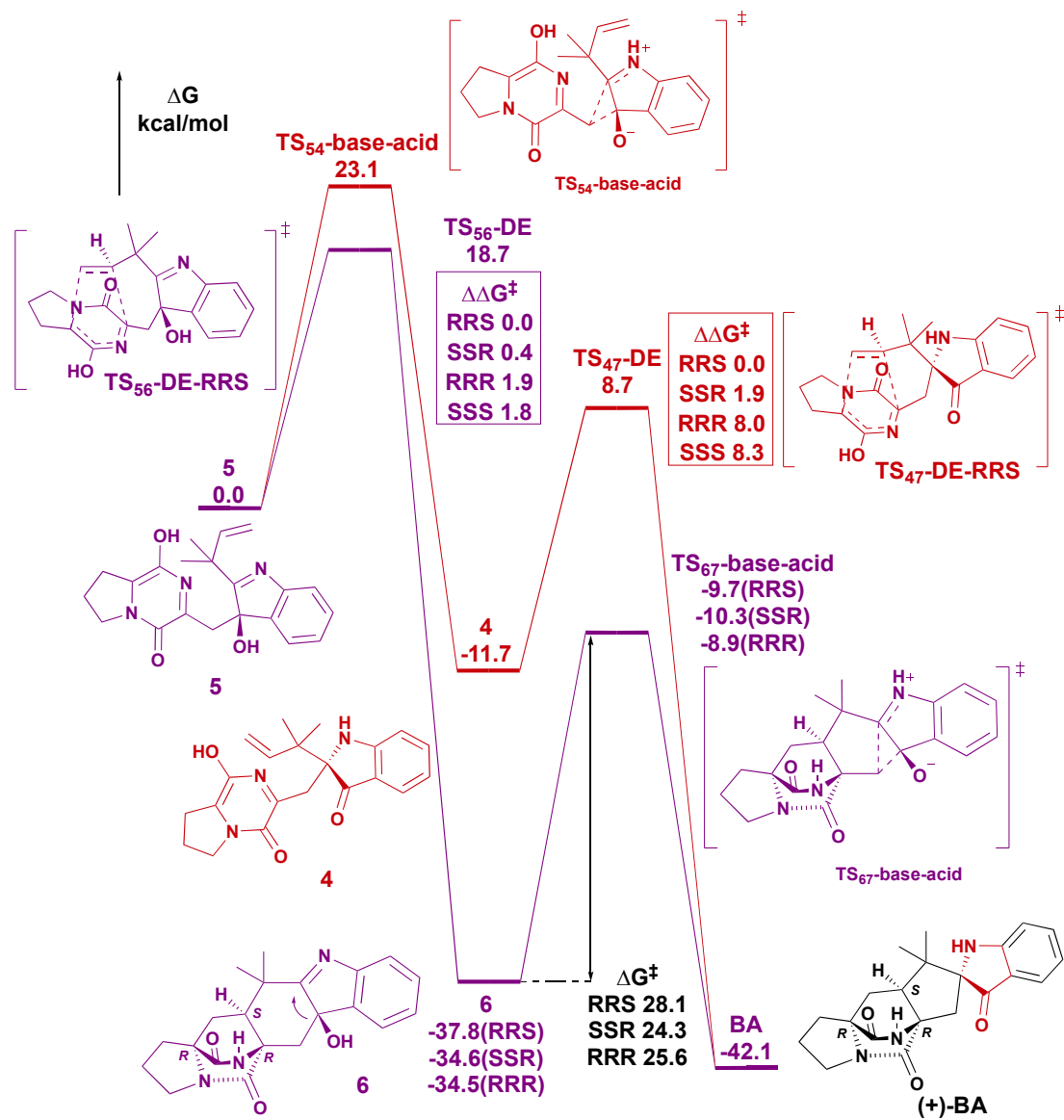


Supplementary Information

Complete details of methods:

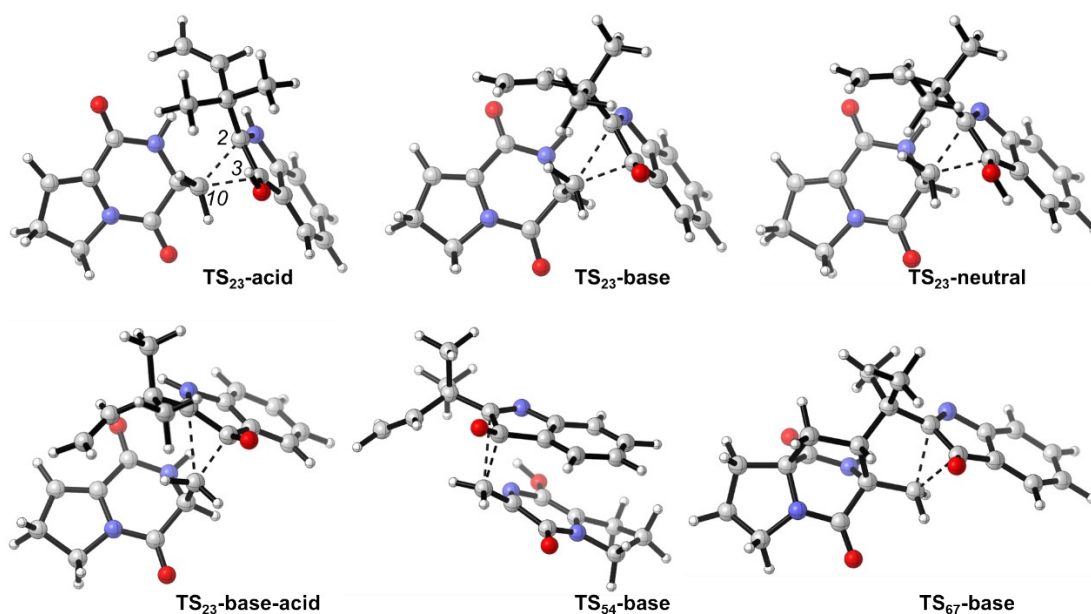
For each structure, we used the CREST¹ tool of Grimme's group to perform conformational sampling, which was pre-optimized using GFN2-xTB². Plausible conformations for the five-membered ring and the orientation of hydroxyl group were added manually for the transition state. We optimize the geometries of all stationary points in gas phase using the range-separated dispersion-corrected M06-2X³ density functional and the 6-31+G(d,p)^{4,8} basis set with Grimme's D3⁹ correction using the original D3 damping function. M06-2X with D3 dispersion is robust, reliable and accurate¹⁰ combination that has been demonstrated in previous studies. We performed vibrational frequency calculations to verify that stationary points were either minima or first-order saddle points on the potential energy surface and to calculate thermal corrections to Gibbs free energies at 298.15 K (25°C). The computed thermochemistry data were corrected using Grimme's quasi-harmonic (QHA) model for entropy¹¹ with a frequency cut-off value of 100.0 cm⁻¹ using the GoodVibes program¹². Also, GoodVibes applied a 1 M concentration correction to account for reactions in solution and a vibrational scaling factor of 0.967 for M062X/6-31+G(d,p) level of theory as suggested¹³. We applied single-point energy corrections to these optimized structures. The single-point energy calculations were obtained using correlated wavefunction theory (WFT) (DLPNO-CCSD(T)/cc-pV(DT)Z)¹⁴⁻²¹. We used the integral equation formalism variant of the polarizable continuum model (IEF-PCM)²²⁻²⁶ with the SMD solvation model (solvent=water)²⁷ to account for solvent effects. Domain-based local pair-natural orbital coupled cluster with perturbative triple excitations (DLPNO-CCSD(T)) calculations were carried out with ORCA 4.2^{28, 29}. DLPNO-CCSD(T) energies with a normal truncation threshold ("normalPNO") show an accuracy of 1 kcal/mol or better compared to CCSD(T)³⁰, which is generally recognized as a "gold standard" in computational chemistry³¹. Extrapolation to the basis set limit was carried out employing cc-pVDZ and cc-pVTZ energies, treating the convergence of SCF and correlation energies separately³². Gaussian 16³³ was employed for all density functional theory (DFT) calculations, using an "ultrafine" pruned (99,590) grid for numerical integration of the exchange-correlation functional and its derivatives. Representations in the main text and supporting information refer to the most stable rotameric conformation found for each step. Structure images of key transition states were generated by CYLview³⁴, while non-covalent interaction analysis were represented using Multiwfn³⁵ and VMD³⁶ graphical interfaces.

Supplementary Scheme 1 Calculations performed by Paton's group for route 2 and 3. Intermediate **5**, due to the high activation barrier, undergoes DA reaction before undergoing the migration reaction, forming the final products. However, the calculated selectivity does not match the experimental results, and the activation barriers of the migration reaction are excessively high.



Supplementary Figure 1 The four possible proton states during the migration reaction of intermediate **2**, along with the substrate free energy, transition state activation barrier, and reaction energy under the same substrate level. Key bond lengths (C2–C10 and C3–C10) are also listed in angstroms. Additionally, the relevant data and structures of intermediates **5** and **6** calculated using the base form are included.

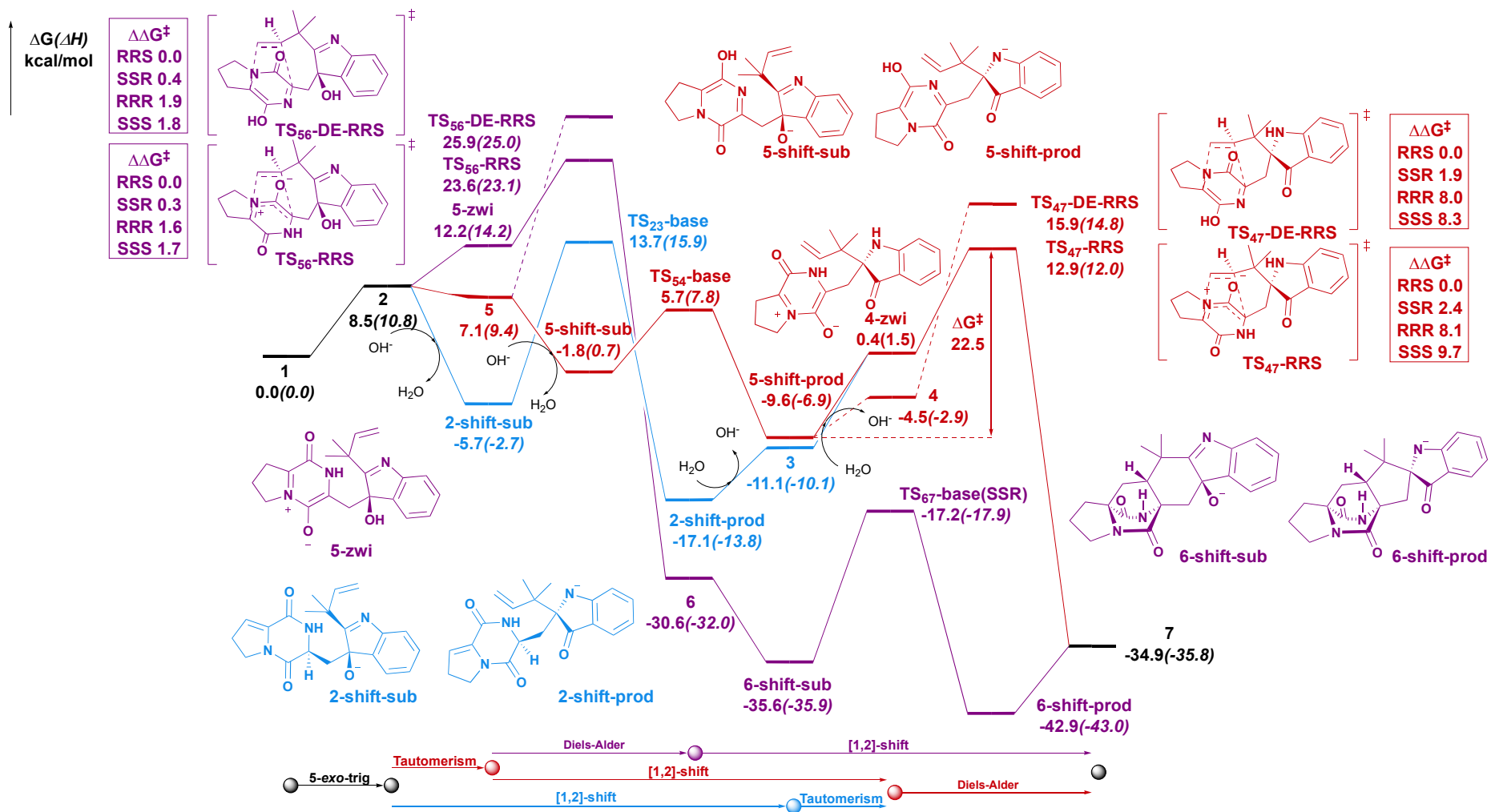
		R ¹	R ²	G _{sub}	ΔG [‡]	ΔG _r	d(C3–C10)	d(C2–C10)
TS ₂₃	acid	H	H ⁺	44.5	72.3	45.4	1.99	2.02
	base	⊖	Lp	-11.0	8.4	-22.4	2.04	2.23
	neutral	H	Lp	0.0	37.6	11.8	2.02	1.95
	base-acid	⊖	H ⁺	11.1	35.1	-8.8	1.82	2.34
TS ₅₄	base	⊖	Lp	-7.2	0.3	-14.9	2.00	2.57
TS ₆₇	base	⊖	Lp	-40.9	-22.5	-48.2	2.03	2.12



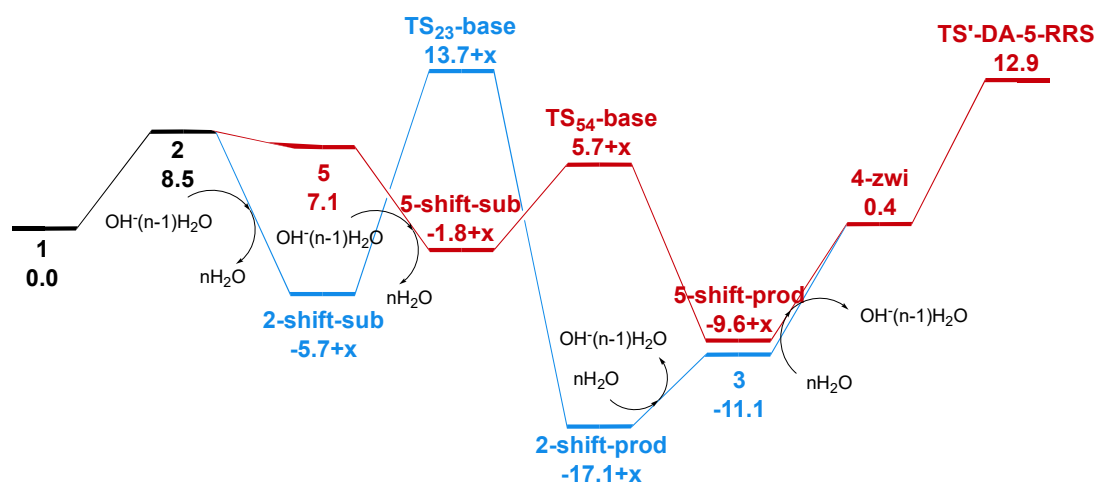
Supplementary Figure 2 The comparison of transition state free energies of three different proton states during the migration of intermediate **2** is performed using different clusters, where the transition state of the base-acid form is consistently found to be lower than that of the neutral form under the same substrate level.

H ₂ O cluster	OH ⁻ cluster	TS_{23⁻} base-acid	TS_{23⁻} base	TS_{23⁻} acid
1H ₂ O	OH ⁻	0.0	-26.7	37.3
2H ₂ O	1H ₂ O+OH ⁻	0.0	-19.0	29.5
3H ₂ O	2H ₂ O+OH ⁻	0.0	-14.4	25.0
4H ₂ O	3H ₂ O+OH ⁻	0.0	-13.3	23.9
5H ₂ O	4H ₂ O+OH ⁻	0.0	-12.8	23.4
6H ₂ O	5H ₂ O+OH ⁻	0.0	-9.5	20.0

Supplementary Figure 3 Complete potential energy surface for the three routes, providing the relative free energy for each configuration in the four DA reactions.

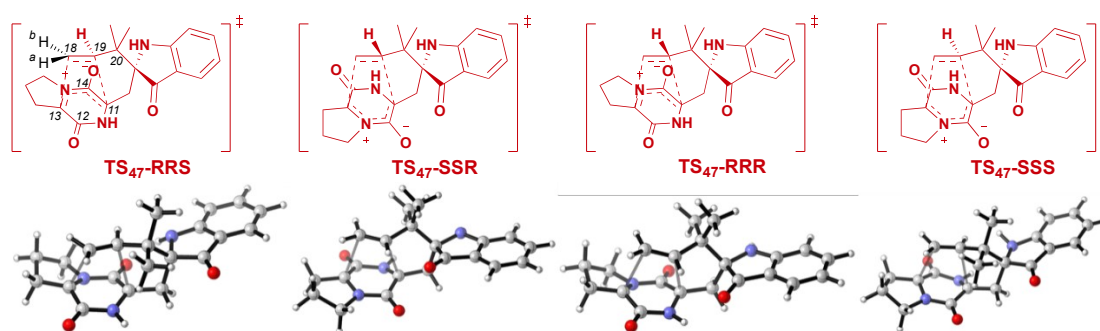


Supplementary Figure 4 Comparison of overall reaction barriers for routes 1 and 3 using the form of cluster hydrated hydroxides. n denotes the number of water molecules in the cluster, and x denotes the free energy of the potential energy surface of the migration reaction that is elevated because of the difference in the clusters.



n	x	ΔG^\ddagger of route 3	ΔG^\ddagger of route 1
1	0.0	22.5	30.0
2	7.7	14.8	24.0
3	12.3	18.0	26.0
4	13.4	19.1	27.1
5	13.9	19.6	27.6
6	17.2	22.9	30.9

Supplementary Figure 5 Structure of the TS_{47} configurations are presented. Key NBO charges, bond lengths (in angstroms), angles and dihedral data for the four structures are also provided.



	NBO charge (C18)	NBO charge (C11)	d(C19-C11)	\angle (Ha-C18-Hb)	\angle (C18-C13-N)	\angle (C19-C11-C14)	\angle (C19-C11-N)	ψ (C13-C12-N-C11)
RRS	-0.496	0.134	2.34	115.6	98.2	84.3	101.7	8.6
SSR	-0.495	0.114	2.35	115.8	97.2	89.4	99.7	-10.2
RRR	-0.485	0.097	2.30	116.8	94.0	102.6	89.4	13.6
SSS	-0.479	0.107	2.30	116.9	93.9	102.6	89.8	-15.2

Supplementary Table 1 Thermodynamic energies and coordinates

Structure	E	ZPE	H	T.S	T.qh-S	G(T)	qh-G(T)	im freq	Ehigh	TCH	H_water	qh-G(T)_water
1	-1203.594133	0.402791	-1203.166955	0.072041	0.069434	-1203.238996	-1203.236389		-1202.592473	0.427178	-1202.165295	-1202.234729
2	-1203.570198	0.400603	-1203.143788	0.077163	0.073088	-1203.220951	-1203.216876		-1202.574497	0.426410	-1202.148087	-1202.221175
2-shift-acid-prod	-1203.948765	0.413368	-1203.509626	0.076939	0.073082	-1203.586565	-1203.582708		-1203.017793	0.439139	-1202.578654	-1202.651736
2-shift-acid-sub	-1203.943903	0.413027	-1203.504662	0.078162	0.073950	-1203.582824	-1203.578612		-1203.018500	0.439241	-1202.579259	-1202.653209
2-shift-base-acid-prod	-1203.591203	0.401083	-1203.164439	0.077540	0.072907	-1203.241980	-1203.237347		-1202.594214	0.426764	-1202.167450	-1202.240357
2-shift-base-acid-sub	-1203.561244	0.401431	-1203.134695	0.074764	0.071379	-1203.209459	-1203.206075		-1202.563743	0.426549	-1202.137194	-1202.208573
2-shift-neutral-prod	-1203.550245	0.400521	-1203.123767	0.078669	0.073763	-1203.202436	-1203.197530		-1202.560199	0.426478	-1202.133721	-1202.207484
2-shift-neutral-sub	-1203.572740	0.400291	-1203.146493	0.077068	0.073263	-1203.223561	-1203.219756		-1202.579254	0.426247	-1202.153007	-1202.226270
2-shift-prod	-1203.047646	0.386695	-1202.635489	0.077435	0.072917	-1202.712924	-1202.708406		-1202.103442	0.412157	-1201.691285	-1201.764202
2-shift-sub	-1203.006933	0.386224	-1202.595204	0.076166	0.072396	-1202.671371	-1202.667600		-1202.085363	0.411729	-1201.673634	-1201.746030
3	-1203.603246	0.401288	-1203.176713	0.073974	0.071135	-1203.250687	-1203.247848		-1202.607847	0.426533	-1202.181314	-1202.252449
4	-1203.595058	0.400783	-1203.168839	0.076091	0.071994	-1203.244930	-1203.240832		-1202.596188	0.426219	-1202.169969	-1202.241963
4-zwi	-1203.578316	0.400908	-1203.152308	0.074702	0.071127	-1203.227010	-1203.223435		-1202.588945	0.426008	-1202.162937	-1202.234064
5	-1203.571572	0.399824	-1203.145899	0.077534	0.073101	-1203.223433	-1203.219000		-1202.575915	0.425673	-1202.150242	-1202.223343
5-shift-prod	-1203.030637	0.386158	-1202.619069	0.075580	0.071858	-1202.694649	-1202.690927		-1202.091952	0.411568	-1201.680384	-1201.752242
5-shift-sub	-1203.002816	0.385323	-1202.592049	0.075085	0.071652	-1202.667134	-1202.663701		-1202.078983	0.410767	-1201.668216	-1201.739868
5-zwi	-1203.552241	0.400070	-1203.126810	0.077023	0.072584	-1203.203833	-1203.199394		-1202.568128	0.425431	-1202.142697	-1202.215281
6-RRR	-1203.631823	0.405348	-1203.202923	0.070139	0.067833	-1203.273063	-1203.270757		-1202.639336	0.428900	-1202.210436	-1202.278269
6-RRS	-1203.639035	0.405622	-1203.210053	0.069134	0.067271	-1203.279187	-1203.277324		-1202.645213	0.428982	-1202.216231	-1202.283502
6-shift-prod-SSR	-1203.089964	0.391334	-1202.675372	0.069764	0.067443	-1202.745135	-1202.742815		-1202.152492	0.414592	-1201.737900	-1201.805343
6-shift-sub-SSR	-1203.060833	0.391240	-1202.646468	0.069596	0.067146	-1202.716064	-1202.713614		-1202.140860	0.414365	-1201.726495	-1201.793641
6-SSR	-1203.629706	0.405194	-1203.200843	0.070510	0.068091	-1203.271353	-1203.268934		-1202.639304	0.428863	-1202.210441	-1202.278532
BA	-1203.642154	0.404945	-1203.213617	0.070499	0.068011	-1203.284116	-1203.281628		-1202.650912	0.428537	-1202.222375	-1202.290386
H2O	-76.394984	0.020905	-76.370298	0.018399	0.018399	-76.388697	-76.388697		-76.391494	0.024686	-76.366808	-76.385207
OH	-75.758884	0.008423	-75.747156	0.016541	0.016541	-75.763698	-75.763698		-75.882596	0.011728	-75.870868	-75.887409

TS23-acid	-1203.899248	0.411449	-1203.462160	0.076049	0.072376	-1203.538209	-1203.534536	-379.82	-1202.973490	0.437088	-1202.536402	-1202.608778
TS23-base-acid	-1203.502637	0.398780	-1203.078669	0.074770	0.071448	-1203.153440	-1203.150118	-262.52	-1202.522898	0.423968	-1202.098930	-1202.170378
TS23-base	-1202.990453	0.385115	-1202.580385	0.074344	0.071133	-1202.654729	-1202.651518	-287.05	-1202.054047	0.410068	-1201.643979	-1201.715112
TS23-neutral	-1203.510677	0.398836	-1203.086481	0.075536	0.071928	-1203.162017	-1203.158409	-538.13	-1202.518607	0.424196	-1202.094411	-1202.166339
TS47-DE-RRR	-1203.554924	0.401526	-1203.129861	0.069446	0.067527	-1203.199307	-1203.197388	-450.59	-1202.554220	0.425063	-1202.129157	-1202.196684
TS47-DE-RRS	-1203.566064	0.401677	-1203.140820	0.069452	0.067702	-1203.210273	-1203.208522	-469.18	-1202.566985	0.425244	-1202.141741	-1202.209443
TS47-DE-SSR	-1203.554863	0.400797	-1203.130090	0.070769	0.068623	-1203.200859	-1203.198713	-441.56	-1202.562497	0.424773	-1202.137724	-1202.206347
TS47-DE-SSS	-1203.547573	0.401087	-1203.122587	0.070649	0.068528	-1203.193237	-1203.191115	-522.38	-1202.552724	0.424986	-1202.127738	-1202.196266
TS47-RRR	-1203.546759	0.400612	-1203.122099	0.070771	0.068718	-1203.192870	-1203.190817	-423.49	-1202.557249	0.424660	-1202.132589	-1202.201307
TS47-RRS	-1203.561754	0.401345	-1203.136723	0.069824	0.068024	-1203.206547	-1203.204747	-351.02	-1202.571200	0.425031	-1202.146169	-1202.214193
TS47-SSR	-1203.545934	0.400327	-1203.121479	0.071203	0.069022	-1203.192682	-1203.190501	-316.74	-1202.565784	0.424455	-1202.141329	-1202.210351
TS47-SSS	-1203.539024	0.400753	-1203.114321	0.070751	0.068627	-1203.185072	-1203.182948	-432.32	-1202.554884	0.424703	-1202.130181	-1202.198808
TS54-base	-1203.000471	0.384422	-1202.590956	0.073901	0.070955	-1202.664857	-1202.661911	-183.67	-1202.066485	0.409515	-1201.656970	-1201.727925
TS54-neu	-1203.506356	0.398230	-1203.083003	0.074679	0.071180	-1203.157682	-1203.154183	-34.84	-1202.538698	0.423353	-1202.115345	-1202.186525
TS56-DE-RRR	-1203.539424	0.400933	-1203.114556	0.070104	0.068290	-1203.184660	-1203.182847	-451.71	-1202.546955	0.424868	-1202.122087	-1202.190377
TS56-DE-RRS	-1203.542461	0.401179	-1203.117518	0.069733	0.067973	-1203.187251	-1203.185492	-464.00	-1202.550412	0.424943	-1202.125469	-1202.193442
TS56-DE-SSR	-1203.546095	0.401448	-1203.120993	0.069722	0.067760	-1203.190715	-1203.188753	-476.44	-1202.550200	0.425102	-1202.125098	-1202.192858
TS56-DE-SSS	-1203.541788	0.401124	-1203.117064	0.069125	0.067592	-1203.186189	-1203.184657	-450.54	-1202.547674	0.424724	-1202.122950	-1202.190542
TS56-RRR	-1203.534732	0.400709	-1203.109960	0.070872	0.068783	-1203.180832	-1203.178743	-345.05	-1202.550559	0.424772	-1202.125787	-1202.194570
TS56-RRS	-1203.539172	0.400732	-1203.114425	0.070336	0.068593	-1203.184761	-1203.183018	-347.48	-1202.553285	0.424747	-1202.128538	-1202.197131
TS56-SSR	-1203.541388	0.401334	-1203.116358	0.069864	0.067960	-1203.186221	-1203.184318	-356.56	-1202.553696	0.425030	-1202.128666	-1202.196626
TS56-SSS	-1203.536102	0.400762	-1203.111670	0.069450	0.067845	-1203.181120	-1203.179515	-364.73	-1202.550965	0.424432	-1202.126533	-1202.194378
TS67-base-SSR	-1203.043429	0.389685	-1202.630961	0.068764	0.066508	-1202.699724	-1202.697468	-316.41	-1202.110329	0.412468	-1201.697861	-1201.764369
TS67-neu-RRR	-1203.571608	0.403639	-1203.145170	0.067874	0.066073	-1203.213044	-1203.211243	-66.97	-1202.597968	0.426438	-1202.171530	-1202.237603
TS67-neu-RRS	-1203.574696	0.403429	-1203.148491	0.067822	0.066145	-1203.216314	-1203.214636	-312.57	-1202.598908	0.426205	-1202.172703	-1202.238848
TS67-neu-SSR	-1203.562614	0.403707	-1203.136094	0.068590	0.066380	-1203.204684	-1203.202474	-71.44	-1202.599898	0.426520	-1202.173378	-1202.239758

I				H	-0.717923	2.503141	1.127264
				H	0.885776	2.585084	1.894967
C	0.281756	-0.295887	1.975883	H	0.291863	3.936147	0.910788
C	2.368314	2.650517	-0.480235	H	0.479931	2.388486	-2.424868
C	-0.825978	-0.660208	1.014105	H	-0.924850	2.650302	-1.382033
C	3.093043	3.448568	0.304527	H	0.325330	3.899303	-1.509084
C	-2.800111	-0.288629	-0.841758	H	1.012502	0.096273	-2.238365
C	-1.410050	0.082925	-1.235390	H	3.140782	0.974818	1.204096
C	-3.869661	-0.439405	-1.626720				
N	-3.144529	-0.376452	0.523382	2			
N	-0.573281	0.198660	-0.161453				
C	-2.248322	-0.516242	1.533205	C	-0.413072	-0.225681	1.441515
O	-2.553830	-0.598096	2.710461	C	-1.909973	-2.581445	-0.640618
C	-4.603585	-0.436867	0.666905	C	0.729399	-0.316955	0.418872
C	-5.093705	-0.707211	-0.779135	C	-1.544776	-3.690334	0.005583
O	-1.115997	0.321151	-2.399689	C	3.367270	-1.007693	-0.368026
C	0.834027	0.680610	-0.242771	C	2.329831	-2.071380	-0.367407
C	2.052930	-1.156352	-0.963200	C	4.617348	-1.050742	-0.832730
C	2.064483	-1.264744	0.429135	N	3.096959	0.213120	0.281219
C	2.557071	-2.181246	-1.762913	N	1.166759	-1.700629	0.240641
C	2.604094	-2.379725	1.053484	C	1.910764	0.581005	0.818661
C	3.084035	-3.306761	-1.128578	O	1.780189	1.581749	1.505880
C	3.117395	-3.412457	0.264790	C	4.340956	0.980293	0.424019
C	0.919240	2.241571	-0.269471	C	5.313994	0.260208	-0.542068
C	0.314623	2.845901	1.002172	O	2.535238	-3.189737	-0.809436
C	0.150702	2.819745	-1.476372	C	-2.369678	-0.196875	-0.250016
N	1.539042	0.078639	-1.369986	C	-1.770593	1.754535	-1.049001
C	1.463382	-0.017863	1.046346	C	-1.343042	1.840601	0.277496
O	2.402426	0.728863	1.777940	C	-1.611850	2.808082	-1.935800
H	0.030594	0.603850	2.542088	C	-0.752816	2.994118	0.764143
H	0.497872	-1.100279	2.680805	C	-1.015420	3.975747	-1.447090
H	2.805560	2.282842	-1.407246	C	-0.596823	4.071050	-0.118570
H	-0.715247	-1.715821	0.715787	C	-2.982818	-1.592826	-0.213361
H	4.101526	3.734438	0.022109	C	-4.101184	-1.672878	-1.272325
H	2.715170	3.838522	1.245297	C	-3.574169	-1.930754	1.159742
H	-3.844357	-0.377311	-2.706129	N	-2.388390	0.501693	-1.327985
H	-4.867233	-1.217675	1.382227	C	-1.663650	0.517153	0.939377
H	-4.971678	0.519832	1.050840	O	-2.501139	0.649774	2.077180
H	-5.433181	-1.741702	-0.908776	H	-0.704506	-1.230187	1.763067
H	-5.931308	-0.058381	-1.046951	H	-0.069016	0.322394	2.323086
H	2.544293	-2.102542	-2.845407	H	-1.451196	-2.350131	-1.604274
H	2.625163	-2.445024	2.138431	H	0.384736	0.087423	-0.548838
H	3.479604	-4.116451	-1.734327	H	-0.802097	-4.360593	-0.418918
H	3.538308	-4.296567	0.731148	H	-1.970904	-3.969667	0.964769

H	5.044786	-1.900766	-1.346523	N	1.521772	-0.590814	-0.717198
H	0.429221	-2.396280	0.193145	C	2.504497	0.545210	1.012104
H	4.157591	2.026954	0.177568	O	2.784406	1.418242	1.948614
H	4.678646	0.925728	1.464404	H	0.116927	1.272974	1.730027
H	5.462810	0.830619	-1.466669	H	0.085866	-0.461520	1.482556
H	6.298277	0.116939	-0.089500	H	0.739440	0.809717	-2.663661
H	-1.946959	2.721371	-2.963980	H	-1.350158	1.504068	-0.374712
H	-0.395709	3.052985	1.787073	H	-0.907587	2.345927	-3.479479
H	-0.877123	4.823101	-2.111463	H	-0.651455	3.483509	-2.048157
H	-0.134382	4.987519	0.233093	H	-6.079066	-0.785999	0.962286
H	-4.880858	-0.936942	-1.053745	H	-2.051156	1.723805	2.043203
H	-3.714631	-1.465213	-2.271231	H	-3.501047	-1.818174	-2.225662
H	-4.540073	-2.674548	-1.255926	H	-3.136209	-2.977012	-0.939126
H	-2.832060	-1.915212	1.961086	H	-5.802344	-1.767349	-1.556936
H	-4.352882	-1.211684	1.424495	H	-5.453520	-3.032609	-0.386680
H	-4.028107	-2.925632	1.120077	H	2.573544	-3.073955	-1.531184
H	-3.155345	1.336880	1.898710	H	4.947667	-0.550210	2.149964
2-shift-acid-prod				H	4.617381	-3.954117	-0.467188
C	0.043128	0.498907	0.955686	H	5.806035	-2.739190	1.322021
C	0.526539	1.707672	-2.086893	H	3.563926	2.264513	-0.587601
C	-1.362586	0.668057	0.335090	H	3.178276	1.118911	-1.894161
C	-0.386828	2.558112	-2.551970	H	2.898906	2.848027	-2.119461
C	-4.016075	-0.441488	0.539667	H	0.033428	3.171771	0.313953
C	-3.609832	0.597581	1.508956	H	1.760029	3.421334	0.690311
C	-5.202110	-1.025359	0.375342	H	1.101157	4.034261	-0.791776
N	-3.053059	-0.957455	-0.359363	H	0.706963	-0.977032	-1.212683
N	-2.280181	0.946056	1.433976	H	2.133089	2.132649	2.008584
C	-1.795665	-0.538266	-0.502929	2-shift-acid-sub			
O	-1.026204	-1.056129	-1.322376	C	-0.038006	-0.648709	1.146720
C	-3.649409	-2.039880	-1.167425	C	1.716054	3.254429	-0.678371
C	-5.136897	-2.045424	-0.733682	C	-0.733141	-0.916083	-0.200795
O	-4.365580	1.075659	2.327987	C	0.723107	3.631163	-1.485261
C	1.315132	0.619726	0.068636	C	-3.321741	0.285810	-0.411102
C	2.585848	-1.275984	-0.293704	C	-2.164204	1.009584	-0.974414
C	3.260716	-0.578317	0.761542	C	-4.584550	0.699587	-0.291643
C	3.076802	-2.526925	-0.742504	N	-3.168027	-1.053514	0.007568
C	4.447410	-1.100342	1.360467	N	-0.990940	0.298727	-0.960222
C	4.214729	-2.999952	-0.140619	C	-2.003186	-1.713831	0.134363
C	4.909449	-2.297896	0.903030	O	-1.900215	-2.855989	0.552642
C	1.410180	1.906472	-0.865065	C	-4.479131	-1.618794	0.376430
C	2.855529	2.035114	-1.391013	C	-5.440392	-0.405785	0.277135
C	1.044309	3.186152	-0.104741	O	-2.239481	2.130918	-1.447669

H	1.804660	4.381680	0.247191	H	4.855007	-0.542160	-1.866000
H	0.512849	-0.240686	-1.691178	H	1.711346	-3.042236	1.109523
2-shift-base-acid-sub				H	5.013788	-3.009484	-1.639366
C	0.026932	-0.437404	1.479010	H	3.454300	-4.253795	-0.181437
C	-0.049686	2.349266	-0.611786	H	2.961199	3.722061	0.311264
C	-0.747958	-1.343297	0.497150	H	2.316911	3.348573	-1.313112
C	-1.314562	2.711555	-0.399245	H	1.532851	4.568615	-0.307734
C	-3.009888	-0.294652	-0.931658	H	-0.007534	2.388697	2.228740
C	-1.677988	-0.257775	-1.585359	H	1.557824	3.183125	2.360447
C	-4.170903	0.185385	-1.379245	H	0.195189	4.035331	1.607300
N	-3.152570	-0.923937	0.318171	2-shift-neutral-prod			
N	-0.690113	-0.865585	-0.878401	C	-0.030538	1.071550	-0.476090
C	-2.164914	-1.496131	1.041116	C	-1.858493	2.635647	1.461313
O	-2.362395	-2.066248	2.103915	C	0.955055	-0.089008	-0.275718
C	-4.568035	-0.945192	0.714288	C	-1.356267	3.860163	1.617794
C	-5.264004	-0.081195	-0.369722	C	3.688549	-0.291289	0.616963
O	-1.505730	0.256877	-2.679728	C	2.602277	-0.351256	1.629981
C	1.872795	1.217023	0.468014	C	5.004228	-0.408968	0.796481
C	3.167340	-0.419699	-0.519916	N	3.364661	-0.063883	-0.733720
C	2.280911	-1.117785	0.315013	N	1.354211	-0.194515	1.123242
C	4.166622	-1.083298	-1.224547	C	2.123963	0.059061	-1.250464
C	2.372039	-2.497742	0.440367	O	1.922316	0.243056	-2.443669
C	4.246631	-2.470503	-1.092215	C	4.587139	-0.012105	-1.548338
C	3.362699	-3.177189	-0.273967	C	5.725506	-0.261170	-0.523498
C	1.110953	2.547811	0.340621	O	2.839677	-0.508218	2.817930
C	2.048177	3.605178	-0.284785	C	-1.490235	0.712462	-0.094306
C	0.682983	3.062756	1.718024	C	-1.996431	-1.279741	0.750870
N	2.855199	0.942476	-0.539785	C	-2.373503	-1.385971	-0.660666
C	1.410104	-0.102537	0.984664	C	-2.184530	-2.440704	1.596848
O	2.208549	0.788083	1.787916	C	-2.917550	-2.605108	-1.195208
H	-0.539858	0.485540	1.629572	C	-2.698556	-3.567612	1.045202
H	0.088013	-0.956194	2.441650	C	-3.072421	-3.659923	-0.357061
H	0.207721	1.886850	-1.566949	C	-2.343781	2.020809	0.163045
H	-0.320607	-2.349635	0.519766	C	-3.820182	1.630049	0.353954
H	-2.064749	2.548471	-1.166840	C	-2.233979	2.999583	-1.010285
H	-1.640665	3.174510	0.528118	N	-1.507887	-0.127504	1.104222
H	-4.288809	0.700730	-2.322812	C	-2.069985	-0.164363	-1.182056
H	0.222681	-0.848859	-1.323091	O	-2.174788	0.289798	-2.434168
H	-4.922290	-1.980012	0.720211	H	0.297236	1.912718	0.143842
H	-4.668995	-0.548419	1.726138	H	-0.006241	1.370933	-1.527573
H	-6.114924	-0.603200	-0.816086	H	-1.960354	1.987955	2.329552
H	-5.646656	0.857461	0.046080				

H	0.465952	-1.027038	-0.582727	C	1.159999	2.596895	0.308299
H	-1.062171	4.212873	2.601101	C	2.013807	3.618219	-0.466297
H	-1.219621	4.549943	0.790126	C	1.117323	2.999601	1.786607
H	5.468245	-0.581779	1.757717	N	2.433697	0.914350	-0.941211
H	0.583191	-0.220115	1.786645	C	1.584998	0.017759	1.088305
H	4.531907	-0.774783	-2.328835	O	2.184966	0.408366	2.319092
H	4.654281	0.962957	-2.037138	H	-0.472306	0.461439	1.600447
H	6.299199	-1.161013	-0.767712	H	0.146645	-1.070812	2.232307
H	6.434922	0.571913	-0.499917	H	-0.219284	2.356485	-1.399776
H	-1.908423	-2.381800	2.644440	H	-0.002994	-2.147797	0.066725
H	-3.201420	-2.682633	-2.241974	H	-2.302849	2.846994	-0.306646
H	-2.843223	-4.447037	1.665860	H	-1.451659	3.086514	1.324941
H	-3.481122	-4.595466	-0.723340	H	-4.492729	0.923549	-1.903101
H	-4.244775	1.234944	-0.575243	H	0.198155	-0.342605	-1.547491
H	-3.929251	0.876048	1.139057	H	-4.643951	-2.377823	0.496981
H	-4.397839	2.512731	0.642979	H	-4.436998	-1.198035	1.798490
H	-1.210509	3.351265	-1.165703	H	-6.080929	-0.811737	-0.579349
H	-2.581979	2.542199	-1.938081	H	-5.635626	0.465756	0.546311
H	-2.860637	3.873482	-0.806131	H	3.931444	-0.690337	-2.671020
H	-2.443498	-0.416704	-3.036458	H	2.324286	-2.820947	1.565970
				H	4.488684	-3.075807	-2.144729
2-shift-neutral-sub				H	3.703904	-4.113788	-0.050830
				H	3.039609	3.620468	-0.085750
C	0.129846	-0.418433	1.350974	H	2.047084	3.377166	-1.529961
C	-0.219681	2.586824	-0.333273	H	1.582267	4.614974	-0.337610
C	-0.564504	-1.223379	0.235142	H	0.514595	2.322445	2.396426
C	-1.379883	2.852995	0.266045	H	2.124715	3.005963	2.208159
C	-3.022948	-0.200427	-0.836222	H	0.696371	4.006557	1.865466
C	-1.760855	0.085509	-1.561956	H	2.463970	-0.387202	2.788935
C	-4.253245	0.243902	-1.096652				
N	-3.008467	-1.082504	0.259579	2-shift-prod			
N	-0.661779	-0.520772	-1.038658				
C	-1.915231	-1.664403	0.797283	C	-0.041507	1.182334	-0.464036
O	-1.971420	-2.456922	1.726742	C	-1.871451	2.494978	1.634238
C	-4.381328	-1.338983	0.717681	C	0.992497	0.050080	-0.416693
C	-5.230295	-0.326091	-0.093599	C	-1.519608	3.751597	1.914500
O	-1.733316	0.782911	-2.563904	C	3.636948	-0.457192	0.598298
C	1.749200	1.207520	0.106047	C	2.472106	-0.637625	1.513606
C	2.836391	-0.445903	-0.834763	C	4.929048	-0.702101	0.826849
C	2.387677	-1.031412	0.351252	N	3.426844	0.066472	-0.686140
C	3.592151	-1.159192	-1.753441	N	1.288113	-0.304084	0.972633
C	2.684905	-2.349431	0.653631	C	2.230869	0.417366	-1.229733
C	3.898011	-2.489971	-1.447742	O	2.165938	0.945514	-2.330421
C	3.455594	-3.078895	-0.262036	C	4.711975	0.308985	-1.347864

C	5.741497	-0.367378	-0.405645	C	2.979929	-0.186540	0.802949
O	2.639520	-1.027132	2.666002	C	1.718997	0.089366	1.543550
C	-1.461872	0.717260	-0.073380	C	4.208212	0.280128	1.041564
C	-1.973833	-1.364190	0.589306	N	2.962697	-1.078322	-0.278014
C	-2.401333	-1.354134	-0.779622	N	0.628953	-0.522961	1.034368
C	-2.153811	-2.586937	1.320209	C	1.868808	-1.740664	-0.744689
C	-2.979176	-2.469111	-1.399049	O	1.967298	-2.629738	-1.578885
C	-2.724183	-3.666744	0.687490	C	4.334052	-1.367309	-0.703936
C	-3.148907	-3.633450	-0.671857	C	5.167719	-0.273102	0.009204
C	-2.355032	1.964952	0.301404	O	1.716487	0.789410	2.550719
C	-3.809808	1.495642	0.498574	C	-1.725470	1.201140	-0.137308
C	-2.325371	3.038642	-0.790869	C	-2.769515	-0.458712	0.824518
N	-1.439632	-0.235290	1.043186	C	-2.408328	-1.007053	-0.409110
C	-2.082002	-0.042578	-1.286793	C	-3.476730	-1.190814	1.771295
O	-2.225099	0.421080	-2.417612	C	-2.775401	-2.302126	-0.731526
H	0.296851	1.976902	0.213478	C	-3.833572	-2.505551	1.448919
H	-0.066684	1.575507	-1.485172	C	-3.493767	-3.054001	0.209222
H	-1.829432	1.736876	2.414889	C	-1.166304	2.607917	-0.328968
H	0.563804	-0.829942	-0.924988	C	-2.074004	3.618781	0.398395
H	-1.202062	4.027990	2.915992	C	-1.067909	2.999455	-1.806668
H	-1.526943	4.540567	1.167168	N	-2.358515	0.900706	0.948554
H	5.310386	-1.105946	1.754129	C	-1.634896	0.056929	-1.205031
H	0.419258	-0.411732	1.520186	O	-2.149206	0.397258	-2.386963
H	4.691018	-0.108654	-2.356444	H	0.489730	0.437885	-1.607406
H	4.872253	1.388893	-1.435980	H	-0.177451	-1.073151	-2.255239
H	6.163091	-1.274263	-0.856310	H	0.140109	2.402916	1.438065
H	6.580968	0.299203	-0.185293	H	-0.077560	-2.141999	-0.055699
H	-1.836412	-2.639984	2.357961	H	2.266237	2.893068	0.431761
H	-3.281202	-2.400178	-2.442212	H	1.477612	3.116462	-1.237267
H	-2.856518	-4.590447	1.248441	H	4.447030	0.979400	1.830606
H	-3.593450	-4.515478	-1.121633	H	-0.246414	-0.284704	1.492861
H	-4.236934	1.160164	-0.452601	H	4.608201	-2.375730	-0.372707
H	-3.850835	0.668252	1.213275	H	4.396922	-1.340009	-1.792974
H	-4.418763	2.323042	0.879355	H	6.077866	-0.686350	0.453397
H	-1.331094	3.483182	-0.901039	H	5.477451	0.512953	-0.691080
H	-2.613265	2.605317	-1.751132	H	-3.745581	-0.743858	2.724409
H	-3.026469	3.842974	-0.537184	H	-2.516073	-2.716188	-1.703542
				H	-4.388746	-3.103552	2.166771
2-shift-sub				H	-3.792863	-4.072276	-0.025672
				H	-3.079742	3.589747	-0.032629
C	-0.137806	-0.429839	-1.369610	H	-2.153502	3.378761	1.460659
C	0.181039	2.633680	0.371850	H	-1.662912	4.627839	0.281947
C	0.523694	-1.245911	-0.238930	H	-0.442413	2.312990	-2.379937
C	1.366504	2.901580	-0.177783	H	-2.054598	2.952806	-2.269993

H	-0.663402	4.017471	-1.877100	H	0.994643	3.289570	1.077693
				H	2.834027	2.221695	-2.670353
3				H	2.777437	3.650708	-0.656246
				H	-3.000544	2.495354	-0.231505
C	-1.513034	-1.259939	0.945004	H	-2.594822	1.744431	-1.794335
C	-3.649434	-0.722244	-1.235631	H	-4.285192	1.861155	-1.273062
C	-0.084238	-1.707771	1.299180	H	-4.113151	-0.641320	1.498165
C	-4.633681	-1.603906	-1.062614	H	-3.627812	1.044447	1.753174
C	2.520147	-0.605926	0.711879	H	-5.047240	0.659616	0.757904
C	1.808881	-0.132716	1.922563	H	-0.768866	-0.961521	-1.616877
C	3.678894	-0.182793	0.208617				
N	1.936999	-1.609446	-0.088679	4			
N	0.605510	-0.733851	2.137852				
C	0.699574	-2.119843	0.053181	C	0.859080	3.072125	-1.249493
O	0.207493	-2.899575	-0.757697	C	0.231466	1.938152	-1.752151
C	2.799193	-1.895793	-1.244706	C	-0.596750	1.212532	-0.883224
C	3.984972	-0.910680	-1.078064	C	-0.750909	1.625047	0.448391
O	2.266820	0.729373	2.653228	C	-0.122888	2.768202	0.940005
C	-1.654090	0.010386	0.087189	C	0.686908	3.499613	0.080193
C	0.138839	0.856411	-1.168439	H	1.501061	3.650643	-1.908205
C	0.096658	1.684852	-0.036131	H	0.368585	1.622961	-2.781933
C	1.132094	1.042830	-2.139500	H	-0.262426	3.054834	1.978263
C	1.038006	2.692804	0.171807	H	1.193628	4.393046	0.428010
C	2.058774	2.057438	-1.926405	C	-1.550544	0.604291	1.133689
C	2.026968	2.878929	-0.785296	C	-1.818851	-0.517259	0.090413
C	-3.170263	0.315742	-0.240557	N	-1.324250	0.074845	-1.159604
C	-3.261216	1.691822	-0.928041	H	-0.923236	-0.570039	-1.835590
C	-4.034584	0.340675	1.024090	O	-1.904427	0.574629	2.294982
N	-0.885832	-0.064290	-1.161351	C	-3.341691	-0.869020	-0.034008
C	-1.000258	1.215394	0.815773	C	-3.575837	-1.709517	-1.293698
O	-1.353035	1.638062	1.899646	H	-3.041629	-2.662815	-1.235502
H	-2.009709	-2.094956	0.439695	H	-4.642958	-1.932589	-1.390477
H	-2.038298	-1.080366	1.888809	H	-3.251181	-1.189949	-2.198084
H	-3.134916	-0.699189	-2.196458	C	-3.835106	-1.657878	1.191838
H	-0.192307	-2.643623	1.865274	H	-3.598630	-1.136197	2.122465
H	-4.908903	-2.288489	-1.858463	H	-4.920719	-1.778800	1.123520
H	-5.200584	-1.673548	-0.139162	H	-3.391575	-2.657997	1.224295
H	4.283417	0.592513	0.659304	C	-4.107381	0.440802	-0.081244
H	0.086013	-0.340784	2.916107	H	-4.179165	0.957265	0.876830
H	3.105497	-2.944393	-1.216177	C	-4.673607	0.994824	-1.151608
H	2.229435	-1.737822	-2.164028	H	-5.196956	1.942429	-1.073352
H	4.943225	-1.436591	-1.029690	H	-4.635803	0.534567	-2.134119
H	4.043362	-0.207403	-1.916176	C	-0.941493	-1.735468	0.502176
H	1.165112	0.426708	-3.033153	H	-1.221584	-2.038603	1.513334

H	-1.113457	-2.559527	-0.197490	C	-3.863710	1.488255	-0.242722
C	0.518699	-1.376729	0.507363	C	-4.074876	-0.450774	1.322132
C	1.251219	-1.412126	-0.763177	N	-1.295086	0.349545	-1.232873
C	2.337208	-0.523713	1.648627	C	-1.259012	1.007584	1.041488
C	3.100007	-0.491242	0.520589	O	-1.506178	1.068135	2.232284
N	1.064829	-0.971436	1.623622	H	-1.693487	-2.178217	-0.191419
N	2.540505	-0.964044	-0.637820	H	-1.728167	-1.640102	1.507555
O	2.838436	-0.087319	2.832174	H	-3.544514	-0.430586	-2.140354
O	0.793248	-1.782126	-1.854058	H	-4.954851	-2.382350	-2.066107
C	3.446854	-0.832366	-1.783635	H	-5.069510	-2.289732	-0.222832
H	3.136426	0.040245	-2.370066	H	4.923042	-1.406588	0.738770
H	3.362597	-1.717913	-2.414430	H	4.603348	0.311917	0.967682
C	4.486546	0.010250	0.249589	H	3.420569	-2.250093	-1.900433
H	4.468565	1.104704	0.176253	H	2.615223	-0.789299	-2.493390
H	5.184331	-0.257887	1.044893	H	5.282606	-0.690083	-1.575578
C	4.813099	-0.645109	-1.109081	H	4.163310	0.669041	-1.371044
H	5.492158	-0.045455	-1.716519	H	0.706663	1.270969	-2.965619
H	5.274552	-1.622826	-0.944052	H	0.732360	2.987990	1.745073
H	2.115611	-0.119576	3.474475	H	2.433784	2.889205	-2.213571
				H	2.465065	3.759476	0.099846
4-zwi				H	-3.364712	1.887661	-1.130616
				H	-4.944807	1.538932	-0.400946
C	-1.336238	-1.417791	0.510538	H	-3.615659	2.118482	0.617867
C	-3.893996	-0.798396	-1.175570	H	-3.893850	-1.512946	1.510056
C	0.160383	-1.418275	0.537134	H	-3.686126	0.120423	2.167572
C	-4.676001	-1.877158	-1.146982	H	-5.158589	-0.306260	1.271287
C	2.858795	-0.887283	0.639784	H	-1.063919	-0.428472	-1.850676
C	2.146563	-0.805206	1.877173	H	0.226242	-0.904624	2.518848
C	4.297621	-0.570234	0.400777				
N	2.247076	-1.250665	-0.489423	5			
N	0.794232	-1.070241	1.688344				
C	0.897372	-1.573706	-0.659236	C	-0.411447	-0.515789	-1.222099
O	0.457078	-1.872870	-1.793215	C	1.946573	0.122553	0.560443
C	3.156260	-1.218104	-1.648761	C	1.521805	0.997565	-0.644661
C	4.335410	-0.383972	-1.130047	C	0.793766	0.194434	-1.760601
O	2.623233	-0.515228	2.976865	H	1.484592	-0.517555	-2.218204
C	-1.879369	-0.025680	0.065655	C	0.347111	1.383761	1.340269
C	-0.265182	1.246477	-1.027143	C	-0.607453	1.901266	2.202733
C	-0.243317	1.741225	0.284881	C	-1.396664	2.957946	1.733355
C	0.709339	1.654827	-1.950262	C	-1.229176	3.466132	0.443912
C	0.730060	2.646128	0.714310	C	-0.273320	2.921693	-0.424091
C	1.671535	2.557146	-1.513431	C	0.510669	1.885206	0.045614
C	1.692304	3.059045	-0.196971	H	-0.723360	1.498718	3.203674
C	-3.442377	0.028306	0.011952	H	-2.148226	3.393835	2.384801

H	-1.854098	4.285848	0.104562	C	-2.781115	-0.603319	-0.707826
H	-0.169256	3.289466	-1.439968	C	-2.038675	0.040614	-1.635751
N	1.266164	0.335948	1.626344	C	-4.161912	-0.371053	-0.171179
H	0.478674	0.922719	-2.512937	N	-2.197392	-1.661032	-0.037322
C	-1.727428	0.098942	-1.465145	N	-0.717984	-0.238203	-1.803888
C	-2.549666	-1.621626	0.050278	C	-0.901976	-2.086650	-0.219826
N	-2.720774	-0.511025	-0.735857	O	-0.471809	-3.111434	0.306713
N	-0.247957	-1.590681	-0.497970	C	-3.079813	-2.221384	0.980201
C	-1.304316	-2.163329	0.126377	C	-4.096564	-1.088976	1.193825
O	-1.088978	-3.290652	0.856500	O	-2.560245	1.057444	-2.384504
C	-3.858037	-2.004916	0.675181	C	1.718761	-0.083176	0.042458
H	-4.311462	-2.830663	0.113334	C	0.050028	0.979378	1.082053
H	-3.734460	-2.334959	1.708324	C	0.418883	1.908988	0.047938
C	-4.678077	-0.705136	0.530488	C	-1.073871	1.335624	1.909645
H	-4.502343	-0.063765	1.398838	C	-0.288346	3.093495	-0.184497
H	-5.750552	-0.886893	0.448520	C	-1.756150	2.500055	1.649615
C	-4.105111	-0.029335	-0.723430	C	-1.386755	3.396798	0.603149
H	-4.602264	-0.348903	-1.646105	C	3.184194	-0.267398	0.575223
H	-4.100955	1.061330	-0.695411	C	3.243112	-1.472402	1.519142
H	-0.132647	-3.408615	0.928618	C	3.571314	0.992950	1.373102
O	2.592659	1.731476	-1.199525	N	0.755571	-0.135555	1.149679
H	3.155283	1.112561	-1.687640	C	1.521512	1.299889	-0.655904
O	-1.951212	1.050020	-2.212680	O	2.173108	1.716354	-1.614632
C	3.156102	-0.800165	0.571058	H	1.694076	-2.161237	-0.663551
C	2.917080	-1.955906	1.556005	H	1.806750	-0.935379	-1.967701
H	3.809665	-2.586519	1.609237	H	4.104559	0.438666	-1.290341
H	2.682058	-1.565559	2.547729	H	5.629971	-1.402266	-1.691330
H	2.074850	-2.568845	1.220229	H	5.037939	-2.275781	-0.169634
C	4.348306	0.043985	1.061109	H	-4.379103	0.696694	-0.090700
H	4.519845	0.917728	0.426064	H	-3.546539	-3.140703	0.603850
H	5.256597	-0.567059	1.083153	H	-2.486275	-2.473500	1.861363
H	4.138824	0.400564	2.072573	H	-5.067711	-1.458106	1.531678
C	3.398899	-1.402643	-0.797019	H	-3.703756	-0.393965	1.941732
C	4.450256	-1.184753	-1.589237	H	-1.370669	0.666387	2.714124
H	2.629283	-2.105387	-1.120631	H	0.030042	3.753773	-0.990150
H	5.254528	-0.508733	-1.311332	H	-2.616118	2.754479	2.268511
H	4.544420	-1.695064	-2.542650	H	-1.962689	4.301796	0.438160
				H	2.956847	-2.405048	1.023063
5-shift-prod				H	4.260060	-1.589994	1.912444
				H	2.547217	-1.312648	2.344264
C	1.350657	-1.182251	-1.003947	H	3.655223	1.866982	0.719504
C	4.139111	-0.396587	-0.590936	H	2.805029	1.191040	2.130499
C	-0.144951	-1.172070	-1.103066	H	4.535640	0.840415	1.871042
C	4.978257	-1.408876	-0.821920	H	-4.917467	-0.825344	-0.825213

H	-1.817029	1.646459	-2.580513	H	-2.616184	-3.593908	-0.441734
				H	2.709208	2.422172	-0.775481
5-shift-sub				H	4.353160	2.085827	-1.372549
				H	2.928305	1.532403	-2.293362
C	0.909308	-0.404796	1.778343	H	4.200271	-1.624030	-0.729822
C	3.872353	0.490304	0.882223	H	3.922465	-0.792338	-2.283624
C	-0.242638	0.430918	1.382012	H	5.293084	-0.298188	-1.247749
C	4.361703	1.599340	1.439179	H	-3.383918	2.277939	-1.716512
C	-2.319995	1.617325	0.041029	H	0.201379	3.184444	-0.851785
C	-1.063991	2.121718	0.027478				
C	-3.581673	1.982922	-0.683267	5-zwi			
N	-2.556873	0.524523	0.853992				
N	-0.042197	1.525195	0.690454	C	-0.971923	-0.541051	0.669981
C	-1.608667	-0.103153	1.620499	C	2.775328	0.154035	0.100327
O	-1.903268	-1.009980	2.400470	C	1.330304	-0.121266	-0.391732
C	-3.935399	0.055175	0.758457	C	0.507131	-0.706315	0.808756
C	-4.405545	0.682999	-0.561946	H	0.840007	-0.229818	1.737885
O	-0.756171	3.227168	-0.715372	C	1.884440	2.138331	-0.132327
C	1.966864	-0.280837	-0.546855	C	1.752874	3.519300	-0.126659
C	0.063931	-0.975788	-1.336830	C	0.580770	4.061758	-0.663350
C	0.235813	-1.790957	-0.210524	C	-0.415052	3.239321	-1.193465
C	-1.073520	-1.061115	-2.131483	C	-0.274345	1.845294	-1.179670
C	-0.714617	-2.738803	0.120602	C	0.880335	1.308156	-0.635599
C	-2.038429	-2.018049	-1.790253	H	2.544594	4.146551	0.269562
C	-1.857242	-2.854228	-0.684598	H	0.447640	5.138847	-0.680031
C	3.342683	0.361769	-0.530500	H	-1.305897	3.685622	-1.623676
C	3.335768	1.686134	-1.291979	H	-1.044681	1.207633	-1.607864
C	4.258943	-0.662713	-1.249775	N	3.022650	1.398822	0.295945
N	1.162751	-0.096886	-1.538826	H	0.742724	-1.773559	0.866807
C	1.505156	-1.316544	0.517413	C	-1.680531	-1.242592	-0.330424
O	2.397566	-2.180074	0.947388	C	-3.700642	-0.166980	0.524987
H	1.741302	0.200692	2.138293	N	-3.048682	-1.007056	-0.288109
H	0.627513	-1.160110	2.512736	N	-1.637027	0.309109	1.487477
H	3.850128	-0.450869	1.433897	C	-3.002693	0.597631	1.508180
H	4.750198	1.582831	2.453668	O	-3.493193	1.408331	2.296417
H	4.377921	2.556142	0.924195	C	-5.162468	-0.144196	0.220667
H	-4.087325	2.821262	-0.186014	H	-5.759699	-0.140539	1.135069
H	-3.936762	-1.036916	0.766084	H	-5.408347	0.774422	-0.327522
H	-4.509060	0.411313	1.623783	C	-5.338043	-1.410700	-0.643459
H	-4.139406	0.010791	-1.383101	H	-6.107075	-1.299731	-1.408497
H	-5.484183	0.855031	-0.582146	H	-5.611304	-2.256300	-0.006730
H	-1.195234	-0.404435	-2.989282	C	-3.952377	-1.657100	-1.256288
H	-0.585413	-3.354437	1.006492	H	-3.661169	-2.702686	-1.358266
H	-2.933082	-2.122073	-2.400572	H	-3.806396	-1.169269	-2.225373

O	1.317423	-0.978918	-1.493548	C	1.508086	-0.267221	1.432493
H	0.450525	-1.439250	-1.541167	C	0.110190	2.461210	0.493867
O	-1.191783	-1.999382	-1.207544	H	-0.634953	3.256923	0.566460
C	3.841431	-0.913910	0.282460	H	1.097399	2.921889	0.385346
C	5.014869	-0.339514	1.092513	H	0.092417	1.896850	1.430498
H	4.689677	-0.019537	2.086949	C	3.131258	-0.225527	-0.355715
H	5.784764	-1.108939	1.203424	N	2.786109	-0.066894	1.062853
H	5.440774	0.529579	0.587237	N	1.417941	-1.861567	-0.361331
C	4.343401	-1.306619	-1.120448	C	2.692379	-1.628465	-0.796695
H	4.761139	-0.424513	-1.614078	O	3.368461	-2.392769	-1.459096
H	3.538353	-1.700291	-1.742433	C	2.250695	0.773808	-1.143099
H	5.134828	-2.057383	-1.024700	H	2.506731	0.738714	-2.206578
C	3.290861	-2.100747	1.048897	H	2.485186	1.777718	-0.773187
C	3.111778	-3.335599	0.583763	C	4.636420	0.026979	-0.385498
H	3.061920	-1.895299	2.097276	H	5.156394	-0.932324	-0.300889
H	3.315022	-3.596797	-0.449953	H	4.951552	0.494588	-1.320815
H	2.741770	-4.125943	1.229578	C	4.886537	0.910124	0.850282
H	-1.100004	0.847410	2.164047	H	5.921367	0.866702	1.194868
6-RRR				H	4.649741	1.955228	0.624124
C	0.687864	-0.707748	0.191890	C	3.898794	0.372960	1.894725
C	0.766107	0.401357	-0.919531	H	4.315204	-0.475219	2.451390
C	-0.218643	1.574842	-0.721324	H	3.553278	1.120283	2.612739
C	-1.586137	0.960869	-0.497282	H	0.427790	-0.124123	-1.816515
C	-1.769248	-0.570152	-0.402819	O	-1.536285	-1.272463	-1.621078
C	-0.743348	-1.075169	0.604303	H	-2.273659	-1.106666	-2.222093
H	-0.942328	-0.625691	1.582619	O	1.061290	-0.121697	2.560539
C	-3.666135	0.699470	0.100676	H	0.895355	-2.611983	-0.798066
C	-4.975156	0.995060	0.446087	6-RRS			
C	-5.832644	-0.077790	0.716528	C	0.357284	1.843012	-0.318597
C	-5.386401	-1.397985	0.640416	C	1.655621	1.087497	-0.194956
C	-4.059284	-1.684942	0.292381	C	1.737168	-0.214176	0.628973
C	-3.211185	-0.622701	0.034653	C	0.700046	-1.180966	0.062617
H	-5.312663	2.024516	0.502253	H	0.676898	-2.095602	0.664604
H	-6.864339	0.120264	0.989664	C	3.690999	0.365071	-0.510488
H	-6.073440	-2.209812	0.855776	C	4.999660	0.297586	-0.961657
H	-3.709241	-2.711832	0.228913	C	5.784813	-0.770544	-0.512778
N	-2.635028	1.637418	-0.206680	C	5.268648	-1.733337	0.356376
H	-0.842526	-2.160097	0.720082	C	3.941736	-1.658395	0.800917
C	-0.247803	2.438741	-1.992157	C	3.167268	-0.603395	0.351977
H	0.724204	2.918917	-2.147877	H	5.391662	1.051735	-1.635823
H	-0.479307	1.834558	-2.875812	H	6.814937	-0.851645	-0.845145
H	-1.009110	3.217011	-1.894817	H	5.901449	-2.549856	0.688549

H	3.535554	-2.406325	1.476506	H	2.030002	-1.756337	1.619722
N	2.729911	1.369478	-0.837033	H	2.158348	-0.179431	2.416797
H	0.986995	-1.472256	-0.952234	H	0.401361	0.751675	1.238767
C	0.049962	2.528168	1.032546	C	-0.564465	-1.068503	0.756952
H	0.909371	3.144286	1.317405	C	-0.337747	-2.499752	0.248615
H	-0.148505	1.822625	1.837913	H	-1.265517	-3.064104	0.363340
H	-0.807646	3.199838	0.939261	H	0.457394	-3.000346	0.815038
C	0.474602	2.927758	-1.394146	H	-0.084698	-2.535011	-0.812326
H	-0.483949	3.444705	-1.508719	C	-1.219927	-1.150894	2.137567
H	1.233454	3.662904	-1.113956	H	-0.630071	-1.795499	2.802738
H	0.767508	2.501013	-2.356942	H	-2.221468	-1.586394	2.041991
O	1.448068	-0.063446	2.015280	H	-1.312654	-0.162953	2.598407
H	2.155524	0.444793	2.431950	C	0.972882	0.138841	-0.708276
C	-0.716920	0.802555	-0.778054	C	1.877105	1.379556	-0.729509
C	-2.173855	1.339946	-0.748154	C	3.164609	-0.290823	0.499748
H	-2.251788	2.285118	-0.203174	N	2.977641	1.102189	0.035556
H	-2.545233	1.510623	-1.762862	N	1.811351	-0.918313	-1.311152
H	-0.456365	0.555577	-1.816350	C	2.996485	-1.201240	-0.730303
C	-0.687732	-0.558530	-0.009373	O	3.800866	-2.049958	-1.096665
C	-1.640989	-1.514809	-0.768823	C	4.584275	-0.289695	1.047601
C	-3.080490	0.292939	-0.070674	C	5.290305	0.777043	0.195024
N	-2.883407	-0.988156	-0.766389	C	4.219848	1.863865	0.016778
N	-1.292308	-0.381786	1.317356	O	1.690688	2.424784	-1.326198
C	-2.546001	0.139697	1.365109	C	-2.127253	0.946132	0.399133
O	-3.142702	0.475266	2.373754	C	-3.532066	0.720987	0.204251
C	-4.586959	0.509109	-0.143043	C	-1.438833	-0.275000	-0.284355
H	-4.943076	1.055768	0.731938	C	-3.633043	-0.502146	-0.551595
H	-4.831697	1.076517	-1.048024	C	-4.652811	1.464292	0.595299
C	-5.148472	-0.920518	-0.232419	C	-4.961913	-0.944589	-0.889411
H	-6.160562	-0.954767	-0.640303	C	-5.916255	1.014671	0.258371
H	-5.163537	-1.368229	0.766483	H	-4.509256	2.384607	1.158608
C	-4.131990	-1.657272	-1.115951	C	-6.041075	-0.196768	-0.487059
H	-4.047499	-2.726848	-0.909954	H	-5.087465	-1.861629	-1.458699
H	-4.349710	-1.526755	-2.182834	H	-6.805066	1.565835	0.548691
O	-1.309775	-2.576085	-1.271695	H	-7.041069	-0.540452	-0.748674
H	-0.714295	-0.414239	2.149028	N	-2.492966	-1.093858	-0.863047
				O	-1.536253	1.873207	0.962103
6-shift-prod-SSR				H	4.237744	2.586854	0.842222
				H	4.296191	2.418707	-0.922474
C	0.705774	-0.197372	0.784225	H	5.547159	0.344253	-0.777483
C	-0.411479	0.233302	-1.344590	H	6.204560	1.159113	0.656277
H	-0.611931	1.266166	-1.642172	H	4.565369	0.007809	2.102543
H	-0.487575	-0.399980	-2.234216	H	5.037637	-1.278695	0.956376
C	2.008786	-0.673400	1.451434	H	1.507207	-1.429611	-2.128285

				H	-0.291705	2.732411	2.574078
6-shift-sub-SSR				H	1.050222	1.559404	2.802303
				H	1.351627	3.144260	2.028412
C	3.522889	0.512024	-0.527381	C	-0.032160	2.814378	-0.223263
C	3.190745	-0.657758	0.170901	H	-0.437555	2.440248	-1.167550
C	1.595534	0.999764	0.330954	H	-0.755576	3.511700	0.212626
C	1.807026	-0.453185	0.792226	H	0.878577	3.372837	-0.454034
N	2.510751	1.514129	-0.417746	H	-0.406868	0.040944	-2.100049
O	1.636213	-0.694590	2.095298				
C	0.333107	1.694834	0.763779	6-SSR			
C	-0.756411	0.587265	0.993921	C	0.705353	-0.429513	0.322362
H	-0.522640	0.140303	1.963898	C	0.730786	0.742033	-0.716121
C	-0.640530	-0.595220	-0.028984	C	-0.392699	1.793817	-0.515524
C	0.757828	-1.223078	-0.107477	C	-1.698101	1.043317	-0.365852
H	1.070633	-1.277598	-1.159654	C	-1.727897	-0.494265	-0.387714
H	0.716381	-2.240272	0.291045	C	-0.696700	-0.971360	0.634280
C	-2.207813	1.133229	0.966995	H	-0.668352	-2.065750	0.637598
H	-2.701272	0.983151	1.933101	C	-3.755715	0.537370	0.141452
H	-2.246275	2.201120	0.734968	C	-5.096395	0.674596	0.464413
C	-1.725708	-1.653520	0.308219	C	-5.847689	-0.495791	0.624485
O	-1.543616	-2.842045	0.510454	C	-5.268931	-1.755766	0.463931
N	-2.950071	-1.065615	0.285265	C	-3.911086	-1.883154	0.139778
N	-1.072070	-0.065688	-1.344912	C	-3.169137	-0.724914	-0.008940
C	-2.286260	0.521941	-1.428148	H	-5.538116	1.658071	0.585244
O	-2.737045	1.115846	-2.400896	H	-6.901056	-0.422438	0.876218
C	-3.018060	0.354316	-0.083376	H	-5.876681	-2.645451	0.592814
C	-4.514095	0.623553	-0.174336	H	-3.455870	-2.861147	0.008494
C	-4.234086	-1.745560	0.217231	N	-2.815794	1.593315	-0.061339
H	-4.113705	-2.715953	-0.272423	H	-1.023692	-0.621697	1.620208
H	-4.633377	-1.919787	1.225087	C	-0.462741	2.693169	-1.761954
C	-5.095845	-0.744984	-0.568038	H	-0.608632	2.098430	-2.669697
H	-4.954615	-0.898780	-1.643088	H	0.464231	3.266604	-1.869678
H	-6.161131	-0.839648	-0.342699	H	-1.296237	3.394180	-1.668185
H	-4.724822	1.406309	-0.905573	C	1.624485	-1.538715	-0.257772
H	-4.886844	0.933378	0.809218	C	-0.221572	2.681141	0.732132
C	4.722644	0.630274	-1.217118	H	-1.070095	3.366350	0.794170
C	5.609496	-0.453259	-1.182638	H	0.696794	3.272434	0.679506
C	4.072838	-1.722126	0.211484	H	-0.194470	2.090837	1.650966
C	5.292715	-1.613998	-0.472750	C	3.107079	0.362957	-0.019303
H	3.821160	-2.614151	0.780205	N	2.852444	-1.012383	-0.488620
H	6.002621	-2.437008	-0.448360	N	1.381201	0.015914	1.552202
H	6.559802	-0.386515	-1.706262	C	2.678683	0.415917	1.458068
H	4.960452	1.543602	-1.755654	O	3.380207	0.772424	2.387839
C	0.632851	2.325540	2.141684				

C	2.166718	1.318256	-0.773102	C	4.628920	-0.054203	1.088339
H	2.505147	1.401103	-1.810183	H	5.351135	0.519030	0.498869
H	2.235067	2.312795	-0.321343	H	4.687143	0.295930	2.121571
C	4.608183	0.529987	-0.211360	C	4.866313	-1.567856	0.944751
H	5.021864	1.226964	0.519586	H	5.925224	-1.831664	0.970058
H	4.805332	0.904600	-1.222024	H	4.362681	-2.109829	1.752688
C	5.145914	-0.901385	-0.047305	C	4.205719	-1.915818	-0.395012
H	5.204990	-1.144305	1.018327	H	3.841662	-2.943630	-0.461966
H	6.136012	-1.036576	-0.487096	H	4.880598	-1.731551	-1.239784
C	4.078316	-1.772721	-0.724092	O	1.696236	-1.947402	-1.988091
H	3.977224	-2.773137	-0.296351	C	-2.563847	1.099332	-0.647771
H	4.258372	-1.874667	-1.800522	C	-3.749068	0.320139	-0.278682
H	0.525786	0.265315	-1.678497	C	-1.340412	0.198111	-0.369227
O	-1.378405	-1.059455	-1.642425	C	-3.319590	-0.987903	-0.005067
H	-2.114906	-0.931110	-2.253315	C	-5.094214	0.679009	-0.209096
O	1.303525	-2.699671	-0.437832	C	-4.244666	-1.965513	0.381078
H	0.968597	-0.115558	2.466233	C	-6.016661	-0.286470	0.172536
BA				H	-5.392675	1.696566	-0.442758
C	-0.553775	0.651576	0.932436	C	-5.580883	-1.591115	0.465223
C	-0.289429	0.231070	-1.502176	H	-3.932058	-2.981941	0.598013
H	-0.437515	-0.603714	-2.191043	H	-7.070119	-0.041673	0.247922
H	-0.393777	1.167876	-2.059494	H	-6.313290	-2.335453	0.763884
C	-0.397995	2.178731	0.973705	N	-1.963449	-1.118806	-0.216371
H	0.364359	2.462194	1.705406	H	-1.456617	-1.882771	0.206882
H	-1.340441	2.642632	1.276731	O	-2.497455	2.225555	-1.095954
H	-0.125976	2.609178	0.010042	H	1.621461	2.079952	-1.648021
C	-1.209996	0.194460	2.236438	H2O			
H	-2.223690	0.597411	2.331562	O	-0.000000	0.000000	0.115587
H	-0.624702	0.560739	3.086866	H	-0.000000	0.768653	-0.462347
H	-1.269442	-0.894966	2.316630	H	-0.000000	-0.768653	-0.462347
C	0.774705	-0.089950	0.678509	OH			
C	2.049103	0.172054	1.498189	O	0.000000	-0.000000	0.107382
H	2.198777	-0.602076	2.257245	H	-0.000000	0.000000	-0.859054
H	2.033587	1.141099	2.008127	TS23-acid			
H	0.544517	-1.161766	0.769857	C	0.056471	-0.277976	0.863852
C	1.079224	0.139366	-0.830708	C	1.087175	3.125474	-0.924888
C	1.973653	-1.054345	-1.204716	C	-0.673751	-0.623676	-0.419802
C	3.238881	0.155939	0.496525	C	-0.034143	3.655149	-1.415712
N	3.083774	-0.986206	-0.428257				
N	1.881560	1.356464	-0.990879				
C	3.076487	1.426123	-0.345278				
O	3.871363	2.345826	-0.404792				

C	-3.460881	-0.069880	-0.203293	H	0.058969	3.876890	1.504169
C	-2.568409	0.970194	-0.758264	H	1.701887	0.984800	-1.864595
C	-4.759277	0.014632	0.090441	H	1.799614	0.942004	2.840598
N	-2.959805	-1.372612	0.018135				
N	-1.298706	0.526208	-1.041716				
C	-1.669407	-1.742296	-0.037925				
O	-1.246901	-2.852080	0.237166	C	-0.191849	-0.124665	-1.458461
C	-4.053758	-2.269159	0.437802	C	1.029262	2.312237	0.591239
C	-5.271116	-1.318627	0.577972	C	0.265710	-1.466763	-0.851274
O	-2.929363	2.109931	-0.991029	C	2.185779	2.562051	-0.019995
C	1.522409	0.955134	0.230311	C	2.417681	-0.808083	0.877590
C	2.584347	-0.714338	-0.906965	C	1.055066	-0.943346	1.446405
C	2.669724	-1.065387	0.447716	C	3.537831	-0.386940	1.469391
C	3.092281	-1.539255	-1.910764	N	2.650146	-1.245283	-0.438079
C	3.283180	-2.255465	0.853717	N	0.187914	-1.559257	0.606712
C	3.704804	-2.714164	-1.496800	C	1.706253	-1.676248	-1.320236
C	3.804489	-3.070683	-0.136679	O	1.983326	-2.108257	-2.425540
C	1.262048	2.461192	0.436464	C	4.091273	-1.229595	-0.720523
C	2.574811	3.025201	1.035312	C	4.689938	-0.472804	0.493526
C	0.090460	2.793559	1.367686	O	0.760467	-0.585056	2.584597
N	1.934168	0.513059	-1.000769	C	-1.196674	1.389708	0.009558
C	2.007854	-0.010247	1.177794	C	-2.456771	-0.296380	0.858865
O	2.096560	0.086026	2.500912	C	-2.630211	-0.381623	-0.519106
H	-0.459096	0.457128	1.478185	C	-3.050717	-1.169933	1.761249
H	0.255010	-1.182467	1.440111	C	-3.473837	-1.347820	-1.048007
H	2.008016	3.222724	-1.502343	C	-3.883191	-2.149990	1.216664
H	0.012190	-1.105915	-1.125029	C	-4.097167	-2.233799	-0.165988
H	-0.020735	4.151741	-2.380908	C	-0.349724	2.645236	0.041693
H	-0.993094	3.621299	-0.904450	C	-1.032285	3.622475	1.031159
H	-5.348250	0.915699	-0.019204	C	-0.299618	3.307608	-1.339712
H	-0.704852	1.236971	-1.456415	N	-1.564547	0.770169	1.121923
H	-4.201546	-3.035323	-0.326862	C	-1.799852	0.692651	-1.191674
H	-3.773289	-2.765528	1.368626	O	-2.150813	1.269567	-2.266170
H	-6.120973	-1.660256	-0.018747	H	0.608893	0.615638	-1.378323
H	-5.617808	-1.246609	1.613956	H	-0.415352	-0.269690	-2.516488
H	3.020303	-1.276349	-2.960515	H	1.048211	1.847762	1.579883
H	3.347290	-2.519294	1.903800	H	-0.331662	-2.282465	-1.262896
H	4.120309	-3.380300	-2.245493	H	3.124479	2.306206	0.461264
H	4.293008	-4.000153	0.132200	H	2.237534	3.021744	-1.002055
H	2.763152	2.662451	2.050681	H	3.590601	-0.026957	2.488178
H	3.436591	2.761122	0.415173	H	-0.725656	-1.750687	0.999454
H	2.505580	4.114879	1.080589	H	4.456982	-2.258913	-0.788774
H	-0.875065	2.482135	0.959868	H	4.270775	-0.741017	-1.679714
H	0.204946	2.348445	2.362816	H	5.550780	-0.999398	0.913456

TS23-base-acid

H	5.034510	0.530557	0.213561	H	-0.087996	2.455330	-1.533017
H	-2.877049	-1.096887	2.830579	H	0.251205	-1.806947	-0.315124
H	-3.635376	-1.394594	-2.120752	H	-2.139805	3.278143	-0.606240
H	-4.378043	-2.852817	1.878659	H	-1.351661	3.512223	1.062017
H	-4.761830	-2.999733	-0.552282	H	-4.835462	0.937407	-1.177266
H	-2.067020	3.811710	0.731657	H	-0.033796	0.146247	-1.687105
H	-1.028014	3.240111	2.056335	H	-4.362800	-2.671502	0.529280
H	-0.483713	4.567695	1.020929	H	-4.000240	-1.805033	2.030067
H	0.164057	2.668782	-2.093829	H	-6.076056	-1.051928	0.175305
H	-1.308790	3.517070	-1.695261	H	-5.402418	0.046420	1.378515
H	0.267329	4.239933	-1.258018	H	2.703615	-1.285543	-2.975038
H	-1.101482	0.872638	2.023266	H	3.343612	-2.350070	1.877961
				H	3.702582	-3.462568	-2.278923
TS23-base				H	4.020695	-4.003989	0.112594
				H	3.238061	3.306043	0.002930
C	0.169536	-0.178672	1.095905	H	2.322643	3.190232	-1.512477
C	-0.110754	2.751767	-0.483651	H	1.976644	4.512655	-0.360361
C	-0.458397	-1.032816	-0.002185	H	0.398994	2.423263	2.294296
C	-1.255683	3.213804	0.021374	H	2.080355	2.896825	2.208631
C	-3.129495	-0.193227	-0.561436	H	0.806669	4.070576	1.757306
C	-2.031715	0.295693	-1.442284				
C	-4.413813	0.173014	-0.539851	TS23-neutral			
N	-2.864352	-1.211404	0.365006	C	-0.116385	0.045754	-0.949106
N	-0.830488	-0.262260	-1.193752	C	-0.025255	2.850389	0.534123
C	-1.645898	-1.770487	0.607300	C	0.505054	-0.877454	0.087578
O	-1.521430	-2.746861	1.332680	C	1.098102	3.396693	0.069542
C	-4.117801	-1.689761	0.951130	C	3.237804	-0.218097	0.537083
C	-5.144123	-0.605638	0.534451	C	2.206943	0.354060	1.443322
O	-2.253531	1.105244	-2.338618	C	4.541676	0.054268	0.473627
C	1.678049	1.134319	0.098815	N	2.874636	-1.231257	-0.373038
C	2.481999	-0.603904	-0.934566	N	0.967234	-0.178517	1.277171
C	2.656291	-0.924335	0.425794	C	1.616524	-1.637258	-0.646855
C	2.852473	-1.524075	-1.925165	O	1.352831	-2.501015	-1.470337
C	3.214209	-2.133371	0.820516	C	4.070672	-1.760265	-1.043614
C	3.406679	-2.736970	-1.525159	C	5.200484	-0.802453	-0.583473
C	3.588429	-3.046958	-0.165765	O	2.482577	1.186846	2.292537
C	1.200094	2.577435	0.255551	C	-1.572251	1.043744	-0.113751
C	2.254774	3.456853	-0.455450	C	-2.394584	-0.645860	0.984696
C	1.113134	3.018396	1.719601	C	-2.649493	-0.974980	-0.375911
N	1.887169	0.640053	-1.120609	C	-2.770168	-1.564246	1.996667
C	2.166984	0.244253	1.206670	C	-3.270799	-2.184442	-0.745858
O	2.444340	0.516972	2.398760	C	-3.387452	-2.735519	1.618763
H	-0.435531	0.706184	1.307739	C	-3.642063	-3.053121	0.256398
H	0.329519	-0.763442	2.002264				

C	-1.275734	2.540807	-0.267138	H	-2.463519	-0.079442	2.080442
C	-2.463902	3.279012	0.387188	H	-2.963025	-1.766576	1.540165
C	-1.172016	2.990676	-1.727426	C	-4.813319	0.380239	0.291430
N	-1.768269	0.548299	1.140270	C	-4.481263	1.748747	0.923430
C	-2.132295	0.130424	-1.105299	C	-3.316766	2.298237	0.080786
O	-2.347271	0.419320	-2.404769	H	-0.819268	-2.164951	0.544916
H	0.462043	0.964925	-1.056178	H	-3.710578	-2.805099	-1.780852
H	-0.196689	-0.447464	-1.918249	O	-0.659727	1.955963	-0.983024
H	-0.080688	2.577809	1.587967	C	0.300563	-0.466421	1.333410
H	-0.218986	-1.643062	0.388066	C	0.045962	0.899083	1.989322
H	1.939966	3.559185	0.735021	H	0.993479	1.343811	2.299453
H	1.218338	3.690624	-0.969941	H	-0.568533	0.757707	2.883720
H	5.035378	0.789595	1.094058	H	-0.448943	1.613746	1.328569
H	0.222283	0.242405	1.830085	C	0.973807	-1.348766	2.407947
H	4.238303	-2.791424	-0.719636	H	0.354178	-1.347863	3.309558
H	3.907528	-1.767025	-2.122995	H	1.959697	-0.946304	2.669792
H	6.057080	-1.353986	-0.186482	H	1.104728	-2.378412	2.072436
H	5.571683	-0.186148	-1.409947	C	2.451396	-1.293155	0.035636
H	-2.572117	-1.331286	3.037899	C	3.643245	-0.458646	-0.099555
H	-3.457865	-2.435496	-1.787618	C	1.223358	-0.336395	0.028226
H	-3.689004	-3.446796	2.381921	C	3.210303	0.872663	-0.215845
H	-4.127779	-3.991083	0.010851	C	4.992535	-0.804274	-0.178696
H	-3.402875	3.001687	-0.104112	C	4.146510	1.894168	-0.442097
H	-2.538603	3.023244	1.445454	C	5.922122	0.204611	-0.386039
H	-2.320449	4.358850	0.284723	H	5.286625	-1.845723	-0.087356
H	-0.398565	2.460723	-2.291304	C	5.485732	1.536893	-0.520982
H	-2.121462	2.839559	-2.244114	H	3.832138	2.927511	-0.545597
H	-0.934738	4.058016	-1.752117	H	6.979658	-0.024841	-0.453225
H	-2.642269	-0.376548	-2.866954	H	6.223547	2.315572	-0.692647
				N	1.853289	0.978221	-0.059583
TS47-DE-RRR				H	1.310002	1.731454	-0.469115
				O	2.369728	-2.504955	0.075179
C	-1.030374	-0.429784	-1.092486	H	-5.202292	-0.346536	1.008140
C	-0.996055	-1.161548	0.934896	H	-5.549165	0.475437	-0.516213
C	0.429467	-0.709129	-1.263447	H	-4.154501	1.609891	1.957761
H	0.538824	-1.780864	-1.452861	H	-5.336123	2.426333	0.930342
H	0.855428	-0.154467	-2.107150	H	-2.575351	2.864165	0.649489
C	-1.408576	0.976453	-0.864306	H	-3.657229	2.921509	-0.752432
C	-3.489608	-0.041445	-0.279525				
N	-2.699940	1.081936	-0.451131	TS47-DE-RRS			
N	-1.956774	-1.307971	-1.546963				
C	-3.180313	-1.122249	-1.121794	C	0.387056	-1.150960	1.006826
O	-4.138973	-2.051283	-1.350020	C	0.382240	-0.594711	-1.449137
C	-2.264400	-0.940806	1.447908	H	0.784519	0.111269	-2.183783

H	0.415861	-1.604529	-1.864955	N	1.635048	0.839165	0.144735
C	0.027866	-2.622501	0.774799	H	1.056139	1.578661	-0.251409
H	-0.518590	-2.997880	1.646627	O	2.708332	-2.444223	-0.654317
H	0.931260	-3.222351	0.654002				
H	-0.598987	-2.765767	-0.108297	TS47-DE-SSR			
C	1.175053	-1.039282	2.324742	C	-0.873585	0.314869	1.127287
H	2.075713	-1.662511	2.283856	C	0.493856	0.260573	-1.351105
H	0.557764	-1.391850	3.156179	H	0.866917	-0.636689	-1.855705
H	1.473069	-0.006369	2.521442	H	0.617546	1.117908	-2.018783
C	-0.847863	-0.262779	1.108039	C	-2.142774	0.740456	1.497920
C	-2.130450	-0.609844	1.533234	H	-2.401434	1.795661	1.545475
H	-2.658508	0.069046	2.196589	H	-2.755115	0.088342	2.113163
H	-2.425718	-1.653314	1.620461	H	-0.635481	-0.723679	1.352786
H	-0.572439	0.777947	1.289991	C	0.384297	1.174191	1.032904
C	-1.045129	-0.269465	-1.104981	C	0.102303	2.636081	0.665130
C	-1.446796	1.134472	-0.940408	H	1.033969	3.207989	0.704144
C	-3.427282	0.100878	-0.072696	H	-0.582227	3.082299	1.393209
N	-2.731606	1.232637	-0.475142	H	-0.342568	2.738047	-0.327921
N	-1.969927	-1.234852	-1.345575	C	1.091373	1.153384	2.401278
C	-3.152320	-1.057669	-0.826918	H	0.502501	1.718920	3.129478
O	-4.083266	-2.035220	-0.869718	H	2.080099	1.619047	2.316420
C	-4.729485	0.538931	0.537539	H	1.210854	0.134340	2.778159
H	-5.511465	0.532092	-0.231010	C	-0.972490	0.126219	-1.062105
H	-5.050146	-0.124099	1.343900	C	-1.550780	-1.225168	-0.918570
C	-4.406407	1.973296	1.005423	C	-3.457938	0.065789	-0.210664
H	-5.285153	2.619661	1.008364	N	-2.856680	-1.146592	-0.486381
H	-4.006098	1.952012	2.023069	N	-1.761869	1.176014	-1.403933
C	-3.324215	2.473190	0.030364	C	-2.991608	1.155738	-0.961178
H	-2.546334	3.081751	0.498081	O	-3.793397	2.240007	-1.098088
H	-3.741475	3.039836	-0.807626	C	-4.829139	-0.193318	0.346660
H	-3.668333	-2.809034	-1.278739	C	-4.697634	-1.632255	0.889339
O	-0.720639	2.122177	-1.110266	C	-3.626493	-2.291217	0.001144
C	2.587841	-1.269239	-0.366797	H	-3.254822	2.943842	-1.486992
C	3.637787	-0.267580	-0.170326	O	-0.972487	-2.288752	-1.103998
C	1.236598	-0.543416	-0.167072	H	-5.567262	-0.133115	-0.462164
C	3.007966	0.963719	0.056755	H	-5.110022	0.538974	1.106889
C	5.026558	-0.381497	-0.247463	H	-4.352968	-1.608359	1.927057
C	3.776034	2.129808	0.186091	H	-5.642918	-2.176326	0.865212
C	5.790994	0.766947	-0.102139	H	-4.057799	-2.826523	-0.850996
H	5.477582	-1.352681	-0.428476	H	-2.960785	-2.976431	0.531248
C	5.156664	2.007060	0.103926	C	1.934808	-0.818352	0.443644
H	3.304141	3.093191	0.349452	C	3.371668	-0.740478	0.144909
H	6.873034	0.718827	-0.154409	C	1.307835	0.523067	-0.042761
H	5.767878	2.899433	0.204156				

C	3.636795	0.543955	-0.340885	H	-4.952305	-0.876444	1.564673
C	4.375888	-1.696515	0.278516	C	-4.454461	-1.155076	-0.530274
C	4.932653	0.895449	-0.733754	H	-4.173402	-2.184722	-0.295257
C	5.666936	-1.354003	-0.104452	H	-5.016140	-1.162828	-1.469751
H	4.132082	-2.682339	0.662874	H	-1.905079	3.652446	-0.432906
C	5.927763	-0.068633	-0.609268	O	-1.973364	-1.918765	-1.746894
H	5.156231	1.886515	-1.115788	C	2.537433	-1.276901	-0.293367
H	6.474190	-2.073197	-0.021856	C	3.698448	-0.383473	-0.199302
H	6.940488	0.183731	-0.909929	C	1.282281	-0.403786	-0.076928
N	2.498473	1.334782	-0.317473	C	3.219207	0.912741	0.024096
H	2.414964	2.063424	-1.014044	C	5.059662	-0.647526	-0.348020
O	1.337344	-1.732604	0.968167	C	4.109719	1.992123	0.075824
TS47-DE-SSS				C	5.948719	0.416730	-0.283467
C	0.394827	-0.888207	1.124929	H	5.394276	-1.665976	-0.521214
C	0.407087	-0.356530	-1.347238	C	5.463901	1.721428	-0.080878
H	0.881262	0.284936	-2.097123	H	3.754871	3.004306	0.242092
H	0.309195	-1.363956	-1.760260	H	7.014489	0.250849	-0.395086
C	-0.112703	-2.323228	0.959399	H	6.170496	2.545347	-0.041394
H	-0.810338	-2.547196	1.774313	N	1.843803	0.932718	0.201438
H	0.718528	-3.027927	1.022603	H	1.335941	1.719560	-0.188191
H	-0.622738	-2.496988	0.011066	O	2.522399	-2.469569	-0.516676
C	1.201083	-0.799862	2.434020	TS47-RRR			
H	2.062752	-1.476117	2.394865	C	-0.406123	-0.344413	-1.370353
H	0.570405	-1.104796	3.274136	C	0.715074	0.212515	1.232134
H	1.561802	0.215473	2.615183	C	0.987203	0.085465	-1.044598
C	-0.719739	0.144336	1.185594	C	1.986605	0.103438	1.744017
C	-2.013788	0.098193	1.688939	C	3.388359	0.711273	-0.090955
H	-2.368460	0.915775	2.309621	C	2.537346	1.833069	-0.436157
H	-2.518572	-0.856826	1.826818	C	4.779786	0.819347	0.445999
H	-0.293313	1.146884	1.231756	N	3.231321	-0.478628	-0.728001
C	-0.963527	0.153000	-0.987622	N	1.376603	1.416396	-1.056993
C	-2.069953	-0.818249	-1.205976	C	2.012592	-0.925535	-1.183822
C	-3.282059	0.839778	0.012438	O	1.855025	-2.094177	-1.574616
N	-3.245225	-0.349448	-0.699559	C	4.380420	-1.374707	-0.544264
N	-1.239596	1.491175	-0.980647	C	5.214577	-0.657195	0.532172
C	-2.386833	1.828022	-0.453329	O	2.787170	3.008785	-0.167566
O	-2.681984	3.126876	-0.195727	C	-1.294615	-0.421635	-0.091903
C	-4.673882	1.023586	0.551398	C	-3.617881	-0.697113	-0.270165
H	-5.253940	1.641507	-0.144708	C	-3.455960	0.676053	-0.030206
H	-4.681133	1.524226	1.521840	C	-4.898182	-1.228730	-0.472656
C	-5.202563	-0.424946	0.600733	C	-4.545468	1.546030	0.024340
H	-6.285028	-0.479883	0.476866	C	-5.975361	-0.353311	-0.412754

C	-5.816717	1.022383	-0.161482	H	-5.108738	-0.127726	1.262161
C	-0.433145	-0.774459	1.174751	H	-5.566587	0.554360	-0.296365
C	0.015839	-2.237146	1.128717	N	-2.749939	1.209844	-0.475079
C	-1.293465	-0.557592	2.435620	N	-2.004843	-1.177563	-1.361078
N	-2.407454	-1.352266	-0.245063	C	-1.440362	1.129583	-0.904255
C	-2.020875	0.942179	0.043329	O	-0.706147	2.134892	-0.964895
O	-1.455708	2.020624	0.103459	C	-3.327923	2.462699	0.034453
H	-0.876898	0.317545	-2.105727	H	-2.542353	3.040438	0.525541
H	-0.325433	-1.341143	-1.813720	H	-3.699920	3.044870	-0.813817
H	0.354448	1.239179	1.173309	C	-4.449500	1.976423	0.968984
H	2.442687	-0.866426	1.937720	H	-4.078972	1.934245	1.997268
H	2.442963	0.963765	2.224118	H	-5.312127	2.643694	0.952916
H	4.808639	1.348216	1.400957	O	-4.065219	-2.077557	-0.876029
H	5.391765	1.396625	-0.259428	C	1.228157	-0.539727	-0.151960
H	0.636386	2.116200	-1.081093	C	2.988148	0.974920	0.070868
H	4.014452	-2.363350	-0.259406	C	3.626296	-0.246932	-0.187940
H	4.904489	-1.469313	-1.500161	C	3.747921	2.145535	0.211076
H	4.965713	-1.057026	1.519118	C	5.015446	-0.346361	-0.288775
H	6.285601	-0.792652	0.375700	C	5.127729	2.036233	0.106264
H	-5.044162	-2.286744	-0.664312	H	3.270014	3.101278	0.399101
H	-4.380451	2.604134	0.203759	C	5.770721	0.805942	-0.133173
H	-6.976005	-0.747253	-0.564862	H	5.732491	2.932015	0.214370
H	-6.688550	1.665441	-0.121391	C	0.402936	-1.174125	1.023805
H	-0.852905	-2.894279	1.232771	C	1.228203	-1.080507	2.322656
H	0.547721	-2.492476	0.208657	H	2.129891	-1.698935	2.247031
H	0.678854	-2.442231	1.975586	H	1.526367	-0.049678	2.527849
H	-1.539146	0.498986	2.584127	H	0.634281	-1.448756	3.163639
H	-2.224905	-1.129208	2.359712	C	0.061636	-2.650252	0.788533
H	-0.744463	-0.901280	3.316739	H	-0.621202	-2.810950	-0.048318
H	-2.276043	-2.226572	-0.732576	H	0.966100	-3.230094	0.599835
				H	-0.426177	-3.050692	1.682309
TS47-RRS				H	5.472889	-1.309544	-0.494326
				H	6.852157	0.769383	-0.202501
C	0.383228	-0.580237	-1.445949	N	1.619506	0.836749	0.175018
H	0.443065	-1.589757	-1.866530	H	1.014780	1.583599	-0.168563
H	0.803787	0.125416	-2.170597	C	2.583899	-1.251435	-0.389112
C	-0.842635	-0.312574	1.198081	O	2.699817	-2.417138	-0.715714
C	-1.036812	-0.231396	-1.128695	H	-0.595652	0.732051	1.398024
C	-2.105428	-0.724345	1.574668	H	-1.728754	-2.080583	-1.732050
H	-2.722172	-0.069313	2.181888				
H	-2.388167	-1.774063	1.581691	TS47-SSR			
C	-3.493092	0.118817	-0.140348				
C	-3.273017	-1.138742	-0.813134	C	-0.499785	-0.284093	-1.344639
C	-4.784831	0.555473	0.474039	H	-0.914977	0.598790	-1.842782

H	-0.633985	-1.141471	-2.015208	H	-2.440497	-2.065031	-1.026680
C	0.877928	-0.445461	1.226495	C	-1.895067	0.777292	0.498158
C	0.955627	-0.083474	-1.091070	O	-1.288715	1.642158	1.087260
C	2.130017	-0.934678	1.505052	H	1.453984	-1.935681	-1.864554
H	2.385341	-1.986702	1.409575				
H	2.828832	-0.329074	2.073159	TS47-SSS			
C	3.519877	0.000223	-0.308181				
C	3.126108	-1.193625	-1.006620	C	0.317150	-0.497221	-1.408974
C	4.874895	0.283630	0.255634	C	-0.670630	0.391588	1.140491
H	5.609526	0.287326	-0.560080	C	-1.059973	-0.011643	-1.089634
H	5.186001	-0.487069	0.964507	C	-1.914122	0.378342	1.727531
N	2.832126	1.155601	-0.471147	C	-3.385329	0.821140	-0.088366
N	1.823428	-1.085635	-1.453756	C	-2.525263	1.857039	-0.622420
C	1.494801	1.232184	-0.851252	C	-4.741729	1.045485	0.501509
O	0.884365	2.300694	-0.883095	N	-3.302441	-0.443015	-0.583639
C	3.546961	2.320416	0.068622	N	-1.427971	1.315302	-1.260513
H	3.907133	2.927596	-0.767698	C	-2.128011	-0.993190	-1.051371
H	2.847564	2.924282	0.650252	O	-2.038223	-2.198719	-1.312607
C	4.684376	1.679735	0.882428	C	-4.466152	-1.266136	-0.229808
H	5.593736	2.281624	0.859429	C	-5.214546	-0.392714	0.793056
H	4.375758	1.578237	1.926926	O	-2.706810	3.070062	-0.492209
O	3.820141	-2.198136	-1.191432	C	1.266723	-0.327135	-0.196946
C	-1.296269	-0.568223	-0.024774	C	3.268443	0.900153	-0.125491
C	-3.620100	-0.509423	-0.361613	C	3.688890	-0.426340	-0.263120
C	-3.323981	0.756130	0.152424	C	4.206862	1.924400	0.038353
C	-4.915920	-0.812954	-0.789220	C	5.039936	-0.770845	-0.270221
C	-4.299266	1.742138	0.281295	C	5.551971	1.571639	0.044174
C	-5.882117	0.181566	-0.671132	C	5.977873	0.241140	-0.114499
H	-5.163058	-1.790252	-1.191647	C	0.477411	-0.606092	1.136332
C	-5.591072	1.448644	-0.138576	C	1.371808	-0.307765	2.357622
H	-6.895176	-0.032390	-0.998815	C	0.002515	-2.059074	1.237056
C	-0.393479	-1.267320	1.037761	N	1.884463	1.014376	-0.206762
H	0.669958	0.586035	1.506259	C	2.488616	-1.263480	-0.365521
C	-0.125670	-2.723222	0.636149	O	2.413944	-2.456791	-0.565878
H	-1.069853	-3.273769	0.596524	H	0.241273	-1.560843	-1.654225
H	0.376984	-2.829044	-0.328351	H	0.751353	0.028547	-2.265934
H	0.505586	-3.210346	1.383936	H	-0.327014	1.412846	0.957747
C	-1.138440	-1.292391	2.388624	H	-2.324312	1.296302	2.137181
H	-1.256019	-0.287351	2.800892	H	-2.377864	-0.553683	2.046210
H	-2.129133	-1.742947	2.260404	H	-5.374555	1.552060	-0.238838
H	-0.572544	-1.890407	3.108285	H	-4.703639	1.688595	1.383316
H	-4.033149	2.712025	0.690353	H	-0.711978	1.983691	-1.530385
H	-6.376069	2.192653	-0.062046	H	-5.047144	-1.456482	-1.137276
N	-2.506816	-1.339583	-0.324797	H	-4.114940	-2.226376	0.154103

H	-6.296367	-0.506181	0.712274	H	-0.767200	1.024710	2.450444
H	-4.921890	-0.678411	1.807303	H	-3.931672	0.575877	1.441307
H	3.897439	2.958936	0.149245	H	-4.930425	-1.324680	2.591892
H	5.330301	-1.810685	-0.386130	H	-4.619978	-2.420271	1.132465
H	6.296914	2.351700	0.170556	H	4.375964	-2.555300	0.010656
H	7.037728	0.012305	-0.110432	H	3.892545	1.311556	0.884112
H	2.262674	-0.944974	2.348836	H	4.481773	-0.068156	1.834085
H	1.699530	0.735324	2.400646	H	4.392504	0.242345	-1.200856
H	0.810567	-0.518217	3.271983	H	5.680717	-0.518535	-0.244803
H	-0.562526	-2.390983	0.365100	H	1.173226	-0.082529	-2.845606
H	0.855960	-2.729651	1.357094	H	0.482687	3.437123	0.650664
H	-0.633033	-2.161758	2.123245	H	2.904197	1.697819	-2.473573
H	1.467212	1.739116	0.361819	H	2.558810	3.436999	-0.753061
				H	-2.846725	-2.466713	-0.549673
TS54-base				H	-4.504131	-2.177407	-1.148224
				H	-3.090459	-1.714423	-2.131307
C	-0.913762	0.210731	1.747285	H	-4.337596	1.575639	-0.842465
C	-4.004605	-0.393256	0.947071	H	-4.031542	0.623688	-2.317119
C	0.278663	-0.467132	1.336166	H	-5.414716	0.212804	-1.263902
C	-4.550628	-1.432736	1.579943	H	3.773202	-2.049042	-1.573137
C	2.523671	-1.460845	0.088576	H	0.180972	-3.244136	-0.887608
C	1.314112	-2.063958	0.009844				
C	3.860981	-1.746827	-0.526182	TS54-neu			
N	2.618960	-0.340446	0.903861	C	-1.304255	2.559938	1.980343
N	0.213219	-1.587115	0.634370	C	-0.597851	1.367917	2.166037
C	1.579050	0.217654	1.591553	C	0.383937	1.087915	1.228800
O	1.741310	1.179918	2.346608	C	0.664016	1.892984	0.129948
C	3.963600	0.221852	0.910645	C	-0.043154	3.070293	-0.042671
C	4.598490	-0.402423	-0.342095	C	-1.021344	3.402076	0.899763
O	1.138890	-3.182358	-0.760515	H	-2.075170	2.838681	2.691648
C	-2.087645	0.220084	-0.543350	H	-0.801706	0.707907	3.004366
C	-0.133052	0.742085	-1.344112	H	0.155386	3.701161	-0.903180
C	-0.324309	1.721479	-0.356404	H	-1.584635	4.322481	0.784843
C	1.031524	0.698369	-2.102926	C	1.664840	1.168417	-0.786953
C	0.629048	2.698925	-0.132352	C	2.023887	-0.023982	0.120495
C	1.993742	1.689019	-1.878619	N	1.261808	-0.031652	1.180341
C	1.795098	2.679124	-0.909123	H	1.252718	-0.780678	1.865482
C	-3.474960	-0.392331	-0.472599	O	2.614780	1.780885	-1.410749
C	-3.484071	-1.778330	-1.114750	C	3.155317	-0.987714	-0.071341
C	-4.379810	0.573572	-1.280216	C	2.978619	-2.244157	0.782513
N	-1.228778	-0.146934	-1.441416	H	2.040610	-2.744987	0.519592
C	-1.638797	1.396339	0.313819	H	3.803099	-2.935800	0.590237
O	-2.422471	2.233298	0.848581	H	2.986168	-2.028567	1.857643
H	-1.765838	-0.431144	1.947567				

C	3.313198	-1.376590	-1.554317	C	-3.100328	0.608185	-0.047304
H	3.402066	-0.479447	-2.172254	H	-4.688057	-2.256895	-0.995235
H	4.225031	-1.971984	-1.652355	H	-6.429095	-0.555946	-1.586490
H	2.461333	-1.979497	-1.882582	H	-6.028765	1.842238	-1.182183
C	4.366271	-0.136449	0.313373	H	-3.868752	2.617157	-0.195448
H	4.453885	0.777090	-0.275573	N	-2.244715	-1.560090	0.170735
C	5.251925	-0.451852	1.256634	H	-0.889038	2.591350	-0.110639
H	6.103327	0.193909	1.445229	C	-0.519037	-1.694416	2.730001
H	5.176770	-1.353027	1.858497	H	0.344994	-2.090427	3.272784
C	0.609302	0.418338	-1.880280	H	-1.292611	-2.465423	2.668273
H	0.291474	1.278736	-2.469487	H	-0.910765	-0.839514	3.289435
H	1.236243	-0.239960	-2.476691	C	0.450610	-2.520367	0.581995
C	-0.545027	-0.295028	-1.289571	H	-0.361191	-3.242382	0.472679
C	-1.850758	0.409077	-1.257305	H	1.251419	-2.984581	1.166095
C	-1.358200	-2.057824	-0.027996	H	0.813213	-2.283859	-0.420513
C	-2.585430	-1.488150	0.089969	C	2.315649	-0.380683	1.546429
N	-0.358583	-1.458232	-0.720190	H	2.929082	0.239842	2.193212
N	-2.804288	-0.290398	-0.557280	H	2.715138	-1.370616	1.341622
O	-0.988280	-3.232604	0.572931	H	0.560469	0.694588	2.023123
O	-2.096172	1.486730	-1.790664	O	-1.669173	1.353227	1.808211
C	-4.155396	0.225036	-0.337296	H	-2.413014	1.023379	2.328566
H	-4.532982	0.661097	-1.263188	C	0.679642	1.168010	-0.349870
H	-4.114385	1.015076	0.421876	C	1.057217	0.082976	-1.280168
C	-3.835501	-1.884954	0.828617	C	3.209435	0.425876	-0.290508
H	-4.055303	-2.954678	0.761054	N	2.396311	-0.190637	-1.224378
H	-3.744731	-1.627046	1.891668	N	1.579733	2.106504	0.025587
C	-4.913366	-1.021487	0.138066	C	2.831546	1.731495	0.071376
H	-5.310472	-1.558656	-0.727790	O	3.770525	2.535683	0.623862
H	-5.744670	-0.775901	0.800281	C	4.590253	-0.161695	-0.395529
H	-1.765424	-3.686860	0.917472	H	5.213412	0.481969	-1.027850
TS56-DE-RRR				H	5.078185	-0.241773	0.578528
C	0.945832	-0.159841	1.472924	C	4.318134	-1.524308	-1.066267
C	-0.082966	-1.275123	1.300428	H	5.162152	-1.876082	-1.661240
C	-1.338333	-0.768806	0.612838	H	4.106615	-2.279439	-0.303256
C	-1.707977	0.728841	0.526618	C	3.062656	-1.290045	-1.922948
C	-0.777822	1.541650	-0.395081	H	2.392191	-2.149529	-1.986971
H	-1.119960	1.401664	-1.425125	H	3.305837	-0.971604	-2.942355
C	-3.333889	-0.753158	-0.266803	H	3.309414	3.313710	0.969718
C	-4.522092	-1.198617	-0.823763	O	0.276709	-0.525798	-2.011955
C	-5.486943	-0.238468	-1.150516	TS56-DE-RRS			
C	-5.261197	1.119894	-0.923653	C	0.359671	1.872939	-0.492033
C	-4.051169	1.559739	-0.368747	C	1.607120	1.030726	-0.306213

C	1.718606	-0.154204	0.684374	H	-3.803961	-0.959792	-2.355835
C	0.753713	-1.262145	0.230568	H	-3.976589	-2.562919	-1.620752
H	0.987800	-1.568568	-0.792799	H	-2.164991	0.947631	3.125077
C	3.633441	0.261327	-0.593229	O	-1.239089	-2.329765	-1.536605
C	4.922418	0.122062	-1.083713				
C	5.730440	-0.863590	-0.506244	TS56-DE-SSR			
C	5.253813	-1.673235	0.526586				
C	3.945810	-1.525732	1.007436	C	0.675135	-0.602450	0.724516
C	3.149598	-0.555433	0.428951	C	0.867351	0.813208	-1.076116
H	5.283294	0.763080	-1.881237	C	-0.338372	1.724635	-0.852883
H	6.747041	-0.997698	-0.862620	C	-1.581098	0.951535	-0.449319
H	5.905599	-2.423507	0.962748	C	-1.654375	-0.583216	-0.336725
H	3.573784	-2.146124	1.818015	C	-0.775187	-0.987625	0.864375
N	2.661112	1.212904	-1.016251	H	-1.167262	-0.507457	1.764294
H	0.907417	-2.140054	0.873295	C	-3.641084	0.550092	0.152416
C	0.040982	2.634154	0.810429	C	-4.963649	0.757284	0.512656
H	-0.686089	3.427675	0.613390	C	-5.762558	-0.372606	0.721596
H	0.952228	3.100846	1.193965	C	-5.244331	-1.660221	0.572036
H	-0.356963	1.984743	1.590954	C	-3.902419	-1.855137	0.217169
C	0.622285	2.914138	-1.598022	C	-3.115972	-0.736896	0.015140
H	1.464886	3.553510	-1.321212	H	-5.356896	1.763015	0.618390
H	-0.272260	3.528875	-1.733068	H	-6.804833	-0.246396	0.997819
H	0.872591	2.430720	-2.544993	H	-5.889238	-2.518880	0.729715
O	1.538429	0.184635	2.042394	H	-3.497985	-2.855930	0.091157
H	0.590762	0.106973	2.239218	N	-2.670296	1.552599	-0.134959
C	-0.809112	1.005475	-0.986074	H	-0.854251	-2.076589	0.984910
C	-2.129256	1.416503	-0.832836	C	-0.656191	2.367287	-2.227211
H	-2.842911	1.189647	-1.619817	H	0.203254	2.952051	-2.569726
H	-2.373302	2.283914	-0.224573	H	-1.526923	3.021247	-2.128729
H	-0.567657	0.428830	-1.880484	H	-0.879889	1.598450	-2.972959
C	-0.692852	-0.852351	0.288059	C	1.519447	-1.525427	-0.044856
C	-1.593224	-1.548125	-0.659212	C	-0.079769	2.841776	0.168490
C	-3.227261	-0.104644	0.340436	H	-0.997854	3.417565	0.300974
N	-2.899491	-1.177259	-0.475272	H	0.704095	3.518205	-0.185287
N	-1.165264	-0.341427	1.453786	H	0.211459	2.429071	1.138672
C	-2.408481	0.073897	1.465166	C	3.214331	0.071074	0.476868
O	-2.890490	0.792647	2.503999	N	2.836686	-1.178571	-0.003901
C	-4.698201	0.196634	0.194874	N	1.193013	0.199738	1.687366
H	-5.186789	0.268496	1.168830	C	2.442075	0.553344	1.552401
H	-4.838257	1.155853	-0.314981	O	2.980435	1.499573	2.352680
C	-5.213743	-0.985375	-0.659673	C	2.184526	1.261815	-0.976237
H	-5.589211	-1.776577	-0.005304	H	2.903605	0.889500	-1.701458
H	-6.017211	-0.694391	-1.337764	H	2.410984	2.247896	-0.578297
C	-3.974851	-1.493156	-1.410329	C	4.695250	0.257959	0.244524

H	5.205894	0.527652	1.171517	N	2.748045	-0.665410	-0.728623
H	4.868665	1.067184	-0.471878	N	1.276229	-1.473659	1.416313
C	5.144091	-1.114005	-0.314286	C	2.534435	-1.157012	1.558993
H	5.533432	-1.733170	0.498091	O	3.169815	-1.349764	2.737529
H	5.921156	-1.023620	-1.074599	C	4.666874	-0.063382	0.474315
C	3.863012	-1.752660	-0.868916	H	5.287058	-0.951054	0.646243
H	3.661696	-1.464534	-1.910054	H	4.936788	0.679202	1.228398
H	3.832475	-2.840527	-0.805472	C	4.797902	0.453534	-0.974075
H	0.677639	0.028981	-1.805811	H	5.794948	0.293578	-1.386322
H	2.274033	1.824336	2.930102	H	4.591023	1.526751	-1.005562
O	-1.292408	-1.246197	-1.524263	C	3.719132	-0.307544	-1.765330
H	-0.590810	-1.897707	-1.339029	H	3.222451	0.284908	-2.537042
O	1.099531	-2.490291	-0.700381	H	4.099082	-1.223121	-2.229120
TS56-DE-SSS				H	2.517235	-1.694514	3.364431
C	0.661951	-1.076324	0.272426	O	-1.536675	-0.420777	-2.016704
C	-0.214505	1.866689	-0.054919	H	-0.634091	-0.737706	-2.227595
C	-1.516088	1.083462	-0.048081	O	1.023168	-1.145672	-2.121164
C	-1.689994	-0.348949	-0.623381	C	0.748629	1.146367	0.892797
C	-0.816151	-1.364454	0.157527	C	2.104707	1.414395	0.998202
H	-1.201139	-1.444568	1.178276	H	2.573941	1.449367	1.977019
C	-3.586433	0.554656	0.423415	H	2.599847	1.993577	0.220981
C	-4.884132	0.650697	0.901595	H	0.257194	0.823490	1.810988
C	-5.744187	-0.425831	0.657509	TS56-RRR			
C	-5.308886	-1.549816	-0.047137	C	3.113844	-0.619581	-0.016317
C	-3.992617	-1.633238	-0.521275	C	3.389412	0.722383	-0.294468
C	-3.143830	-0.572853	-0.266129	C	4.605225	1.109256	-0.835460
H	-5.212644	1.535797	1.436432	C	5.553224	0.109609	-1.083230
H	-6.768821	-0.383356	1.013702	C	5.284722	-1.229700	-0.797097
H	-6.000368	-2.365368	-0.234050	C	4.046492	-1.610934	-0.261586
H	-3.654528	-2.498099	-1.085409	C	1.696085	-0.677611	0.499334
N	-2.564627	1.540893	0.534746	C	1.369988	0.838142	0.535451
H	-0.958461	-2.341602	-0.326694	N	2.312265	1.576099	0.074667
C	0.337132	2.057762	-1.476577	C	0.798753	-1.450846	-0.487928
H	1.232507	2.688491	-1.443502	C	0.131107	1.442273	1.179636
H	-0.408572	2.572632	-2.088751	C	0.604394	1.995378	2.551793
H	0.583107	1.122721	-1.978170	C	-0.393402	2.614087	0.341082
C	1.448489	-0.977984	-0.964443	C	-0.920604	0.388356	1.487414
C	-0.463373	3.260761	0.555086	C	-0.661626	-1.138314	-0.395292
H	-1.227648	3.792197	-0.018509	C	-2.273782	0.604535	1.563528
H	0.470197	3.831004	0.535005	C	-3.272232	-0.533987	-0.234572
H	-0.815997	3.186744	1.585976	C	-2.871175	-1.774352	0.388990
C	3.215761	-0.448294	0.550969	C	-4.675026	-0.019682	-0.307561

N	-2.524376	0.016143	-1.222889	C	0.326983	1.898882	-0.443730
N	-1.533704	-2.036212	0.167957	C	0.022868	2.600018	0.897358
C	-1.159793	-0.165143	-1.333306	C	0.615866	2.992527	-1.493453
O	-0.470136	0.484753	-2.132122	C	-0.868680	1.102318	-0.980484
C	-3.248964	1.049281	-1.975209	C	-0.699322	-0.945495	0.318703
C	-4.510544	1.277705	-1.124750	C	-2.165179	1.491938	-0.741628
O	-3.597348	-2.494057	1.077777	C	-3.283426	-0.236083	0.441655
O	1.556150	-1.318619	1.761054	C	-2.488463	0.077707	1.599897
H	4.805263	2.153153	-1.052315	C	-4.747119	0.032715	0.299932
H	6.516837	0.380957	-1.502888	N	-2.901338	-1.214437	-0.421185
H	6.040940	-1.982769	-0.993397	N	-1.215713	-0.441018	1.481201
H	3.831840	-2.653695	-0.042041	C	-1.584060	-1.568970	-0.637073
H	1.114675	-1.192909	-1.503239	O	-1.243686	-2.286475	-1.586318
H	0.989588	-2.516175	-0.313863	C	-3.968420	-1.598129	-1.354494
H	1.394107	2.735919	2.397700	C	-5.070007	-0.553920	-1.090595
H	-0.240620	2.462394	3.066395	O	-2.856315	0.747859	2.569423
H	0.990243	1.194060	3.190983	O	1.448014	0.120122	2.020047
H	0.423939	3.313167	0.152006	H	5.243640	0.844124	-1.899952
H	-0.769240	2.275736	-0.627352	H	6.732288	-0.926586	-0.937067
H	-1.182983	3.142404	0.884513	H	5.915704	-2.419901	0.844291
H	-0.532666	-0.462796	2.041026	H	3.583687	-2.204981	1.710774
H	-2.888962	-0.001184	2.222287	H	0.959237	-1.633241	-0.766614
H	-2.707724	1.543066	1.226561	H	0.954276	-2.166204	0.915153
H	-5.303394	-0.760957	-0.817736	H	0.942675	3.032226	1.305045
H	-5.101157	0.131694	0.686911	H	-0.673722	3.425984	0.730396
H	-2.607909	1.925599	-2.088151	H	-0.414461	1.941214	1.648632
H	-3.469666	0.659831	-2.973956	H	1.471569	3.599902	-1.185585
H	-4.350729	2.123577	-0.450201	H	0.852273	2.555678	-2.466221
H	-5.382289	1.501666	-1.740875	H	-0.266700	3.629708	-1.591800
H	2.260627	-1.010538	2.345442	H	-0.655380	0.535082	-1.887489
H	-1.155926	-2.816158	0.697659	H	-2.402240	2.276955	-0.028693
				H	-2.934905	1.261709	-1.470983
TS56-RRS				H	-5.286109	-0.476922	1.108509
				H	-4.968110	1.098801	0.392629
C	3.138634	-0.563772	0.382337	H	-3.566102	-1.589733	-2.369970
C	3.606393	0.288184	-0.618856	H	-4.280684	-2.621109	-1.124910
C	4.894615	0.178296	-1.117844	H	-5.024729	0.233075	-1.848076
C	5.716305	-0.814505	-0.571914	H	-6.065890	-0.996548	-1.135746
C	5.254696	-1.661927	0.436888	H	2.112025	0.742579	2.342202
C	3.946500	-1.546124	0.926281	H	-0.555507	-0.175905	2.209765
C	1.704525	-0.179851	0.651617				
C	1.565751	1.030549	-0.307609	TS56-SSR			
N	2.621674	1.240101	-1.008838				
C	0.749988	-1.309438	0.256720	C	-3.582489	0.563205	0.204265

C	-3.099744	-0.723711	-0.044087	H	3.485160	-2.122914	-1.657474
C	-1.522595	0.953996	-0.416208	H	5.011408	-0.287900	-1.669891
C	-1.633228	-0.584355	-0.378912	H	6.002035	-1.278911	-0.603187
N	-2.589902	1.556993	-0.033114	H	5.217464	-0.096295	1.369239
O	-1.249977	-1.221129	-1.567650	H	4.960843	1.205715	0.212861
C	-0.301291	1.731549	-0.878291				
C	0.925828	0.861321	-1.131987	TS56-SSS			
H	0.766802	0.068350	-1.859561				
C	0.645005	-0.694022	0.747234	C	-3.576172	0.559325	0.389635
C	-0.803431	-1.061321	0.838532	C	-3.129203	-0.600323	-0.240322
H	-1.246125	-0.635600	1.744812	C	-1.510226	1.081379	-0.122551
H	-0.894494	-2.153922	0.893947	C	-1.675304	-0.390158	-0.606194
C	2.216117	1.313631	-0.945395	N	-2.563264	1.558784	0.436252
H	3.003438	0.927772	-1.585891	O	-1.503753	-0.567948	-1.982548
H	2.422862	2.266246	-0.465572	C	-0.231317	1.901777	-0.204491
C	1.511297	-1.552754	-0.001821	C	0.757050	1.320849	0.803399
O	1.126508	-2.487105	-0.737475	H	0.281307	1.041660	1.745565
N	2.835078	-1.200918	0.107125	C	0.657108	-1.080037	0.329571
N	1.171664	0.141121	1.699881	C	-0.817413	-1.362478	0.255593
C	2.457334	0.640380	1.662298	H	-1.226024	-1.349618	1.272612
O	2.853453	1.542308	2.399121	H	-0.983633	-2.369056	-0.155210
C	3.231314	-0.005207	0.624714	C	2.104844	1.571985	0.861253
C	4.705229	0.167251	0.435631	H	2.614169	2.039819	0.020708
C	3.889376	-1.860106	-0.677437	H	2.611554	1.615006	1.820838
C	5.021223	-0.814669	-0.712261	C	1.450982	-1.073466	-0.861702
C	-4.892116	0.779003	0.604631	O	1.045362	-1.251790	-2.034181
C	-5.720812	-0.340958	0.737422	N	2.771426	-0.785683	-0.621777
C	-3.913849	-1.832724	0.086135	N	1.305771	-1.330620	1.522884
C	-5.244193	-1.627112	0.476951	C	2.604115	-0.951018	1.790951
H	-3.540217	-2.831027	-0.125122	O	3.103753	-0.979979	2.914619
H	-5.913113	-2.476097	0.574996	C	3.260795	-0.461967	0.597171
H	-6.754705	-0.207252	1.039968	C	4.705004	-0.089642	0.489209
H	-5.254077	1.784006	0.794909	C	3.731290	-0.532173	-1.707607
H	-0.513371	-1.841686	-1.399025	H	4.068484	-1.495501	-2.101221
C	-0.698076	2.308897	-2.265177	H	3.221370	0.003052	-2.510974
H	-0.963115	1.504815	-2.958293	C	4.845744	0.263435	-1.005520
H	-1.561596	2.969271	-2.147427	H	5.831163	0.019977	-1.404189
H	0.141093	2.873748	-2.681933	H	4.681043	1.334461	-1.150731
C	-0.020926	2.901781	0.075996	H	5.318199	-0.952685	0.778237
H	0.657734	3.619860	-0.393042	H	4.964430	0.728254	1.165076
H	-0.958866	3.410412	0.304807	C	-4.872681	0.672310	0.867274
H	0.437837	2.575534	1.015391	C	-5.725804	-0.421767	0.684700
H	0.542752	0.614159	2.341574	C	-3.970638	-1.679354	-0.435022
H	4.172668	-2.785694	-0.168694	C	-5.285844	-1.578860	0.038930

H	-3.629615	-2.569800	-0.956018	C	-5.075943	-0.842698	-0.632130
H	-5.973126	-2.406774	-0.103206	H	-4.905871	-0.971331	-1.706306
H	-6.749548	-0.366908	1.041498	H	-6.143004	-0.970921	-0.433531
H	-5.205780	1.583131	1.353763	H	-4.756475	1.325349	-0.915796
H	-0.581294	-0.857901	-2.165024	H	-4.945812	0.810255	0.783625
C	0.322466	1.968741	-1.636209	C	4.338521	0.357748	-1.721687
H	-0.446866	2.358831	-2.308307	C	5.376341	-0.550214	-1.542327
H	1.173002	2.658211	-1.667205	C	4.390836	-1.385946	0.513309
H	0.640167	1.000941	-2.023547	C	5.412701	-1.418012	-0.434136
C	-0.529967	3.340460	0.266469	H	4.396789	-2.042041	1.380506
H	-1.305170	3.788138	-0.361341	H	6.241130	-2.112336	-0.322868
H	-0.888611	3.357315	1.297589	H	6.181313	-0.590478	-2.272730
H	0.386030	3.933969	0.195413	H	4.312641	1.028219	-2.576765
H	0.749381	-1.548275	2.343829	C	0.622058	2.311925	2.149847
				H	-0.280772	2.778483	2.566749
TS67-base-SSR				H	1.018011	1.577372	2.855438
				H	1.368780	3.098722	1.996422
C	3.313053	0.405247	-0.763047	C	-0.080503	2.753192	-0.188997
C	3.343797	-0.489195	0.332462	H	-0.462140	2.397501	-1.147014
C	1.512791	0.883112	0.329294	H	-0.819759	3.432062	0.250268
C	2.154517	-0.172683	1.163945	H	0.824254	3.327135	-0.401426
N	2.202631	1.233345	-0.760967	H	-0.331104	0.218154	-1.978277
O	1.943982	-0.477156	2.367294				
C	0.285701	1.636819	0.803285	TS67-neu-RRR			
C	-0.820632	0.565657	1.058378	C	0.598679	0.820704	-0.306465
H	-0.593923	0.113261	2.030671	C	0.875353	0.358467	1.165630
C	-0.649685	-0.573406	0.003414	C	-0.034542	-0.861891	1.530533
C	0.770913	-1.073575	-0.016176	C	-1.332648	-0.572409	0.854577
H	1.158344	-1.256698	-1.020052	C	-1.897689	0.823955	0.772822
H	0.869888	-1.951139	0.621641	C	-0.868336	1.135875	-0.565705
C	-2.281647	1.077560	1.021647	H	-1.197171	0.654750	-1.489309
H	-2.795230	0.885010	1.969399	C	-3.266411	-0.795718	-0.295208
H	-2.339323	2.151067	0.819816	C	-4.311313	-1.354868	-1.014360
C	-1.696960	-1.676939	0.295843	C	-5.372124	-0.503524	-1.329249
O	-1.474503	-2.856797	0.510276	C	-5.364873	0.839140	-0.932763
N	-2.937683	-1.125905	0.246427	C	-4.286703	1.377671	-0.225495
N	-1.052593	-0.023335	-1.306918	C	-3.224208	0.543819	0.083296
C	-2.275895	0.547494	-1.392827	H	-4.313630	-2.398328	-1.313597
O	-2.712276	1.189084	-2.340383	H	-6.219314	-0.894157	-1.883113
C	-3.040072	0.304243	-0.077453	H	-6.214213	1.467916	-1.180211
C	-4.541196	0.532407	-0.196955	H	-4.268093	2.415930	0.091377
C	-4.204148	-1.834657	0.152415	N	-2.085394	-1.423127	0.191789
H	-4.054610	-2.795418	-0.347736	H	-1.049880	2.211704	-0.604255
H	-4.614534	-2.030472	1.152066				

C	-0.331482	-0.792096	3.049475	C	3.193367	-0.408554	0.593016
H	0.617631	-0.831183	3.595058	H	5.101221	0.316811	-2.166095
H	-0.851581	0.141137	3.283703	H	6.592338	-1.294333	-0.993705
H	-0.942479	-1.643971	3.363622	H	5.933749	-2.292621	1.161937
C	1.092828	-0.344875	-1.194417	H	3.722513	-1.720438	2.206431
C	0.506537	-2.256795	1.185364	N	2.579613	1.052681	-1.024982
H	-0.238848	-3.013899	1.456129	H	0.909500	-1.853001	0.538989
H	1.392933	-2.480869	1.783450	C	0.012459	2.612490	0.965144
H	0.756852	-2.380516	0.128645	H	-0.812880	3.316244	0.830216
C	3.090228	0.357605	-0.022387	H	0.894646	3.191155	1.256921
N	2.415013	-0.508896	-1.002722	H	-0.209213	1.929912	1.783593
N	1.471154	1.968630	-0.573479	C	0.490623	2.926098	-1.465434
C	2.813107	1.810686	-0.420864	H	1.283163	3.637407	-1.212064
O	3.658958	2.676688	-0.546365	H	-0.439455	3.491128	-1.578862
C	2.396113	0.156360	1.348531	H	0.709242	2.475548	-2.440819
H	2.805885	0.876754	2.062819	O	1.353390	0.127581	2.133873
H	2.644268	-0.844230	1.714771	C	-0.797619	0.868142	-0.819054
C	4.547658	-0.080822	-0.110069	C	-2.262866	1.352663	-0.693120
H	5.061175	0.546147	-0.845596	H	-2.694564	1.555174	-1.677784
H	5.064121	0.033547	0.845547	H	-2.350033	2.263214	-0.093077
C	4.458651	-1.542749	-0.582514	H	-0.584561	0.657610	-1.876692
H	5.383076	-1.893900	-1.044534	C	-0.654478	-0.492651	-0.084148
H	4.233045	-2.201391	0.263612	C	-1.577646	-1.483588	-0.833796
C	3.277402	-1.542778	-1.562255	C	-3.078679	0.227853	-0.017447
H	3.588112	-1.268264	-2.577059	N	-2.844065	-1.017571	-0.767017
H	2.737990	-2.492403	-1.614094	N	-1.193312	-0.386185	1.275045
H	0.519827	1.188364	1.781559	C	-2.464908	0.073122	1.388202
O	-1.741762	1.704518	1.701731	O	-3.035838	0.377219	2.421851
O	0.379229	-1.063288	-1.885901	C	-4.595665	0.361698	-0.014588
H	1.085488	2.889076	-0.736487	H	-4.936564	0.863243	0.892873
H	-1.769373	-2.336351	-0.117759	H	-4.916600	0.937799	-0.890123
TS67-neu-RRS				C	-5.079968	-1.094694	-0.118709
C	0.307373	1.877044	-0.358907	H	-5.017412	-1.568897	0.865925
C	1.555243	1.055042	-0.162458	H	-6.108363	-1.176700	-0.476037
C	1.823551	0.101643	0.946575	C	-4.070560	-1.747102	-1.073619
C	0.776230	-0.970406	-0.088663	H	-4.350382	-1.600256	-2.123889
H	1.123537	-1.185112	-1.102064	H	-3.915560	-2.815238	-0.904489
C	3.595547	0.168417	-0.608740	O	-1.212740	-2.506625	-1.388942
C	4.806744	-0.131311	-1.222202	H	-0.508210	-0.300689	2.033632
C	5.633878	-1.033699	-0.556969	H	2.541758	1.466007	-1.947351
C	5.256400	-1.603558	0.668210	TS67-neu-SSR			
C	4.030638	-1.295624	1.256202	C	-0.646835	-0.602032	-0.176798

C	-0.831194	0.486453	0.935819	H	-0.640278	-0.027090	1.880930
C	0.256783	1.620794	0.843246	O	1.564233	-0.806351	2.042408
C	1.515941	0.950994	0.426671	O	-1.517833	-2.865279	0.296936
C	1.774046	-0.513860	0.772473	H	-0.407039	-0.025111	-2.268158
C	0.754062	-1.218495	-0.226531	H	2.540601	2.417922	-0.599390
H	0.705095	-2.248912	0.138434				
C	3.572606	0.520007	-0.420325				
C	4.786596	0.710026	-1.057201				
C	5.661204	-0.380504	-1.053300				
C	5.308556	-1.581219	-0.430263				
C	4.067489	-1.735982	0.197273				
C	3.186363	-0.667826	0.190554				
H	5.055639	1.650202	-1.529087				
H	6.629797	-0.286887	-1.532735				
H	6.016018	-2.404312	-0.430487				
H	3.794542	-2.660754	0.696348				
N	2.508759	1.468360	-0.240834				
H	1.118627	-1.234850	-1.261960				
C	0.509002	2.136403	2.285416				
H	0.887284	1.319610	2.905387				
H	-0.439637	2.506975	2.688873				
H	1.226442	2.963644	2.281590				
C	-1.732013	-1.689749	0.061646				
C	-0.060637	2.817014	-0.069018				
H	0.794484	3.503184	-0.098841				
H	-0.885540	3.406892	0.334593				
H	-0.312231	2.520715	-1.090162				
C	-3.029980	0.324962	-0.283958				
N	-2.954135	-1.121615	-0.042758				
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C	-2.240480	0.594872	-1.572807				
O	-2.657597	1.193364	-2.548558				
C	-2.284952	1.020245	0.875001				
H	-2.820262	0.787661	1.800809				
H	-2.334897	2.102482	0.733667				
C	-4.530562	0.592102	-0.378527				
H	-4.793157	1.579299	0.009044				
H	-4.828324	0.555330	-1.430875				
C	-5.162496	-0.561094	0.422294				
H	-5.136188	-0.338343	1.494125				
H	-6.201356	-0.745301	0.142117				
C	-4.252613	-1.760058	0.123896				
H	-4.203569	-2.496991	0.928658				
H	-4.547025	-2.274779	-0.799036				

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