

## **Supplementary Material for**

### **Modelling the Effect of Conformation on Hydrogen-Atom Abstraction from Peptides**

Bun Chan,<sup>A</sup> and Leo Radom<sup>B</sup>

<sup>A</sup> Graduate School of Engineering, Nagasaki University, Bunkyo 1-14, Nagasaki 852-8521, Japan

<sup>B</sup> School of Chemistry, University of Sydney, NSW 2006, Australia

Email: [bun.chan@nagasaki-u.ac.jp](mailto:bun.chan@nagasaki-u.ac.jp); [radom@chem.usyd.edu.au](mailto:radom@chem.usyd.edu.au)

**Table S1. Structure Numbers (Num) Used in the Main Text, DSD-PBE-P86 Vibrationless Energy ( $E_e$ ), M05-2X Gas-Phase (Gas) and Aqueous-Phase ( $H_2O$ ) Energies (hartree), Zero-Point Vibrational Energy (ZPVE), Thermal Correction for 298 K Enthalpy ( $\Delta H$ ) (kJ mol<sup>-1</sup>), and 298 K Entropy (S) (J mol<sup>-1</sup> K<sup>-1</sup>)**

Species <sup>a</sup>	Num	$E_e$	Gas	$H_2O$	ZPVE	$\Delta H$	S
OH		-75.65315	-75.70892	-75.71829	21.4	8.7	178.2
H <sub>2</sub> O		-76.34811	-76.39388	-76.40814	53.6	9.9	188.8
GA_1	<b>1</b>	-455.93091	-456.46178	-456.48841	406.3	31.2	437.0
GA_2	<b>2</b>	-455.93480	-456.46619	-456.49068	408.0	30.7	431.6
GA_3	<b>3</b>	-455.92905	-456.45926	-456.49145	407.3	31.0	434.0
GA_4	<b>4</b>	-455.93348	-456.46444	-456.49108	405.3	32.0	451.1
GA_5	<b>5</b>	-455.92016	-456.45054	-456.48063	408.3	30.2	434.8
GA_6	<b>6</b>	-455.92867	-456.45906	-456.48762	407.1	30.6	427.8
GA_7	<b>7</b>	-455.91888	-456.44891	-456.47876	408.6	29.8	418.7
GA_8	<b>8</b>	-455.92427	-456.45538	-456.48823	407.2	30.7	431.8
GB_1		-455.28890	-455.82202	-455.84467	372.9	30.9	437.5
GB_2		-455.27859	-455.81112	-455.83619	373.4	30.6	441.7
GB_3		-455.27856	-455.81107	-455.83617	374.0	30.3	435.1
GB_4	<b>10</b>	-455.29137	-455.82446	-455.84805	372.6	31.3	442.4
GB_5		-455.27315	-455.80540	-455.83158	374.8	29.7	422.4
GB_6		-455.27237	-455.80496	-455.83023	372.0	30.6	430.2
GB_7		-455.27315	-455.80540	-455.83158	374.8	29.7	422.5
GB_8		-455.27544	-455.80798	-455.83484	372.3	30.8	433.4
GT1_1		-531.59032	-532.18010	-532.20685	423.0	36.1	484.4
GT1_2		-531.59032	-532.18010	-532.20685	423.0	36.1	484.4
GT1_3		-531.58374	-532.17229	-532.20508	423.3	36.2	483.3
GT1_4	<b>9</b>	-531.59193	-532.18083	-532.20898	422.0	36.8	490.0
GT1_5		-531.56906	-532.15727	-532.19399	425.8	34.9	461.7
GT1_6		-531.58366	-532.17348	-532.20304	422.9	35.4	470.6
GT1_7		-531.56984	-532.15708	-532.19311	423.9	35.6	469.0
GT1_8		-531.57935	-532.16814	-532.20271	422.7	35.9	473.8
GT2_1		-531.59030	-532.18006	-532.20685	422.7	36.0	493.8
GT2_2		-531.58374	-532.17229	-532.20508	423.3	36.2	483.1
GT2_3		-531.58104	-532.16959	-532.20697	422.2	36.2	491.2
GT2_4		-531.59193	-532.18083	-532.20898	422.0	36.8	490.0
GT2_5		-531.56570	-532.15307	-532.19356	422.8	35.3	467.1
GT2_6		-531.58228	-532.17029	-532.20156	422.7	35.9	479.3
GT2_7		-531.57485	-532.16201	-532.19579	423.9	35.0	468.4
GT2_8		-531.58045	-532.16941	-532.20259	421.1	37.0	490.0
PA_1	<b>11</b>	-572.47605	-573.18204	-573.21252	573.9	36.8	478.3
PA_2	<b>12</b>	-572.48110	-573.18733	-573.21225	573.2	36.8	473.9
PA_3	<b>13</b>	-572.48366	-573.19091	-573.21018	574.8	36.1	470.6

PA_4	<b>14</b>	-572.48619	-573.19401	-573.21344	574.1	36.2	468.7
PA_5	<b>15</b>	-572.47933	-573.18481	-573.20949	572.7	37.3	482.8
PB1_1	<b>17</b>	-571.82872	-572.53705	-572.56220	539.8	37.0	479.0
PB1_2		-571.82707	-572.53551	-572.55907	539.2	36.9	479.8
PB1_3		-571.83097	-572.53970	-572.56236	539.9	36.3	474.0
PB1_4		-571.83056	-572.53939	-572.56232	540.4	36.2	474.4
PB1_5		-571.82702	-572.53531	-572.55858	539.5	36.8	479.1
PB2_1		-571.80953	-572.51509	-572.54580	535.2	37.9	488.9
PB2_2		-571.81372	-572.51910	-572.54385	535.2	37.8	489.0
PB2_3		-571.81648	-572.52314	-572.54391	535.8	37.4	486.2
PB2_4		-571.81703	-572.52373	-572.54376	536.5	37.0	480.7
PB2_5		-571.81381	-572.51914	-572.54411	534.6	38.2	491.3
PB3_1		-571.80952	-572.51492	-572.54586	534.9	37.7	494.5
PB3_2		-571.81474	-572.52008	-572.54519	534.7	37.6	486.0
PB3_3		-571.81855	-572.52530	-572.54552	535.4	37.2	482.2
PB3_4		-571.81855	-572.52530	-572.54552	535.4	37.2	482.2
PB3_5		-571.81474	-572.52008	-572.54519	534.7	37.6	486.0
PB4_1		-571.81956	-572.52508	-572.55476	536.8	37.5	488.7
PB4_2		-571.82511	-572.53112	-572.55414	535.5	37.7	485.6
PB4_3	<b>18</b>	-571.82260	-572.52777	-572.55589	537.2	37.1	479.0
PB4_4		-571.83125	-572.53962	-572.55615	537.3	36.6	476.9
PB4_5		-571.82234	-572.52832	-572.55063	536.7	37.3	483.5
PT1_1		-648.13435	-648.89875	-648.92938	588.2	42.5	523.6
PT1_2		-648.13784	-648.90246	-648.92915	588.5	42.4	524.4
PT1_3		-648.13219	-648.89545	-648.92600	588.8	42.2	523.4
PT1_4		-648.13424	-648.89723	-648.92754	587.3	42.6	533.2
PT1_5		-648.13841	-648.90297	-648.92959	588.1	42.2	526.8
PT2_1		-648.12532	-648.88592	-648.92525	588.4	42.6	530.1
PT2_2		-648.12937	-648.89059	-648.92449	586.6	43.2	536.0
PT2_3		-648.13060	-648.89366	-648.92535	590.2	41.7	516.0
PT2_4		-648.13397	-648.89622	-648.92609	589.6	41.6	519.7
PT2_5		-648.12937	-648.89020	-648.92484	588.3	42.5	528.5
PT3_1	<b>19</b>	-648.12641	-648.88981	-648.92460	588.3	42.2	526.2
PT3_2	<b>20</b>	-648.12304	-648.88353	-648.92201	587.8	42.6	523.2
PT3_3	<b>21</b>	-648.12089	-648.88010	-648.92559	586.2	43.1	534.0
PT3_4	<b>22</b>	-648.13849	-648.86810	-648.88417	589.2	41.0	511.2
PT3_5	<b>23</b>	-648.13212	-648.89539	-648.92459	587.3	41.9	520.3
PT4_1		-648.11979	-648.88160	-648.92619	587.2	42.4	523.6
PT4_2		-648.13347	-648.89751	-648.92761	588.7	41.1	508.7
PT4_3		-648.12869	-648.89012	-648.92042	588.2	42.3	526.9
PT4_4		-648.12983	-648.89137	-648.92629	588.4	41.7	517.6
PT4_5		-648.12495	-648.88466	-648.91934	586.2	43.4	540.6
PT5_1		-648.12200	-648.88210	-648.92293	586.5	43.5	546.5

PT5_2		-648.12681	-648.88717	-648.92241	586.6	43.1	533.0
PT5_3		-648.13325	-648.89666	-648.92507	589.8	41.7	522.2
PT5_4		-648.13208	-648.89388	-648.92353	586.8	42.8	530.5
PT5_5		-648.12987	-648.89244	-648.92334	589.1	42.2	527.3
PT6_1		-648.12625	-648.88761	-648.92873	590.4	42.2	527.9
PT6_2		-648.12994	-648.89142	-648.92830	588.4	42.5	528.6
PT6_3		-648.12821	-648.88909	-648.92739	587.4	43.1	534.7
PT6_4		-648.13843	-648.90309	-648.93056	589.4	42.1	525.1
PT6_5		-648.12408	-648.88465	-648.92242	587.4	43.5	539.0
PT7_1		-648.13076	-648.89426	-648.93368	591.2	41.3	515.0
PT7_2		-648.13298	-648.89772	-648.93130	591.1	41.6	515.0
PT7_3	<b>16</b>	-648.14114	-648.90516	-648.93773	591.4	41.2	516.2
PT7_4		-648.13623	-648.89956	-648.92816	588.1	42.3	531.2
PT7_5		-648.14176	-648.90848	-648.93227	591.4	41.1	508.8

<sup>a</sup> First letter: G = Gly, P = Pro; second letter: A = reactant, B = product; Tn = TS for abstracting hydrogen *n*; suffix = conformer number

---

**Table S2. Optimized geometries (Å)****GA\_1**

C	0.286309	-0.347664	0.000651
H	0.372844	-0.991286	-0.878616
H	0.373058	-0.990230	0.880673
N	-0.972079	0.355904	0.000306
H	-0.933670	1.365164	0.000599
C	1.410505	0.669189	0.000039
O	1.176673	1.886308	-0.000016
C	-2.139239	-0.300102	-0.000050
O	-2.190610	-1.539717	-0.000150
N	2.650450	0.171155	-0.000390
H	3.395078	0.852791	-0.000651
C	2.992599	-1.244361	-0.000139
H	4.075722	-1.322997	-0.000229
H	2.607823	-1.744817	0.888453
H	2.607646	-1.745183	-0.888452
C	-3.385586	0.543569	-0.000298
H	-3.975149	0.289788	-0.882006
H	-3.172499	1.611019	-0.000280
H	-3.975480	0.289830	0.881203

**GA\_2**

C	-0.095999	-1.316305	0.484028
H	0.063808	-1.132694	1.547530
H	-0.262265	-2.378084	0.330056
N	1.097094	-0.924664	-0.244269
H	1.399357	-1.499480	-1.015399
C	-1.364503	-0.589891	0.050814
O	-2.386951	-1.217425	-0.256527
C	1.830940	0.145670	0.095404
O	1.483506	0.912153	1.010031
N	-1.306613	0.744716	0.053642
H	-0.462657	1.186597	0.396015
C	-2.466587	1.540286	-0.307894
H	-2.190512	2.590077	-0.267179
H	-2.796419	1.297128	-1.317691
H	-3.292982	1.360478	0.380807
C	3.095568	0.374514	-0.683915
H	3.245634	-0.364326	-1.468556
H	3.935983	0.343770	0.010800
H	3.057730	1.372701	-1.120655

**GA\_3**

C	0.070292	-1.361023	-0.445460
H	0.338564	-1.953968	-1.318766
H	-0.136517	-2.042617	0.378682
N	-1.102523	-0.580001	-0.761634
H	-1.428372	-0.526682	-1.713913
C	1.298190	-0.556410	-0.047707
O	2.241708	-1.127693	0.517050
C	-1.789088	0.045585	0.215886
O	-1.416000	-0.006818	1.394090
N	1.326400	0.735690	-0.375376
H	0.515337	1.148551	-0.808578
C	2.472869	1.564562	-0.045444
H	2.277969	2.575255	-0.391945
H	3.371587	1.185793	-0.531926
H	2.639433	1.580498	1.031836
C	-3.016365	0.808393	-0.200493

H	-3.222778	0.724190	-1.265898
H	-3.866677	0.430750	0.367980
H	-2.876733	1.857850	0.061792

**GA\_4**

C	0.054623	-0.656872	-0.062861
H	0.021481	-1.251992	-0.978755
H	0.021761	-1.350593	0.779452
N	-1.047318	0.271500	-0.007931
H	-0.818629	1.255477	-0.005642
C	1.354739	0.125433	-0.028831
O	1.371250	1.362739	-0.072556
C	-2.316786	-0.153372	0.009814
O	-2.599228	-1.361295	-0.014738
N	2.464121	-0.611484	0.040949
H	2.383606	-1.615948	0.083683
C	3.778481	0.008401	0.053785
H	3.882554	0.669950	0.913600
H	4.526188	-0.776784	0.114773
H	3.939582	0.587097	-0.855625
C	-3.381728	0.908618	0.061026
H	-4.012124	0.810936	-0.823624
H	-2.968924	1.914875	0.103779
H	-4.005270	0.732066	0.937987

**GA\_5**

C	0.310287	0.382752	1.171781
H	0.846150	-0.062514	2.009932
H	-0.092639	1.337002	1.503288
N	-0.760270	-0.522275	0.797033
H	-0.649697	-1.505271	1.002726
C	1.299836	0.692242	0.052542
O	1.534629	1.869410	-0.257536
C	-1.772059	-0.226375	-0.050275
O	-2.553692	-1.106036	-0.429908
N	1.899551	-0.336329	-0.560298
H	2.521992	-0.076371	-1.312235
C	1.776484	-1.751209	-0.238297
H	2.673072	-2.252360	-0.594293
H	0.908612	-2.204661	-0.717614
H	1.714312	-1.899407	0.838630
C	-1.922547	1.212655	-0.467345
H	-2.755342	1.281644	-1.162290
H	-1.016082	1.589162	-0.942747
H	-2.124848	1.835623	0.406579

**GA\_6**

C	-0.012417	-1.258646	-0.440305
H	-0.242304	-1.945492	-1.253949
H	0.278359	-1.866380	0.415146
N	1.075051	-0.400462	-0.852395
H	1.154986	-0.166694	-1.832453
C	-1.316926	-0.564579	-0.076397
O	-2.281672	-1.251380	0.288883
C	1.985917	0.184774	-0.039859
O	2.858451	0.926753	-0.503928
N	-1.369792	0.762536	-0.185246
H	-0.544736	1.264607	-0.473595
C	-2.585919	1.488209	0.139587
H	-3.408345	1.156625	-0.494005
H	-2.862003	1.329622	1.182028

H	-2.410074	2.546800	-0.027368
C	1.899948	-0.124240	1.431476
H	0.897917	0.060790	1.820496
H	2.617742	0.503608	1.952861
H	2.143789	-1.174097	1.607678

H	2.513727	-1.802980	0.888344
H	2.515371	-1.803244	-0.888558
C	-3.377719	0.515519	0.000103
H	-3.965976	0.258730	-0.881857
H	-3.168967	1.583371	0.000586
H	-3.966231	0.258048	0.881693

**GA\_7**

C	-0.423790	-1.015821	0.382810
H	-0.150503	-0.712242	1.392521
H	-0.577965	-2.094020	0.376363
N	0.618025	-0.622970	-0.545871
H	0.379630	-0.592000	-1.528497
C	-1.762643	-0.388526	0.017999
O	-2.751027	-1.108838	-0.174892
C	1.853100	-0.168105	-0.247209
O	2.606298	0.232844	-1.144051
N	-1.823513	0.946114	-0.085408
H	-2.729551	1.306911	-0.348342
C	-0.774390	1.907298	0.227744
H	-1.254166	2.856650	0.452632
H	-0.086068	2.049895	-0.605246
H	-0.215346	1.594802	1.107367
C	2.282565	-0.186298	1.196745
H	3.337048	0.074648	1.235980
H	2.130657	-1.171134	1.640164
H	1.713460	0.541139	1.779022

**GB\_2**

C	0.076227	-1.353789	-0.053534
H	0.196611	-2.423925	-0.094513
N	-1.234450	-0.957506	0.105185
H	-1.862123	-1.725650	0.305582
C	1.335388	-0.625481	-0.020973
O	2.383373	-1.299386	-0.152206
C	-1.854131	0.246890	-0.090462
O	-1.256644	1.261211	-0.455722
N	1.375049	0.701063	0.191991
H	0.514114	1.220941	0.077766
C	2.650932	1.390837	0.159821
H	2.474005	2.446205	0.348385
H	3.314456	0.999495	0.930310
H	3.143434	1.277522	-0.808095
C	-3.327663	0.254251	0.200658
H	-3.781863	-0.728610	0.085734
H	-3.807908	0.968254	-0.465167
H	-3.473259	0.590019	1.230129

**GA\_8**

C	0.044142	1.128386	0.365530
H	-0.095265	1.018653	1.441270
H	0.417731	2.136180	0.191965
N	-1.216125	0.973758	-0.319156
H	-1.265070	1.342471	-1.259604
C	1.082292	0.104253	-0.086240
O	0.759691	-0.945364	-0.655249
C	-2.092392	-0.032801	-0.080344
O	-2.989103	-0.290700	-0.890797
N	2.349067	0.408943	0.206410
H	2.551539	1.285756	0.661569
C	3.431784	-0.512354	-0.095112
H	4.364219	-0.069213	0.241912
H	3.490570	-0.697737	-1.167500
H	3.280786	-1.463025	0.416276
C	-1.968541	-0.768815	1.227769
H	-2.793446	-1.472902	1.300891
H	-2.007015	-0.072504	2.067383
H	-1.023051	-1.310090	1.273801

**GB\_3**

C	0.076067	-1.352117	0.048994
H	0.194066	-2.422487	0.090959
N	-1.232329	-0.953843	-0.126066
H	-1.859891	-1.722194	-0.325222
C	1.336879	-0.626016	0.024630
O	2.382834	-1.301741	0.162545
C	-1.852744	0.250354	0.062570
O	-1.257679	1.268253	0.422850
N	1.379895	0.700286	-0.187099
H	0.517987	1.221246	-0.084776
C	2.656614	1.388129	-0.151195
H	2.481281	2.444441	-0.335904
H	3.320773	0.998932	-0.922337
H	3.147611	1.270436	0.816895
C	-3.336992	0.246909	-0.168298
H	-3.688926	-0.654717	-0.665351
H	-3.833240	0.341957	0.799579
H	-3.592804	1.121632	-0.765053

**GB\_1**

C	0.276858	-0.224168	0.000193
H	0.319620	-1.298994	0.000476
N	-0.947975	0.369879	0.000710
H	-0.953199	1.383844	0.000022
C	1.416217	0.664997	-0.000084
O	1.249894	1.907391	-0.000334
C	-2.131607	-0.319884	-0.000004
O	-2.150064	-1.549757	-0.000631
N	2.642613	0.108103	-0.000033
H	3.412995	0.758791	-0.001474
C	2.921495	-1.319282	0.000224
H	4.000080	-1.447611	0.001161

**GB\_4**

C	0.063018	-0.518704	0.003151
H	-0.068526	-1.587419	0.007277
N	-1.041205	0.278611	-0.002413
H	-0.872449	1.278199	-0.004620
C	1.345544	0.144375	0.000716
O	1.433181	1.392955	-0.004393
C	-2.326538	-0.192554	-0.005195
O	-2.561540	-1.400566	-0.004712
N	2.431717	-0.650912	0.004034
H	2.310374	-1.651401	0.006543
C	3.766293	-0.084301	-0.000142
H	3.927029	0.536231	0.882135
H	4.484415	-0.899183	0.002495

H	3.924761	0.528485	-0.888246
C	-3.405741	0.850028	0.004603
H	-4.107278	0.631388	-0.800494
H	-3.014062	1.858562	-0.112407
H	-3.946427	0.779071	0.950017

C	2.657107	-1.068794	0.445435
H	3.731754	-0.930100	0.525703
H	2.445451	-1.903431	-0.226064
H	2.239822	-1.306117	1.425497

**GB\_5**

C	0.190589	0.754818	0.061091
H	-0.210144	1.722110	0.311801
N	-0.691578	-0.251165	-0.219910
H	-0.351320	-1.131573	-0.588042
C	1.625271	0.668409	-0.095526
O	2.272892	1.732064	-0.206404
C	-2.061359	-0.197338	-0.091882
O	-2.728729	-1.175800	-0.419303
N	2.251443	-0.536308	-0.163104
H	3.251113	-0.434073	-0.262252
C	1.795714	-1.780096	0.453644
H	2.670023	-2.306509	0.828696
H	1.291754	-2.435708	-0.258215
H	1.135155	-1.580272	1.296043
C	-2.657169	1.068909	0.445108
H	-3.731881	0.930410	0.524830
H	-2.444990	1.903591	-0.226151
H	-2.240340	1.306016	1.425429

**GB\_8**

C	0.047288	1.195472	0.247848
H	0.356615	2.171819	0.589049
N	-1.283494	1.048027	-0.051962
H	-1.794865	1.881346	-0.320705
C	1.036062	0.204748	-0.142803
O	0.772650	-0.761116	-0.885633
C	-2.075405	-0.074482	0.029220
O	-3.209619	-0.033512	-0.446227
N	2.277699	0.417937	0.335577
H	2.453328	1.222449	0.916809
C	3.376285	-0.447916	-0.046513
H	4.278110	-0.095883	0.445946
H	3.528910	-0.431096	-1.126519
H	3.180672	-1.475937	0.259304
C	-1.565641	-1.280641	0.762077
H	-2.410560	-1.702928	1.304506
H	-0.762239	-1.038856	1.455107
H	-1.205193	-2.018720	0.047096

**GB\_6**

C	0.001222	-1.416586	-0.066614
H	-0.095189	-2.489838	-0.011518
N	1.227623	-0.923229	-0.460835
H	1.797380	-1.531068	-1.040067
C	-1.224565	-0.641494	0.059091
O	-2.202799	-1.124941	0.664169
C	1.925193	0.165592	0.016422
O	3.023228	0.426441	-0.468939
N	-1.281585	0.569252	-0.525050
H	-0.503342	0.907705	-1.068069
C	-2.476414	1.384821	-0.409416
H	-3.332648	0.890404	-0.870157
H	-2.708649	1.577026	0.638374
H	-2.296053	2.329573	-0.914553
C	1.331628	0.975255	1.132762
H	0.827507	1.852004	0.723503
H	2.157633	1.318126	1.753545
H	0.625273	0.406385	1.734830

**GT1\_1**

C	0.293135	0.028728	-0.196360
H	0.346551	0.921166	0.578733
H	0.384025	0.523674	-1.162835
N	-0.939807	-0.657244	-0.051216
H	-0.901932	-1.594865	0.327974
C	1.445945	-0.895578	0.115841
O	1.236459	-2.038979	0.541765
C	-2.115200	-0.028228	-0.239568
O	-2.156260	1.166891	-0.569800
N	2.667297	-0.391924	-0.075476
H	3.433976	-1.020515	0.117555
C	2.961784	0.929045	-0.616832
H	4.016861	1.127771	-0.452556
H	2.756412	0.977911	-1.686752
H	2.382723	1.695002	-0.103833
C	-3.359796	-0.843957	-0.044964
H	-3.996890	-0.337170	0.680056
H	-3.146970	-1.855639	0.295030
H	-3.896219	-0.884387	-0.993987
O	-0.072965	2.177640	1.106327
H	-0.884038	2.206740	0.552434

**GB\_7**

C	-0.190604	-0.754872	0.061049
H	0.210130	-1.722154	0.311798
N	0.691568	0.251113	-0.219950
H	0.351281	1.131410	-0.588330
C	-1.625263	-0.668387	-0.095611
O	-2.272956	-1.731986	-0.206510
C	2.061332	0.197329	-0.091893
O	2.728730	1.175666	-0.419637
N	-2.251326	0.536399	-0.163186
H	-3.251001	0.434201	-0.262342
C	-1.795657	1.780046	0.453907
H	-2.670011	2.306380	0.828967
H	-1.291614	2.435828	-0.257736
H	-1.135181	1.580024	1.296322

**GT1\_2**

C	0.293135	0.028728	-0.196360
H	0.346551	0.921166	0.578733
H	0.384025	0.523674	-1.162835
N	-0.939807	-0.657244	-0.051216
H	-0.901932	-1.594865	0.327974
C	1.445945	-0.895578	0.115841
O	1.236459	-2.038979	0.541765
C	-2.115200	-0.028228	-0.239568
O	-2.156260	1.166891	-0.569800
N	2.667297	-0.391924	-0.075476
H	3.433976	-1.020515	0.117555
C	2.961784	0.929045	-0.616832

H	4.016861	1.127771	-0.452556
H	2.756412	0.977911	-1.686752
H	2.382723	1.695002	-0.103833
C	-3.359796	-0.843957	-0.044964
H	-3.996890	-0.337170	0.680056
H	-3.146970	-1.855639	0.295030
H	-3.896219	-0.884387	-0.993987
O	-0.072965	2.177640	1.106327
H	-0.884038	2.206740	0.552434

**GT1\_3**

C	-0.014836	0.650828	0.204244
H	-0.163575	1.708681	-0.305732
H	0.248991	0.881089	1.234720
N	1.028785	-0.082820	-0.411235
H	0.890596	-0.435069	-1.348419
C	-1.389511	0.018085	0.150617
O	-2.398970	0.724965	0.300238
C	2.268673	-0.195380	0.145499
O	2.530083	0.284096	1.247844
N	-1.447337	-1.299050	-0.025378
H	-0.589235	-1.824218	-0.095465
C	-2.724939	-1.993944	-0.034755
H	-2.541175	-3.044354	-0.239018
H	-3.370629	-1.582885	-0.809708
H	-3.224185	-1.894920	0.929043
C	3.290397	-0.928762	-0.676702
H	4.005803	-0.199558	-1.061636
H	3.827262	-1.619147	-0.027412
H	2.848477	-1.470473	-1.511064
O	-0.864722	2.907673	-0.569780
H	-1.712302	2.515112	-0.268845

**GT1\_4**

C	-0.122205	0.276250	0.339079
H	-0.017201	1.242175	-0.332068
H	-0.075729	0.661825	1.356809
N	0.929590	-0.630690	0.044988
H	0.675424	-1.480547	-0.442334
C	-1.456265	-0.344832	-0.002065
O	-1.522799	-1.398662	-0.646993
C	2.220263	-0.284531	0.206378
O	2.533874	0.828281	0.657002
N	-2.527236	0.327700	0.417269
H	-2.399583	1.177287	0.945997
C	-3.868776	-0.139730	0.109129
H	-4.045129	-1.119392	0.552798
H	-4.580679	0.571443	0.516857
H	-4.008983	-0.211823	-0.969278
C	3.249093	-1.310315	-0.169015
H	3.946942	-0.859093	-0.874509
H	2.806783	-2.202792	-0.607048
H	3.806512	-1.583046	0.728253
O	0.670025	2.388280	-0.843678
H	1.493712	2.200645	-0.342966

**GT1\_5**

C	-0.197027	0.176939	-0.659695
H	-0.242249	-0.973911	-0.833639
H	0.170491	0.587904	-1.595462
N	0.661795	0.506585	0.434144

H	0.266964	0.613700	1.359734
C	-1.618015	0.673174	-0.458495
O	-2.073523	1.532640	-1.220971
C	2.020555	0.414230	0.399274
O	2.679854	0.605175	1.422022
N	-2.328609	0.146878	0.545338
H	-3.250955	0.543431	0.662141
C	-1.911328	-0.889117	1.481827
H	-2.790427	-1.462432	1.765709
H	-1.466678	-0.464925	2.382994
H	-1.204147	-1.564883	1.006964
C	2.647369	0.091575	-0.927573
H	3.718412	-0.021829	-0.782618
H	2.459122	0.898951	-1.638621
H	2.227623	-0.826875	-1.341776
O	0.059800	-2.423123	-1.011010
H	0.801174	-2.421715	-0.374171

**GT1\_6**

C	-0.054369	0.697584	-1.002359
H	0.214430	0.956135	-2.025212
H	-0.273138	1.739620	-0.484817
N	-1.201012	-0.140859	-1.010975
H	-1.665592	-0.299962	-1.895091
C	1.180423	0.165269	-0.289739
O	1.982178	0.949036	0.239841
C	-1.912819	-0.528989	0.090745
O	-2.959311	-1.159868	-0.047799
N	1.371554	-1.150298	-0.333784
H	0.654506	-1.734220	-0.737188
C	2.515976	-1.759557	0.325409
H	2.470733	-2.832651	0.165469
H	3.444246	-1.371864	-0.092094
H	2.495277	-1.551369	1.395557
C	-1.355419	-0.171414	1.440445
H	-0.544822	-0.857159	1.698174
H	-2.151650	-0.281920	2.172590
H	-0.967551	0.847240	1.464142
O	-0.021367	2.890885	0.288018
H	0.875023	2.566468	0.524285

**GT1\_7**

C	0.179424	-0.121181	-0.613298
H	0.282362	1.037161	-0.607112
H	-0.198746	-0.379472	-1.598301
N	-0.707523	-0.556333	0.420461
H	-0.320576	-0.775218	1.330187
C	1.557893	-0.743801	-0.460961
O	1.877028	-1.693549	-1.184057
C	-2.061515	-0.404078	0.394341
O	-2.734298	-0.686528	1.386589
N	2.360923	-0.249502	0.487399
H	3.271352	-0.685818	0.539349
C	2.139204	0.944747	1.294942
H	2.722237	0.845724	2.206947
H	1.092571	1.039814	1.571563
H	2.452777	1.845835	0.767873
C	-2.665659	0.106117	-0.882688
H	-3.739783	0.194659	-0.743152
H	-2.458045	-0.579003	-1.706869
H	-2.241425	1.080319	-1.133574



O	-0.016076	2.486646	-0.675221
H	-0.345844	2.473459	-1.594435

### GT1\_8

C	0.075719	0.593928	0.948570
H	-0.115847	1.547402	0.302369
H	-0.176253	0.886230	1.966574
N	1.440670	0.210421	0.904721
H	1.993080	0.304002	1.745789
C	-0.911122	-0.475414	0.489848
O	-0.691198	-1.674677	0.692098
C	2.121572	-0.207103	-0.196989
O	3.312860	-0.508995	-0.108492
N	-2.023483	-0.008640	-0.074121
H	-2.068185	0.978207	-0.295127
C	-3.074080	-0.913524	-0.508025
H	-3.899096	-0.322143	-0.894258
H	-3.425111	-1.515500	0.329357
H	-2.712143	-1.580383	-1.291660
C	1.366818	-0.285299	-1.495026
H	2.091471	-0.355128	-2.302615
H	0.726636	0.584464	-1.648581
H	0.742996	-1.181468	-1.501102
O	-0.804162	2.666419	-0.349926
H	-1.091285	3.104348	0.475343

### GT2\_1

C	-0.293270	0.028563	-0.197477
H	-0.384797	0.524027	-1.163774
H	-0.345001	0.920412	0.578136
N	0.939667	-0.658323	-0.054341
H	0.902454	-1.596245	0.323692
C	-1.446615	-0.894150	0.116769
O	-1.238324	-2.035856	0.547945
C	2.114848	-0.028810	-0.241508
O	2.155470	1.167138	-0.569358
N	-2.667634	-0.391082	-0.078040
H	-3.434714	-1.017625	0.119322
C	-2.962386	0.929680	-0.620027
H	-4.019740	1.123611	-0.465020
H	-2.391474	1.697623	-0.100716
H	-2.747535	0.981160	-1.688031
C	3.359790	-0.844118	-0.047373
H	3.903988	-0.871397	-0.992381
H	3.146842	-1.860401	0.278608
H	3.989908	-0.345041	0.689181
O	0.077314	2.173330	1.112645
H	0.885953	2.205842	0.555493

### GT2\_2

C	0.014852	0.650845	0.204222
H	-0.248998	0.880967	1.234724
H	0.163513	1.708761	-0.305676
N	-1.028688	-0.082892	-0.411275
H	-0.890515	-0.435068	-1.348488
C	1.389525	0.018113	0.150605
O	2.399015	0.724962	0.300131
C	-2.268587	-0.195399	0.145464
O	-2.529948	0.284091	1.247811
N	1.447291	-1.299041	-0.025308
H	0.589178	-1.824177	-0.095446

C	2.724867	-1.993982	-0.034763
H	2.541034	-3.044420	-0.238812
H	3.370465	-1.583086	-0.809880
H	3.224253	-1.894811	0.928945
C	-3.290349	-0.928837	-0.676637
H	-4.006347	-0.199806	-1.060790
H	-3.826527	-1.619865	-0.027456
H	-2.848565	-1.469865	-1.511511
O	0.864469	2.907830	-0.569688
H	1.712161	2.515398	-0.268902

### GT2\_3

C	0.026612	0.727179	1.007474
H	0.306151	0.965275	2.031703
H	-0.146297	1.770379	0.471771
N	-1.165633	-0.041747	0.982815
H	-1.687570	-0.172247	1.836841
C	1.214129	0.124752	0.273677
O	2.056855	0.860114	-0.263059
C	-1.754811	-0.337858	-0.207649
O	-1.210621	-0.027223	-1.267978
N	1.334604	-1.199572	0.317497
H	0.592036	-1.744178	0.728760
C	2.445910	-1.870526	-0.337455
H	2.344530	-2.939146	-0.172969
H	3.393100	-1.530609	0.079612
H	2.439571	-1.667675	-1.408638
C	-3.076420	-1.047012	-0.147203
H	-3.355649	-1.327281	0.866643
H	-3.838704	-0.387313	-0.564697
H	-3.021742	-1.936953	-0.774093
O	0.111704	2.863578	-0.360745
H	0.995754	2.508010	-0.595922

### GT2\_4

C	0.122237	0.276415	0.338847
H	0.075741	0.662194	1.356493
H	0.017142	1.242221	-0.332515
N	-0.929503	-0.630655	0.044968
H	-0.675340	-1.480432	-0.442496
C	1.456309	-0.344647	-0.002267
O	1.522862	-1.398222	-0.647608
C	-2.220200	-0.284631	0.206531
O	-2.533870	0.828157	0.657173
N	2.527267	0.327609	0.417550
H	2.399602	1.176996	0.946597
C	3.868812	-0.139825	0.109452
H	4.009193	-0.211478	-0.968962
H	4.580727	0.571099	0.517601
H	4.044969	-1.119697	0.552736
C	-3.248946	-1.310530	-0.168775
H	-2.806524	-2.203050	-0.606609
H	-3.946744	-0.859466	-0.874424
H	-3.806454	-1.583150	0.728472
O	-0.670476	2.388215	-0.843834
H	-1.494056	2.200203	-0.343081

### GT2\_5

C	-0.196347	0.575720	-0.918515
H	-0.683313	0.643511	-1.890507
H	0.405760	1.577150	-0.811541

N	0.659638	-0.559953	-0.909444
H	0.683313	-1.144480	-1.734559
C	-1.237271	0.664320	0.194072
O	-1.337569	1.693472	0.870439
C	1.412319	-1.001179	0.135316
O	2.049567	-2.050789	0.033487
N	-2.038686	-0.394609	0.362032
H	-2.708765	-0.301187	1.112671
C	-2.059396	-1.624030	-0.421309
H	-3.042579	-2.072352	-0.303000
H	-1.304306	-2.334114	-0.083294
H	-1.906805	-1.410842	-1.477654
C	1.425960	-0.168264	1.387367
H	2.299300	-0.453322	1.969364
H	0.531348	-0.381032	1.977634
H	1.451938	0.899135	1.171379
O	1.259158	2.705461	-0.610817
H	2.086606	2.194923	-0.705065

**GT2\_6**

C	-0.047686	0.608921	0.170041
H	0.062679	1.679199	-0.316681
H	-0.343555	0.810551	1.197039
N	-1.008460	-0.178750	-0.513763
H	-0.791164	-0.473372	-1.458504
C	1.365239	0.056239	0.167057
O	2.324355	0.818517	0.364496
C	-2.301828	-0.402870	-0.133973
O	-3.061554	-1.005704	-0.890824
N	1.503663	-1.253206	-0.015722
H	0.678999	-1.822250	-0.130867
C	2.817379	-1.876443	0.014626
H	2.698094	-2.935164	-0.194523
H	3.463402	-1.429645	-0.740105
H	3.279808	-1.751096	0.993478
C	-2.731022	0.091837	1.218349
H	-2.109871	-0.342262	2.003806
H	-3.767041	-0.198534	1.370225
H	-2.644032	1.178464	1.274602
O	0.715240	2.921318	-0.558680
H	1.569434	2.568639	-0.228606

**GT2\_7**

C	0.399681	0.495199	0.318887
H	0.096364	0.364418	1.356196
H	0.841946	1.586240	0.265781
N	-0.694632	0.349812	-0.573517
H	-0.492237	0.235212	-1.559025
C	1.568087	-0.421628	-0.022559
O	2.694490	0.043839	-0.253877
C	-2.017954	0.334985	-0.251841
O	-2.860740	0.181157	-1.136960
N	1.317305	-1.732187	-0.056080
H	2.109297	-2.308399	-0.305766
C	0.071192	-2.401146	0.299789
H	0.317847	-3.415291	0.603369
H	-0.621919	-2.441419	-0.540054
H	-0.406934	-1.900791	1.139017
C	-2.387801	0.509436	1.194671
H	-3.472017	0.539702	1.263450
H	-1.967989	1.433422	1.595195

H	-2.010565	-0.324384	1.790656
O	1.786397	2.628742	0.101260
H	2.487097	1.976951	-0.118707

**GT2\_8**

C	-0.050300	0.162762	0.278072
H	-0.188070	0.505555	1.304535
H	0.023410	1.143323	-0.345992
N	-1.110386	-0.665718	-0.171869
H	-0.860164	-1.506468	-0.677251
C	1.284979	-0.541050	0.131464
O	1.355783	-1.771095	0.031089
C	-2.431850	-0.380808	-0.053319
O	-3.282089	-1.148822	-0.509185
N	2.345663	0.265836	0.142088
H	2.185587	1.262359	0.078782
C	3.690202	-0.272613	0.023053
H	3.887616	-0.975813	0.831104
H	4.395582	0.550672	0.085969
H	3.820608	-0.786771	-0.929786
C	-2.781605	0.900438	0.651130
H	-3.859056	1.036702	0.610425
H	-2.281117	1.748667	0.179170
H	-2.458142	0.856587	1.693650
O	0.460944	2.524984	-0.646467
H	0.141148	2.911454	0.191970

**PA\_1**

N	-1.207623	0.117506	-0.248622
C	0.109628	0.386832	-0.806886
C	1.211697	-0.102688	0.133839
O	1.001678	-0.311253	1.335948
C	0.121901	1.923157	-0.892467
C	-0.662184	2.336782	0.355797
C	-1.769121	1.283868	0.451437
H	0.230962	-0.073515	-1.787116
H	-0.408496	2.223986	-1.797050
H	1.133004	2.325626	-0.927958
H	-1.064119	3.345850	0.284219
H	-0.019043	2.281463	1.234591
H	-2.685027	1.605976	-0.046634
H	-2.013137	1.018291	1.479116
N	2.414295	-0.257808	-0.425774
H	2.526516	-0.065989	-1.409739
C	3.568208	-0.641718	0.369900
H	3.406117	-1.615532	0.831810
H	4.433907	-0.696141	-0.283635
H	3.755973	0.090853	1.154862
C	-1.735405	-1.107655	-0.067192
O	-2.793937	-1.257284	0.562193
C	-1.001541	-2.277809	-0.671090
H	-0.064167	-2.451070	-0.137876
H	-1.629783	-3.160218	-0.576506
H	-0.770440	-2.103780	-1.722459

**PA\_2**

N	1.015666	0.172620	-0.017537
C	-0.096101	0.475046	0.878262
C	-1.437252	-0.110784	0.440168
O	-2.433778	0.059417	1.157541
C	-0.155711	2.010188	0.825864

C	0.223345	2.310439	-0.627261
C	1.323383	1.289111	-0.927811
H	0.091430	0.110751	1.887192
H	-1.135695	2.385571	1.113644
H	0.593885	2.413501	1.508002
H	-0.635067	2.143602	-1.280061
H	0.570668	3.331836	-0.771458
H	1.321121	0.949182	-1.962728
H	2.316306	1.678013	-0.694976
N	-1.486493	-0.766599	-0.719942
H	-0.639543	-0.871929	-1.257103
C	-2.734505	-1.332628	-1.203337
H	-2.544872	-1.821770	-2.154325
H	-3.123291	-2.063239	-0.494077
H	-3.480274	-0.550098	-1.343206
C	1.822473	-0.906412	0.043589
O	2.792504	-1.011414	-0.720505
C	1.512789	-1.952549	1.083727
H	2.132914	-2.823596	0.887028
H	0.461319	-2.239580	1.071667
H	1.746562	-1.562871	2.077261

**PA\_3**

N	0.925104	0.132534	0.143327
C	-0.051021	-0.685326	-0.607868
C	-1.463250	-0.572738	-0.012151
O	-2.008372	-1.505566	0.592888
C	0.506712	-2.112198	-0.529735
C	1.982541	-1.926910	-0.171207
C	1.944750	-0.726432	0.768372
H	-0.086200	-0.313355	-1.632748
H	0.352412	-2.648439	-1.464346
H	-0.006578	-2.650419	0.265972
H	2.568483	-1.675935	-1.057319
H	2.415536	-2.807653	0.300726
H	2.895606	-0.207977	0.841748
H	1.621262	-1.020455	1.768844
N	-2.067557	0.601612	-0.207805
H	-1.518773	1.343018	-0.627790
C	-3.379729	0.866044	0.354345
H	-3.672291	1.877166	0.085658
H	-4.113429	0.165269	-0.043675
H	-3.366296	0.773825	1.441204
C	1.077786	1.440193	-0.135787
O	0.293309	2.037567	-0.896088
C	2.229310	2.169101	0.506715
H	2.068720	3.236158	0.374098
H	2.310442	1.935435	1.567938
H	3.166176	1.887926	0.020526

**PA\_4**

N	0.987204	0.004831	0.024872
C	-0.114799	0.587484	0.810526
C	-1.473827	0.329850	0.142876
O	-2.202120	1.249243	-0.255336
C	0.239455	2.071362	0.843131
C	0.908845	2.291975	-0.515665
C	1.766357	1.038677	-0.682359
H	-0.129009	0.127973	1.799264
H	0.953425	2.247478	1.649195
H	-0.637625	2.693777	1.000989

H	1.508452	3.199456	-0.558157
H	0.150352	2.333880	-1.298919
H	2.739367	1.161690	-0.202526
H	1.919514	0.762710	-1.724345
N	-1.818075	-0.955792	0.036228
H	-1.159354	-1.651463	0.367013
C	-3.061806	-1.345142	-0.603921
H	-3.132949	-2.428991	-0.587228
H	-3.915916	-0.923218	-0.073900
H	-3.090626	-1.000519	-1.638101
C	1.374834	-1.270089	0.184467
O	0.716013	-2.071413	0.875531
C	2.637095	-1.689387	-0.519434
H	2.821511	-2.738758	-0.304268
H	2.537306	-1.548269	-1.597103
H	3.483572	-1.090040	-0.178892

**PA\_5**

N	1.010887	-0.059329	-0.068632
C	-0.014605	0.625019	0.718104
C	-1.446984	0.228149	0.395475
O	-2.350772	0.521473	1.190466
C	0.177597	2.119214	0.356368
C	1.612944	2.192671	-0.168331
C	1.772103	0.871046	-0.913115
H	0.132936	0.457015	1.784860
H	-0.519497	2.392790	-0.438151
H	-0.010495	2.758193	1.216096
H	2.319586	2.230756	0.662417
H	1.778425	3.055087	-0.812034
H	1.336699	0.919119	-1.914220
H	2.801551	0.531445	-0.991785
N	-1.677207	-0.350040	-0.785292
H	-0.893487	-0.588751	-1.373673
C	-3.027369	-0.699711	-1.193680
H	-2.981402	-1.156446	-2.177957
H	-3.471162	-1.405218	-0.490898
H	-3.654948	0.190109	-1.239357
C	1.386192	-1.346643	0.094110
O	2.290086	-1.843915	-0.591646
C	0.673421	-2.142088	1.158747
H	-0.404528	-2.164281	0.994312
H	1.060220	-3.157847	1.139509
H	0.856043	-1.702784	2.141711

**PB1\_1**

N	-1.143562	0.045190	0.077009
C	0.117391	0.545583	-0.199852
C	1.331935	-0.147747	0.201577
O	1.328604	-1.107530	0.999567
C	-0.009561	1.996882	-0.548975
C	-1.260583	2.400374	0.252430
C	-2.127456	1.140610	0.249051
H	-0.186984	2.115377	-1.623431
H	0.871209	2.577418	-0.280132
H	-1.783043	3.250695	-0.180738
H	-0.971389	2.648511	1.273674
H	-2.826403	1.115467	-0.587322
H	-2.682878	0.999768	1.172987
N	2.480239	0.328181	-0.322046
H	2.452015	1.081870	-0.989665

C	3.757713	-0.243826	0.057673
H	3.808247	-1.298756	-0.214547
H	4.543041	0.295872	-0.463855
H	3.917898	-0.155985	1.132776
C	-1.618451	-1.231256	-0.093157
O	-2.793475	-1.472923	0.197812
C	-0.727171	-2.283775	-0.687812
H	-0.202312	-2.819838	0.101509
H	-1.370623	-2.980497	-1.222289
H	0.010561	-1.860953	-1.368350

**PB1\_2**

N	-1.018812	-0.191397	0.126122
C	-0.064908	0.722543	-0.309509
C	1.379076	0.595207	-0.185565
O	2.126067	1.383801	-0.802917
C	-0.732010	2.038420	-0.545060
C	-1.881403	1.988404	0.476791
C	-2.265721	0.508545	0.530258
H	-0.053591	2.876230	-0.400616
H	-1.128360	2.085161	-1.565432
H	-1.515711	2.313232	1.451003
H	-2.727882	2.611185	0.194742
H	-2.573993	0.177722	1.519023
H	-3.049041	0.255190	-0.184091
N	1.878580	-0.347862	0.635979
H	1.258993	-0.928340	1.177586
C	3.312852	-0.525931	0.767979
H	3.493207	-1.363675	1.435819
H	3.764298	-0.736958	-0.201846
H	3.781531	0.367975	1.181897
C	-1.104663	-1.536719	-0.143228
O	-2.089174	-2.163811	0.252013
C	-0.021127	-2.202643	-0.945044
H	-0.496609	-2.996164	-1.519104
H	0.712733	-2.659652	-0.279528
H	0.488332	-1.513973	-1.616660

**PB1\_3**

N	1.012024	0.105593	0.099823
C	-0.062641	-0.752621	-0.127587
C	-1.498945	-0.516619	-0.032139
O	-2.257814	-1.502441	-0.174272
C	0.424105	-2.171876	-0.133022
C	1.948385	-2.033513	-0.173897
C	2.197343	-0.692372	0.507300
H	0.018381	-2.731651	-0.976187
H	0.090644	-2.677051	0.779609
H	2.294880	-1.985532	-1.206650
H	2.463517	-2.846027	0.333836
H	3.112577	-0.213058	0.177959
H	2.204046	-0.784368	1.594098
N	-1.990667	0.700854	0.276384
H	-1.393787	1.497089	0.097132
C	-3.429533	0.893910	0.295304
H	-3.631109	1.931221	0.549136
H	-3.880489	0.667916	-0.673452
H	-3.887557	0.250689	1.045353
C	1.091538	1.441236	-0.184834
O	0.171799	2.040823	-0.754194
C	2.354996	2.153090	0.212475

H	2.156177	3.221365	0.175710
H	2.685752	1.869673	1.211181
H	3.154111	1.920146	-0.495050

**PB1\_4**

N	1.020012	-0.092514	-0.049649
C	-0.068167	0.738825	0.215738
C	-1.498574	0.485407	0.098759
O	-2.287017	1.409920	0.400398
C	0.431765	2.138516	0.389386
C	1.713341	2.136023	-0.450912
C	2.249314	0.721654	-0.266322
H	0.664418	2.325348	1.444366
H	-0.300454	2.874470	0.068707
H	2.437322	2.882803	-0.131869
H	1.466513	2.306884	-1.499108
H	2.883213	0.645068	0.617418
H	2.793702	0.353683	-1.132018
N	-1.956621	-0.681777	-0.406164
H	-1.343794	-1.481540	-0.325553
C	-3.389841	-0.917531	-0.430534
H	-3.565748	-1.903948	-0.851510
H	-3.825662	-0.871470	0.570030
H	-3.883466	-0.174107	-1.054533
C	1.114310	-1.439078	0.189556
O	0.163773	-2.092719	0.631782
C	2.436819	-2.085064	-0.114135
H	2.345947	-3.146557	0.100627
H	2.705391	-1.943987	-1.162345
H	3.231024	-1.656731	0.499823

**PB1\_5**

N	1.001111	-0.210672	-0.195302
C	0.071387	0.747217	0.189062
C	-1.378522	0.636761	0.126676
O	-2.081891	1.523283	0.656728
C	0.724440	2.096012	0.260525
C	2.212898	1.784723	0.037378
C	2.200735	0.466569	-0.738282
H	0.322337	2.742217	-0.526086
H	0.529166	2.589728	1.214064
H	2.711811	1.635251	0.995156
H	2.729557	2.571576	-0.507957
H	2.068720	0.625317	-1.808870
H	3.074427	-0.154463	-0.570241
N	-1.934610	-0.387735	-0.547708
H	-1.355885	-1.038760	-1.052993
C	-3.378097	-0.508198	-0.640573
H	-3.610536	-1.418079	-1.187011
H	-3.821549	-0.564838	0.353605
H	-3.810721	0.344929	-1.165417
C	1.056725	-1.543526	0.136096
O	1.951380	-2.252792	-0.327582
C	0.043658	-2.099248	1.099198
H	-0.730137	-2.643175	0.555719
H	0.573165	-2.812360	1.729884
H	-0.421117	-1.334286	1.717577

**PB2\_1**

N	-1.213962	0.035021	-0.283748
C	0.074277	0.534842	-0.752303

C	1.219861	0.036912	0.144878
O	1.017292	-0.305766	1.315951
C	-0.057651	2.014056	-0.579453
C	-1.370310	2.371085	0.025978
C	-1.900177	1.032283	0.549425
H	0.269499	0.244991	-1.789385
H	0.681827	2.707804	-0.946605
H	-2.049054	2.784453	-0.730725
H	-1.287952	3.114159	0.821721
H	-2.976873	0.927098	0.444472
H	-1.632645	0.879765	1.597280
N	2.431582	0.050579	-0.412056
H	2.526119	0.323106	-1.378641
C	3.612589	-0.306078	0.356796
H	3.538849	-1.332370	0.716233
H	4.482418	-0.214546	-0.286888
H	3.727358	0.358093	1.213177
C	-1.491451	-1.277177	-0.112031
O	-2.446913	-1.636162	0.588708
C	-0.615219	-2.279162	-0.817438
H	0.249004	-2.502804	-0.187365
H	-1.187173	-3.194680	-0.953169
H	-0.259255	-1.919400	-1.781866

**PB2\_2**

N	-1.046889	0.139927	-0.040284
C	0.071229	0.468104	-0.917132
C	1.428540	-0.084758	-0.455936
O	2.367429	-0.132898	-1.260744
C	0.128269	1.959786	-0.835938
C	-0.603646	2.438883	0.370154
C	-1.576422	1.296946	0.699803
H	-0.079373	0.102083	-1.935326
H	0.861744	2.529065	-1.385789
H	0.088707	2.606423	1.205163
H	-1.127416	3.380687	0.198790
H	-1.618265	1.074296	1.764730
H	-2.588353	1.511860	0.354459
N	1.548280	-0.410853	0.832183
H	0.728367	-0.385149	1.419596
C	2.815134	-0.881849	1.366886
H	2.684409	-1.094279	2.423921
H	3.134738	-1.789636	0.854808
H	3.586058	-0.121163	1.245552
C	-1.688723	-1.046143	-0.004463
O	-2.683464	-1.203173	0.716707
C	-1.162449	-2.146342	-0.889466
H	-1.697001	-3.062444	-0.650869
H	-0.091986	-2.303305	-0.751900
H	-1.334688	-1.891150	-1.937569

**PB2\_3**

N	0.967615	0.093781	-0.007654
C	-0.050422	-0.667302	-0.746818
C	-1.429921	-0.561096	-0.064572
O	-1.943289	-1.516108	0.531570
C	0.490474	-2.054349	-0.720790
C	1.770672	-2.125761	0.037531
C	1.802775	-0.798317	0.808339
H	-0.141689	-0.249476	-1.754198
H	0.018875	-2.875525	-1.235511

H	2.631472	-2.191207	-0.640219
H	1.824221	-2.984171	0.710058
H	2.805933	-0.395237	0.911151
H	1.361831	-0.914110	1.800037
N	-2.021641	0.631363	-0.172564
H	-1.486004	1.382385	-0.592153
C	-3.285473	0.897360	0.491765
H	-3.575226	1.923332	0.283379
H	-4.059167	0.226029	0.119977
H	-3.196742	0.761761	1.570509
C	1.129086	1.414505	-0.182616
O	0.374856	2.065648	-0.930457
C	2.260107	2.079471	0.556741
H	2.188335	3.151866	0.394375
H	2.208909	1.864103	1.624723
H	3.221111	1.720850	0.183021

**PB2\_4**

N	0.986703	-0.054473	0.012239
C	-0.070500	0.604155	0.799756
C	-1.433059	0.471340	0.085965
O	-1.940288	1.418896	-0.528298
C	0.385333	2.018956	0.847477
C	1.323452	2.276682	-0.279749
C	1.965140	0.906554	-0.534177
H	-0.146530	0.130753	1.782078
H	-0.151359	2.780375	1.391674
H	2.071152	3.039831	-0.062699
H	0.765864	2.603401	-1.167867
H	2.909717	0.814678	0.003315
H	2.141994	0.716703	-1.591123
N	-2.013674	-0.726981	0.183897
H	-1.459079	-1.475494	0.582094
C	-3.248419	-1.013874	-0.525509
H	-3.536598	-2.039889	-0.315096
H	-4.040832	-0.345540	-0.190279
H	-3.121042	-0.890018	-1.601958
C	1.214136	-1.374629	0.135188
O	0.443334	-2.112761	0.775030
C	2.444457	-1.916664	-0.540147
H	2.451992	-2.997975	-0.429545
H	2.453327	-1.653296	-1.598771
H	3.342577	-1.497549	-0.081462

**PB2\_5**

N	1.052278	0.083615	0.039196
C	-0.055790	0.572089	0.850570
C	-1.445281	0.076262	0.426348
O	-2.403632	0.253232	1.188933
C	-0.004952	2.050027	0.626474
C	1.097452	2.421597	-0.303424
C	1.519546	1.084749	-0.929380
H	0.060139	0.293402	1.901788
H	-0.678510	2.730523	1.121728
H	1.937573	2.866800	0.244270
H	0.790332	3.145374	-1.060765
H	1.037529	0.927001	-1.896935
H	2.594524	0.991191	-1.058143
N	-1.567225	-0.460969	-0.788601
H	-0.744230	-0.595479	-1.355631
C	-2.864817	-0.889276	-1.284954

H	-2.733607	-1.292069	-2.284932
H	-3.287770	-1.659325	-0.639852
H	-3.554937	-0.046663	-1.323969
C	1.564083	-1.164991	0.076003
O	2.445014	-1.515248	-0.720616
C	1.040009	-2.092534	1.142813
H	-0.043267	-2.206599	1.080199
H	1.512504	-3.062725	1.011734
H	1.281789	-1.701361	2.133109

**PB3\_1**

N	-1.218356	0.182488	-0.264086
C	0.111822	0.440059	-0.803479
C	1.186336	-0.102733	0.140990
O	0.939272	-0.367861	1.324174
C	0.179181	1.981848	-0.847340
C	-0.724118	2.380578	0.268413
C	-1.679298	1.286563	0.590078
H	0.232362	0.001501	-1.792883
H	-0.195753	2.329883	-1.818367
H	1.200816	2.351300	-0.743744
H	-0.822368	3.383547	0.652393
H	-2.719615	1.534248	0.354743
H	-1.650616	0.989483	1.644719
N	2.401956	-0.244197	-0.392815
H	2.543075	-0.005248	-1.362621
C	3.530811	-0.676069	0.414557
H	3.345451	-1.666486	0.829909
H	4.411934	-0.713819	-0.219221
H	3.707351	0.020149	1.234434
C	-1.736063	-1.052656	-0.086512
O	-2.729592	-1.224253	0.632457
C	-1.079311	-2.193383	-0.819508
H	-0.105164	-2.414835	-0.377347
H	-1.715318	-3.070394	-0.726754
H	-0.930953	-1.955697	-1.873194

**PB3\_2**

N	1.032240	0.239124	0.012774
C	-0.106628	0.556198	0.867456
C	-1.418851	-0.092472	0.430769
O	-2.426880	0.050254	1.136921
C	-0.230612	2.088528	0.731676
C	0.318066	2.341382	-0.631585
C	1.242155	1.246312	-1.037390
H	0.071680	0.252448	1.897065
H	-1.259654	2.422496	0.868419
H	0.377717	2.570288	1.507896
H	0.257544	3.282426	-1.154914
H	1.015811	0.833115	-2.027260
H	2.295111	1.548436	-1.049985
N	-1.435045	-0.759711	-0.723969
H	-0.582243	-0.854065	-1.253290
C	-2.659539	-1.373281	-1.210358
H	-2.447407	-1.858838	-2.158358
H	-3.025086	-2.114716	-0.500043
H	-3.431888	-0.618459	-1.356883
C	1.803566	-0.865758	0.080439
O	2.707545	-1.054089	-0.745055
C	1.532882	-1.831183	1.205232
H	2.189549	-2.688969	1.084158

H	0.494053	-2.164020	1.202622
H	1.732889	-1.353703	2.166573

**PB3\_3**

N	1.007495	-0.030224	-0.071870
C	-0.097497	-0.636788	-0.829049
C	-1.422161	-0.387756	-0.094800
O	-2.020347	-1.279053	0.521387
C	0.268582	-2.121903	-0.863573
C	1.075219	-2.298390	0.377615
C	1.668297	-1.002481	0.812831
H	-0.144054	-0.180427	-1.816153
H	0.863742	-2.326218	-1.762900
H	-0.617127	-2.755396	-0.900559
H	1.382554	-3.246942	0.788557
H	2.753756	-0.966065	0.669480
H	1.469554	-0.777575	1.866352
N	-1.869840	0.870112	-0.162973
H	-1.264397	1.559661	-0.591898
C	-3.053147	1.282194	0.571915
H	-3.231016	2.335522	0.374918
H	-3.920368	0.707870	0.247410
H	-2.920017	1.134967	1.644646
C	1.338410	1.263951	-0.202731
O	0.700563	2.026262	-0.952935
C	2.520104	1.745491	0.595352
H	2.631659	2.814929	0.436095
H	2.374195	1.544868	1.658150
H	3.429367	1.232017	0.276825

**PB3\_4**

N	1.007548	0.030152	0.071943
C	-0.097404	0.636786	0.829128
C	-1.421997	0.387891	0.094715
O	-2.019844	1.279144	-0.521864
C	0.268855	2.121847	0.863776
C	1.075426	2.298325	-0.377461
C	1.668193	1.002345	-0.812927
H	-0.144077	0.180346	1.816183
H	0.864133	2.325992	1.763068
H	-0.616752	2.755465	0.900932
H	1.382880	3.246874	-0.788338
H	2.753698	0.965731	-0.670015
H	1.469010	0.777532	-1.866393
N	-1.870008	-0.869851	0.163218
H	-1.264828	-1.559399	0.592512
C	-3.053235	-1.281861	-0.571830
H	-3.230961	-2.335276	-0.375169
H	-3.920559	-0.707748	-0.247213
H	-2.920062	-1.134295	-1.644507
C	1.338249	-1.264080	0.202739
O	0.700266	-2.026304	0.952911
C	2.519790	-1.745789	-0.595466
H	2.631487	-2.815163	-0.435888
H	2.373505	-1.545555	-1.658291
H	3.429102	-1.232113	-0.277423

**PB3\_5**

N	1.032387	0.239031	0.012827
C	-0.106546	0.556032	0.867448
C	-1.418836	-0.092490	0.430761

O	-2.426681	0.049963	1.137224
C	-0.230444	2.088409	0.731851
C	0.318370	2.341392	-0.631325
C	1.242663	1.246474	-1.037036
H	0.071711	0.252190	1.897023
H	-1.259449	2.422456	0.868624
H	0.377914	2.569955	1.508191
H	0.257430	3.282313	-1.154816
H	1.016759	0.833503	-2.027094
H	2.295628	1.548626	-1.049154
N	-1.435378	-0.759194	-0.724298
H	-0.582730	-0.853438	-1.253880
C	-2.660030	-1.372537	-1.210568
H	-2.448203	-1.857733	-2.158824
H	-3.025392	-2.114249	-0.500444
H	-3.432393	-0.617628	-1.356555
C	1.803551	-0.865990	0.080340
O	2.707745	-1.054192	-0.744939
C	1.532363	-1.831713	1.204750
H	0.493435	-2.164225	1.201855
H	2.188794	-2.689655	1.083507
H	1.732363	-1.354591	2.166273

**PB4\_1**

N	-1.215643	0.133417	-0.182200
C	0.092077	0.402169	-0.786073
C	1.202582	-0.061028	0.154222
O	1.030478	-0.131691	1.377181
C	0.097452	1.939607	-0.906484
C	-0.759434	2.397678	0.284761
C	-1.722396	1.271375	0.430998
H	0.186576	-0.082646	-1.755388
H	-0.384255	2.214872	-1.844388
H	1.108243	2.343101	-0.898221
H	-1.248481	3.354986	0.100214
H	-0.141947	2.510189	1.184625
H	-2.531653	1.175800	1.133159
N	2.369866	-0.337982	-0.431202
H	2.448357	-0.267140	-1.434271
C	3.534309	-0.701676	0.359090
H	3.336230	-1.605547	0.934812
H	4.364928	-0.883027	-0.316523
H	3.798671	0.101304	1.047041
C	-1.763023	-1.105326	-0.040121
O	-2.823231	-1.253911	0.584633
C	-1.032833	-2.258053	-0.675003
H	-0.065766	-2.419418	-0.192645
H	-1.641419	-3.150297	-0.549550
H	-0.859427	-2.083880	-1.737898

**PB4\_2**

N	1.058185	0.274036	0.006003
C	-0.083684	0.519912	0.893653
C	-1.365614	-0.181070	0.453877
O	-2.334568	-0.188408	1.225169
C	-0.260675	2.046881	0.795438
C	0.183188	2.368762	-0.642814
C	1.201691	1.313815	-0.904866
H	0.126868	0.195241	1.909486
H	-1.283375	2.343487	1.018309
H	0.410816	2.521789	1.510106

H	-0.663149	2.297021	-1.337494
H	0.590812	3.376512	-0.734510
H	1.877479	1.213029	-1.734581
N	-1.407228	-0.720685	-0.765332
H	-0.592790	-0.678490	-1.358565
C	-2.619996	-1.359032	-1.250416
H	-2.433916	-1.732050	-2.253199
H	-2.898145	-2.190361	-0.602979
H	-3.443438	-0.645501	-1.277956
C	1.845053	-0.840868	0.020867
O	2.752256	-0.973211	-0.811702
C	1.575801	-1.858714	1.096545
H	2.220384	-2.715445	0.916446
H	0.534472	-2.184480	1.099093
H	1.801208	-1.439380	2.079715

**PB4\_3**

N	-1.144117	0.030890	0.115385
C	0.071950	-0.688891	0.513288
C	1.295782	-0.133122	-0.198571
O	1.266887	0.148207	-1.403129
C	-0.211179	-2.131234	0.053787
C	-1.744242	-2.238080	0.069739
C	-2.162374	-0.842584	-0.245708
H	0.193033	-0.620576	1.595265
H	0.283065	-2.857414	0.694864
H	0.152311	-2.249904	-0.967659
H	-2.100617	-2.541412	1.062423
H	-2.118519	-2.966129	-0.650479
H	-3.171130	-0.477518	-0.341261
N	2.408454	-0.064374	0.535258
H	2.359670	-0.258957	1.523199
C	3.659270	0.391077	-0.046183
H	4.434252	0.328143	0.712116
H	3.934478	-0.236320	-0.893371
H	3.573806	1.423017	-0.388021
C	-1.190205	1.385576	0.187607
O	-0.204078	2.022202	0.592073
C	-2.472817	2.042806	-0.234656
H	-2.338282	3.120709	-0.193680
H	-2.744999	1.742272	-1.248259
H	-3.287009	1.751909	0.432998

**PB4\_4**

N	1.026771	0.042552	0.049232
C	-0.093748	0.610007	0.831447
C	-1.422848	0.326179	0.117195
O	-2.085208	1.223400	-0.419775
C	0.240788	2.100776	0.859931
C	0.965807	2.340486	-0.476341
C	1.637961	1.031082	-0.712467
H	-0.108804	0.147693	1.816369
H	0.919135	2.291564	1.691209
H	-0.652185	2.708298	0.979723
H	1.674001	3.168769	-0.426461
H	0.245640	2.569683	-1.270685
H	2.300716	0.766200	-1.518184
N	-1.809509	-0.951612	0.123237
H	-1.174282	-1.635381	0.517294
C	-3.013837	-1.368850	-0.573347
H	-3.131986	-2.440796	-0.443627

H	-3.886504	-0.861276	-0.162950
H	-2.947413	-1.141093	-1.637900
C	1.405421	-1.253688	0.176124
O	0.762030	-2.039774	0.897539
C	2.623829	-1.675633	-0.592456
H	2.858250	-2.704135	-0.330279
H	2.436501	-1.608602	-1.666637
H	3.471273	-1.028661	-0.357772

**PB4\_5**

N	1.081966	-0.159608	0.016146
C	0.129049	0.705878	0.731766
C	-1.328120	0.398946	0.412996
O	-2.191653	0.488677	1.293943
C	0.506246	2.129517	0.260702
C	1.957524	2.005168	-0.230328
C	2.026899	0.587323	-0.678818
H	0.255178	0.593674	1.807524
H	-0.137020	2.418131	-0.570458
H	0.380945	2.850377	1.064840
H	2.661002	2.188734	0.591648
H	2.187167	2.715205	-1.024924
H	2.875885	0.078818	-1.102142
N	-1.613336	0.090450	-0.855045
H	-0.862414	0.012922	-1.525031
C	-2.972905	-0.235189	-1.251736
H	-2.973122	-0.477976	-2.310335
H	-3.340171	-1.092214	-0.685821
H	-3.636996	0.611083	-1.077147
C	1.099168	-1.523413	0.075475
O	1.942907	-2.164933	-0.565109
C	0.062490	-2.205345	0.927918
H	-0.855378	-2.353048	0.353071
H	0.454101	-3.182834	1.202078
H	-0.181721	-1.646042	1.830474

**PT1\_1**

N	1.277286	-0.036048	0.091617
C	-0.015543	0.498724	0.409171
C	-1.107863	0.098391	-0.579200
O	-0.864318	0.027382	-1.790249
C	0.201826	2.020359	0.428940
C	1.364279	2.215417	-0.547937
C	2.252411	1.007330	-0.266833
H	-0.362400	0.147396	1.461287
H	0.498057	2.315063	1.437344
H	-0.701927	2.563327	0.156850
H	1.887116	3.157832	-0.395822
H	0.998377	2.171552	-1.574405
H	2.934296	1.184710	0.567309
H	2.830283	0.682753	-1.129066
N	-2.315630	-0.092561	-0.052962
H	-2.404596	-0.080612	0.955446
C	-3.454701	-0.406056	-0.898547
H	-3.292721	-1.344697	-1.429680
H	-4.335238	-0.497864	-0.269420
H	-3.615911	0.386144	-1.629133
C	1.590132	-1.352233	0.003345
O	2.731761	-1.703990	-0.312138
C	0.500861	-2.349844	0.294690
H	-0.195099	-2.388734	-0.546699

H	0.961681	-3.327602	0.413036
H	-0.057179	-2.095598	1.196374
O	-1.194417	0.009825	2.676565
H	-1.248943	0.968319	2.860793

**PT1\_2**

N	-1.141980	-0.036993	-0.103717
C	0.039178	-0.592366	0.490912
C	1.369918	-0.044832	-0.009592
O	2.376754	-0.113813	0.712111
C	-0.091371	-2.106256	0.268347
C	-0.968107	-2.200938	-0.984297
C	-1.951069	-1.046370	-0.810037
H	0.077070	-0.398138	1.650463
H	0.881506	-2.584821	0.169036
H	-0.607275	-2.537653	1.127533
H	-0.364933	-2.041557	-1.879670
H	-1.473423	-3.161110	-1.068478
H	-2.310196	-0.635053	-1.750715
H	-2.810367	-1.326079	-0.197257
N	1.397338	0.425078	-1.253897
H	0.535130	0.470041	-1.776700
C	2.630615	0.929087	-1.837989
H	2.416577	1.270134	-2.846522
H	3.017279	1.761042	-1.249225
H	3.383647	0.142249	-1.875028
C	-1.591303	1.237320	0.054567
O	-2.672673	1.577576	-0.432847
C	-0.718976	2.197624	0.818534
H	-1.318640	3.068112	1.073631
H	0.115254	2.518075	0.190334
H	-0.310962	1.750791	1.725040
O	0.682365	-0.337772	2.936834
H	1.576948	-0.260175	2.539399

**PT1\_3**

N	-0.889136	0.198644	-0.479080
C	0.066206	-0.683107	0.176800
C	1.533587	-0.530223	-0.249435
O	2.118675	-1.453353	-0.829559
C	-0.478274	-2.090664	-0.043404
C	-1.975929	-1.862407	-0.228636
C	-2.001890	-0.585361	-1.061124
H	0.031230	-0.425811	1.313403
H	-0.225177	-2.746710	0.788619
H	-0.039910	-2.501100	-0.953450
H	-2.453277	-1.678775	0.735891
H	-2.476197	-2.690719	-0.727014
H	-2.937703	-0.041932	-0.981430
H	-1.794982	-0.793487	-2.111903
N	2.133076	0.615578	0.067782
H	1.565969	1.339860	0.492159
C	3.513468	0.858049	-0.312582
H	3.798401	1.845054	0.040137
H	4.169276	0.113108	0.137972
H	3.631986	0.815730	-1.395872
C	-1.007779	1.495917	-0.101977
O	-0.206993	2.012595	0.690713
C	-2.146616	2.291668	-0.678467
H	-1.923271	3.346675	-0.539753
H	-2.296717	2.076656	-1.735723



H -3.068842 2.053791 -0.142959  
O -0.542660 -0.364798 2.663777  
H -0.657186 -1.330680 2.752516

**PT1\_4**

N 0.982919 -0.036292 -0.291860  
C -0.079463 0.595699 0.469617  
C -1.466796 0.435597 -0.166536  
O -2.063945 1.406692 -0.647324  
C 0.372416 2.042058 0.606036  
C 1.165066 2.271272 -0.683821  
C 1.924582 0.957991 -0.848292  
H -0.139101 0.070650 1.511910  
H 1.033747 2.116018 1.471743  
H -0.466008 2.721209 0.734372  
H 1.838404 3.124395 -0.626077  
H 0.478135 2.414279 -1.519439  
H 2.848546 0.958698 -0.266737  
H 2.156087 0.722646 -1.885244  
N -1.968312 -0.798768 -0.160984  
H -1.373721 -1.542897 0.184811  
C -3.239925 -1.087614 -0.801297  
H -4.037867 -0.505290 -0.341072  
H -3.203162 -0.849521 -1.865017  
H -3.454153 -2.145255 -0.678168  
C 1.243581 -1.359393 -0.194833  
O 0.490400 -2.123366 0.428566  
C 2.486016 -1.854616 -0.880118  
H 2.554179 -2.929585 -0.734779  
H 2.448856 -1.628444 -1.947129  
H 3.371534 -1.370971 -0.463320  
O 0.116206 -0.277500 2.888893  
H 0.068113 0.636924 3.228436

**PT1\_5**

N -1.075820 0.288146 -0.161439  
C -0.100343 -0.725778 0.121248  
C 1.356422 -0.335608 -0.089920  
O 2.247172 -0.824675 0.621108  
C -0.520536 -1.922326 -0.742251  
C -2.030053 -1.723145 -0.889287  
C -2.167033 -0.208175 -1.018251  
H -0.159313 -1.051931 1.244744  
H -0.030295 -1.848894 -1.716093  
H -0.235561 -2.862160 -0.274024  
H -2.542381 -2.064683 0.011522  
H -2.440172 -2.247633 -1.750168  
H -2.010362 0.127763 -2.045400  
H -3.117705 0.178804 -0.660346  
N 1.607975 0.487186 -1.105185  
H 0.832920 0.873242 -1.623826  
C 2.964455 0.925839 -1.393453  
H 2.929753 1.613410 -2.233373  
H 3.390324 1.433174 -0.527343  
H 3.594573 0.074729 -1.649632  
C -1.131831 1.519415 0.415198  
O -2.027520 2.310372 0.107384  
C -0.070343 1.871491 1.424486  
H 0.819876 2.241806 0.910583  
H -0.461358 2.669261 2.052310  
H 0.213456 1.020881 2.044207

O 0.333756 -1.550341 2.512119  
H 1.259470 -1.478219 2.191699

**PT2\_1**

N 0.957627 0.499036 0.039452  
C -0.039133 -0.456338 -0.425386  
C -1.413282 -0.171331 0.185963  
O -1.529400 0.348484 1.302272  
C 0.491238 -1.782848 0.116220  
C 1.232436 -1.414516 1.388517  
C 1.865710 -0.065967 1.049040  
H -0.109810 -0.472292 -1.513066  
H 1.271346 -2.159844 -0.683003  
H -0.251665 -2.574782 0.191064  
H 1.970069 -2.160026 1.680947  
H 0.511621 -1.299235 2.201126  
H 2.864659 -0.184318 0.624289  
H 1.929799 0.601531 1.906045  
N -2.457495 -0.557088 -0.549314  
H -2.299089 -0.953747 -1.462880  
C -3.816265 -0.409564 -0.054526  
H -4.041431 0.639929 0.135296  
H -4.499416 -0.791927 -0.807100  
H -3.950467 -0.969645 0.870788  
C 0.940794 1.822698 -0.208583  
O 1.777575 2.576672 0.310107  
C -0.133112 2.350834 -1.124757  
H -1.075276 2.421502 -0.575579  
H 0.156995 3.348072 -1.447323  
H -0.287934 1.714099 -1.995448  
O 2.315873 -2.179945 -1.627033  
H 3.026984 -1.952467 -0.997824

**PT2\_2**

N 0.665440 0.428970 0.302419  
C -0.044432 -0.470185 -0.601791  
C -1.569892 -0.404148 -0.497288  
O -2.256500 -1.125983 -1.232723  
C 0.436510 -1.841457 -0.139585  
C 0.624333 -1.685026 1.358980  
C 1.178554 -0.264887 1.498674  
H 0.210194 -0.281831 -1.644454  
H -0.167302 -2.677010 -0.485252  
H 1.509582 -1.991613 -0.616844  
H -0.346501 -1.771564 1.853880  
H 1.294208 -2.429953 1.784473  
H 0.846142 0.236361 2.406300  
H 2.269379 -0.255218 1.472214  
N -2.090025 0.423823 0.407444  
H -1.466430 0.990106 0.962308  
C -3.529264 0.535877 0.577223  
H -3.727297 1.264171 1.358040  
H -3.999277 0.864624 -0.349663  
H -3.955092 -0.425403 0.864558  
C 1.116379 1.664777 -0.010072  
O 1.852547 2.279077 0.771970  
C 0.702153 2.244537 -1.337407  
H 0.941534 3.305134 -1.336531  
H -0.361721 2.105551 -1.529367  
H 1.260532 1.754103 -2.138787  
O 2.832941 -1.725500 -0.989783

H 2.746199 -0.754684 -1.058033

**PT2\_3**

N -1.127802 0.203917 0.112687  
C 0.247242 0.451389 -0.307976  
C 1.246553 -0.666683 -0.092011  
O 2.381604 -0.539801 -0.589189  
C 0.658373 1.664855 0.529637  
C -0.638413 2.413042 0.771449  
C -1.622160 1.260246 1.016782  
H 0.276868 0.689801 -1.373782  
H 1.472058 2.281828 -0.113962  
H 1.180119 1.385552 1.445237  
H -0.934799 2.960485 -0.124760  
H -0.586856 3.098908 1.613924  
H -2.645083 1.532098 0.769482  
H -1.580997 0.921820 2.053016  
N 0.906439 -1.693165 0.677157  
H -0.043162 -1.755231 1.011147  
C 1.847149 -2.766743 0.955442  
H 2.137323 -3.272707 0.034676  
H 2.740639 -2.370321 1.436120  
H 1.367040 -3.478407 1.620328  
C -1.893337 -0.656437 -0.596841  
O -1.396750 -1.339744 -1.501863  
C -3.351000 -0.744844 -0.232918  
H -3.765959 -1.637672 -0.694283  
H -3.492792 -0.782341 0.847180  
H -3.878652 0.131666 -0.616337  
O 2.478026 2.333195 -0.995703  
H 2.634315 1.361095 -1.004234

**PT2\_4**

N 0.609982 0.496498 0.281476  
C -0.030620 -0.562382 -0.515554  
C -1.494010 -0.770261 -0.096281  
O -1.883041 -1.814115 0.444515  
C 0.816752 -1.780416 -0.202451  
C 1.319208 -1.545097 1.210749  
C 1.604703 -0.044470 1.227001  
H -0.006199 -0.285623 -1.570666  
H 1.737753 -1.717745 -0.939258  
H 0.339041 -2.735518 -0.401442  
H 2.199353 -2.134087 1.462584  
H 0.518823 -1.788357 1.914170  
H 2.612081 0.163554 0.861038  
H 1.484802 0.398884 2.213574  
N -2.306439 0.253361 -0.364637  
H -1.893872 1.090848 -0.759316  
C -3.704630 0.219915 0.027495  
H -4.217265 -0.611823 -0.455504  
H -3.803589 0.109374 1.108101  
H -4.170286 1.151730 -0.280425  
C 0.536898 1.786326 -0.091390  
O -0.226812 2.157014 -1.001632  
C 1.412841 2.757643 0.651293  
H 1.211347 3.759514 0.281009  
H 1.211575 2.713216 1.722896  
H 2.466038 2.514327 0.496327  
O 2.853771 -1.214844 -1.626318  
H 3.467395 -1.269302 -0.868650

**PT2\_5**

N 0.665704 -0.477303 -0.283713  
C -0.004818 0.483740 0.584216  
C -1.531830 0.479632 0.482937  
O -2.187192 1.217529 1.230977  
C 0.527799 1.820052 0.075952  
C 0.763540 1.595810 -1.408040  
C 1.261094 0.150422 -1.475778  
H 0.242398 0.326045 1.633713  
H -0.070265 2.683182 0.358688  
H 1.572002 1.961566 0.609935  
H 1.476757 2.297321 -1.837131  
H -0.184850 1.701105 -1.941069  
H 0.944949 -0.367299 -2.379972  
H 2.349162 0.092529 -1.404780  
N -2.089273 -0.306414 -0.437268  
H -1.493521 -0.895860 -0.998758  
C -3.532926 -0.354973 -0.599644  
H -4.010847 -0.684704 0.322944  
H -3.919975 0.629405 -0.862409  
H -3.765894 -1.056557 -1.395161  
C 0.987062 -1.746997 0.047749  
O 1.685753 -2.434937 -0.707671  
C 0.482078 -2.273679 1.365709  
H -0.577030 -2.060744 1.511854  
H 0.647518 -3.347935 1.389985  
H 1.039174 -1.807538 2.181942  
O 2.841377 1.658585 1.121899  
H 3.283899 1.562045 0.256854

**PT3\_1**

N -1.389402 0.201585 -0.200330  
C -0.053652 0.177693 -0.790998  
C 0.960255 -0.525690 0.105892  
O 0.979590 -0.315458 1.328828  
C 0.316885 1.669011 -0.858178  
C -0.529688 2.352343 0.203957  
C -1.827549 1.546411 0.193625  
H -0.063696 -0.271796 -1.784357  
H 0.209104 2.078151 -1.861058  
H 1.474433 1.818095 -0.600080  
H -0.692679 3.407073 -0.006658  
H -0.047736 2.254857 1.177492  
H -2.541929 1.935550 -0.534490  
H -2.309333 1.508561 1.168229  
N 1.864212 -1.280556 -0.512650  
H 1.806232 -1.397472 -1.512968  
C 3.010204 -1.808389 0.209371  
H 2.683082 -2.452731 1.024364  
H 3.617555 -2.383853 -0.482787  
H 3.604089 -0.990195 0.619643  
C -2.171563 -0.872802 0.017070  
O -3.300590 -0.744895 0.513203  
C -1.614946 -2.225720 -0.342111  
H -0.856484 -2.517213 0.388624  
H -2.428228 -2.946723 -0.308911  
H -1.160360 -2.232457 -1.333203  
O 2.639260 1.872069 0.122259  
H 2.296515 1.372081 0.890930

**PT3\_2**

N	1.172217	-0.483904	-0.011060
C	-0.013513	-0.276775	-0.838336
C	-0.904107	0.882603	-0.391677
O	-1.742490	1.339038	-1.179438
C	-0.756030	-1.610066	-0.681512
C	-0.377325	-2.109511	0.704503
C	1.082427	-1.672277	0.851928
H	0.246910	-0.086235	-1.878055
H	-1.930612	-1.418053	-0.756334
H	-0.526405	-2.306645	-1.485979
H	-0.994481	-1.613161	1.455263
H	-0.496756	-3.185581	0.810945
H	1.346273	-1.417611	1.877145
H	1.774515	-2.436301	0.493841
N	-0.765397	1.319218	0.860184
H	-0.041362	0.922573	1.439681
C	-1.623466	2.371057	1.379834
H	-1.363829	2.544243	2.420070
H	-1.485674	3.293899	0.815959
H	-2.669346	2.071375	1.313391
C	2.325460	0.211547	-0.105548
O	3.304043	-0.098348	0.586528
C	2.374458	1.345964	-1.095445
H	3.294392	1.902022	-0.932644
H	1.519410	2.015196	-0.994554
H	2.372085	0.945449	-2.111947
O	-3.219822	-1.228667	-0.351748
H	-3.274128	-2.029803	0.204135

**PT3\_3**

N	1.151510	-0.289366	0.264173
C	-0.099791	0.184328	0.840688
C	-1.299916	-0.208180	-0.018745
O	-1.232598	-0.235500	-1.252227
C	0.086965	1.701007	0.877258
C	1.591656	1.910459	0.898642
C	2.093955	0.800172	-0.021412
H	-0.231084	-0.210189	1.851773
H	-0.492753	2.209189	1.643652
H	-0.303741	2.126113	-0.158941
H	1.967284	1.756525	1.913293
H	1.888484	2.902169	0.560404
H	3.115330	0.497372	0.197694
H	2.021677	1.100308	-1.069334
N	-2.429148	-0.444779	0.652540
H	-2.413411	-0.445057	1.660467
C	-3.662260	-0.764320	-0.046814
H	-3.934469	0.041879	-0.727629
H	-3.551698	-1.684768	-0.620551
H	-4.451163	-0.893580	0.688245
C	1.309822	-1.590989	-0.027642
O	0.425252	-2.415709	0.253344
C	2.603430	-1.991262	-0.684982
H	2.543646	-3.042939	-0.954112
H	2.789508	-1.391203	-1.577148
H	3.437485	-1.841003	0.003730
O	-0.370363	2.692941	-1.436817
H	0.236882	3.433056	-1.244886

**PT3\_4**

N	1.040268	-0.539724	0.005077
C	-0.217250	-0.256045	-0.710742
C	-0.978679	0.873437	0.000107
O	-2.019587	0.689511	0.653777
C	-0.908231	-1.610403	-0.663550
C	-0.495658	-2.203398	0.671713
C	0.981209	-1.805564	0.762171
H	0.012079	0.065198	-1.726062
H	-0.624579	-2.225977	-1.516964
H	-2.101105	-1.535031	-0.760360
H	-0.629256	-3.281609	0.723256
H	-1.062512	-1.732782	1.476025
H	1.615947	-2.552650	0.283318
H	1.315181	-1.659940	1.788093
N	-0.420707	2.075954	-0.120201
H	0.479177	2.130689	-0.585059
C	-0.971829	3.229098	0.571887
H	-0.366554	4.097053	0.327147
H	-1.998231	3.407098	0.253048
H	-0.962525	3.075985	1.651610
C	2.169315	0.136546	-0.273275
O	2.162616	1.135647	-1.014505
C	3.434493	-0.370077	0.363081
H	4.254449	0.279502	0.067838
H	3.340850	-0.372680	1.450433
H	3.641107	-1.392425	0.040787
O	-3.406319	-1.379393	-0.517497
H	-3.224849	-0.583723	0.030197

**PT3\_5**

N	1.172153	0.289233	-0.070456
C	0.040701	0.303933	0.849505
C	-1.077679	-0.676302	0.513018
O	-2.048501	-0.758953	1.283428
C	-0.516944	1.736800	0.729993
C	0.512380	2.526456	-0.064164
C	1.170272	1.467477	-0.944501
H	0.354457	0.097942	1.873236
H	-1.511117	1.705009	0.084364
H	-0.823592	2.165825	1.679877
H	1.251456	2.948405	0.621354
H	0.067980	3.337976	-0.638458
H	0.579597	1.271547	-1.842866
H	2.189166	1.709361	-1.232810
N	-1.002674	-1.343829	-0.633998
H	-0.212716	-1.185576	-1.241336
C	-2.129296	-2.135139	-1.101083
H	-2.384383	-2.900438	-0.369743
H	-2.997797	-1.494337	-1.262641
H	-1.851653	-2.610262	-2.037279
C	2.195282	-0.594653	-0.042983
O	3.123051	-0.526457	-0.858763
C	2.161503	-1.647445	1.035672
H	1.219604	-2.196674	1.037499
H	2.983335	-2.337754	0.863534
H	2.282560	-1.178638	2.014707
O	-2.756391	1.458739	-0.502315
H	-3.015831	0.776383	0.150204

**PT4\_1**

N	1.337963	0.315496	0.315229
---	----------	----------	----------

C	0.128112	-0.079905	1.017250
C	-0.843311	-0.765255	0.045365
O	-0.570400	-0.913871	-1.150900
C	-0.420117	1.273072	1.495470
C	-0.095465	2.189816	0.325028
C	1.204128	1.657994	-0.268214
H	0.342420	-0.749716	1.849160
H	0.137578	1.586879	2.380254
H	-1.480016	1.245452	1.744307
H	-0.087338	3.252444	0.554959
H	-0.947053	2.070252	-0.482400
H	2.056654	2.275974	0.017522
H	1.177154	1.600107	-1.357563
N	-1.994995	-1.185220	0.578139
H	-2.191167	-0.982054	1.546761
C	-3.054379	-1.705461	-0.271170
H	-2.720957	-2.603624	-0.789848
H	-3.908218	-1.950494	0.353862
H	-3.349466	-0.960507	-1.011831
C	2.253639	-0.542684	-0.182996
O	3.100181	-0.156309	-1.000413
C	2.233424	-1.958271	0.333186
H	1.327188	-2.472387	0.008870
H	3.100972	-2.478484	-0.065515
H	2.265409	-1.975185	1.423569
O	-2.141571	1.854902	-1.215349
H	-2.665811	1.535797	-0.455910

**PT4\_2**

N	1.133873	0.339727	-0.034199
C	0.161051	0.168192	1.039574
C	-1.027711	-0.706499	0.628006
O	-2.079707	-0.665492	1.288575
C	-0.320074	1.605094	1.273998
C	-0.366072	2.154714	-0.143189
C	0.818048	1.516322	-0.859809
H	0.613823	-0.269552	1.927672
H	-1.274454	1.644060	1.793420
H	0.429261	2.143217	1.858550
H	-1.370177	1.775490	-0.648986
H	-0.417065	3.237247	-0.232402
H	0.591776	1.226703	-1.886656
H	1.678227	2.188331	-0.875040
N	-0.892289	-1.477436	-0.447572
H	-0.046638	-1.410245	-0.992708
C	-2.019539	-2.242216	-0.953958
H	-1.683553	-2.828788	-1.803985
H	-2.401397	-2.909129	-0.182717
H	-2.818832	-1.569866	-1.269883
C	2.296252	-0.326393	-0.198427
O	3.074532	-0.015187	-1.109901
C	2.604848	-1.439067	0.770554
H	3.483627	-1.968872	0.411672
H	1.770047	-2.133834	0.865235
H	2.815493	-1.022768	1.758206
O	-2.638794	1.269413	-0.994357
H	-2.790290	0.771209	-0.165019

**PT4\_3**

N	-0.271675	0.793620	-0.019191
C	0.127983	-0.372762	0.794883

C	1.216447	-1.197269	0.089987
O	0.997913	-2.312413	-0.400408
C	-1.171424	-1.167849	0.999976
C	-2.273949	-0.193004	0.617517
C	-1.658769	0.650884	-0.485200
H	0.533994	-0.003999	1.736963
H	-1.258564	-1.535561	2.019700
H	-1.177181	-2.018285	0.318464
H	-2.658653	0.402756	1.444534
H	-3.201101	-0.798295	0.196905
H	-2.134814	1.618790	-0.604262
H	-1.682876	0.116555	-1.437264
N	2.419836	-0.620491	0.052292
H	2.491131	0.333140	0.387455
C	3.523918	-1.249945	-0.650101
H	4.396192	-0.607841	-0.566157
H	3.751497	-2.220485	-0.209558
H	3.285353	-1.394727	-1.704719
C	0.412851	1.950825	0.063430
O	1.492523	2.017449	0.677570
C	-0.165529	3.162558	-0.618504
H	0.596015	3.938365	-0.630659
H	-0.478568	2.935780	-1.637535
H	-1.034618	3.524638	-0.064871
O	-4.032692	-1.487506	-0.662163
H	-4.196070	-0.743610	-1.272616

**PT4\_4**

N	1.066439	-0.005066	-0.173319
C	-0.065205	-0.133247	-1.107699
C	-1.404205	0.269544	-0.469929
O	-2.393597	-0.474139	-0.495951
C	-0.035154	-1.613060	-1.482156
C	0.498528	-2.274836	-0.222530
C	1.546420	-1.312838	0.303341
H	0.104221	0.522172	-1.963156
H	0.677522	-1.767228	-2.296296
H	-1.011193	-1.977053	-1.790831
H	0.839128	-3.302236	-0.323835
H	-0.382967	-2.301337	0.563241
H	2.525152	-1.536994	-0.128316
H	1.629144	-1.330173	1.389602
N	-1.435154	1.484396	0.081711
H	-0.607126	2.064233	0.009795
C	-2.652492	1.992110	0.689003
H	-3.453584	2.066984	-0.047541
H	-2.981083	1.334191	1.493598
H	-2.448813	2.978526	1.095893
C	1.726329	1.152707	-0.006669
O	1.303593	2.216303	-0.497827
C	2.989518	1.104878	0.808869
H	3.387172	2.113107	0.890006
H	2.787855	0.708158	1.805352
H	3.727278	0.456654	0.331525
O	-1.092899	-2.124521	1.767894
H	-0.370907	-2.437003	2.345918

**PT4\_5**

N	0.173926	0.971691	-0.038703
C	-0.085473	-0.160379	-0.928525
C	-1.149419	-1.133187	-0.443242

O	-1.628611	-1.950884	-1.240624
C	1.273140	-0.907384	-0.991233
C	2.280498	0.137461	-0.540406
C	1.539314	0.956075	0.502355
H	-0.387090	0.180127	-1.918689
H	1.266133	-1.734803	-0.277977
H	1.463729	-1.302461	-1.985557
H	2.686620	0.740328	-1.351853
H	3.218901	-0.375909	-0.026212
H	1.562821	0.464145	1.477884
H	1.907341	1.973116	0.604367
N	-1.458934	-1.112608	0.854141
H	-1.052900	-0.401763	1.443329
C	-2.420513	-2.052720	1.405589
H	-2.533797	-1.845911	2.465714
H	-3.387065	-1.945361	0.913050
H	-2.072156	-3.077143	1.274310
C	-0.639835	2.040328	0.118589
O	-0.326088	2.979508	0.860749
C	-1.927063	2.044462	-0.666050
H	-2.512841	1.141290	-0.492192
H	-2.505886	2.913867	-0.364737
H	-1.709982	2.107154	-1.734785
O	3.973747	-1.199125	0.774362
H	3.674955	-2.034175	0.366920

**PT5\_1**

N	0.565554	0.929570	-0.221986
C	-0.151180	-0.215425	-0.768588
C	-1.315829	-0.610650	0.138430
O	-1.315572	-0.337329	1.346099
C	0.924164	-1.317759	-0.750140
C	1.712415	-0.994954	0.510905
C	1.704264	0.525323	0.618216
H	-0.507222	-0.021422	-1.779817
H	1.558989	-1.196999	-1.629426
H	0.496142	-2.318360	-0.755144
H	2.831304	-1.356422	0.397002
H	1.339020	-1.495419	1.402311
H	2.625786	0.965496	0.234052
H	1.557557	0.868194	1.641710
N	-2.297643	-1.296893	-0.450101
H	-2.237860	-1.490082	-1.438177
C	-3.420921	-1.811801	0.315531
H	-3.078844	-2.507700	1.081700
H	-3.958871	-0.995862	0.797728
H	-4.091222	-2.329116	-0.364673
C	0.051551	2.171276	-0.102601
O	0.639345	3.039545	0.557272
C	-1.245127	2.456403	-0.815185
H	-2.065032	1.914678	-0.337826
H	-1.442779	3.523598	-0.750116
H	-1.199321	2.154637	-1.862045
O	4.053878	-1.690782	-0.169327
H	3.719751	-2.449899	-0.684422

**PT5\_2**

N	-0.350993	0.825910	0.054890
C	0.173024	-0.199872	0.949176
C	1.408867	-0.927497	0.423154
O	1.953398	-1.781198	1.137261

C	-1.004329	-1.186643	1.052551
C	-1.611467	-1.117686	-0.341217
C	-1.466881	0.337822	-0.771108
H	0.436486	0.212801	1.921741
H	-0.679936	-2.182774	1.343705
H	-1.713557	-0.808072	1.789983
H	-1.179206	-1.825435	-1.046914
H	-2.758128	-1.404023	-0.277312
H	-1.240853	0.446126	-1.831412
H	-2.365221	0.915269	-0.545501
N	1.834118	-0.632892	-0.805859
H	1.362931	0.088933	-1.329373
C	2.993812	-1.301517	-1.372556
H	3.880029	-1.113626	-0.766123
H	2.825551	-2.377050	-1.423663
H	3.156941	-0.915945	-2.374706
C	0.020497	2.122556	0.011641
O	-0.537022	2.909288	-0.765762
C	1.110649	2.565944	0.952828
H	1.383388	3.587841	0.701160
H	1.989954	1.924415	0.883847
H	0.747223	2.533490	1.982365
O	-4.129606	-1.306176	-0.151949
H	-4.266672	-0.767039	-0.954221

**PT5\_3**

N	0.548298	0.253839	0.465844
C	-0.231425	-0.648796	-0.410921
C	-1.729538	-0.621003	-0.088573
O	-2.343493	-1.623898	0.298904
C	0.395779	-2.033279	-0.203118
C	1.745576	-1.737351	0.422551
C	1.488034	-0.522681	1.287445
H	-0.107392	-0.302717	-1.438810
H	0.459215	-2.591642	-1.135295
H	-0.211248	-2.606710	0.499917
H	2.484345	-1.363662	-0.422217
H	2.243388	-2.571618	0.912173
H	2.384342	0.046834	1.510711
H	1.013183	-0.817429	2.226941
N	-2.325024	0.558616	-0.275840
H	-1.751925	1.333500	-0.588908
C	-3.737128	0.735522	0.011765
H	-4.001478	1.770607	-0.185290
H	-4.344278	0.085698	-0.618936
H	-3.950871	0.504639	1.055733
C	0.762500	1.526858	0.069257
O	0.091103	2.031793	-0.846934
C	1.826856	2.323956	0.774729
H	1.703394	3.368858	0.501602
H	1.765701	2.213353	1.856962
H	2.810957	1.981668	0.446266
O	3.066598	-0.465103	-1.348798
H	2.302164	-0.420263	-1.955060

**PT5\_4**

N	-0.313383	0.756505	0.060642
C	0.134709	-0.408086	0.841198
C	1.281954	-1.129942	0.121703
O	1.142831	-2.248461	-0.391046
C	-1.124130	-1.271354	0.922789

C	-1.808898	-0.986122	-0.404511
C	-1.579193	0.499378	-0.648907
H	0.484170	-0.071814	1.817133
H	-1.745035	-0.912033	1.745110
H	-0.893235	-2.322030	1.074801
H	-2.969693	-1.198091	-0.304199
H	-1.463382	-1.618941	-1.220099
H	-2.382861	1.092756	-0.208062
H	-1.493910	0.744209	-1.706217
N	2.435629	-0.458522	0.091279
H	2.439474	0.483853	0.463528
C	3.587025	-0.982141	-0.622849
H	4.403296	-0.271794	-0.526722
H	3.895335	-1.938546	-0.200973
H	3.358813	-1.125433	-1.679819
C	0.276754	1.957478	0.176016
O	1.313728	2.110122	0.848385
C	-0.369796	3.102191	-0.555193
H	0.197068	4.007272	-0.352803
H	-0.377799	2.908003	-1.629445
H	-1.403215	3.234436	-0.229792
O	-4.309203	-1.044034	-0.011580
H	-4.474153	-0.327155	-0.653435

**PT5\_5**

N	0.530409	0.318742	0.433662
C	-0.221358	-0.525273	-0.505743
C	-1.731241	-0.374257	-0.428194
O	-2.443395	-1.046291	-1.188981
C	0.176299	-1.979160	-0.138520
C	1.413953	-1.806797	0.721624
C	1.159622	-0.514461	1.467720
H	0.070725	-0.307406	-1.531332
H	-0.612419	-2.447722	0.455611
H	0.340636	-2.584481	-1.027172
H	2.311553	-1.587496	-0.022058
H	1.706306	-2.663219	1.325244
H	0.463873	-0.680392	2.294526
H	2.051548	-0.023599	1.844919
N	-2.224320	0.454953	0.490542
H	-1.577591	0.983060	1.056419
C	-3.657438	0.634510	0.647211
H	-4.100001	1.018194	-0.272107
H	-4.135291	-0.312723	0.896488
H	-3.829281	1.344508	1.450748
C	1.115059	1.489613	0.059875
O	1.988771	2.023026	0.751601
C	0.660606	2.112542	-1.234036
H	-0.415279	2.035906	-1.384461
H	0.960040	3.157731	-1.229366
H	1.163218	1.606332	-2.062576
O	3.029780	-0.852664	-0.990581
H	3.365079	-0.167418	-0.380246

**PT6\_1**

N	0.816584	0.379694	-0.053489
C	-0.268699	-0.368698	-0.680034
C	-1.567336	-0.193047	0.108005
O	-1.567106	0.111087	1.307792
C	0.231182	-1.822069	-0.574497
C	1.003798	-1.823526	0.746931

C	1.676811	-0.459873	0.743195
H	-0.417215	-0.067083	-1.716198
H	0.907310	-2.018376	-1.408838
H	-0.585600	-2.541095	-0.606835
H	1.729095	-2.632092	0.815439
H	0.317369	-1.893172	1.592092
H	2.711866	-0.548989	0.229326
H	1.886751	-0.025708	1.719385
N	-2.686725	-0.424338	-0.581390
H	-2.620337	-0.669273	-1.557524
C	-3.990030	-0.376676	0.060422
H	-4.056079	-1.118979	0.856040
H	-4.167815	0.610503	0.486684
H	-4.749046	-0.584551	-0.688013
C	0.917008	1.730833	-0.003366
O	1.833653	2.268195	0.627617
C	-0.118030	2.528588	-0.749951
H	-1.098556	2.406062	-0.284889
H	0.166130	3.577167	-0.708671
H	-0.188889	2.208237	-1.790194
O	3.823321	-1.156927	-0.574388
H	3.228830	-1.462163	-1.286055

**PT6\_2**

N	-0.637781	0.292247	-0.098789
C	0.258903	-0.394247	0.832714
C	1.737418	-0.295606	0.464437
O	2.577941	-0.797751	1.223985
C	-0.213346	-1.854575	0.729475
C	-0.627587	-1.968738	-0.739751
C	-1.297295	-0.628063	-0.997430
H	0.158099	-0.005353	1.844340
H	0.564812	-2.553162	1.029289
H	-1.084083	-1.986249	1.374220
H	0.250079	-2.076069	-1.381389
H	-1.301704	-2.801466	-0.933455
H	-1.305968	-0.278843	-2.028813
H	-2.414720	-0.682822	-0.686220
N	2.062946	0.310374	-0.677485
H	1.331215	0.701361	-1.250418
C	3.451301	0.417876	-1.094247
H	3.486757	0.959829	-2.034690
H	4.033499	0.956352	-0.346487
H	3.887612	-0.571422	-1.231876
C	-1.072531	1.575792	0.005824
O	-1.961402	1.990821	-0.743352
C	-0.446759	2.437763	1.068112
H	-0.751243	3.467027	0.895297
H	0.641072	2.368052	1.059885
H	-0.801243	2.120482	2.051669
O	-3.622792	-0.913528	0.148866
H	-3.360946	-1.813613	0.421763

**PT6\_3**

N	0.712585	-0.102266	-0.050948
C	-0.420810	0.688944	0.427436
C	-1.734777	0.171312	-0.143680
O	-1.842699	-0.140023	-1.336413
C	-0.112959	2.084635	-0.136178
C	1.417149	2.136408	-0.149750
C	1.820190	0.708449	-0.500385

H	-0.453395	0.689306	1.519503
H	-0.566950	2.872470	0.461363
H	-0.498157	2.140312	-1.155928
H	1.792275	2.383759	0.844846
H	1.813489	2.858261	-0.860836
H	2.777848	0.441010	0.096890
H	2.070885	0.537512	-1.548232
N	-2.770317	0.171052	0.698527
H	-2.615761	0.388986	1.670233
C	-4.091613	-0.237769	0.254447
H	-4.778496	-0.150219	1.091165
H	-4.434671	0.400579	-0.559454
H	-4.078693	-1.271171	-0.093086
C	0.701339	-1.452844	0.027875
O	-0.265081	-2.045432	0.522935
C	1.910387	-2.170920	-0.503093
H	1.737225	-3.241802	-0.433378
H	2.097069	-1.891848	-1.541868
H	2.790657	-1.898978	0.081688
O	4.025688	0.176741	0.833659
H	4.474090	-0.239255	0.072549

**PT6\_4**

N	0.591361	0.242297	0.151194
C	-0.290204	-0.560742	-0.721111
C	-1.726765	-0.572371	-0.179798
O	-2.271360	-1.607080	0.227201
C	0.358268	-1.942273	-0.677189
C	0.952092	-1.998900	0.732483
C	1.503921	-0.593981	0.901041
H	-0.299342	-0.121238	-1.718569
H	1.161343	-1.979135	-1.415204
H	-0.358714	-2.733166	-0.881004
H	1.726645	-2.754620	0.848896
H	0.166414	-2.177841	1.469743
H	2.550747	-0.565413	0.402829
H	1.652975	-0.251437	1.923699
N	-2.345134	0.610319	-0.190322
H	-1.821492	1.417709	-0.506377
C	-3.695070	0.750926	0.326160
H	-3.996146	1.789605	0.224163
H	-4.386947	0.121726	-0.234006
H	-3.740390	0.466288	1.377988
C	0.756499	1.572311	-0.040611
O	0.010125	2.206763	-0.800927
C	1.876831	2.231467	0.713945
H	1.892459	3.287348	0.456846
H	1.728899	2.117384	1.789517
H	2.831899	1.770757	0.454066
O	3.698313	-0.564887	-0.559710
H	3.258006	0.046743	-1.180730

**PT6\_5**

N	-0.652489	0.132576	-0.089061
C	0.269292	-0.740636	0.645048
C	1.742579	-0.418539	0.434348
O	2.554492	-0.636302	1.342092
C	-0.061073	-2.136106	0.080581
C	-1.542889	-2.031810	-0.289174
C	-1.684198	-0.601663	-0.787284
H	0.084859	-0.695601	1.719027

H	0.535794	-2.313417	-0.815393
H	0.151556	-2.917538	0.806616
H	-2.158515	-2.163549	0.602687
H	-1.846026	-2.761844	-1.036554
H	-1.639361	-0.467433	-1.869252
H	-2.717562	-0.152174	-0.483023
N	2.103731	0.029400	-0.770980
H	1.387365	0.245525	-1.447755
C	3.483625	0.396503	-1.041406
H	3.809782	1.187991	-0.365093
H	4.139097	-0.464612	-0.915481
H	3.550810	0.749949	-2.066181
C	-0.728595	1.485071	0.016409
O	-1.587064	2.108174	-0.216392
C	0.262525	2.185200	0.908066
H	1.184630	2.376016	0.354356
H	-0.169701	3.140656	1.197554
H	0.506979	1.608754	1.800048
O	-3.883737	0.201178	0.298498
H	-4.095525	-0.719074	0.545615

**PT7\_1**

N	1.032812	0.037367	-0.615453
C	-0.338299	-0.181116	-1.057294
C	-1.330772	0.099401	0.070643
O	-0.988692	0.129057	1.264411
C	-0.323753	-1.674562	-1.425782
C	0.632585	-2.280462	-0.390687
C	1.653209	-1.175371	-0.136413
H	-0.578689	0.444530	-1.915670
H	0.084696	-1.775494	-2.431383
H	-1.318747	-2.115598	-1.404531
H	1.102551	-3.197769	-0.739098
H	0.098036	-2.496871	0.535581
H	2.644481	-1.325310	-0.564103
H	1.845732	-1.071393	1.015609
N	-2.591952	0.287477	-0.310752
H	-2.814746	0.256220	-1.294494
C	-3.653781	0.492585	0.661762
H	-3.727348	-0.361702	1.334389
H	-3.461318	1.388936	1.250912
H	-4.590775	0.609992	0.125798
C	1.574835	1.247385	-0.325466
O	2.680869	1.319566	0.218620
C	0.784997	2.467269	-0.716078
H	-0.149705	2.516449	-0.153225
H	1.382719	3.347005	-0.491130
H	0.542884	2.449492	-1.779654
O	1.464917	-0.763412	2.372105
H	0.603329	-0.394859	2.069230

**PT7\_2**

N	0.986253	-0.129366	-0.471251
C	-0.245701	-0.248308	-1.245111
C	-1.494655	0.278937	-0.543088
O	-2.530199	0.433578	-1.207492
C	-0.349697	-1.768579	-1.452458
C	0.234400	-2.341920	-0.153267
C	1.324458	-1.344107	0.230361
H	-0.168663	0.284780	-2.190913
H	-1.374778	-2.081813	-1.641961

H	0.269513	-2.047070	-2.305321
H	-0.531171	-2.369074	0.624235
H	0.632100	-3.346880	-0.276846
H	1.310769	-1.118274	1.364375
H	2.349628	-1.657161	0.028972
N	-1.430524	0.515961	0.767479
H	-0.589121	0.298779	1.291731
C	-2.614190	0.943553	1.495181
H	-2.977802	1.895329	1.108529
H	-3.411351	0.204293	1.409068
H	-2.345771	1.062163	2.541515
C	1.711741	1.002580	-0.287357
O	2.694406	0.994715	0.460329
C	1.280902	2.227222	-1.048043
H	1.894670	3.064282	-0.725302
H	0.228513	2.456434	-0.874653
H	1.420340	2.067086	-2.119331
O	0.734717	-0.510204	2.614635
H	0.128085	-1.260025	2.775223

**PT7\_3**

N	0.969896	0.172841	-0.589574
C	-0.260873	-0.558511	-0.892558
C	-1.378186	-0.132303	0.048541
O	-1.159477	0.076789	1.254885
C	0.117721	-2.030575	-0.618012
C	1.645962	-2.048718	-0.716809
C	2.023962	-0.698416	-0.137527
H	-0.553826	-0.393614	-1.929990
H	-0.374043	-2.706408	-1.313756
H	-0.178653	-2.290995	0.399746
H	1.969107	-2.096202	-1.759196
H	2.096524	-2.874846	-0.169893
H	3.017120	-0.327885	-0.381459
H	1.980780	-0.765934	1.030462
N	-2.600463	-0.078169	-0.470196
H	-2.720830	-0.221410	-1.461246
C	-3.754849	0.237069	0.355858
H	-3.658639	1.235009	0.783238
H	-4.643098	0.197487	-0.267409
H	-3.850053	-0.485131	1.165957
C	0.948246	1.521675	-0.459845
O	-0.057783	2.163840	-0.781605
C	2.187995	2.169218	0.089741
H	2.015942	3.239834	0.165191
H	2.409956	1.757780	1.076789
H	3.044804	1.979340	-0.559099
O	1.365635	-0.651606	2.356369
H	0.492001	-0.378549	1.985522

**PT7\_4**

N	0.738353	0.079135	-0.533081
C	-0.502164	-0.505951	-1.069946
C	-1.659872	-0.367462	-0.071351
O	-2.205911	-1.348358	0.450440
C	-0.102211	-1.958432	-1.307498
C	0.871658	-2.245616	-0.157770
C	1.622103	-0.926972	0.013743
H	-0.769367	0.022064	-1.984956
H	0.411814	-2.027748	-2.266711
H	-0.962292	-2.623238	-1.313709

H	1.551497	-3.069430	-0.364433
H	0.313249	-2.472603	0.751129
H	2.610804	-0.898914	-0.444532
H	1.797770	-0.727489	1.143490
N	-2.037707	0.887564	0.183377
H	-1.524315	1.639053	-0.261010
C	-3.092624	1.170574	1.140771
H	-4.032830	0.720943	0.820752
H	-2.836850	0.778428	2.125628
H	-3.217723	2.247665	1.206396
C	1.033218	1.391204	-0.661699
O	0.214784	2.186716	-1.149350
C	2.387802	1.829264	-0.181059
H	2.465911	2.906783	-0.300236
H	2.519649	1.558847	0.867720
H	3.173200	1.337613	-0.758729
O	2.136971	-0.371900	2.530917
H	3.080751	-0.210180	2.339927

**PT7\_5**

N	0.948669	0.041360	-0.568876
C	-0.102886	-0.930676	-0.897738
C	-1.476020	-0.531285	-0.367954
O	-2.494570	-0.802638	-1.016976
C	0.380456	-2.232898	-0.213575
C	1.876274	-2.010537	0.028920
C	1.967432	-0.516995	0.278367
H	-0.194396	-1.051251	-1.976075
H	-0.131750	-2.355089	0.741420
H	0.169642	-3.101859	-0.832328
H	2.454953	-2.250031	-0.865984
H	2.260781	-2.597114	0.860833
H	1.694129	-0.270013	1.388889
H	2.935843	-0.052200	0.111386
N	-1.508777	0.061752	0.828147
H	-0.645575	0.256412	1.328697
C	-2.775620	0.470280	1.410548
H	-3.418938	-0.392488	1.586540
H	-2.573025	0.964183	2.356973
H	-3.294773	1.164093	0.748023
C	0.855680	1.383233	-0.743468
O	1.634736	2.141527	-0.148921
C	-0.208493	1.907359	-1.666723
H	0.173132	2.813528	-2.134015
H	-0.496842	1.189146	-2.432445
H	-1.092121	2.173622	-1.081652
O	1.069708	0.673034	2.364438
H	1.299770	1.461004	1.826247