

## Supporting Information

### **Base-controlled, product switch in the ruthenium-catalyzed protodecarbonylation of phthalimides: a mechanistic study**

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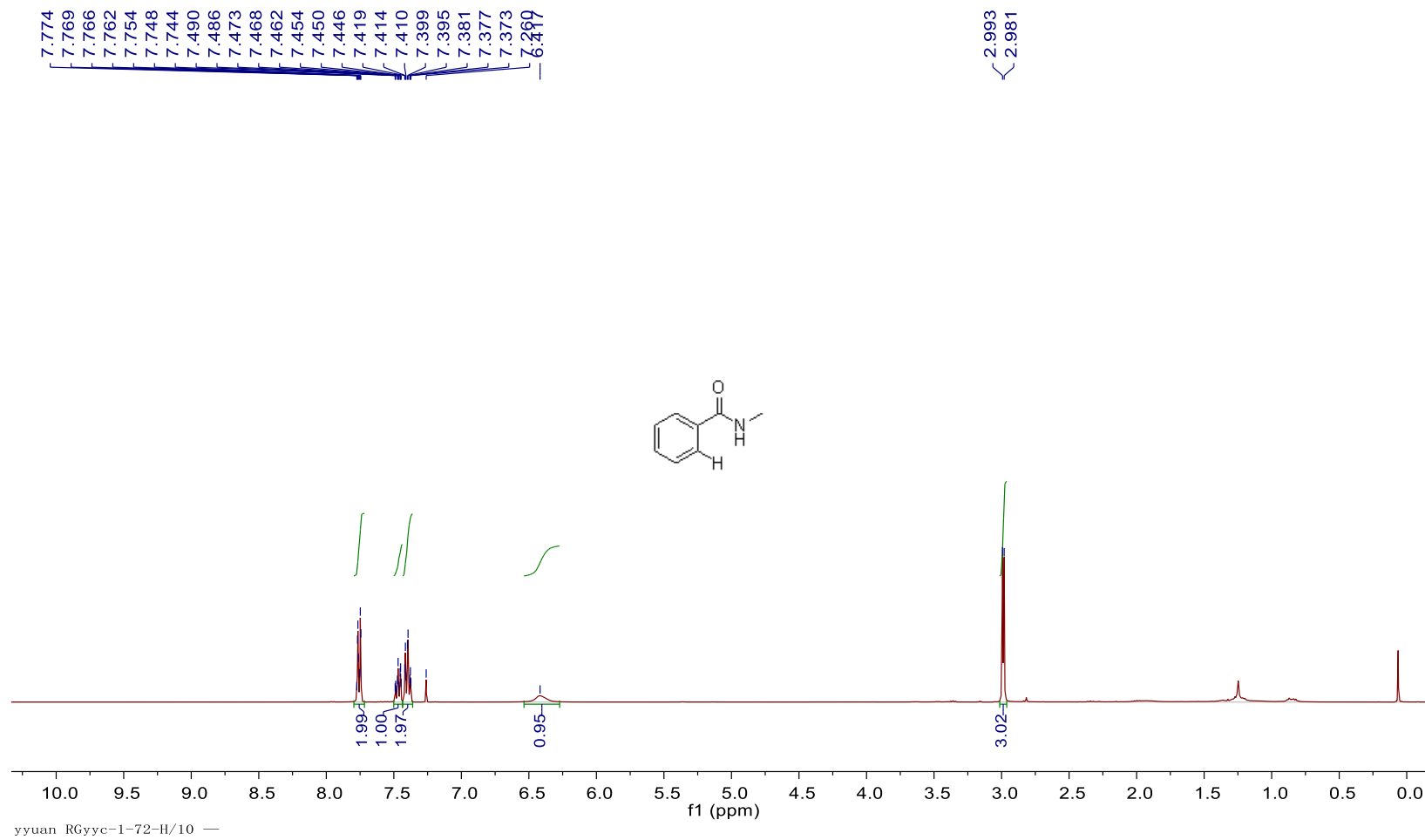
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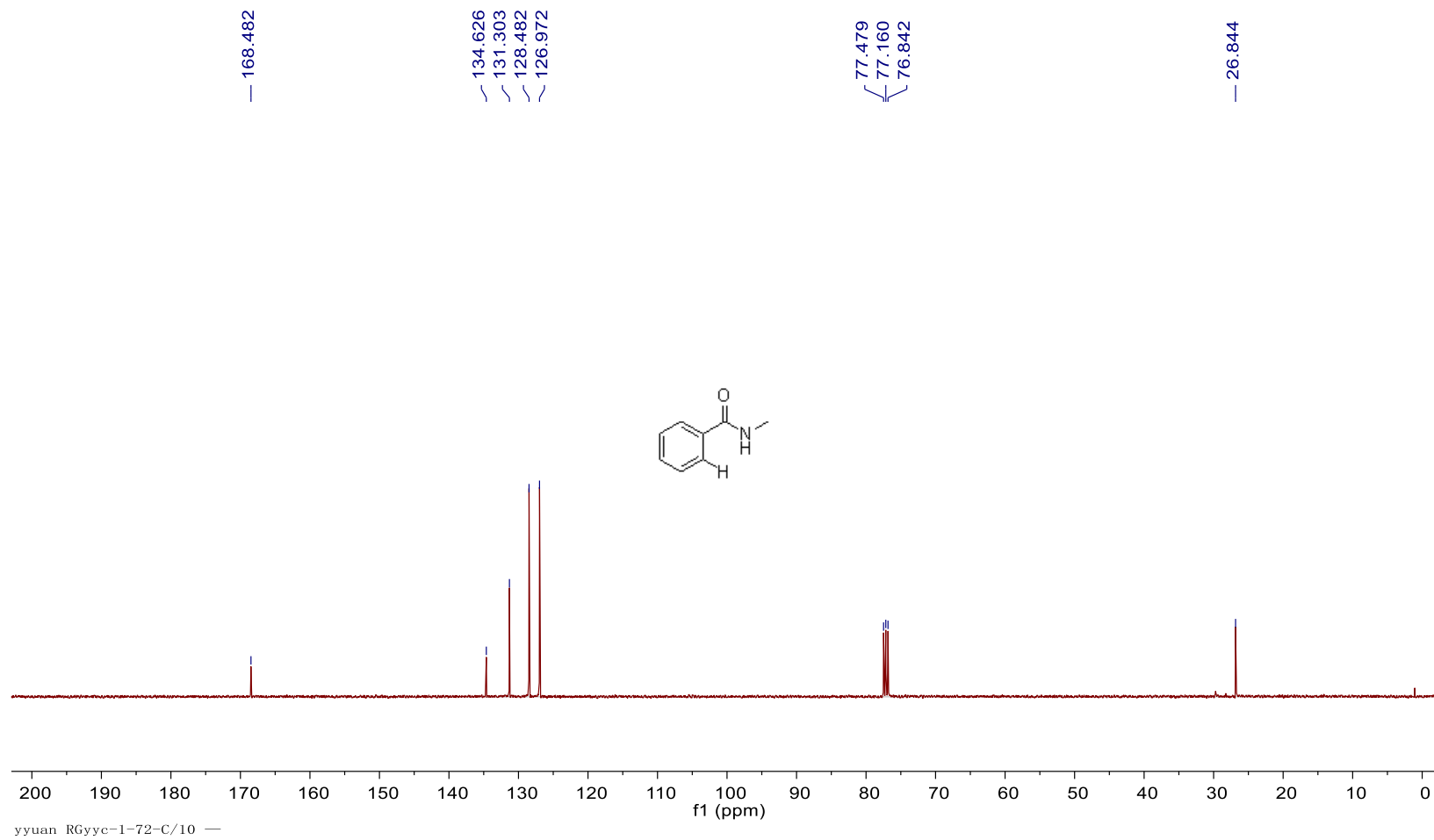
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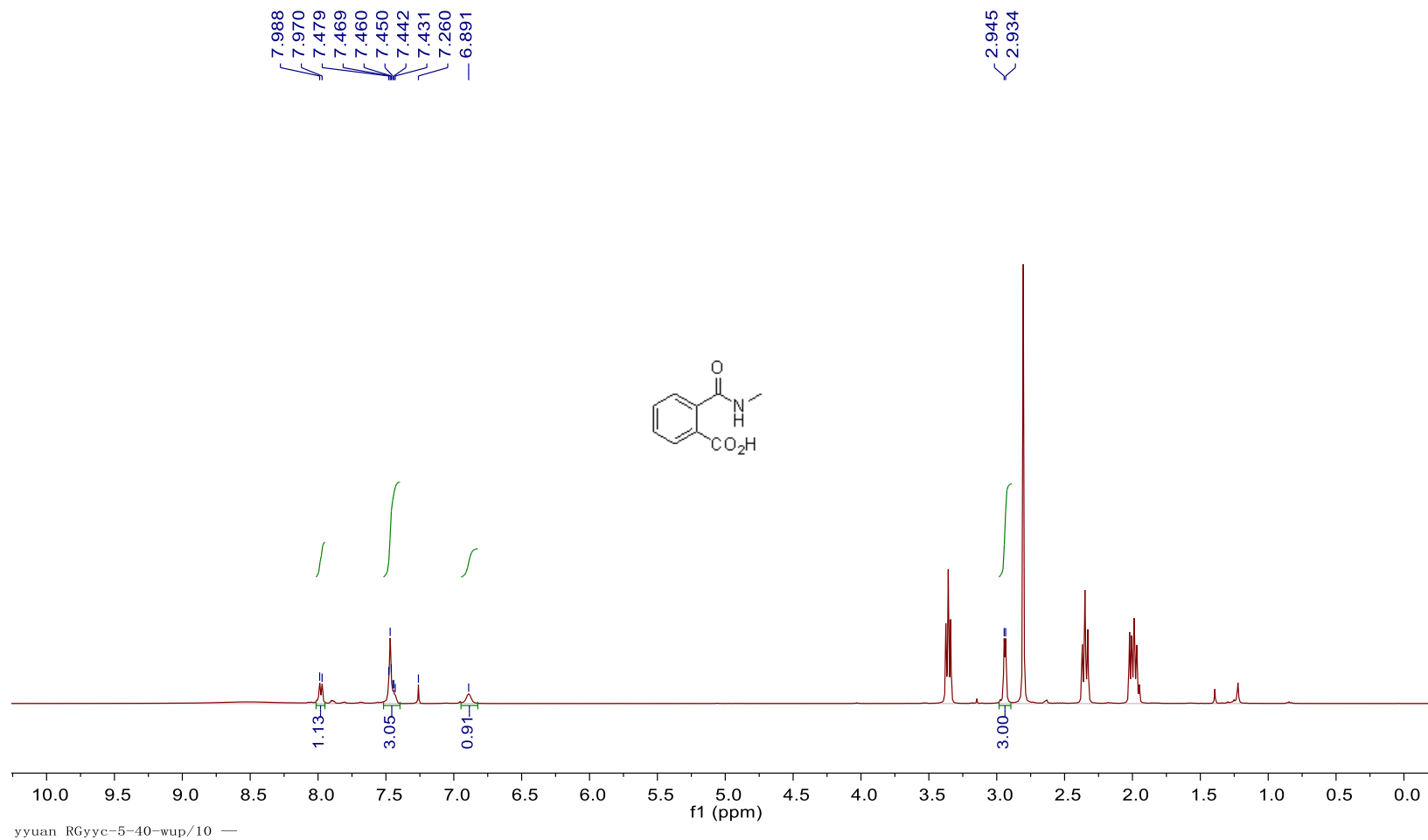
# 1. NMR spectra of products 2 and 3.



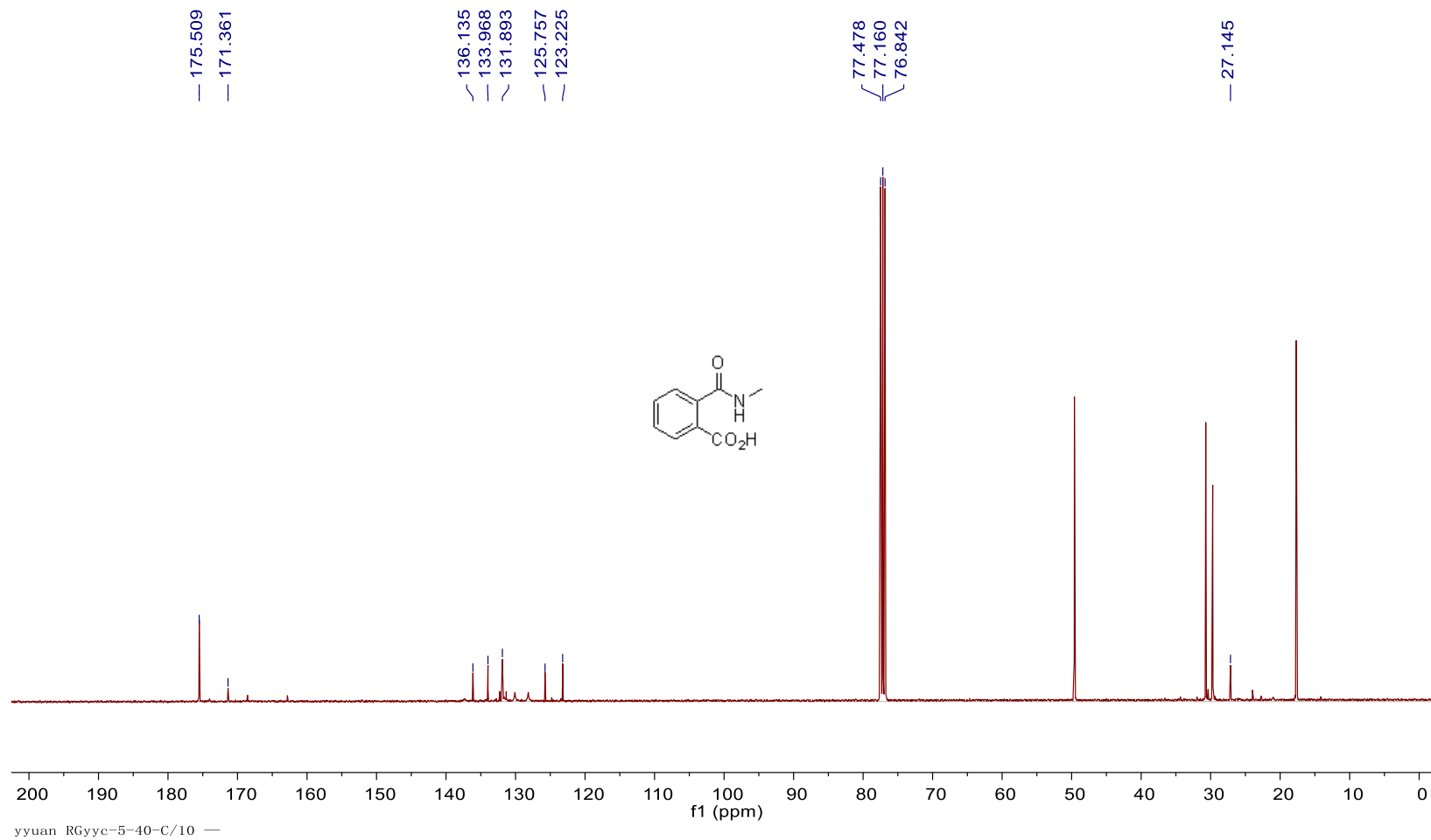
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of 2.



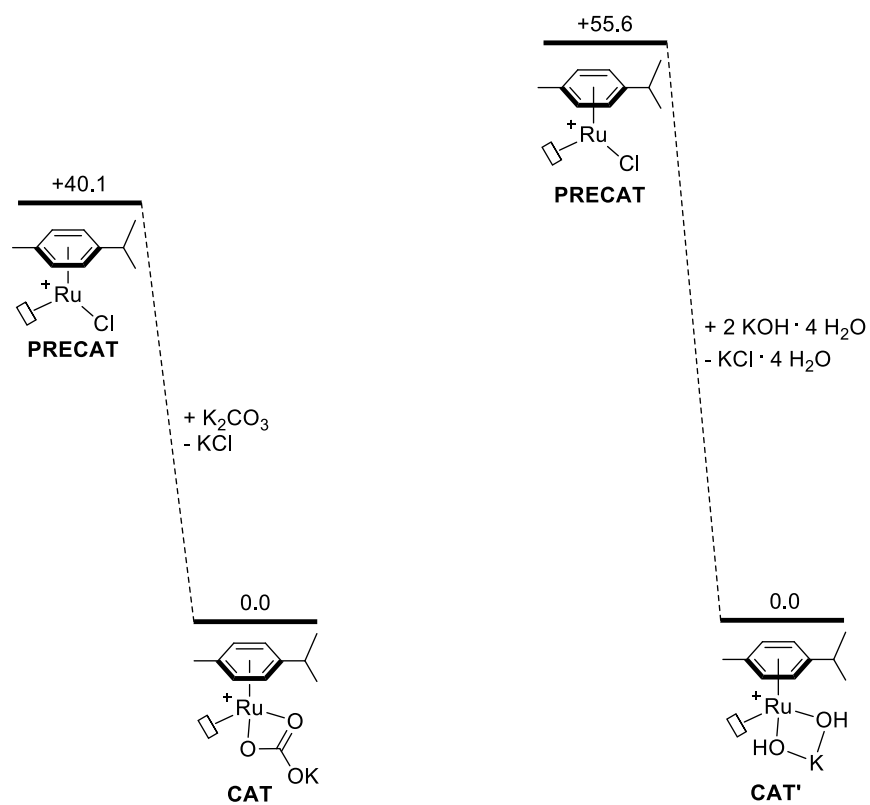
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of **2**.



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of **3**.



## 2. Computed reaction profile for the formation of CAT and CAT'



**Figure S1.** Computed, minimum free energy reaction profile (kcal/mol) for the formation of the catalysts **CAT** (left) and **CAT'** (right).

### 3. XYZ Cartesian coordinates

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PRECAT

Ru	1.411217	-0.227193	0.243011
Cl	0.065406	1.062369	-0.969473
C	1.836154	-2.377440	0.636972
C	2.514208	-1.611654	1.642451
H	2.292178	-1.802907	2.704604
C	3.341455	-0.507899	1.293176
H	3.746301	0.132740	2.094031
C	3.558416	-0.121782	-0.081281
C	2.906779	-0.911388	-1.101499
H	2.973682	-0.605028	-2.156537
C	2.050046	-2.009281	-0.744756
H	1.477975	-2.523406	-1.534484
C	0.876406	-3.473472	0.999018
H	0.435748	-3.322882	2.003342
H	0.061995	-3.571303	0.254807
H	1.431458	-4.438200	1.014626
C	4.410617	1.086949	-0.408673
H	4.322563	1.780321	0.457492
C	5.882283	0.599479	-0.483388
H	6.021278	-0.111902	-1.323843
H	6.547388	1.469202	-0.657393
H	6.207162	0.101102	0.452462
C	3.988388	1.839709	-1.679686
H	4.172311	1.243184	-2.597603
H	2.917292	2.127751	-1.653205
H	4.586953	2.766586	-1.777286

3

H<sub>2</sub>O

O	-5.472327	3.804012	0.000000
H	-4.498778	3.866335	0.000000
H	-5.738556	4.742524	0.000000

3

CO<sub>2</sub>

C	-4.761905	2.036862	0.026664
O	-3.586530	2.036862	0.026664
O	-5.937280	2.036862	0.026664

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K<sub>2</sub>CO<sub>3</sub>

O	-1.133488	1.395819	-0.002195
C	0.000233	0.785594	0.002442
O	0.000705	-0.574917	0.006602
O	1.133681	1.396403	0.002370
K	2.458361	-0.599653	0.009110



K	-2.456761	-0.601227	0.002013
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2

KCl

Cl	-2.318170	2.262017	0.029611
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K	-4.994889	2.262017	0.029611
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KOH\*4H<sub>2</sub>O

O	-0.449565	0.052059	-1.403510
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K	-0.944333	0.859955	1.035624
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H	0.047186	0.461495	-2.133841
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O	-0.042611	0.260177	3.550212
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H	-0.274336	-0.636035	3.195391
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H	0.790376	0.455186	3.047248
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O	1.691749	0.829935	1.459868
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H	1.642952	-0.069897	0.904766
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H	2.612138	1.137888	1.410876
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O	-0.761081	-1.712030	1.746491
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H	-1.147450	-2.601325	1.676126
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H	0.061703	-1.692236	1.086848
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O	1.136349	-1.242808	0.151354
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H	0.244639	-0.556144	-0.937312
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H	1.777458	-1.931394	-0.098099
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CAT

Ru	0.057702	0.572746	0.181355
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C	0.754949	2.558635	-0.416207
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C	0.908469	1.694094	-1.551119
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H	0.398893	1.941525	-2.495040
---	----------	----------	-----------

C	1.552762	0.435569	-1.404581
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H	1.540453	-0.281115	-2.241491
---	----------	-----------	-----------

C	2.130255	0.022684	-0.139788
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C	2.094811	0.950719	0.955673
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H	2.468248	0.645800	1.943997
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C	1.387764	2.177025	0.830862
---	----------	----------	----------

H	1.235839	2.806583	1.722080
---	----------	----------	----------

C	-0.049213	3.826635	-0.502967
---	-----------	----------	-----------

H	-0.815489	3.771153	-1.300147
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H	-0.547651	4.057967	0.459042
---	-----------	----------	----------

H	0.630629	4.674353	-0.740364
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C	2.751417	-1.357759	-0.007687
---	----------	-----------	-----------

H	2.254029	-1.998514	-0.770137
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C	4.250419	-1.250940	-0.376300
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H	4.789137	-0.608404	0.351181
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H	4.718028	-2.256224	-0.354891
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H	4.399808	-0.823689	-1.388941
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C	2.540172	-2.004396	1.371344
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H	3.120254	-1.487398	2.164097
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H	1.470637	-2.001856	1.667115
H	2.891944	-3.055053	1.351806
C	-1.969792	-0.608298	0.966086
O	-1.783086	-0.172927	-0.317048
O	-0.916314	-0.308493	1.716843
O	-2.988585	-1.195814	1.321562
K	-4.210054	-1.224901	-0.944325

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INT1

Ru	-1.269954	-0.664897	0.725022
C	-2.761801	-1.899560	-0.378589
C	-1.827872	-1.352748	-1.304128
H	-1.243688	-2.034790	-1.941751
C	-1.536531	0.060486	-1.337401
H	-0.749053	0.434561	-2.010924
C	-2.186372	0.977260	-0.455828
C	-3.121772	0.426060	0.501596
H	-3.567654	1.076379	1.268110
C	-3.393033	-0.975576	0.542509
H	-4.041191	-1.371899	1.340055
C	-3.036711	-3.377397	-0.295775
H	-2.224334	-3.969330	-0.760198
H	-3.151294	-3.701552	0.757844
H	-3.982877	-3.617026	-0.827062
C	-1.884989	2.465434	-0.530653
H	-0.847978	2.555406	-0.924149
C	-2.839749	3.106777	-1.563713
H	-3.896415	3.012569	-1.235779
H	-2.614416	4.187148	-1.674877
H	-2.747326	2.630485	-2.561111
C	-1.952030	3.186093	0.826561
H	-2.998175	3.280682	1.186659
H	-1.370486	2.659400	1.610086
H	-1.557832	4.217320	0.725424
O	0.729952	-1.348000	0.442864
C	1.774697	-0.781938	0.041083
C	2.139286	0.656838	-0.053336
N	2.834882	-1.514241	-0.448118
C	1.481430	1.815301	0.374203
C	3.410602	0.727320	-0.667669
C	3.888260	-0.660513	-0.932901
C	2.869368	-2.963487	-0.543155
C	2.115261	3.052732	0.129346
H	0.534614	1.753233	0.924027
C	4.045766	1.946615	-0.907000
O	4.914415	-1.065851	-1.437297
H	2.797474	-3.421136	0.463698
H	2.029738	-3.334605	-1.164914
H	3.833283	-3.240340	-1.010784

C	3.370616	3.121350	-0.507530
H	1.622148	3.980643	0.457982
H	5.037557	1.978244	-1.382708
H	3.838650	4.102781	-0.680326
O	-0.518058	0.434968	2.322607
C	-0.538656	-0.586626	3.153273
O	-1.060140	-1.677591	2.560000
O	-0.143055	-0.587344	4.330869
K	-0.635350	-3.019695	4.792731

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TS1

Ru	1.347034	-0.767810	0.114659
C	2.139480	-2.766557	0.484067
C	2.606899	-1.920086	1.539567
H	2.348812	-2.160344	2.582381
C	3.195439	-0.656353	1.234911
H	3.399835	0.050305	2.056234
C	3.459979	-0.233760	-0.130321
C	3.096822	-1.131759	-1.179514
H	3.174506	-0.809868	-2.227789
C	2.394271	-2.343002	-0.882906
H	1.984768	-2.940501	-1.713518
C	1.361463	-4.021242	0.769108
H	0.818930	-3.950957	1.731408
H	0.629441	-4.233928	-0.034720
H	2.059418	-4.884686	0.827000
C	4.053435	1.139753	-0.392280
H	3.706315	1.790661	0.442282
C	5.594324	1.036191	-0.304742
H	5.989093	0.381564	-1.109581
H	6.049230	2.040111	-0.426201
H	5.929780	0.623962	0.669064
C	3.587225	1.769618	-1.714445
H	4.025997	1.251565	-2.593094
H	2.482288	1.741486	-1.811582
H	3.919915	2.825373	-1.767131
O	-0.254790	-0.656953	1.344360
C	-1.441312	-0.291426	0.953653
C	-2.315967	-1.095125	0.021905
N	-2.322174	0.276489	1.901662
C	-2.003975	-1.987438	-1.005035
C	-3.649575	-0.737355	0.296600
C	-3.645730	0.245911	1.425215
C	-1.862208	1.208255	2.917163
C	-3.074915	-2.517135	-1.758914
H	-0.961500	-2.257669	-1.231347
C	-4.717206	-1.249357	-0.449408
O	-4.559743	0.962212	1.819126
H	-1.311084	2.050579	2.447859

H	-2.751642	1.594302	3.449576
H	-1.191370	0.690839	3.629725
C	-4.410486	-2.152637	-1.489627
H	-2.863317	-3.225263	-2.574947
H	-5.754762	-0.966252	-0.212691
H	-5.222157	-2.587020	-2.093448
C	-0.636963	1.038802	-1.265333
O	-1.231109	1.193579	-0.077352
O	0.393267	0.212009	-1.365569
O	-1.054551	1.679496	-2.246886
K	-3.317146	2.440938	-1.171096

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#### Ring Opening Without Nucleophilic Attack

Ru	0.621412	0.648725	0.162904
C	2.627235	1.614267	0.435491
C	2.577671	1.109034	-0.903847
H	2.740329	1.790610	-1.752465
C	2.213965	-0.243368	-1.138558
H	2.076138	-0.595246	-2.171896
C	1.992901	-1.175880	-0.049344
C	2.079306	-0.683277	1.285341
H	1.803212	-1.328950	2.130020
C	2.343971	0.697072	1.521593
H	2.286932	1.087790	2.549438
C	2.890400	3.066555	0.715708
H	2.641158	3.705771	-0.153193
H	2.321784	3.420840	1.597730
H	3.972425	3.200026	0.938187
C	1.709992	-2.634183	-0.359677
H	1.176505	-2.652995	-1.333008
C	3.069641	-3.347409	-0.558266
H	3.664744	-3.333271	0.378773
H	2.898861	-4.406688	-0.838700
H	3.675073	-2.875735	-1.359349
C	0.837972	-3.334900	0.693259
H	1.409195	-3.544760	1.622185
H	-0.034643	-2.715197	0.983450
H	0.488721	-4.311572	0.302190
N	-0.726737	1.601424	-0.984217
C	-2.082910	1.776840	-0.560340
C	-0.805789	-0.568500	-1.117303
C	-0.328638	2.254865	-2.227636
C	-2.735920	0.515878	-0.085006
O	-2.660941	2.843631	-0.688945
C	-2.091832	-0.702834	-0.402602
O	-0.428371	-1.063440	-2.141868
H	0.044745	1.485925	-2.940800
H	-1.190651	2.784645	-2.678923
H	0.484023	2.987930	-2.044371

C	-3.994323	0.501534	0.530490
C	-2.674549	-1.941090	-0.083954
C	-4.584461	-0.735400	0.857145
H	-4.498756	1.458249	0.732847
C	-3.930167	-1.947919	0.551309
H	-2.158078	-2.878422	-0.335601
H	-5.580768	-0.754903	1.327683
H	-4.415224	-2.909679	0.782585
O	-0.728577	0.872529	1.567160
C	-0.998227	0.098840	2.662089
O	-1.513557	0.709088	3.636118
O	-0.805509	-1.155664	2.562073
K	-2.774806	-1.404891	4.230607

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INT2

Ru	1.487841	-0.446525	0.025918
C	2.456050	-2.375481	-0.139319
C	2.754617	-1.848103	1.163153
H	2.444595	-2.406197	2.059936
C	3.237609	-0.513431	1.294754
H	3.308718	-0.065495	2.299575
C	3.544396	0.312736	0.139431
C	3.366919	-0.266000	-1.155543
H	3.494205	0.355175	-2.053740
C	2.789370	-1.562386	-1.295556
H	2.517282	-1.923114	-2.300451
C	1.788657	-3.712482	-0.306578
H	1.152476	-3.959331	0.564943
H	1.164636	-3.741254	-1.221446
H	2.565713	-4.502033	-0.403126
C	4.008364	1.745983	0.337852
H	3.582923	2.078243	1.311767
C	5.549825	1.753484	0.463493
H	6.021609	1.416016	-0.482998
H	5.908942	2.780559	0.677541
H	5.903390	1.089907	1.279050
C	3.512414	2.709490	-0.752621
H	4.013347	2.524029	-1.725761
H	2.417178	2.622155	-0.907073
H	3.744822	3.754889	-0.467499
O	-0.121585	-0.687617	1.159322
C	-1.320709	-0.186911	0.795392
C	-2.153237	-0.970086	-0.221896
N	-2.248459	0.005789	1.897214
C	-1.786343	-1.617683	-1.402754
C	-3.500486	-0.878198	0.168973
C	-3.567929	-0.133380	1.467996
C	-1.869060	0.761362	3.076927
C	-2.817511	-2.174119	-2.191920

H	-0.732575	-1.685378	-1.713447
C	-4.532041	-1.415971	-0.611127
O	-4.559806	0.344113	2.017421
H	-1.496761	1.773403	2.805487
H	-2.765453	0.860765	3.717959
H	-1.071031	0.225108	3.626228
C	-4.170584	-2.071493	-1.806301
H	-2.561269	-2.696204	-3.126884
H	-5.580010	-1.341541	-0.281124
H	-4.949947	-2.519561	-2.441911
C	-0.620912	1.425449	-0.996190
O	-1.202408	1.230080	0.253138
O	0.441143	0.738471	-1.280231
O	-1.162853	2.262308	-1.723094
K	-3.527591	2.496895	-0.496868

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TS2

Ru	-1.602934	0.717922	0.147227
C	-3.590888	1.654642	0.100973
C	-3.490128	0.835506	1.277526
H	-3.616750	1.289120	2.272453
C	-3.033950	-0.512299	1.162884
H	-2.818444	-1.086522	2.078555
C	-2.766918	-1.121888	-0.126573
C	-2.973168	-0.317362	-1.297537
H	-2.704278	-0.716216	-2.286126
C	-3.353394	1.047118	-1.189667
H	-3.392330	1.673525	-2.094488
C	-3.907620	3.121334	0.207663
H	-3.562493	3.544359	1.170758
H	-3.451814	3.698251	-0.620680
H	-5.009588	3.259680	0.148248
C	-2.282340	-2.564489	-0.172116
H	-1.471028	-2.643791	0.587975
C	-3.443024	-3.492237	0.261385
H	-4.287162	-3.425963	-0.456126
H	-3.097853	-4.545641	0.286014
H	-3.830735	-3.241060	1.269557
C	-1.711557	-2.997139	-1.529590
H	-2.502948	-3.044673	-2.307122
H	-0.910374	-2.324076	-1.893039
H	-1.281669	-4.015173	-1.445806
O	-0.247154	1.184270	1.462299
C	0.942915	0.896416	0.797752
C	1.382150	-0.543176	1.054556
N	0.332864	0.701427	-0.770221
C	1.867966	-1.069409	2.254718
C	1.245988	-1.354988	-0.087145
C	0.853953	-0.529701	-1.251047

C	0.465085	1.876529	-1.651445
C	2.207222	-2.438222	2.287283
H	1.993249	-0.426825	3.138969
C	1.589089	-2.717310	-0.064416
O	1.039021	-0.781607	-2.446205
H	1.539470	2.051813	-1.862445
H	-0.090968	1.700929	-2.591443
H	0.063991	2.767933	-1.131401
C	2.064440	-3.256736	1.144523
H	2.596742	-2.876615	3.219400
H	1.472117	-3.337866	-0.966780
H	2.332135	-4.323008	1.203022
C	3.337848	1.566938	0.339387
O	1.835400	1.865566	0.887056
O	4.163793	2.093722	1.030397
O	3.282759	0.879865	-0.707267
K	3.796291	-0.552764	-2.612511

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INT3

Ru	-1.062049	0.295684	0.001143
C	-2.823814	1.183650	1.039691
C	-2.306836	0.132399	1.862363
H	-1.998544	0.347149	2.896216
C	-2.035659	-1.151792	1.288770
H	-1.485973	-1.895862	1.889491
C	-2.393283	-1.496616	-0.067872
C	-2.937318	-0.443202	-0.866147
H	-3.126655	-0.619891	-1.935660
C	-3.124996	0.883361	-0.342352
H	-3.477455	1.686930	-1.006846
C	-2.974166	2.585833	1.557711
H	-2.369329	2.750810	2.469061
H	-2.661937	3.324093	0.793412
H	-4.040784	2.775654	1.804812
C	-2.143308	-2.898297	-0.597485
H	-1.288676	-3.299032	-0.007811
C	-3.377480	-3.780294	-0.306064
H	-4.266562	-3.406572	-0.856389
H	-3.191795	-4.824998	-0.628971
H	-3.626991	-3.794751	0.774774
C	-1.749734	-2.928282	-2.082866
H	-2.604434	-2.667548	-2.742096
H	-0.922595	-2.219985	-2.296105
H	-1.425072	-3.947733	-2.372167
O	0.006443	2.119080	0.256942
C	1.169245	1.668218	0.617956
C	1.116743	0.170751	0.907759
N	-0.116429	0.400509	-1.841216
C	1.291560	-0.373599	2.217728

C	1.098865	-0.711647	-0.232758
C	1.113824	-0.063251	-1.614035
C	-0.478627	1.212984	-2.985898
C	1.397514	-1.750206	2.385750
H	1.355059	0.310760	3.077572
C	1.253618	-2.116072	-0.029824
O	2.159640	0.052582	-2.301397
H	-0.578507	2.280727	-2.690706
H	0.297711	1.126229	-3.774140
H	-1.449305	0.877690	-3.406134
C	1.380736	-2.622936	1.259502
H	1.526219	-2.170242	3.395513
H	1.284987	-2.779616	-0.907078
H	1.495841	-3.707294	1.413196
O	2.233216	2.305778	0.644164
K	3.777128	1.836231	-1.393761

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TS3

Ru	-0.671174	0.447694	-0.072569
C	-1.446010	2.371679	0.552259
C	-1.727215	1.405614	1.595382
H	-1.295829	1.560935	2.595391
C	-2.441821	0.209982	1.310056
H	-2.566871	-0.546877	2.098994
C	-2.813175	-0.117689	-0.033530
C	-2.600271	0.873950	-1.068637
H	-2.868671	0.640930	-2.110334
C	-1.966292	2.111567	-0.768761
H	-1.747114	2.822385	-1.580851
C	-0.659325	3.618111	0.853799
H	-1.351237	4.420357	1.191937
H	0.076176	3.433963	1.660152
H	-0.126296	3.987890	-0.044347
C	-3.391491	-1.485677	-0.375768
H	-3.440959	-2.054724	0.578042
C	-4.827667	-1.336312	-0.919171
H	-4.839758	-0.818788	-1.901438
H	-5.284312	-2.336132	-1.066124
H	-5.472700	-0.764436	-0.221582
C	-2.483650	-2.274545	-1.341734
H	-2.353133	-1.744155	-2.308145
H	-1.476737	-2.440243	-0.904556
H	-2.929571	-3.265455	-1.562478
O	1.177364	1.207080	2.651374
C	1.702072	0.802608	1.643718
C	0.708856	-0.785142	0.955124
N	0.798146	0.573081	-1.411570
C	0.383302	-1.611195	2.064407
C	1.270984	-1.407169	-0.207865



C	1.660416	-0.482353	-1.326078
C	1.014404	1.617057	-2.401715
C	0.568481	-2.998704	1.999009
H	0.012521	-1.134342	2.986374
C	1.461481	-2.799752	-0.274280
O	2.670501	-0.671295	-2.042035
H	0.101132	1.760902	-3.014305
H	1.244333	2.580894	-1.897105
H	1.852144	1.348962	-3.076612
C	1.100214	-3.590678	0.829913
H	0.313518	-3.631075	2.863990
H	1.877648	-3.248165	-1.190293
H	1.242375	-4.682224	0.789266
O	2.694667	0.930283	0.933578
K	4.608315	0.207508	-0.614320

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INT4

Ru	0.875176	-0.458934	0.028001
C	1.841669	-2.388712	0.409449
C	2.273174	-1.473801	1.433996
H	2.079989	-1.712698	2.490668
C	2.774130	-0.194691	1.072588
H	2.968561	0.558870	1.851829
C	2.876192	0.194182	-0.318655
C	2.661553	-0.825376	-1.330617
H	2.778867	-0.565965	-2.393948
C	2.154115	-2.090174	-0.975544
H	1.874630	-2.812238	-1.758858
C	1.169664	-3.687542	0.771588
H	0.634433	-3.610875	1.737852
H	0.446968	-3.998536	-0.008592
H	1.933265	-4.490835	0.865075
C	3.339647	1.595119	-0.690889
H	3.183477	2.226545	0.211373
C	4.852815	1.559247	-0.999605
H	5.062152	0.936373	-1.895076
H	5.230935	2.582029	-1.202957
H	5.432661	1.140874	-0.151776
C	2.530012	2.219176	-1.840312
H	2.665488	1.664757	-2.792862
H	1.447813	2.230296	-1.598636
H	2.863306	3.260995	-2.020882
C	-0.267711	0.634054	1.331184
N	-0.518351	0.228174	-1.272124
C	-0.111577	0.814979	2.720396
C	-1.390913	1.247469	0.710740
C	-1.509364	1.014628	-0.757986
C	-0.521199	0.017549	-2.715373

C	-1.038394	1.582973	3.459113
H	0.738435	0.356128	3.252067
C	-2.317406	2.010569	1.435833
O	-2.434836	1.506860	-1.464782
H	-1.509047	-0.353560	-3.067469
H	-0.294542	0.957684	-3.268225
H	0.244865	-0.734006	-2.979132
C	-2.138964	2.182930	2.822350
H	-0.895911	1.714968	4.543879
H	-3.175141	2.466822	0.914765
H	-2.855359	2.782845	3.404637
K	-4.221208	2.434728	-2.733415

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TS4

Ru	-0.450100	-0.658257	-0.203979
C	-1.828511	-2.427254	-0.423210
C	-2.112224	-1.455503	-1.462766
H	-2.078341	-1.766153	-2.519085
C	-2.386186	-0.101896	-1.137847
H	-2.551028	0.624171	-1.949421
C	-2.331400	0.375546	0.228480
C	-2.056394	-0.593193	1.247511
H	-1.948195	-0.264517	2.291488
C	-1.845270	-1.983898	0.928332
H	-1.591133	-2.691898	1.731260
C	-1.484442	-3.847105	-0.783254
H	-2.413222	-4.422170	-0.987801
H	-0.860427	-3.889082	-1.698900
H	-0.939507	-4.353977	0.036373
C	-2.578785	1.844913	0.531783
H	-2.255890	2.404482	-0.374182
C	-4.095446	2.066593	0.723638
H	-4.463245	1.516775	1.615464
H	-4.312685	3.143625	0.874137
H	-4.677690	1.719067	-0.154514
C	-1.763997	2.376913	1.720423
H	-2.103880	1.943168	2.684301
H	-0.684189	2.157599	1.598584
H	-1.886796	3.475201	1.801831
C	0.619686	1.132905	-0.842918
N	1.053359	-0.540442	1.215455
C	0.193260	2.096983	-1.787240
C	1.574177	1.513462	0.140285
C	1.995821	0.426564	1.087164
C	1.263263	-1.626933	2.160844
C	0.681416	3.413617	-1.721210
H	-0.510842	1.809718	-2.585025
C	2.094030	2.814817	0.187095
O	3.147727	0.401847	1.603885

H	0.405186	-1.701789	2.861792
H	1.343347	-2.609223	1.639535
H	2.180437	-1.451395	2.761429
C	1.625232	3.770143	-0.735758
H	0.337427	4.166269	-2.448042
H	2.843007	3.071290	0.952714
H	2.004444	4.803357	-0.693611
H	0.964409	-0.063072	-1.341165
O	1.299230	-1.371794	-1.398992
H	0.953299	-1.680001	-2.260560
K	3.879755	-1.274501	-0.282999

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INT5

Ru	0.814781	-0.992118	0.169589
C	1.057042	-3.011504	1.024685
C	1.790574	-2.086657	1.824517
H	1.550352	-1.988688	2.894217
C	2.720565	-1.166887	1.218941
H	3.187284	-0.388634	1.844681
C	3.007142	-1.189925	-0.182908
C	2.292098	-2.159448	-0.979388
H	2.430998	-2.168102	-2.069901
C	1.327777	-3.030994	-0.401911
H	0.735150	-3.690240	-1.055972
C	-0.012489	-3.894882	1.606450
H	0.374015	-4.929654	1.726247
H	-0.344843	-3.531295	2.597692
H	-0.894759	-3.933323	0.937391
C	4.043086	-0.254989	-0.788859
H	4.114956	0.622519	-0.106740
C	5.416060	-0.964027	-0.785200
H	5.392791	-1.865546	-1.433264
H	6.202864	-0.286499	-1.175321
H	5.710465	-1.285508	0.234806
C	3.669005	0.257927	-2.189661
H	3.719345	-0.552507	-2.947103
H	2.643422	0.679977	-2.203368
H	4.383422	1.041585	-2.512159
C	1.535934	2.440699	0.047491
N	0.279082	0.237566	-1.488552
C	2.061697	3.509683	0.791611
C	0.271271	2.543882	-0.574026
C	-0.346819	1.442374	-1.407002
C	-0.167132	-0.600483	-2.605293
C	1.336845	4.713605	0.917119
H	3.051947	3.412442	1.264698
C	-0.442173	3.760952	-0.457086
O	-1.405087	1.714011	-2.051587
H	0.673756	-1.230329	-2.954126

H	-0.993747	-1.295381	-2.321736
H	-0.514218	0.021861	-3.455787
C	0.083817	4.838214	0.282646
H	1.758635	5.558656	1.484277
H	-1.406114	3.847745	-0.981713
H	-0.474152	5.786602	0.344421
H	2.096827	1.502642	-0.048198
K	-3.344001	0.263675	-1.169930
O	-1.334548	-1.071362	0.270987
C	-1.377493	-0.020152	1.056648
O	-0.177483	0.384323	1.441906
O	-2.434755	0.601137	1.360649
K	-1.080227	2.524576	2.611582

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TS5

Ru	-1.319428	-0.207332	0.638874
C	-3.332581	-0.529044	-0.174677
C	-3.027242	-1.455216	0.895202
H	-3.666612	-1.468837	1.792789
C	-1.874367	-2.313458	0.840981
H	-1.643463	-2.952533	1.708080
C	-0.938301	-2.218879	-0.232964
C	-1.215911	-1.242681	-1.260212
H	-0.432217	-1.005394	-2.004998
C	-2.422141	-0.470790	-1.273495
H	-2.562289	0.278844	-2.063472
C	-4.544125	0.381477	-0.069610
H	-4.771593	0.475467	1.015542
C	0.341351	-3.009794	-0.242939
H	0.597596	-3.383690	0.767661
C	4.029874	0.013683	-0.586229
N	0.994006	0.801239	-2.435053
C	5.123112	-0.872382	-0.583754
C	2.888763	-0.232885	-1.386778
C	1.712475	0.714195	-1.342696
C	-0.077651	1.768145	-2.438793
C	5.086421	-2.031230	-1.380334
H	6.016270	-0.646893	0.021294
C	2.891493	-1.372673	-2.221851
O	1.510607	1.349747	-0.206989
H	-0.716392	1.749715	-1.514526
H	0.310762	2.814561	-2.547994
H	-0.744431	1.609203	-3.312059
C	3.971887	-2.270236	-2.206966
H	5.935843	-2.731880	-1.378345
H	2.032523	-1.529146	-2.892226
H	3.951769	-3.160095	-2.855959
H	4.082803	0.960169	-0.021046
K	0.404154	3.673606	0.228913

O	-1.281627	1.759784	1.271950
C	-0.298955	1.481128	2.136422
O	0.452771	2.317374	2.648966
O	-0.157282	0.151994	2.283377
K	2.480259	0.250546	2.102814
C	-4.297469	1.794765	-0.622028
H	-4.165191	1.791371	-1.724452
H	-5.170203	2.442268	-0.404692
H	-3.400315	2.250614	-0.155846
C	-5.743485	-0.312278	-0.755403
H	-5.942374	-1.315386	-0.325548
H	-6.660106	0.299829	-0.633457
H	-5.556914	-0.436416	-1.842840
H	0.233681	-3.889599	-0.913172
H	1.183942	-2.404180	-0.632236

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P

C	-3.176011	1.872197	-1.094329
N	-1.916965	-0.136864	-2.660519
C	-3.739992	2.914008	-0.341523
C	-1.898970	1.361812	-0.766720
C	-1.249032	0.253415	-1.578312
C	-1.369957	-1.280630	-3.361274
C	-3.040509	3.457727	0.754454
H	-4.736716	3.304579	-0.605134
C	-1.207836	1.907177	0.337935
O	-0.067664	-0.135525	-1.221122
H	-2.125493	-1.694753	-4.062675
H	-0.470948	-1.061003	-4.016159
H	-1.025467	-2.095484	-2.679351
C	-1.774034	2.948658	1.094112
H	-3.486954	4.273194	1.346562
H	-0.225159	1.478729	0.591271
H	-1.227901	3.361720	1.958202
H	-3.701909	1.422259	-1.950224
K	0.740295	1.112751	-3.160912

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CAT'

Ru	0.627891	-0.694577	-0.379172
C	1.727208	1.144347	-0.034060
C	1.169238	0.696267	1.226017
H	1.847033	0.489944	2.069573
C	-0.217334	0.407246	1.348295
H	-0.604670	-0.022986	2.285801
C	-1.085775	0.485835	0.201351
C	-0.547176	1.029896	-1.028197

H	-1.185764	1.084701	-1.922764
C	0.827610	1.380735	-1.132730
H	1.237123	1.698529	-2.104746
C	3.207225	1.378428	-0.176930
H	3.444935	2.424354	0.116447
H	3.788753	0.702655	0.480380
H	3.543563	1.232890	-1.221861
C	-2.539018	0.048815	0.308109
H	-2.602101	-0.613870	1.199513
C	-3.412414	1.296465	0.569379
H	-3.373906	1.994053	-0.293769
H	-4.470532	1.000182	0.719469
H	-3.079182	1.849583	1.470980
C	-3.031253	-0.753554	-0.908896
H	-3.083750	-0.129308	-1.825440
H	-2.367595	-1.618633	-1.116744
H	-4.054081	-1.137335	-0.721503
O	0.787729	-2.524403	0.410728
H	0.642285	-2.515945	1.376103
K	1.269628	-4.166549	-1.455501
O	0.992136	-1.721425	-2.055612
H	0.994227	-1.140966	-2.840568

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TS1'

Ru	1.293769	0.623046	0.100731
C	2.940272	1.497426	-1.105550
C	2.486905	0.279310	-1.740682
H	2.140602	0.313490	-2.784175
C	2.372657	-0.926385	-1.000103
H	1.911322	-1.808595	-1.471551
C	2.719345	-0.986533	0.406234
C	3.212808	0.215777	1.009810
H	3.427975	0.229491	2.089352
C	3.345915	1.442396	0.262884
H	3.680687	2.357802	0.775586
C	2.943630	2.786872	-1.885859
H	2.001941	2.902481	-2.460278
C	2.491762	-2.276611	1.177329
H	1.576249	-2.729638	0.734634
O	-0.341897	1.770984	-0.736606
C	-1.369786	0.985691	-0.821259
C	-2.604599	1.027970	0.023980
N	-1.728840	0.388863	-2.012684
C	-2.818464	1.494424	1.326384
C	-3.648472	0.429543	-0.709214
C	-3.101609	-0.017746	-2.023466
C	-0.817286	0.106520	-3.100604
C	-4.120590	1.380512	1.859847
H	-1.977640	1.863173	1.935647

C	-4.939265	0.306292	-0.188306
O	-3.638828	-0.591741	-2.949766
H	-0.163522	-0.751378	-2.839576
H	-1.420029	-0.155862	-3.990521
H	-0.192781	0.997316	-3.307279
C	-5.168210	0.802712	1.112119
H	-4.319780	1.732750	2.883981
H	-5.737976	-0.166739	-0.779544
H	-6.172241	0.725101	1.556827
O	-0.383094	-0.581123	0.163191
H	-0.694512	-0.465753	1.089676
O	0.462617	1.406986	1.826410
H	1.002754	1.135626	2.592905
K	0.055967	3.746706	0.899847
C	2.226372	-2.063471	2.674613
H	1.934744	-3.021289	3.149611
H	3.128890	-1.700909	3.210995
H	1.400618	-1.339951	2.840255
C	3.679578	-3.233650	0.934992
H	3.494557	-4.211187	1.424802
H	3.844474	-3.420576	-0.146025
H	4.617162	-2.812121	1.354758
H	3.076736	3.668521	-1.227161
H	3.781546	2.788491	-2.615230

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INT1'

Ru	-1.140574	-0.687874	-0.227524
C	-2.985395	-1.080869	0.922672
C	-3.293021	-0.929748	-0.477957
H	-3.783694	-1.761709	-1.010287
C	-2.866319	0.205275	-1.226315
H	-3.058466	0.248123	-2.309604
C	-2.107612	1.266791	-0.590813
C	-1.837685	1.158289	0.808103
H	-1.225580	1.916490	1.316294
C	-2.231472	-0.020115	1.529727
H	-1.875044	-0.145133	2.565188
C	-3.386906	-2.309151	1.696186
H	-3.410855	-3.208834	1.048515
H	-2.686630	-2.499565	2.532895
H	-4.403575	-2.181204	2.125958
C	-1.640970	2.438113	-1.440136
H	-1.274655	1.995216	-2.394103
C	-2.858549	3.338903	-1.753614
H	-3.266527	3.783181	-0.821586
H	-2.558994	4.169801	-2.424208
H	-3.678431	2.779790	-2.249384
C	-0.492180	3.244747	-0.823317
H	-0.811625	3.780769	0.094958

H	0.367664	2.595980	-0.572738
H	-0.140240	4.013081	-1.540187
O	0.550978	-0.247765	-1.419758
C	1.529150	-0.461765	-0.502274
C	2.156882	0.821308	0.020155
N	0.806298	-1.031176	0.763951
C	2.946215	1.744028	-0.677927
C	1.728240	1.084801	1.331327
C	0.949567	-0.054968	1.852803
C	1.081864	-2.420278	1.183090
C	3.305611	2.934569	-0.017465
H	3.268717	1.547727	-1.711851
C	2.071827	2.276326	1.993918
O	0.506650	-0.240092	2.970993
H	2.156969	-2.547022	1.428134
H	0.473994	-2.619275	2.085260
H	0.776688	-3.104024	0.373040
C	2.867243	3.202399	1.300735
H	3.934179	3.675038	-0.536365
H	1.726556	2.458923	3.022920
H	3.159710	4.145840	1.786657
O	2.472549	-1.382904	-1.030564
H	3.334909	-1.258514	-0.585992
K	0.761345	-2.299823	-3.024846
O	-0.805678	-2.553731	-1.052773
H	-1.573138	-3.120146	-0.848669

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TS2'

Ru	-1.068458	0.241647	-0.031699
C	-2.333234	1.412188	1.283407
C	-2.638904	1.756002	-0.088499
H	-3.667714	1.602203	-0.457217
C	-1.635627	2.156386	-1.009274
H	-1.897709	2.325815	-2.064117
C	-0.254999	2.251656	-0.582282
C	0.057753	1.996755	0.791794
H	1.098587	2.032725	1.138854
C	-0.958050	1.540789	1.692044
H	-0.665388	1.204306	2.700717
C	-3.401802	0.942999	2.233795
H	-4.175853	0.345099	1.712806
H	-2.973499	0.324002	3.045908
H	-3.906951	1.815886	2.699915
C	0.798510	2.651856	-1.608736
H	0.662958	1.961137	-2.472163
C	0.514410	4.094450	-2.091885
H	0.605149	4.812971	-1.251165
H	1.250684	4.385463	-2.868619
H	-0.498019	4.207839	-2.528822



C	2.243439	2.527536	-1.109367
H	2.458526	3.260695	-0.304123
H	2.468403	1.515544	-0.726181
H	2.949831	2.736425	-1.937372
O	0.148696	-0.899388	-1.494440
C	1.041807	-1.576409	-0.929638
C	2.204279	-1.030188	-0.169472
N	-0.252993	-1.389297	1.122725
C	3.446909	-0.909805	-0.829978
C	2.057951	-0.615688	1.170211
C	0.795903	-0.955290	1.924743
C	-1.251965	-2.162934	1.866797
C	4.535298	-0.332545	-0.152611
H	3.555753	-1.239954	-1.875362
C	3.156085	-0.044199	1.837066
O	0.781215	-0.918957	3.160137
H	-0.796068	-3.096277	2.265407
H	-1.643960	-1.602135	2.744450
H	-2.094616	-2.411626	1.196510
C	4.384560	0.112352	1.174184
H	5.503761	-0.229971	-0.665982
H	3.026088	0.238426	2.893441
H	5.240065	0.562172	1.701540
O	1.153176	-2.868734	-1.350032
K	-1.587958	-3.032242	-2.078961
H	1.921056	-3.287285	-0.903039
O	-2.423201	-1.172283	-0.676710
H	-3.318749	-0.812151	-0.542834

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INT2'

Ru	0.807737	-0.368989	-0.120462
C	1.176465	-1.624502	1.639517
C	2.176539	-1.836920	0.618169
H	3.238434	-1.668442	0.855072
C	1.792453	-2.241498	-0.712816
H	2.574614	-2.365178	-1.480929
C	0.426893	-2.361824	-1.094984
C	-0.557158	-2.062887	-0.071510
H	-1.623765	-2.034858	-0.346215
C	-0.203122	-1.778195	1.280816
H	-0.989701	-1.534628	2.010836
C	1.557016	-1.183480	3.025961
H	2.593170	-0.796864	3.061924
H	0.872457	-0.389917	3.384146
H	1.489156	-2.046324	3.722005
C	0.020235	-2.766279	-2.503715
H	0.942597	-2.725162	-3.124679
C	-0.480777	-4.226750	-2.486371
H	-1.402950	-4.322268	-1.874066

H	-0.722197	-4.566776	-3.514152
H	0.279188	-4.915956	-2.065189
C	-1.008722	-1.812832	-3.135807
H	-1.974387	-1.825146	-2.586356
H	-0.637533	-0.769542	-3.144191
H	-1.227136	-2.122184	-4.177621
O	-0.786716	0.835775	-1.248139
C	-1.972786	0.952546	-0.884015
C	-2.399169	0.830168	0.524178
N	0.885414	1.344733	1.135964
C	-3.622007	0.210665	0.874929
C	-1.520425	1.326327	1.520981
C	-0.239022	2.087109	1.204979
C	2.166176	2.024573	1.331344
C	-3.972597	0.072279	2.224764
H	-4.278547	-0.207433	0.093284
C	-1.903193	1.203639	2.869843
O	-0.309585	3.339030	1.101789
H	2.694845	2.261993	0.381121
H	2.026546	2.957813	1.915279
H	2.846821	1.349442	1.888846
C	-3.111696	0.576458	3.219571
H	-4.912048	-0.428547	2.502720
H	-1.243718	1.609209	3.652741
H	-3.387501	0.480140	4.281317
O	-2.878925	1.225552	-1.830280
K	0.854407	3.197447	-1.402617
H	-3.744388	1.433703	-1.416124
O	1.921638	0.806555	-1.342799
H	2.577833	0.274871	-1.830513

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TS3'

Ru	-0.997722	-0.431355	0.411628
C	-1.249587	0.910720	2.138587
C	-2.158310	-0.204884	2.229636
H	-2.137484	-0.860697	3.113127
C	-3.044741	-0.501297	1.137279
H	-3.666847	-1.410457	1.199478
C	-3.066560	0.267337	-0.072244
C	-2.109671	1.342345	-0.152746
H	-1.982085	1.876608	-1.106783
C	-1.251610	1.698353	0.937595
H	-0.506137	2.496747	0.802468
C	-0.278324	1.195574	3.250221
H	0.030260	0.264395	3.762916
H	0.626828	1.706194	2.871716
H	-0.762263	1.858185	3.999180
C	-4.015181	-0.079894	-1.209698
H	-4.295539	-1.148666	-1.067829

C	-5.298815	0.768312	-1.074594
H	-5.067686	1.848417	-1.191914
H	-6.033010	0.491024	-1.858362
H	-5.781520	0.629157	-0.085576
C	-3.378454	0.058589	-2.603195
H	-3.178853	1.121122	-2.857483
H	-2.420860	-0.495591	-2.670290
H	-4.070501	-0.330281	-3.376793
O	1.950827	-1.122506	-1.922952
C	1.050865	-0.246528	-1.622390
C	1.497155	1.107326	-1.146021
N	0.956079	-0.853504	1.136351
C	1.379264	2.280244	-1.913775
C	1.976678	1.158203	0.184176
C	2.072188	-0.125577	0.971811
C	1.134495	-2.079130	1.921739
C	1.779478	3.509740	-1.360079
H	0.983342	2.228616	-2.940052
C	2.413027	2.388691	0.714125
O	3.223084	-0.483806	1.380776
H	1.659459	-2.864209	1.332104
H	1.756014	-1.879787	2.819269
H	0.150459	-2.482997	2.217040
C	2.302434	3.561936	-0.052629
H	1.692404	4.431628	-1.955576
H	2.821860	2.419385	1.736293
H	2.623635	4.525895	0.371652
O	-0.183529	-0.524968	-1.616948
K	4.561905	-0.926106	-0.698693
O	-1.012102	-2.502101	0.047429
H	1.433078	-2.197469	-1.722196
H	-1.830651	-2.741852	-0.426893
H	-0.089149	-2.837232	-0.668608
O	0.850555	-3.163582	-1.372654
H	1.419624	-3.782630	-0.879822

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INT3'

Ru	-1.062049	0.295684	0.001143
C	-2.823814	1.183650	1.039691
C	-2.306836	0.132399	1.862363
H	-1.998544	0.347149	2.896216
C	-2.035659	-1.151792	1.288770
H	-1.485973	-1.895862	1.889491
C	-2.393283	-1.496616	-0.067872
C	-2.937318	-0.443202	-0.866147
H	-3.126655	-0.619891	-1.935660
C	-3.124996	0.883361	-0.342352
H	-3.477455	1.686930	-1.006846
C	-2.974166	2.585833	1.557711

H	-2.369329	2.750810	2.469061
H	-2.661937	3.324093	0.793412
H	-4.040784	2.775654	1.804812
C	-2.143308	-2.898297	-0.597485
H	-1.288676	-3.299032	-0.007811
C	-3.377480	-3.780294	-0.306064
H	-4.266562	-3.406572	-0.856389
H	-3.191795	-4.824998	-0.628971
H	-3.626991	-3.794751	0.774774
C	-1.749734	-2.928282	-2.082866
H	-2.604434	-2.667548	-2.742096
H	-0.922595	-2.219985	-2.296105
H	-1.425072	-3.947733	-2.372167
O	0.006443	2.119080	0.256942
C	1.169245	1.668218	0.617956
C	1.116743	0.170751	0.907759
N	-0.116429	0.400509	-1.841216
C	1.291560	-0.373599	2.217728
C	1.098865	-0.711647	-0.232758
C	1.113824	-0.063251	-1.614035
C	-0.478627	1.212984	-2.985898
C	1.397514	-1.750206	2.385750
H	1.355059	0.310760	3.077572
C	1.253618	-2.116072	-0.029824
O	2.159640	0.052582	-2.301397
H	-0.578507	2.280727	-2.690706
H	0.297711	1.126229	-3.774140
H	-1.449305	0.877690	-3.406134
C	1.380736	-2.622936	1.259502
H	1.526219	-2.170242	3.395513
H	1.284987	-2.779616	-0.907078
H	1.495841	-3.707294	1.413196
O	2.233216	2.305778	0.644164
K	3.777128	1.836231	-1.393761

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TS4'

Ru	-0.671174	0.447694	-0.072569
C	-1.446010	2.371679	0.552259
C	-1.727215	1.405614	1.595382
H	-1.295829	1.560935	2.595391
C	-2.441821	0.209982	1.310056
H	-2.566871	-0.546877	2.098994
C	-2.813175	-0.117689	-0.033530
C	-2.600271	0.873950	-1.068637
H	-2.868671	0.640930	-2.110334
C	-1.966292	2.111567	-0.768761
H	-1.747114	2.822385	-1.580851
C	-0.659325	3.618111	0.853799
H	-1.351237	4.420357	1.191937

H	0.076176	3.433963	1.660152
H	-0.126296	3.987890	-0.044347
C	-3.391491	-1.485677	-0.375768
H	-3.440959	-2.054724	0.578042
C	-4.827667	-1.336312	-0.919171
H	-4.839758	-0.818788	-1.901438
H	-5.284312	-2.336132	-1.066124
H	-5.472700	-0.764436	-0.221582
C	-2.483650	-2.274545	-1.341734
H	-2.353133	-1.744155	-2.308145
H	-1.476737	-2.440243	-0.904556
H	-2.929571	-3.265455	-1.562478
O	1.177364	1.207080	2.651374
C	1.702072	0.802608	1.643718
C	0.708856	-0.785142	0.955124
N	0.798146	0.573081	-1.411570
C	0.383302	-1.611195	2.064407
C	1.270984	-1.407169	-0.207865
C	1.660416	-0.482353	-1.326078
C	1.014404	1.617057	-2.401715
C	0.568481	-2.998704	1.999009
H	0.012521	-1.134342	2.986374
C	1.461481	-2.799752	-0.274280
O	2.670501	-0.671295	-2.042035
H	0.101132	1.760902	-3.014305
H	1.244333	2.580894	-1.897105
H	1.852144	1.348962	-3.076612
C	1.100214	-3.590678	0.829913
H	0.313518	-3.631075	2.863990
H	1.877648	-3.248165	-1.190293
H	1.242375	-4.682224	0.789266
O	2.694667	0.930283	0.933578
K	4.608315	0.207508	-0.614320

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INT4'

Ru	0.875176	-0.458934	0.028001
C	1.841669	-2.388712	0.409449
C	2.273174	-1.473801	1.433996
H	2.079989	-1.712698	2.490668
C	2.774130	-0.194691	1.072588
H	2.968561	0.558870	1.851829
C	2.876192	0.194182	-0.318655
C	2.661553	-0.825376	-1.330617
H	2.778867	-0.565965	-2.393948
C	2.154115	-2.090174	-0.975544
H	1.874630	-2.812238	-1.758858
C	1.169664	-3.687542	0.771588
H	0.634433	-3.610875	1.737852
H	0.446968	-3.998536	-0.008592

H	1.933265	-4.490835	0.865075
C	3.339647	1.595119	-0.690889
H	3.183477	2.226545	0.211373
C	4.852815	1.559247	-0.999605
H	5.062152	0.936373	-1.895076
H	5.230935	2.582029	-1.202957
H	5.432661	1.140874	-0.151776
C	2.530012	2.219176	-1.840312
H	2.665488	1.664757	-2.792862
H	1.447813	2.230296	-1.598636
H	2.863306	3.260995	-2.020882
C	-0.267711	0.634054	1.331184
N	-0.518351	0.228174	-1.272124
C	-0.111577	0.814979	2.720396
C	-1.390913	1.247469	0.710740
C	-1.509364	1.014628	-0.757986
C	-0.521199	0.017549	-2.715373
C	-1.038394	1.582973	3.459113
H	0.738435	0.356128	3.252067
C	-2.317406	2.010569	1.435833
O	-2.434836	1.506860	-1.464782
H	-1.509047	-0.353560	-3.067469
H	-0.294542	0.957684	-3.268225
H	0.244865	-0.734006	-2.979132
C	-2.138964	2.182930	2.822350
H	-0.895911	1.714968	4.543879
H	-3.175141	2.466822	0.914765
H	-2.855359	2.782845	3.404637
K	-4.221208	2.434728	-2.733415

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TS5'

Ru	-0.450100	-0.658257	-0.203979
C	-1.828511	-2.427254	-0.423210
C	-2.112224	-1.455503	-1.462766
H	-2.078341	-1.766153	-2.519085
C	-2.386186	-0.101896	-1.137847
H	-2.551028	0.624171	-1.949421
C	-2.331400	0.375546	0.228480
C	-2.056394	-0.593193	1.247511
H	-1.948195	-0.264517	2.291488
C	-1.845270	-1.983898	0.928332
H	-1.591133	-2.691898	1.731260
C	-1.484442	-3.847105	-0.783254
H	-2.413222	-4.422170	-0.987801
H	-0.860427	-3.889082	-1.698900
H	-0.939507	-4.353977	0.036373
C	-2.578785	1.844913	0.531783
H	-2.255890	2.404482	-0.374182
C	-4.095446	2.066593	0.723638

H	-4.463245	1.516775	1.615464
H	-4.312685	3.143625	0.874137
H	-4.677690	1.719067	-0.154514
C	-1.763997	2.376913	1.720423
H	-2.103880	1.943168	2.684301
H	-0.684189	2.157599	1.598584
H	-1.886796	3.475201	1.801831
C	0.619686	1.132905	-0.842918
N	1.053359	-0.540442	1.215455
C	0.193260	2.096983	-1.787240
C	1.574177	1.513462	0.140285
C	1.995821	0.426564	1.087164
C	1.263263	-1.626933	2.160844
C	0.681416	3.413617	-1.721210
H	-0.510842	1.809718	-2.585025
C	2.094030	2.814817	0.187095
O	3.147727	0.401847	1.603885
H	0.405186	-1.701789	2.861792
H	1.343347	-2.609223	1.639535
H	2.180437	-1.451395	2.761429
C	1.625232	3.770143	-0.735758
H	0.337427	4.166269	-2.448042
H	2.843007	3.071290	0.952714
H	2.004444	4.803357	-0.693611
H	0.964409	-0.063072	-1.341165
O	1.299230	-1.371794	-1.398992
H	0.953299	-1.680001	-2.260560
K	3.879755	-1.274501	-0.282999

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INT5'

Ru	-1.074169	0.173734	-1.013745
C	-3.067165	0.581377	-1.881593
C	-2.974590	1.181502	-0.594493
H	-3.107582	2.271149	-0.500902
C	-2.611823	0.413148	0.570912
H	-2.525518	0.918076	1.546570
C	-2.318457	-0.981411	0.472901
C	-2.382860	-1.599018	-0.834198
H	-2.106874	-2.656267	-0.960804
C	-2.745083	-0.832850	-1.977062
H	-2.724168	-1.311512	-2.970376
C	-3.388746	1.385335	-3.111934
H	-4.451795	1.246280	-3.403412
H	-3.210684	2.464697	-2.940920
H	-2.759587	1.071366	-3.969606
C	-2.092035	-1.815463	1.728251
H	-1.872335	-1.105517	2.557510
C	-3.420945	-2.525047	2.076089
H	-3.697406	-3.250984	1.282724

H	-3.329274	-3.083248	3.030711
H	-4.253993	-1.800114	2.176527
C	-0.929917	-2.817631	1.639394
H	-1.100547	-3.574288	0.846053
H	0.028603	-2.310118	1.415514
H	-0.829675	-3.370651	2.596128
C	0.554999	0.684056	2.213864
N	0.750088	-0.859864	-0.583523
C	0.605958	1.668533	3.217070
C	1.609464	0.544916	1.285545
C	1.691867	-0.622633	0.326483
C	0.974561	-2.059071	-1.397743
C	1.710480	2.536184	3.308813
H	-0.226562	1.761382	3.933019
C	2.733654	1.399598	1.409134
O	2.728415	-1.368870	0.491999
H	0.729715	-2.981045	-0.823546
H	0.339787	-2.009820	-2.299679
H	2.037978	-2.147632	-1.704947
C	2.775684	2.399104	2.397234
H	1.743188	3.313619	4.087763
H	3.577073	1.282592	0.707242
H	3.642134	3.077233	2.456761
H	-0.312953	0.020301	2.129541
K	3.596077	-1.455413	2.783434
O	-0.124133	0.385041	-2.863972
K	1.786591	1.793081	-2.325100
H	-0.679591	-0.045180	-3.537241
O	0.026443	1.883051	-0.621809
H	-0.350030	2.322531	0.161251

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TS6'

Ru	-1.044659	0.214509	-0.785129
C	-2.312856	0.726675	0.906673
C	-1.255786	-0.105768	1.399288
H	-0.572899	0.266834	2.179577
C	-0.944724	-1.328881	0.729096
H	-0.031392	-1.870527	1.009626
C	-1.740041	-1.850868	-0.358159
C	-2.834053	-1.051414	-0.802391
H	-3.410452	-1.349069	-1.691612
C	-3.085646	0.245564	-0.222081
H	-3.861211	0.893943	-0.660401
C	-2.573900	2.092908	1.483514
H	-3.388599	2.036813	2.236879
H	-1.675827	2.498001	1.991431
H	-2.887288	2.806479	0.695672
C	-1.334250	-3.165186	-1.004458
H	-0.224584	-3.191791	-0.933594



C	-1.911485	-4.338782	-0.183078
H	-3.021711	-4.332141	-0.212517
H	-1.565332	-5.310503	-0.591738
H	-1.601661	-4.285899	0.881121
C	-1.713875	-3.270224	-2.488395
H	-2.813884	-3.318127	-2.634459
H	-1.316826	-2.410552	-3.066129
H	-1.290666	-4.196074	-2.927522
C	2.283563	-0.758990	1.528245
N	1.574382	-1.129990	-1.261312
C	2.297581	-0.433128	2.895621
C	2.347142	0.253343	0.543155
C	2.317298	-0.094194	-0.931827
C	1.620609	-1.581369	-2.640744
C	2.374216	0.913730	3.299601
H	2.247903	-1.232906	3.651588
C	2.460199	1.601547	0.960433
O	3.055630	0.644933	-1.722229
H	1.425005	-2.673457	-2.684296
H	0.818671	-1.093583	-3.243585
H	2.595136	-1.372772	-3.142819
C	2.460743	1.929750	2.327893
H	2.377071	1.171082	4.370402
H	2.511789	2.389426	0.193181
H	2.524281	2.984477	2.640521
H	2.215775	-1.805543	1.192189
K	5.262490	0.411909	-0.618003
O	-0.891119	0.425050	-2.784667
K	1.136198	1.950868	-3.093873
H	-1.562996	-0.109514	-3.247198
O	-0.013193	1.952711	-0.831225
H	0.000588	2.353678	0.057300

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INT3''

Ru	1.182216	-0.413132	-0.593177
C	2.903170	0.504004	0.489431
C	3.350522	-0.360385	-0.556887
H	3.999403	0.052891	-1.347863
C	2.934410	-1.741744	-0.647407
H	3.264332	-2.358657	-1.497183
C	2.000071	-2.270953	0.295343
C	1.524151	-1.413109	1.355067
H	0.761377	-1.775674	2.060736
C	1.957818	-0.057249	1.424220
H	1.508591	0.587814	2.188865
C	3.378483	1.950651	0.556957
H	3.291839	2.353115	-0.477879
C	1.487389	-3.682481	0.173575
H	1.496639	-4.032265	-0.877646

O	-3.108354	-2.341298	-0.541056
C	-2.748220	-1.064029	-0.270829
C	-2.118437	-0.891655	1.064067
N	-0.110591	1.294734	-0.449675
C	-2.293178	-1.890529	2.052982
C	-1.404956	0.295761	1.385769
C	-1.128462	1.416834	0.403893
C	0.161002	2.481871	-1.265907
C	-1.820143	-1.698895	3.358916
H	-2.830238	-2.813614	1.791000
C	-0.994213	0.498158	2.720206
O	-1.870571	2.451659	0.499287
H	0.864433	2.203497	-2.072193
H	-0.772519	2.901881	-1.705994
H	0.607467	3.299236	-0.658450
C	-1.186740	-0.488491	3.700329
H	-1.968458	-2.482867	4.117289
H	-0.500940	1.448049	2.980100
H	-0.839781	-0.314954	4.730894
O	-3.159298	-0.127202	-0.993848
K	-1.210813	-0.030244	-3.131973
O	1.195311	0.087109	-2.614150
H	2.111337	0.032423	-2.939832
O	-0.555438	-1.425034	-1.163197
H	-0.507288	-2.336329	-0.821672
K	-4.251776	2.131448	0.064888
C	2.529364	2.834363	1.484728
H	2.671018	2.553454	2.550060
H	2.833689	3.895649	1.386287
H	1.448018	2.765154	1.250238
C	4.866903	1.993349	0.968068
H	5.503946	1.407738	0.274177
H	5.241048	3.037755	0.975095
H	5.004148	1.575276	1.987755
H	2.130609	-4.367783	0.766031
H	0.457893	-3.775299	0.577650
H	-3.637569	-2.319401	-1.366742

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TS3''

Ru	1.730608	-0.244451	-0.823646
C	2.993579	0.734313	0.719285
C	3.821786	0.082095	-0.244110
H	4.570101	0.668399	-0.802113
C	3.575050	-1.284532	-0.627446
H	4.146359	-1.720588	-1.462965
C	2.576217	-2.090638	0.043547
C	1.769453	-1.448147	1.028143
H	0.916533	-1.984078	1.468010
C	1.928658	-0.047026	1.301332

H	1.175871	0.445725	1.932064
C	3.182128	2.213698	1.022777
H	3.477561	2.694803	0.061809
C	2.324889	-3.514026	-0.379053
H	2.445421	-3.631961	-1.474886
O	-2.429101	-2.516368	-1.453105
C	-2.623122	-1.383481	-0.739512
C	-2.037203	-1.434874	0.620624
N	-1.164666	1.753850	0.130377
C	-1.780699	-2.704049	1.206349
C	-1.783154	-0.244378	1.359705
C	-2.077966	1.164089	0.870547
C	-1.461987	3.145731	-0.194134
C	-1.311463	-2.803819	2.520718
H	-1.981278	-3.614560	0.623062
C	-1.303189	-0.371923	2.681845
O	-3.192086	1.649241	1.292043
H	-0.608937	3.597148	-0.746420
H	-2.384341	3.269968	-0.822781
H	-1.649374	3.771215	0.708814
C	-1.072929	-1.628052	3.262119
H	-1.136235	-3.792776	2.970739
H	-1.122069	0.546371	3.262187
H	-0.703636	-1.694136	4.297659
O	-3.277537	-0.440804	-1.217070
K	-0.988461	1.118772	-2.539426
O	1.527120	1.192496	-2.191823
H	2.257870	1.838271	-2.146566
O	0.171332	-1.026724	-1.805119
H	-0.039493	-1.929059	-1.497216
K	-5.208775	1.040122	0.142916
C	1.902751	2.901856	1.524510
H	1.666108	2.599970	2.567127
H	2.037894	4.002032	1.531422
H	1.027062	2.648443	0.892721
C	4.351803	2.384816	2.016870
H	5.292125	1.941493	1.629660
H	4.535290	3.460094	2.218787
H	4.116231	1.892111	2.983861
H	3.049263	-4.195753	0.115694
H	1.304965	-3.844402	-0.097598
H	-2.885322	-2.401454	-2.315686

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P'

O	0.991729	2.120823	0.448938
C	-0.166194	1.871105	0.102444
C	-0.780175	0.526478	-0.064241
N	2.385001	-0.477340	-0.630822
C	-2.173791	0.430207	-0.316081

C	0.002128	-0.661344	0.033737
C	1.492200	-0.646990	0.330303
C	1.924080	-0.335508	-2.002460
C	-2.790533	-0.815000	-0.475076
H	-2.770253	1.351415	-0.380189
C	-0.640359	-1.906306	-0.132759
O	1.784600	-0.743185	1.574103
H	1.411409	0.642033	-2.198135
H	2.790464	-0.383608	-2.696684
H	1.205199	-1.127423	-2.326472
C	-2.017042	-1.989086	-0.384575
H	-3.872968	-0.873229	-0.668391
H	-0.033867	-2.822380	-0.055745
H	-2.493533	-2.974929	-0.510555
O	-1.029286	2.890933	-0.158454
H	-0.517543	3.712239	0.005719
K	3.361896	1.135472	1.201831