
H	-0.482579	-4.270100	-2.896893
C	-1.976685	-3.049946	4.802932
C	-1.669100	-3.876304	3.723602
C	-1.006217	-3.363473	2.603121
C	-0.642578	-2.009393	2.533300
C	-0.980905	-1.182476	3.624207
C	-1.627660	-1.697384	4.748515
H	-2.486829	-3.450879	5.674916
H	-1.941206	-4.928655	3.747040
H	-0.775662	-4.031671	1.781666
H	-1.863764	-1.038453	5.580599
C	4.745448	-3.043861	-2.068998
C	4.070404	-2.191914	-1.223413
H	5.361494	-3.836670	-1.652867
H	4.158442	-2.325432	-0.152342
C	4.641881	-2.901146	-3.472674
C	3.849879	-1.906783	-3.997271
H	5.182768	-3.577672	-4.129060
H	3.752680	-1.785211	-5.073756
C	6.359787	0.938858	0.685512
C	5.117013	0.578024	0.214036
H	7.104572	1.325176	-0.005445
H	4.899780	0.687345	-0.841432
C	6.676943	0.810500	2.058623

C	5.730135	0.326783	2.930366
H	7.662100	1.095539	2.418081
H	5.952613	0.225965	3.990202
H	-0.747000	-0.123345	3.573876
C	-5.100402	2.790043	0.754988
H	-4.776575	3.839157	0.784198
H	-5.501626	2.607336	-0.251973
C	-5.419096	0.127938	2.021409
H	-5.734583	-0.922289	1.964741
H	-5.000756	0.279236	3.028875
C	-6.625004	1.062047	1.821152
H	-7.114803	0.817238	0.867967
H	-7.368452	0.889561	2.609371
C	-6.195817	2.537366	1.804621
H	-5.818002	2.817244	2.799168
H	-7.061290	3.181915	1.607626
H	-2.987323	-0.251566	-2.601423
C	-3.736317	0.738364	-2.394625
C	-1.982650	-0.229387	-3.755337
C	-1.181573	-0.962435	-3.635326
C	-2.525923	-0.443915	-4.687006
H	-1.539613	0.760883	-3.849112
O	-3.504818	-1.628267	-2.328541
H	-3.327022	-2.822706	-2.976887
C	-4.433440	-1.796035	-1.333123
O	-4.185353	-3.778015	-2.344234
C	-2.673736	-2.998127	-3.819197
H	-4.829493	-3.102304	-1.354854
H	-4.306751	-4.822195	-2.597238
H	-5.568022	-3.380277	-0.617977

TSu₈

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.428679	-0.457723	0.259387
H	-1.921369	0.823770	-0.999784
H	-1.265817	-1.672209	1.362917
N	-3.201183	0.248822	1.332329
H	-3.007381	0.624882	2.258885
H	-3.572809	1.015676	0.744154

N	-3.069062	-1.746121	-0.557188
H	-3.095663	-1.758801	-1.575427
H	-2.828596	-2.693725	-0.269096
P	0.096340	0.755203	1.488520
P	0.237768	-1.472862	-0.971070
C	-4.401379	-1.365451	-0.017641
H	-4.753041	-0.525454	-0.626376
C	-4.223637	-0.819254	1.404339
H	-3.815256	-1.611801	2.045161
C	4.261536	-2.346693	1.342814
C	3.405096	-3.391124	0.922584
C	2.256690	-3.116696	0.223337
C	1.876178	-1.786529	-0.109435
C	2.713496	-0.725804	0.256261
C	3.920115	-0.998319	1.001336
H	3.670442	-4.419747	1.156760
H	1.633770	-3.943016	-0.093550
C	3.211804	2.679871	-1.458505
C	2.196618	3.442436	-0.831793
C	1.345134	2.864640	0.074813
C	1.456353	1.493327	0.439637
C	2.457554	0.706579	-0.140777
C	3.339405	1.292799	-1.122315
H	2.093235	4.495214	-1.084176
H	0.569473	3.470586	0.527106
C	-1.961648	4.390200	3.636866
C	-0.995377	3.655995	4.326248
C	-0.346926	2.582367	3.710356
C	-0.653173	2.219225	2.387748
C	-1.640179	2.958486	1.714084
C	-2.281873	4.037113	2.324984
H	-2.464816	5.223692	4.120674
H	-0.742567	3.914521	5.351646
H	0.393951	2.027876	4.273338
H	-1.912559	2.689190	0.702654
H	-3.036789	4.586108	1.768734
C	2.306184	-1.123667	5.159475
C	2.816694	0.024766	4.550639
C	2.182075	0.563955	3.431043
C	1.027833	-0.033399	2.897614
C	0.527537	-1.185718	3.517607
C	1.161021	-1.726920	4.638703
H	2.801477	-1.546127	6.030077
H	3.714734	0.496992	4.939838

H	2.589859	1.457504	2.967368
H	-0.355436	-1.659716	3.100663
H	0.758428	-2.624202	5.102631
C	1.833707	0.203711	-5.029442
C	2.308747	-1.020791	-4.551189
C	1.841753	-1.522885	-3.337290
C	0.874428	-0.822597	-2.595139
C	0.411755	0.406274	-3.078239
C	0.894541	0.918288	-4.286634
H	2.205985	0.602674	-5.969585
H	3.050923	-1.577826	-5.117592
H	2.230213	-2.467555	-2.965282
H	-0.308594	0.964911	-2.487284
H	0.544140	1.884690	-4.638433
C	-1.542043	-5.671585	-2.100735
C	-1.176423	-4.782836	-3.110124
C	-0.590370	-3.551947	-2.793968
C	-0.362211	-3.178788	-1.460078
C	-0.763991	-4.077882	-0.450167
C	-1.332605	-5.312517	-0.765809
H	-1.990469	-6.630281	-2.347553
H	-1.341485	-5.043124	-4.152680
H	-0.310859	-2.883030	-3.599934
H	-1.618138	-5.992118	0.033473
C	5.193854	1.136343	-2.706863
C	4.351983	0.545371	-1.790976
H	5.954918	0.537898	-3.200715
H	4.454557	-0.511715	-1.578404
C	5.075090	2.511912	-3.014888
C	4.098018	3.262649	-2.403835
H	5.749193	2.967669	-3.735339
H	3.984788	4.319376	-2.635454
C	5.951046	-0.256977	2.144340
C	4.807831	0.030720	1.432348
H	6.606193	0.551621	2.457949
H	4.576013	1.061972	1.195960
C	6.280948	-1.593404	2.472411
C	5.448081	-2.613846	2.078135
H	7.186689	-1.807577	3.033477
H	5.683114	-3.647158	2.323049
H	-0.642814	-3.792971	0.590911
C	-5.574210	-0.349503	1.970259
H	-5.437165	0.017453	2.996164
H	-5.930494	0.500196	1.371464

C	-5.431002	-2.503042	-0.060991
H	-5.558111	-2.851069	-1.094877
H	-5.047486	-3.359031	0.516096
C	-6.780561	-2.053137	0.523850
H	-7.216047	-1.282950	-0.128309
H	-7.485101	-2.894014	0.530303
C	-6.614226	-1.482495	1.940817
H	-6.296122	-2.286562	2.620899
H	-7.577475	-1.117979	2.318182
H	-3.206559	1.717928	-1.707633
C	-4.102447	1.814465	-0.824359
C	-3.417430	0.784800	-2.906429
C	-2.484952	0.515158	-3.408246
C	-3.929216	-0.123055	-2.584210
H	-4.073772	1.290724	-3.628018
O	-2.430502	2.941322	-2.077238
H	-1.797526	3.340540	-3.227262
C	-2.399669	3.965984	-1.171552
O	-1.339260	4.678261	-3.008218
C	-1.685556	2.756358	-4.128944
H	-1.729978	5.002315	-1.744120
H	-0.801479	5.311334	-3.700603
H	-1.625870	5.886638	-1.133664

Pf8

Coordinates (Angstroms)			
	X	Y	Z

Ru		1.00396600	0.49551600 -0.93987900
H		2.40348100	0.00378400 2.25453100
H		0.40286200	0.87842100 -2.34802600
N		2.60419200	1.77349800 -0.66260800
H		2.40976200	2.76942100 -0.55580700
H		3.37676100	1.44227500 0.94607800
N		2.64994900	-0.57193700 -1.99651600
H		2.71825100	-1.57122800 -1.80354100
H		2.40317300	-0.49678300 -2.98412000
P		-0.63597200	1.82200100 0.01291400
P		-0.39349600	-1.37325700 -1.05123100
C		3.95407100	0.09975400 -1.74133100
H		4.27343700	-0.23865300 -0.74923100

C	3.67815600	1.60128100	-1.64474500
H	3.35926800	1.94378400	-2.65017000
C	-5.04233300	-0.68622300	-1.39854900
C	-4.30582700	-1.33191300	-2.41962400
C	-2.96000400	-1.55687100	-2.27639200
C	-2.25118500	-1.16363700	-1.10543700
C	-2.94568100	-0.54331000	-0.06159600
C	-4.36057100	-0.28981500	-0.20271100
H	-4.82108200	-1.65070800	-3.32294500
H	-2.42662900	-2.05604800	-3.07563800
C	-2.23104600	-0.62486700	3.71148500
C	-1.41489700	0.52170700	3.85356700
C	-1.04701000	1.25984500	2.75717600
C	-1.46867200	0.92165700	1.43863700
C	-2.31495300	-0.18138600	1.25992300
C	-2.69183200	-0.98095500	2.40250000
H	-1.08143600	0.81493900	4.84648200
H	-0.42486900	2.13346600	2.90417700
C	0.95004800	5.81379800	1.92145100
C	-0.22326500	5.83382700	1.16705300
C	-0.72469500	4.65784900	0.60327400
C	-0.06372500	3.43129100	0.78354700
C	1.12712300	3.43230000	1.53254900
C	1.62562200	4.60588900	2.10038300
H	1.33846000	6.73112500	2.35647300
H	-0.75572300	6.76875500	1.01066200
H	-1.63440300	4.70851800	0.01751400
H	1.69322400	2.51869500	1.66440700
H	2.55187800	4.56506900	2.66710700
C	-4.08183900	3.56860400	-2.60925700
C	-4.26664200	3.41109800	-1.23415900
C	-3.25315700	2.85719400	-0.45137300
C	-2.04192000	2.44277500	-1.02781800
C	-1.86794400	2.60932200	-2.40896400
C	-2.87934700	3.16824500	-3.19345500
H	-4.87089800	3.99940800	-3.22025500
H	-5.20167600	3.71176900	-0.76937300
H	-3.40661500	2.74767700	0.61792400
H	-0.93442300	2.29684900	-2.86525100
H	-2.72539000	3.28929500	-4.26280300
C	0.33205900	-4.68255500	2.16057800
C	-0.84471200	-4.71380300	1.40773800
C	-1.09591900	-3.72305300	0.45751200
C	-0.17482800	-2.68501700	0.24702600

C	1.00108300	-2.66514700	1.00946800
C	1.25660200	-3.65634200	1.95984100
H	0.52415100	-5.45353800	2.90231000
H	-1.57028900	-5.50792800	1.56428300
H	-2.01210700	-3.75720900	-0.12548900
H	1.72307900	-1.86794200	0.85538500
H	2.17447800	-3.62107000	2.54063800
C	0.67028700	-3.68339800	-5.00064400
C	0.65421400	-4.37374400	-3.78977500
C	0.30221700	-3.71827800	-2.60482000
C	-0.03245100	-2.35516200	-2.60555200
C	0.00042400	-1.66924700	-3.83609600
C	0.33698700	-2.32583500	-5.01995800
H	0.94129200	-4.19445100	-5.92073800
H	0.91344400	-5.42914000	-3.76012000
H	0.29006400	-4.28024900	-1.67757100
H	0.34357200	-1.77527300	-5.95744500
C	-3.87006300	-2.87815400	3.39879800
C	-3.52103300	-2.13561700	2.29290000
H	-4.50199500	-3.75436200	3.27965800
H	-3.88115100	-2.43624900	1.31684800
C	-3.41391200	-2.51383400	4.68773000
C	-2.60857800	-1.40926700	4.83488300
H	-3.69839400	-3.10690200	5.55274000
H	-2.24536700	-1.11453400	5.81673500
C	-6.47961700	0.59044100	0.64404400
C	-5.13215400	0.35682300	0.80733300
H	-7.03813500	1.08611500	1.43375800
H	-4.64687700	0.67313600	1.72272400
C	-7.14410300	0.18996200	-0.53950300
C	-6.43421800	-0.43463900	-1.53770600
H	-8.20831900	0.37700900	-0.65502300
H	-6.92683100	-0.74743400	-2.45548800
H	-0.23856700	-0.61000300	-3.85777900
C	4.98125300	2.34885900	-1.30071100
H	4.78305700	3.42856000	-1.26654000
H	5.30352700	2.05441900	-0.29329700
C	5.04108700	-0.23165100	-2.77071900
H	5.22726700	-1.31463600	-2.79437300
H	4.68868300	0.05185100	-3.77467800
C	6.33930900	0.53051100	-2.44844100
H	6.74875900	0.15304700	-1.50057700
H	7.09365500	0.32794400	-3.21929500
C	6.08856800	2.04229100	-2.32379100

H	5.79965900	2.44230200	-3.30730100
H	7.01751300	2.55349700	-2.04102200
C	3.38177400	0.35036900	2.62923500
O	3.83758600	1.43941300	1.84118000
C	3.20522100	0.83315500	4.07086800
H	2.86208100	0.02681000	4.72824400
H	4.15290400	1.22586400	4.45521900
H	2.47128300	1.64364600	4.09515700
C	4.33189200	-0.81685200	2.56622800
C	5.22869700	-1.36787800	3.43510500
O	4.36258800	-1.51889800	1.38410400
C	5.85433100	-2.46639400	2.75510300
H	5.42520600	-1.03426400	4.44393300
C	5.29344400	-2.51087600	1.51782100
H	6.61767400	-3.12809700	3.14092400
H	5.42838900	-3.14842400	0.65722800

Pu8

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.14790100	0.91085100	0.30714100
H	4.27081800	-0.99007500	-1.39567200
H	0.56973000	2.19682900	1.01664800
N	2.90694200	0.52476600	1.34081100
H	2.81585800	0.21079000	2.30787600
H	3.86354600	-0.92163400	0.73034300
N	2.61843700	2.24679000	-0.71737800
H	2.61234300	2.20665000	-1.73660100
H	2.29832700	3.18612700	-0.47994400
P	-0.23754400	-0.35305000	1.66239600
P	-0.53489900	1.30183000	-1.26148900
C	3.99189300	2.03090700	-0.18394900
H	4.38493300	1.15229700	-0.71165300
C	3.84807000	1.64622000	1.29067100
H	3.44382100	2.53506500	1.81609000
C	-4.87277500	1.83500400	0.50665500
C	-4.18901400	2.90450000	-0.11784900
C	-2.94889200	2.71366100	-0.67328800
C	-2.29890300	1.44730800	-0.64917000
C	-2.95510100	0.35514500	-0.07156700
C	-4.25746200	0.54150800	0.52392200

H	-4.66206700	3.88317000	-0.15833500
H	-2.46050600	3.55182500	-1.15337900
C	-2.72688400	-3.36613400	-0.98375100
C	-1.69870900	-3.79301600	-0.11016600
C	-1.04056200	-2.89356500	0.69096300
C	-1.37059500	-1.50754800	0.70436200
C	-2.41467300	-1.05210800	-0.11174800
C	-3.08887800	-1.98020300	-0.98985300
H	-1.43594200	-4.84830100	-0.07566200
H	-0.25494300	-3.25531100	1.34165800
C	2.20162200	-3.18825900	4.48793800
C	1.10963100	-2.48962100	5.00507600
C	0.34942900	-1.65424400	4.18264600
C	0.66580100	-1.50573500	2.82234300
C	1.77219900	-2.21217700	2.31797800
C	2.53202800	-3.04574600	3.13923200
H	2.79550700	-3.83055600	5.13336100
H	0.84687000	-2.58731400	6.05559300
H	-0.48653700	-1.11506900	4.61263400
H	2.05971500	-2.10556600	1.27918800
H	3.39286800	-3.55499700	2.71619800
C	-2.96956000	1.76609800	4.79960500
C	-3.29300600	0.48418200	4.35077100
C	-2.49938000	-0.14096300	3.38826500
C	-1.37461200	0.50545100	2.85178500
C	-1.05810300	1.79105200	3.31390800
C	-1.84917500	2.41625500	4.28015400
H	-3.58788000	2.25452000	5.54837100
H	-4.16702500	-0.02854400	4.74314700
H	-2.75734700	-1.14095900	3.05300800
H	-0.18926000	2.29893700	2.90855000
H	-1.58849800	3.41366700	4.62518500
C	-0.85533900	-1.54681200	-4.94339200
C	-1.82998500	-0.56223500	-4.75766700
C	-1.76469700	0.28698200	-3.65294600
C	-0.72005900	0.16899200	-2.72135100
C	0.24735400	-0.82534400	-2.91511200
C	0.18144300	-1.67997000	-4.01896900
H	-0.91018800	-2.21100000	-5.80210500
H	-2.64469600	-0.46060400	-5.47010800
H	-2.52883400	1.04773700	-3.51491100
H	1.04614500	-0.94298200	-2.18778000
H	0.93561200	-2.45195400	-4.14635100
C	0.50200300	5.43688000	-3.22901500

C	0.37159600	4.30786600	-4.03577700
C	0.01044500	3.07549700	-3.47930800
C	-0.22027300	2.94402900	-2.10122800
C	-0.06332900	4.09174900	-1.29672800
C	0.28014100	5.32383300	-1.85312700
H	0.77734600	6.39425500	-3.66332200
H	0.54664600	4.37935300	-5.10635300
H	-0.08945100	2.21441400	-4.13055800
H	0.37928200	6.19524900	-1.21055900
C	-4.76223600	-2.48597700	-2.69940500
C	-4.12491800	-1.57820100	-1.88333000
H	-5.54626700	-2.14615800	-3.37098700
H	-4.41233000	-0.53473400	-1.92435800
C	-4.40651500	-3.85528300	-2.67440600
C	-3.40557100	-4.28104000	-1.83332000
H	-4.92087000	-4.56215700	-3.31991900
H	-3.11430100	-5.32853100	-1.80330900
C	-6.22088000	-0.31141400	1.70690800
C	-4.98116300	-0.51911400	1.14407800
H	-6.74531400	-1.14197300	2.17214000
H	-4.54583800	-1.51049600	1.17346700
C	-6.81921000	0.97076200	1.68414100
C	-6.15344500	2.01942300	1.09478400
H	-7.79883300	1.12130900	2.12974800
H	-6.59694400	3.01211400	1.06743500
H	-0.21126600	4.01217100	-0.22326400
C	5.23142600	1.35169200	1.90238900
H	5.11267600	1.13077700	2.97170900
H	5.63689700	0.44294500	1.44007800
C	4.94171900	3.21574200	-0.39691400
H	5.04295600	3.43618300	-1.46869600
H	4.50848600	4.11295900	0.07159500
C	6.31902700	2.92709100	0.22772600
H	6.79884800	2.10638400	-0.32535800
H	6.97116800	3.80226500	0.11414100
C	6.19535100	2.53442500	1.70874300
H	5.83216300	3.40117700	2.28103200
H	7.18465600	2.28740000	2.11438000
C	4.64225200	-1.87653600	-0.85302500
O	4.50339100	-1.67440700	0.54434000
C	6.12486500	-2.06503700	-1.18059600
H	6.28589400	-2.22957700	-2.25196700
H	6.68165300	-1.17569600	-0.87118800
H	6.52536800	-2.92087900	-0.62679600

C	3.82881300	-3.05447900	-1.31500400
C	4.12124100	-4.29584800	-1.80115500
O	2.46672000	-2.91039400	-1.23378400
C	2.86896800	-4.95987600	-2.03036700
H	5.10974300	-4.69609200	-1.97651300
C	1.90087300	-4.07633200	-1.66724900
H	2.71762300	-5.96066100	-2.41125900
H	0.82238000	-4.10300700	-1.64883300

ABS₉

Coordinates (Angstroms)			
	X	Y	Z
Ru	-0.566213	0.847579	-0.600848
H	-1.394267	0.045750	0.683471
H	0.035880	1.732123	-1.937587
N	-2.364305	0.465598	-1.857497
H	-2.115462	0.015572	-2.735976
H	-2.991286	-0.168520	-1.359162
N	-1.838197	2.637358	-0.194180
H	-1.910389	2.824786	0.803566
H	-1.356571	3.435553	-0.606595
P	0.525658	-1.069812	-1.178545
P	1.167369	1.583647	0.688409
C	-3.189733	2.486953	-0.784066
H	-3.754399	1.837055	-0.102957
C	-3.061258	1.743769	-2.121457
H	-2.394644	2.325728	-2.771676
C	5.424000	0.576338	-1.078303
C	4.928517	1.901140	-1.039186
C	3.705834	2.175636	-0.480108
C	2.891553	1.156232	0.088480
C	3.356555	-0.163737	0.096610
C	4.632456	-0.471320	-0.505742
H	5.531978	2.704009	-1.457128
H	3.359447	3.201229	-0.464207
C	2.602481	-2.990380	2.590948
C	1.454510	-3.566059	1.995764
C	0.903843	-3.020446	0.863762
C	1.463095	-1.874891	0.230957
C	2.619615	-1.296068	0.765835
C	3.192903	-1.839956	1.974168

H	1.012088	-4.451232	2.447896
H	0.023932	-3.484491	0.435453
C	-2.662364	-4.238283	-2.557960
C	-1.529156	-4.027251	-3.342153
C	-0.547062	-3.116609	-2.939000
C	-0.679314	-2.393468	-1.742548
C	-1.840511	-2.603131	-0.972869
C	-2.814502	-3.519819	-1.369435
H	-3.423728	-4.947679	-2.872429
H	-1.401867	-4.571630	-4.274723
H	0.322049	-2.972598	-3.569776
H	-1.974049	-2.017731	-0.067524
H	-3.701134	-3.660795	-0.756543
C	3.551764	-1.255571	-4.737633
C	3.470681	-2.325518	-3.842699
C	2.590834	-2.266833	-2.761771
C	1.774394	-1.141113	-2.560197
C	1.867447	-0.072877	-3.460654
C	2.750864	-0.129874	-4.541942
H	4.241109	-1.299003	-5.577252
H	4.099275	-3.201565	-3.980641
H	2.538581	-3.103617	-2.070042
H	1.248587	0.803831	-3.284928
H	2.815155	0.710388	-5.229297
C	1.454072	0.694992	5.270569
C	2.525676	1.311165	4.618597
C	2.460855	1.556491	3.247000
C	1.321763	1.197406	2.506658
C	0.256927	0.575093	3.168500
C	0.323349	0.324542	4.541953
H	1.506795	0.498404	6.338560
H	3.414637	1.593600	5.177061
H	3.301031	2.034036	2.749160
H	-0.608336	0.278298	2.579806
H	-0.508442	-0.166675	5.041737
C	0.924548	6.282626	0.682931
C	0.974296	5.601600	1.897988
C	1.093575	4.207499	1.925985
C	1.157018	3.462148	0.738196
C	1.082294	4.164374	-0.482446
C	0.979990	5.555870	-0.510090
H	0.838221	7.366052	0.662818
H	0.923809	6.152004	2.834363
H	1.135730	3.705830	2.885835

H	0.938285	6.072349	-1.466268
C	4.880605	-1.828499	3.743239
C	4.344593	-1.279454	2.599515
H	5.759215	-1.375846	4.195553
H	4.805746	-0.400222	2.166369
C	4.297926	-2.972953	4.336773
C	3.178946	-3.536277	3.769520
H	4.732320	-3.398941	5.237375
H	2.713558	-4.412741	4.215007
C	6.383505	-2.058647	-1.133154
C	5.157739	-1.795258	-0.563185
H	6.755024	-3.079779	-1.160125
H	4.577719	-2.611742	-0.150909
C	7.162280	-1.014773	-1.686113
C	6.685134	0.274572	-1.659939
H	8.129158	-1.234973	-2.130940
H	7.266689	1.089490	-2.085174
H	1.081781	3.596407	-1.408896
C	-4.430296	1.574508	-2.804007
H	-4.293189	1.088620	-3.779271
H	-5.047659	0.899555	-2.196168
C	-3.929787	3.824346	-0.946035
H	-4.045999	4.303584	0.035227
H	-3.308237	4.499499	-1.554306
C	-5.296198	3.644457	-1.626201
H	-5.955450	3.058667	-0.969378
H	-5.777341	4.620704	-1.763244
C	-5.150654	2.922068	-2.973441
H	-4.581279	3.558520	-3.666653
H	-6.135426	2.765806	-3.430811
C	-5.229903	-0.983257	0.987941
O	-4.941974	-0.740130	-0.178179
C	-4.212731	-0.843987	2.097829
H	-4.075648	-1.800296	2.618107
H	-3.255873	-0.514074	1.679480
H	-4.557705	-0.119451	2.846674
C	-8.854780	-1.994008	0.613025
C	-7.562955	-1.582363	0.294370
C	-6.627618	-1.430177	1.325891
C	-7.047937	-1.703885	2.632865
C	-8.367635	-2.109595	2.842986
H	-9.600144	-2.120817	-0.170019
H	-7.269151	-1.380266	-0.729875
H	-6.374177	-1.607012	3.477772

H	-8.718814	-2.327205	3.850159
N	-9.265448	-2.256308	1.862342

INTf₉

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.857504	0.464983	0.743006
H	-1.511367	-0.000008	-0.787866
H	-0.451561	0.981638	2.322776
N	-2.367762	2.096444	0.793389
H	-1.926476	2.985145	1.021039
H	-2.783255	2.203919	-0.132314
N	-2.615129	-0.535656	1.682118
H	-2.795545	-1.441235	1.254122
H	-2.368310	-0.716531	2.654588
P	0.782898	1.702816	-0.257000
P	0.498709	-1.358396	0.962814
C	-3.827029	0.313002	1.601024
H	-4.210300	0.205583	0.578292
C	-3.418462	1.781184	1.786175
H	-2.944094	1.882228	2.771355
C	5.000319	-0.334869	1.935919
C	4.147876	-0.933413	2.893557
C	2.853998	-1.258890	2.573054
C	2.316472	-1.022536	1.276537
C	3.133799	-0.456009	0.291224
C	4.492032	-0.091011	0.619290
H	4.532312	-1.135595	3.890940
H	2.230365	-1.717584	3.330042
C	2.977993	-0.877626	-3.529210
C	2.080407	0.162448	-3.871228
C	1.501395	0.936171	-2.897674
C	1.785746	0.744773	-1.516068
C	2.688975	-0.253644	-1.135442
C	3.284540	-1.095375	-2.146638
H	1.855758	0.342593	-4.920439
H	0.815426	1.721692	-3.191076
C	-1.225890	5.219378	-2.645174
C	-0.066982	5.473870	-1.911913
C	0.573906	4.444037	-1.215807

C	0.070141	3.133641	-1.242930
C	-1.104904	2.896737	-1.981195
C	-1.746331	3.923245	-2.675184
H	-1.725153	6.024516	-3.178482
H	0.342930	6.480214	-1.872227
H	1.465150	4.674509	-0.644019
H	-1.518598	1.892757	-1.980859
H	-2.665720	3.707627	-3.212892
C	3.994243	4.040191	2.208364
C	4.187370	3.840311	0.839305
C	3.249824	3.118845	0.099629
C	2.103292	2.588304	0.714068
C	1.923149	2.790406	2.088307
C	2.862103	3.511893	2.829930
H	4.726919	4.598175	2.786169
H	5.072674	4.236752	0.348882
H	3.412983	2.965600	-0.963829
H	1.047506	2.354340	2.562790
H	2.709946	3.655162	3.897163
C	0.684998	-4.760558	-2.244277
C	1.586337	-4.767400	-1.176422
C	1.554049	-3.744718	-0.228202
C	0.615750	-2.703474	-0.326287
C	-0.279013	-2.704397	-1.402621
C	-0.243768	-3.725479	-2.356227
H	0.714587	-5.553430	-2.987492
H	2.319810	-5.564791	-1.087119
H	2.262948	-3.758270	0.595750
H	-0.981672	-1.877474	-1.481179
H	-0.937572	-3.707950	-3.194049
C	-1.041604	-3.725956	4.726964
C	-0.887187	-4.394957	3.514082
C	-0.389539	-3.723589	2.391626
C	-0.042038	-2.364989	2.455145
C	-0.225589	-1.697090	3.683589
C	-0.706863	-2.370960	4.806888
H	-1.423296	-4.250226	5.599344
H	-1.151614	-5.446527	3.433374
H	-0.276434	-4.272015	1.463681
H	-0.825260	-1.833855	5.745058
C	4.752781	-2.930802	-2.819968
C	4.184902	-2.154862	-1.833870
H	5.435482	-3.731328	-2.547113
H	4.424592	-2.353983	-0.796587

C	4.454604	-2.698428	-4.183229
C	3.580632	-1.692980	-4.524813
H	4.911888	-3.315050	-4.952558
H	3.334516	-1.503136	-5.567258
C	6.668700	0.845691	0.015266
C	5.374132	0.517335	-0.320966
H	7.315388	1.308013	-0.726042
H	5.015379	0.728159	-1.320922
C	7.164287	0.590019	1.315638
C	6.340755	0.014229	2.254227
H	8.188445	0.851699	1.568190
H	6.701778	-0.184983	3.260731
H	-0.006542	-0.634005	3.735939
C	-4.641069	2.709364	1.696794
H	-4.326350	3.748009	1.863177
H	-5.043957	2.660223	0.674355
C	-4.923552	-0.092759	2.599710
H	-5.223688	-1.132394	2.414836
H	-4.503785	-0.061101	3.616987
C	-6.142514	0.840858	2.522762
H	-6.630741	0.715949	1.545763
H	-6.881533	0.553044	3.280538
C	-5.732498	2.309875	2.703033
H	-5.357807	2.460381	3.726004
H	-6.604385	2.965971	2.590900
C	-4.318658	0.476027	-2.620424
O	-4.449023	1.605204	-2.165535
C	-5.261491	-0.615233	-2.185149
H	-6.462372	-0.267319	-1.553208
H	-4.990988	-1.976382	-2.367332
H	-7.326868	-1.281036	-1.145455
C	-6.705012	0.778830	-1.399701
C	-5.917945	-2.912984	-1.903474
C	-4.074842	-2.312921	-2.841295
C	-7.070473	-2.587280	-1.306979
C	-8.272824	-1.036828	-0.665017
H	-5.723902	-3.977687	-2.021092
H	-3.219732	0.137227	-3.601101
H	-2.388000	-0.313474	-3.042089
H	-3.549980	-0.564233	-4.373477
N	-2.855140	1.056143	-4.064373

TSf₉

	Coordinates (Angstroms)		
	X	Y	Z

Ru	-1.142956	0.505190	0.342394
H	-1.772136	-0.084102	-1.266673
H	-0.846505	1.047680	1.882193
N	-2.593342	2.140409	0.124301
H	-2.165912	3.064952	0.141063
H	-3.029392	2.019784	-0.802580
N	-3.011382	-0.361022	1.210431
H	-3.264889	-1.235833	0.752208
H	-2.803737	-0.589111	2.182039
P	0.675794	1.727230	-0.388063
P	0.177146	-1.311042	0.867130
C	-4.153943	0.588008	1.134141
H	-4.602686	0.443685	0.146585
C	-3.627705	2.026995	1.176609
H	-3.120358	2.192302	2.135412
C	4.450671	-0.273891	2.593219
C	3.440954	-0.843932	3.403523
C	2.216705	-1.166528	2.874414
C	1.906746	-0.948378	1.502769
C	2.889984	-0.421017	0.657652
C	4.179555	-0.065486	1.202523
H	3.648074	-1.029481	4.455168
H	1.475632	-1.614570	3.523233
C	3.404193	-0.966720	-3.113720
C	2.597403	0.069630	-3.643044
C	1.861686	0.877473	-2.813573
C	1.895291	0.730580	-1.397338
C	2.703569	-0.261003	-0.830188
C	3.452649	-1.144707	-1.692711
H	2.566187	0.217430	-4.720332
H	1.246507	1.656590	-3.247659
C	-0.600972	5.204948	-3.279706
C	0.482802	5.402157	-2.422247
C	0.894400	4.388100	-1.553905
C	0.230844	3.149489	-1.527106
C	-0.866061	2.972531	-2.387427
C	-1.277266	3.984503	-3.256937
H	-0.919504	5.998422	-3.951096
H	1.012423	6.351728	-2.422505

H	1.732523	4.575672	-0.893609
H	-1.419797	2.042379	-2.365706
H	-2.135190	3.810382	-3.900754
C	3.321658	4.155998	2.610415
C	3.830574	3.810181	1.357152
C	3.059874	3.053027	0.473942
C	1.768930	2.625322	0.825462
C	1.272856	2.974821	2.088570
C	2.041685	3.734693	2.973144
H	3.921915	4.743410	3.300590
H	4.831611	4.119656	1.068843
H	3.469665	2.791079	-0.497069
H	0.286391	2.623932	2.375483
H	1.639672	3.992149	3.950136
C	1.167112	-4.758428	-2.132482
C	1.595452	-4.854552	-0.805285
C	1.314883	-3.828444	0.096654
C	0.582093	-2.699404	-0.308287
C	0.173138	-2.607467	-1.642417
C	0.463803	-3.629148	-2.551236
H	1.392626	-5.555042	-2.836627
H	2.156069	-5.725604	-0.475349
H	1.663507	-3.909270	1.123104
H	-0.357645	-1.713947	-1.955853
H	0.146732	-3.537728	-3.587143
C	-2.144817	-3.467865	4.334407
C	-1.890435	-4.149918	3.146025
C	-1.148302	-3.545458	2.125392
C	-0.647648	-2.241699	2.266740
C	-0.939257	-1.555193	3.463992
C	-1.665022	-2.163916	4.488794
H	-2.716439	-3.940595	5.128585
H	-2.267116	-5.159878	3.005279
H	-0.964052	-4.102502	1.213921
H	-1.861323	-1.614794	5.406482
C	4.969278	-3.030231	-2.037721
C	4.252995	-2.212458	-1.192088
H	5.567187	-3.838137	-1.624190
H	4.290453	-2.388655	-0.124110
C	4.931702	-2.832720	-3.437965
C	4.159448	-1.821790	-3.960585
H	5.506073	-3.481571	-4.093837
H	4.110247	-1.660540	-5.035119
C	6.441731	0.831342	0.957221

C	5.221567	0.500535	0.410800
H	7.214317	1.261154	0.324987
H	5.048899	0.675871	-0.644022
C	6.699799	0.617567	2.331985
C	5.719313	0.076437	3.129610
H	7.667280	0.881042	2.750936
H	5.897531	-0.093870	4.188924
H	-0.609293	-0.526726	3.576752
C	-4.784577	3.030192	1.030943
H	-4.394321	4.055190	1.085818
H	-5.232985	2.914154	0.033731
C	-5.224059	0.343660	2.206820
H	-5.606414	-0.681378	2.119603
H	-4.760212	0.428192	3.201841
C	-6.374575	1.358171	2.089597
H	-6.914773	1.181682	1.148467
H	-7.097760	1.199307	2.898915
C	-5.854453	2.803665	2.112081
H	-5.423107	3.019963	3.100543
H	-6.683646	3.508107	1.973219
C	-3.145606	0.032140	-2.534386
O	-3.592818	1.197337	-2.450493
C	-2.228606	-0.340439	-3.697032
H	-1.759904	-1.318582	-3.576423
H	-2.850212	-0.372222	-4.604142
H	-1.456449	0.416818	-3.839656
C	-4.012315	-1.104672	-2.007634
C	-5.395268	-0.891640	-1.935997
C	-3.547026	-2.379974	-1.660410
C	-6.228478	-1.932107	-1.522125
C	-5.798597	0.078566	-2.207183
H	-4.464497	-3.348123	-1.250354
H	-2.488335	-2.613716	-1.681978
H	-5.788826	-3.148162	-1.174413
H	-7.306099	-1.780659	-1.467832
N	-4.116086	-4.340363	-0.966364

TSu₉

Coordinates (Angstroms)

X	Y	Z
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Ru	-1.318733	-0.657799	0.199127
H	-1.950718	0.694612	-0.928090
H	-1.063090	-1.926652	1.218692
N	-3.138058	-0.223575	1.333646
H	-2.961754	0.072331	2.292364
H	-3.603995	0.553221	0.839715
N	-2.831985	-2.019876	-0.739288
H	-2.877058	-1.923738	-1.752284
H	-2.489254	-2.962878	-0.557988
P	0.082869	0.604772	1.518912
P	0.447492	-1.489791	-1.048964
C	-4.187344	-1.837415	-0.151171
H	-4.641746	-0.994938	-0.683182
C	-4.037829	-1.399933	1.312097
H	-3.528426	-2.196325	1.870328
C	4.555969	-2.002084	1.216919
C	3.817343	-3.117161	0.756335
C	2.638639	-2.943388	0.075807
C	2.111234	-1.650395	-0.199740
C	2.826663	-0.519222	0.208373
C	4.062676	-0.686736	0.937228
H	4.196999	-4.118683	0.946231
H	2.104849	-3.819722	-0.268744
C	2.962816	3.010216	-1.308527
C	1.916945	3.643370	-0.594969
C	1.136769	2.932548	0.282219
C	1.358786	1.549472	0.532225
C	2.414124	0.895452	-0.114890
C	3.215197	1.619294	-1.072010
H	1.731669	4.703166	-0.753900
H	0.336150	3.443741	0.802359
C	-2.348673	3.821049	3.925339
C	-1.402083	3.044866	4.593567
C	-0.643080	2.099557	3.898158
C	-0.819627	1.907367	2.517459
C	-1.796393	2.679563	1.864347
C	-2.542820	3.634705	2.555305
H	-2.933984	4.559774	4.466837
H	-1.247006	3.172231	5.662069
H	0.085441	1.512031	4.443183
H	-1.971412	2.523328	0.806352
H	-3.277305	4.227478	2.017952
C	2.518288	-1.270481	5.043918
C	2.866644	-0.014680	4.541466

C	2.162972	0.527639	3.466080
C	1.100188	-0.173603	2.871492
C	0.761257	-1.431763	3.385129
C	1.464860	-1.976531	4.462194
H	3.067875	-1.695475	5.879972
H	3.691903	0.540019	4.979858
H	2.443266	1.506112	3.086197
H	-0.052177	-1.981796	2.922273
H	1.189050	-2.956551	4.844100
C	1.728182	0.267504	-5.182099
C	2.460852	-0.786894	-4.628867
C	2.105168	-1.310451	-3.386021
C	1.003781	-0.793485	-2.683092
C	0.284446	0.265624	-3.242166
C	0.641814	0.796292	-4.484751
H	2.009316	0.677491	-6.148662
H	3.313060	-1.197434	-5.164607
H	2.682665	-2.128788	-2.963711
H	-0.548441	0.663970	-2.671245
H	0.074980	1.623102	-4.906433
C	-0.883222	-5.841916	-2.223665
C	-0.584468	-4.917511	-3.222952
C	-0.132910	-3.635182	-2.891371
C	0.022974	-3.245276	-1.551834
C	-0.304566	-4.185547	-0.553160
C	-0.739270	-5.469618	-0.883755
H	-1.228495	-6.839433	-2.482237
H	-0.697916	-5.189225	-4.269451
H	0.097505	-2.939337	-3.689880
H	-0.970699	-6.178328	-0.092318
C	5.025434	1.725621	-2.710429
C	4.269911	1.007880	-1.810296
H	5.819090	1.228654	-3.262134
H	4.473487	-0.046038	-1.665193
C	4.777832	3.101943	-2.926846
C	3.763918	3.726233	-2.238833
H	5.384845	3.657898	-3.636399
H	3.555130	4.781986	-2.396071
C	6.003873	0.226651	2.110808
C	4.830630	0.415643	1.414729
H	6.565021	1.089004	2.461166
H	4.481496	1.423989	1.229244
C	6.485640	-1.077273	2.375190
C	5.770614	-2.166443	1.936089

H	7.414035	-1.212912	2.923517
H	6.122468	-3.176621	2.132645
H	-0.230711	-3.894556	0.490267
C	-5.416826	-1.138399	1.939895
H	-5.294470	-0.845865	2.991392
H	-5.886019	-0.289708	1.423255
C	-5.082930	-3.078333	-0.275067
H	-5.199502	-3.348441	-1.333099
H	-4.588592	-3.931003	0.216405
C	-6.458637	-2.840839	0.372319
H	-6.998113	-2.073578	-0.200756
H	-7.061211	-3.755846	0.316887
C	-6.319679	-2.378242	1.830614
H	-5.892422	-3.194077	2.432299
H	-7.307518	-2.162114	2.255598
C	-3.454469	1.545820	-1.535316
O	-4.364177	1.290279	-0.709183
C	-3.473836	0.838600	-2.890453
H	-2.538743	0.921666	-3.445187
H	-3.725696	-0.216228	-2.762830
H	-4.270769	1.300108	-3.491541
C	-2.913015	2.969098	-1.565611
C	-3.671194	3.965084	-0.936117
C	-1.771644	3.386008	-2.259991
C	-3.261386	5.295433	-1.023288
C	-4.570702	3.683401	-0.399422
H	-1.447289	4.741945	-2.283365
H	-1.120922	2.674743	-2.753783
H	-2.167958	5.699353	-1.682875
H	-3.845657	6.080231	-0.543488
N	-0.557042	5.076836	-2.814146

Pf9

Coordinates (Angstroms)				
	X	Y	Z	

Ru		0.86801200	0.46541900	-0.83359200
H		0.25125700	0.80756500	-2.24521200
N		2.44446400	1.79122800	-0.59124100
H		2.21073200	2.77938000	-0.48660800
N		2.52750600	-0.56380000	-1.91117200

H	2.63945100	-1.55833000	-1.71383900
H	2.24652900	-0.51181500	-2.89112000
P	-0.79159700	1.79054000	0.09280100
P	-0.52628800	-1.40616100	-0.94937100
C	3.81314600	0.16087800	-1.71639100
H	4.19348500	-0.15704400	-0.73815100
C	3.48113500	1.65208900	-1.61887700
H	3.10307900	1.96769400	-2.61184000
C	-5.12611600	-0.64525500	-1.64007900
C	-4.33229600	-1.30912300	-2.60505400
C	-3.00356500	-1.55748700	-2.36828300
C	-2.37068800	-1.16778700	-1.15413200
C	-3.12593500	-0.53501400	-0.16131800
C	-4.52253100	-0.25818600	-0.39997200
H	-4.79001000	-1.62548500	-3.53969700
H	-2.42827100	-2.07601700	-3.12484100
C	-2.67331500	-0.66477100	3.64967500
C	-1.83853500	0.45808600	3.85895500
C	-1.37717900	1.19569500	2.79823000
C	-1.72176500	0.88377600	1.45113700
C	-2.58093500	-0.19553100	1.20341700
C	-3.05008600	-0.99906200	2.30849000
H	-1.56576700	0.73341900	4.87530000
H	-0.74070700	2.04864800	2.99619200
C	0.82411200	5.67253400	2.18380900
C	-0.31379800	5.75202500	1.38035100
C	-0.82535900	4.60917800	0.76054000
C	-0.20880100	3.35856200	0.93255700
C	0.94643900	3.29864100	1.73260600
C	1.45420800	4.43928600	2.35631500
H	1.22066200	6.56438000	2.66234600
H	-0.80990900	6.70760700	1.22948200
H	-1.70681700	4.70428100	0.13804400
H	1.47866500	2.36424700	1.86461100
H	2.35316300	4.35250400	2.96032800
C	-4.05753000	3.69628300	-2.64481800
C	-4.31398800	3.50538900	-1.28565200
C	-3.35399000	2.90479500	-0.47055800
C	-2.12570500	2.47689800	-0.99886500
C	-1.87864300	2.67895200	-2.36417800
C	-2.83673700	3.28380000	-3.18070400
H	-4.80509800	4.16285800	-3.28114200
H	-5.26368500	3.81633000	-0.85899800
H	-3.56181900	2.76984300	0.58647100

H	-0.93101200	2.35740700	-2.78320600
H	-2.62692700	3.43132200	-4.23712100
C	-0.25374500	-4.58153900	2.46634000
C	-1.20418600	-4.74633800	1.45507200
C	-1.31413700	-3.79984900	0.43603800
C	-0.46887200	-2.67846200	0.40628400
C	0.47442900	-2.52324900	1.42893900
C	0.58310800	-3.46508300	2.45486300
H	-0.17357800	-5.31611900	3.26326600
H	-1.86489700	-5.60937600	1.46446300
H	-2.06074500	-3.93421100	-0.34244600
H	1.11613800	-1.64612000	1.42222800
H	1.31352700	-3.32166200	3.24715800
C	0.91400900	-3.78716300	-4.72940100
C	0.92165300	-4.41166600	-3.48359700
C	0.44584900	-3.74106500	-2.35095000
C	-0.04027100	-2.42733800	-2.43935400
C	-0.02116100	-1.80308900	-3.70345600
C	0.43682200	-2.47705100	-4.83536300
H	1.27944300	-4.31045300	-5.60889600
H	1.29559500	-5.42760500	-3.38475600
H	0.45731800	-4.25313900	-1.39534300
H	0.42661100	-1.97608800	-5.80016900
C	-4.32871500	-2.88244000	3.20092000
C	-3.88874100	-2.13816200	2.12909200
H	-4.96432400	-3.74713200	3.02909400
H	-4.18025700	-2.42797300	1.12709900
C	-3.96085400	-2.53548400	4.52237500
C	-3.14631500	-1.44863200	4.73649700
H	-4.31879000	-3.12866500	5.35958500
H	-2.84789700	-1.16896200	5.74423900
C	-6.68134400	0.65214700	0.30037500
C	-5.35211400	0.39818400	0.55605500
H	-7.28606300	1.15471200	1.05069500
H	-4.92683600	0.70444000	1.50419400
C	-7.26815000	0.26348000	-0.92741300
C	-6.50082100	-0.37156900	-1.87524900
H	-8.31877000	0.46716000	-1.11594900
H	-6.93372400	-0.67667600	-2.82514100
H	-0.36564400	-0.77700700	-3.79499700
C	4.76483700	2.45878700	-1.34441500
H	4.52207700	3.52955500	-1.31646100
H	5.14119400	2.19498700	-0.34764600
C	4.86967100	-0.13741500	-2.78684500

H	5.09868000	-1.21161700	-2.80685500
H	4.46376500	0.12141400	-3.77722700
C	6.14785700	0.67948100	-2.52489000
H	6.60943300	0.32849100	-1.59142800
H	6.87777800	0.49761100	-3.32360400
C	5.84149500	2.18171300	-2.40789800
H	5.49700700	2.55749500	-3.38286100
H	6.75925000	2.73411800	-2.16941400
C	4.88326700	-2.00351500	1.81891600
C	6.07623800	-2.66393700	1.52177400
C	4.89546500	-0.61594100	2.00265600
H	3.95611900	-2.56784200	1.89949000
H	6.08075600	-3.74309500	1.37076700
C	6.12814400	0.03273900	1.87526900
C	7.26445300	-0.72062400	1.57910700
H	6.18424000	1.10947400	1.99610200
H	8.23286500	-0.23141600	1.47897100
C	3.62913000	0.15612200	2.36470400
H	2.77609200	-0.37086700	1.90378900
O	3.66929300	1.49273100	1.91831200
H	3.26267700	1.54453200	0.99390000
C	3.42238100	0.16155800	3.88608200
H	3.40811500	-0.85563500	4.29368800
H	4.23495200	0.71540200	4.36884600
H	2.47542300	0.65451600	4.12899900
N	7.25964600	-2.04921700	1.39917600

Pu9

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.84433000	1.19075500	-0.54391800
H	-2.68507300	-0.92822800	1.66229500
H	-0.07878000	2.07288000	-1.60576700
N	-2.75062500	0.88744000	-1.27587200
H	-2.86966900	0.28492500	-2.09013200
H	-3.70732500	0.15562600	0.06380400
N	-1.90536400	3.04197100	0.11151200
H	-1.75846400	3.31173400	1.08398000
H	-1.47379400	3.78016200	-0.44565500
P	0.13410900	-0.66380700	-1.51628000
P	1.01408000	1.63665300	0.79910400

C	-3.36071700	2.95462500	-0.19713100
H	-3.80854900	2.36763400	0.61320900
C	-3.50104000	2.13129600	-1.48116500
H	-3.06036300	2.72756000	-2.30498700
C	5.22955600	0.38203300	-0.89247900
C	4.89512600	1.73695900	-0.65923500
C	3.67876700	2.07568300	-0.12187600
C	2.70959000	1.09205400	0.22571700
C	3.01043500	-0.26121800	0.03733900
C	4.28355300	-0.63235100	-0.53434300
H	5.61760200	2.51072700	-0.90897800
H	3.45758800	3.12173900	0.04950000
C	1.78736100	-3.32343700	2.00651100
C	0.65437600	-3.69450500	1.24522400
C	0.25191300	-2.93877200	0.17295600
C	0.95020400	-1.76442800	-0.23130500
C	2.10383300	-1.38663600	0.47003800
C	2.52472000	-2.15848800	1.61604500
H	0.10450500	-4.59338000	1.51513600
H	-0.61727300	-3.25983200	-0.38618200
C	-2.93173900	-3.46019000	-3.71768300
C	-1.74925300	-3.09563800	-4.36101500
C	-0.81329600	-2.28272200	-3.71654100
C	-1.04158300	-1.81221200	-2.41277300
C	-2.25176600	-2.16922500	-1.78943700
C	-3.18087400	-2.99293300	-2.42615200
H	-3.65573800	-4.09728800	-4.21881800
H	-1.54661600	-3.44493300	-5.37037200
H	0.09630600	-2.01719200	-4.24124000
H	-2.47789500	-1.79598500	-0.79738100
H	-4.09808500	-3.25971200	-1.90904100
C	3.26163900	-0.16178100	-4.94398200
C	3.23753900	-1.33751100	-4.19088700
C	2.32710200	-1.47805500	-3.14319200
C	1.43250700	-0.44439800	-2.82364600
C	1.46354100	0.72926600	-3.58988500
C	2.37118200	0.86948100	-4.64215900
H	3.97076200	-0.05117500	-5.76031400
H	3.93072000	-2.14406900	-4.41352300
H	2.31099400	-2.40066900	-2.57102300
H	0.77174000	1.53153100	-3.35537500
H	2.38091300	1.78690100	-5.22528900
C	0.84361800	0.29210300	5.26844700
C	2.06068800	0.71776300	4.73005300

C	2.13840600	1.10219600	3.39098300
C	1.00045600	1.06889500	2.56917700
C	-0.21303100	0.63839900	3.12171000
C	-0.29435400	0.25256100	4.46161200
H	0.78515600	-0.01117000	6.31046700
H	2.95147200	0.74543800	5.35227100
H	3.08971100	1.43200600	2.98227800
H	-1.09749400	0.60182400	2.49040900
H	-1.24426200	-0.08087700	4.87134200
C	1.27519400	6.30701600	1.22197000
C	1.23811100	5.51856700	2.37074500
C	1.20569400	4.12302700	2.27240700
C	1.20059200	3.48731800	1.02128700
C	1.22146300	4.29969300	-0.13043100
C	1.27025400	5.69013900	-0.03274200
H	1.30421000	7.39057100	1.30004700
H	1.23746900	5.98500800	3.35269900
H	1.18447800	3.53282400	3.18155800
H	1.29881700	6.29236000	-0.93745000
C	4.05204600	-2.57501500	3.47994500
C	3.66725900	-1.81565600	2.39747000
H	4.92707000	-2.28450400	4.05542000
H	4.24306700	-0.93620100	2.13600100
C	3.32064900	-3.72792000	3.85168700
C	2.20938400	-4.08874700	3.12705600
H	3.63731900	-4.32045500	4.70575700
H	1.63301200	-4.97025900	3.39817600
C	5.87336300	-2.31354400	-1.32588200
C	4.65446000	-1.98823500	-0.77347300
H	6.12487000	-3.35726200	-1.49507300
H	3.96106700	-2.77986100	-0.51674700
C	6.80162300	-1.30350500	-1.67364400
C	6.48035600	0.01619000	-1.45972000
H	7.76111700	-1.57321400	-2.10662600
H	7.18033800	0.80624000	-1.72169400
H	1.19634000	3.83115300	-1.11004800
C	-4.99199700	1.93044800	-1.81295100
H	-5.08261200	1.36475200	-2.75013600
H	-5.45333300	1.32113300	-1.02517900
C	-4.06365100	4.31356900	-0.29969800
H	-3.96523800	4.86636100	0.64487900
H	-3.56943600	4.91936500	-1.07527800
C	-5.54882900	4.12876800	-0.66172900
H	-6.06150400	3.63415300	0.17544500

H	-6.02686400	5.10854900	-0.78703000
C	-5.72119800	3.27974200	-1.93256200
H	-5.32310400	3.83524500	-2.79478000
H	-6.78810400	3.11838300	-2.13231600
C	-3.78640700	-0.94830400	1.73266200
O	-4.35338800	-0.04065400	0.81505200
C	-4.18534100	-0.51343300	3.15179700
H	-3.79613400	-1.20257900	3.90987100
H	-3.80237300	0.49292900	3.35328900
H	-5.27715400	-0.48788900	3.23679200
C	-4.24052800	-2.38380300	1.47708200
C	-5.41951600	-2.65656300	0.77687700
C	-3.52034400	-3.47948700	1.96707500
C	-5.82041900	-3.98361200	0.61425700
H	-5.99961800	-1.83791000	0.36476400
C	-4.00589900	-4.76835600	1.74595100
H	-2.58679700	-3.33537400	2.50671800
N	-5.13885900	-5.03765800	1.08389100
H	-6.74017200	-4.21367400	0.07695800
H	-3.45473700	-5.63160900	2.11809500

ABS₁₀

Coordinates (Angstroms)			
	X	Y	Z
Ru	-0.471869	0.825983	-0.603043
H	-1.278434	0.016657	0.688975
H	0.105959	1.714074	-1.948849
N	-2.276093	0.424957	-1.846038
H	-2.029903	-0.024130	-2.725764
H	-2.899511	-0.211461	-1.344513
N	-1.763345	2.596952	-0.179795
H	-1.836027	2.771202	0.820249
H	-1.291989	3.405526	-0.583875
P	0.645459	-1.076205	-1.180676
P	1.257694	1.589079	0.676987
C	-3.114444	2.437750	-0.768965
H	-3.673256	1.782487	-0.088506
C	-2.982019	1.698773	-2.108190
H	-2.319635	2.286684	-2.757420
C	5.533639	0.600320	-1.054338
C	5.025832	1.920855	-1.032556

C	3.796779	2.189779	-0.484904
C	2.987682	1.168742	0.088188
C	3.463525	-0.147225	0.111169
C	4.747081	-0.448906	-0.477769
H	5.624901	2.724846	-1.454655
H	3.440569	3.212173	-0.482038
C	2.703972	-2.965563	2.614035
C	1.564765	-3.550922	2.011358
C	1.021558	-3.014358	0.871574
C	1.580283	-1.869188	0.237539
C	2.728347	-1.280796	0.780173
C	3.293446	-1.814932	1.996716
H	1.122945	-4.435888	2.464525
H	0.147588	-3.484743	0.437906
C	-2.480969	-4.291086	-2.594173
C	-1.331679	-4.080095	-3.354804
C	-0.367585	-3.154986	-2.941789
C	-0.533174	-2.418143	-1.757839
C	-1.708484	-2.630149	-1.011254
C	-2.666040	-3.559216	-1.418768
H	-3.229476	-5.010067	-2.917743
H	-1.178518	-4.634843	-4.277349
H	0.513284	-3.010262	-3.555804
H	-1.866749	-2.037205	-0.115299
H	-3.566663	-3.696862	-0.825727
C	3.701007	-1.211287	-4.717032
C	3.637596	-2.278809	-3.817878
C	2.748960	-2.235008	-2.743366
C	1.906752	-1.126746	-2.551900
C	1.981939	-0.060872	-3.456899
C	2.873450	-0.103129	-4.532177
H	4.397039	-1.242902	-5.551678
H	4.286971	-3.140924	-3.947004
H	2.710817	-3.069568	-2.048069
H	1.342395	0.802495	-3.289424
H	2.923350	0.735107	-5.223223
C	1.537601	0.763652	5.271991
C	2.610218	1.371255	4.613625
C	2.548290	1.597148	3.238518
C	1.411156	1.226676	2.500655
C	0.345628	0.612683	3.169088
C	0.408911	0.381835	4.546149
H	1.588026	0.582491	6.342843
H	3.497727	1.662368	5.170002

H	3.389182	2.068790	2.736275
H	-0.517411	0.305460	2.582560
H	-0.423804	-0.102917	5.050640
C	0.990176	6.287379	0.615856
C	1.055862	5.622341	1.838993
C	1.181622	4.229279	1.883647
C	1.235872	3.468804	0.704973
C	1.145690	4.154903	-0.523728
C	1.036625	5.545492	-0.568144
H	0.898431	7.370070	0.582707
H	1.012536	6.184514	2.768737
H	1.235688	3.740578	2.849524
H	0.982181	6.049242	-1.530468
C	4.964358	-1.784294	3.781519
C	4.435777	-1.244368	2.629989
H	5.835917	-1.323954	4.239708
H	4.895638	-0.364640	2.196480
C	4.382876	-2.929061	4.375579
C	3.272535	-3.501838	3.800799
H	4.811136	-3.347699	5.282562
H	2.807934	-4.378576	4.246611
C	6.517127	-2.026316	-1.076705
C	5.284674	-1.768563	-0.518690
H	6.898005	-3.044273	-1.090919
H	4.708892	-2.586422	-0.103188
C	7.290749	-0.980774	-1.633749
C	6.801847	0.304385	-1.623461
H	8.262986	-1.196432	-2.069054
H	7.379279	1.120471	-2.052080
H	1.137495	3.574664	-1.442527
C	-4.350673	1.521328	-2.789611
H	-4.210438	1.040159	-3.766854
H	-4.962314	0.840233	-2.183488
C	-3.863952	3.770250	-0.926281
H	-3.982492	4.246090	0.056435
H	-3.248017	4.451551	-1.533471
C	-5.229489	3.582555	-1.606016
H	-5.883785	2.989440	-0.950394
H	-5.718176	4.555669	-1.739454
C	-5.079663	2.864776	-2.955261
H	-4.515131	3.507609	-3.646685
H	-6.063728	2.703224	-3.412395
C	-5.101517	-0.989854	0.967514
O	-4.817395	-0.756716	-0.200296

C	-4.018138	-1.269261	1.990922
H	-4.314302	-0.964259	3.000364
H	-3.821911	-2.349657	2.021440
H	-3.089132	-0.769717	1.691309
C	-6.554777	-1.032659	1.435135
C	-7.539712	-0.560048	0.355458
C	-6.925529	-2.452993	1.937836
H	-6.622911	-0.358036	2.305059
C	-8.993305	-0.621880	0.848689
H	-7.419572	-1.192404	-0.533637
H	-7.283945	0.458432	0.039696
C	-8.382589	-2.511839	2.423442
H	-6.786576	-3.166012	1.112061
H	-6.249485	-2.764125	2.742986
C	-9.362704	-2.027902	1.344931
H	-9.672575	-0.311657	0.044763
H	-9.132229	0.098802	1.668550
H	-8.627188	-3.536282	2.731546
H	-8.487454	-1.882074	3.319327
H	-10.388500	-2.038212	1.734318
H	-9.342066	-2.728270	0.496952

INTf₁₀

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.635656	0.610514	0.788205
H	-1.409591	-0.140373	-0.555780
H	-0.101680	1.426844	2.198661
N	-2.161106	2.220891	0.626711
H	-1.721877	3.138665	0.594755
H	-2.675612	2.107080	-0.248053
N	-2.292439	-0.162692	2.064720
H	-2.511071	-1.132048	1.845269
H	-1.944909	-0.151568	3.022942
P	0.909246	1.601695	-0.568886
P	0.736702	-1.157076	1.242831
C	-3.509878	0.674055	1.943629
H	-4.003556	0.364607	1.012704
C	-3.088710	2.140815	1.774894
H	-2.501911	2.429581	2.657200

C	5.310072	-0.050815	1.588655
C	4.547843	-0.430440	2.718753
C	3.229692	-0.787780	2.586819
C	2.576171	-0.801687	1.322716
C	3.299329	-0.455174	0.175644
C	4.683401	-0.061696	0.300563
H	5.021705	-0.437976	3.697953
H	2.676864	-1.076083	3.472060
C	2.792060	-1.605308	-3.459249
C	1.876534	-0.627690	-3.918023
C	1.390681	0.331272	-3.065884
C	1.794838	0.401535	-1.702786
C	2.724238	-0.524495	-1.216588
C	3.218604	-1.560799	-2.092280
H	1.560848	-0.646883	-4.959038
H	0.685467	1.061357	-3.444344
C	-1.301179	4.640363	-3.393775
C	-0.088063	5.013390	-2.815700
C	0.612193	4.121674	-1.996931
C	0.114357	2.833572	-1.742961
C	-1.115891	2.476632	-2.327184
C	-1.815838	3.366036	-3.142963
H	-1.846492	5.339021	-4.023434
H	0.318739	6.005781	-2.994727
H	1.546596	4.443364	-1.552398
H	-1.521392	1.493501	-2.105598
H	-2.775539	3.068399	-3.557035
C	4.327966	4.315000	1.106332
C	4.400239	3.847944	-0.208364
C	3.400983	3.012584	-0.708778
C	2.312693	2.632727	0.094264
C	2.254214	3.101799	1.412629
C	3.254877	3.937759	1.914773
H	5.108712	4.962344	1.498137
H	5.239209	4.125643	-0.841267
H	3.469575	2.652249	-1.731765
H	1.422450	2.782637	2.036042
H	3.197253	4.289209	2.942337
C	0.608522	-5.122186	-1.237161
C	1.601624	-4.944009	-0.270263
C	1.663064	-3.755311	0.457054
C	0.729280	-2.728794	0.235881
C	-0.257890	-2.915826	-0.738735
C	-0.316994	-4.104765	-1.471153

H	0.564262	-6.045885	-1.808887
H	2.332796	-5.727762	-0.088414
H	2.441594	-3.626240	1.204699
H	-0.956994	-2.102054	-0.920752
H	-1.084446	-4.233117	-2.231289
C	-0.460922	-2.714477	5.519166
C	-0.421804	-3.609892	4.451705
C	-0.025681	-3.181114	3.179850
C	0.332210	-1.844197	2.945272
C	0.266055	-0.946468	4.030641
C	-0.113698	-1.377690	5.302376
H	-0.763115	-3.050441	6.507859
H	-0.696998	-4.650991	4.602477
H	0.000731	-3.900969	2.370061
H	-0.142716	-0.666039	6.124235
C	4.601028	-3.531730	-2.518102
C	4.131702	-2.564566	-1.657177
H	5.295716	-4.284114	-2.153718
H	4.458907	-2.567044	-0.624712
C	4.185557	-3.557953	-3.870148
C	3.295744	-2.613126	-4.325247
H	4.565866	-4.323971	-4.540873
H	2.959673	-2.621369	-5.359806
C	6.797680	0.690973	-0.670750
C	5.476900	0.329307	-0.817289
H	7.374863	0.982687	-1.544397
H	5.029055	0.342844	-1.803323
C	7.409735	0.688789	0.604895
C	6.674629	0.327632	1.709409
H	8.453222	0.974737	0.707744
H	7.126241	0.325282	2.698952
H	0.494756	0.100866	3.853131
C	-4.316243	3.058306	1.644303
H	-3.985601	4.101845	1.558430
H	-4.842365	2.813708	0.710393
C	-4.480851	0.501580	3.123625
H	-4.799973	-0.547120	3.189761
H	-3.941036	0.725071	4.056723
C	-5.700488	1.430695	3.008770
H	-6.308301	1.127999	2.144098
H	-6.339328	1.318380	3.893501
C	-5.271261	2.895107	2.837744
H	-4.770434	3.236874	3.755432
H	-6.151277	3.536337	2.705187

C	-4.549545	0.121273	-2.258394
O	-4.464252	1.234063	-1.758905
C	-3.627708	-0.299762	-3.386223
H	-2.976898	-1.114532	-3.043933
H	-4.190958	-0.667408	-4.250349
H	-3.002552	0.541475	-3.687297
C	-5.556903	-0.904556	-1.716833
C	-6.710096	-0.219151	-0.960865
C	-6.101238	-1.894456	-2.771019
H	-4.971363	-1.498058	-0.990570
C	-7.675267	-1.238768	-0.339745
H	-7.258057	0.422787	-1.665545
H	-6.305171	0.449050	-0.195557
C	-7.073312	-2.908436	-2.144709
H	-6.622945	-1.331574	-3.559480
H	-5.279425	-2.431879	-3.257586
C	-8.218300	-2.216936	-1.391604
H	-8.502073	-0.714495	0.156148
H	-7.151308	-1.805969	0.444419
H	-7.471770	-3.568117	-2.925721
H	-6.517672	-3.551666	-1.446383
H	-8.867827	-2.965063	-0.919951
H	-8.844098	-1.665841	-2.109181

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Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.822762	-1.263516	0.187153
H	-1.707996	0.106695	-0.371713
H	-0.158253	-2.734182	0.762116
N	-2.518104	-1.688402	1.559892
H	-2.201472	-1.775796	2.523547
H	-3.177145	-0.909219	1.529235
N	-2.162756	-2.545503	-1.062239
H	-2.331837	-2.127388	-1.974475
H	-1.655830	-3.413831	-1.230234
P	0.355768	0.022823	1.658338
P	0.804179	-1.120582	-1.409283
C	-3.452116	-2.817101	-0.380636
H	-4.077955	-1.929119	-0.534388

C	-3.198381	-2.929055	1.128801
H	-2.482438	-3.743496	1.300088
C	5.198154	-1.144938	0.308061
C	4.674222	-2.241233	-0.417017
C	3.408551	-2.191276	-0.944436
C	2.575380	-1.046889	-0.797412
C	3.064996	0.070304	-0.110481
C	4.388908	0.026553	0.464516
H	5.289660	-3.127872	-0.553352
H	3.040130	-3.047549	-1.495132
C	2.142899	3.779066	-0.551856
C	1.041815	3.882128	0.332296
C	0.580081	2.780348	1.007015
C	1.188042	1.501079	0.865243
C	2.294776	1.359936	0.020709
C	2.776220	2.504483	-0.716662
H	0.565968	4.850327	0.473419
H	-0.265473	2.891319	1.675009
C	-2.612295	1.785254	4.853308
C	-1.372856	1.302026	5.271478
C	-0.456035	0.802008	4.341577
C	-0.757589	0.778113	2.970127
C	-2.017434	1.260531	2.566167
C	-2.932437	1.759919	3.493865
H	-3.325999	2.167235	5.578995
H	-1.113731	1.306123	6.327477
H	0.494274	0.422440	4.697549
H	-2.274660	1.213789	1.511736
H	-3.904706	2.106317	3.153021
C	3.656089	-1.765187	4.446745
C	3.561805	-0.380216	4.289850
C	2.599748	0.162180	3.437328
C	1.714059	-0.668771	2.731020
C	1.821630	-2.055990	2.892046
C	2.786232	-2.599888	3.744168
H	4.408560	-2.188717	5.107394
H	4.243825	0.277515	4.822486
H	2.539212	1.240882	3.319372
H	1.150914	-2.694741	2.322372
H	2.859969	-3.679358	3.853789
C	0.768141	2.167796	-4.737295
C	1.886082	1.341096	-4.596896
C	1.918629	0.373788	-3.592131
C	0.832171	0.211963	-2.715717

C	-0.278791	1.050556	-2.861377
C	-0.311161	2.022327	-3.865194
H	0.745332	2.925370	-5.516753
H	2.735903	1.455044	-5.265228
H	2.795102	-0.261353	-3.491498
H	-1.098678	0.936025	-2.155989
H	-1.178479	2.671831	-3.960304
C	0.508060	-5.037134	-4.003010
C	0.512824	-3.795782	-4.636918
C	0.644068	-2.618734	-3.891568
C	0.766532	-2.656011	-2.493667
C	0.739520	-3.918674	-1.866050
C	0.623522	-5.093148	-2.611005
H	0.410554	-5.950875	-4.583715
H	0.416342	-3.734827	-5.718260
H	0.647768	-1.668853	-4.413389
H	0.617871	-6.053701	-2.101063
C	4.326513	3.543349	-2.296514
C	3.876174	2.431286	-1.620074
H	5.168451	3.452955	-2.977973
H	4.366310	1.478499	-1.779027
C	3.703243	4.800369	-2.115754
C	2.630486	4.909115	-1.262013
H	4.070162	5.671330	-2.652410
H	2.134762	5.866051	-1.114237
C	6.212306	1.044915	1.736838
C	4.944167	1.111684	1.203730
H	6.605308	1.890621	2.295255
H	4.352821	2.006945	1.351882
C	7.006744	-0.113699	1.568418
C	6.503096	-1.185394	0.869502
H	8.006435	-0.153915	1.992875
H	7.096125	-2.087105	0.734110
H	0.786019	-3.961171	-0.780922
C	-4.502691	-3.211349	1.891369
H	-4.284655	-3.319254	2.962206
H	-5.168480	-2.342617	1.786735
C	-4.176660	-4.059887	-0.923590
H	-4.386870	-3.926972	-1.993306
H	-3.501121	-4.925542	-0.841775
C	-5.473231	-4.352186	-0.151133
H	-6.194031	-3.541667	-0.330443
H	-5.934439	-5.271894	-0.531849
C	-5.207613	-4.468702	1.357002

H	-4.578098	-5.350218	1.548536
H	-6.147388	-4.632694	1.898314
C	-4.764266	1.227930	-0.449882
O	-4.929203	0.449633	0.479476
C	-4.774888	0.731868	-1.884903
H	-5.148820	1.476453	-2.594008
H	-3.738072	0.495294	-2.157825
H	-5.370901	-0.181530	-1.955407
C	-4.536292	2.715063	-0.199091
C	-3.299555	3.274375	-0.937328
C	-5.800038	3.539217	-0.553641
H	-4.370638	2.809386	0.881615
C	-3.094504	4.762788	-0.616201
H	-3.436795	3.159444	-2.022330
H	-2.408765	2.695609	-0.667904
C	-5.590699	5.030588	-0.243143
H	-6.028788	3.422373	-1.622790
H	-6.664932	3.153756	0.000866
C	-4.345610	5.590273	-0.948422
H	-2.225652	5.143048	-1.167561
H	-2.858906	4.871982	0.452528
H	-6.483424	5.598023	-0.535788
H	-5.480880	5.158846	0.843497
H	-4.194351	6.640811	-0.669448
H	-4.509591	5.576294	-2.036435

TSf₁₀

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.054469	0.671676	0.377844
H	-1.876986	-0.168731	-1.053447
H	-0.606779	1.468268	1.755311
N	-2.433349	2.319108	-0.038832
H	-1.969317	3.200809	-0.250869
H	-2.956378	2.026383	-0.884528
N	-2.889861	0.117860	1.542672
H	-3.222649	-0.814870	1.304130
H	-2.595860	0.077471	2.517741
P	0.763487	1.638373	-0.671194
P	0.226157	-1.090422	1.145266

C	-3.984466	1.110500	1.371183
H	-4.526909	0.819899	0.464614
C	-3.375381	2.488351	1.087640
H	-2.781798	2.798869	1.957178
C	4.648356	-0.005017	2.407963
C	3.667377	-0.354405	3.365291
C	2.396316	-0.692010	2.974059
C	2.007764	-0.709720	1.605350
C	2.957031	-0.404143	0.622718
C	4.296366	-0.036135	1.020081
H	3.934082	-0.356673	4.419876
H	1.677558	-0.967626	3.734625
C	3.190505	-1.639312	-3.012483
C	2.383564	-0.679240	-3.670294
C	1.738675	0.299307	-2.958048
C	1.871091	0.410638	-1.544161
C	2.677677	-0.502665	-0.856096
C	3.331159	-1.562817	-1.588500
H	2.278591	-0.728717	-4.751887
H	1.119757	1.014238	-3.487224
C	-0.457032	4.638981	-4.080991
C	0.736809	4.847655	-3.387264
C	1.126702	3.975072	-2.369202
C	0.332710	2.866956	-2.024786
C	-0.869956	2.678035	-2.724932
C	-1.261554	3.550956	-3.742892
H	-0.758622	5.323244	-4.870125
H	1.369273	5.697185	-3.633270
H	2.051290	4.172050	-1.839900
H	-1.523093	1.853668	-2.469311
H	-2.202443	3.372371	-4.256617
C	3.677633	4.424980	1.707999
C	4.116350	3.795836	0.541728
C	3.264904	2.933664	-0.150848
C	1.962807	2.678438	0.309494
C	1.537905	3.312968	1.484860
C	2.386364	4.179849	2.177000
H	4.340237	5.095272	2.249663
H	5.124914	3.965482	0.174347
H	3.621436	2.450884	-1.055752
H	0.543016	3.099467	1.862832
H	2.037583	4.659166	3.088640
C	0.923401	-5.078589	-1.189503
C	1.422635	-4.942841	0.109500

C	1.226701	-3.754793	0.812244
C	0.509308	-2.691525	0.235991
C	0.027328	-2.834051	-1.068482
C	0.234308	-4.019746	-1.779510
H	1.082768	-6.002110	-1.740180
H	1.972134	-5.759688	0.570785
H	1.630542	-3.655385	1.816581
H	-0.499262	-1.998918	-1.518237
H	-0.140487	-4.111833	-2.795737
C	-1.967065	-2.448996	5.071786
C	-1.825424	-3.344507	4.013087
C	-1.122505	-2.975853	2.860673
C	-0.549459	-1.700155	2.737945
C	-0.727482	-0.796262	3.805990
C	-1.413842	-1.169657	4.962506
H	-2.506597	-2.739070	5.969482
H	-2.258983	-4.339329	4.078175
H	-1.024206	-3.694353	2.054808
H	-1.521105	-0.457048	5.776747
C	4.753626	-3.548742	-1.680071
C	4.124815	-2.561905	-0.953589
H	5.349620	-4.297269	-1.164602
H	4.227978	-2.548367	0.124399
C	4.627629	-3.601436	-3.087955
C	3.855610	-2.665447	-3.735682
H	5.133179	-4.382101	-3.650181
H	3.737724	-2.695879	-4.816544
C	6.580015	0.661043	0.487975
C	5.311292	0.312399	0.081094
H	7.329738	0.920417	-0.255015
H	5.078790	0.303138	-0.976674
C	6.917513	0.684449	1.862021
C	5.965656	0.358322	2.798959
H	7.922533	0.959742	2.170431
H	6.204272	0.372641	3.859983
H	-0.338775	0.213815	3.713540
C	-4.480382	3.523774	0.825923
H	-4.027968	4.507956	0.645750
H	-5.015927	3.247058	-0.093390
C	-4.967529	1.161594	2.549820
H	-5.412611	0.170166	2.706659
H	-4.412858	1.408944	3.468206
C	-6.065659	2.212590	2.313517
H	-6.694140	1.893286	1.469864

H	-6.723603	2.268629	3.189461
C	-5.466684	3.593541	2.004078
H	-4.942791	3.970207	2.895022
H	-6.265309	4.312632	1.784724
C	-3.212480	-0.170712	-2.208597
O	-3.654347	1.011242	-2.219068
C	-2.369252	-0.635757	-3.399850
H	-1.823964	-1.561895	-3.208451
H	-3.045508	-0.806779	-4.250663
H	-1.659656	0.138763	-3.692194
C	-4.128240	-1.241260	-1.562038
C	-5.427204	-1.343279	-2.402560
C	-3.540285	-2.640537	-1.330655
H	-4.427937	-0.836155	-0.587396
C	-6.451444	-2.286594	-1.752827
H	-5.182389	-1.717168	-3.407854
H	-5.847366	-0.340082	-2.530028
C	-4.562597	-3.581304	-0.669376
H	-3.233995	-3.079847	-2.290591
H	-2.636906	-2.570262	-0.717166
C	-5.857527	-3.678416	-1.489794
H	-7.343631	-2.366480	-2.388005
H	-6.787452	-1.852201	-0.798763
H	-4.121305	-4.577250	-0.533210
H	-4.802923	-3.208885	0.339148
H	-6.589574	-4.317256	-0.978332
H	-5.636458	-4.164028	-2.452069

TSu₁₀

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.231126	-0.838094	0.161976
H	-2.018782	0.728354	-0.528451
H	-0.813318	-2.290549	0.813335
N	-3.004002	-0.913137	1.445635
H	-2.803333	-0.864728	2.443074
H	-3.564910	-0.082721	1.183425
N	-2.697067	-2.010793	-1.055675
H	-2.814689	-1.624064	-1.990661
H	-2.282596	-2.934536	-1.176141

P	0.174338	0.190299	1.678044
P	0.504973	-1.226311	-1.327711
C	-4.019490	-2.125308	-0.383587
H	-4.565947	-1.205108	-0.616827
C	-3.800871	-2.121053	1.133650
H	-3.191442	-2.991296	1.410085
C	4.778397	-1.996874	0.531536
C	4.056761	-3.021981	-0.123512
C	2.824354	-2.770345	-0.671982
C	2.221177	-1.482476	-0.612684
C	2.913875	-0.432920	0.000677
C	4.207493	-0.684923	0.592539
H	4.492895	-4.016164	-0.190910
H	2.307575	-3.576465	-1.176028
C	2.751625	3.352729	-0.653891
C	1.702305	3.725404	0.220469
C	1.017730	2.776517	0.936753
C	1.348543	1.393480	0.860757
C	2.405691	0.985751	0.038961
C	3.104612	1.967806	-0.755975
H	1.438020	4.776313	0.311937
H	0.206890	3.088994	1.584196
C	-2.085290	2.797009	4.873378
C	-0.830488	2.271291	5.187881
C	-0.133509	1.497665	4.257901
C	-0.673686	1.236129	2.986807
C	-1.938524	1.767754	2.689127
C	-2.638423	2.541162	3.618704
H	-2.627032	3.394929	5.601856
H	-0.390537	2.457892	6.164456
H	0.830958	1.090619	4.537025
H	-2.379700	1.572438	1.720705
H	-3.616285	2.935210	3.354355
C	2.754544	-2.364442	4.628335
C	3.176622	-1.080923	4.277885
C	2.434970	-0.323945	3.369339
C	1.264325	-0.836157	2.788094
C	0.855922	-2.129349	3.144034
C	1.591990	-2.885690	4.058326
H	3.331329	-2.955496	5.335220
H	4.088636	-0.669393	4.701919
H	2.777759	0.671875	3.105914
H	-0.033139	-2.543116	2.678418
H	1.258362	-3.887076	4.319759

C	1.465104	1.501634	-4.994513
C	2.295485	0.411983	-4.714491
C	2.035266	-0.400824	-3.611712
C	0.932922	-0.142639	-2.778988
C	0.111550	0.950757	-3.066862
C	0.375825	1.772311	-4.166607
H	1.673408	2.138678	-5.850313
H	3.149885	0.200191	-5.352574
H	2.689164	-1.243176	-3.401142
H	-0.723549	1.152432	-2.404083
H	-0.266771	2.625259	-4.369581
C	-0.627522	-5.271311	-3.446719
C	-0.430024	-4.121776	-4.209522
C	-0.043329	-2.923126	-3.599598
C	0.146981	-2.843912	-2.210909
C	-0.078331	-4.010860	-1.451576
C	-0.448048	-5.210430	-2.061606
H	-0.921983	-6.203327	-3.921908
H	-0.572544	-4.150300	-5.286909
H	0.109068	-2.047319	-4.219532
H	-0.600803	-6.097508	-1.451691
C	4.815952	2.582794	-2.389033
C	4.154435	1.622813	-1.655951
H	5.609559	2.286291	-3.069820
H	4.430847	0.581901	-1.770113
C	4.471610	3.949674	-2.267950
C	3.456237	4.321385	-1.418212
H	5.004831	4.697740	-2.848542
H	3.171372	5.366206	-1.317928
C	6.189429	0.055790	1.820269
C	4.960662	0.325715	1.259655
H	6.736768	0.849606	2.321859
H	4.556643	1.328325	1.328528
C	6.746768	-1.242993	1.748132
C	6.050018	-2.245510	1.115908
H	7.718547	-1.442922	2.191570
H	6.460186	-3.250864	1.053228
H	0.022853	-3.965590	-0.371447
C	-5.148173	-2.185897	1.872950
H	-4.974144	-2.207733	2.957176
H	-5.714830	-1.269213	1.658018
C	-4.832275	-3.345295	-0.837609
H	-5.003049	-3.296570	-1.921339
H	-4.246080	-4.258575	-0.650604

C	-6.171861	-3.433867	-0.086142
H	-6.803656	-2.581978	-0.374879
H	-6.710864	-4.340734	-0.387068
C	-5.961978	-3.415243	1.435629
H	-5.433296	-4.330329	1.741231
H	-6.929737	-3.427618	1.951836
C	-3.533313	1.571543	-0.777778
O	-4.332955	1.109231	0.085996
C	-3.732318	1.139961	-2.236806
H	-2.845700	1.271052	-2.859491
H	-4.054461	0.097325	-2.280388
H	-4.544598	1.742295	-2.668739
C	-3.082379	3.040870	-0.569631
C	-1.988461	3.586012	-1.499610
C	-4.347974	3.935215	-0.645223
H	-2.711359	3.111780	0.458875
C	-1.672352	5.062164	-1.199546
H	-2.311685	3.503584	-2.548039
H	-1.079474	2.987293	-1.390439
C	-4.027612	5.406990	-0.344866
H	-4.788162	3.866050	-1.651641
H	-5.095293	3.548291	0.055057
C	-2.926782	5.944571	-1.270192
H	-0.906608	5.428622	-1.896018
H	-1.236974	5.137713	-0.192001
H	-4.937251	6.015307	-0.438445
H	-3.696315	5.499030	0.700415
H	-2.679944	6.982707	-1.010697
H	-3.300753	5.961286	-2.305186

Pf₁₀

Coordinates (Angstroms)			
	X	Y	Z

Ru		-0.60012800	0.54344900 1.06092300
H		-3.33642700	-0.72465300 -1.01392500
H		0.20887700	1.03363200 2.32570700
N		-2.23139400	1.80023000 0.88276400
H		-2.05853200	2.77615300 0.63843900
H		-3.24068600	1.36851600 -0.59018200
N		-2.06930500	-0.37851100 2.46717000

H	-2.14821800	-1.39488800	2.43453900
H	-1.68270500	-0.16330500	3.38699600
P	0.88071700	1.75879500	-0.24425800
P	0.82624100	-1.30150900	1.15817300
C	-3.40197500	0.26527300	2.31969700
H	-3.85323900	-0.17914900	1.42290200
C	-3.15264300	1.74597500	2.01959000
H	-2.69425400	2.18583600	2.92870200
C	5.46333800	-0.46112500	1.05795100
C	4.83490500	-1.01825600	2.19677200
C	3.49163900	-1.29864800	2.18876700
C	2.67764400	-1.04843700	1.04758700
C	3.26525000	-0.52699900	-0.10985500
C	4.67586900	-0.21931100	-0.11396400
H	5.43192000	-1.22581500	3.08200000
H	3.04573200	-1.73280800	3.07441600
C	2.24183600	-1.05592400	-3.77378000
C	1.35575400	0.03046000	-3.96344600
C	1.04700600	0.87230900	-2.92525900
C	1.60232500	0.70652700	-1.62315200
C	2.51281400	-0.33610700	-1.40269400
C	2.82847700	-1.24482900	-2.48061700
H	0.92244100	0.19590300	-4.94725900
H	0.36943000	1.69584600	-3.10982200
C	-1.09532100	5.39568900	-2.45928100
C	0.14620800	5.56343600	-1.84457600
C	0.76681700	4.49286300	-1.19576600
C	0.15695100	3.22796200	-1.14942900
C	-1.09908100	3.07859300	-1.76405300
C	-1.71686200	4.14692800	-2.41565100
H	-1.57639300	6.23217000	-2.95993600
H	0.63882400	6.53249800	-1.86479400
H	1.72728700	4.65585500	-0.72178000
H	-1.62099400	2.13020000	-1.72764700
H	-2.69157500	3.99189200	-2.86989900
C	4.47338500	3.96393000	1.76034200
C	4.53971900	3.61497700	0.41006900
C	3.48416800	2.92435100	-0.18651400
C	2.34995300	2.56154300	0.55613100
C	2.29314100	2.92219100	1.91014400
C	3.34607900	3.61862900	2.50730000
H	5.29544900	4.50108700	2.22638300
H	5.41520800	3.87281500	-0.17961300
H	3.54319400	2.66733500	-1.23970700

H	1.41872700	2.65158500	2.49274700
H	3.28396000	3.88907500	3.55845000
C	0.02018200	-4.83207900	-1.79064300
C	1.18560000	-4.83850600	-1.01946700
C	1.45390000	-3.78334300	-0.14740100
C	0.55970900	-2.70689100	-0.02861500
C	-0.60315900	-2.71160000	-0.80949500
C	-0.87343000	-3.76585600	-1.68531000
H	-0.18518300	-5.65167600	-2.47428600
H	1.88932800	-5.66265800	-1.10265600
H	2.36485400	-3.79639300	0.44522700
H	-1.29632500	-1.87672500	-0.73711200
H	-1.77819800	-3.74850200	-2.28726300
C	0.05270300	-3.30574100	5.33373400
C	-0.10805000	-4.05926100	4.17237400
C	0.16589500	-3.49872400	2.91956900
C	0.59805400	-2.16873700	2.80123300
C	0.73663400	-1.41479500	3.98450300
C	0.48052200	-1.97815500	5.23442000
H	-0.15600900	-3.74340100	6.30629600
H	-0.44490700	-5.09110200	4.23350600
H	0.03886000	-4.10990300	2.03303800
H	0.60949100	-1.37759900	6.13152100
C	4.01218400	-3.19155800	-3.36889800
C	3.71773900	-2.34802200	-2.32086400
H	4.69342000	-4.02397700	-3.21288700
H	4.16845100	-2.52839000	-1.35273300
C	3.43574400	-2.98838500	-4.64498500
C	2.56564800	-1.94116700	-4.83708800
H	3.67931700	-3.65933300	-5.46439200
H	2.10864400	-1.77057700	-5.80908300
C	6.68725600	0.62222500	-1.22149800
C	5.34128500	0.33145500	-1.24848400
H	7.16367200	1.04234600	-2.10342500
H	4.77466800	0.52728300	-2.15082900
C	7.45612700	0.37820700	-0.05862600
C	6.85078600	-0.15280800	1.05583900
H	8.51774500	0.61012000	-0.05069500
H	7.42490800	-0.34641300	1.95903400
H	1.04507700	-0.37539000	3.91867300
C	-4.49368000	2.47037000	1.79085900
H	-4.30360900	3.53924000	1.62539600
H	-4.94836400	2.08772700	0.86804100
C	-4.33899500	0.05419500	3.51537700

H	-4.51368800	-1.01840800	3.67879500
H	-3.85425800	0.43928400	4.42556500
C	-5.67288800	0.79057500	3.29548300
H	-6.20790900	0.32049700	2.45754400
H	-6.31367900	0.67576300	4.17874400
C	-5.44799000	2.27848600	2.98164700
H	-5.02849900	2.77387000	3.86993600
H	-6.40898400	2.76763900	2.77840800
C	-3.93437400	-0.12653900	-1.72583100
O	-3.79054800	1.25419900	-1.42157900
C	-3.37852700	-0.38112300	-3.13239100
H	-3.52063800	-1.42038100	-3.45258800
H	-3.86675000	0.27441400	-3.86129500
H	-2.30522500	-0.16349700	-3.15347700
C	-5.41191700	-0.54430900	-1.52862300
C	-6.39279200	0.23028800	-2.42698300
C	-5.65193500	-2.06005800	-1.65788200
H	-5.64834200	-0.26729500	-0.48742300
C	-7.85214400	-0.12732200	-2.10206600
H	-6.19488400	-0.01028500	-3.48196600
H	-6.21948300	1.30513000	-2.30735900
C	-7.10820700	-2.42959900	-1.32855200
H	-5.42907900	-2.38521800	-2.68452300
H	-4.96191200	-2.60979200	-1.00127600
C	-8.09832900	-1.64136700	-2.20112400
H	-8.53369700	0.41120200	-2.77369000
H	-8.08869200	0.21131700	-1.08212600
H	-7.26449400	-3.50896400	-1.45675900
H	-7.30568200	-2.20958000	-0.26870900
H	-9.13102900	-1.88197100	-1.91609500
H	-7.98206300	-1.95597300	-3.24919000

Pf₁₀

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.56378300	1.50475800	0.35293700
H	3.01379400	-0.88335500	-0.93821400
H	-0.42640800	2.56690300	0.97602800
N	2.36039300	1.67632300	1.34468400
H	2.40424000	1.39131400	2.32341500
H	3.60125300	0.43383500	0.70065400

N	1.55075700	3.19148900	-0.73091400
H	1.48115000	3.17373800	-1.74841500
H	1.01730600	4.00938200	-0.43366400
P	-0.39518400	-0.08095800	1.74589800
P	-1.09614400	1.26460100	-1.26819100
C	2.96698900	3.32807200	-0.29583600
H	3.52283700	2.54762000	-0.83124200
C	3.01550600	2.97617700	1.19252000
H	2.45914100	3.77030800	1.73134300
C	-5.40519500	0.07027400	0.22093100
C	-5.14988000	1.32471200	-0.38204400
C	-3.89761600	1.63525400	-0.84950400
C	-2.81118700	0.72033200	-0.75383700
C	-3.02617700	-0.54059400	-0.18765500
C	-4.33709500	-0.87969900	0.31360300
H	-5.96218100	2.04222100	-0.47416600
H	-3.73798000	2.60120300	-1.31200900
C	-1.24600000	-3.86210800	-0.93549100
C	-0.20689800	-3.82959600	0.02409100
C	-0.04334300	-2.74112200	0.84308000
C	-0.90512700	-1.60832000	0.77872800
C	-1.97034100	-1.61663600	-0.13206800
C	-2.14004200	-2.74562500	-1.01707900
H	0.46296100	-4.68241000	0.10895000
H	0.76000300	-2.75286600	1.56839100
C	2.49292000	-1.68291500	5.08809400
C	1.17772600	-1.35425900	5.41819900
C	0.29375900	-0.89539700	4.43834100
C	0.70534800	-0.75847600	3.10178900
C	2.03885800	-1.07916100	2.78964600
C	2.92106800	-1.54088200	3.76763500
H	3.17879200	-2.03605000	5.85395500
H	0.83215000	-1.45037500	6.44455200
H	-0.71800300	-0.63995200	4.72845300
H	2.41634200	-0.95381800	1.78255800
H	3.94518500	-1.76874000	3.48532500
C	-4.05291500	1.05669000	4.41376300
C	-3.82704700	-0.27977200	4.07810200
C	-2.75606200	-0.62181800	3.25184300
C	-1.89810400	0.36400500	2.73918700
C	-2.13339700	1.70169400	3.08683800
C	-3.20185900	2.04538300	3.91795500
H	-4.88737000	1.32457200	5.05677000
H	-4.48745000	-1.05730500	4.45216500

H	-2.58664700	-1.66538300	3.00448800
H	-1.47284000	2.47090700	2.70073100
H	-3.36816600	3.08820800	4.17629900
C	-0.16731900	-1.43030500	-4.96755800
C	-1.46349900	-0.93966100	-4.78804400
C	-1.76566900	-0.14926100	-3.67894100
C	-0.77555500	0.16743300	-2.73470200
C	0.51905800	-0.33145000	-2.92646800
C	0.82418900	-1.12637800	-4.03391100
H	0.06522000	-2.05145600	-5.82860600
H	-2.24090700	-1.17910500	-5.50903300
H	-2.77725700	0.22489700	-3.54520000
H	1.28839100	-0.10023700	-2.19389800
H	1.83282100	-1.51080700	-4.16135200
C	-1.62744100	5.49631400	-3.23642500
C	-1.32148700	4.40073100	-4.04168500
C	-1.20746900	3.12161300	-3.48534500
C	-1.38759700	2.91259300	-2.10914000
C	-1.67659800	4.03468600	-1.30631500
C	-1.80803000	5.30682200	-1.86291200
H	-1.72073600	6.48841700	-3.67011600
H	-1.17316800	4.53337000	-5.11046900
H	-0.97644300	2.28574700	-4.13596600
H	-2.04604200	6.15217100	-1.22197400
C	-3.32566800	-3.90159200	-2.81586700
C	-3.17888800	-2.80848100	-1.99138700
H	-4.12753200	-3.91715400	-3.54936700
H	-3.86427200	-1.97537500	-2.08553100
C	-2.44338000	-5.00359500	-2.71952200
C	-1.42360400	-4.97784400	-1.79753200
H	-2.57233200	-5.86174000	-3.37364100
H	-0.73237500	-5.81303800	-1.71116500
C	-5.88819700	-2.43226600	1.39258000
C	-4.62977000	-2.13833800	0.91637500
H	-6.07769800	-3.40135100	1.84672600
H	-3.84409900	-2.87900500	1.00234400
C	-6.93647600	-1.48653700	1.29551700
C	-6.69390400	-0.26139300	0.72028500
H	-7.92550000	-1.73090400	1.67368000
H	-7.48675400	0.47846600	0.63732400
H	-1.79493800	3.90401900	-0.23457300
C	4.47179800	3.01996300	1.69518700
H	4.49003600	2.80493400	2.77189300
H	5.04055400	2.21877900	1.20530800

C	3.59472000	4.69440800	-0.59843900
H	3.56651500	4.89674000	-1.67818300
H	2.99788900	5.48123500	-0.11200000
C	5.04241400	4.75210400	-0.07674100
H	5.65912700	4.04838700	-0.65412300
H	5.46194600	5.75096100	-0.25066800
C	5.11989700	4.38613000	1.41422200
H	4.60808200	5.16208100	2.00277100
H	6.16614000	4.38446600	1.74501100
C	4.09114100	-0.91208700	-0.69578800
O	4.31684200	-0.24588100	0.53985100
C	4.85286300	-0.20398200	-1.82557800
H	4.73612200	-0.71333700	-2.79006700
H	4.48172700	0.82060500	-1.94215400
H	5.92056400	-0.14271200	-1.59130800
C	4.46129500	-2.40027200	-0.50554800
C	4.07472600	-3.28778400	-1.70356200
C	5.93796200	-2.62055000	-0.12680300
H	3.85668900	-2.73371500	0.35258600
C	4.36040700	-4.77226400	-1.41891900
H	4.64460100	-2.98219600	-2.59351600
H	3.01175600	-3.15067300	-1.94743900
C	6.22728600	-4.10165900	0.16550600
H	6.58456700	-2.29097000	-0.95347700
H	6.18702300	-1.99748900	0.73903100
C	5.82626300	-4.99851300	-1.01614200
H	4.10823300	-5.38194100	-2.29670800
H	3.70572700	-5.11370500	-0.60287300
H	7.29036900	-4.24077700	0.40267200
H	5.66596500	-4.41087300	1.06007600
H	5.99398800	-6.05531400	-0.76961400
H	6.47445400	-4.77178400	-1.87618700

ABS₁₁

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.006871	0.414940	-0.626504
H	-1.589889	0.071354	0.959720
H	-0.668071	0.788422	-2.263360
N	-2.855285	-0.552761	-1.407680
H	-2.636294	-1.262390	-2.103877

H	-3.347865	-1.019075	-0.642824
N	-2.461406	2.108274	-0.679512
H	-2.457428	2.615865	0.202600
H	-2.139051	2.760962	-1.393361
P	0.275497	-1.471018	-0.627897
P	0.728036	1.730212	0.061700
C	-3.831544	1.635280	-0.989806
H	-4.232090	1.220440	-0.056112
C	-3.734013	0.481521	-1.998108
H	-3.210908	0.853024	-2.889548
C	4.901009	0.531610	-1.781669
C	4.232163	1.719491	-2.161151
C	3.040262	2.069281	-1.578524
C	2.430862	1.269109	-0.571562
C	3.070921	0.098299	-0.149620
C	4.318029	-0.291501	-0.764354
H	4.677091	2.356531	-2.922565
H	2.557095	2.986273	-1.891514
C	2.913097	-1.644420	3.275051
C	1.799389	-2.496859	3.084314
C	1.086450	-2.466310	1.912733
C	1.436651	-1.599658	0.839167
C	2.552667	-0.765520	0.972711
C	3.295898	-0.765084	2.210917
H	1.514382	-3.180200	3.881519
H	0.237279	-3.129003	1.800530
C	-2.522428	-5.238266	-0.331577
C	-1.479662	-5.237291	-1.257212
C	-0.612658	-4.143833	-1.347603
C	-0.771412	-3.024888	-0.514146
C	-1.841334	-3.033752	0.401428
C	-2.700498	-4.128616	0.497996
H	-3.195396	-6.089342	-0.263335
H	-1.335008	-6.089368	-1.917008
H	0.187031	-4.170358	-2.078152
H	-1.995718	-2.156974	1.023788
H	-3.520726	-4.106432	1.211004
C	2.959699	-2.668382	-4.264512
C	3.132510	-3.313197	-3.037212
C	2.355781	-2.943570	-1.938865
C	1.392860	-1.926610	-2.048872
C	1.230363	-1.284996	-3.283276
C	2.008874	-1.653933	-4.383458
H	3.568219	-2.952515	-5.119549

H	3.878544	-4.096754	-2.932063
H	2.499937	-3.450760	-0.988443
H	0.498970	-0.483315	-3.355698
H	1.874537	-1.142219	-5.333617
C	1.540225	2.638244	4.577056
C	2.465848	3.048814	3.613955
C	2.246958	2.759564	2.266978
C	1.096314	2.063336	1.860016
C	0.179553	1.650293	2.833918
C	0.400536	1.935645	4.184131
H	1.713522	2.858468	5.627566
H	3.361939	3.586932	3.912942
H	2.975103	3.080435	1.526381
H	-0.691463	1.085246	2.509061
H	-0.316725	1.601834	4.930478
C	-0.100908	6.053419	-1.604306
C	0.186214	5.886784	-0.250515
C	0.476423	4.617628	0.262489
C	0.478407	3.484829	-0.566371
C	0.164492	3.667163	-1.928862
C	-0.109938	4.935180	-2.443251
H	-0.320978	7.040802	-2.002284
H	0.188593	6.745602	0.416406
H	0.700295	4.519517	1.318299
H	-0.336259	5.048162	-3.500999
C	5.116248	0.056301	3.621793
C	4.417273	0.085573	2.435416
H	5.966071	0.719527	3.761094
H	4.722070	0.773193	1.656089
C	4.737342	-0.824715	4.661805
C	3.654401	-1.654191	4.487374
H	5.298594	-0.840533	5.592411
H	3.344182	-2.334360	5.277601
C	6.208136	-1.824707	-1.002697
C	5.015252	-1.482067	-0.405732
H	6.714224	-2.739514	-0.705203
H	4.595273	-2.131213	0.352856
C	6.779804	-0.999993	-2.000191
C	6.132871	0.152326	-2.380189
H	7.722514	-1.280184	-2.462792
H	6.553942	0.796555	-3.148828
H	0.115754	2.790863	-2.570203
C	-5.126424	-0.043047	-2.391513
H	-5.017737	-0.825835	-3.154196

H	-5.585500	-0.515743	-1.513331
C	-4.757827	2.753755	-1.492780
H	-4.843272	3.535739	-0.726355
H	-4.295006	3.226021	-2.373097
C	-6.146059	2.218320	-1.877962
H	-6.654094	1.842409	-0.977674
H	-6.766086	3.034375	-2.269397
C	-6.034430	1.084750	-2.907659
H	-5.626236	1.487142	-3.846540
H	-7.028555	0.686468	-3.145620
C	-5.254219	-1.164396	2.042001
O	-5.089889	-1.308821	0.838307
C	-4.120578	-0.757928	2.957914
H	-3.800939	-1.637241	3.534995
H	-3.268743	-0.386053	2.378524
H	-4.448739	-0.008743	3.688337
C	-6.632933	-1.375303	2.675225
C	-7.447805	-2.431619	1.921106
C	-7.367323	-0.015844	2.708676
H	-6.479104	-1.698788	3.714091
H	-6.946187	-3.405405	1.931645
H	-8.435612	-2.552451	2.379212
H	-7.581152	-2.139423	0.875492
H	-6.803262	0.744367	3.260701
H	-7.532998	0.354492	1.690438
H	-8.343521	-0.126232	3.193112

INTf₁₁

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.128047	0.106014	-0.746833
H	1.710557	-0.110726	0.867361
H	0.799183	0.334315	-2.410531
N	2.824148	1.514018	-1.042298
H	2.502530	2.394487	-1.439334
H	3.239170	1.729839	-0.134647
N	2.768676	-1.245998	-1.426993
H	2.830812	-2.078478	-0.844890
H	2.514287	-1.563332	-2.361827
P	-0.385683	1.686220	-0.089018

P	-0.414209	-1.573401	-0.638821
C	4.071294	-0.540668	-1.450507
H	4.410630	-0.490118	-0.408591
C	3.843578	0.901808	-1.922739
H	3.399946	0.866620	-2.926865
C	-4.770442	-0.323547	-1.949124
C	-3.978071	-1.194225	-2.734075
C	-2.730984	-1.579510	-2.310816
C	-2.183423	-1.132625	-1.075639
C	-2.945674	-0.293051	-0.254968
C	-4.254107	0.132291	-0.693097
H	-4.371608	-1.558699	-3.680501
H	-2.154364	-2.250861	-2.934559
C	-2.872610	0.075426	3.572475
C	-1.881643	1.075789	3.720636
C	-1.216411	1.569814	2.627438
C	-1.501265	1.121357	1.306857
C	-2.495608	0.156541	1.112159
C	-3.182123	-0.396727	2.255612
H	-1.653254	1.449803	4.716497
H	-0.459122	2.330434	2.773869
C	1.936934	5.426408	1.559900
C	0.836715	5.625472	0.726168
C	0.104421	4.535632	0.245218
C	0.455302	3.220782	0.591879
C	1.573155	3.037891	1.427170
C	2.304871	4.124462	1.907178
H	2.508601	6.275411	1.926383
H	0.544403	6.632948	0.440036
H	-0.738867	4.720923	-0.409295
H	1.871863	2.023959	1.674682
H	3.177416	3.946977	2.530366
C	-3.303819	3.768084	-3.090281
C	-3.533966	3.873797	-1.716414
C	-2.686851	3.228620	-0.814890
C	-1.594820	2.471240	-1.269916
C	-1.376455	2.368738	-2.649580
C	-2.225639	3.012818	-3.553238
H	-3.966187	4.266679	-3.793680
H	-4.378511	4.449512	-1.346592
H	-2.876765	3.315440	0.251612
H	-0.543219	1.762220	-2.996002
H	-2.045356	2.919098	-4.621611
C	-0.990539	-4.209672	3.182465

C	-1.861210	-4.362726	2.099884
C	-1.712134	-3.564949	0.965433
C	-0.686157	-2.607273	0.891079
C	0.175466	-2.457890	1.983664
C	0.023648	-3.253566	3.122757
H	-1.110314	-4.827350	4.069125
H	-2.660647	-5.098261	2.142608
H	-2.397235	-3.690170	0.130628
H	0.948645	-1.694780	1.922976
H	0.695971	-3.121082	3.967419
C	0.944764	-4.796693	-3.785951
C	0.731694	-5.178661	-2.462641
C	0.281326	-4.248355	-1.519073
C	0.042233	-2.911926	-1.875979
C	0.286258	-2.536193	-3.213154
C	0.718671	-3.467953	-4.157749
H	1.288417	-5.521764	-4.519312
H	0.911420	-6.206125	-2.155440
H	0.119143	-4.576263	-0.498748
H	0.884537	-3.152871	-5.185335
C	-4.827964	-1.909130	3.246048
C	-4.176032	-1.411467	2.139587
H	-5.580225	-2.683953	3.122850
H	-4.418468	-1.801915	1.158786
C	-4.526268	-1.424980	4.540650
C	-3.563823	-0.454662	4.695072
H	-5.050386	-1.822894	5.405643
H	-3.313395	-0.074653	5.683093
C	-6.323379	1.393557	-0.365348
C	-5.076782	1.007545	0.074779
H	-6.925255	2.062105	0.244813
H	-4.710599	1.379193	1.024038
C	-6.827036	0.931281	-1.604172
C	-6.060144	0.092073	-2.377694
H	-7.812849	1.241894	-1.940156
H	-6.428442	-0.269699	-3.335092
H	0.154920	-1.494907	-3.494016
C	5.166877	1.685424	-1.962293
H	4.979809	2.700097	-2.338007
H	5.540914	1.788291	-0.934229
C	5.134401	-1.251512	-2.303650
H	5.303374	-2.264736	-1.915089
H	4.745719	-1.368338	-3.327058
C	6.453301	-0.462592	-2.348319

H	6.898544	-0.441952	-1.342996
H	7.173179	-0.974026	-2.999249
C	6.221197	0.977608	-2.828307
H	5.886385	0.961618	-3.875936
H	7.162006	1.541315	-2.809913
C	4.634454	0.520139	2.561319
O	4.727709	1.362285	1.679304
C	3.596511	0.654775	3.658011
H	2.656955	0.238140	3.269570
H	3.860705	0.117380	4.573185
H	3.425415	1.710684	3.881450
C	5.549080	-0.705634	2.568748
C	4.753902	-2.018650	2.684085
C	6.604409	-0.581592	3.686045
H	6.069803	-0.682993	1.603908
H	3.966411	-2.080418	1.924747
H	5.424787	-2.875765	2.555428
H	4.277987	-2.117426	3.666330
H	7.188966	0.339177	3.582875
H	6.142433	-0.583704	4.680212
H	7.297616	-1.429316	3.641645

INTu₁₁

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.201277	0.546210	-0.606815
H	-1.773713	-0.290494	0.791418
H	-0.875374	1.414530	-2.046288
N	-2.983445	-0.254003	-1.667176
H	-2.721387	-0.704470	-2.541761
H	-3.417276	-0.968235	-1.081113
N	-2.753827	2.100427	-0.199184
H	-2.769461	2.357037	0.785595
H	-2.478155	2.936588	-0.713173
P	0.194250	-1.171419	-1.166228
P	0.448473	1.682134	0.486913
C	-4.097513	1.644640	-0.627981
H	-4.449660	0.951022	0.144801
C	-3.953584	0.833135	-1.922424
H	-3.497786	1.477079	-2.686456

C	4.717550	1.314331	-1.486577
C	3.990226	2.527990	-1.506601
C	2.768176	2.622648	-0.889717
C	2.184940	1.522236	-0.201227
C	2.882432	0.310700	-0.134796
C	4.161573	0.190307	-0.793946
H	4.413922	3.390064	-2.017268
H	2.240065	3.567266	-0.921713
C	2.768165	-2.411903	2.579003
C	1.711994	-3.220963	2.094750
C	1.018797	-2.865628	0.965194
C	1.336528	-1.691989	0.225366
C	2.395722	-0.881902	0.649341
C	3.114236	-1.225757	1.853546
H	1.456790	-4.132989	2.630255
H	0.214351	-3.503941	0.620085
C	-2.404813	-4.948521	-2.213665
C	-1.329820	-4.613137	-3.035808
C	-0.517681	-3.516824	-2.729384
C	-0.760986	-2.732285	-1.590254
C	-1.857627	-3.078238	-0.777209
C	-2.667335	-4.173037	-1.081789
H	-3.038435	-5.797759	-2.456853
H	-1.119042	-5.201288	-3.925718
H	0.304110	-3.275616	-3.392758
H	-2.078668	-2.456798	0.085970
H	-3.517412	-4.403611	-0.444996
C	3.012678	-1.003761	-4.893010
C	3.194209	-2.002622	-3.933088
C	2.376345	-2.042078	-2.803608
C	1.361244	-1.088932	-2.617375
C	1.191486	-0.089673	-3.583495
C	2.012540	-0.047434	-4.713390
H	3.653164	-0.968971	-5.770861
H	3.978823	-2.744392	-4.058348
H	2.528626	-2.821096	-2.061124
H	0.419025	0.658086	-3.420660
H	1.871592	0.738370	-5.451859
C	1.200439	1.224703	5.082277
C	2.080683	1.987635	4.310177
C	1.878257	2.109260	2.935424
C	0.787932	1.479331	2.311592
C	-0.083357	0.712450	3.093543
C	0.122528	0.584450	4.470077

H	1.361727	1.124267	6.152748
H	2.929068	2.481098	4.777822
H	2.571157	2.701969	2.343407
H	-0.906081	0.206322	2.592963
H	-0.557465	-0.022494	5.063616
C	-0.655710	6.245761	0.180965
C	-0.407776	5.683943	1.432160
C	-0.032107	4.340625	1.545188
C	0.096194	3.526014	0.408957
C	-0.180543	4.103825	-0.847360
C	-0.539156	5.447670	-0.961025
H	-0.942322	7.290753	0.094371
H	-0.502527	6.289146	2.330549
H	0.159849	3.933196	2.531012
H	-0.733482	5.869955	-1.944185
C	4.855437	-0.787230	3.512806
C	4.176006	-0.427809	2.370047
H	5.659351	-0.155122	3.880998
H	4.449583	0.484042	1.853476
C	4.515459	-1.967962	4.213966
C	3.488945	-2.758985	3.753405
H	5.061492	-2.242940	5.112562
H	3.209162	-3.667421	4.282325
C	6.138096	-1.103436	-1.425885
C	4.916432	-1.018925	-0.795789
H	6.687866	-2.040931	-1.408034
H	4.517227	-1.890866	-0.292271
C	6.683150	0.015935	-2.098162
C	5.980696	1.197660	-2.127409
H	7.649117	-0.062486	-2.590034
H	6.380395	2.067424	-2.644024
H	-0.134507	3.474646	-1.732098
C	-5.321627	0.327590	-2.411443
H	-5.194152	-0.218700	-3.355404
H	-5.711159	-0.390307	-1.675930
C	-5.107384	2.791917	-0.790699
H	-5.218014	3.325061	0.163083
H	-4.704096	3.519288	-1.512293
C	-6.471345	2.285713	-1.287862
H	-6.925885	1.648719	-0.515529
H	-7.152679	3.132530	-1.436712
C	-6.324012	1.479494	-2.586724
H	-5.981216	2.145862	-3.391953
H	-7.297600	1.084560	-2.902009

C	-4.538331	-1.702804	1.962991
O	-4.851737	-1.691719	0.781370
C	-4.593515	-0.432694	2.792458
H	-4.753747	-0.617796	3.858541
H	-3.625895	0.072539	2.672985
H	-5.376489	0.225867	2.407704
C	-4.073599	-2.991765	2.641450
C	-5.192982	-3.539907	3.550984
C	-2.755073	-2.809035	3.413547
H	-3.914853	-3.708269	1.827705
H	-6.121321	-3.700094	2.991557
H	-4.886806	-4.500164	3.981228
H	-5.407959	-2.858693	4.382747
H	-1.966310	-2.398446	2.774524
H	-2.880828	-2.139675	4.272655
H	-2.413895	-3.776750	3.798793

TSf₁₁

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.406019	0.166188	-0.299984
H	1.961672	-0.367811	1.392007
H	1.209177	0.609474	-1.879535
N	3.069078	1.590867	-0.185376
H	2.783970	2.564666	-0.275491
H	3.468656	1.465139	0.762591
N	3.151912	-1.015118	-1.059979
H	3.273108	-1.888692	-0.550184
H	2.917546	-1.272904	-2.017901
P	-0.235476	1.697745	0.242736
P	-0.157460	-1.482309	-0.715394
C	4.416223	-0.231896	-1.031000
H	4.828051	-0.345522	-0.022339
C	4.093239	1.256881	-1.197809
H	3.633500	1.412030	-2.182319
C	-4.191796	-0.025116	-2.698216
C	-3.249061	-0.798493	-3.414972
C	-2.096997	-1.234902	-2.810832
C	-1.797581	-0.936013	-1.452233
C	-2.720262	-0.203778	-0.695994

C	-3.933358	0.270846	-1.320957
H	-3.450630	-1.049212	-4.454098
H	-1.408074	-1.838086	-3.387364
C	-3.403590	-0.299589	3.087432
C	-2.460308	0.649610	3.550744
C	-1.592470	1.256654	2.679431
C	-1.618061	0.984968	1.281389
C	-2.549909	0.070867	0.776925
C	-3.443224	-0.606006	1.688208
H	-2.430092	0.890999	4.610977
H	-0.874607	1.971314	3.064043
C	1.363565	5.274608	2.842343
C	0.281524	5.488492	1.985947
C	-0.217545	4.447413	1.200412
C	0.351846	3.163252	1.258510
C	1.445228	2.967777	2.117713
C	1.946456	4.008833	2.902834
H	1.751375	6.089389	3.448680
H	-0.176904	6.472345	1.921767
H	-1.049459	4.649234	0.536487
H	1.926437	1.999699	2.168062
H	2.798216	3.817255	3.549994
C	-2.368737	4.172973	-3.110683
C	-3.000683	3.983371	-1.880527
C	-2.388093	3.214577	-0.889611
C	-1.137239	2.615045	-1.108764
C	-0.517019	2.810267	-2.350484
C	-1.125083	3.583639	-3.341638
H	-2.845566	4.769993	-3.883916
H	-3.976153	4.424024	-1.692582
H	-2.893396	3.077969	0.061611
H	0.437960	2.329665	-2.537724
H	-0.626595	3.719528	-4.298479
C	-1.766087	-4.465922	2.502017
C	-2.158149	-4.612561	1.167852
C	-1.689346	-3.724676	0.200584
C	-0.802953	-2.689596	0.547439
C	-0.427293	-2.546228	1.886403
C	-0.907693	-3.427153	2.859843
H	-2.137931	-5.153370	3.257428
H	-2.836476	-5.413148	0.883408
H	-2.012444	-3.839708	-0.830972
H	0.236075	-1.729566	2.152268
H	-0.611414	-3.297752	3.897682

C	1.933349	-4.247599	-3.886326
C	1.556077	-4.773159	-2.651759
C	0.878872	-3.979332	-1.719355
C	0.567600	-2.639134	-1.998196
C	0.982987	-2.114723	-3.239994
C	1.643981	-2.910886	-4.176501
H	2.452782	-4.867090	-4.612632
H	1.783944	-5.807467	-2.406430
H	0.595122	-4.415401	-0.768345
H	1.937701	-2.483668	-5.132266
C	-5.239316	-2.199502	2.146570
C	-4.383274	-1.587210	1.258169
H	-5.943343	-2.945010	1.786288
H	-4.419161	-1.861545	0.211044
C	-5.208521	-1.872382	3.522449
C	-4.302548	-0.943810	3.979221
H	-5.893210	-2.358834	4.212148
H	-4.256378	-0.686863	5.035109
C	-6.056427	1.483754	-1.245889
C	-4.909380	1.042442	-0.624285
H	-6.779866	2.069307	-0.684530
H	-4.744882	1.287180	0.417841
C	-6.302633	1.182617	-2.606437
C	-5.384094	0.443645	-3.313742
H	-7.212178	1.535169	-3.085402
H	-5.554255	0.203063	-4.360695
H	0.800526	-1.066498	-3.458199
C	5.374954	2.099976	-1.092934
H	5.131103	3.160898	-1.236881
H	5.781465	2.002866	-0.076176
C	5.457776	-0.702090	-2.055703
H	5.691751	-1.761864	-1.888863
H	5.025167	-0.628476	-3.065450
C	6.736923	0.149035	-1.980580
H	7.231319	-0.028704	-1.014818
H	7.443736	-0.169099	-2.756780
C	6.425138	1.647153	-2.121434
H	6.049708	1.846487	-3.135972
H	7.342436	2.237442	-2.006996
C	3.201073	-0.268558	2.654351
O	3.862212	0.773778	2.396293
C	2.211494	-0.228810	3.822255
H	1.499269	-1.055993	3.812957
H	2.786563	-0.283297	4.758688

H	1.661797	0.712875	3.826654
C	3.931504	-1.621090	2.431604
C	3.088062	-2.893851	2.539532
C	5.128033	-1.673526	3.406880
H	4.354286	-1.574281	1.422258
H	2.242412	-2.877053	1.847310
H	3.702164	-3.774439	2.310700
H	2.690999	-3.035325	3.551841
H	5.747119	-0.778327	3.301267
H	4.791159	-1.736262	4.449191
H	5.746251	-2.557648	3.208150

TSu₁₁

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.467095	-0.065754	-0.248294
H	1.900945	0.054387	1.626003
H	1.397243	-0.156539	-1.883689
N	3.263262	1.162251	-0.479866
H	3.095797	2.082897	-0.882222
H	3.627783	1.286207	0.482817
N	3.104362	-1.578964	-0.485007
H	3.114790	-2.277712	0.255934
H	2.871793	-2.076658	-1.343722
P	-0.070980	1.649115	-0.400042
P	-0.204503	-1.678220	-0.257687
C	4.444638	-0.945332	-0.607982
H	4.793537	-0.755999	0.412864
C	4.281644	0.429737	-1.265681
H	3.875235	0.298979	-2.277266
C	-4.225399	-0.692177	-2.534385
C	-3.339649	-1.695729	-2.991290
C	-2.182633	-1.972288	-2.307524
C	-1.823345	-1.275517	-1.119518
C	-2.685990	-0.296028	-0.615703
C	-3.902337	0.014842	-1.331532
H	-3.587749	-2.250240	-3.893580
H	-1.535174	-2.754685	-2.681412
C	-3.243922	0.939903	2.983196
C	-2.279041	1.973933	3.057323

C	-1.419156	2.204482	2.013472
C	-1.478152	1.445043	0.810552
C	-2.447859	0.445045	0.675909
C	-3.327049	0.158978	1.784472
H	-2.221526	2.580235	3.958456
H	-0.678971	2.991066	2.103756
C	1.766255	5.865512	0.562718
C	0.712539	5.777434	-0.348709
C	0.135893	4.541402	-0.647469
C	0.599439	3.362852	-0.037476
C	1.664338	3.468394	0.871313
C	2.240870	4.704599	1.173422
H	2.214882	6.829032	0.790647
H	0.336164	6.673792	-0.835451
H	-0.672391	4.504140	-1.367683
H	2.040277	2.570187	1.345710
H	3.059340	4.751639	1.886482
C	-2.052595	2.757743	-4.490949
C	-2.710604	3.056973	-3.296715
C	-2.143133	2.692072	-2.074849
C	-0.915265	2.013253	-2.021756
C	-0.266921	1.717241	-3.228689
C	-0.828583	2.088166	-4.452388
H	-2.493083	3.041044	-5.443523
H	-3.670390	3.566368	-3.312716
H	-2.664743	2.935433	-1.154350
H	0.675099	1.179196	-3.198065
H	-0.309204	1.848012	-5.377028
C	-1.859437	-3.805163	3.557900
C	-2.378968	-4.139625	2.303265
C	-1.906028	-3.500388	1.158141
C	-0.894542	-2.528005	1.249036
C	-0.387218	-2.197449	2.507646
C	-0.868122	-2.829776	3.658366
H	-2.233869	-4.298730	4.451096
H	-3.157392	-4.893977	2.218952
H	-2.320849	-3.762560	0.188296
H	0.374082	-1.427639	2.568534
H	-0.471732	-2.553507	4.631959
C	1.695725	-5.271940	-2.619860
C	1.289023	-5.448225	-1.298663
C	0.670861	-4.404220	-0.601309
C	0.452028	-3.156667	-1.206895
C	0.891621	-2.987788	-2.536090

C	1.492662	-4.034018	-3.237352
H	2.170047	-6.085078	-3.162948
H	1.447363	-6.401829	-0.801250
H	0.359155	-4.572243	0.423180
H	1.807463	-3.879065	-4.266459
C	-5.132319	-1.127368	2.812909
C	-4.296480	-0.884720	1.745655
H	-5.856947	-1.935226	2.754535
H	-4.367385	-1.505867	0.861257
C	-5.054859	-0.339420	3.985431
C	-4.124816	0.670727	4.065034
H	-5.723650	-0.538252	4.818614
H	-4.044567	1.281188	4.961597
C	-5.963333	1.303715	-1.607930
C	-4.815214	1.022456	-0.900910
H	-6.636770	2.078744	-1.251409
H	-4.600565	1.582188	0.001208
C	-6.275947	0.593100	-2.791029
C	-5.419464	-0.383726	-3.240930
H	-7.186689	0.821717	-3.338051
H	-5.640119	-0.938280	-4.150145
H	0.772403	-2.020375	-3.014188
C	5.637986	1.149449	-1.349518
H	5.510161	2.122956	-1.841668
H	5.995343	1.350208	-0.330046
C	5.468443	-1.810607	-1.355508
H	5.587841	-2.773946	-0.842015
H	5.084681	-2.034649	-2.363193
C	6.824134	-1.092003	-1.470089
H	7.259879	-0.984900	-0.466684
H	7.524134	-1.703990	-2.052330
C	6.670820	0.297857	-2.106746
H	6.352128	0.184838	-3.153649
H	7.638804	0.813241	-2.129560
C	3.229142	0.161639	2.751169
O	4.135676	0.802071	2.146688
C	3.418568	-1.355885	2.923834
H	2.489838	-1.897064	3.112314
H	3.909970	-1.781563	2.048096
H	4.091919	-1.520750	3.778286
C	2.613019	0.819468	4.025505
C	1.244399	0.303508	4.479958
C	2.645044	2.349995	4.013087
H	3.344626	0.502122	4.790193

H	1.241660	-0.778973	4.643714
H	0.963773	0.774216	5.430715
H	0.471028	0.544664	3.744490
H	3.565902	2.709256	3.546134
H	1.791018	2.763181	3.468456
H	2.594668	2.736635	5.038266

Pf₁₂

Coordinates (Angstroms)			
	X	Y	Z
Ru		1.09904900	0.07456500 -0.94146700
H		3.49152200	-0.66966700 1.79480300
H		0.46475100	0.13080900 -2.38795700
N		2.79923000	1.24568700 -0.91902800
H		2.69459400	2.25784000 -0.99533300
H		3.54760000	1.21538100 0.77198000
N		2.64347400	-1.30862900 -1.75948900
H		2.62078700	-2.25847300 -1.38876900
H		2.39872300	-1.39229500 -2.74677900
P		-0.40029100	1.72511000 -0.30832600
P		-0.45634900	-1.62945700 -0.61408500
C		3.99991000	-0.71360300 -1.62484800
H		4.29326400	-0.87229500 -0.57887600
C		3.85048600	0.79579700 -1.83262300
H		3.55433100	0.94831200 -2.89066300
C		-4.94694400	-0.58412200 -1.58606700
C		-4.22665400	-1.53520000 -2.34697300
C		-2.93580700	-1.86425500 -2.01694100
C		-2.27031900	-1.27442500 -0.90532600
C		-2.95749200	-0.35383800 -0.10699400
C		-4.31239200	0.00910200 -0.44696200
H		-4.71138000	-2.00877900 -3.19784100
H		-2.41811400	-2.60330500 -2.61542300
C		-2.53764100	0.30555700 3.65177800
C		-1.57635800	1.34327700 3.63710800
C		-1.03428200	1.78017000 2.45481500
C		-1.41257500	1.22760900 1.19684100
C		-2.38743900	0.22160700 1.16515400
C		-2.95009300	-0.26457000 2.40405800
H		-1.27166600	1.79700400 4.57749700

H	-0.30541400	2.57964000	2.48336500
C	1.69636200	5.72957300	0.95017400
C	0.59553100	5.77521900	0.09404600
C	-0.06152500	4.59995500	-0.27972600
C	0.36982000	3.35171300	0.19872600
C	1.49081100	3.32130200	1.04798700
C	2.14352400	4.49549400	1.42507500
H	2.20625400	6.64608700	1.23616300
H	0.24238900	6.72890500	-0.29054000
H	-0.90965700	4.66640000	-0.95060700
H	1.88125800	2.37797600	1.41134000
H	3.01115500	4.42805000	2.07535100
C	-3.47124500	3.38960100	-3.40503300
C	-3.72052400	3.52413200	-2.03771700
C	-2.82325500	2.99735500	-1.10818600
C	-1.66666400	2.32042300	-1.52686700
C	-1.42513700	2.19705800	-2.90243700
C	-2.32046200	2.72699200	-3.83418300
H	-4.17020700	3.79854500	-4.13012100
H	-4.61623400	4.03338800	-1.69263200
H	-3.02393200	3.11635400	-0.04774900
H	-0.53113200	1.68153400	-3.23675900
H	-2.11654500	2.62037400	-4.89667900
C	-0.42097000	-3.77359000	3.53175100
C	-1.39298600	-4.12568400	2.59126000
C	-1.43171800	-3.48583400	1.35243700
C	-0.49233600	-2.49189000	1.03110800
C	0.47280200	-2.14489000	1.98486000
C	0.50932500	-2.77887700	3.22897400
H	-0.39599100	-4.26821900	4.49926600
H	-2.12629100	-4.89263800	2.82687000
H	-2.19674300	-3.76003900	0.63050000
H	1.18741900	-1.35967400	1.75034600
H	1.25959000	-2.48999700	3.96011800
C	0.69650900	-5.03646600	-3.63023300
C	0.63404000	-5.32345400	-2.26783100
C	0.24345300	-4.33924500	-1.35254300
C	-0.08542700	-3.04375000	-1.78048800
C	0.00596700	-2.76398500	-3.15973900
C	0.37794800	-3.74934800	-4.07401600
H	0.99461700	-5.80331400	-4.34023700
H	0.88595900	-6.31776400	-1.90766800
H	0.19775400	-4.59035600	-0.29879100
H	0.42553500	-3.50959400	-5.13339700

C	-4.44572000	-1.74848000	3.64531500
C	-3.91760500	-1.31089500	2.45112700
H	-5.18052500	-2.54933600	3.64567800
H	-4.24005300	-1.77485300	1.52718600
C	-4.04040000	-1.16930000	4.87090500
C	-3.10130300	-0.16495000	4.86845300
H	-4.46774600	-1.52120800	5.80605600
H	-2.77231100	0.28924800	5.80027400
C	-6.36088900	1.28027100	-0.03868800
C	-5.07000100	0.95054800	0.30967000
H	-6.91112100	2.00198500	0.55936200
H	-4.61891500	1.41620000	1.17764800
C	-6.97860600	0.68797200	-1.16589600
C	-6.28063900	-0.22479700	-1.92104400
H	-7.99857100	0.95482600	-1.42926600
H	-6.73889300	-0.69025200	-2.79063900
H	-0.21159100	-1.76010000	-3.51371300
C	5.21001700	1.49377600	-1.63670500
H	5.09770200	2.56760800	-1.83756900
H	5.50555600	1.40301200	-0.58341200
C	5.05680600	-1.33381300	-2.54646500
H	5.15164800	-2.41042800	-2.34821800
H	4.72894400	-1.23072500	-3.59234500
C	6.41301500	-0.62939100	-2.36192500
H	6.79010700	-0.83841900	-1.35025600
H	7.14903400	-1.04574400	-3.06115200
C	6.28924400	0.89128800	-2.55286900
H	6.03597500	1.10167200	-3.60266000
H	7.25740500	1.37239500	-2.36488500
C	4.02962900	0.10554000	2.36890000
O	3.95939400	1.34477600	1.67581300
C	3.32375600	0.26605000	3.72050400
H	3.38347500	-0.64344200	4.33061700
H	3.76686700	1.09118900	4.28816800
H	2.26621600	0.50320800	3.56156000
C	5.50712200	-0.35491200	2.46938700
C	5.64921900	-1.76821700	3.05400900
C	6.38690700	0.65718300	3.21608100
H	5.86402000	-0.38983500	1.42881500
H	5.01067500	-2.49057100	2.52852900
H	6.68476300	-2.12016400	2.97257500
H	5.37942100	-1.79701100	4.11671300
H	6.24783300	1.66027400	2.80213500
H	6.14524500	0.69026800	4.28577200

H	7.44725300	0.39004600	3.12899200
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Pu₁₂

Coordinates (Angstroms)			
	X	Y	Z
Ru	-1.18391100	0.67422100	-0.73147800
H	-3.04244400	-1.01034400	1.96593000
H	-0.64567800	1.52221300	-1.95014900
N	-2.96804800	-0.14774500	-1.36504300
H	-2.93465400	-0.84606100	-2.10845200
H	-3.71726000	-1.25796000	-0.07043700
N	-2.63124900	2.32704200	-0.33809000
H	-2.53252200	2.81179100	0.55393700
H	-2.39717100	3.01655800	-1.05366300
P	0.21395100	-1.04216400	-1.40932100
P	0.50335500	1.73085500	0.48938300
C	-4.02634000	1.84842700	-0.53219100
H	-4.28184700	1.29381500	0.38057500
C	-3.99984700	0.84045100	-1.68417200
H	-3.74245000	1.40729400	-2.60224800
C	4.97370800	1.11515000	-0.86419800
C	4.36238400	2.39121000	-0.88240200
C	3.07199400	2.55548900	-0.44532500
C	2.30005700	1.46457400	0.04612800
C	2.87464300	0.19081900	0.10607600
C	4.22815600	0.00109100	-0.35920700
H	4.92998000	3.24474100	-1.24632200
H	2.63529600	3.54620900	-0.46795400
C	2.16407600	-2.68110300	2.55379800
C	1.17231800	-3.39794100	1.84381200
C	0.69056600	-2.92978500	0.64739400
C	1.16700500	-1.72271500	0.05903800
C	2.18348100	-1.00756400	0.70739300
C	2.67950900	-1.47296300	1.98160200
H	0.79376400	-4.32982100	2.25761800
H	-0.06621200	-3.50651000	0.13136500
C	-2.03488200	-4.73674800	-3.24152100
C	-0.90132600	-4.23648200	-3.88257700
C	-0.20201300	-3.15318400	-3.34467500
C	-0.62104200	-2.54518000	-2.14889800
C	-1.77635400	-3.05078200	-1.52453600

C	-2.47090200	-4.13699300	-2.05932200
H	-2.57748600	-5.57864800	-3.66401100
H	-0.55442500	-4.68720700	-4.80920200
H	0.67055800	-2.78622600	-3.87082900
H	-2.16400900	-2.59253900	-0.62249500
H	-3.36128700	-4.49374200	-1.54902800
C	3.36339900	-0.36123600	-4.78604900
C	3.54388500	-1.39389300	-3.86349400
C	2.62356200	-1.57781300	-2.83137700
C	1.51299400	-0.72958100	-2.69681400
C	1.34124000	0.30121400	-3.63128500
C	2.25919200	0.48392300	-4.66811500
H	4.07989300	-0.21670100	-5.59059000
H	4.40398200	-2.05330600	-3.94152200
H	2.77011700	-2.38971400	-2.12536100
H	0.48294200	0.95878200	-3.54012600
H	2.10926200	1.28862400	-5.38356800
C	0.41639500	1.22797600	5.13153700
C	1.53338800	1.81356800	4.53002100
C	1.58996500	1.95276000	3.14286900
C	0.52979100	1.51024300	2.33538500
C	-0.58155800	0.92028600	2.95106800
C	-0.64179400	0.77989800	4.33959500
H	0.37490900	1.11707000	6.21191000
H	2.36330200	2.15787000	5.14178400
H	2.46289800	2.40966300	2.68414400
H	-1.39909500	0.56134700	2.33010300
H	-1.51142800	0.31751300	4.79915700
C	-0.25667700	6.34162400	0.01905300
C	-0.19862900	5.78610500	1.29592200
C	0.07647300	4.42427900	1.46478000
C	0.28930800	3.58743900	0.35820500
C	0.21173700	4.16229900	-0.92639800
C	-0.04566900	5.52264100	-1.09445100
H	-0.46672000	7.39999000	-0.11077300
H	-0.36386100	6.41026900	2.17056600
H	0.12436900	4.01952100	2.46951200
H	-0.08712000	5.94240100	-2.09649800
C	4.14232100	-1.24463300	3.92756600
C	3.68144300	-0.77517200	2.71779800
H	4.90449300	-0.68647600	4.46496300
H	4.08359500	0.14783300	2.31858400
C	3.63295600	-2.44400400	4.47906900
C	2.66126500	-3.14294100	3.80243400

H	4.00752000	-2.80561900	5.43293400
H	2.25443300	-4.06452300	4.21227200
C	6.16440100	-1.42393000	-0.80628500
C	4.87411700	-1.26998900	-0.35000500
H	6.62754300	-2.40696400	-0.78605400
H	4.33676100	-2.13399600	0.02173700
C	6.89360000	-0.31565200	-1.29921900
C	6.30458500	0.92650800	-1.32603900
H	7.91203400	-0.44976200	-1.65375300
H	6.84830800	1.78965800	-1.70306200
H	0.35171700	3.53145900	-1.79911600
C	-5.40608600	0.24551900	-1.89504200
H	-5.38320000	-0.44055300	-2.75225700
H	-5.66909500	-0.36054200	-1.01818400
C	-5.05305800	2.96588200	-0.75022800
H	-5.05968700	3.65047000	0.10941300
H	-4.75735900	3.56153500	-1.62758800
C	-6.45606800	2.37503500	-0.98016400
H	-6.79544200	1.88714600	-0.05487100
H	-7.17106000	3.18097600	-1.18810000
C	-6.45465800	1.34674100	-2.12358600
H	-6.24160200	1.86362500	-3.07120500
H	-7.45291700	0.90353100	-2.22929100
C	-3.89064200	-1.71095900	1.87042100
O	-4.13805700	-1.96874600	0.49436300
C	-5.12501300	-1.05754700	2.50700600
H	-4.98315600	-0.85071400	3.57465400
H	-5.34512500	-0.10776000	2.00641100
H	-6.00350100	-1.70076400	2.39062400
C	-3.45178700	-3.03547600	2.54222300
C	-4.51885400	-4.13373400	2.42675000
C	-3.00094300	-2.84015700	3.99726300
H	-2.57548900	-3.36467200	1.96582700
H	-4.85604400	-4.23357200	1.39076700
H	-4.11687200	-5.10022700	2.75479200
H	-5.39393900	-3.91571500	3.05185300
H	-2.22505300	-2.06829800	4.07868900
H	-3.83616000	-2.55163200	4.64737900
H	-2.58290900	-3.77051700	4.40056100

ABS₁₂

Coordinates (Angstroms)

	X	Y	Z

Ru	-1.034456	0.537675	-0.524432
H	-1.587625	0.113125	1.051717
H	-0.727644	1.011372	-2.142165
N	-2.926638	-0.315707	-1.317534
H	-2.742415	-0.998613	-2.049689
H	-3.427448	-0.798409	-0.568277
N	-2.431873	2.277715	-0.438393
H	-2.403587	2.722726	0.476404
H	-2.090916	2.965618	-1.108996
P	0.168122	-1.392140	-0.686217
P	0.771424	1.734879	0.198295
C	-3.821234	1.875643	-0.768189
H	-4.235389	1.421428	0.140863
C	-3.770864	0.779722	-1.842590
H	-3.240859	1.182853	-2.715913
C	4.820076	0.499093	-1.884317
C	4.192637	1.738983	-2.151343
C	3.039687	2.095801	-1.498692
C	2.431254	1.251864	-0.527404
C	3.034813	0.028774	-0.212922
C	4.238401	-0.369182	-0.904689
H	4.638177	2.410514	-2.882152
H	2.588112	3.053089	-1.726415
C	2.946148	-1.953567	3.080365
C	1.796145	-2.752611	2.874324
C	1.037297	-2.609139	1.740441
C	1.374829	-1.675243	0.720650
C	2.525339	-0.892001	0.867218
C	3.316601	-1.008508	2.069380
H	1.519961	-3.485766	3.629269
H	0.161911	-3.234144	1.615077
C	-2.805392	-5.032722	-0.534133
C	-1.828856	-4.991754	-1.528317
C	-0.910339	-3.938181	-1.576658
C	-0.952120	-2.898223	-0.633797
C	-1.960180	-2.942324	0.348968
C	-2.867140	-4.000972	0.405709
H	-3.516425	-5.854271	-0.496181
H	-1.774977	-5.781822	-2.273432
H	-0.161624	-3.934003	-2.359852
H	-2.030419	-2.120782	1.056158
H	-3.632168	-4.012307	1.178027

C	2.665727	-2.480791	-4.485649
C	2.836108	-3.219490	-3.311931
C	2.116309	-2.883782	-2.165115
C	1.212607	-1.808265	-2.173369
C	1.053410	-1.071584	-3.353694
C	1.775955	-1.405960	-4.502140
H	3.229913	-2.739132	-5.378449
H	3.535751	-4.051082	-3.286940
H	2.258061	-3.462685	-1.256177
H	0.369551	-0.226010	-3.344508
H	1.645497	-0.820941	-5.409578
C	1.775043	2.259330	4.736322
C	2.679461	2.714705	3.773218
C	2.401934	2.541311	2.417260
C	1.213152	1.917449	2.001817
C	0.317438	1.459624	2.975169
C	0.597175	1.628852	4.334055
H	1.994266	2.388584	5.793364
H	3.604499	3.197412	4.078577
H	3.114221	2.896293	1.676703
H	-0.585543	0.953245	2.641300
H	-0.104591	1.260972	5.079100
C	0.055634	6.198251	-1.109785
C	0.370788	5.917268	0.218561
C	0.631267	4.603409	0.623546
C	0.575427	3.539168	-0.290150
C	0.234578	3.837613	-1.625757
C	-0.010523	5.150036	-2.032365
H	-0.141626	7.220101	-1.423877
H	0.418320	6.720650	0.949773
H	0.877619	4.415780	1.662202
H	-0.258683	5.352587	-3.071689
C	5.221818	-0.357336	3.456199
C	4.475986	-0.214646	2.307262
H	6.099790	0.265312	3.607512
H	4.771405	0.520393	1.568614
C	4.855064	-1.303013	4.442541
C	3.736511	-2.080623	4.254454
H	5.453659	-1.408712	5.343529
H	3.435138	-2.808902	5.004198
C	6.044909	-1.962001	-1.328465
C	4.892437	-1.612129	-0.660555
H	6.518246	-2.917699	-1.118412
H	4.470911	-2.297237	0.064698

C	6.616670	-1.092422	-2.286968
C	6.010043	0.111533	-2.557642
H	7.527414	-1.379053	-2.806227
H	6.431470	0.791123	-3.295004
H	0.142059	3.018358	-2.334199
C	-5.182227	0.328949	-2.256925
H	-5.104166	-0.411875	-3.064086
H	-5.656824	-0.176168	-1.405730
C	-4.706312	3.055469	-1.201838
H	-4.760674	3.794469	-0.391335
H	-4.228182	3.559772	-2.055838
C	-6.114372	2.594708	-1.611128
H	-6.633743	2.187138	-0.731620
H	-6.704161	3.454244	-1.953199
C	-6.047285	1.518180	-2.704434
H	-5.624429	1.957393	-3.620029
H	-7.056396	1.172981	-2.961736
C	-5.263664	-1.114868	2.108210
O	-5.136624	-1.103478	0.887293
C	-4.179478	-0.608740	3.032724
H	-3.306417	-0.281206	2.459318
H	-4.566534	0.222700	3.637523
H	-3.887901	-1.397542	3.738644
C	-6.510582	-1.635130	2.740603
C	-7.824025	-1.428345	1.993001
C	-7.224749	-2.789627	2.043271
H	-6.545529	-1.610069	3.826053
H	-7.751549	-0.881113	1.058039
H	-8.703497	-1.215798	2.593705
H	-7.678777	-3.543361	2.679827
H	-6.745784	-3.161869	1.142659

INTf₁₂

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.073482	0.209783	-0.730694
H	-1.684749	0.035915	0.875953
H	-0.711759	0.398939	-2.391952
N	-2.829042	-0.972848	-1.411808
H	-2.538247	-1.745758	-2.007220

H	-3.305476	-1.378284	-0.603357
N	-2.627151	1.779784	-1.042715
H	-2.680556	2.408355	-0.244044
H	-2.320829	2.341543	-1.836354
P	0.332071	-1.573582	-0.480224
P	0.556819	1.711082	-0.176570
C	-3.957248	1.181657	-1.309276
H	-4.356826	0.875829	-0.334215
C	-3.765907	-0.092326	-2.144292
H	-3.259305	0.185333	-3.078408
C	4.863209	0.574991	-1.731104
C	4.135616	1.659439	-2.276107
C	2.901792	1.995299	-1.778658
C	2.306123	1.285109	-0.698724
C	3.002056	0.220604	-0.114427
C	4.294006	-0.155961	-0.638693
H	4.568373	2.227309	-3.096893
H	2.372576	2.831894	-2.217120
C	2.831125	-1.117420	3.487242
C	1.781756	-2.060126	3.366800
C	1.110790	-2.213526	2.180128
C	1.445688	-1.456220	1.022520
C	2.498281	-0.536196	1.088749
C	3.193662	-0.341214	2.338949
H	1.512634	-2.664392	4.230631
H	0.308515	-2.939134	2.121846
C	-2.223041	-5.469105	0.154078
C	-1.125965	-5.509745	-0.705917
C	-0.328304	-4.376521	-0.892354
C	-0.610926	-3.176239	-0.220422
C	-1.730926	-3.148003	0.631988
C	-2.524227	-4.279903	0.821880
H	-2.843709	-6.350641	0.293999
H	-0.885833	-6.425446	-1.240890
H	0.512895	-4.435931	-1.572729
H	-1.982230	-2.214101	1.125547
H	-3.391187	-4.222866	1.475038
C	3.212161	-2.965629	-3.891166
C	3.391071	-3.454676	-2.594755
C	2.555861	-3.023110	-1.563846
C	1.526287	-2.099670	-1.811328
C	1.360444	-1.611796	-3.113563
C	2.197812	-2.041887	-4.146118
H	3.865872	-3.297908	-4.693893

H	4.186948	-4.164351	-2.383828
H	2.708440	-3.406491	-0.558322
H	0.578442	-0.877641	-3.292123
H	2.058926	-1.648900	-5.150605
C	1.161946	3.252899	4.199019
C	2.099559	3.581292	3.216215
C	1.943857	3.104212	1.914648
C	0.845677	2.297254	1.572079
C	-0.083610	1.969550	2.566084
C	0.073550	2.443816	3.871354
H	1.286496	3.619644	5.214926
H	2.956208	4.202529	3.465563
H	2.680715	3.364667	1.159101
H	-0.912863	1.320007	2.295558
H	-0.652800	2.173951	4.634641
C	-0.493219	5.729653	-2.393291
C	-0.243990	5.749695	-1.022105
C	0.112776	4.576242	-0.348352
C	0.221250	3.353701	-1.029730
C	-0.054511	3.346740	-2.412745
C	-0.395644	4.520020	-3.087171
H	-0.765427	6.642966	-2.916248
H	-0.323386	6.681042	-0.466530
H	0.304841	4.623553	0.717197
H	-0.590427	4.487036	-4.156639
C	4.904735	0.760403	3.694183
C	4.247503	0.605729	2.493815
H	5.703591	1.492605	3.778812
H	4.533187	1.219088	1.648022
C	4.548700	-0.021209	4.818371
C	3.529009	-0.937957	4.712015
H	5.077141	0.107621	5.759344
H	3.236814	-1.543598	5.567073
C	6.283141	-1.578390	-0.629210
C	5.048866	-1.246586	-0.116248
H	6.832884	-2.415759	-0.207180
H	4.639214	-1.827844	0.700556
C	6.841263	-0.842617	-1.701131
C	6.139019	0.209805	-2.239834
H	7.817061	-1.112827	-2.096148
H	6.548443	0.783395	-3.068419
H	-0.020312	2.400056	-2.945475
C	-5.116109	-0.757728	-2.463623
H	-4.946926	-1.635557	-3.101520

H	-5.557719	-1.123575	-1.527274
C	-4.938050	2.156849	-1.980255
H	-5.085374	3.033992	-1.336002
H	-4.486736	2.525276	-2.914464
C	-6.283823	1.485558	-2.297769
H	-6.784837	1.214450	-1.357132
H	-6.943937	2.195060	-2.812076
C	-6.083886	0.221755	-3.147296
H	-5.685963	0.506264	-4.132540
H	-7.047346	-0.269887	-3.330776
C	-5.145120	-1.098827	2.050429
O	-4.963836	-1.536547	0.917685
C	-3.975077	-0.947535	3.003106
H	-3.149362	-0.464452	2.463566
H	-4.204705	-0.389874	3.914656
H	-3.628421	-1.947171	3.292639
C	-6.523645	-0.731505	2.477991
C	-6.984730	-0.905885	3.921292
C	-6.789965	0.470278	3.381231
H	-7.259208	-0.928066	1.703322
H	-6.265483	-1.286874	4.640236
H	-7.995709	-1.276481	4.062420
H	-7.664647	1.066801	3.139242
H	-5.938043	1.049307	3.725197

TSf₁₂

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.387272	0.196293	-0.324221
H	1.854655	-0.193188	1.396068
H	1.254542	0.561919	-1.935724
N	3.072819	1.599904	-0.234077
H	2.813669	2.571059	-0.399223
H	3.438127	1.530048	0.730737
N	3.129942	-1.068738	-0.916411
H	3.212908	-1.881305	-0.308251
H	2.932145	-1.417700	-1.853608
P	-0.272232	1.735728	0.111560
P	-0.142378	-1.495299	-0.683417
C	4.405949	-0.305586	-0.899055

H	4.771104	-0.359479	0.129977
C	4.120745	1.172607	-1.186231
H	3.692990	1.265177	-2.192463
C	-4.313875	-0.248800	-2.505770
C	-3.378027	-1.009920	-3.244683
C	-2.181200	-1.381546	-2.686022
C	-1.829359	-1.025791	-1.353571
C	-2.735789	-0.294173	-0.578543
C	-3.996647	0.110885	-1.156054
H	-3.620139	-1.301264	-4.264340
H	-1.493012	-1.971502	-3.277771
C	-3.213145	-0.182477	3.236703
C	-2.314582	0.855303	3.583059
C	-1.525281	1.444842	2.628542
C	-1.588767	1.062394	1.258417
C	-2.494213	0.069535	0.865319
C	-3.303465	-0.586563	1.864758
H	-2.254566	1.178984	4.619785
H	-0.840713	2.230998	2.924205
C	1.309594	5.575937	2.322976
C	0.233095	5.691439	1.441959
C	-0.261629	4.567847	0.775956
C	0.307452	3.298486	0.977928
C	1.398197	3.202152	1.859334
C	1.892015	4.324894	2.527860
H	1.693466	6.453143	2.837721
H	-0.225824	6.661204	1.265475
H	-1.091074	4.692726	0.090479
H	1.879266	2.246383	2.024661
H	2.737359	4.209327	3.201105
C	-2.615371	3.822411	-3.361170
C	-3.185942	3.743425	-2.089382
C	-2.508815	3.091246	-1.057981
C	-1.253352	2.501159	-1.277361
C	-0.694651	2.584102	-2.559917
C	-1.368292	3.240432	-3.592502
H	-3.142503	4.328686	-4.165908
H	-4.163051	4.179627	-1.899755
H	-2.966102	3.038676	-0.074390
H	0.265120	2.110150	-2.741313
H	-0.917803	3.291349	-4.580913
C	-1.335113	-4.601080	2.599442
C	-1.951146	-4.654517	1.345476
C	-1.621186	-3.721289	0.362984

C	-0.659402	-2.727653	0.614596
C	-0.056708	-2.679568	1.874949
C	-0.391345	-3.608755	2.864119
H	-1.597916	-5.325197	3.366349
H	-2.694128	-5.419995	1.135721
H	-2.110460	-3.769583	-0.606547
H	0.663281	-1.890501	2.064897
H	0.081535	-3.551873	3.841498
C	1.843727	-4.247007	-3.938546
C	1.472315	-4.791443	-2.710535
C	0.833619	-4.001402	-1.748202
C	0.557520	-2.646420	-1.989811
C	0.960208	-2.105772	-3.228385
C	1.583559	-2.897293	-4.194026
H	2.335001	-4.862811	-4.687338
H	1.675174	-5.837241	-2.493426
H	0.551979	-4.453588	-0.804344
H	1.870532	-2.456558	-5.145689
C	-4.982382	-2.237730	2.520059
C	-4.210540	-1.639463	1.549041
H	-5.662095	-3.040597	2.246825
H	-4.287480	-1.979344	0.523554
C	-4.897165	-1.821143	3.869483
C	-4.025465	-0.815427	4.215839
H	-5.514752	-2.298702	4.625526
H	-3.940847	-0.486344	5.249062
C	-6.154329	1.254753	-1.017298
C	-4.961999	0.878093	-0.439902
H	-6.868033	1.839191	-0.442472
H	-4.752423	1.172359	0.581092
C	-6.459731	0.888591	-2.349641
C	-5.552697	0.152854	-3.075046
H	-7.404927	1.189979	-2.793218
H	-5.767340	-0.135683	-4.101485
H	0.796720	-1.049359	-3.418543
C	5.415972	1.997472	-1.101753
H	5.199536	3.049480	-1.330401
H	5.790241	1.967328	-0.068392
C	5.472195	-0.870241	-1.847934
H	5.679522	-1.917800	-1.592488
H	5.075571	-0.867154	-2.875026
C	6.765028	-0.038349	-1.794415
H	7.224286	-0.149788	-0.801710
H	7.490561	-0.427039	-2.519614

C	6.487283	1.449443	-2.059343
H	6.146202	1.576502	-3.097309
H	7.412080	2.031061	-1.961730
C	3.006315	-0.082160	2.722932
O	3.779043	0.874795	2.458285
C	1.930854	0.102257	3.797215
H	1.195515	-0.705978	3.801164
H	2.437252	0.108588	4.773413
H	1.409127	1.051767	3.680274
C	3.537974	-1.509309	2.665694
C	4.967756	-1.784103	2.275440
C	4.567644	-1.882852	3.722216
H	2.802826	-2.278598	2.448406
H	5.569208	-0.921293	2.007140
H	5.198934	-2.698407	1.733585
H	4.494121	-2.862989	4.186401
H	4.913708	-1.093058	4.383679

TSu₁₂

	Coordinates (Angstroms)		
	X	Y	Z

Ru	-1.443297	0.116656	-0.377723
H	-1.904412	0.005199	1.399477
H	-1.315732	0.246569	-2.023200
N	-3.223029	-1.134390	-0.653116
H	-3.037012	-2.035919	-1.089460
H	-3.577535	-1.306536	0.302750
N	-3.086869	1.617276	-0.619115
H	-3.097466	2.315406	0.122528
H	-2.864726	2.118012	-1.478709
P	0.086218	-1.601285	-0.465525
P	0.224009	1.704385	-0.197785
C	-4.421867	0.970877	-0.728467
H	-4.751801	0.765735	0.295921
C	-4.256862	-0.393168	-1.410095
H	-3.861766	-0.241453	-2.423276
C	4.271269	0.757598	-2.439147
C	3.413471	1.799142	-2.863630
C	2.255267	2.074549	-2.181115
C	1.867489	1.338076	-1.027086

C	2.703735	0.320343	-0.553211
C	3.919702	0.010624	-1.268651
H	3.684841	2.384623	-3.739323
H	1.629031	2.885653	-2.529745
C	3.180094	-1.010730	3.024288
C	2.180360	-2.012670	3.067476
C	1.336114	-2.205951	2.003594
C	1.440711	-1.433852	0.812050
C	2.436365	-0.455153	0.713144
C	3.307274	-0.214739	1.839540
H	2.089418	-2.630435	3.958265
H	0.575690	-2.974783	2.068977
C	-1.963553	-5.744932	0.372174
C	-1.023933	-5.647275	-0.653792
C	-0.379066	-4.434490	-0.910043
C	-0.660917	-3.290344	-0.144565
C	-1.625509	-3.400026	0.873305
C	-2.262034	-4.614814	1.135370
H	-2.464084	-6.689249	0.570527
H	-0.788351	-6.516179	-1.263360
H	0.341394	-4.388940	-1.717251
H	-1.883273	-2.523310	1.457007
H	-2.997510	-4.672199	1.932962
C	2.351476	-2.687200	-4.411863
C	2.835458	-3.137120	-3.181520
C	2.182342	-2.781382	-2.001196
C	1.034452	-1.971524	-2.026646
C	0.559907	-1.526930	-3.267298
C	1.213515	-1.880845	-4.450258
H	2.861747	-2.960165	-5.332107
H	3.727694	-3.755962	-3.137819
H	2.570106	-3.138461	-1.051370
H	-0.318362	-0.889184	-3.289756
H	0.831982	-1.521702	-5.403097
C	1.739550	3.354148	3.904248
C	2.284925	3.852429	2.717239
C	1.852811	3.358300	1.486774
C	0.855189	2.369932	1.423550
C	0.326788	1.870975	2.617399
C	0.765251	2.357543	3.852293
H	2.081370	3.736090	4.862788
H	3.052779	4.621343	2.751137
H	2.290957	3.747549	0.571214
H	-0.420615	1.087072	2.553684

H	0.347316	1.954404	4.771388
C	-1.524819	5.526446	-2.297840
C	-1.147346	5.588515	-0.957647
C	-0.573402	4.477457	-0.329567
C	-0.370986	3.275705	-1.026099
C	-0.785072	3.220932	-2.373140
C	-1.340502	4.334356	-3.004711
H	-1.963643	6.392380	-2.786456
H	-1.293724	6.504876	-0.391281
H	-0.284081	4.556919	0.712005
H	-1.635325	4.267765	-4.049171
C	5.142109	0.990685	2.913908
C	4.311854	0.795986	1.832415
H	5.896351	1.772368	2.877898
H	4.417271	1.428378	0.959507
C	5.021121	0.187006	4.071823
C	4.054636	-0.790266	4.122199
H	5.685971	0.347281	4.916429
H	3.941304	-1.412832	5.006907
C	5.958490	-1.306558	-1.569347
C	4.805937	-1.031678	-0.867253
H	6.612127	-2.108236	-1.235524
H	4.566321	-1.623230	0.007859
C	6.299744	-0.557223	-2.720091
C	5.467555	0.452116	-3.143168
H	7.213134	-0.782215	-3.264258
H	5.710699	1.036580	-4.027597
H	-0.683154	2.287730	-2.919310
C	-5.608648	-1.121979	-1.491272
H	-5.478353	-2.085279	-2.002377
H	-5.951203	-1.344221	-0.471122
C	-5.465660	1.837507	-1.446993
H	-5.585490	2.791700	-0.916771
H	-5.098651	2.080512	-2.456597
C	-6.816504	1.109366	-1.554465
H	-7.236561	0.979764	-0.547022
H	-7.530289	1.725603	-2.115100
C	-6.659332	-0.266771	-2.219060
H	-6.355940	-0.131423	-3.267840
H	-7.622660	-0.790963	-2.238434
C	-3.177630	-0.171126	2.576816
O	-4.118261	-0.801160	2.023884
C	-3.357687	1.326519	2.849236
H	-2.419014	1.837256	3.074316

H	-3.850173	1.822276	2.010054
H	-4.019674	1.428107	3.720877
C	-2.352000	-0.866042	3.648882
C	-3.103256	-1.258605	4.914888
C	-2.603667	-2.313947	3.966971
H	-1.344056	-0.489671	3.795845
H	-4.174813	-1.077917	4.936062
H	-2.601700	-1.124035	5.869991
H	-1.762564	-2.934396	4.264320
H	-3.355017	-2.807319	3.358586

Pf₁₂

Coordinates (Angstroms)			
	X	Y	Z

Ru		-1.15373400	0.12174900 -0.84537400
H		-3.44511100	0.51128600 2.01245100
H		-0.59485300	0.27011900 -2.31494200
N		-2.88664500	-0.99131500 -0.97991800
H		-2.80660600	-1.97445200 -1.24099400
H		-3.61626700	-1.18950100 0.70435000
N		-2.67980400	1.67101200 -1.34515600
H		-2.63584500	2.53311400 -0.80183200
H		-2.44548500	1.93850000 -2.30195500
P		0.31068200	-1.64924300 -0.56327500
P		0.47285600	1.71944400 -0.34191400
C		-4.04828000	1.08718700 -1.30398300
H		-4.33067200	1.05363400 -0.24386700
C		-3.93155900	-0.36011500 -1.78881800
H		-3.64182400	-0.32094800 -2.85865800
C		4.91797400	0.69520400 -1.52312000
C		4.21839300	1.76550600 -2.12918900
C		2.94007600	2.07676800 -1.73917200
C		2.26691800	1.34830400 -0.71802400
C		2.93198700	0.30008500 -0.07345800
C		4.27497000	-0.04306100 -0.47752100
H		4.70896200	2.34463500 -2.90837000
H		2.43722700	2.90795900 -2.21735900
C		2.53815100	-0.95437100 3.53366500
C		1.56287900	-1.96439100 3.36117700
C		0.99445500	-2.18724700 2.13232300

C	1.36148100	-1.43443200	0.97949400
C	2.35493800	-0.45307900	1.09884600
C	2.94019900	-0.18712300	2.39258800
H	1.26661700	-2.56712800	4.21665900
H	0.25299500	-2.97018500	2.03794600
C	-1.81667000	-5.79658200	0.02363800
C	-0.71295600	-5.70542700	-0.82483000
C	-0.05234700	-4.48693200	-0.99967400
C	-0.48132000	-3.33003500	-0.32757800
C	-1.60484600	-3.43594200	0.51285200
C	-2.26097900	-4.65480500	0.69184400
H	-2.32994900	-6.74563800	0.15587500
H	-0.36001600	-6.58461000	-1.35823700
H	0.79845100	-4.44707400	-1.66900000
H	-1.99464200	-2.56528700	1.02596500
H	-3.12840900	-4.69458900	1.34490700
C	3.26197500	-2.79057900	-3.99613700
C	3.55692300	-3.15058200	-2.67964800
C	2.69569700	-2.78447800	-1.64463400
C	1.53155700	-2.04451400	-1.90469100
C	1.24527400	-1.69145800	-3.23134400
C	2.10308200	-2.06244500	-4.26907200
H	3.93257800	-3.07502000	-4.80293300
H	4.46068600	-3.71044000	-2.45500700
H	2.93201400	-3.07720300	-0.62612600
H	0.34667700	-1.12148100	-3.44408000
H	1.86439000	-1.77947800	-5.29122900
C	0.59004800	3.45391400	3.99022300
C	1.60403700	3.79495000	3.09088900
C	1.59857200	3.26995600	1.79860000
C	0.57651800	2.40055300	1.38387900
C	-0.43102300	2.06304600	2.29626600
C	-0.42636100	2.58489700	3.59206700
H	0.59786600	3.85923400	4.99867300
H	2.40243600	4.46520100	3.39884300
H	2.39219000	3.53821900	1.10619900
H	-1.21549200	1.37669400	1.98720100
H	-1.21226700	2.30675100	4.28932500
C	-0.65166300	5.49611400	-2.89503600
C	-0.56440100	5.60771000	-1.50856400
C	-0.17760800	4.50985500	-0.73143900
C	0.12108700	3.27337000	-1.32472800
C	0.00886400	3.17263900	-2.72640800
C	-0.35924400	4.27125500	-3.50274700

H	-0.94745100	6.35064100	-3.49779400
H	-0.79336600	6.55236500	-1.02166600
H	-0.11042700	4.62655700	0.34441400
H	-0.42350000	4.16875700	-4.58320000
C	4.47494400	1.04958700	3.83966300
C	3.92338800	0.82482900	2.59810600
H	5.22048400	1.83087700	3.96229500
H	4.23853500	1.43381300	1.75986100
C	4.08044300	0.27647700	4.95712000
C	3.12766100	-0.70266500	4.80204300
H	4.52667500	0.46113500	5.93060800
H	2.80663000	-1.30362600	5.64972000
C	6.28985200	-1.41598100	-0.28709700
C	5.01140300	-1.10714900	0.12135400
H	6.82349100	-2.23350700	0.19056300
H	4.55437600	-1.68583400	0.91482100
C	6.91622400	-0.67893400	-1.32010300
C	6.23857800	0.35445200	-1.92305700
H	7.92630100	-0.93083700	-1.63181000
H	6.70284000	0.93182500	-2.71928500
H	0.20967700	2.22019700	-3.20803000
C	-5.30327300	-1.05725800	-1.71557400
H	-5.21369000	-2.07642200	-2.11493500
H	-5.58974400	-1.15934200	-0.66083200
C	-5.09909200	1.88706300	-2.08248900
H	-5.17157300	2.90929100	-1.68585100
H	-4.78078200	1.97560700	-3.13270300
C	-6.46774800	1.18549700	-2.01799600
H	-6.83270800	1.20789800	-0.98105300
H	-7.20015900	1.73916300	-2.61885300
C	-6.37640800	-0.27442800	-2.49183200
H	-6.13484200	-0.29001400	-3.56507300
H	-7.35261700	-0.76436000	-2.38633700
C	-3.83663900	-0.38724300	2.52414100
O	-4.06909000	-1.41138700	1.57119200
C	-2.79832700	-0.84595600	3.55719600
H	-2.63783400	-0.08408400	4.33163800
H	-3.14599100	-1.76247300	4.04677800
H	-1.83451000	-1.05351500	3.07953600
C	-5.14354800	-0.00007900	3.21096700
C	-6.45010900	0.03384500	2.46144400
C	-6.19618900	-1.04406000	3.48981500
H	-5.01440900	0.76430500	3.97717500
H	-6.43700400	-0.27312000	1.42020100

H	-7.16089300	0.82209900	2.69758200
H	-6.73402600	-1.00264800	4.43361700
H	-6.00779100	-2.04406200	3.11166300

Pu₁₂

Coordinates (Angstroms)			
	X	Y	Z
Ru	-1.16762300	0.61469300	-0.77161800
H	-2.64461700	-1.32051300	2.26882300
H	-0.54667700	1.30033400	-2.05373800
N	-2.97354100	-0.24504600	-1.24943100
H	-2.98462700	-1.07248100	-1.84609400
H	-3.71319000	-1.05295100	0.29694500
N	-2.56742800	2.34357200	-0.63888200
H	-2.44666800	2.95663300	0.16747200
H	-2.32196600	2.90937700	-1.45204900
P	0.18149100	-1.21461600	-1.21524000
P	0.53619800	1.76019200	0.33463200
C	-3.97821500	1.88442200	-0.75091300
H	-4.24977800	1.50017300	0.23996300
C	-3.99301900	0.69723800	-1.71576800
H	-3.74038900	1.09165600	-2.72120300
C	4.95904000	0.99961600	-1.09848200
C	4.34464700	2.26740400	-1.23023800
C	3.07226400	2.48069300	-0.76305700
C	2.32113200	1.45029900	-0.12992000
C	2.90149600	0.18959000	0.04677400
C	4.23738200	-0.05129800	-0.44496700
H	4.89625200	3.07599300	-1.70465200
H	2.63510700	3.46514300	-0.87320900
C	2.28559800	-2.37249900	2.84037300
C	1.25526700	-3.15374900	2.26660100
C	0.72563300	-2.82567300	1.04453400
C	1.18886600	-1.70719800	0.29280900
C	2.23573300	-0.93017000	0.80769800
C	2.78319800	-1.24705900	2.10677900
H	0.88449900	-4.02172700	2.80702100
H	-0.06255600	-3.44542100	0.63682900
C	-2.15937800	-5.10664600	-2.42723100
C	-1.00794700	-4.74952700	-3.12875700
C	-0.28609500	-3.60846100	-2.77055500

C	-0.69721500	-2.79894600	-1.69817500
C	-1.86684000	-3.16695100	-1.00779600
C	-2.58675700	-4.30843600	-1.36542000
H	-2.72224900	-5.99245500	-2.71012300
H	-0.66558500	-5.35715600	-3.96277100
H	0.59955100	-3.35280300	-3.33933400
H	-2.24051500	-2.55793200	-0.19323800
H	-3.49094800	-4.55812700	-0.81708600
C	3.18679900	-1.04396900	-4.78454800
C	3.42716100	-1.91047600	-3.71643800
C	2.55067600	-1.94276200	-2.63114500
C	1.42606300	-1.10397300	-2.58825300
C	1.19238200	-0.24325000	-3.67027200
C	2.06556400	-0.21323300	-4.75968100
H	3.86964000	-1.01704500	-5.62986500
H	4.30071400	-2.55666500	-3.72151000
H	2.74413900	-2.62726900	-1.81101400
H	0.32188700	0.40389200	-3.65092600
H	1.86800400	0.46170000	-5.58871600
C	0.54354800	1.55728600	4.99784900
C	1.62377100	2.15182600	4.34004200
C	1.65188600	2.20434100	2.94630600
C	0.59808000	1.66729200	2.18906900
C	-0.47653100	1.07091000	2.86055200
C	-0.50600500	1.01427500	4.25587700
H	0.52510200	1.51272000	6.08365900
H	2.44772800	2.56892200	4.91328700
H	2.49791600	2.66521200	2.44316700
H	-1.28735200	0.63925600	2.27887100
H	-1.34549600	0.54252000	4.75981200
C	-0.24078700	6.32135000	-0.46433200
C	-0.18304900	5.85665000	0.84834200
C	0.09957700	4.51164900	1.11281800
C	0.32089300	3.60048600	0.06831100
C	0.23956700	4.08322200	-1.25389600
C	-0.02437700	5.42715200	-1.51725100
H	-0.45592100	7.36688900	-0.66831800
H	-0.35411600	6.53933000	1.67691300
H	0.14619100	4.17815600	2.14346300
H	-0.06693800	5.77516300	-2.54638700
C	4.32986400	-0.80628500	3.94891600
C	3.81867200	-0.47694400	2.71337900
H	5.11765900	-0.19667900	4.38373200
H	4.20688000	0.38968400	2.19270700

C	3.83975100	-1.92774500	4.65888600
C	2.83513100	-2.69060400	4.11178000
H	4.25460700	-2.17910900	5.63133100
H	2.44097600	-3.55340300	4.64379900
C	6.16259000	-1.51669600	-0.80219300
C	4.88997500	-1.31274300	-0.31677200
H	6.63118800	-2.49071900	-0.68822600
H	4.37202600	-2.12916800	0.17182900
C	6.86661000	-0.47116700	-1.44569500
C	6.27138600	0.76002300	-1.58856900
H	7.87113900	-0.64403300	-1.82243200
H	6.79640300	1.57548000	-2.08073200
H	0.38187300	3.39355400	-2.08096800
C	-5.41641400	0.11262700	-1.80212000
H	-5.42629900	-0.71445200	-2.52455200
H	-5.68266600	-0.31765600	-0.82769600
C	-4.97197100	2.98032100	-1.15346400
H	-4.94855000	3.80333700	-0.42570000
H	-4.66946900	3.40455400	-2.12326700
C	-6.39397000	2.40046000	-1.26611600
H	-6.73391300	2.09200500	-0.26701300
H	-7.08903200	3.17831300	-1.60644400
C	-6.43739900	1.18851700	-2.21140400
H	-6.22333100	1.52419400	-3.23709800
H	-7.44907800	0.76387300	-2.22846300
C	-3.74697300	-1.39966400	2.27099100
O	-4.21486300	-1.61826600	0.95044000
C	-4.32859100	-0.10797200	2.86533700
H	-4.01022300	0.03261700	3.90672500
H	-4.00322800	0.76942800	2.29475400
H	-5.42309700	-0.14859500	2.84221900
C	-4.12387100	-2.59639100	3.13568300
C	-5.42428600	-3.32876900	2.91057800
C	-4.10819800	-4.00140000	2.59419500
H	-3.81247000	-2.48287900	4.17368600
H	-6.02840400	-3.01220000	2.06614100
H	-5.98742000	-3.66599200	3.77722700
H	-3.76183100	-4.80032100	3.24536600
H	-3.85900000	-4.12800100	1.54577500

ABS₁₃

Coordinates (Angstroms)

	X	Y	Z

Ru	-0.720485	0.365410	-0.910046
H	-1.495712	0.196564	0.623766
H	-0.182218	0.573116	-2.522809
N	-2.479636	-0.663561	-1.803753
H	-2.196055	-1.453652	-2.379914
H	-3.066836	-1.031847	-1.054886
N	-2.125038	2.052704	-1.316096
H	-2.223769	2.643694	-0.493600
H	-1.704203	2.631066	-2.042516
P	0.491294	-1.533861	-0.571296
P	0.967881	1.711754	-0.170502
C	-3.455998	1.561073	-1.750854
H	-3.986408	1.248656	-0.843553
C	-3.257597	0.304354	-2.609060
H	-2.620918	0.566387	-3.464758
C	5.239124	0.248898	-1.540572
C	4.642476	1.413900	-2.078233
C	3.420042	1.846045	-1.629100
C	2.706627	1.159033	-0.607169
C	3.274753	0.018967	-0.027113
C	4.551113	-0.459944	-0.503268
H	5.167393	1.967173	-2.854016
H	2.994129	2.742500	-2.061716
C	2.812340	-1.364855	3.529652
C	1.688516	-2.204409	3.341148
C	1.065390	-2.277553	2.120985
C	1.521573	-1.534904	0.995697
C	2.648499	-0.716086	1.130808
C	3.298855	-0.607431	2.415282
H	1.323729	-2.795225	4.178721
H	0.207022	-2.928568	2.011632
C	-2.497027	-5.136235	-0.119599
C	-1.412673	-5.255111	-0.987414
C	-0.488366	-4.212836	-1.113733
C	-0.633185	-3.024919	-0.379332
C	-1.748984	-2.911116	0.473482
C	-2.661815	-3.957190	0.612320
H	-3.211223	-5.949859	-0.019273
H	-1.277462	-6.162323	-1.571395
H	0.346736	-4.334000	-1.793530
H	-1.894758	-1.978653	1.012468
H	-3.509879	-3.844721	1.283135

C	3.434860	-3.238647	-3.778578
C	3.447164	-3.760617	-2.482411
C	2.592548	-3.238527	-1.511367
C	1.708521	-2.191334	-1.820808
C	1.708017	-1.672828	-3.121386
C	2.566422	-2.193035	-4.093834
H	4.104782	-3.641564	-4.534200
H	4.128889	-4.567446	-2.225515
H	2.612443	-3.648424	-0.504866
H	1.038063	-0.846019	-3.345017
H	2.558793	-1.775238	-5.097856
C	1.403133	2.952972	4.317369
C	2.411440	3.286580	3.409167
C	2.303718	2.900861	2.072864
C	1.183267	2.183142	1.621370
C	0.182480	1.848450	2.541196
C	0.292185	2.230107	3.881297
H	1.490027	3.248332	5.360092
H	3.285532	3.839771	3.743564
H	3.095456	3.163151	1.375592
H	-0.665425	1.267204	2.185410
H	-0.489704	1.956175	4.585721
C	0.377987	5.892444	-2.244167
C	0.511009	5.828878	-0.858109
C	0.732369	4.602460	-0.221860
C	0.818382	3.410171	-0.957605
C	0.658997	3.488633	-2.356733
C	0.453874	4.713986	-2.992387
H	0.211337	6.846733	-2.737363
H	0.445653	6.735626	-0.261567
H	0.836411	4.584553	0.856768
H	0.347819	4.746521	-4.074251
C	5.040092	0.305298	3.868741
C	4.428528	0.232830	2.636916
H	5.899638	0.956648	4.004233
H	4.811085	0.828721	1.817351
C	4.559691	-0.456848	4.959640
C	3.464910	-1.271371	4.788541
H	5.052940	-0.393505	5.926061
H	3.077373	-1.860414	5.616870
C	6.401083	-2.058272	-0.448966
C	5.177287	-1.630593	0.015962
H	6.850651	-2.955426	-0.031210
H	4.677024	-2.197822	0.791272

C	7.077025	-1.344652	-1.466646
C	6.500818	-0.216125	-2.000726
H	8.043298	-1.691141	-1.823728
H	7.002062	0.342876	-2.787767
H	0.675916	2.567902	-2.934228
C	-4.602158	-0.250573	-3.109114
H	-4.419690	-1.117936	-3.758160
H	-5.178250	-0.607918	-2.245653
C	-4.280667	2.626215	-2.491151
H	-4.442884	3.490178	-1.832844
H	-3.698128	2.991298	-3.351519
C	-5.622807	2.065473	-2.988227
H	-6.247828	1.800877	-2.123738
H	-6.166763	2.837321	-3.546971
C	-5.410698	0.819552	-3.860811
H	-4.877538	1.105428	-4.779673
H	-6.376799	0.406365	-4.176327
H	-6.769573	2.591950	3.055967
C	-6.369300	1.571206	3.059188
C	-4.952441	1.537058	2.466178
H	-7.064651	0.940049	2.493443
H	-6.367713	1.220245	4.099705
C	-4.365726	0.103259	2.438622
H	-5.010395	1.875133	1.422551
C	-4.013180	2.481352	3.228677
C	-5.155099	-0.834852	1.541343
H	-4.309240	-0.290775	3.461617
H	-3.346286	0.149043	2.028317
H	-3.923733	2.180117	4.280806
H	-3.006566	2.483813	2.795670
H	-4.394102	3.509793	3.212033
O	-5.180882	-0.653979	0.323939
C	-5.894548	-1.959980	2.172756
H	-5.833418	-2.060808	3.254681
C	-6.624251	-2.820559	1.444434
H	-6.646067	-2.662685	0.366076
C	-7.410682	-3.971366	1.985265
H	-7.326069	-4.054648	3.073252
H	-8.473398	-3.869565	1.726046
H	-7.074512	-4.915974	1.536633

INTf₁₃

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.842897	0.551264	-0.710006
H	-1.504328	-0.446875	0.531258
H	-0.419217	1.576771	-2.016823
N	-2.473826	-0.212315	-2.006570
H	-2.112135	-0.668639	-2.841646
H	-2.996544	-0.914636	-1.481035
N	-2.499885	2.018211	-0.354716
H	-2.699464	2.120661	0.637864
H	-2.146163	2.918317	-0.676350
P	0.676383	-1.041765	-1.295776
P	0.639875	1.622735	0.659638
C	-3.738934	1.650940	-1.085445
H	-4.278218	0.936838	-0.452403
C	-3.363440	0.908403	-2.375685
H	-2.757409	1.579096	-2.998430
C	5.083497	1.620764	-0.925541
C	4.306956	2.802877	-0.884446
C	3.032026	2.786137	-0.377812
C	2.439173	1.597201	0.132517
C	3.183272	0.411677	0.137628
C	4.520145	0.409263	-0.408964
H	4.734815	3.730149	-1.259443
H	2.467446	3.709758	-0.360531
C	2.962086	-2.599426	2.519067
C	2.001541	-3.394047	1.848505
C	1.395541	-2.942572	0.703225
C	1.711095	-1.677507	0.132021
C	2.684377	-0.877404	0.741405
C	3.308235	-1.324738	1.964272
H	1.749929	-4.372489	2.252182
H	0.665984	-3.576458	0.214608
C	-1.630484	-4.776638	-2.981235
C	-0.562241	-4.250013	-3.705589
C	0.164387	-3.163292	-3.208494
C	-0.166305	-2.573596	-1.977393
C	-1.264928	-3.101708	-1.270683
C	-1.978874	-4.196617	-1.758943
H	-2.191471	-5.624239	-3.366632
H	-0.285681	-4.683543	-4.663608
H	0.991436	-2.777455	-3.792443

H	-1.560759	-2.627122	-0.339010
H	-2.815415	-4.590976	-1.187767
C	3.823382	-0.406866	-4.694780
C	3.945267	-1.498675	-3.831494
C	3.026775	-1.676263	-2.796798
C	1.969683	-0.769997	-2.610509
C	1.858430	0.322040	-3.479999
C	2.780717	0.502745	-4.514300
H	4.541617	-0.264990	-5.498590
H	4.760488	-2.206470	-3.957991
H	3.131940	-2.527658	-2.129358
H	1.048657	1.029491	-3.318385
H	2.684365	1.359171	-5.177590
C	0.946258	0.691983	5.233534
C	1.881297	1.542984	4.637875
C	1.813256	1.807609	3.269957
C	0.805092	1.233183	2.476921
C	-0.122420	0.378593	3.083291
C	-0.051807	0.108564	4.452722
H	1.003486	0.480094	6.298381
H	2.668221	1.993821	5.237420
H	2.547594	2.468754	2.816764
H	-0.880907	-0.081041	2.454238
H	-0.774638	-0.564761	4.907670
C	-0.612546	6.157786	0.720206
C	-0.442994	5.479161	1.925851
C	-0.027357	4.143092	1.936111
C	0.221131	3.452856	0.739352
C	0.025701	4.147649	-0.472270
C	-0.374513	5.484654	-0.481710
H	-0.930792	7.197201	0.714326
H	-0.631196	5.986936	2.868791
H	0.100303	3.642714	2.888983
H	-0.505369	5.999205	-1.430838
C	4.868857	-1.005375	3.818776
C	4.276801	-0.546985	2.662819
H	5.603233	-0.386554	4.327870
H	4.548458	0.427648	2.276232
C	4.529241	-2.271162	4.351649
C	3.590944	-3.046973	3.712122
H	5.006204	-2.623124	5.262606
H	3.312268	-4.020411	4.109577
C	6.601326	-0.736653	-0.989037
C	5.326677	-0.764845	-0.468153

H	7.189520	-1.650240	-1.018869
H	4.925938	-1.700447	-0.097911
C	7.151365	0.467529	-1.488218
C	6.401338	1.619589	-1.457374
H	8.158966	0.477310	-1.895466
H	6.804429	2.554023	-1.841417
H	0.169006	3.612168	-1.407292
C	-4.623828	0.476229	-3.143144
H	-4.332919	-0.032802	-4.071735
H	-5.175843	-0.254827	-2.535404
C	-4.649996	2.853500	-1.381644
H	-4.933960	3.342549	-0.440300
H	-4.080316	3.595154	-1.962704
C	-5.901937	2.438822	-2.172999
H	-6.529973	1.793268	-1.542119
H	-6.503640	3.324426	-2.412762
C	-5.528052	1.679629	-3.454622
H	-5.004937	2.361200	-4.141153
H	-6.433521	1.345677	-3.976158
H	-2.537164	-5.219366	2.202429
C	-2.616847	-4.158013	2.467275
C	-3.851726	-3.521380	1.815332
H	-1.693349	-3.659166	2.152236
H	-2.674110	-4.094463	3.562083
C	-3.926901	-2.017447	2.154890
H	-3.750213	-3.591573	0.725163
C	-5.136440	-4.258560	2.222722
C	-4.979416	-1.268293	1.355927
H	-2.968246	-1.540003	1.893336
H	-4.085796	-1.880947	3.232584
H	-5.296664	-4.199158	3.307568
H	-6.018707	-3.836517	1.727450
H	-5.081198	-5.320411	1.954718
O	-5.031750	-1.373978	0.130678
C	-5.919333	-0.387361	2.100903
H	-5.767242	-0.282315	3.173531
C	-6.940785	0.235312	1.492273
H	-7.052190	0.073594	0.419892
C	-7.945665	1.118357	2.161086
H	-7.752555	1.223315	3.233264
H	-7.945863	2.119476	1.708838
H	-8.961193	0.720955	2.028500

TSf₁₃

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.157862	-0.592009	0.466876
H	-1.863712	0.841275	-0.413346
H	-0.752829	-1.973338	1.286613
N	-2.756673	-0.264803	1.933707
H	-2.427208	-0.045124	2.872110
H	-3.282823	0.552423	1.578703
N	-2.872184	-1.753421	-0.368441
H	-3.116452	-1.395099	-1.291581
H	-2.564801	-2.717924	-0.487422
P	0.477329	0.543118	1.632437
P	0.336164	-1.279390	-1.151481
C	-4.076714	-1.688953	0.502907
H	-4.626349	-0.796661	0.186160
C	-3.648474	-1.444054	1.953295
H	-3.046098	-2.293358	2.298773
C	4.680678	-2.276150	0.407745
C	3.799929	-3.289058	-0.038747
C	2.552906	-2.972642	-0.515712
C	2.091539	-1.628205	-0.586464
C	2.941691	-0.592975	-0.181354
C	4.253675	-0.911078	0.332355
H	4.124931	-4.326518	-0.003020
H	1.911406	-3.773636	-0.859288
C	3.072446	3.059789	-1.379115
C	2.139597	3.659245	-0.498922
C	1.448543	2.900627	0.411545
C	1.650652	1.495544	0.528130
C	2.582820	0.866402	-0.304952
C	3.293229	1.646746	-1.290922
H	1.974364	4.732886	-0.554540
H	0.735740	3.386291	1.067347
C	-1.243788	3.849807	4.505940
C	-0.038461	3.223877	4.828294
C	0.494351	2.240367	3.992499
C	-0.163572	1.861041	2.809377
C	-1.381136	2.494056	2.505357
C	-1.914815	3.478872	3.340625
H	-1.657522	4.613041	5.160198

H	0.491811	3.496434	5.737501
H	1.424638	1.764284	4.277731
H	-1.928944	2.215643	1.613939
H	-2.859917	3.944133	3.073276
C	3.195074	-1.704401	4.706870
C	3.643326	-0.514508	4.130441
C	2.856579	0.144467	3.184459
C	1.612002	-0.374217	2.792676
C	1.177555	-1.573267	3.374306
C	1.960564	-2.231485	4.325046
H	3.807621	-2.219524	5.442515
H	4.609934	-0.102325	4.407397
H	3.219130	1.067649	2.742540
H	0.229564	-1.994182	3.053779
H	1.606251	-3.161723	4.762733
C	1.139087	1.070896	-5.111813
C	1.857630	-0.097940	-4.844252
C	1.640676	-0.795697	-3.656464
C	0.691335	-0.344321	-2.723568
C	-0.015150	0.830884	-2.998506
C	0.207554	1.536891	-4.184154
H	1.313447	1.618135	-6.034661
H	2.592966	-0.461111	-5.557865
H	2.210021	-1.699648	-3.455568
H	-0.725983	1.189723	-2.261619
H	-0.343768	2.453708	-4.378202
C	-1.355569	-5.360344	-2.760825
C	-1.121566	-4.313268	-3.650413
C	-0.571113	-3.108379	-3.199919
C	-0.247032	-2.920414	-1.847128
C	-0.514523	-3.980542	-0.955952
C	-1.049031	-5.187933	-1.407821
H	-1.777599	-6.297863	-3.113209
H	-1.364289	-4.427883	-4.703928
H	-0.397598	-2.313162	-3.915536
H	-1.231141	-5.992763	-0.699734
C	4.902483	1.840894	-3.120729
C	4.224468	1.070099	-2.202734
H	5.605051	1.369554	-3.803012
H	4.396629	0.001205	-2.175251
C	4.691014	3.238091	-3.187621
C	3.789526	3.829919	-2.334200
H	5.235240	3.835900	-3.913912
H	3.607094	4.901332	-2.376569

C	6.411776	-0.246604	1.272623
C	5.167135	0.085665	0.785585
H	7.083698	0.538544	1.609443
H	4.874819	1.127909	0.746834
C	6.824818	-1.598536	1.338234
C	5.971222	-2.589383	0.914111
H	7.810195	-1.847834	1.722760
H	6.269010	-3.634467	0.959218
H	-0.316617	-3.839908	0.102754
C	-4.881426	-1.292576	2.859956
H	-4.561044	-1.134882	3.898512
H	-5.439953	-0.394645	2.558998
C	-4.986927	-2.918219	0.381267
H	-5.307283	-3.041474	-0.661747
H	-4.410931	-3.819145	0.643961
C	-6.209363	-2.801209	1.308011
H	-6.849286	-1.979111	0.956702
H	-6.813428	-3.715036	1.248938
C	-5.790879	-2.528937	2.761178
H	-5.256212	-3.405414	3.156061
H	-6.678010	-2.394782	3.392149
H	-3.050632	6.566013	-0.879760
C	-2.443390	5.652887	-0.916609
C	-3.330790	4.399540	-0.964385
H	-1.790203	5.647380	-0.035603
H	-1.802515	5.717763	-1.806358
C	-2.450455	3.126816	-0.962763
H	-3.929866	4.364900	-0.044827
C	-4.292466	4.466525	-2.160120
C	-3.262844	1.842725	-0.682428
H	-1.691190	3.239706	-0.186143
H	-1.914735	3.045270	-1.917549
H	-3.738208	4.475737	-3.108922
H	-4.974869	3.611811	-2.181332
H	-4.897547	5.381053	-2.122660
O	-3.970646	1.798977	0.361390
C	-3.690665	1.087738	-1.912946
H	-2.966462	1.018550	-2.723293
C	-4.928085	0.596965	-2.075770
H	-5.634903	0.732824	-1.257135
C	-5.437461	-0.083879	-3.314333
H	-4.657107	-0.175760	-4.077869
H	-5.819368	-1.091002	-3.094524
H	-6.276571	0.473264	-3.753660

TSu₁₃

	Coordinates (Angstroms)		
	X	Y	Z

Ru	1.118781	0.477831	-0.641392
H	1.901559	-0.293690	0.857560
H	0.702316	1.202497	-2.062382
N	2.695386	1.973652	-0.375383
H	2.350564	2.921619	-0.234074
H	3.196002	1.680904	0.484192
N	2.814135	-0.356055	-1.838277
H	3.015065	-1.331707	-1.623190
H	2.487955	-0.341428	-2.804130
P	-0.552472	1.689576	0.385336
P	-0.340944	-1.226538	-1.203668
C	4.048501	0.461357	-1.698370
H	4.524030	0.147859	-0.762277
C	3.646880	1.929256	-1.508057
H	3.101519	2.268572	-2.398967
C	-4.796513	0.035023	-2.128912
C	-3.938214	-0.455707	-3.140597
C	-2.655332	-0.841940	-2.844134
C	-2.133213	-0.771198	-1.521934
C	-2.959142	-0.321918	-0.485345
C	-4.308432	0.098218	-0.783866
H	-4.309173	-0.527246	-4.160661
H	-2.031508	-1.222630	-3.642467
C	-2.900726	-1.195234	3.259183
C	-2.016397	-0.202577	3.746735
C	-1.401670	0.671806	2.886657
C	-1.643656	0.639984	1.484005
C	-2.539955	-0.300656	0.963453
C	-3.161925	-1.253964	1.851327
H	-1.826600	-0.142472	4.816176
H	-0.719135	1.411361	3.287456
C	1.192984	5.028964	3.190438
C	0.072231	5.316620	2.410740
C	-0.482727	4.339561	1.580416
C	0.072408	3.050279	1.513526
C	1.210778	2.780915	2.292749

C	1.761125	3.755543	3.127623
H	1.623602	5.791717	3.834275
H	-0.375399	6.306907	2.442813
H	-1.348166	4.594497	0.980872
H	1.668845	1.800328	2.245623
H	2.640772	3.515579	3.718950
C	-3.523036	4.316632	-2.096248
C	-3.861061	3.915375	-0.802095
C	-2.993866	3.100313	-0.073699
C	-1.776442	2.667035	-0.624518
C	-1.449920	3.076946	-1.923940
C	-2.315492	3.895015	-2.653928
H	-4.198956	4.949584	-2.665663
H	-4.804149	4.227324	-0.361391
H	-3.268265	2.797630	0.932672
H	-0.515931	2.735264	-2.359333
H	-2.044864	4.199475	-3.662120
C	-0.905170	-5.089122	1.364605
C	-1.638287	-4.931431	0.184573
C	-1.491949	-3.774948	-0.580648
C	-0.597694	-2.764605	-0.186197
C	0.123139	-2.929772	1.000031
C	-0.029350	-4.083961	1.773815
H	-1.024689	-5.988280	1.963542
H	-2.329404	-5.707279	-0.135370
H	-2.072164	-3.660339	-1.492721
H	0.794501	-2.134796	1.306717
H	0.534905	-4.194288	2.696518
C	1.357648	-2.931774	-5.238487
C	1.238861	-3.769333	-4.130927
C	0.680743	-3.294735	-2.938517
C	0.236070	-1.968078	-2.824481
C	0.386602	-1.127233	-3.946710
C	0.926688	-1.605316	-5.141164
H	1.785362	-3.303400	-6.165906
H	1.577258	-4.800875	-4.188089
H	0.595159	-3.970611	-2.095287
H	1.016017	-0.938085	-5.995017
C	-4.632648	-3.162609	2.260099
C	-4.041849	-2.274980	1.388554
H	-5.295131	-3.933189	1.874693
H	-4.240631	-2.358950	0.327182
C	-4.383122	-3.084817	3.650510
C	-3.530531	-2.120382	4.134676

H	-4.859700	-3.788276	4.328074
H	-3.319889	-2.050559	5.199467
C	-6.479316	0.993811	-0.101019
C	-5.198761	0.595672	0.212673
H	-7.132366	1.368241	0.683007
H	-4.858915	0.665567	1.238741
C	-6.953206	0.920983	-1.432411
C	-6.123042	0.451786	-2.422897
H	-7.966452	1.236333	-1.666654
H	-6.467653	0.391451	-3.452702
H	0.090193	-0.085319	-3.869862
C	4.894154	2.807268	-1.309152
H	4.592414	3.857495	-1.199227
H	5.385174	2.515000	-0.370709
C	5.030933	0.288010	-2.864741
H	5.327131	-0.766237	-2.947481
H	4.521419	0.547816	-3.805978
C	6.270516	1.181726	-2.689733
H	6.844561	0.835238	-1.818736
H	6.930310	1.081512	-3.560430
C	5.875506	2.651880	-2.482761
H	5.408263	3.035838	-3.401762
H	6.769048	3.263736	-2.308478
H	6.040426	-3.043148	3.644018
C	5.046524	-2.737589	3.293832
C	5.100779	-2.293531	1.824405
H	4.687527	-1.937639	3.946887
H	4.374158	-3.598007	3.416917
C	3.726863	-1.833511	1.276883
H	5.773840	-1.429089	1.749526
C	5.666633	-3.422659	0.948491
C	3.281648	-0.465383	1.839648
H	2.971951	-2.606358	1.465595
H	3.820773	-1.738557	0.191671
H	5.007156	-4.300984	0.961115
H	5.777439	-3.105467	-0.096255
H	6.652539	-3.744950	1.305936
O	4.037490	0.528134	1.627855
C	2.488045	-0.533750	3.114932
H	1.733063	-1.314678	3.190304
C	2.723143	0.279819	4.152332
H	3.505502	1.029039	4.031572
C	1.997303	0.246468	5.465264
H	1.233874	-0.538983	5.486182

H	2.689010	0.072422	6.301334
H	1.501877	1.207024	5.666588

Pf₁₃

Coordinates (Angstroms)			
	X	Y	Z

Ru		0.83102700	1.03012400 0.49099600
H		3.07002000	-0.75525600 -1.13582900
H		0.11435900	2.24440500 1.19697900
N		2.53845400	0.73395300 1.63028300
H		2.40889000	0.39178100 2.58320300
H		3.49164300	-0.61837600 0.93807200
N		2.26258300	2.49908400 -0.39623500
H		2.31740400	2.50560500 -1.41474100
H		1.86858400	3.40451400 -0.13802000
P		-0.56870500	-0.36737900 1.69854100
P		-0.75672500	1.35768400 -1.19040400
C		3.61655900	2.34674500 0.20655100
H		4.09762800	1.51685200 -0.32604100
C		3.41377000	1.90774100 1.65933600
H		2.93043500	2.75330700 2.18912200
C		-5.28573300	1.31386200 0.11930600
C		-4.66811200	2.48794000 -0.37259800
C		-3.36040000	2.46992000 -0.78837200
C		-2.57429500	1.28371000 -0.74795200
C		-3.15487300	0.09435400 -0.29505200
C		-4.52711300	0.09936700 0.15311900
H		-5.24542100	3.40852700 -0.42204800
H		-2.92337900	3.38451800 -1.16881200
C		-2.33892500	-3.51233600 -1.33363600
C		-1.35501000	-3.85077200 -0.37507200
C		-0.92223300	-2.92629500 0.54169400
C		-1.44273700	-1.60035300 0.58412700
C		-2.44364900	-1.23519700 -0.32589600
C		-2.89030400	-2.19026900 -1.31369400
H		-0.94393500	-4.85772900 -0.37028900
H		-0.17132100	-3.22242500 1.26290000
C		1.67755800	-3.03759700 4.84236300
C		0.47745900	-2.42261000 5.19998800
C		-0.21840600	-1.63670800 4.27805700

C	0.27191000	-1.44909500	2.97484900
C	1.49173000	-2.06221200	2.63532600
C	2.18337800	-2.85245000	3.55487700
H	2.21730600	-3.64702900	5.56273800
H	0.07585200	-2.55030200	6.20222700
H	-1.14480500	-1.16841300	4.58762400
H	1.93027000	-1.91505700	1.65546300
H	3.12527600	-3.30493100	3.25727700
C	-3.85729500	1.45048100	4.46837300
C	-3.99869400	0.14780700	3.98602900
C	-3.03713100	-0.38913100	3.12924000
C	-1.92357100	0.36761900	2.73200100
C	-1.79167200	1.67348500	3.22585000
C	-2.75042200	2.21050900	4.08758500
H	-4.60621100	1.86984200	5.13528800
H	-4.86047900	-0.45018800	4.26959100
H	-3.15411800	-1.40626300	2.76794400
H	-0.93313500	2.26658200	2.92862200
H	-2.63091600	3.22495200	4.45969200
C	-0.52933300	-1.26965900	-5.04413400
C	-1.58178200	-0.36182200	-4.89677100
C	-1.67543000	0.41979400	-3.74542000
C	-0.71158200	0.31494900	-2.72890000
C	0.33588300	-0.60027400	-2.88803600
C	0.42757300	-1.39081000	-4.03620800
H	-0.46167500	-1.88413100	-5.93806100
H	-2.33452000	-0.26963400	-5.67553900
H	-2.50122300	1.11805200	-3.63633000
H	1.07364100	-0.70197400	-2.09616100
H	1.24224400	-2.10310400	-4.13731000
C	0.01381200	5.69948300	-2.80284500
C	0.07313200	4.62147200	-3.68408700
C	-0.20562600	3.32438800	-3.23846700
C	-0.54221600	3.07654000	-1.89869000
C	-0.57536300	4.17554900	-1.01574000
C	-0.31477900	5.47073100	-1.46315600
H	0.22567300	6.70678100	-3.15135000
H	0.33407200	4.78313000	-4.72698700
H	-0.15785800	2.50503200	-3.94675000
H	-0.36228900	6.30120800	-0.76311600
C	-4.29480800	-2.81131700	-3.21626100
C	-3.87625900	-1.87740600	-2.29480200
H	-5.04746000	-2.53965500	-3.95175000
H	-4.30097100	-0.88146900	-2.31825100

C	-3.75332700	-4.11846900	-3.21820200
C	-2.79125500	-4.45555300	-2.29543900
H	-4.09470300	-4.84714500	-3.94856100
H	-2.35822500	-5.45313200	-2.28467100
C	-6.49219300	-1.03464300	1.06554500
C	-5.18221800	-1.06892500	0.64174500
H	-6.96195000	-1.94354100	1.43230300
H	-4.63660200	-2.00391700	0.68049200
C	-7.23307600	0.17052300	1.02636100
C	-6.63624300	1.31894500	0.56223900
H	-8.26665200	0.18400500	1.36163900
H	-7.18891400	2.25490200	0.52533400
H	-0.80283000	4.00785500	0.03311600
C	4.77739600	1.66996100	2.33483900
H	4.61914800	1.39533000	3.38634200
H	5.26429700	0.81121900	1.85477400
C	4.49741300	3.59705500	0.08994000
H	4.64395400	3.86299600	-0.96605100
H	3.98300100	4.44750000	0.56377400
C	5.85460900	3.37042700	0.78081500
H	6.41265500	2.60209300	0.22679500
H	6.45470700	4.28799600	0.73588200
C	5.67655700	2.91402000	2.23788300
H	5.22980400	3.73345800	2.82045600
H	6.65587700	2.71024400	2.68925800
H	3.86673700	-6.17611700	-0.24940200
C	3.28853100	-5.31240400	-0.60088500
C	4.18204900	-4.07144900	-0.76073500
H	2.48142700	-5.13271300	0.11972800
H	2.82535300	-5.59241900	-1.55715000
C	3.34634900	-2.86656600	-1.24865100
H	4.57451500	-3.80893200	0.22993100
C	5.36808800	-4.38975500	-1.68499700
C	3.85846900	-1.46784400	-0.82122700
H	2.32865800	-2.95463400	-0.84590100
H	3.24892800	-2.89932800	-2.34531400
H	5.01624600	-4.66851100	-2.68823200
H	6.04036700	-3.53368300	-1.78871500
H	5.95224200	-5.23287900	-1.29490800
O	3.99185200	-1.42122400	0.58354300
C	5.12584800	-1.04580600	-1.53773700
H	5.06714500	-1.05087100	-2.62922800
C	6.26309300	-0.67640600	-0.94156200
H	6.29371300	-0.69937400	0.14642900

C	7.51664800	-0.25250300	-1.65450700
H	7.38838400	-0.26005000	-2.74292800
H	7.82481000	0.76013600	-1.35775300
H	8.35801200	-0.91556400	-1.40917200

Pu₁₃

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.78899400	0.90651100	-0.86182200
H	-2.43032500	-1.22981600	1.01858100
H	-0.06556600	1.85783900	-1.89042200
N	-2.50543600	0.32002300	-1.85988600
H	-2.39357500	-0.26128600	-2.69088000
H	-3.45782700	-0.78691000	-0.80997200
N	-2.18486500	2.59237800	-0.42831900
H	-2.20368300	2.93094700	0.53373200
H	-1.80287000	3.35940700	-0.98311100
P	0.60035900	-0.79622300	-1.58506800
P	0.77603400	1.68547100	0.69419600
C	-3.55718900	2.26047300	-0.89784900
H	-3.98580100	1.60211200	-0.13145300
C	-3.41235500	1.42758200	-2.17358800
H	-2.98253000	2.09121000	-2.95099900
C	5.35236400	0.86077600	-0.07135300
C	4.83442000	2.17592100	-0.00712200
C	3.50499600	2.39233500	0.25474600
C	2.59748500	1.31801600	0.47791600
C	3.07329500	0.00265900	0.45048500
C	4.46784000	-0.24070000	0.16594500
H	5.50476700	3.01725900	-0.16803000
H	3.14116800	3.41120100	0.29947500
C	1.78367400	-3.06897100	2.36327800
C	0.85546600	-3.59312100	1.43331000
C	0.60479000	-2.94379000	0.25120900
C	1.26646400	-1.73248600	-0.10152600
C	2.21945500	-1.19743300	0.77648600
C	2.47545800	-1.85772500	2.03522100
H	0.33591700	-4.51957600	1.66636700
H	-0.11655600	-3.37336600	-0.43178300
C	-1.48720100	-4.04177700	-4.26979600
C	-0.23111100	-3.55404800	-4.62998900

C	0.41448900	-2.60494200	-3.83406700
C	-0.18085600	-2.12100200	-2.65651300
C	-1.45643600	-2.60940300	-2.31728200
C	-2.09731900	-3.56348400	-3.10978200
H	-1.98855300	-4.77995100	-4.89055500
H	0.25438000	-3.90945400	-5.53550700
H	1.38656200	-2.24217600	-4.14390600
H	-1.97370900	-2.24212900	-1.43926300
H	-3.08132600	-3.91929500	-2.81710800
C	4.25847400	0.13110600	-4.33227400
C	4.25209700	-1.02597000	-3.55050400
C	3.17820300	-1.28888400	-2.69958700
C	2.09681100	-0.39839600	-2.60753200
C	2.11391200	0.75769900	-3.40018200
C	3.18603800	1.02076200	-4.25572600
H	5.09470700	0.33717300	-4.99540800
H	5.08514000	-1.72210700	-3.59589500
H	3.18101100	-2.19655400	-2.10378700
H	1.28044900	1.45003400	-3.34229300
H	3.18097300	1.92278700	-4.86252100
C	-0.00728200	0.76222100	5.20684700
C	1.23985900	1.25741100	4.81731300
C	1.50164000	1.51707900	3.47169000
C	0.52095300	1.28639600	2.49346800
C	-0.72405800	0.78699700	2.89773200
C	-0.98962000	0.52679900	4.24422500
H	-0.20914500	0.55716800	6.25491900
H	2.01113200	1.43741700	5.56181700
H	2.47382800	1.90442900	3.17965100
H	-1.48714400	0.59416300	2.14802800
H	-1.96134500	0.13785000	4.53707000
C	0.44367300	6.37058600	0.65001800
C	0.29476500	5.68700100	1.85548500
C	0.43534200	4.29546600	1.90309200
C	0.71796400	3.55793200	0.74296400
C	0.85191500	4.26300000	-0.46992200
C	0.72848500	5.65149100	-0.51486100
H	0.33806200	7.45166300	0.61478100
H	0.07131500	6.23307500	2.76857100
H	0.32315300	3.78844800	2.85492800
H	0.84927200	6.17186800	-1.46177000
C	3.63493300	-2.00830800	4.18306100
C	3.40378100	-1.35440600	2.99346800
H	4.34755500	-1.59601800	4.89261500

H	3.93524000	-0.43472700	2.78212300
C	2.95347000	-3.20917200	4.49244200
C	2.04476700	-3.72307200	3.59765800
H	3.14710200	-3.71705200	5.43342400
H	1.50741400	-4.64229300	3.81925400
C	6.35384700	-1.75670800	-0.18764000
C	5.02168900	-1.55286400	0.09632600
H	6.74403900	-2.77002700	-0.23437100
H	4.37931600	-2.40804100	0.26801500
C	7.21983500	-0.66094200	-0.41639600
C	6.72337200	0.61996300	-0.35827400
H	8.26967500	-0.83498600	-0.63646000
H	7.37284000	1.47451700	-0.53358300
H	1.05235600	3.71203800	-1.38391100
C	-4.80366800	0.98466400	-2.66714000
H	-4.69372000	0.41945900	-3.60225300
H	-5.23588500	0.29448200	-1.93031200
C	-4.46978900	3.47793200	-1.08767300
H	-4.56823400	4.03134500	-0.14330600
H	-4.00764500	4.16635800	-1.81198400
C	-5.85315400	3.04188500	-1.60291800
H	-6.35830100	2.45682600	-0.82068300
H	-6.47886100	3.92447800	-1.78579800
C	-5.73742000	2.18922800	-2.87706600
H	-5.35063500	2.81459400	-3.69551300
H	-6.73195400	1.84749400	-3.19040100
H	-7.29676600	-2.33402800	2.87714600
C	-6.20737300	-2.20376700	2.89757600
C	-5.78806600	-0.98332200	2.06272100
H	-5.75013200	-3.12365700	2.52418500
H	-5.90984100	-2.07891200	3.94826900
C	-4.25887400	-0.77131600	2.03154100
H	-6.10579700	-1.14589200	1.02491100
C	-6.49470700	0.27887800	2.58375500
C	-3.46803900	-1.62061200	0.99813100
H	-3.83756700	-0.93449900	3.03616700
H	-4.05907500	0.28079700	1.78339800
H	-6.17645100	0.51770400	3.60804800
H	-6.27352900	1.15124000	1.95572400
H	-7.58364200	0.14646600	2.60011000
O	-4.00088900	-1.46667900	-0.30075500
C	-3.37771500	-3.08237300	1.37557600
H	-2.98021100	-3.27834100	2.37379200
C	-3.72539500	-4.10535800	0.59055200

H	-4.12738400	-3.87448900	-0.39415400
C	-3.61752800	-5.55687100	0.96522800
H	-3.20464600	-5.68705200	1.97224700
H	-4.59876400	-6.05125600	0.93721500
H	-2.97454000	-6.10477800	0.26213000

TSf₁₄

Coordinates (Angstroms)			
	X	Y	Z
Ru	0.982261	0.469346	-0.500286
H	1.843859	-0.222635	1.100827
H	0.551792	1.078726	-1.957877
N	2.465833	2.076306	-0.355355
H	2.054393	3.001155	-0.240000
H	3.014415	1.875799	0.501362
N	2.728413	-0.335427	-1.640353
H	3.056249	-1.226576	-1.269119
H	2.387864	-0.515974	-2.583643
P	-0.768219	1.715962	0.373363
P	-0.430028	-1.286394	-1.045307
C	3.870882	0.615887	-1.677658
H	4.466700	0.403932	-0.785366
C	3.351771	2.049683	-1.538565
H	2.728626	2.288947	-2.409757
C	-4.818674	-0.155308	-2.394100
C	-3.875873	-0.690413	-3.302177
C	-2.612814	-1.024750	-2.883696
C	-2.194155	-0.857302	-1.533661
C	-3.106757	-0.364009	-0.594580
C	-4.436780	0.006954	-1.023442
H	-4.165282	-0.838669	-4.340203
H	-1.925876	-1.446050	-3.605233
C	-3.380699	-0.987855	3.188795
C	-2.554284	0.047898	3.687626
C	-1.862339	0.865267	2.830237
C	-1.966466	0.731847	1.416102
C	-2.809883	-0.248089	0.879650
C	-3.505596	-1.147301	1.770122
H	-2.467594	0.184380	4.763193
H	-1.224251	1.639439	3.239277
C	0.639259	5.204402	3.189029

C	-0.575700	5.325666	2.510530
C	-1.022012	4.303116	1.671937
C	-0.266004	3.129593	1.499856
C	0.952968	3.023233	2.187443
C	1.402810	4.049454	3.022846
H	0.987118	6.005992	3.835855
H	-1.178607	6.222908	2.627158
H	-1.959917	4.432435	1.144850
H	1.564200	2.136118	2.075972
H	2.354721	3.934109	3.534500
C	-3.436897	4.291318	-2.487199
C	-3.958863	3.833123	-1.276730
C	-3.182352	3.031596	-0.438010
C	-1.874874	2.664319	-0.793254
C	-1.365419	3.129808	-2.013805
C	-2.137164	3.936973	-2.851986
H	-4.040287	4.914307	-3.142547
H	-4.974513	4.088206	-0.986298
H	-3.604329	2.684638	0.499862
H	-0.363969	2.835312	-2.310325
H	-1.721719	4.284357	-3.794974
C	-1.302607	-4.946514	1.722133
C	-1.856385	-4.907363	0.438697
C	-1.611930	-3.817030	-0.394943
C	-0.791874	-2.758820	0.034574
C	-0.250731	-2.804906	1.321670
C	-0.506608	-3.890806	2.164719
H	-1.500798	-5.792735	2.374892
H	-2.485614	-5.723145	0.091363
H	-2.056815	-3.791395	-1.386426
H	0.361620	-1.970069	1.648997
H	-0.085490	-3.907328	3.166298
C	1.562384	-3.245951	-4.823597
C	1.397847	-3.994598	-3.659568
C	0.754613	-3.443476	-2.545960
C	0.265043	-2.128058	-2.568018
C	0.466760	-1.374656	-3.743295
C	1.093293	-1.929512	-4.860246
H	2.055603	-3.677444	-5.690526
H	1.766358	-5.016264	-3.611423
H	0.637211	-4.050644	-1.655718
H	1.219939	-1.329431	-5.758027
C	-4.992458	-3.045241	2.170753
C	-4.328382	-2.211305	1.298949

H	-5.607253	-3.851434	1.779268
H	-4.421863	-2.373266	0.232245
C	-4.878608	-2.867168	3.569616
C	-4.084108	-1.859156	4.063522
H	-5.412259	-3.528865	4.246712
H	-3.976588	-1.712685	5.135866
C	-6.672319	0.892656	-0.570667
C	-5.412803	0.546059	-0.134182
H	-7.391153	1.300987	0.134913
H	-5.158160	0.687603	0.908936
C	-7.040272	0.720968	-1.926234
C	-6.126466	0.207914	-2.815966
H	-8.038092	0.995282	-2.257952
H	-6.388248	0.071501	-3.862763
H	0.140342	-0.339020	-3.771050
C	4.526505	3.040476	-1.469188
H	4.142800	4.066288	-1.388455
H	5.103974	2.844243	-0.554660
C	4.766889	0.459351	-2.913972
H	5.146182	-0.568961	-2.966715
H	4.165753	0.627778	-3.821056
C	5.934915	1.460262	-2.875435
H	6.597010	1.201058	-2.037231
H	6.535885	1.371633	-3.788965
C	5.436675	2.903491	-2.701686
H	4.878383	3.205731	-3.599999
H	6.287407	3.590950	-2.618409
C	3.346475	-0.073412	2.135621
O	3.628890	1.153702	2.069068
C	6.089501	-2.713419	0.027482
C	6.520129	-1.525854	0.621055
C	5.604400	-0.693212	1.269461
C	4.243332	-1.031518	1.346280
C	3.824767	-2.231814	0.751253
C	4.736692	-3.061642	0.094713
H	6.797720	-3.362555	-0.480921
H	7.569796	-1.244776	0.579727
H	5.928567	0.239404	1.720732
H	2.774130	-2.501646	0.784985
H	4.388337	-3.982995	-0.366022
C	2.882843	-0.608156	3.544968
C	2.646857	-2.126033	3.629412
C	4.061036	-0.263036	4.494845
C	1.629977	0.125687	4.039731

H	1.861168	-2.461450	2.950887
H	3.551974	-2.699615	3.407793
H	2.335653	-2.383719	4.649705
H	4.248361	0.813880	4.497693
H	3.821274	-0.583814	5.516294
H	4.983754	-0.772825	4.192853
H	1.374504	-0.213022	5.052045
H	1.795539	1.204451	4.079930
H	0.776063	-0.068981	3.384988

TSu₁₄

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.060581	0.765407	0.366148
H	2.015817	-0.525089	-0.784996
H	0.572297	1.981890	1.338631
N	2.778928	0.492049	1.685775
H	2.548225	0.089988	2.592915
H	3.403027	-0.166359	1.185561
N	2.510511	2.328956	-0.335362
H	2.714076	2.270158	-1.330098
H	2.023793	3.212001	-0.189884
P	-0.386008	-0.558472	1.595759
P	-0.643152	1.445968	-1.056206
C	3.782007	2.304388	0.434874
H	4.414905	1.558052	-0.055506
C	3.502316	1.773329	1.846557
H	2.821603	2.464064	2.361714
C	-5.003336	1.758902	0.745418
C	-4.286009	2.905611	0.332207
C	-3.026630	2.789374	-0.199664
C	-2.388568	1.527603	-0.362986
C	-3.076986	0.364328	-0.000801
C	-4.399298	0.471881	0.573445
H	-4.747258	3.885167	0.437133
H	-2.515860	3.688419	-0.518187
C	-2.862807	-3.215476	-1.381784
C	-1.854172	-3.758674	-0.549271
C	-1.196897	-2.971235	0.362288
C	-1.522959	-1.596325	0.537213

C	-2.549578	-1.030798	-0.228216
C	-3.210316	-1.833484	-1.230189
H	-1.601663	-4.812594	-0.644244
H	-0.413300	-3.409917	0.968324
C	1.854147	-3.597520	4.393495
C	0.701255	-2.966189	4.861777
C	0.003583	-2.071672	4.047350
C	0.444578	-1.788358	2.742649
C	1.615562	-2.421560	2.292445
C	2.309688	-3.322037	3.103781
H	2.394867	-4.293591	5.029848
H	0.339275	-3.165688	5.867417
H	-0.883561	-1.592560	4.442191
H	1.984667	-2.210825	1.295964
H	3.203655	-3.802059	2.717571
C	-3.200272	1.326770	4.828841
C	-3.514871	0.091253	4.260128
C	-2.697231	-0.450455	3.267619
C	-1.554864	0.231964	2.817631
C	-1.250259	1.469839	3.399659
C	-2.065005	2.012852	4.395980
H	-3.837022	1.751363	5.600805
H	-4.401803	-0.448950	4.580132
H	-2.952787	-1.414676	2.838791
H	-0.374802	2.009846	3.053736
H	-1.811275	2.976381	4.831439
C	-1.690457	-0.585961	-5.131216
C	-2.337453	0.598938	-4.766587
C	-2.034132	1.216358	-3.554082
C	-1.060772	0.671223	-2.697721
C	-0.427405	-0.516290	-3.069471
C	-0.741404	-1.146253	-4.277579
H	-1.933680	-1.071779	-6.072601
H	-3.084624	1.036879	-5.423870
H	-2.554688	2.128697	-3.274638
H	0.308652	-0.935141	-2.390713
H	-0.243949	-2.073752	-4.548443
C	0.573069	5.828454	-2.225719
C	0.502505	4.841747	-3.207593
C	0.081632	3.547195	-2.883887
C	-0.272264	3.207399	-1.568504
C	-0.165863	4.209581	-0.581949
C	0.236533	5.505598	-0.907808
H	0.892830	6.835552	-2.479654

H	0.771903	5.073909	-4.234863
H	0.031606	2.801211	-3.669059
H	0.293385	6.261822	-0.128715
C	-4.836614	-2.101422	-3.034469
C	-4.212360	-1.308942	-2.097068
H	-5.591934	-1.669007	-3.685291
H	-4.477063	-0.261272	-2.024438
C	-4.502086	-3.470099	-3.162029
C	-3.531194	-4.010420	-2.351558
H	-5.006630	-4.086145	-3.901602
H	-3.254149	-5.058403	-2.441687
C	-6.407079	-0.531432	1.546994
C	-5.150021	-0.663120	0.999697
H	-6.951264	-1.418479	1.860565
H	-4.721567	-1.652038	0.893218
C	-6.997013	0.745076	1.704323
C	-6.302798	1.864784	1.311318
H	-7.990754	0.835722	2.134666
H	-6.736777	2.855331	1.427102
H	-0.386963	3.962885	0.452298
C	4.810338	1.655902	2.645774
H	4.593722	1.293792	3.659846
H	5.451834	0.903286	2.166935
C	4.505135	3.657501	0.479498
H	4.720544	3.998852	-0.541755
H	3.839513	4.410145	0.930804
C	5.804767	3.563961	1.297382
H	6.511874	2.906185	0.772522
H	6.280649	4.550535	1.359511
C	5.545273	3.005691	2.705358
H	4.939044	3.725114	3.275526
H	6.491085	2.895008	3.249863
C	3.641538	-1.263758	-1.085873
O	4.399702	-0.687567	-0.256666
C	2.959536	-5.485184	-0.310356
C	1.951429	-4.743503	-0.932183
C	2.121177	-3.379475	-1.169877
C	3.301340	-2.725316	-0.790893
C	4.298266	-3.476194	-0.146173
C	4.134037	-4.843998	0.086254
H	2.825989	-6.548833	-0.130096
H	1.024022	-5.226545	-1.229517
H	1.317116	-2.810517	-1.621696
H	5.204302	-2.966223	0.165202

H	4.925305	-5.407224	0.575774
C	3.917235	-0.937400	-2.608186
C	5.397916	-1.347909	-2.825427
C	3.060852	-1.707783	-3.626176
C	3.782915	0.563559	-2.896371
H	6.055046	-0.786324	-2.156069
H	5.546257	-2.416856	-2.633950
H	5.693167	-1.149194	-3.863378
H	2.001602	-1.463385	-3.534567
H	3.372218	-1.428977	-4.641125
H	3.178329	-2.791023	-3.531711
H	4.130154	0.785549	-3.913159
H	2.734732	0.872694	-2.821747
H	4.392509	1.149160	-2.201845

Pf₁₄

Coordinates (Angstroms)			
	X	Y	Z

Ru		-0.60472600	0.43382300 -1.05865500
H		-2.87002500	-0.90466300 1.55915900
H		0.12373300	1.12810600 -2.27409500
N		-2.22131700	-0.56124400 -1.88740900
H		-2.01695100	-1.37021300 -2.47548600
H		-3.23713700	-1.44446300 -0.58841700
N		-2.14430800	2.04338100 -1.18913300
H		-2.28193800	2.59512500 -0.34245600
H		-1.75624900	2.68917200 -1.87739900
P		0.94584400	-1.27659700 -1.24341500
P		0.82675000	1.75544700 0.23344800
C		-3.44346700	1.50130300 -1.67637100
H		-3.94720100	1.08833900 -0.79512900
C		-3.12507500	0.33512900 -2.61391700
H		-2.62970900	0.76142500 -3.50939400
C		5.45757700	1.34636500 -0.55357600
C		4.76338800	2.54919100 -0.82416100
C		3.42373600	2.66206100 -0.54873900
C		2.67921300	1.58914400 0.01812000
C		3.33281000	0.39130300 0.32605900
C		4.74037300	0.25508400 0.03517300
H		5.30682800	3.38898100 -1.25147300

H	2.92617100	3.59992500	-0.76093600
C	2.53354900	-2.12920600	3.11116900
C	1.65897300	-3.01026000	2.43235200
C	1.28744400	-2.76674200	1.13420700
C	1.76526100	-1.63731900	0.40806400
C	2.66163500	-0.75967600	1.03270200
C	3.04187900	-0.98973400	2.40748800
H	1.28302100	-3.88875100	2.95178900
H	0.61675700	-3.46288000	0.64694400
C	-0.87376900	-5.40002700	-2.56394100
C	0.35232200	-4.99389800	-3.09182800
C	0.92403700	-3.77978900	-2.70374900
C	0.28189200	-2.94503800	-1.77384800
C	-0.95824100	-3.36352400	-1.25959200
C	-1.52851600	-4.57762700	-1.64605100
H	-1.31804100	-6.34312200	-2.87192500
H	0.87032600	-5.62061600	-3.81361400
H	1.87270100	-3.48862800	-3.13814800
H	-1.50238500	-2.73770400	-0.56268500
H	-2.49330100	-4.86168800	-1.23473300
C	4.37259400	-0.96461200	-4.39891400
C	4.54791900	-1.75565400	-3.26189300
C	3.54327600	-1.82482300	-2.29585800
C	2.35155900	-1.09790100	-2.44226500
C	2.18646800	-0.30981900	-3.59068900
C	3.18811800	-0.24446600	-4.56158000
H	5.15453900	-0.91005500	-5.15198200
H	5.46878100	-2.31493300	-3.12069300
H	3.68860900	-2.45148100	-1.42145200
H	1.26767900	0.25310700	-3.71793200
H	3.04115100	0.37200700	-5.44487600
C	0.27924000	1.68573800	4.87098400
C	1.35059800	2.39524500	4.32172100
C	1.54402900	2.41328900	2.94021300
C	0.66411700	1.72986400	2.08510500
C	-0.40226400	1.01880000	2.64926000
C	-0.59544300	0.99380700	4.03253600
H	0.13338800	1.66658100	5.94780200
H	2.04047800	2.92837500	4.97084800
H	2.38369400	2.96357300	2.52367700
H	-1.07483300	0.47142800	1.99305000
H	-1.42336800	0.42909300	4.45366900
C	-0.19123400	6.20533400	-0.86594300
C	-0.28629700	5.78954800	0.46089500

C	0.06020400	4.48248900	0.82145100
C	0.50115600	3.56020700	-0.14012800
C	0.57252500	3.99141100	-1.48049800
C	0.24377200	5.29905000	-1.83767700
H	-0.45618700	7.22202000	-1.14366200
H	-0.62783600	6.48187700	1.22633500
H	-0.01539800	4.18755400	1.86203800
H	0.32186000	5.60834500	-2.87699000
C	4.27469200	-0.36783200	4.42544000
C	3.91984300	-0.11973300	3.11815300
H	4.94428200	0.31702900	4.93912400
H	4.31167300	0.75804100	2.61937600
C	3.77542400	-1.50246200	5.10735600
C	2.91926500	-2.36122400	4.45902300
H	4.06610200	-1.68884400	6.13774600
H	2.52062100	-3.23604000	4.96756500
C	6.81266200	-1.04351400	0.01218000
C	5.47092000	-0.93954000	0.30486400
H	7.33978800	-1.96857300	0.23055200
H	4.95846500	-1.78443600	0.74896300
C	7.51210700	0.04193200	-0.56714700
C	6.84258800	1.21079500	-0.84277200
H	8.57128900	-0.05181600	-0.79121300
H	7.36266800	2.05523100	-1.28917400
H	0.88699800	3.29004000	-2.24798900
C	-4.43168100	-0.32380300	-3.09359000
H	-4.19394700	-1.13746300	-3.79208200
H	-4.93486000	-0.78352700	-2.23294900
C	-4.35185700	2.54834500	-2.33232100
H	-4.58069100	3.35254600	-1.61989600
H	-3.81852700	3.01186900	-3.17721700
C	-5.65050900	1.89528500	-2.83932400
H	-6.23364500	1.54986800	-1.97487400
H	-6.26573800	2.64187100	-3.35764600
C	-5.36025200	0.70262300	-3.76573700
H	-4.88905000	1.06872000	-4.69022800
H	-6.30111800	0.22365100	-4.06563600
C	-3.80756000	-1.44021400	1.32550800
O	-3.70808600	-2.05619500	0.05534900
C	-7.01098900	1.50356000	1.42521200
C	-7.15967200	0.32200300	0.69344700
C	-6.12916400	-0.61934700	0.65680200
C	-4.93393300	-0.40568600	1.35927100
C	-4.79417800	0.78863700	2.08116000

C	-5.82079300	1.73586200	2.11694200
H	-7.81212100	2.23766900	1.45032100
H	-8.08094000	0.13364300	0.14734100
H	-6.23325600	-1.52355800	0.06618400
H	-3.86869800	0.98255100	2.61989900
H	-5.68829600	2.65500600	2.68257200
C	-3.93690100	-2.56816600	2.40840200
C	-4.02974600	-1.95293100	3.81703800
C	-5.17528600	-3.44614800	2.14931600
C	-2.67398700	-3.44961500	2.33956400
H	-3.15684900	-1.32419400	4.03811100
H	-4.92757900	-1.33906600	3.94057000
H	-4.06000500	-2.74724000	4.57274300
H	-5.14956600	-3.86275200	1.13775200
H	-5.20410900	-4.27923400	2.86278900
H	-6.10529600	-2.87898300	2.26470900
H	-2.70419200	-4.21827500	3.12200700
H	-2.59403300	-3.94918600	1.37115900
H	-1.76352900	-2.85518500	2.49051800

Pu₁₄

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.48979200	1.15755100	-0.78868500
H	-3.06531600	-0.74710600	1.51204700
H	0.40976600	1.97836400	-1.79399900
N	-2.30345200	0.84942900	-1.72817100
H	-2.33027900	0.20383200	-2.51751400
H	-3.56386900	0.21675000	-0.45440100
N	-1.57806900	3.06361000	-0.37036600
H	-1.55444400	3.38895700	0.59614000
H	-1.05756500	3.76006800	-0.90489700
P	0.58264600	-0.74689000	-1.54677700
P	1.20552500	1.64140600	0.74077900
C	-2.98098900	2.98950600	-0.86456800
H	-3.54593700	2.45496800	-0.09321200
C	-2.97154400	2.09939700	-2.11022100
H	-2.39501800	2.63438200	-2.89159800
C	5.58985800	0.34707400	-0.41184900
C	5.22834500	1.70831800	-0.27601300
C	3.95853300	2.06103700	0.10624600

C	2.95780700	1.08693700	0.38350800
C	3.28217800	-0.27073200	0.29046700
C	4.61199700	-0.65749300	-0.11772100
H	5.97290000	2.47586600	-0.47515300
H	3.71824700	3.11172500	0.20868500
C	1.83282400	-3.23239900	2.26005900
C	0.77144700	-3.62368000	1.41029800
C	0.49005100	-2.91737200	0.26829800
C	1.25049900	-1.77743300	-0.12344400
C	2.33173300	-1.37675600	0.67289400
C	2.62331900	-2.09592000	1.89143200
H	0.17924700	-4.49827500	1.67043800
H	-0.32981300	-3.24827000	-0.35652900
C	-2.18664600	-3.70681400	-3.91636500
C	-0.90675100	-3.43345000	-4.39867200
C	-0.05783200	-2.56986600	-3.70268900
C	-0.47264400	-1.95756600	-2.50803300
C	-1.77359000	-2.22948300	-2.04717000
C	-2.61915300	-3.10116600	-2.73571600
H	-2.84455800	-4.38115500	-4.45868200
H	-0.56080500	-3.89252800	-5.32152700
H	0.92950500	-2.37574900	-4.10347100
H	-2.13683500	-1.74926600	-1.14555600
H	-3.61311600	-3.29670800	-2.34539800
C	4.05452900	-0.36473600	-4.64553700
C	3.98304100	-1.48806800	-3.81943600
C	2.96857000	-1.59282800	-2.86710000
C	2.01502000	-0.57383500	-2.71476500
C	2.09552000	0.54678500	-3.55389500
C	3.10608200	0.65024900	-4.51213000
H	4.84480600	-0.28195500	-5.38725500
H	4.72016000	-2.28134900	-3.90914700
H	2.91884500	-2.47653100	-2.23834300
H	1.36025100	1.33776200	-3.45034500
H	3.15121700	1.52709400	-5.15319800
C	0.54032800	0.39211700	5.19055700
C	1.79455700	0.86458500	4.79546400
C	2.02084800	1.22278300	3.46616800
C	0.99568600	1.11903000	2.51231800
C	-0.25612200	0.64165000	2.92113000
C	-0.48502000	0.27935200	4.25070100
H	0.36622900	0.10837000	6.22516300
H	2.59874300	0.94792900	5.52196400
H	3.00008200	1.58737000	3.16753000

H	-1.05176700	0.55137600	2.18508100
H	-1.46184500	-0.09163800	4.54991700
C	1.39986100	6.32291700	1.04912000
C	1.20052500	5.56937200	2.20457000
C	1.18767200	4.17122700	2.14623800
C	1.36436400	3.49748200	0.92799000
C	1.54584500	4.27488500	-0.23393300
C	1.57595400	5.66803500	-0.17363600
H	1.41393200	7.40854000	1.09668300
H	1.05685800	6.06534300	3.16124400
H	1.03820800	3.60888100	3.06104900
H	1.73126900	6.24259200	-1.08344700
C	3.94906000	-2.43597200	3.91792600
C	3.68461400	-1.72531300	2.76830800
H	4.76518700	-2.12561700	4.56513400
H	4.29466200	-0.86387500	2.52603100
C	3.16877500	-3.56354800	4.26650600
C	2.13017000	-3.94769200	3.45139900
H	3.38965800	-4.11772100	5.17480900
H	1.51592800	-4.80874800	3.70471300
C	6.28421200	-2.35990700	-0.65299000
C	5.01077700	-2.01980800	-0.25373900
H	6.55546500	-3.40813900	-0.74737600
H	4.29470700	-2.80447400	-0.04107900
C	7.24312400	-1.35916700	-0.93934700
C	6.89693700	-0.03387600	-0.81983600
H	8.24534200	-1.64033700	-1.25139300
H	7.61967700	0.74934600	-1.03673400
H	1.66059300	3.77658200	-1.19241000
C	-4.40567300	1.92539600	-2.64797700
H	-4.37867400	1.32190300	-3.56550300
H	-4.99682700	1.36541400	-1.91277200
C	-3.62498400	4.35662800	-1.12358900
H	-3.64114600	4.95300500	-0.20060200
H	-3.01410800	4.91341900	-1.85144500
C	-5.05065000	4.18491500	-1.67818100
H	-5.68463300	3.73400400	-0.90157100
H	-5.48394300	5.16707200	-1.90618600
C	-5.06520100	3.28751500	-2.92598700
H	-4.52930300	3.79573600	-3.74167100
H	-6.09658500	3.14525100	-3.27310600
C	-4.12637700	-0.76602500	1.20627300
O	-4.34918800	0.16801400	0.16600300
C	-5.08604400	-4.82441400	-0.02714200

C	-4.03368200	-4.59074700	0.85985600
C	-3.71746500	-3.28534500	1.24367700
C	-4.44519900	-2.19150700	0.75445500
C	-5.48114500	-2.43714900	-0.15868500
C	-5.80540600	-3.74100500	-0.53911300
H	-5.33598400	-5.83920600	-0.32579500
H	-3.45469600	-5.42406700	1.25036400
H	-2.88958500	-3.11380100	1.92853300
H	-6.01813700	-1.59197400	-0.57632200
H	-6.61902800	-3.91109600	-1.24036500
C	-4.94772200	-0.29756900	2.46028900
C	-6.45363900	-0.23644600	2.14367600
C	-4.71011400	-1.25121500	3.64580800
C	-4.46607600	1.11299000	2.85581900
H	-6.64130400	0.40705800	1.27863400
H	-6.86262200	-1.22955500	1.92940400
H	-7.00381600	0.17216500	3.00053600
H	-3.64237400	-1.33257300	3.89009800
H	-5.22542400	-0.87765900	4.53899800
H	-5.08332500	-2.25966900	3.44162800
H	-4.98451500	1.45270600	3.76102000
H	-3.38883700	1.12397700	3.06705300
H	-4.66300900	1.83258900	2.05714000

Tsf₁₅

Coordinates (Angstroms)			
	X	Y	Z
Ru	0.632947	0.711069	-0.830650
H	1.530579	0.771605	0.830977
H	0.106791	0.799791	-2.381367
N	1.654367	2.615936	-1.159915
H	1.029215	3.413377	-1.265505
H	2.236990	2.769760	-0.319712
N	2.590942	0.093274	-1.705744
H	3.104557	-0.491531	-1.045282
H	2.387313	-0.480348	-2.523297
P	-1.366898	1.643845	-0.166857
P	-0.261600	-1.427567	-0.852348
C	3.438786	1.260358	-2.082392
H	4.035151	1.491825	-1.195365
C	2.547777	2.483548	-2.333658

H	1.904488	2.288435	-3.200705
C	-4.818855	-1.715096	-2.062588
C	-3.792811	-2.208214	-2.902001
C	-2.477690	-2.136730	-2.516892
C	-2.086423	-1.573392	-1.269791
C	-3.071894	-1.099738	-0.396396
C	-4.460067	-1.157925	-0.792804
H	-4.059052	-2.650265	-3.859587
H	-1.721558	-2.534361	-3.181298
C	-3.069335	-0.847863	3.440595
C	-2.516123	0.443154	3.617478
C	-2.087971	1.177096	2.539815
C	-2.204173	0.689824	1.207817
C	-2.778659	-0.567010	0.983830
C	-3.197218	-1.366083	2.110543
H	-2.429410	0.849143	4.622805
H	-1.657252	2.155796	2.710782
C	-0.693729	5.982569	1.497881
C	-1.734924	5.754368	0.598155
C	-1.977721	4.468862	0.106389
C	-1.178300	3.382941	0.501851
C	-0.117760	3.635102	1.390443
C	0.115023	4.915639	1.893833
H	-0.509936	6.982860	1.881752
H	-2.366599	6.577599	0.273489
H	-2.793720	4.323086	-0.590785
H	0.531509	2.820205	1.688650
H	0.933477	5.069410	2.590986
C	-4.804080	2.540665	-3.207574
C	-5.073228	2.506854	-1.837525
C	-4.056642	2.200880	-0.932707
C	-2.753628	1.922113	-1.378253
C	-2.497060	1.960300	-2.754863
C	-3.514177	2.265671	-3.662758
H	-5.596293	2.775779	-3.913802
H	-6.076502	2.709341	-1.472280
H	-4.278723	2.180089	0.130453
H	-1.494658	1.734884	-3.105541
H	-3.296211	2.285135	-4.727840
C	0.048221	-4.449399	2.701041
C	-0.674785	-4.803990	1.558371
C	-0.793158	-3.906565	0.496945
C	-0.179677	-2.644095	0.556760
C	0.534444	-2.299546	1.707027

C	0.649474	-3.192611	2.776453
H	0.133949	-5.147357	3.529789
H	-1.151843	-5.778898	1.497037
H	-1.361044	-4.191807	-0.384785
H	0.986533	-1.315076	1.745507
H	1.201102	-2.903603	3.667872
C	2.030320	-3.716778	-4.259313
C	2.039251	-4.222402	-2.960691
C	1.323324	-3.580548	-1.944582
C	0.586165	-2.414141	-2.202330
C	0.610088	-1.900865	-3.515617
C	1.310760	-2.550033	-4.532995
H	2.582854	-4.218991	-5.048981
H	2.605494	-5.120678	-2.728467
H	1.348605	-3.997460	-0.944748
H	1.298716	-2.139224	-5.539605
C	-4.154460	-3.406359	3.057065
C	-3.747381	-2.672882	1.965016
H	-4.566974	-4.401379	2.912260
H	-3.839824	-3.098735	0.973450
C	-4.038998	-2.879566	4.365186
C	-3.503044	-1.626332	4.547724
H	-4.368493	-3.466561	5.218362
H	-3.400499	-1.207488	5.546316
C	-6.832966	-0.738562	-0.374036
C	-5.517923	-0.670314	0.029463
H	-7.614766	-0.357768	0.277975
H	-5.282515	-0.234524	0.992582
C	-7.176448	-1.297931	-1.627500
C	-6.184387	-1.772795	-2.452442
H	-8.218018	-1.347958	-1.933450
H	-6.427725	-2.202502	-3.421476
H	0.083759	-0.975782	-3.730617
C	3.413299	3.722767	-2.611374
H	2.769309	4.592357	-2.800059
H	4.006642	3.951643	-1.715068
C	4.364947	0.991554	-3.275091
H	5.008801	0.129424	-3.057509
H	3.758127	0.721419	-4.153479
C	5.218718	2.230224	-3.599797
H	5.916231	2.411828	-2.769770
H	5.832519	2.040333	-4.489061
C	4.347762	3.479562	-3.809194
H	3.743619	3.352843	-4.719765

H	4.981699	4.359048	-3.976511
C	2.986166	1.283633	1.613932
O	3.517562	2.191340	0.913105
C	1.592800	2.542561	5.526722
C	1.126029	1.334887	5.001114
C	1.530692	0.914178	3.734037
C	2.407193	1.693720	2.966813
C	2.864202	2.908025	3.500566
C	2.462736	3.329159	4.769471
H	1.278761	2.867190	6.515473
H	0.438667	0.719171	5.575772
H	1.129139	-0.008857	3.331218
H	3.543788	3.503775	2.900435
H	2.835437	4.269240	5.169535
C	3.558207	-0.103636	1.585229
C	4.726876	-0.383448	0.976726
H	3.024615	-0.868593	2.138561
H	5.252221	0.452437	0.516793
C	5.401032	-1.686641	0.904693
C	4.776704	-2.900027	1.258087
C	6.733559	-1.740854	0.454239
C	5.465275	-4.107563	1.178677
H	3.740494	-2.899883	1.584675
C	7.423041	-2.949915	0.374581
H	7.232084	-0.815937	0.172702
C	6.792452	-4.140775	0.738898
H	4.961861	-5.030204	1.456513
H	8.453256	-2.961355	0.027889
H	7.325635	-5.085649	0.676758

TSu₁₅

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.931174	-1.062507	0.503674
H	-1.868785	0.411748	-0.130324
H	-0.397922	-2.510418	1.082123
N	-2.404103	-1.017719	2.119124
H	-1.991977	-0.940799	3.047460
H	-2.968929	-0.166146	1.954804
N	-2.626368	-2.237411	-0.345637

H	-2.935664	-1.849157	-1.236843
H	-2.268940	-3.172172	-0.538364
P	0.730473	-0.028344	1.726817
P	0.491843	-1.407048	-1.283597
C	-3.781228	-2.298350	0.590618
H	-4.366014	-1.393153	0.404663
C	-3.278256	-2.208712	2.035685
H	-2.648629	-3.081601	2.250800
C	4.964101	-2.391835	-0.123633
C	4.107748	-3.370445	-0.680232
C	2.821131	-3.053849	-1.037116
C	2.293363	-1.742901	-0.870982
C	3.116876	-0.735958	-0.352801
C	4.469347	-1.057830	0.039327
H	4.483534	-4.380626	-0.827419
H	2.199437	-3.826815	-1.470061
C	3.016251	3.057183	-0.987237
C	2.098250	3.468250	0.009830
C	1.493096	2.546518	0.826285
C	1.775612	1.155039	0.724356
C	2.689349	0.705928	-0.235861
C	3.308834	1.660984	-1.124370
H	1.868291	4.525542	0.117082
H	0.786043	2.890296	1.571558
C	-1.122438	2.533747	5.196878
C	0.019089	1.773141	5.452102
C	0.608499	1.018262	4.434905
C	0.068206	1.011035	3.137475
C	-1.091738	1.769448	2.900145
C	-1.676882	2.526927	3.916049
H	-1.580730	3.117852	5.990974
H	0.455594	1.760336	6.447804
H	1.488340	0.429709	4.664921
H	-1.550881	1.756742	1.918778
H	-2.575733	3.098216	3.701604
C	3.845451	-2.507923	4.184261
C	4.099958	-1.168323	3.882857
C	3.188877	-0.438088	3.119308
C	2.008010	-1.030843	2.641618
C	1.765196	-2.375360	2.951564
C	2.676387	-3.108323	3.715819
H	4.556560	-3.079081	4.775683
H	5.012392	-0.692959	4.232798
H	3.399657	0.603009	2.891971

H	0.861844	-2.843259	2.572412
H	2.471797	-4.152291	3.940924
C	1.066997	1.654858	-4.769285
C	1.712962	0.416536	-4.827246
C	1.558257	-0.503035	-3.790058
C	0.737766	-0.207592	-2.687746
C	0.114342	1.042797	-2.631126
C	0.275598	1.969711	-3.665015
H	1.192443	2.373032	-5.575342
H	2.344539	0.170800	-5.677291
H	2.076500	-1.457138	-3.840941
H	-0.478490	1.280139	-1.753408
H	-0.215175	2.938135	-3.606082
C	-1.162321	-5.258142	-3.407323
C	-1.070909	-4.064031	-4.120082
C	-0.530075	-2.920402	-3.522614
C	-0.072046	-2.943310	-2.196137
C	-0.200231	-4.151203	-1.479394
C	-0.724366	-5.296477	-2.080250
H	-1.576295	-6.147607	-3.874809
H	-1.418557	-4.014980	-5.148965
H	-0.469670	-2.006598	-4.102189
H	-0.795907	-6.218194	-1.507976
C	4.807828	2.213963	-2.974354
C	4.215242	1.278372	-2.155463
H	5.493940	1.888964	-3.752114
H	4.437256	0.228268	-2.300254
C	4.529369	3.591999	-2.816864
C	3.646166	3.999325	-1.844394
H	5.007920	4.320687	-3.465856
H	3.412497	5.053525	-1.713539
C	6.644323	-0.427167	0.962535
C	5.357862	-0.094374	0.600637
H	7.296118	0.332042	1.386965
H	5.011402	0.921113	0.748140
C	7.125379	-1.746617	0.789536
C	6.296228	-2.706519	0.259044
H	8.143175	-1.996128	1.077377
H	6.646303	-3.727058	0.121630
H	0.100211	-4.180344	-0.435956
C	-4.462986	-2.178793	3.015733
H	-4.088926	-2.135459	4.047338
H	-5.037474	-1.257392	2.845696
C	-4.682742	-3.522972	0.381275

H	-5.053243	-3.534871	-0.651783
H	-4.087290	-4.439003	0.519282
C	-5.859216	-3.519128	1.372605
H	-6.516606	-2.668870	1.142219
H	-6.462305	-4.426191	1.242112
C	-5.372312	-3.404440	2.825257
H	-4.817005	-4.314743	3.095484
H	-6.228143	-3.347303	3.509028
C	-3.357417	1.341007	-0.086719
O	-3.852505	1.211562	1.066923
C	-5.630745	-0.428759	-3.339105
C	-6.226240	-0.109717	-2.117312
C	-5.460456	0.436205	-1.085108
C	-4.087831	0.674539	-1.253124
C	-3.501269	0.359341	-2.487818
C	-4.264908	-0.191430	-3.519316
H	-6.223283	-0.855122	-4.144445
H	-7.289433	-0.281684	-1.967644
H	-5.909637	0.690413	-0.130325
H	-2.439836	0.523535	-2.638698
H	-3.789621	-0.436162	-4.466043
C	-2.654254	2.610813	-0.459644
C	-2.713418	3.699304	0.328989
H	-2.168002	2.640142	-1.429714
H	-3.287186	3.599367	1.249000
C	-2.120780	5.017496	0.079895
C	-1.180305	5.262944	-0.940374
C	-2.497208	6.099517	0.897751
C	-0.656719	6.537459	-1.140962
H	-0.842729	4.443367	-1.567703
C	-1.973449	7.375952	0.698484
H	-3.216591	5.930059	1.695642
C	-1.051334	7.602651	-0.324675
H	0.067134	6.701165	-1.935576
H	-2.284915	8.193514	1.343611
H	-0.639369	8.595781	-0.482484

Pf₁₅

Coordinates (Angstroms)

X	Y	Z
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Ru	-0.23576000	-0.98419700	0.98954300
H	-2.14770900	1.28171900	-0.27540800
H	0.55705100	-2.10360100	1.76344400
N	-1.68621500	-0.43468200	2.37387800
H	-1.35450100	0.01035900	3.23042100
H	-2.72004800	0.80506200	1.73081800
N	-1.84133100	-2.49008200	0.61504600
H	-2.08618900	-2.65119200	-0.36222700
H	-1.43706200	-3.36789500	0.94387600
P	1.39958400	0.51884400	1.65448500
P	0.97623000	-1.65920300	-0.88849300
C	-3.05745600	-2.16376800	1.41134000
H	-3.58415600	-1.38278300	0.84905800
C	-2.58043900	-1.54216700	2.72684600
H	-2.03717600	-2.33235700	3.28259800
C	5.67789200	-1.39143600	-0.69772800
C	5.00618300	-2.62948200	-0.83094600
C	3.63850900	-2.67668100	-0.93017900
C	2.84071600	-1.49721100	-0.90605400
C	3.46614700	-0.25053000	-0.79848300
C	4.90471600	-0.18578800	-0.68866000
H	5.58885500	-3.54758800	-0.85710400
H	3.15668500	-3.64047300	-1.03658900
C	2.30745100	3.15719900	-2.14115900
C	1.57101900	3.64354400	-1.03583400
C	1.40200400	2.87303700	0.08663900
C	1.95816900	1.56656300	0.19950600
C	2.72228300	1.05965800	-0.86103000
C	2.89247500	1.85194400	-2.05646000
H	1.13023000	4.63609200	-1.08429000
H	0.83092000	3.28010700	0.91084900
C	-0.02507300	3.62202200	4.88156300
C	1.22031000	3.00889700	5.02157400
C	1.67276800	2.09694200	4.06499200
C	0.88755200	1.77620800	2.94470400
C	-0.37349500	2.38868800	2.82946400
C	-0.82160800	3.30681600	3.78011200
H	-0.37393300	4.33188500	5.62721600
H	1.84843600	3.23748200	5.87902900
H	2.64253700	1.63489800	4.20313700
H	-1.03130600	2.14561300	2.00477000
H	-1.80012200	3.76113400	3.65264800
C	5.28221600	-0.99071700	3.76015700
C	5.28465600	0.23754500	3.09600900

C	4.13790300	0.67673500	2.43378200
C	2.97248000	-0.10580700	2.41527400
C	2.98175800	-1.33508300	3.08923300
C	4.12722200	-1.77405300	3.75705200
H	6.17518300	-1.33413600	4.27605500
H	6.18038900	0.85252300	3.08570400
H	4.15032500	1.63778100	1.92868600
H	2.08471100	-1.94526700	3.08695800
H	4.11481000	-2.73004700	4.27450600
C	-0.38001500	0.04431200	-5.02407900
C	0.86708900	-0.57606600	-4.91947300
C	1.30190900	-1.07448900	-3.69042000
C	0.49928700	-0.95800800	-2.54478800
C	-0.74995400	-0.33356800	-2.66436300
C	-1.18984500	0.16309700	-3.89341900
H	-0.71646300	0.43493300	-5.98079000
H	1.50460100	-0.66817800	-5.79490000
H	2.27272600	-1.55731600	-3.62179200
H	-1.38050600	-0.23647100	-1.78394700
H	-2.16220800	0.64378100	-3.96645000
C	0.15694000	-6.24688200	-1.47926500
C	-0.04908400	-5.37355000	-2.54590700
C	0.22641300	-4.00875800	-2.40772000
C	0.70485900	-3.48753700	-1.19587900
C	0.89455600	-4.38165200	-0.12301400
C	0.63504200	-5.74485200	-0.26520100
H	-0.05444900	-7.30724900	-1.58878400
H	-0.42335600	-5.74979200	-3.49466900
H	0.06436500	-3.35203600	-3.25499800
H	0.80156200	-6.41462700	0.57484100
C	3.78639800	2.17195700	-4.31039500
C	3.63202800	1.39235600	-3.18588900
H	4.35657600	1.79099300	-5.15366000
H	4.08180200	0.40758000	-3.15800100
C	3.21021600	3.46261900	-4.38038000
C	2.48378900	3.93928200	-3.31483900
H	3.34195600	4.06896400	-5.27250000
H	2.03125000	4.92760700	-3.34939000
C	6.98497800	1.07784800	-0.44991900
C	5.61253700	1.04539600	-0.56055700
H	7.49343600	2.03357900	-0.35361400
H	5.05787100	1.97565800	-0.54868900
C	7.73925600	-0.11950800	-0.46200800
C	7.09307800	-1.32713700	-0.58263700

H	8.82184900	-0.08059000	-0.37627200
H	7.65543900	-2.25797100	-0.59235800
H	1.24753700	-3.99883700	0.83016800
C	-3.79117700	-1.12986900	3.58632300
H	-3.43567100	-0.72658000	4.54396800
H	-4.32314700	-0.31377800	3.08010500
C	-3.99695500	-3.35630500	1.63029200
H	-4.34148700	-3.75162900	0.66495200
H	-3.44091400	-4.16690200	2.12669000
C	-5.19787700	-2.95062700	2.50331300
H	-5.81719800	-2.23337500	1.94626900
H	-5.83109700	-3.82582800	2.69573500
C	-4.74256400	-2.31429100	3.82645500
H	-4.23222300	-3.07530100	4.43546000
H	-5.61525300	-1.98731700	4.40599500
C	-3.09702200	1.76380500	0.03101900
O	-3.31436500	1.56561000	1.40421300
C	-2.80523700	5.99248400	-0.91071700
C	-2.16718600	5.04998400	-1.71941200
C	-2.24577200	3.69045100	-1.40712300
C	-2.96541400	3.25653500	-0.28755200
C	-3.60127700	4.20705600	0.51996100
C	-3.51994500	5.56552700	0.21146500
H	-2.74302900	7.05098200	-1.15030000
H	-1.60302600	5.37124600	-2.59180500
H	-1.73139800	2.96442600	-2.03381200
H	-4.14766200	3.86673300	1.39340000
H	-4.01599100	6.29368500	0.84876400
C	-4.20628900	1.17359000	-0.82845800
C	-5.32698300	0.62965800	-0.33242700
H	-4.05002300	1.25917800	-1.90401700
H	-5.42322200	0.61879600	0.75158800
C	-6.45602500	0.05553800	-1.08043200
C	-6.47427500	-0.08021000	-2.48216000
C	-7.58254100	-0.39250000	-0.36624800
C	-7.57097100	-0.63550800	-3.13539400
H	-5.61999700	0.24986600	-3.06659800
C	-8.68237200	-0.94939000	-1.01850400
H	-7.59172700	-0.29288300	0.71695600
C	-8.68246400	-1.07404200	-2.40826400
H	-7.55979700	-0.72855600	-4.21856200
H	-9.53942000	-1.28475400	-0.43996700
H	-9.53659800	-1.50776800	-2.92130800

Pu ₁₅			

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.15913500	-1.54194900	0.45208600
H	-3.05462300	0.05558100	-0.74997000
H	0.87403400	-2.67792400	0.81770400
N	-1.77490800	-1.76024300	1.73390900
H	-1.63183700	-1.54369200	2.72111400
H	-2.97729700	-0.48996800	1.34640700
N	-1.37349900	-3.11197800	-0.56322300
H	-1.50962600	-2.98568500	-1.56603800
H	-0.80110200	-3.95170500	-0.47046100
P	1.10765200	-0.11034800	1.76277400
P	1.22249900	-1.22692500	-1.40311900
C	-2.67696700	-3.31114800	0.12840900
H	-3.34104300	-2.52015900	-0.24060700
C	-2.43877800	-3.06141900	1.61959600
H	-1.77992100	-3.87547400	1.98340100
C	5.81104900	-0.57969700	-0.54675500
C	5.33765500	-1.73736900	-1.20857000
C	4.00364700	-1.88454100	-1.49482700
C	3.04559400	-0.89200600	-1.14377500
C	3.47536400	0.28103500	-0.51430100
C	4.87478600	0.44866300	-0.20387500
H	6.04716200	-2.51067400	-1.49452400
H	3.67822500	-2.77792700	-2.01247800
C	1.92853200	3.78630500	-0.76450900
C	1.01468500	3.75486200	0.31491300
C	0.86616300	2.62210900	1.07406000
C	1.61840700	1.43742600	0.82564700
C	2.55371100	1.43661800	-0.21814100
C	2.70739600	2.61582300	-1.03884700
H	0.42389700	4.64071100	0.53621400
H	0.15720100	2.63694400	1.89141500
C	-1.16679400	1.53183400	5.52732300
C	0.16456700	1.13417400	5.65391400
C	0.86996900	0.65652600	4.54656300
C	0.25730100	0.56851000	3.28572700
C	-1.08843900	0.96202000	3.17657000
C	-1.79188100	1.44230200	4.28246200
H	-1.71380400	1.89930000	6.39184100

H	0.66189000	1.19134100	6.61903400
H	1.90046700	0.34864800	4.67763000
H	-1.60489500	0.88169400	2.22724200
H	-2.83354200	1.72850600	4.16380500
C	4.95962200	-1.71947000	3.85225800
C	4.83481700	-0.35489600	3.58463300
C	3.70152000	0.12864100	2.92947100
C	2.67902100	-0.74190600	2.52119600
C	2.81454900	-2.10978200	2.79982600
C	3.94521700	-2.59442500	3.46076900
H	5.84227000	-2.09748700	4.36171900
H	5.62170800	0.33476300	3.87757900
H	3.61222800	1.19292800	2.73519500
H	2.02851500	-2.79221700	2.49379900
H	4.03191300	-3.65809000	3.66807200
C	-0.07022500	2.02452100	-4.49062200
C	1.13275700	1.33997500	-4.68638700
C	1.54824700	0.37667400	-3.76698100
C	0.76034300	0.07390200	-2.64427300
C	-0.43979400	0.77066300	-2.45807400
C	-0.85404600	1.74283800	-3.37127900
H	-0.38757800	2.78132800	-5.20319400
H	1.75242800	1.56424900	-5.55078800
H	2.49013700	-0.14313700	-3.92290200
H	-1.04028300	0.55935000	-1.57731500
H	-1.78074100	2.28386900	-3.19941900
C	0.95772300	-5.22902300	-3.84276400
C	0.59209800	-4.03034000	-4.45254900
C	0.71491900	-2.81757900	-3.76444100
C	1.19862300	-2.77897600	-2.44758300
C	1.54322100	-4.00319300	-1.83826600
C	1.43774200	-5.20989400	-2.52962000
H	0.86652700	-6.16942300	-4.37966900
H	0.21157700	-4.03005500	-5.47089700
H	0.42913200	-1.89927100	-4.26522000
H	1.72453700	-6.13705600	-2.03958100
C	3.74527000	3.81624300	-2.89936200
C	3.61255300	2.67568900	-2.13907300
H	4.44356400	3.82729500	-3.73221200
H	4.20514500	1.80339200	-2.38601800
C	2.98074500	4.97114600	-2.61070500
C	2.08821400	4.94956900	-1.56497200
H	3.09734600	5.86566200	-3.21667600
H	1.48504400	5.82382200	-1.33169000

C	6.72562600	1.74255800	0.73386600
C	5.38557100	1.61119600	0.44455800
H	7.08286300	2.64195900	1.22855200
H	4.70295400	2.40780000	0.71483800
C	7.64209600	0.71972900	0.39179100
C	7.18817100	-0.41652200	-0.23552200
H	8.69733400	0.83588800	0.62387800
H	7.87759300	-1.21276600	-0.50679100
H	1.89256600	-4.00525000	-0.80954100
C	-3.76899200	-3.17656700	2.38933900
H	-3.58236700	-3.03158400	3.46202500
H	-4.43526600	-2.36411000	2.07134100
C	-3.32840300	-4.67231100	-0.14111500
H	-3.50777800	-4.80173700	-1.21731100
H	-2.63577400	-5.47166500	0.16530600
C	-4.64707100	-4.80519300	0.64315100
H	-5.37529200	-4.08565200	0.24400200
H	-5.07392000	-5.80408600	0.48710300
C	-4.43978900	-4.53889400	2.14325200
H	-3.81235900	-5.33627400	2.56900200
H	-5.40217900	-4.58679700	2.66830200
C	-3.89927300	0.43922600	-0.14633300
O	-3.62822600	0.27610600	1.22408400
C	-7.46145100	-1.70163500	-1.41462600
C	-7.36812500	-1.19008500	-0.11668300
C	-6.22061100	-0.50890000	0.29098100
C	-5.14741200	-0.33442500	-0.59110600
C	-5.24816000	-0.84834400	-1.88944300
C	-6.39775300	-1.52761000	-2.30204800
H	-8.35571600	-2.23257600	-1.73051400
H	-8.19334000	-1.32148500	0.57899100
H	-6.13403800	-0.11654200	1.29937400
H	-4.41956700	-0.71866600	-2.58449400
H	-6.45911800	-1.92468400	-3.31236300
C	-4.06300900	1.90551600	-0.49396400
C	-3.88841900	2.91248500	0.37289100
H	-4.34411100	2.09626800	-1.52923400
H	-3.60431200	2.64734300	1.38858500
C	-4.01898500	4.35238600	0.10062900
C	-4.52333900	4.87338500	-1.10657000
C	-3.61882500	5.26768700	1.09124100
C	-4.60980800	6.24721200	-1.31463800
H	-4.86122100	4.19605200	-1.88586200
C	-3.70465600	6.64439000	0.88500800

H	-3.23269800	4.88636700	2.03396000
C	-4.19924100	7.14208600	-0.32132700
H	-5.00504100	6.62380500	-2.25488800
H	-3.38676700	7.32791100	1.66836000
H	-4.27025200	8.21394700	-0.48592400