

Supporting Information

Origins of enantioselectivity in chiral Brønsted acid catalyzed hydrophosphonylation of imines

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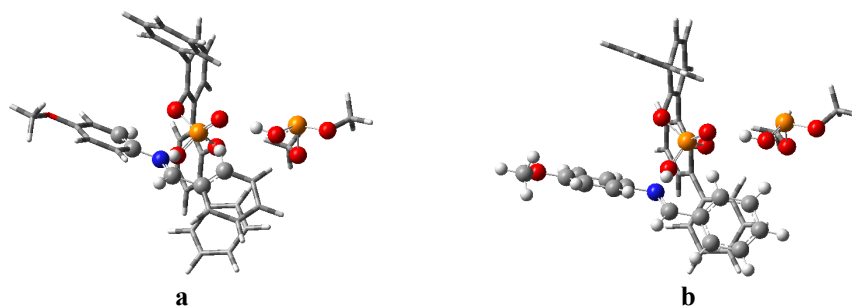
ONIOM evaluation

S-Table 1. Selected distances (in Å) in the test complexes.

	<i>R-complex</i>			<i>S-complex</i>		
	N-H...O	O-H...O	C-H...O	N-H...O	O-H...O	C-H...O
B3LYP/6-31G*	1.597	1.756	2.525	1.593	1.790	2.375
B3LYP/6-31G*/ HF/STO-3G ^a	1.537	1.777	2.379	1.518	1.804	2.415
B3LYP/6-31G*/ AM1 ^a	1.654	1.767	2.362	1.672	1.780	2.251
B3LYP/6-31G*/ AM1 ^b	1.605	1.753	2.384	1.615	1.752	2.275
B3LYP/D95**/ AM1 ^b	1.540	1.708	2.240	1.546	1.718	2.293

^a Part imine was treated at the B3LYP/6-31G* level (**a** in **S-Figure 1**).

^b Whole imine was treated at the B3LYP/6-31G* level (**b** in **S-Figure 1**).

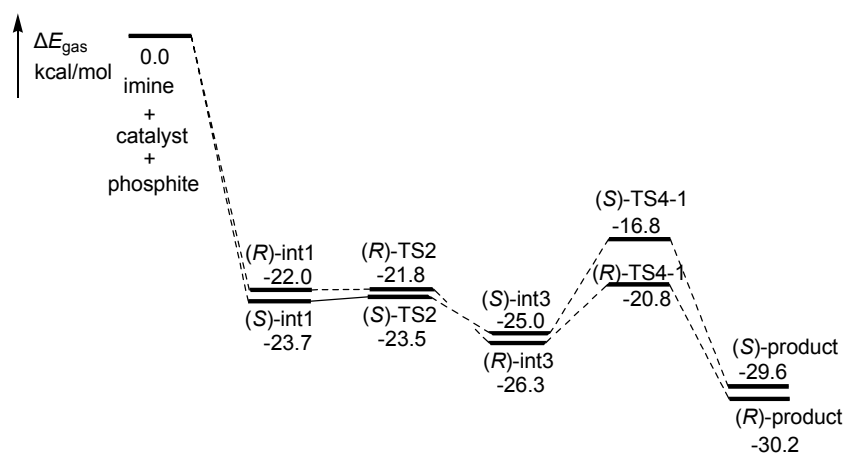


S-Figure 1. The test *R*-complex. (high layer is shown ball and bond type and low layer is shown in tube type)

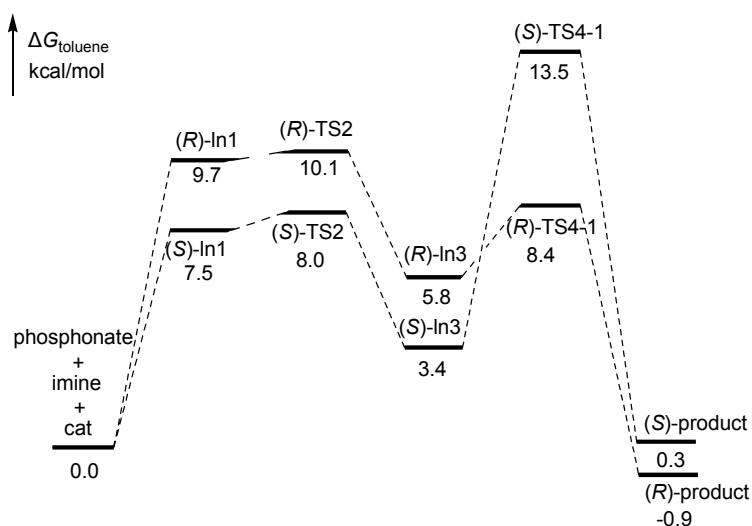
S-Table 2. The energy difference (kcal/mol) computed at the B3LYP/D95** levels.

	E_R (au)	E_S (au)	ΔE (kcal/mol)
B3LYP/6-31G*	-2886.2666954	-2886.2628500	2.413
B3LYP/6-31G*/ AM1 ^a	-2886.2401161	-2886.2397281	0.243
B3LYP/6-31G*/ AM1 ^b	-2886.2452782	-2886.2425108	1.737
B3LYP/D95**/ AM1 ^b	-2886.2455694	-2886.2448364	0.460

Both combinations of B3LYP/6-31G* with HF/STO-3G and AM1 reproduce the results from density functional theory (B3LYP/6-31G*). In contrast, the combination of B3LYP/6-31G* with B3LYP/STO-3G fail since it optimized the test complex to a zwitterionic complex of iminium salt. Among all the test combinations, B3LYP/6-31G*/ AM1^b gives the best result.

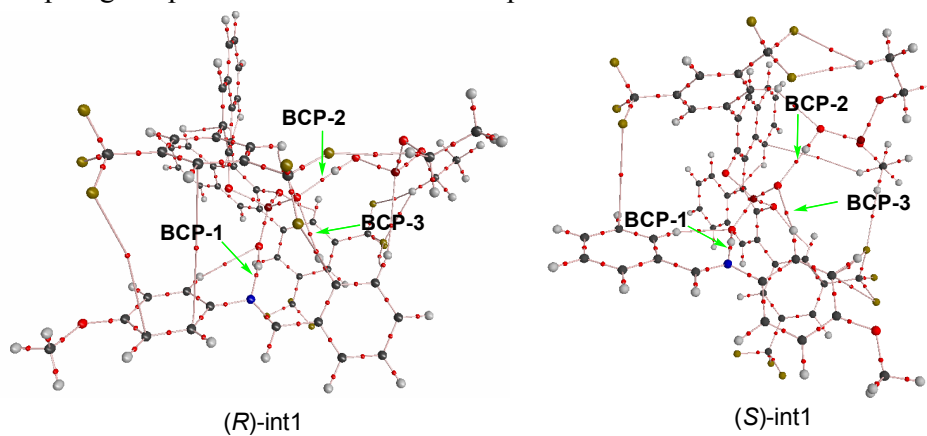


S-Figure 2. Potential energy surfaces of chiral Brønsted acid catalyzed enantioselective hydrophosphonylation of aldimine in dicoordination pathway (kcal/mol in terms of electronic energy).

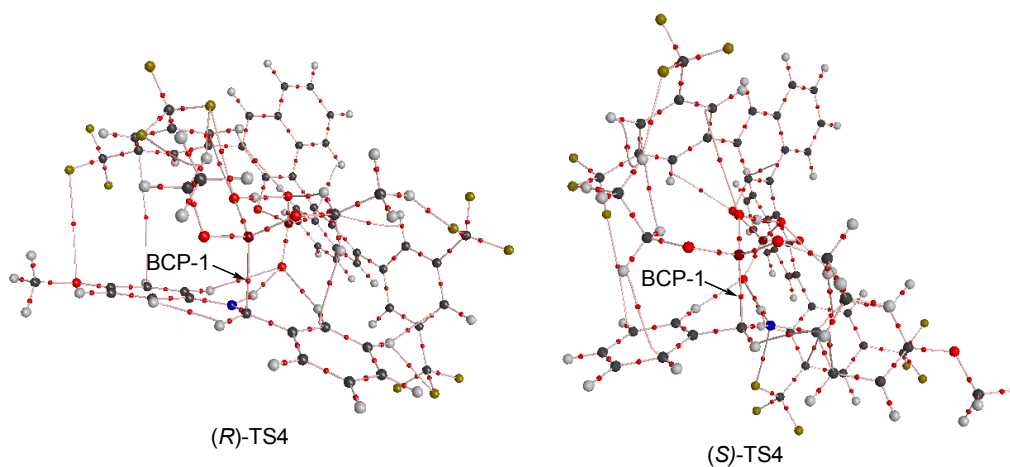


S-Figure 3. Potential energy surfaces of chiral Brønsted acid catalyzed enantioselective hydrophosphonylation of aldimine in dicoordination pathway (Part imine was treated at the B3LYP/D95** level, a in S-Figure 1).

Selected topological parameters at bond critical points in **int1** and **TS4**

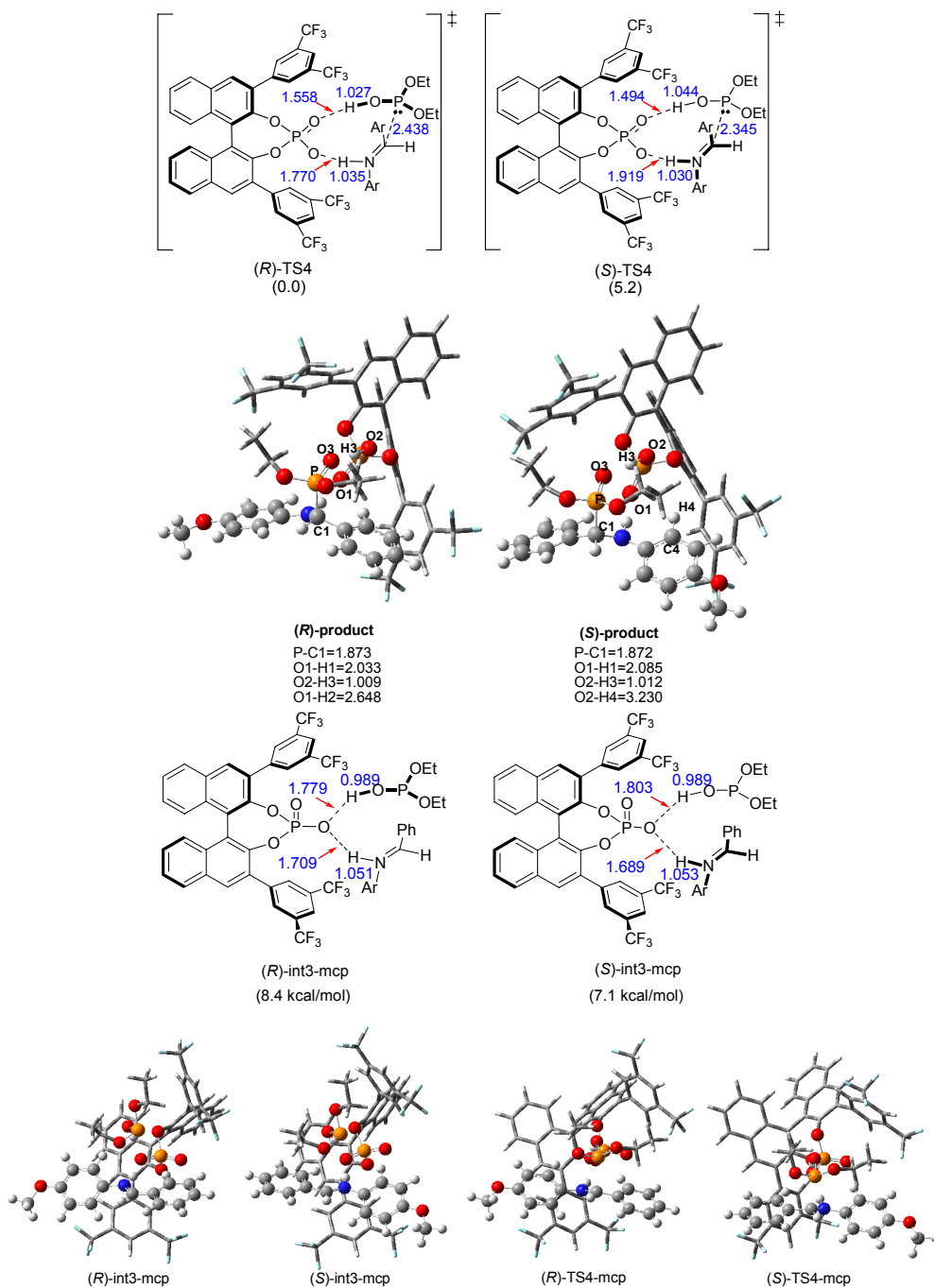


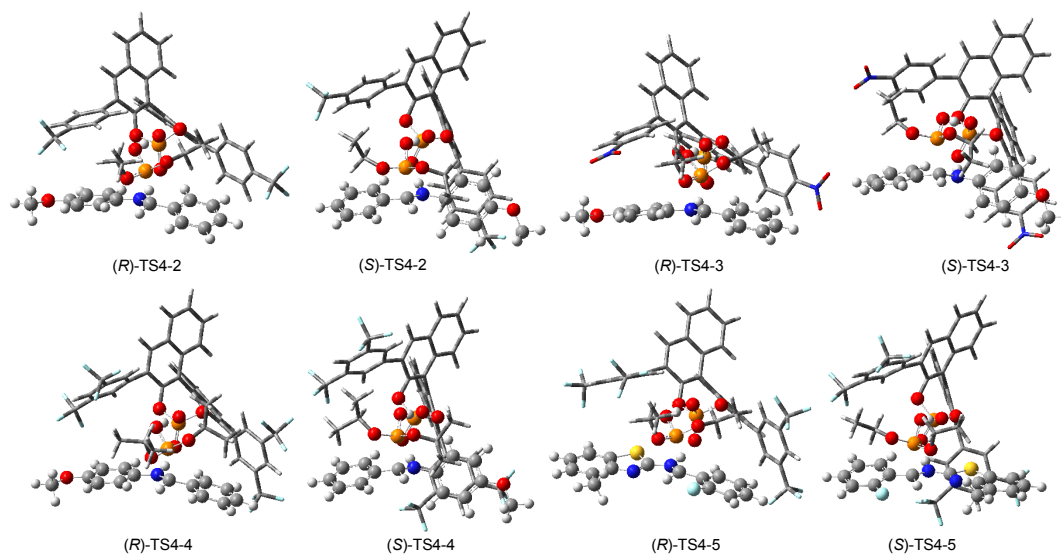
	<i>(R)</i> -int1 (au)		<i>(S)</i> -int1 (au)	
	<i>charge density</i>	<i>Laplacian</i>	<i>charge density</i>	<i>Laplacian</i>
BCP-1	0.1006	-0.0021	0.1059	-0.0248
BCP-2	0.0342	0.1062	0.0349	0.1098
BCP-3	0.0116	0.0428	0.0133	0.0495



	<i>(R)</i> -TS4 (au)		<i>(S)</i> -TS4 (au)	
	<i>charge density</i>	<i>Laplacian</i>	<i>charge density</i>	<i>Laplacian</i>
BCP-1	0.0583	0.0383	0.0708	0.0190

Optimized structures of the investigated system





Cartesian coordinates

Catalyst				diethyl phosphite			
C	2.190211	5.266865	-2.741303	P	0.033055	0.011241	-0.116104
C	3.012732	4.241149	-2.347262	O	0.020738	-0.003972	1.583831
C	2.517848	3.192906	-1.522379	O	1.675869	-0.023168	-0.327439
C	1.169399	3.223679	-1.083835	O	-0.420874	1.583898	-0.414862
C	0.339396	4.294587	-1.520642	C	2.677694	0.538251	0.549838
C	0.836693	5.287531	-2.328542	H	2.335271	0.485648	1.588810
H	4.411465	2.128293	-1.465015	H	2.831419	1.592818	0.283361
H	2.568464	6.076839	-3.382905	C	3.969580	-0.248739	0.364472
H	4.065705	4.206875	-2.666370	H	4.762921	0.178071	0.990694
C	3.356451	2.113389	-1.145219	H	3.827076	-1.296562	0.649131
C	0.678207	2.169237	-0.253018	H	4.296222	-0.215961	-0.680378
H	-0.715814	4.309272	-1.203834	C	0.096482	2.743671	0.269946
H	0.186414	6.10859	-2.667074	H	1.030384	3.053542	-0.218586
C	1.502100	1.07138	0.007675	H	0.313579	2.495478	1.316237
C	2.875858	1.061217	-0.395572	C	-0.939369	3.858927	0.186865
C	-0.702955	2.178446	0.244309	H	-0.554067	4.768421	0.664353
C	-1.198644	3.248866	1.050515	H	-1.174850	4.088711	-0.857746
C	-1.526641	1.076254	0.001014	H	-1.865546	3.566160	0.692895
C	-0.370793	4.327322	1.472223	H	-0.787772	-0.434468	1.895777
C	-2.550987	3.226631	1.478491				
C	-2.904364	1.074312	0.388939				
C	-0.873116	5.335242	2.258074				
H	0.686097	4.335017	1.160731				
C	-3.050448	4.290393	2.280564				
C	-3.388904	2.141794	1.114241				
C	-2.229583	5.322349	2.661675				
H	-0.225005	6.162326	2.585884				
H	-4.105618	4.262739	2.593159				
H	-4.446538	2.164487	1.42493				
H	-2.611694	6.143895	3.286153				
O	-1.070005	-0.005518	-0.741752				
O	1.070509	-0.000933	0.774121				
P	-0.048999	-1.041342	0.090451				
O	-0.583027	-1.980071	1.104839				
O	0.63432	-1.736601	-1.204695				
H	0.725099	-2.690075	-1.044549				
C	-3.795651	-0.024421	0.017703				
C	-4.670763	-0.569086	0.968145				
C	-3.806403	-0.520257	-1.293535				
C	-5.551088	-1.588145	0.601439				

H	-4.662741	-0.197152	2.006739
C	-4.691056	-1.541729	-1.643991
H	-3.111309	-0.104354	-2.044669
C	-5.569651	-2.082391	-0.703892
H	-6.273773	-2.883096	-0.988688
C	3.774534	-0.027021	-0.010486
C	4.635455	-0.592017	-0.961364
C	3.812717	-0.486676	1.314130
C	5.527407	-1.597775	-0.584591
H	4.603691	-0.25123	-2.010084
C	4.711720	-1.491052	1.675436
H	3.126627	-0.055126	2.065320
C	5.575764	-2.05305	0.733461
H	6.285551	-2.845368	1.027658
C	-4.681801	-2.080416	-3.070542
C	-6.496306	-2.180669	1.641434
C	6.473155	-2.189692	-1.624083
C	4.746989	-1.993357	3.115657
F	-3.717547	-3.031477	-3.302283
F	-4.453933	-1.127457	-4.033107
F	-5.852041	-2.683753	-3.461034
F	-7.699495	-2.606975	1.133486
F	-5.997017	-3.279501	2.295654
F	-6.843359	-1.313924	2.649506
F	6.873987	-3.476597	-1.363016
F	7.647877	-1.491662	-1.770466
F	5.954759	-2.245017	-2.894857
F	5.985854	-2.412431	3.536558
F	3.927964	-3.070344	3.351220
F	4.367295	-1.063263	4.051287

(R)-int1

C	0.46618	-7.247457	-2.007983
C	1.44236	-6.552117	-1.339451
C	1.406818	-5.130971	-1.279437
C	0.366802	-4.427522	-1.938924
C	-0.63741	-5.179415	-2.61245
C	-0.589109	-6.551291	-2.644211
H	3.215122	-4.976584	-0.084655
H	0.488727	-8.346455	-2.05353
H	2.265927	-7.079133	-0.834003
C	2.394129	-4.413477	-0.557824
C	0.338014	-2.999653	-1.881345

(S)-int1

O	0.795229	-0.692256	-1.499687
H	0.989653	-1.772615	-1.4156
N	1.365855	-3.161899	-1.440911
C	0.944377	6.038174	-4.358022
C	1.941749	5.301829	-3.769219
C	1.637892	4.353023	-2.753502
C	0.293889	4.185263	-2.332372
C	-0.718198	4.957838	-2.969443
C	-0.400847	5.857763	-3.956778
H	3.706992	3.751567	-2.469112
H	1.175713	6.769873	-5.146353

H	-1.460997	-4.638077	-3.105236	H	2.991783	5.427236	-4.074356
H	-1.372387	-7.124791	-3.16269	C	2.663622	3.571385	-2.163158
C	1.264906	-2.335557	-1.072498	C	-0.008354	3.229787	-1.314075
C	2.340136	-3.040999	-0.442886	H	-1.765122	4.814978	-2.656373
C	-0.704295	-2.234446	-2.577577	H	-1.189532	6.447034	-4.44863
C	-0.887454	-2.332446	-3.990826	C	1.009152	2.392683	-0.84791
C	-1.474602	-1.316885	-1.856765	C	2.374453	2.606293	-1.222851
C	-0.035112	-3.121842	-4.813817	C	-1.375691	3.049429	-0.811093
C	-1.928455	-1.593164	-4.609099	C	-2.094363	4.126024	-0.206277
C	-2.550493	-0.603901	-2.472146	C	-1.945023	1.772963	-0.81963
C	-0.227547	-3.184617	-6.171858	C	-1.52439	5.419458	-0.035411
H	0.791078	-3.67553	-4.339856	C	-3.4076	3.898336	0.279465
C	-2.114912	-1.686261	-6.016521	C	-3.283227	1.553048	-0.366618
C	-2.762422	-0.755221	-3.824269	C	-2.235215	6.430084	0.563378
C	-1.283254	-2.465442	-6.781267	H	-0.494433	5.59374	-0.38506
H	0.441311	-3.789877	-6.802334	C	-4.127005	4.965349	0.88652
H	-2.932787	-1.111534	-6.477427	C	-3.985386	2.606904	0.175137
H	-3.581969	-0.211365	-4.321581	C	-3.554221	6.204841	1.024155
H	-1.420372	-2.533577	-7.870746	H	-1.784314	7.424897	0.697679
O	-1.294283	-1.162391	-0.488148	H	-5.14657	4.769863	1.252685
O	1.269535	-0.954619	-0.943199	H	-5.011055	2.453977	0.548783
P	0.043476	-0.251737	-0.075373	H	-4.10542	7.029976	1.499039
O	-0.04536	1.185908	-0.454685	O	-1.272053	0.693166	-1.377045
O	0.249089	-0.596741	1.424047	O	0.764194	1.401466	0.091016
H	-0.230233	0.008117	2.194578	P	-0.056221	0.050605	-0.433773
N	-0.884816	0.558774	3.377275	O	-0.485126	-0.731627	0.755314
C	-3.43215	0.264355	-1.684008	C	-3.909429	0.232588	-0.469218
C	-3.063136	1.581942	-1.378048	C	-4.277073	-0.464537	0.690421
C	-4.667987	-0.231524	-1.24967	C	-4.16938	-0.321998	-1.728867
C	-3.938344	2.389254	-0.647462	C	-4.928537	-1.695516	0.576865
H	-2.080622	1.9812	-1.697864	H	-4.033358	-0.053474	1.690765
C	-5.53151	0.590557	-0.523098	C	-4.822428	-1.55188	-1.823178
H	-4.956854	-1.272146	-1.473089	H	-3.852112	0.212942	-2.639933
C	-5.17525	1.904501	-0.218492	C	-5.209713	-2.244741	-0.674425
H	-5.861321	2.551201	0.354164	H	-5.73518	-3.210901	-0.759262
C	3.381725	-2.33168	0.300486	C	3.454499	1.840069	-0.601483
C	3.789823	-2.807531	1.553899	C	4.475891	1.292816	-1.389099
C	3.999628	-1.194627	-0.24147	C	3.49346	1.674997	0.791203
C	4.81067	-2.156731	2.24934	C	5.524384	0.595924	-0.784975
H	3.298282	-3.68896	1.998727	H	4.446809	1.399597	-2.486446
C	5.020364	-0.557171	0.465479	C	4.552696	0.983146	1.380458

H	3.669308	-0.804359	-1.221932	H	2.675198	2.079402	1.414402
C	5.4347	-1.03067	1.712176	C	5.574343	0.43821	0.600583
H	6.242691	-0.520877	2.26395	H	6.402953	-0.117728	1.071405
C	-0.436035	1.522829	4.111634	C	1.11935	-3.994569	-2.396911
H	-0.854402	1.651841	5.115823	H	1.45228	-5.030107	-2.272284
C	0.604423	2.471633	3.7371	C	0.423662	-3.725102	-3.651577
C	1.216341	3.211352	4.767584	C	0.20347	-4.826118	-4.501892
C	0.989515	2.702192	2.402635	C	-0.02505	-2.451548	-4.054958
C	2.215418	4.134726	4.476741	C	-0.451152	-4.66827	-5.719777
H	0.909402	3.048304	5.798343	H	0.548102	-5.811675	-4.197315
C	1.979034	3.63775	2.114634	C	-0.677409	-2.300429	-5.27388
H	0.497402	2.18196	1.588593	H	0.136099	-1.588211	-3.420761
C	2.596911	4.347986	3.14918	C	-0.893481	-3.402333	-6.108105
H	2.689111	4.692683	5.279596	H	-0.617013	-5.528251	-6.362264
H	2.250132	3.820991	1.077377	H	-1.022152	-1.315766	-5.576164
H	3.368568	5.07799	2.918513	H	-1.406926	-3.27293	-7.057039
C	-1.98677	-0.218645	3.816172	C	2.139335	-3.583858	-0.325291
C	-3.063723	0.335418	4.51902	C	3.259807	-4.410497	-0.469628
C	-2.016356	-1.588796	3.498161	C	1.78243	-3.128916	0.956407
C	-4.134883	-0.457288	4.932108	C	4.001946	-4.809513	0.64235
H	-3.092613	1.404174	4.711151	H	3.586377	-4.713985	-1.460425
C	-3.071506	-2.382801	3.915947	C	2.509822	-3.533567	2.064374
H	-1.198733	-2.02206	2.932714	H	0.921973	-2.478123	1.077781
C	-4.139365	-1.827133	4.639964	C	3.622188	-4.379328	1.920365
H	-4.962033	0.005259	5.458118	H	4.875461	-5.434965	0.49828
H	-3.098232	-3.443111	3.686184	H	2.234976	-3.201532	3.060609
P	2.031192	3.82597	-1.892717	P	-1.285914	0.002475	4.290478
O	1.603136	2.33228	-2.377899	O	-2.113697	-0.049884	2.883866
O	0.796035	4.698466	-2.610734	O	-2.598097	0.042567	5.329064
O	3.237356	4.09622	-3.013756	O	-0.910193	1.63335	4.311361
C	0.452677	5.864128	-1.885735	C	-2.720602	-1.145279	6.090213
C	0.755447	7.102603	-2.703204	C	-4.038889	-1.824253	5.784128
H	0.989447	5.896527	-0.900051	H	-2.700029	-0.83513	7.174746
H	-0.658509	5.798577	-1.69407	H	-1.860425	-1.83971	5.894241
H	0.332834	7.999184	-2.190947	H	-4.157314	-2.719468	6.439195
H	1.854775	7.243332	-2.830661	H	-4.884348	-1.119639	5.97058
H	0.297398	7.010868	-3.717098	H	-4.090349	-2.145834	4.714708
C	4.477793	4.152343	-2.327976	C	0.291063	1.798087	5.0488
C	5.555006	4.451275	-3.34417	C	0.595008	3.276385	5.118126
H	4.65959	3.164687	-1.820392	H	1.115896	1.236653	4.530321
H	4.426745	4.954853	-1.543137	H	0.151055	1.366806	6.076543

H	6.545811	4.493525	-2.833344	H	1.54305	3.434813	5.684346
H	5.577903	3.655632	-4.126605	H	0.705398	3.697319	4.090513
H	5.356285	5.428614	-3.844767	H	-0.235292	3.818406	5.630331
H	1.004376	1.911968	-1.716395	H	-1.519939	-0.310889	2.140055
C	-6.884246	0.056828	-0.068943	C	-5.121356	-2.163931	-3.185317
C	-3.541173	3.816703	-0.287281	C	-5.327115	-2.451394	1.839383
C	5.258801	-2.693345	3.603617	C	6.636758	0.014389	-1.649334
C	5.688754	0.683014	-0.117021	C	4.601627	0.840079	2.897818
F	-6.934973	-1.304792	0.103441	F	-4.34776	-3.257431	-3.493742
F	-7.913631	0.322389	-0.940202	F	-4.944972	-1.317428	-4.252497
F	-7.322352	0.564914	1.130382	F	-6.410322	-2.619376	-3.327854
F	-4.596423	4.696977	-0.229817	F	-6.315335	-3.389471	1.652269
F	-2.946526	3.936366	0.94644	F	-4.305532	-3.15927	2.423555
F	-2.656838	4.408596	-1.152226	F	-5.81008	-1.65558	2.848483
F	5.770026	-1.743443	4.453574	F	7.245856	-1.098973	-1.12377
F	6.24783	-3.645038	3.528617	F	7.674237	0.884248	-1.886606
F	4.26543	-3.301008	4.332319	F	6.237362	-0.379271	-2.903338
F	7.017029	0.815596	0.210156	F	5.339843	-0.227174	3.347769
F	5.125719	1.86823	0.293353	F	3.37506	0.681093	3.494589
F	5.667855	0.758368	-1.48695	F	5.151292	1.922917	3.541864
O	-5.128129	-2.692747	4.992864	O	4.268142	-4.708996	3.071684
C	-6.250971	-2.185585	5.699614	C	5.406847	-5.55294	2.990749
H	-6.789588	-1.431518	5.110976	H	6.207657	-5.093088	2.396811
H	-6.904631	-3.041812	5.873746	H	5.751435	-5.687658	4.017382
H	-5.957023	-1.751078	6.664037	H	5.153509	-6.531082	2.561154

(R)-TS2

O	0.266206	-0.660089	1.373366
H	-0.231706	-0.129369	2.248938
N	-0.831333	0.257148	3.406478
C	0.314499	-7.067562	-2.517932
C	1.312716	-6.437596	-1.818004
C	1.30384	-5.023728	-1.658209
C	0.267408	-4.258006	-2.250493
C	-0.759997	-4.943671	-2.958989
C	-0.737142	-6.310505	-3.087238
H	3.130714	-4.984623	-0.483139
H	0.316461	-8.16082	-2.640659
H	2.133964	-7.012698	-1.363871
C	2.313789	-4.375527	-0.903355
C	0.265901	-2.83754	-2.093381

(S)-TS2

O	0.811727	-0.55384	-1.529723
H	1.04828	-1.665988	-1.561838
N	1.444472	-2.961665	-1.714274
C	0.933622	6.430257	-3.754814
C	1.930442	5.649541	-3.225333
C	1.623029	4.606437	-2.307851
C	0.275612	4.388676	-1.921979
C	-0.735704	5.209954	-2.496405
C	-0.414695	6.201821	-3.38995
H	3.693797	3.996931	-2.055616
H	1.167752	7.235212	-4.467214
H	2.982928	5.811738	-3.503442
C	2.648603	3.780689	-1.780828
C	-0.030034	3.339266	-1.002155

H	-1.580412	-4.354892	-3.399937	H	-1.784937	5.029701	-2.211638
H	-1.53803	-6.832763	-3.632208	H	-1.202678	6.828768	-3.83396
C	1.216749	-2.24658	-1.255743	C	0.989385	2.470654	-0.602066
C	2.286422	-3.013681	-0.691932	C	2.356904	2.729254	-0.939015
C	-0.772349	-2.007513	-2.717684	C	-1.401661	3.100083	-0.536858
C	-0.977118	-2.003016	-4.13126	C	-2.138598	4.108	0.157652
C	-1.515873	-1.130608	-1.921691	C	-1.957665	1.825056	-0.673976
C	-0.150727	-2.746965	-5.020509	C	-1.583907	5.38451	0.45748
C	-2.013626	-1.205306	-4.680433	C	-3.455191	3.823673	0.602715
C	-2.587749	-0.358933	-2.469983	C	-3.29943	1.552031	-0.261719
C	-0.363729	-2.711546	-6.376423	C	-2.311949	6.327421	1.140154
H	0.672315	-3.345932	-4.599064	H	-0.55166	5.600248	0.139112
C	-2.221857	-1.196605	-6.087864	C	-4.192456	4.821786	1.298932
C	-2.821496	-0.411217	-3.826006	C	-4.018754	2.542953	0.368721
C	-1.415234	-1.934138	-6.917859	C	-3.633948	6.047717	1.560695
H	0.285171	-3.282299	-7.057821	H	-1.87275	7.308976	1.373821
H	-3.036	-0.577571	-6.494768	H	-5.214218	4.583321	1.631943
H	-3.638534	0.179445	-4.271267	H	-5.047256	2.346181	0.712754
H	-1.569154	-1.923771	-8.007123	H	-4.199008	6.81907	2.104599
O	-1.313931	-1.075876	-0.549664	O	-1.26752	0.808537	-1.320427
O	1.247797	-0.878736	-1.034541	O	0.741613	1.396295	0.238088
P	0.048804	-0.219446	-0.089472	P	-0.056434	0.0884	-0.422977
O	-0.022636	1.241235	-0.382733	O	-0.502026	-0.789683	0.692779
C	-3.445002	0.465414	-1.611022	C	-3.910479	0.242211	-0.500329
C	-3.045963	1.748119	-1.20786	C	-4.293906	-0.564672	0.580442
C	-4.689111	-0.033907	-1.207378	C	-4.138138	-0.193669	-1.811718
C	-3.900507	2.516019	-0.413592	C	-4.931704	-1.783822	0.337116
H	-2.056389	2.149464	-1.50321	H	-4.072103	-0.248864	1.619772
C	-5.532207	0.749503	-0.415137	C	-4.775853	-1.415031	-2.035792
H	-5.007119	-1.045443	-1.509096	H	-3.808022	0.427372	-2.661483
C	-5.146976	2.028073	-0.015118	C	-5.181317	-2.215257	-0.96617
H	-5.817037	2.649308	0.603376	H	-5.697149	-3.172545	-1.151674
C	3.348978	-2.377845	0.087329	C	3.436104	1.914839	-0.380714
C	3.767291	-2.954787	1.2941	C	4.471498	1.454447	-1.204819
C	3.975423	-1.209999	-0.373414	C	3.459423	1.614352	0.989551
C	4.806523	-2.373574	2.023155	C	5.518239	0.709111	-0.65841
H	3.269311	-3.861473	1.676542	H	4.459257	1.675914	-2.285208
C	5.013939	-0.642531	0.366541	C	4.518365	0.877564	1.522258
H	3.637498	-0.740311	-1.315823	H	2.629603	1.949028	1.638449
C	5.438848	-1.217227	1.566242	C	5.553895	0.418959	0.706068
H	6.261301	-0.762444	2.144013	H	6.387426	-0.164476	1.132612

C	-0.388272	1.173679	4.205319	C	1.264391	-3.672589	-2.778952
H	-0.797912	1.212798	5.219434	H	1.618278	-4.707569	-2.761063
C	0.626647	2.168998	3.896198	C	0.625887	-3.26644	-4.02545
C	1.225538	2.84341	4.978921	C	0.515552	-4.25199	-5.02639
C	1.002298	2.506786	2.581253	C	0.125563	-1.973551	-4.281738
C	2.202998	3.807344	4.756383	C	-0.078941	-3.962361	-6.25056
H	0.925595	2.597189	5.995093	H	0.899127	-5.251521	-4.835004
C	1.970437	3.482561	2.363329	C	-0.467939	-1.69177	-5.507348
H	0.520931	2.039478	1.729741	H	0.199979	-1.19858	-3.52829
C	2.575618	4.126754	3.447466	C	-0.572815	-2.6791	-6.492825
H	2.666783	4.314419	5.597763	H	-0.158971	-4.733686	-7.011114
H	2.235044	3.747904	1.342192	H	-0.854325	-0.694373	-5.695853
H	3.330624	4.888534	3.270807	H	-1.040799	-2.447762	-7.445873
C	-1.91027	-0.581503	3.787995	C	2.166773	-3.497595	-0.61257
C	-2.979514	-0.120595	4.565215	C	3.296862	-4.304713	-0.788233
C	-1.920151	-1.913209	3.334933	C	1.744002	-3.178449	0.689749
C	-4.025867	-0.972123	4.91951	C	3.983155	-4.819989	0.311276
H	-3.024142	0.922765	4.864016	H	3.676028	-4.500932	-1.787339
C	-2.951778	-2.764994	3.692223	C	2.417523	-3.697557	1.78374
H	-1.108004	-2.269534	2.711395	H	0.876925	-2.541723	0.836796
C	-4.012866	-2.305735	4.49028	C	3.538463	-4.525649	1.607186
H	-4.848617	-0.581833	5.507266	H	4.865584	-5.427444	0.14629
H	-2.965593	-3.797005	3.356936	H	2.092546	-3.470236	2.794126
P	2.046711	3.964947	-1.616246	P	-1.346086	-0.433361	4.258237
O	1.622127	2.513041	-2.213913	O	-2.159329	-0.321537	2.84778
O	0.818456	4.889567	-2.278578	O	-2.667883	-0.524898	5.282259
O	3.261647	4.32347	-2.703448	O	-0.981648	1.18576	4.475871
C	0.49476	6.020105	-1.491753	C	-2.781117	-1.791933	5.904088
C	0.807004	7.295401	-2.246704	C	-4.087668	-2.448542	5.511011
H	1.039335	5.99524	-0.510127	H	-2.773795	-1.605516	7.016778
H	-0.615615	5.958255	-1.294557	H	-1.910253	-2.449611	5.640104
H	0.404882	8.170032	-1.682665	H	-4.199945	-3.412662	6.060942
H	1.906844	7.42559	-2.380969	H	-4.943889	-1.779401	5.76634
H	0.33535	7.264166	-3.25802	H	-4.125854	-2.649415	4.411973
C	4.501043	4.28625	-2.014794	C	0.207699	1.269971	5.245105
C	5.586607	4.665279	-2.994765	C	0.499343	2.73169	5.491955
H	4.662733	3.249217	-1.609172	H	1.044055	0.778403	4.676474
H	4.4632	5.006354	-1.152976	H	0.056871	0.720004	6.212938
H	6.576772	4.635796	-2.481823	H	1.440343	2.828371	6.083268
H	5.595744	3.952725	-3.853827	H	0.616761	3.27177	4.522461
H	5.408537	5.692069	-3.393818	H	-0.340322	3.203911	6.055415

H	1.02626	2.039136	-1.585319	H	-1.559251	-0.503239	2.084795
C	-6.882124	0.182809	0.005756	C	-5.029688	-1.896879	-3.45791
C	-3.469248	3.902741	0.050971	C	-5.349591	-2.660096	1.512425
C	5.264566	-3.019695	3.325122	C	6.627923	0.191109	-1.565334
C	5.689801	0.632181	-0.125601	C	4.551692	0.588642	3.019108
F	-6.80125	-0.971465	0.747367	F	-4.135505	-2.842555	-3.900523
F	-7.701763	-0.153442	-1.044913	F	-4.979319	-0.91527	-4.417571
F	-7.64921	1.022037	0.776262	F	-6.256379	-2.487322	-3.645589
F	-4.506575	4.790842	0.215014	F	-6.347846	-3.560833	1.22273
F	-2.835651	3.910343	1.271235	F	-4.341222	-3.438441	2.025934
F	-2.601413	4.551951	-0.789131	F	-5.830181	-1.967234	2.595656
F	5.805078	-2.146545	4.237134	F	6.391815	-1.059225	-2.084884
F	6.234916	-3.979638	3.162642	F	7.853669	0.073862	-0.956363
F	4.271008	-3.664238	4.021336	F	6.872367	0.971572	-2.669207
F	7.02287	0.725707	0.19578	F	5.292252	-0.513299	3.371588
F	5.144315	1.787401	0.382622	F	3.32011	0.365232	3.583905
F	5.655306	0.814429	-1.485089	F	5.0874	1.606663	3.771421
O	-4.977388	-3.221107	4.774025	O	4.127413	-4.975492	2.747516
C	-6.100297	-2.807518	5.540008	C	5.270316	-5.810705	2.635971
H	-6.737422	-3.688404	5.633141	H	6.098915	-5.294351	2.133816
H	-5.802058	-2.46775	6.540419	H	5.563348	-6.052465	3.65893
H	-6.657511	-2.00763	5.035423	H	5.039934	-6.737841	2.094967

(R)-int3

C	-0.626405	-5.260015	5.311685
C	-1.604139	-4.914909	4.413147
C	-1.508988	-3.707013	3.666876
C	-0.40519	-2.840584	3.873402
C	0.598187	-3.234586	4.80449
C	0.490788	-4.41185	5.502178
H	-3.368663	-4.034388	2.594174
H	-0.695525	-6.194046	5.888281
H	-2.476244	-5.565901	4.249697
C	-2.500042	-3.366671	2.712368
C	-0.31664	-1.625564	3.12832
H	1.468132	-2.574326	4.951047
H	1.272895	-4.710268	6.216292
C	-1.256146	-1.371509	2.123018
C	-2.391367	-2.22749	1.944132
C	0.791178	-0.684201	3.334644
C	1.038441	-0.09116	4.60988
C	1.561399	-0.286602	2.236377
C	0.197383	-0.329116	5.734256

(S)-int3

C	-2.782076	6.685507	2.043361
C	-3.493584	5.672738	1.451065
C	-2.822732	4.570558	0.851116
C	-1.404872	4.532636	0.845599
C	-0.696717	5.594502	1.477733
C	-1.367371	6.640160	2.061918
H	-4.656012	3.577374	0.241876
H	-3.297668	7.537709	2.509950
H	-4.593749	5.691725	1.431885
C	-3.556562	3.50771	0.266320
C	-0.733704	3.427469	0.239658
H	0.404661	5.557065	1.490318
H	-0.812678	7.454420	2.551903
C	-1.487654	2.345127	-0.226409
C	-2.918999	2.407959	-0.265800
C	0.731468	3.364004	0.171055
C	1.490854	4.367263	-0.505597
C	1.389663	2.241811	0.682327
C	0.876641	5.469354	-1.165498

C	2.135811	0.794063	4.764899	C	2.903687	4.251598	-0.561183
C	2.691607	0.575148	2.404912	C	2.817424	2.143783	0.653191
C	0.452993	0.265243	6.945006	C	1.631881	6.411289	-1.819229
H	-0.672232	-0.993925	5.609943	H	-0.221996	5.547647	-1.150518
C	2.386458	1.387371	6.033538	C	3.664217	5.246728	-1.236165
C	2.96232	1.093003	3.651347	C	3.545321	3.135571	0.035451
C	1.564083	1.128063	7.100961	C	3.042631	6.304874	-1.850331
H	-0.20726	0.082881	7.806095	H	1.147882	7.255702	-2.332358
H	3.246869	2.066066	6.135069	H	4.759463	5.141027	-1.264282
H	3.823934	1.763647	3.799305	H	4.643989	3.066753	-0.015283
H	1.750952	1.590693	8.08111	H	3.627563	7.071992	-2.37854
O	1.330937	-0.809647	0.978517	O	0.694827	1.235900	1.326662
O	-1.199265	-0.230932	1.34944	O	-0.892565	1.229255	-0.776714
P	-0.000521	-0.159981	0.162781	P	-0.129862	0.156201	0.300186
O	0.169739	1.300824	-0.140989	O	0.765733	-0.715349	-0.546374
O	-0.260652	-1.128825	-0.963785	O	-1.136987	-0.524340	1.230351
H	0.23871	-1.084507	-2.507408	H	-1.237342	-1.934793	1.706227
N	0.540403	-1.346732	-3.491408	N	-1.432617	-2.946443	2.077601
C	3.570736	0.893274	1.274353	C	3.494379	0.998514	1.264468
C	3.224367	1.884712	0.344833	C	4.330378	0.177707	0.493175
C	4.779678	0.200304	1.134192	C	3.309042	0.721094	2.624624
C	4.09639	2.174474	-0.707765	C	5.003062	-0.885166	1.101137
H	2.260376	2.425207	0.432795	H	4.428908	0.352630	-0.596957
C	5.639512	0.504506	0.076613	C	3.981968	-0.351648	3.213231
H	5.053817	-0.585506	1.857679	H	2.620615	1.343736	3.220969
C	5.307535	1.494406	-0.848024	C	4.839224	-1.155400	2.460633
H	5.996684	1.741933	-1.672724	H	5.382226	-1.990102	2.934869
C	-3.433618	-1.902427	0.970537	C	-3.699106	1.331852	-0.876692
C	-3.942754	-2.902928	0.131903	C	-4.850006	0.849050	-0.240245
C	-3.944346	-0.598396	0.877185	C	-3.313223	0.784590	-2.110378
C	-4.955393	-2.601662	-0.781272	C	-5.603987	-0.165257	-0.834667
H	-3.535806	-3.926593	0.18205	H	-5.154639	1.258111	0.737382
C	-4.957336	-0.314347	-0.040047	C	-4.079742	-0.225329	-2.693276
H	-3.532017	0.199604	1.523023	H	-2.390497	1.142699	-2.603602
C	-5.472488	-1.309563	-0.873085	C	-5.22909	-0.707748	-2.063818
H	-6.274723	-1.077037	-1.593288	H	-5.82431	-1.512973	-2.526356
C	0.140763	-0.647837	-4.517487	C	-1.842777	-3.143294	3.302501
H	0.365127	-1.067709	-5.496376	H	-2.014079	-4.180896	3.599897
C	-0.568463	0.604715	-4.495424	C	-2.079658	-2.141231	4.337747
C	-1.070485	1.067322	-5.733629	C	-2.478455	-2.623166	5.590357
C	-0.759711	1.382202	-3.330933	C	-1.919187	-0.722202	4.157742
C	-1.767818	2.265365	-5.804921	C	-2.715914	-1.750081	6.649615
H	-0.913324	0.473965	-6.631477	H	-2.606608	-3.706075	5.750989
C	-1.45093	2.585375	-3.414816	C	-2.160109	0.124242	5.229628
H	-0.358466	1.077454	-2.370077	H	-1.615314	-0.327602	3.188531

C	-1.957156	3.023106	-4.644218	C	-2.555758	-0.377942	6.471786
H	-2.156825	2.612642	-6.757598	H	-3.027403	-2.149277	7.626567
H	-1.581857	3.188723	-2.519066	H	-2.033632	1.211027	5.096241
H	-2.494991	3.966146	-4.698617	H	-2.739436	0.312246	7.309938
C	1.309206	-2.539612	-3.555245	C	-1.231484	-3.976369	1.118915
C	2.133441	-2.839089	-4.64408	C	-1.727756	-5.276077	1.287936
C	1.236281	-3.423486	-2.464372	C	-0.493939	-3.653224	-0.069649
C	2.853857	-4.030653	-4.672214	C	-1.505411	-6.254373	0.321805
H	2.255596	-2.134912	-5.461656	H	-2.319743	-5.557345	2.173268
C	1.952796	-4.607058	-2.492853	C	-0.275417	-4.630541	-1.019414
H	0.620734	-3.159456	-1.611129	H	-0.089832	-2.649621	-0.219672
C	2.761625	-4.927704	-3.596793	C	-0.778849	-5.936026	-0.829762
H	3.49759	-4.237137	-5.518939	H	-1.908433	-7.265115	0.477735
H	1.90842	-5.304718	-1.663163	H	0.294821	-4.401256	-1.934422
P	-1.460625	4.463465	0.036562	P	2.565622	-0.79128	-3.707086
O	-1.192281	3.29327	1.123507	O	2.882196	-0.283365	-2.177287
O	-0.160408	5.45679	0.392815	O	4.146774	-0.660426	-4.292773
O	-2.65199	5.313294	0.845443	O	1.956644	0.656288	-4.337202
C	0.214143	6.284368	-0.691385	C	4.673045	-1.902067	-4.712430
C	0.022167	7.742554	-0.329892	C	5.893369	-2.254918	-3.887793
H	-0.369385	6.024722	-1.615035	H	4.973012	-1.778562	-5.793135
H	1.308135	6.080522	-0.883356	H	3.899406	-2.713136	-4.642249
H	0.441005	8.386237	-1.139138	H	6.337391	-3.205657	-4.266324
H	-1.058957	7.983653	-0.195981	H	6.653365	-1.440687	-3.96214
H	0.548922	7.969609	0.627748	H	5.630397	-2.379021	-2.808493
C	-3.891675	5.056872	0.207006	C	1.003370	0.338607	-5.33401
C	-4.952893	5.871028	0.909539	C	0.529359	1.631930	-5.955784
H	-4.115822	3.955975	0.26945	H	0.150360	-0.219249	-4.858591
H	-3.811829	5.344375	-0.876651	H	1.481721	-0.325710	-6.103778
H	-5.943553	5.680924	0.433292	H	-0.238078	1.411164	-6.734644
H	-5.002924	5.588407	1.988192	H	0.082915	2.293952	-5.176113
H	-4.714973	6.959248	0.843711	H	1.385681	2.172607	-6.424557
H	-0.709831	2.532041	0.705654	H	2.101224	-0.417008	-1.581495
C	6.944206	-0.264213	-0.084314	C	3.760557	-0.663700	4.686372
C	3.719469	3.230471	-1.739394	C	5.913173	-1.777845	0.266114
C	-5.509723	-3.699311	-1.680105	C	-6.857019	-0.676700	-0.135586
C	-5.499461	1.105395	-0.152894	C	-3.667892	-0.803314	-4.042614
F	6.848261	-1.370177	-0.8959	F	2.725764	-1.538016	4.926768
F	7.469835	-0.753916	1.086316	F	3.459798	0.426234	5.466539
F	7.971087	0.462937	-0.636604	F	4.834156	-1.242979	5.318671
F	4.792144	3.862514	-2.324158	F	6.904693	-2.406236	0.983726
F	3.011636	2.736828	-2.811157	F	5.26721	-2.808736	-0.372204
F	2.944731	4.257601	-1.265108	F	6.58933	-1.12796	-0.735995
F	-5.981511	-3.260174	-2.893692	F	-7.182004	-1.980087	-0.424163
F	-6.568108	-4.38956	-1.139469	F	-7.997744	0.027975	-0.437068

F	-4.605106	-4.680363	-2.008069	F	-6.797829	-0.642963	1.237075
F	-6.812303	1.1823	-0.553301	F	-4.031377	-2.115263	-4.232372
F	-4.831114	1.889926	-1.063684	F	-2.316701	-0.789489	-4.285006
F	-5.457464	1.832496	1.009814	F	-4.211408	-0.147544	-5.121364
O	3.421058	-6.109508	-3.521917	O	-0.495556	-6.818077	-1.844800
C	4.277624	-6.4846	-4.594188	C	-0.993727	-8.144739	-1.693456
H	4.690308	-7.455564	-4.317163	H	-0.643244	-8.657351	-2.625469
H	3.722137	-6.58009	-5.535782	H	-0.554878	-8.627944	-0.787213
H	5.095684	-5.764681	-4.722898	H	-2.109256	-8.14166	-1.639169

(*R*)-int3-mcp

C	1.728777	-3.717632	1.073032
P	-1.898971	-3.150166	-0.906445
C	1.727658	5.698809	-4.103547
C	2.600077	4.939015	-3.366011
C	2.146279	4.215818	-2.227217
C	0.784641	4.299598	-1.84075
C	-0.096429	5.091689	-2.631738
C	0.362326	5.769284	-3.73361
H	4.105246	3.420698	-1.747496
H	2.073213	6.255254	-4.987127
H	3.662786	4.869777	-3.643298
C	3.03804	3.414965	-1.472824
C	0.333674	3.571953	-0.69977
H	-1.158825	5.14251	-2.343542
H	-0.326291	6.372378	-4.3443
C	1.205476	2.67409	-0.071564
C	2.596974	2.653869	-0.411799
C	-1.049825	3.700113	-0.225021
C	-1.57795	4.961868	0.177258
C	-1.832856	2.550288	-0.078668
C	-0.788977	6.147217	0.192922
C	-2.927651	5.045038	0.60795
C	-3.202354	2.641271	0.316922
C	-1.323525	7.345765	0.595165
H	0.265325	6.081925	-0.119892
C	-3.461103	6.302029	1.008864
C	-3.725885	3.873941	0.644985
C	-2.677143	7.428195	1.001984
H	-0.704755	8.255458	0.609456
H	-4.512775	6.347809	1.330089
H	-4.780173	3.963922	0.952803
H	-3.085246	8.400321	1.315028
O	-1.339207	1.316945	-0.43441
O	0.80855	1.885039	0.985439

(*S*)-int3-mcp

C	1.092554	6.502283	-3.494082
C	2.060246	5.657026	-3.012942
C	1.764731	4.738196	-1.967328
C	0.464067	4.713374	-1.402399
C	-0.519824	5.597124	-1.931664
C	-0.213996	6.464883	-2.950332
H	3.7733	3.916621	-1.900212
H	1.316246	7.211482	-4.304451
H	3.079268	5.670573	-3.428062
C	2.754474	3.845269	-1.486366
C	0.170754	3.79119	-0.352377
H	-1.537179	5.564608	-1.5093
H	-0.982005	7.139446	-3.357728
C	1.130995	2.839163	0.009001
C	2.462859	2.909798	-0.516575
C	-1.147903	3.769011	0.292813
C	-1.671037	4.918659	0.957948
C	-1.863406	2.567156	0.336979
C	-0.932946	6.130944	1.076773
C	-2.957517	4.852777	1.551626
C	-3.172814	2.51244	0.912306
C	-1.460216	7.217475	1.729216
H	0.076649	6.177694	0.6385
C	-3.486591	5.997144	2.211121
C	-3.697067	3.643542	1.496701
C	-2.755073	7.154817	2.297454
H	-0.880577	8.148138	1.821308
H	-4.491185	5.929278	2.655516
H	-4.703662	3.620967	1.944349
H	-3.159507	8.039729	2.81023
O	-1.376466	1.435136	-0.283455
O	0.886124	1.882059	0.969738
P	-0.165469	0.614026	0.562801
O	-0.618121	0.01077	1.842792

P	-0.276119	0.614487	0.68249	O	0.436696	-0.268121	-0.530665
O	-0.90663	0.295217	1.990413	H	1.390356	-1.654196	-0.383419
O	0.356046	-0.492479	-0.149082	N	1.876655	-2.588198	-0.360848
H	1.232054	-1.910766	0.228642	C	-3.965834	1.278434	0.878145
N	1.826407	-2.776252	0.179839	C	-3.752983	0.261028	1.819553
C	-4.071842	1.45894	0.354296	C	-4.961843	1.129465	-0.095128
C	-3.99768	0.54098	1.412503	C	-4.552699	-0.883499	1.787141
C	-5.011378	1.26769	-0.669008	H	-2.944012	0.348887	2.571416
C	-4.866014	-0.550912	1.435995	C	-5.750715	-0.022682	-0.113406
H	-3.247854	0.670564	2.218914	H	-5.116863	1.914615	-0.853701
C	-5.879848	0.174361	-0.622637	C	-5.554433	-1.034264	0.826416
H	-5.066781	1.979007	-1.510021	H	-6.177774	-1.943811	0.806693
C	-5.813683	-0.740874	0.427819	C	3.521911	2.035569	-0.012853
H	-6.501199	-1.601826	0.466352	C	4.417604	1.429592	-0.903642
C	3.564568	1.89398	0.377189	C	3.676749	1.82837	1.367465
C	4.644821	1.260466	-0.252641	C	5.459258	0.636862	-0.416953
C	3.459438	1.841334	1.776064	H	4.302207	1.579206	-1.990119
C	5.615628	0.607781	0.510827	C	4.730948	1.045091	1.838228
H	4.729619	1.274404	-1.352118	H	2.955216	2.282424	2.072319
C	4.427107	1.169933	2.523404	C	5.63083	0.446263	0.954064
H	2.605782	2.331354	2.281409	H	6.470173	-0.159059	1.335116
C	5.515282	0.556056	1.901849	C	2.261307	-3.149322	-1.472998
H	6.286909	0.0431	2.500147	H	2.629355	-4.167892	-1.38337
H	2.328129	-4.60586	0.880878	C	2.267569	-2.580139	-2.800129
C	0.922367	-3.720802	2.267549	C	2.716207	-3.42449	-3.839174
C	1.007684	-4.864322	3.092693	C	1.866604	-1.261062	-3.105157
C	0.061142	-2.663162	2.627666	C	2.767785	-2.966696	-5.150491
C	0.250395	-4.945728	4.254923	H	3.022439	-4.441681	-3.607087
H	1.66773	-5.681651	2.812631	C	1.921078	-0.815094	-4.419767
C	-0.695867	-2.756041	3.78641	H	1.500936	-0.602344	-2.324915
H	-0.037472	-1.770898	2.024802	C	2.370714	-1.658935	-5.441552
C	-0.60284	-3.89158	4.599937	H	3.11623	-3.623625	-5.941958
H	0.318936	-5.825079	4.887991	H	1.603639	0.19691	-4.651732
H	-1.363364	-1.937875	4.038188	H	2.409488	-1.296744	-6.465251
H	-1.200033	-3.956465	5.505526	C	1.978026	-3.175985	0.931165
C	2.675081	-2.844495	-0.972902	C	2.94068	-4.148435	1.220828
C	3.907648	-3.490819	-0.922848	C	1.092348	-2.7387	1.93067
C	2.23867	-2.2409	-2.162984	C	3.000833	-4.720347	2.488522
C	4.706875	-3.571484	-2.065834	H	3.676873	-4.44278	0.478675
H	4.277598	-3.90387	0.0109	C	1.155949	-3.307278	3.191236
C	3.03107	-2.319514	-3.29551	H	0.360563	-1.960022	1.734804
H	1.276196	-1.742286	-2.197432	C	2.099026	-4.306782	3.482136
C	4.269075	-2.987794	-3.260687	H	3.762298	-5.462396	2.69705
H	5.670677	-4.063032	-2.001288	H	0.477823	-2.984073	3.973713
H	2.712191	-1.870505	-4.230097	P	-1.603117	-3.171424	-1.254372

O	-1.370282	-1.86887	-1.794076	O	-1.361662	-1.756748	-2.039781
O	-0.826114	-4.366882	-1.32764	O	-0.685363	-4.252023	-2.162131
O	-3.216264	-3.451264	-1.89037	O	-3.146761	-3.411973	-1.860566
C	-0.6219	-4.53896	-2.71935	C	-0.903073	-4.216227	-3.564881
C	-1.08061	-5.916417	-3.136876	C	-1.537073	-5.509411	-4.030735
H	0.485476	-4.425392	-2.9016	H	0.113062	-4.092722	-4.038945
H	-1.170431	-3.741518	-3.288996	H	-1.545849	-3.334456	-3.830859
H	-0.830671	-6.08268	-4.211206	H	-1.582824	-5.521462	-5.145427
H	-0.577756	-6.698203	-2.519775	H	-0.940575	-6.384804	-3.680254
H	-2.184423	-6.017298	-3.001933	H	-2.573934	-5.604956	-3.625815
C	-4.123137	-4.27906	-1.175352	C	-3.776469	-4.411393	-1.069117
C	-5.32825	-4.507057	-2.0567	C	-5.185116	-4.588625	-1.58429
H	-4.407468	-3.765675	-0.216472	H	-3.771675	-4.081441	0.005779
H	-3.605673	-5.244924	-0.929702	H	-3.183771	-5.361592	-1.161011
H	-6.076143	-5.128089	-1.509636	H	-5.707527	-5.364294	-0.976074
H	-5.792978	-3.530218	-2.337366	H	-5.748687	-3.625719	-1.517184
H	-5.028722	-5.033395	-2.994199	H	-5.16846	-4.908985	-2.653383
H	-0.834896	-1.267063	-1.220072	H	-0.813726	-1.143151	-1.490111
C	-6.901378	-0.032771	-1.732775	C	-6.845761	-0.179639	-1.160466
C	-4.806487	-1.581491	2.555726	C	-4.330436	-2.004848	2.794516
C	6.818143	-0.037388	-0.168086	C	6.414759	-0.043895	-1.38806
C	4.296085	1.09371	4.040081	C	4.909591	0.824153	3.336557
F	-6.462558	-0.825131	-2.765922	F	-7.066834	-1.474577	-1.563675
F	-7.316989	1.123633	-2.346408	F	-6.62952	0.508587	-2.328514
F	-8.068962	-0.633705	-1.32538	F	-8.083476	0.25324	-0.744439
F	-5.995518	-1.746525	3.2291	F	-5.489613	-2.598205	3.239384
F	-4.495014	-2.852284	2.124189	F	-3.593199	-3.058806	2.30766
F	-3.894108	-1.334543	3.547928	F	-3.682766	-1.636018	3.945444
F	7.113743	-1.303247	0.284936	F	6.085467	-1.350117	-1.670138
F	7.995197	0.653873	-0.00784	F	7.715397	-0.117416	-0.953707
F	6.70436	-0.189847	-1.528466	F	6.502261	0.550094	-2.623075
F	5.495724	1.06978	4.711012	F	6.221642	0.757375	3.742243
F	3.645608	-0.031833	4.486362	F	4.360532	-0.347852	3.798364
F	3.609274	2.135298	4.610614	F	4.359107	1.797561	4.131035
O	4.96258	-3.00142	-4.423528	O	2.072735	-4.794616	4.746769
C	6.233483	-3.636092	-4.447918	C	3.011623	-5.796804	5.114056
H	6.153082	-4.702872	-4.204122	H	4.042838	-5.431484	5.026237
H	6.60049	-3.525373	-5.468527	H	2.799714	-6.03269	6.157877
H	6.93454	-3.154743	-3.754514	H	2.891327	-6.701759	4.504805
<i>(R)</i> -TS4-mcp				<i>(S)</i> -TS4-mcp			
C	1.623192	-3.634992	0.380754	C	-0.264367	-3.730707	1.507548
P	-0.354022	-3.871817	-1.030322	P	1.483317	-2.509627	2.56263
C	1.595459	5.728492	-4.0249	C	-3.916157	5.134413	3.535431
C	2.443544	5.033687	-3.199812	C	-4.446282	4.072687	2.846693

C	1.936064	4.303908	-2.088745	C	-3.714605	3.453633	1.795014
C	0.543506	4.313217	-1.821591	C	-2.436331	3.95523	1.44101
C	-0.310145	5.039275	-2.700613	C	-1.911245	5.052967	2.181375
C	0.202242	5.72472	-3.773976	C	-2.630397	5.623815	3.201846
H	3.890798	3.637537	-1.424737	H	-5.270597	2.010456	1.340754
H	1.983596	6.290147	-4.887235	H	-4.477219	5.613031	4.351409
H	3.528413	5.023798	-3.383977	H	-5.442687	3.678245	3.09668
C	2.805778	3.570906	-1.243311	C	-4.248232	2.34167	1.096868
C	0.037465	3.576514	-0.708102	C	-1.704756	3.33264	0.384467
H	-1.394324	5.033121	-2.503576	H	-0.909331	5.430736	1.920944
H	-0.464694	6.276869	-4.453036	H	-2.214439	6.466895	3.773633
C	0.902293	2.740168	0.007033	C	-2.195	2.148122	-0.178268
C	2.319286	2.800561	-0.207735	C	-3.519189	1.688722	0.12551
C	-1.384139	3.630382	-0.345208	C	-0.417222	3.871709	-0.070811
C	-2.012307	4.867975	-0.009599	C	-0.30372	5.206215	-0.566207
C	-2.108664	2.438863	-0.22831	C	0.697719	3.027891	-0.117427
C	-1.297775	6.099594	0.028919	C	-1.425556	6.077213	-0.674386
C	-3.389608	4.87944	0.328769	C	0.960963	5.683439	-0.996657
C	-3.503251	2.457973	0.092631	C	1.969674	3.511677	-0.559989
C	-1.928994	7.272528	0.360546	C	-1.284073	7.356045	-1.152724
H	-0.221835	6.092569	-0.207341	H	-2.4159	5.701527	-0.371615
C	-4.023631	6.110324	0.656585	C	1.083852	7.017919	-1.474846
C	-4.117263	3.662531	0.354105	C	2.085742	4.819376	-0.97335
C	-3.309943	7.282062	0.670993	C	-0.013759	7.837783	-1.549663
H	-1.367463	8.218198	0.392717	H	-2.157624	8.019732	-1.236942
H	-5.095834	6.098787	0.904609	H	2.076722	7.373223	-1.789909
H	-5.190659	3.695805	0.600898	H	3.058459	5.211425	-1.31112
H	-3.795889	8.234682	0.927722	H	0.077143	8.868481	-1.922423
O	-1.53066	1.227052	-0.541618	O	0.629324	1.740956	0.371391
O	0.455456	1.935	1.031894	O	-1.495753	1.450276	-1.139529
P	-0.49246	0.589134	0.633662	P	-0.109062	0.611066	-0.652587
O	-1.177029	0.168963	1.882861	O	0.662952	0.313676	-1.885164
O	0.314593	-0.426359	-0.178046	O	-0.455642	-0.506345	0.334973
H	1.695908	-1.616085	0.196883	H	-0.604627	-2.375015	0.034909
N	2.172516	-2.491006	-0.061319	N	-0.285236	-3.335047	0.215898
C	-4.293586	1.222811	0.138362	C	3.138219	2.625516	-0.602043
C	-4.265286	0.392444	1.268077	C	3.38364	1.84505	-1.741479
C	-5.11257	0.891286	-0.947896	C	4.020085	2.569954	0.48352
C	-5.077624	-0.743158	1.307228	C	4.535477	1.057465	-1.803389
H	-3.592398	0.619587	2.118234	H	2.657218	1.828836	-2.576119
C	-5.913763	-0.251533	-0.893643	C	5.153937	1.757411	0.414384
H	-5.120527	1.526089	-1.849467	H	3.814069	3.156784	1.394239
C	-5.906135	-1.073458	0.233056	C	5.426934	1.008125	-0.730979
H	-6.544466	-1.971802	0.274447	H	6.335355	0.385641	-0.784843
C	3.25567	2.113779	0.68202	C	-4.124969	0.577973	-0.609034

C	4.409721	1.510628	0.162013	C	-4.904331	-0.371091	0.065953
C	3.040316	2.099077	2.069651	C	-3.973981	0.477101	-2.001678
C	5.338539	0.919214	1.020045	C	-5.536655	-1.392923	-0.64517
H	4.588003	1.504441	-0.926455	H	-5.020688	-0.312784	1.161129
C	3.975861	1.499387	2.913715	C	-4.612328	-0.54954	-2.698166
H	2.12604	2.560459	2.488221	H	-3.343175	1.209758	-2.539227
C	5.132645	0.910854	2.399996	C	-5.400351	-1.488902	-2.030079
H	5.877732	0.455737	3.073635	H	-5.914688	-2.288176	-2.589591
H	2.08046	-4.534687	-0.019899	H	0.199407	-4.699562	1.661381
C	1.056728	-3.765051	1.740879	C	-1.381406	-3.443212	2.439523
C	1.209125	-4.999195	2.395047	C	-1.647507	-4.390846	3.440974
C	0.381766	-2.717965	2.389079	C	-2.169007	-2.282648	2.361667
C	0.719199	-5.175412	3.687863	C	-2.695385	-4.19859	4.337669
H	1.720677	-5.817841	1.89359	H	-1.032767	-5.284948	3.513624
C	-0.112275	-2.903302	3.677379	C	-3.211839	-2.09496	3.265637
H	0.203163	-1.767943	1.900544	H	-1.953679	-1.522679	1.617393
C	0.059176	-4.126402	4.332059	C	-3.481688	-3.048727	4.25056
H	0.851768	-6.130068	4.189318	H	-2.897304	-4.944809	5.100814
H	-0.63962	-2.08362	4.154723	H	-3.81728	-1.195446	3.20099
H	-0.326781	-4.264272	5.338548	H	-4.300758	-2.894787	4.947798
C	2.957066	-2.41169	-1.246729	C	0.614707	-3.855754	-0.755009
C	3.960107	-3.345407	-1.514661	C	0.906872	-5.222275	-0.810922
C	2.729194	-1.359789	-2.148534	C	1.195131	-2.985127	-1.694297
C	4.717948	-3.256477	-2.682858	C	1.788054	-5.723657	-1.770099
H	4.181204	-4.132953	-0.799607	H	0.42257	-5.91738	-0.13069
C	3.488583	-1.263504	-3.304491	C	2.065728	-3.485436	-2.65165
H	1.947554	-0.637881	-1.934258	H	0.971749	-1.921053	-1.683104
C	4.484418	-2.212129	-3.586548	C	2.375881	-4.853737	-2.697375
H	5.495915	-3.988955	-2.863289	H	1.989792	-6.788247	-1.793699
H	3.3215	-0.460636	-4.01527	H	2.532033	-2.817487	-3.370682
O	-1.033155	-2.433719	-1.244238	O	1.396685	-0.979668	2.110993
O	0.134017	-4.415645	-2.492694	O	1.236236	-2.584295	4.171621
O	-1.639507	-4.873062	-0.762505	O	3.096619	-2.859795	2.503141
C	-0.733829	-4.189906	-3.599797	C	1.849905	-1.58119	4.977251
C	-1.314202	-5.497978	-4.089679	C	2.943976	-2.186661	5.828069
H	-0.090646	-3.727501	-4.400927	H	1.028489	-1.175223	5.632965
H	-1.541872	-3.468256	-3.306057	H	2.246217	-0.760108	4.322641
H	-1.892089	-5.315799	-5.026922	H	3.326077	-1.415048	6.538203
H	-0.49813	-6.22936	-4.300729	H	2.548277	-3.053295	6.40933
H	-1.995474	-5.942379	-3.324562	H	3.790019	-2.545267	5.19351
C	-2.260223	-4.543322	0.477205	C	3.584748	-2.704089	1.173784
C	-3.409368	-5.497015	0.692982	C	5.077608	-2.924015	1.197011
H	-2.616483	-3.478316	0.426799	H	3.3294	-1.66949	0.816378
H	-1.490178	-4.633807	1.291659	H	3.063422	-3.457494	0.521865
H	-3.979083	-5.174639	1.598342	H	5.461666	-2.952041	0.149562

H	-4.090379	-5.489063	-0.191463	H	5.582332	-2.094172	1.750016
H	-3.03567	-6.537743	0.839528	H	5.322397	-3.887131	1.70484
H	-0.524746	-1.64052	-0.857741	H	0.651968	-0.751589	1.444713
C	-6.820044	-0.594066	-2.068839	C	6.117886	1.670988	1.590216
C	-5.057849	-1.650689	2.530654	C	4.821766	0.231241	-3.051432
C	6.597257	0.268219	0.461032	C	-6.379987	-2.425551	0.091705
C	3.733583	1.474204	4.419028	C	-4.444789	-0.661843	-4.210007
F	-6.346686	-0.192091	-3.293916	F	6.420971	0.385117	1.972887
F	-8.071791	-0.029487	-1.994499	F	5.683605	2.272402	2.745288
F	-7.069598	-1.935829	-2.226965	F	7.345411	2.243835	1.355613
F	-6.268107	-2.239294	2.817093	F	6.160263	0.03882	-3.305467
F	-4.195805	-2.717252	2.428777	F	4.310553	-1.043815	-3.018623
F	-4.701674	-1.036236	3.704169	F	4.334619	0.76504	-4.21773
F	6.570639	-1.106656	0.470688	F	-5.72159	-3.60228	0.359845
F	7.747025	0.581314	1.144891	F	-7.510119	-2.821802	-0.58082
F	6.883826	0.587304	-0.843649	F	-6.844149	-2.017316	1.319078
F	4.879934	1.507629	5.176954	F	-5.549109	-1.15515	-4.863815
F	3.076918	0.350308	4.860075	F	-3.426438	-1.497336	-4.599769
F	2.982484	2.518453	4.896553	F	-4.178466	0.524393	-4.846363
O	5.166322	-2.025826	-4.750469	O	3.245078	-5.234998	-3.674363
C	6.202738	-2.93897	-5.079802	C	3.577513	-6.610021	-3.78332
H	5.819213	-3.962213	-5.18661	H	2.691333	-7.224138	-3.991395
H	6.603475	-2.602279	-6.037308	H	4.271897	-6.683659	-4.621979
H	7.002695	-2.928302	-4.327787	H	4.068214	-6.980587	-2.873284

(R)-TS4

C	0.206199	-3.735622	1.396088
P	1.120592	-3.627412	-0.861516
C	-2.919922	6.541624	2.872822
C	-3.660685	5.41436	2.62092
C	-3.178945	4.415987	1.728934
C	-1.930173	4.598411	1.082111
C	-1.183859	5.776905	1.369043
C	-1.664994	6.720309	2.242553
H	-4.928597	3.147812	1.938761
H	-3.287036	7.313354	3.565266
H	-4.63589	5.25899	3.106611
C	-3.932647	3.24249	1.476553
C	-1.446417	3.589283	0.195992
H	-0.206804	5.912357	0.87801
H	-1.079211	7.624863	2.464895
C	-2.144919	2.382617	0.083274
C	-3.446481	2.239542	0.664455
C	-0.190311	3.758272	-0.543036
C	-0.020292	4.841789	-1.456693

(S)-TS4

C	-0.185816	-3.743843	0.633496
P	1.64998	-3.510402	-0.806538
C	1.675031	6.816657	-3.347356
C	2.568534	5.829481	-3.015779
C	2.227227	4.836795	-2.055238
C	0.960441	4.882589	-1.419851
C	0.052685	5.914366	-1.793736
C	0.400367	6.853364	-2.732851
H	4.133725	3.807584	-2.198532
H	1.933586	7.582983	-4.09275
H	3.560661	5.782793	-3.489768
C	3.13611	3.799099	-1.730089
C	0.622416	3.882786	-0.458272
H	-0.940586	5.939257	-1.317695
H	-0.309468	7.643079	-3.021251
C	1.489555	2.803392	-0.256086
C	2.794262	2.796268	-0.847573
C	-0.656148	3.919112	0.260969
C	-1.012956	5.036007	1.075016

C	0.811735	2.787798	-0.426823	C	-1.491726	2.796577	0.224882
C	-1.056682	5.78141	-1.726064	C	-0.141727	6.14644	1.269042
C	1.208855	4.980213	-2.149644	C	-2.264074	5.03867	1.742475
C	2.063499	2.954281	-1.097733	C	-2.758093	2.810511	0.889251
C	-0.8649	6.807538	-2.617234	C	-0.512813	7.204793	2.06024
H	-2.021997	5.664802	-1.208215	H	0.842523	6.136739	0.773941
C	1.387077	6.059337	-3.059885	C	-2.631412	6.154319	2.545917
C	2.242106	4.034379	-1.935333	C	-3.126153	3.920741	1.618079
C	0.372943	6.954665	-3.288253	C	-1.775383	7.215147	2.700694
H	-1.672925	7.525441	-2.82332	H	0.168497	8.056053	2.208501
H	2.35263	6.154072	-3.579454	H	-3.612701	6.142365	3.043999
H	3.200367	4.174049	-2.461477	H	-4.100977	3.948187	2.13123
H	0.505125	7.787927	-3.993833	H	-2.053904	8.077687	3.323729
O	0.677004	1.719934	0.435669	O	-1.175521	1.701268	-0.554552
O	-1.667192	1.343197	-0.690288	O	1.173313	1.774264	0.610103
P	-0.363953	0.477199	-0.040724	P	0.009076	0.672826	0.065933
O	0.17772	-0.2874	-1.225744	O	-0.458966	-0.076943	1.278815
O	-0.722766	-0.236285	1.231839	O	0.475418	-0.103541	-1.148079
H	-0.049018	-1.758658	1.831789	H	-0.970238	-1.843077	0.729725
N	0.545522	-2.589453	1.99525	N	-1.123907	-2.799659	0.380744
C	3.184285	2.026295	-0.909622	C	-3.682179	1.673135	0.824099
C	3.301996	0.871716	-1.696592	C	-3.529178	0.58337	1.692066
C	4.190287	2.347465	0.010057	C	-4.762369	1.704668	-0.066623
C	4.458357	0.094583	-1.605987	C	-4.481789	-0.439098	1.691579
H	2.478592	0.568899	-2.371162	H	-2.649558	0.519005	2.360572
C	5.324637	1.538948	0.112423	C	-5.696256	0.666098	-0.064698
H	4.088928	3.236886	0.653796	H	-4.874509	2.545185	-0.771808
C	5.472716	0.41661	-0.701539	C	-5.5701	-0.40626	0.81907
H	6.375517	-0.212493	-0.632632	H	-6.317246	-1.217782	0.821614
C	-4.28689	1.079822	0.370127	C	3.779585	1.768664	-0.512268
C	-5.015934	0.458262	1.393204	C	4.540373	1.170391	-1.526992
C	-4.415639	0.617838	-0.948883	C	4.004816	1.408199	0.823992
C	-5.876429	-0.598735	1.091728	C	5.525518	0.237401	-1.200916
H	-4.903839	0.798846	2.436559	H	4.349616	1.424735	-2.583381
C	-5.288419	-0.433115	-1.235032	C	4.997894	0.47719	1.133932
H	-3.819083	1.087166	-1.752936	H	3.382018	1.850801	1.62207
C	-6.025305	-1.047772	-0.221422	C	5.762565	-0.116171	0.128084
H	-6.719388	-1.872581	-0.453682	H	6.531038	-0.867561	0.376511
H	0.862604	-4.574269	1.609248	H	-0.445849	-4.719035	0.227273
C	-1.204063	-4.116766	1.166262	C	0.510482	-3.805998	1.947815
C	-1.486605	-5.486841	1.035695	C	1.007136	-5.05115	2.36972
C	-2.256338	-3.18724	1.107747	C	0.669791	-2.682966	2.777134
C	-2.795929	-5.928529	0.863483	C	1.641626	-5.179332	3.603613
H	-0.673617	-6.208602	1.072524	H	0.89366	-5.92193	1.728197
C	-3.564239	-3.638278	0.939448	C	1.305315	-2.820572	4.010715

H	-2.056965	-2.122964	1.190489	H	0.302079	-1.709326	2.46791
C	-3.839906	-5.003054	0.81868	C	1.790689	-4.062139	4.428445
H	-2.999861	-6.991428	0.769868	H	2.013652	-6.149484	3.920906
H	-4.379876	-2.918232	0.908948	H	1.421695	-1.948276	4.647516
H	-4.864772	-5.341711	0.692509	C	-2.077484	-2.963524	-0.666548
C	1.822332	-2.280809	2.52326	C	-2.933469	-4.069375	-0.663474
C	2.903276	-3.166155	2.499604	C	-2.182663	-2.015565	-1.698815
C	1.980141	-1.018984	3.124406	C	-3.878715	-4.247011	-1.675101
C	4.118312	-2.814869	3.093111	H	-2.886547	-4.783139	0.155194
H	2.833806	-4.12981	2.005694	C	-3.132892	-2.181862	-2.698136
C	3.183719	-0.670967	3.712166	H	-1.50963	-1.164585	-1.720659
H	1.152868	-0.317112	3.1108	C	-3.985299	-3.296759	-2.699224
C	4.263496	-1.569088	3.712931	H	-4.53385	-5.10989	-1.640236
H	4.940235	-3.52064	3.057056	H	-3.227828	-1.45609	-3.499592
H	3.31485	0.299149	4.180656	O	2.135854	-2.016252	-1.01722
O	1.85708	-2.247528	-1.204758	O	2.955777	-4.315874	-0.247544
O	2.311923	-4.741078	-0.868723	O	1.631989	-4.294167	-2.255226
O	0.26126	-4.088454	-2.201345	C	3.686977	-3.681136	0.794293
C	3.209201	-4.740261	-1.976474	C	5.158492	-3.710414	0.448993
C	3.003028	-5.977166	-2.821338	H	3.495493	-4.272849	1.736226
H	4.244177	-4.73653	-1.530172	H	3.331867	-2.625016	0.931109
H	3.069535	-3.799774	-2.575703	H	5.736959	-3.24	1.281486
H	3.795035	-6.020893	-3.606506	H	5.503043	-4.761937	0.306056
H	3.065502	-6.894763	-2.189331	H	5.35529	-3.14564	-0.495109
H	2.002506	-5.957922	-3.317046	C	0.402843	-4.234344	-2.960525
C	-0.85709	-3.220911	-2.374425	C	-0.16207	-5.630165	-3.116233
C	-1.608241	-3.670101	-3.603353	H	0.638215	-3.803112	-3.975648
H	-0.48074	-2.165181	-2.481167	H	-0.324528	-3.556115	-2.436143
H	-1.499159	-3.294228	-1.453442	H	-1.013782	-5.606616	-3.836781
H	-2.527812	-3.046231	-3.718728	H	0.626506	-6.319062	-3.504509
H	-0.969471	-3.555162	-4.511177	H	-0.526118	-6.030167	-2.140251
H	-1.900728	-4.743198	-3.512836	H	1.420559	-1.255741	-1.041446
H	1.234494	-1.430879	-1.173262	C	-6.881837	0.718449	-1.020237
C	6.426166	1.910069	1.096579	C	-4.330703	-1.589737	2.678678
C	4.661829	-1.107881	-2.519866	C	6.365577	-0.404283	-2.298731
C	-6.687493	-1.268297	2.194175	C	5.267406	0.11475	2.588628
C	-5.440578	-0.921405	-2.671227	F	-7.394353	-0.509581	-1.362982
F	7.193959	0.853076	1.522728	F	-6.618096	1.322768	-2.22482
F	5.982634	2.495575	2.257022	F	-7.966264	1.40694	-0.530411
F	7.342839	2.806805	0.600419	F	-4.561299	-1.240696	3.987497
F	3.575848	-1.472838	-3.271066	F	-5.178347	-2.650733	2.463619
F	5.661856	-0.926244	-3.449573	F	-3.082698	-2.16286	2.698473
F	5.036346	-2.258648	-1.867521	F	6.620559	-1.740806	-2.108148
F	-8.018303	-0.927592	2.200869	F	7.614318	0.154476	-2.442762
F	-6.26352	-0.997416	3.471433	F	5.823524	-0.335436	-3.557721

F	-6.694105	-2.641945	2.125182	F	6.196904	0.916743	3.20619
F	-4.569137	-1.926262	-3.017909	F	5.750151	-1.159176	2.778442
F	-5.243482	0.0435	-3.626927	F	4.169631	0.179474	3.411205
F	-6.678765	-1.441006	-2.964557	H	2.283078	-4.158873	5.392369
O	5.39643	-1.13333	4.330806	O	-4.873875	-3.363794	-3.72962
C	6.530259	-1.986601	4.339	C	-5.797709	-4.441276	-3.754984
H	6.87731	-2.205502	3.320466	H	-6.437939	-4.444236	-2.863032
H	7.309369	-1.442095	4.875464	H	-6.414701	-4.284043	-4.641347
H	6.321153	-2.930107	4.860733	H	-5.286645	-5.409967	-3.836436

(R)-TS4-mcp

C	-2.276212	-3.272056	-0.095349
P	-0.110664	-4.024105	0.651677
C	-1.150356	5.772313	3.975905
C	-2.044824	5.112846	3.171024
C	-1.592134	4.35264	2.056772
C	-0.205572	4.293227	1.765391
C	0.696704	4.984239	2.623956
C	0.236388	5.700822	3.700604
H	-3.588434	3.775133	1.429834
H	-1.496178	6.357891	4.840364
H	-3.125573	5.156059	3.373733
C	-2.51083	3.657963	1.230876
C	0.246992	3.524645	0.649969
H	1.775822	4.925762	2.408137
H	0.940696	6.22591	4.363269
C	-0.66953	2.729956	-0.047918
C	-2.077945	2.862992	0.190928
C	1.665454	3.502282	0.271752
C	2.35403	4.700391	-0.087268
C	2.326191	2.273469	0.167081
C	1.705448	5.967585	-0.132515
C	3.725728	4.633863	-0.442027
C	3.715229	2.213256	-0.173987
C	2.393705	7.101123	-0.487089
H	0.634058	6.020444	0.117981
C	4.419604	5.825132	-0.79377
C	4.388081	3.37959	-0.460626
C	3.768921	7.03301	-0.814841
H	1.882988	8.074983	-0.524256
H	5.486424	5.753623	-1.05476
H	5.457939	3.3528	-0.723057
H	4.30146	7.95505	-1.090142
O	1.68809	1.101903	0.508053
O	-0.287511	1.896399	-1.074045

(S)-TS4-mcp

C	-0.182070	-3.880299	1.368074
P	1.334568	-2.585006	2.686164
C	-3.891903	5.000821	3.652190
C	-4.442117	3.973575	2.927668
C	-3.719443	3.373769	1.858878
C	-2.428934	3.857679	1.527288
C	-1.884112	4.921375	2.302053
C	-2.595294	5.474242	3.337989
H	-5.310386	1.997170	1.336976
H	-4.445398	5.463957	4.482165
H	-5.447294	3.592155	3.162135
C	-4.274263	2.301542	1.117052
C	-1.706415	3.25153	0.455177
H	-0.874192	5.286722	2.055507
H	-2.164382	6.29016	3.937449
C	-2.211126	2.089000	-0.139103
C	-3.552270	1.657584	0.133400
C	-0.420484	3.799104	0.007304
C	-0.320738	5.143143	-0.465599
C	0.699934	2.963981	-0.054812
C	-1.450288	6.006437	-0.555006
C	0.937774	5.638728	-0.892281
C	1.966246	3.468687	-0.488965
C	-1.321467	7.293926	-1.013238
H	-2.436435	5.618534	-0.254114
C	1.047816	6.981432	-1.350178
C	2.069251	4.784181	-0.882747
C	-0.05703	7.792842	-1.407868
H	-2.200913	7.951523	-1.082871
H	2.036467	7.349965	-1.663248
H	3.038544	5.190265	-1.214057
H	0.02342	8.830013	-1.764762
O	0.642877	1.669386	0.411126
O	-1.514128	1.398826	-1.104598

P	0.61507	0.494009	-0.680188	P	-0.107634	0.545784	-0.637951
O	1.289569	0.048604	-1.935917	O	0.654994	0.274541	-1.896146
O	-0.247706	-0.477694	0.160888	O	-0.450343	-0.606701	0.335489
H	-1.826755	-1.312854	0.251388	H	-0.385251	-2.442142	-0.069791
N	-2.410603	-2.104847	0.568212	N	-0.052787	-3.402907	0.107892
C	4.430512	0.932953	-0.216307	C	3.154694	2.61018	-0.541628
C	4.346086	0.100767	-1.341932	C	3.430421	1.864281	-1.696815
C	5.226065	0.552333	0.870976	C	4.041257	2.571182	0.540968
C	5.076988	-1.089259	-1.374833	C	4.621461	1.139605	-1.781374
H	3.691418	0.367882	-2.194808	H	2.701621	1.833065	-2.528862
C	5.944474	-0.644592	0.823694	C	5.214449	1.818862	0.449689
H	5.286992	1.195037	1.764754	H	3.81355	3.131993	1.462950
C	5.878723	-1.471396	-0.297897	C	5.520463	1.112252	-0.714204
H	6.457931	-2.409261	-0.335795	H	6.464421	0.547392	-0.790858
C	-3.057515	2.22323	-0.686859	C	-4.19042	0.597499	-0.646918
C	-4.211774	1.635171	-0.152248	C	-5.074549	-0.295013	-0.024671
C	-2.87708	2.238747	-2.079421	C	-3.977579	0.494854	-2.031490
C	-5.172269	1.080625	-1.000814	C	-5.743986	-1.261252	-0.777563
H	-4.366569	1.612422	0.939557	H	-5.243293	-0.236533	1.063736
C	-3.848541	1.684675	-2.914197	C	-4.646506	-0.482852	-2.768900
H	-1.960777	2.686397	-2.507913	H	-3.276689	1.188468	-2.533360
C	-5.003589	1.105574	-2.385456	C	-5.536051	-1.365219	-2.152950
H	-5.775637	0.683673	-3.050912	H	-6.067884	-2.129895	-2.743422
H	-2.797417	-4.119991	0.349563	H	0.321035	-4.831166	1.544414
C	-2.116975	-3.320108	-1.571176	C	-1.418769	-3.685441	2.171984
C	-2.272742	-4.561372	-2.196927	C	-1.615946	-4.546805	3.256670
C	-1.845359	-2.170285	-2.369569	C	-2.421475	-2.719628	1.859612
C	-2.160898	-4.675092	-3.581835	C	-2.777487	-4.470032	4.023128
H	-2.488687	-5.462108	-1.59952	H	-0.848348	-5.292391	3.521362
C	-1.735758	-2.301874	-3.745843	C	-3.571667	-2.66221	2.632870
H	-1.711593	-1.197493	-1.909337	H	-2.272985	-2.023887	1.038117
C	-1.889749	-3.549562	-4.356759	C	-3.756636	-3.529893	3.712360
H	-2.284258	-5.659411	-4.058763	H	-2.914147	-5.152987	4.875100
H	-1.523656	-1.40944	-4.360665	H	-4.356713	-1.927884	2.386286
H	-1.793223	-3.639894	-5.450092	H	-4.676155	-3.467894	4.314841
C	-2.845424	-1.989426	1.914143	C	0.953971	-3.856017	-0.789619
C	-3.763204	-2.88597	2.476502	C	1.394444	-5.1867	-0.774571
C	-2.372751	-0.888276	2.701377	C	1.484431	-2.955207	-1.774019
C	-4.212597	-2.716325	3.785082	C	2.345060	-5.635367	-1.689375
H	-4.159788	-3.736183	1.898689	H	0.987841	-5.917219	-0.056947
C	-2.823723	-0.722596	3.99399	C	2.423391	-3.408233	-2.677608
H	-1.642976	-0.209197	2.263537	H	1.144672	-1.918348	-1.815765
C	-3.747649	-1.638805	4.543235	C	2.860554	-4.75063	-2.639952
H	-4.931201	-3.436433	4.201853	H	2.671360	-6.684419	-1.652535
H	-2.465917	0.115145	4.612561	H	2.850188	-2.721065	-3.428843

O	0.796718	-2.713486	0.857475	O	1.125021	-1.044653	2.291052
O	-0.354003	-4.713768	2.128997	O	1.031713	-2.747723	4.295813
O	0.921332	-5.143285	-0.022149	O	2.987014	-2.802963	2.689096
C	0.702575	-4.626046	3.075555	C	1.402423	-1.667398	5.142580
C	1.310447	-5.990211	3.31707	C	2.561984	-2.06574	6.028891
H	0.230656	-4.240421	4.023444	H	0.492386	-1.449822	5.770782
H	1.474734	-3.892564	2.71982	H	1.651877	-0.764117	4.524214
H	2.062652	-5.91768	4.138326	H	2.762661	-1.247672	6.761040
H	0.519458	-6.720801	3.610327	H	2.320602	-3.002327	6.585677
H	1.814813	-6.370489	2.396279	H	3.483512	-2.244652	5.424121
C	1.388148	-4.674273	-1.282371	C	3.512591	-2.548535	1.393137
C	2.337312	-5.706227	-1.841449	C	5.013403	-2.694434	1.459851
H	1.905203	-3.686815	-1.131123	H	3.214594	-1.510051	1.082907
H	0.497343	-4.526622	-1.952219	H	3.056769	-3.288817	0.678321
H	2.865917	-5.270382	-2.723847	H	5.434300	-2.648393	0.427412
H	3.092229	-5.993467	-1.070684	H	5.455022	-1.870605	2.072493
H	1.785441	-6.623993	-2.152714	H	5.290044	-3.669422	1.927014
H	0.388549	-1.807288	0.573199	H	0.454490	-0.838216	1.526604
C	6.79669	-1.059094	2.015863	C	6.179660	1.751874	1.626054
C	4.988617	-1.994163	-2.597834	C	4.950468	0.368374	-3.053875
C	-6.417204	0.42776	-0.413117	C	-6.733078	-2.204018	-0.104232
C	-3.639312	1.706146	-4.424513	C	-4.40127	-0.601396	-4.269821
F	6.128549	-1.804631	2.95722	F	6.145114	0.56141	2.313370
F	7.322797	-0.011101	2.732534	F	5.981180	2.70519	2.593938
F	7.889872	-1.828358	1.696761	F	7.502329	1.894511	1.279758
F	6.111395	-2.758589	-2.818586	F	6.296223	0.268247	-3.320674
F	3.971802	-2.917141	-2.548905	F	4.519841	-0.936468	-3.054719
F	4.797291	-1.336587	-3.786902	F	4.421344	0.902599	-4.201692
F	-6.307381	-0.932532	-0.241619	F	-6.643813	-3.510802	-0.518358
F	-7.551761	0.576438	-1.172534	F	-8.051669	-1.876375	-0.307382
F	-6.777017	0.892016	0.828376	F	-6.615469	-2.27699	1.263740
F	-4.795255	1.618106	-5.162027	F	-5.486218	-1.050809	-4.984645
F	-2.865779	0.671369	-4.89543	F	-3.396250	-1.476097	-4.604433
F	-3.020067	2.835463	-4.897666	F	-4.053916	0.573775	-4.887192
O	-4.125261	-1.370403	5.838913	O	3.799171	-5.080512	-3.589405
C	-5.043479	-2.283525	6.433601	C	4.252573	-6.431089	-3.591672
H	-4.604943	-3.309787	6.477174	H	3.404420	-7.130633	-3.788414
H	-5.186283	-1.869154	7.464068	H	4.988548	-6.452801	-4.435511
H	-6.009278	-2.290073	5.872611	H	4.752760	-6.679471	-2.624409
<i>(R)</i> -product				<i>(S)</i> -product			
C	-4.425634	5.265827	3.725723	C	0.173827	-3.934791	1.075299
C	-4.845889	4.029951	3.301889	P	1.385549	-3.603672	-0.312861
C	-4.14858	3.343694	2.268841	C	2.171089	7.033436	-2.914974

C	-3.021629	3.952933	1.660393	C	2.984588	5.955954	-2.668783
C	-2.606338	5.231506	2.128945	C	2.558447	4.910433	-1.802889
C	-3.289365	5.868839	3.135302	C	1.291419	4.995876	-1.171611
H	-5.470867	1.619767	2.297936	C	0.466919	6.120929	-1.457529
H	-4.959709	5.797395	4.527499	C	0.89529	7.111028	-2.306962
H	-5.723805	3.545163	3.755669	H	4.377307	3.74713	-2.046379
C	-4.566082	2.057051	1.844438	H	2.495456	7.84181	-3.587154
C	-2.321789	3.255262	0.628851	H	3.976391	5.877312	-3.139623
H	-1.719556	5.699141	1.671865	C	3.382106	3.77984	-1.573302
H	-2.958196	6.854293	3.496707	C	0.870125	3.943159	-0.302434
C	-2.691985	1.943898	0.31858	H	-0.528111	6.180065	-0.988037
C	-3.869426	1.357453	0.881662	H	0.249297	7.974451	-2.527392
C	-1.156216	3.850744	-0.03458	C	1.663498	2.79947	-0.178314
C	-1.25738	5.080563	-0.754485	C	2.961247	2.735389	-0.777756
C	0.056654	3.157515	-0.03835	C	-0.429347	3.998935	0.377204
C	-2.496832	5.760079	-0.923172	C	-0.753249	5.060827	1.275896
C	-0.096919	5.631417	-1.355896	C	-1.334895	2.947402	0.209931
C	1.24365	3.755434	-0.568473	C	0.183438	6.076498	1.618939
C	-2.567196	6.928935	-1.640467	C	-2.036401	5.092256	1.879064
H	-3.4027	5.32511	-0.471237	C	-2.657466	3.02076	0.751546
C	-0.194691	6.849234	-2.084665	C	-0.150818	7.072946	2.502595
C	1.147513	4.963788	-1.223796	H	1.187042	6.043531	1.165401
C	-1.40352	7.48429	-2.223981	C	-2.361919	6.142295	2.782233
H	-3.530377	7.444886	-1.772571	C	-2.9796	4.077755	1.57669
H	0.718006	7.265965	-2.537334	C	-1.439198	7.11144	3.087374
H	2.048013	5.433357	-1.652225	H	0.580934	7.850758	2.768784
H	-1.483388	8.423965	-2.790721	H	-3.365781	6.155381	3.233615
O	0.189679	1.921754	0.579066	H	-3.989669	4.149679	2.012644
O	-2.00964	1.212678	-0.645504	H	-1.685974	7.922123	3.789165
P	-0.523348	0.623473	-0.187752	O	-1.028461	1.855978	-0.595092
O	0.094966	0.429315	-1.622869	O	1.282223	1.736792	0.628003
O	-0.488208	-0.544656	0.720925	P	0.041208	0.770931	0.073812
H	0.428689	-2.354609	0.59418	O	-0.434399	-0.083614	1.184194
N	0.907911	-3.250526	0.649488	O	0.478278	0.032092	-1.24937
C	2.553667	3.13203	-0.380062	H	-0.831265	-2.110606	0.896891
C	3.404482	2.921931	-1.472954	N	-1.009759	-3.113155	0.907962
C	2.9831	2.79146	0.910702	C	-3.68151	2.032587	0.414226
C	4.675449	2.382634	-1.267752	C	-4.498653	1.492847	1.41728
H	3.065876	3.169429	-2.493286	C	-3.897059	1.668096	-0.921911
C	4.266255	2.276885	1.101797	C	-5.531806	0.617884	1.077735
H	2.29791	2.918948	1.76741	H	-4.320331	1.749177	2.475287
C	5.118206	2.062917	0.016998	C	-4.939031	0.796855	-1.245786
H	6.122746	1.63242	0.169444	H	-3.235934	2.063635	-1.713117
C	-4.372281	0.059437	0.432527	C	-5.76342	0.26531	-0.253025
C	-4.766828	-0.905139	1.370075	H	-6.579048	-0.431841	-0.512571

C	-4.524488	-0.203663	-0.935859	C	3.854007	1.598927	-0.551216
C	-5.327108	-2.10817	0.937336	C	4.485027	0.981527	-1.639755
H	-4.62605	-0.720043	2.448528	C	4.117029	1.148866	0.750602
C	-5.095669	-1.407795	-1.351897	C	5.374337	-0.07194	-1.422444
H	-4.181542	0.538497	-1.678608	H	4.268783	1.317951	-2.667859
C	-5.50082	-2.367735	-0.422944	C	5.021619	0.105908	0.951809
H	-5.942685	-3.322066	-0.757421	H	3.594063	1.612829	1.606025
C	1.304592	-3.823384	-0.615301	C	5.650807	-0.515736	-0.128955
H	1.856726	-4.747466	-0.429373	H	6.344649	-1.357188	0.037553
C	0.138449	-4.163084	-1.534706	H	-0.108393	-4.980312	0.925915
C	0.223063	-5.29899	-2.352946	C	0.829442	-3.807694	2.443098
C	-1.003185	-3.355344	-1.613328	C	1.417255	-4.936634	3.031935
C	-0.811524	-5.627249	-3.228926	C	0.873042	-2.584045	3.125159
H	1.105437	-5.932704	-2.29997	C	2.030582	-4.850941	4.282487
C	-2.035697	-3.683422	-2.493444	H	1.386905	-5.891709	2.511623
H	-1.099049	-2.481344	-0.977806	C	1.484687	-2.502637	4.377277
C	-1.94514	-4.816449	-3.303071	H	0.425329	-1.696797	2.690143
H	-0.733549	-6.518187	-3.846341	C	2.064765	-3.630957	4.95967
H	-2.916744	-3.047365	-2.551253	H	2.471579	-5.738262	4.729096
H	-2.755111	-5.066831	-3.983118	H	1.508024	-1.54899	4.89762
C	1.579901	-3.454921	1.865013	H	2.538213	-3.560738	5.935366
C	2.515405	-4.473273	2.092281	C	-2.080912	-3.522962	0.089062
C	1.252996	-2.609666	2.948885	C	-2.619281	-4.814887	0.166377
C	3.093394	-4.658349	3.35547	C	-2.683092	-2.612491	-0.799245
H	2.818839	-5.142869	1.294135	C	-3.705406	-5.197509	-0.623417
C	1.825194	-2.792745	4.197088	H	-2.205706	-5.53453	0.867383
H	0.538934	-1.806463	2.792089	C	-3.778627	-2.981201	-1.571055
C	2.750779	-3.823395	4.418539	H	-2.281574	-1.605986	-0.882797
H	3.810657	-5.461582	3.483236	C	-4.297128	-4.27983	-1.497692
H	1.567518	-2.138717	5.02479	H	-4.088116	-6.207907	-0.531561
P	2.538485	-2.706367	-1.474016	H	-4.239134	-2.272862	-2.256491
O	2.079465	-1.27595	-1.566424	O	1.713508	-2.142894	-0.493929
O	3.938528	-2.952261	-0.692991	O	2.670776	-4.57956	-0.103554
O	2.969852	-3.401467	-2.88024	O	0.739623	-4.345804	-1.603844
C	4.247086	-2.01469	0.338653	C	3.685711	-4.060727	0.756516
C	5.669054	-1.539494	0.152289	C	5.032339	-4.246222	0.097684
H	4.142144	-2.559818	1.321157	H	3.638762	-4.647758	1.718442
H	3.523375	-1.155859	0.294728	H	3.490506	-2.972611	0.963994
H	5.957532	-0.898883	1.021518	H	5.826345	-3.885021	0.795937
H	6.361533	-2.412988	0.09309	H	5.205086	-5.323738	-0.135368
H	5.77274	-0.944784	-0.787927	H	5.095965	-3.666011	-0.854952
C	2.158414	-2.91923	-3.954993	C	0.310123	-3.395418	-2.582751
C	2.739671	-3.423291	-5.251454	C	-0.124673	-4.146332	-3.81486
H	2.152775	-1.794666	-3.917133	H	1.168173	-2.70169	-2.800584
H	1.117874	-3.312467	-3.788593	H	-0.537734	-2.808855	-2.1318

H	2.108389	-3.068178	-6.100592	H	-0.483025	-3.417975	-4.581054
H	3.781467	-3.04442	-5.382877	H	0.727713	-4.733271	-4.232953
H	2.770003	-4.53903	-5.256266	H	-0.950679	-4.854959	-3.566542
H	0.841398	-0.249359	-1.630792	H	0.94849	-0.837486	-1.03193
C	4.753935	1.96989	2.513681	C	-5.174275	0.443503	-2.71009
C	5.607551	2.138517	-2.449049	C	-6.43543	0.059804	2.171977
C	-5.780512	-3.142339	1.962485	C	6.061568	-0.748422	-2.602768
C	-5.303916	-1.658506	-2.840781	C	5.34917	-0.371534	2.36181
F	3.767619	1.592949	3.390072	F	-6.076441	-0.569061	-2.92319
F	5.369077	3.03195	3.132225	F	-4.045032	0.033782	-3.377448
F	5.68065	0.957698	2.58634	F	-5.651365	1.487026	-3.466421
F	6.632009	3.049206	-2.550512	F	-7.531591	0.846742	2.439174
F	6.243262	0.920517	-2.418307	F	-6.968341	-1.175376	1.899527
F	5.001964	2.17573	-3.680351	F	-5.82728	-0.089512	3.393701
F	-5.080741	-3.121163	3.143091	F	6.174548	-2.112671	-2.482604
F	-5.695546	-4.443864	1.534305	F	7.350607	-0.322953	-2.818674
F	-7.092952	-3.000434	2.34836	F	5.440368	-0.564419	-3.813221
F	-6.436193	-1.07437	-3.354643	F	6.598649	-0.002183	2.799845
F	-5.421138	-2.982938	-3.187486	F	5.338239	-1.739182	2.50476
F	-4.289711	-1.191901	-3.641327	F	4.501554	0.080699	3.340942
O	3.255506	-3.916212	5.691974	O	-5.368211	-4.547445	-2.310346
C	4.182072	-4.951158	5.958551	C	-5.935623	-5.843024	-2.252362
H	4.447149	-4.856332	7.013718	H	-6.321257	-6.073576	-1.24958
H	3.74463	-5.944285	5.783941	H	-6.764073	-5.841474	-2.963722
H	5.09126	-4.851753	5.348519	H	-5.212294	-6.617741	-2.54297

(R)-TS4-2

C	1.417228	-3.370829	1.19031
P	2.190388	-2.936917	-1.006427
C	-4.723663	5.534005	2.854318
C	-5.135341	4.246293	2.619627
C	-4.409567	3.404161	1.731561
C	-3.263229	3.909467	1.067339
C	-2.857601	5.247271	1.339486
C	-3.567248	6.035983	2.210606
H	-5.741132	1.7089	1.988741
H	-5.279963	6.186321	3.543223
H	-6.028952	3.83948	3.11652
C	-4.816959	2.065559	1.505744
C	-2.537235	3.059508	0.178814
H	-1.955887	5.635333	0.839121
H	-3.243536	7.066396	2.420298
C	-2.889451	1.708919	0.083389
C	-4.08778	1.218749	0.697309
C	-1.380088	3.557473	-0.574494

(S)-TS4-2

C	0.751406	-3.624905	-0.629093
P	-0.921453	-3.730266	1.059215
C	-2.701259	6.334843	3.565914
C	-3.448515	5.247323	3.188933
C	-2.982838	4.364682	2.174972
C	-1.74371	4.62427	1.536428
C	-0.989511	5.757231	1.955082
C	-1.454975	6.587473	2.944436
H	-4.731416	3.079111	2.257906
H	-3.056196	7.016272	4.352792
H	-4.416687	5.034183	3.66664
C	-3.742908	3.229909	1.794603
C	-1.276153	3.730223	0.526064
H	-0.018377	5.949722	1.471707
H	-0.86283	7.45653	3.267699
C	-1.978692	2.545052	0.283991
C	-3.272685	2.330342	0.861269
C	-0.034968	3.992516	-0.211945

C	-1.513592	4.65643	-1.476702	C	0.119038	5.186327	-0.979605
C	-0.152493	2.892232	-0.477165	C	0.96756	3.015659	-0.245684
C	-2.768819	5.275542	-1.741745	C	-0.920977	6.152136	-1.104231
C	-0.368889	5.138285	-2.160322	C	1.335709	5.416758	-1.669984
C	1.007154	3.401591	-1.144818	C	2.199508	3.259941	-0.930457
C	-2.866152	6.327333	-2.618413	C	-0.74244	7.289568	-1.85132
H	-3.665609	4.888295	-1.232334	H	-1.878118	5.965471	-0.591438
C	-0.493615	6.23831	-3.053974	C	1.501094	6.610234	-2.427129
C	0.884476	4.508309	-1.956086	C	2.366676	4.4465	-1.612087
C	-1.71527	6.821478	-3.277807	C	0.485058	7.527807	-2.515136
H	-3.840792	6.795766	-2.821232	H	-1.552786	8.027842	-1.945356
H	0.409571	6.604105	-3.565347	H	2.458436	6.775382	-2.944056
H	1.769019	4.914341	-2.472765	H	3.312749	4.65162	-2.138583
H	-1.816388	7.669284	-3.970938	H	0.607544	8.449809	-3.101974
O	0.012843	1.817489	0.372588	O	0.852839	1.855301	0.492904
O	-2.165998	0.83467	-0.70517	O	-1.511561	1.601671	-0.611258
P	-0.672748	0.348235	-0.090122	P	-0.195482	0.676383	-0.097901
O	0.016631	-0.246494	-1.30253	O	0.320487	-0.008543	-1.331508
O	-0.776154	-0.45123	1.176791	O	-0.495178	-0.154528	1.132144
H	0.441069	-1.643937	1.693605	H	1.107167	-1.606027	-0.826575
N	1.306173	-2.193577	1.828296	N	1.495937	-2.505376	-0.499171
C	2.329924	2.787581	-0.983381	C	3.305068	2.294514	-0.937236
C	2.650837	1.595016	-1.64215	C	3.288048	1.193894	-1.80436
C	3.301474	3.427397	-0.198682	C	4.427162	2.52036	-0.126821
C	3.927301	1.04671	-1.518295	C	4.398239	0.355001	-1.891078
H	1.895825	1.068378	-2.252472	H	2.39174	0.981448	-2.413096
C	4.578786	2.886372	-0.082019	C	5.532233	1.676738	-0.205746
H	3.050387	4.359218	0.329852	H	4.434147	3.369818	0.572968
C	4.890774	1.697282	-0.746972	C	5.521551	0.604144	-1.100931
C	-4.575715	-0.139006	0.454605	C	-4.12208	1.214844	0.443328
C	-5.104026	-0.895894	1.512233	C	-4.853834	0.487185	1.393254
C	-4.575034	-0.676706	-0.841153	C	-4.259874	0.901918	-0.917972
C	-5.640889	-2.15836	1.276036	C	-5.727724	-0.520246	0.989994
H	-5.087184	-0.491947	2.53616	H	-4.727278	0.703293	2.465268
C	-5.1149	-1.938393	-1.079778	C	-5.135552	-0.10129	-1.322672
H	-4.134088	-0.09563	-1.668734	H	-3.66007	1.450674	-1.6628
C	-5.652363	-2.674498	-0.021912	C	-5.874525	-0.80526	-0.368303
H	2.325578	-3.922112	1.419911	H	1.245581	-4.51643	-0.248933
C	0.231938	-4.236814	0.970535	C	-0.089462	-3.857019	-1.833011
C	0.448046	-5.620792	0.87256	C	-0.399936	-5.184453	-2.173233
C	-1.076158	-3.734031	0.869324	C	-0.563203	-2.809065	-2.640692
C	-0.621006	-6.494793	0.687979	C	-1.160147	-5.466053	-3.306302
H	1.46	-6.013233	0.943958	H	-0.044464	-5.998501	-1.545939
C	-2.140041	-4.615244	0.683847	C	-1.323082	-3.100034	-3.77261
H	-1.264027	-2.665868	0.932371	H	-0.344792	-1.774927	-2.39124

C	-1.919845	-5.992272	0.593575	C	-1.623095	-4.422211	-4.110099
H	-0.439245	-7.563637	0.620003	H	-1.387678	-6.497461	-3.56097
H	-3.153075	-4.226142	0.606075	H	-1.682877	-2.285169	-4.39389
H	-2.760872	-6.665746	0.448252	C	2.571507	-2.430049	0.434392
C	2.380742	-1.441245	2.359438	C	3.670277	-3.284374	0.304915
C	3.717361	-1.842337	2.284838	C	2.552141	-1.481927	1.471224
C	2.061675	-0.236475	3.012286	C	4.745819	-3.20316	1.190324
C	4.722723	-1.068489	2.871237	H	3.704718	-3.994209	-0.517309
H	4.008099	-2.741313	1.751543	C	3.625325	-1.393016	2.348205
C	3.057508	0.529554	3.5927	H	1.696656	-0.824097	1.58516
H	1.028819	0.094489	3.040683	C	4.732062	-2.244733	2.213128
C	4.399353	0.120021	3.533754	H	5.594284	-3.864296	1.055278
H	5.751543	-1.400177	2.788432	H	3.630726	-0.657242	3.145781
H	2.819822	1.461368	4.095337	O	-1.690233	-2.370338	1.327873
O	2.263804	-1.396049	-1.397445	O	-2.077521	-4.815003	0.661045
O	3.736906	-3.450603	-1.017138	O	-0.56641	-4.447148	2.503399
O	1.575951	-3.755973	-2.307244	C	-3.157798	-4.34318	-0.133382
C	4.568246	-3.003028	-2.086048	C	-4.461347	-4.685284	0.552651
C	5.019709	-4.186631	-2.91128	H	-3.085731	-4.879574	-1.123029
H	5.452898	-2.495399	-1.60473	H	-3.071941	-3.235515	-0.293184
H	4.011058	-2.257132	-2.71312	H	-5.314134	-4.313303	-0.067708
H	5.750816	-3.841595	-3.680673	H	-4.553989	-5.789431	0.68302
H	5.50904	-4.949407	-2.259931	H	-4.511334	-4.207768	1.5603
H	4.151311	-4.666448	-3.423428	C	0.711337	-4.136657	3.032453
C	0.215004	-3.380543	-2.512267	C	1.553654	-5.392607	3.106676
C	-0.273955	-4.070369	-3.761898	H	0.537071	-3.733646	4.071176
H	0.157052	-2.259777	-2.609135	H	1.216357	-3.34452	2.415036
H	-0.37162	-3.703786	-1.608647	H	2.472965	-5.18757	3.70499
H	-1.342984	-3.801448	-3.935594	H	0.973752	-6.211853	3.596125
H	0.332007	-3.750505	-4.642965	H	1.855408	-5.737886	2.08944
H	-0.184928	-5.177878	-3.657883	H	-1.176065	-1.469886	1.193518
H	1.361915	-0.8732	-1.301167	H	-2.215736	-4.638219	-4.995039
O	5.300107	0.945234	4.139509	O	5.736128	-2.062655	3.115418
C	6.679973	0.633399	4.021608	C	6.970263	-2.729716	2.88956
H	6.998601	0.615829	2.9694	H	7.384041	-2.473548	1.904134
H	7.211636	1.42829	4.547598	H	7.646249	-2.378433	3.670945
H	6.91818	-0.331188	4.489574	H	6.86416	-3.819776	2.969413
H	-5.126657	-2.351677	-2.100757	H	6.414382	1.851906	0.429202
H	-6.063849	-2.747446	2.104727	H	4.389607	-0.500359	-2.584812
H	4.154175	0.085936	-2.010985	H	-5.249616	-0.343133	-2.390597
H	5.341186	3.386598	0.534747	H	-6.29659	-1.092998	1.739291
C	6.294248	1.122571	-0.638457	C	-6.846401	-1.880583	-0.830208
C	-6.247693	-4.051444	-0.27525	C	6.757206	-0.275249	-1.219616
F	-5.373556	-5.091307	-0.049743	F	-6.340566	-2.730601	-1.786885
F	-7.332546	-4.361502	0.508956	F	-7.293459	-2.72747	0.155297

F	-6.688638	-4.26624	-1.558165	F	-8.000201	-1.396109	-1.399556
F	6.394315	-0.224414	-0.896811	F	7.301778	-0.665437	-0.01749
F	7.209285	1.688963	-1.494359	F	6.569845	-1.459645	-1.891568
F	6.879524	1.26001	0.599459	F	7.810775	0.313774	-1.8778
(R)-TS4-3				(S)-TS4-3			
C	-2.784868	2.424084	1.194783	C	-3.618676	0.974813	-0.670719
P	-3.257424	1.759798	-1.036428	P	-3.02606	2.448074	1.059877
C	6.672896	-2.744912	2.90276	C	6.817689	-0.272143	3.566531
C	6.453806	-1.413442	2.653413	C	6.16565	0.86849	3.170171
C	5.434202	-1.003452	1.749681	C	5.179832	0.820616	2.145534
C	4.65311	-1.982976	1.084202	C	4.884422	-0.415472	1.515809
C	4.899438	-3.355574	1.372812	C	5.573384	-1.58153	1.95532
C	5.880598	-3.725318	2.258999	C	6.511995	-1.511321	2.954819
H	5.832566	1.118019	2.006321	H	4.771683	2.954302	2.209502
H	7.457758	-3.064795	3.603781	H	7.576861	-0.239114	4.36168
H	7.057337	-0.639132	3.150712	H	6.387712	1.838293	3.640601
C	5.187068	0.37299	1.513973	C	4.489271	1.993995	1.74858
C	3.6291	-1.568542	0.178911	C	3.88833	-0.461339	0.493517
H	4.279791	-4.117183	0.872669	H	5.331086	-2.545421	1.479822
H	6.06018	-4.787991	2.480828	H	7.034568	-2.418275	3.293917
C	3.333796	-0.206405	0.064362	C	3.130242	0.683989	0.230018
C	4.165182	0.781659	0.685328	C	3.488386	1.948139	0.802401
C	2.824141	-2.540993	-0.570515	C	3.589615	-1.699723	-0.235507
C	3.439198	-3.479582	-1.454225	C	4.603729	-2.37405	-0.981196
C	1.427817	-2.484958	-0.493989	C	2.271294	-2.167721	-0.287033
C	4.842576	-3.487828	-1.69793	C	5.932389	-1.871134	-1.088065
C	2.63252	-4.421719	-2.141584	C	4.282642	-3.572606	-1.667585
C	0.6193	-3.452165	-1.174049	C	1.955088	-3.382007	-0.974958
C	5.405276	-4.400036	-2.555667	C	6.885673	-2.542336	-1.812463
H	5.470691	-2.740192	-1.187779	H	6.180844	-0.92537	-0.580419
C	3.241333	-5.365806	-3.01464	C	5.292169	-4.257267	-2.400349
C	1.225492	-4.401109	-1.966025	C	2.953898	-4.064761	-1.633731
C	4.598466	-5.35673	-3.216802	C	6.566742	-3.75452	-2.470347
H	6.489723	-4.395148	-2.741805	H	7.908149	-2.143767	-1.892733
H	2.598456	-6.096517	-3.528402	H	5.024829	-5.193306	-2.913652
H	0.617336	-5.155237	-2.490916	H	2.72692	-5.005167	-2.161274
H	5.072106	-6.082319	-3.894148	H	7.349055	-4.278901	-3.038376
O	0.789657	-1.593615	0.343597	O	1.267648	-1.554694	0.434376
O	2.306397	0.242503	-0.742601	O	2.089691	0.668492	-0.678331
P	0.747996	0.02521	-0.132206	P	0.671432	-0.097768	-0.169042

O	-0.123637	0.23821	-1.352676	O	-0.158977	-0.264568	-1.408631
O	0.480918	0.793273	1.129769	O	0.056304	0.544173	1.05569
H	-1.161372	1.280916	1.679018	H	-1.950976	-0.215708	-0.906509
N	-2.180923	1.388012	1.801179	N	-2.930135	-0.18752	-0.584106
C	-0.841546	-3.451175	-1.038008	C	0.590732	-3.92168	-1.004517
C	-1.618929	-2.518328	-1.734812	C	-0.347611	-3.423444	-1.919129
C	-1.468374	-4.402139	-0.218355	C	0.237219	-4.977273	-0.152442
C	-3.005189	-2.509826	-1.597882	C	-1.618576	-3.984991	-2.001265
H	-1.141984	-1.756157	-2.377811	H	-0.09027	-2.56393	-2.563614
C	-2.851291	-4.411451	-0.072957	C	-1.034742	-5.539004	-0.209243
H	-0.859415	-5.139775	0.326624	H	0.969321	-5.361248	0.575044
C	-3.618234	-3.453778	-0.759331	C	-1.960194	-5.042046	-1.141588
C	3.949611	2.205177	0.426469	C	2.838722	3.182598	0.362545
C	3.915235	3.121788	1.48794	C	2.425188	4.142576	1.297477
C	3.793926	2.665898	-0.889754	C	2.659334	3.431182	-1.007399
C	3.715262	4.477186	1.247493	C	1.840891	5.334454	0.879466
H	4.028708	2.762995	2.52302	H	2.543869	3.944277	2.374398
C	3.613298	4.02026	-1.150483	C	2.087772	4.620884	-1.443572
H	3.793631	1.938992	-1.719995	H	2.960481	2.662836	-1.739554
C	3.565658	4.923495	-0.07607	C	1.676417	5.572076	-0.494836
H	-3.847679	2.51064	1.406027	H	-4.645517	0.889353	-0.31984
C	-2.096225	3.730358	1.047148	C	-3.447743	1.874971	-1.844065
C	-2.897187	4.879996	0.950399	C	-4.504292	2.740596	-2.170986
C	-0.697427	3.863412	1.0339	C	-2.285168	1.876087	-2.633221
C	-2.317525	6.143354	0.856351	C	-4.411506	3.586353	-3.274215
H	-3.980677	4.782275	0.953822	H	-5.401391	2.751295	-1.556365
C	-0.125489	5.131523	0.945267	C	-2.199717	2.726955	-3.734136
H	-0.058585	2.987112	1.092229	H	-1.453675	1.218348	-2.397823
C	-0.92733	6.272749	0.857551	C	-3.256638	3.580944	-4.059231
H	-2.950334	7.02386	0.788333	H	-5.239115	4.246142	-3.519937
H	0.957953	5.230938	0.950021	H	-1.299958	2.719853	-4.342253
H	-0.468224	7.25625	0.791178	C	-3.333573	-1.234994	0.29592
C	-2.825349	0.216257	2.265078	C	-4.556666	-1.882376	0.097623
C	-4.197284	-0.016565	2.133409	C	-2.494959	-1.650322	1.344052
C	-2.025045	-0.746559	2.906226	C	-4.947418	-2.938327	0.921873
C	-4.769481	-1.18503	2.64374	H	-5.192026	-1.586766	-0.733373
H	-4.841556	0.683186	1.611226	C	-2.879448	-2.703903	2.163471
C	-2.592281	-1.902322	3.41386	H	-1.54681	-1.148017	1.506993
H	-0.955389	-0.582386	2.983221	C	-4.101029	-3.363161	1.956125
C	-3.971995	-2.135387	3.29047	H	-5.891259	-3.437617	0.731287
H	-5.835026	-1.343034	2.517612	H	-2.236567	-3.044656	2.968514

H	-1.981069	-2.650821	3.907256	O	-1.469687	2.533976	1.344948
O	-2.652905	0.339866	-1.43337	O	-3.49832	3.972525	0.717501
O	-4.871243	1.550691	-1.080846	O	-3.837245	2.369178	2.493902
O	-3.026417	2.781984	-2.317387	C	-2.551288	4.838881	0.106259
C	-5.405272	0.778475	-2.156092	C	-2.299972	6.029942	1.004031
C	-6.335556	1.637869	-2.98137	H	-3.021301	5.174938	-0.86196
H	-5.967933	-0.07722	-1.683466	H	-1.597192	4.287162	-0.104178
H	-4.567726	0.368758	-2.780842	H	-1.617381	6.748814	0.487791
H	-6.829683	1.004575	-3.75625	H	-3.261624	6.543801	1.242041
H	-7.119077	2.095582	-2.33162	H	-1.827546	5.709036	1.962989
H	-5.773094	2.459506	-3.486236	C	-4.131371	1.062503	2.958244
C	-1.635034	3.064848	-2.455939	C	-5.63068	0.856675	2.996971
C	-1.458979	3.94938	-3.665471	H	-3.710695	0.994682	4.002357
H	-1.078273	2.092381	-2.569549	H	-3.631084	0.290244	2.313058
H	-1.291473	3.580558	-1.51707	H	-5.860631	-0.088178	3.544416
H	-0.376865	4.192377	-3.789131	H	-6.11939	1.712218	3.522587
H	-1.824771	3.428376	-4.582298	H	-6.056904	0.789421	1.967956
H	-2.037453	4.89612	-3.545247	H	-0.871562	1.696654	1.165779
H	-1.617376	0.25613	-1.344843	H	-3.180212	4.239799	-4.920255
O	-4.427339	-3.305448	3.81797	O	-4.370626	-4.39689	2.798728
C	-5.787188	-3.657968	3.599211	C	-5.441001	-5.273645	2.466237
H	-6.014991	-3.730325	2.525481	H	-5.304566	-5.702115	1.462812
H	-5.918178	-4.636599	4.064135	H	-5.411661	-6.071609	3.210059
H	-6.471206	-2.940241	4.07124	H	-6.413384	-4.766876	2.52176
H	-3.601746	-1.739583	-2.12028	H	-1.313546	-6.361984	0.47
H	-3.339793	-5.153414	0.580359	H	-2.349499	-3.60024	-2.73232
H	3.504413	4.379561	-2.187832	H	1.957816	4.815631	-2.521381
H	3.67193	5.193121	2.085429	H	1.504025	6.080528	1.618949
N	-5.088558	-3.419524	-0.575189	N	-3.322813	-5.62479	-1.206285
O	-5.600844	-4.166926	0.218992	O	-4.058708	-5.301482	-2.101339
O	-5.744805	-2.634409	-1.208644	O	-3.674046	-6.39853	-0.352729
N	3.342092	6.366541	-0.340834	N	1.046511	6.834723	-0.952856
O	3.437554	6.780185	-1.465109	O	0.970999	7.057661	-2.132799
O	3.052687	7.087865	0.578765	O	0.612255	7.604088	-0.135749
<i>(R)</i> -TS4-4				<i>(S)</i> -TS4-4			
C	0.545147	-3.649607	1.099816	C	-0.251746	-3.661138	0.711743
P	1.498797	-3.340339	-1.091146	P	1.602558	-3.461783	-0.751129
C	-3.771827	6.509617	2.382714	C	1.448851	6.813359	-3.527302
C	-4.358327	5.272187	2.293889	C	2.372582	5.875841	-3.139156
C	-3.762338	4.243261	1.512725	C	2.051127	4.912201	-2.142878

C	-2.558248	4.505125	0.810866	C	0.772014	4.936065	-1.531797
C	-1.974111	5.798729	0.925604	C	-0.166428	5.91671	-1.963011
C	-2.564033	6.772444	1.692765	C	0.162959	6.827832	-2.935611
H	-5.33292	2.798506	1.913089	H	4.001086	3.9614	-2.198884
H	-4.227338	7.306188	2.989174	H	1.691937	7.556719	-4.300644
H	-5.295309	5.05147	2.827224	H	3.374142	5.847125	-3.59433
C	-4.362054	2.962494	1.417908	C	2.992826	3.926839	-1.754953
C	-1.95499	3.463894	0.043141	C	0.453718	3.96412	-0.535719
H	-1.033331	5.999961	0.388561	H	-1.167886	5.923983	-1.503812
H	-2.102893	7.767491	1.782522	H	-0.570288	7.577492	-3.268858
C	-2.491977	2.173716	0.091707	C	1.351956	2.9215	-0.281507
C	-3.763369	1.94154	0.709995	C	2.670986	2.945304	-0.840787
C	-0.73215	3.701965	-0.731349	C	-0.831003	3.992375	0.172587
C	-0.706211	4.659775	-1.78983	C	-1.223927	5.131418	0.938104
C	0.394939	2.909679	-0.491855	C	-1.633148	2.845366	0.179698
C	-1.862123	5.396509	-2.176056	C	-0.388799	6.276299	1.085237
C	0.49684	4.86639	-2.511634	C	-2.475956	5.123527	1.60383
C	1.632638	3.193695	-1.15234	C	-2.895424	2.844271	0.85166
C	-1.813065	6.291418	-3.215923	C	-0.79592	7.356429	1.82778
H	-2.801575	5.228736	-1.625593	H	0.597338	6.276361	0.593888
C	0.523648	5.805209	-3.580157	C	-2.881462	6.26162	2.355827
C	1.660419	4.139514	-2.154186	C	-3.299466	3.972498	1.532218
C	-0.606504	6.502909	-3.92517	C	-2.060434	7.355294	2.464434
H	-2.712427	6.851887	-3.512196	H	-0.142269	8.234533	1.939534
H	1.468288	5.954675	-4.124662	H	-3.863423	6.240315	2.852276
H	2.600611	4.351866	-2.688259	H	-4.272738	3.988869	2.048796
H	-0.590601	7.22676	-4.753111	H	-2.368468	8.235557	3.047489
O	0.39001	1.921097	0.470228	O	-1.288091	1.734794	-0.564302
O	-1.896312	1.118099	-0.565721	O	1.051362	1.908113	0.608011
P	-0.463059	0.505063	0.099148	P	-0.073806	0.757462	0.080694
O	0.137995	-0.25235	-1.060516	O	-0.522777	0.020367	1.308548
O	-0.663454	-0.178118	1.421801	O	0.419723	-0.026513	-1.116202
H	0.183454	-1.736631	1.73021	H	-1.021379	-1.753902	0.772273
N	0.820497	-2.548162	1.810815	N	-1.171761	-2.712109	0.426707
C	2.884641	2.555406	-0.741369	C	-3.774561	1.670006	0.853913
C	3.639744	1.806089	-1.653112	C	-3.586284	0.650754	1.797899
C	3.372682	2.767789	0.555176	C	-4.847591	1.596777	-0.042266
C	4.884105	1.302309	-1.270964	C	-4.500663	-0.403225	1.868337
H	3.247277	1.609794	-2.665447	H	-2.710775	0.670236	2.474068
C	4.630113	2.277329	0.913958	C	-5.742232	0.526294	0.030543
H	2.760443	3.320062	1.288329	H	-4.986119	2.379882	-0.806359

C	5.39234	1.539951	0.007877	C	-5.582847	-0.473992	0.990034
H	6.382259	1.147004	0.29351	H	-6.302635	-1.307514	1.051997
C	-4.473027	0.674463	0.540838	C	3.695308	1.983806	-0.434111
C	-5.123868	0.075098	1.62765	C	4.553749	1.427428	-1.393488
C	-4.570452	0.089039	-0.731111	C	3.867932	1.655239	0.918654
C	-5.885033	-1.078767	1.432603	C	5.586693	0.577293	-0.996161
H	-5.034195	0.513789	2.635926	H	4.405909	1.651014	-2.463678
C	-5.350783	-1.054172	-0.912486	C	4.904444	0.801345	1.299476
H	-4.018385	0.531891	-1.580334	H	3.172065	2.063937	1.673907
C	-6.016922	-1.643495	0.163006	C	5.772099	0.259116	0.349744
H	-6.641032	-2.540606	0.014441	H	6.58493	-0.420465	0.655585
H	1.237968	-4.471957	1.252456	H	-0.511536	-4.639023	0.313459
C	-0.847179	-4.084824	0.845434	C	0.433632	-3.706551	2.029359
C	-1.04171	-5.400705	0.392385	C	0.840839	-4.96161	2.510302
C	-1.963644	-3.274554	1.104967	C	0.65126	-2.561955	2.814224
C	-2.325412	-5.906396	0.2098	C	1.43904	-5.079482	3.762954
H	-0.178498	-6.03019	0.186196	H	0.682791	-5.84915	1.901912
C	-3.24632	-3.791818	0.930049	C	1.255747	-2.687861	4.064052
H	-1.83839	-2.250637	1.441777	H	0.345852	-1.581653	2.460652
C	-3.433526	-5.102441	0.485554	C	1.647535	-3.940433	4.543406
H	-2.460325	-6.927181	-0.136733	H	1.73985	-6.057529	4.127856
H	-4.10884	-3.167127	1.15484	H	1.417825	-1.798998	4.66723
H	-4.438117	-5.496495	0.357467	C	-2.124994	-2.887716	-0.618996
C	2.060369	-2.252583	2.425561	C	-2.984006	-3.990911	-0.60129
C	3.156112	-3.11998	2.410696	C	-2.227055	-1.952988	-1.663252
C	2.161706	-1.030537	3.11485	C	-3.928216	-4.180206	-1.611739
C	4.327976	-2.792423	3.097013	H	-2.940859	-4.691942	0.228447
H	3.132678	-4.052938	1.857805	C	-3.176207	-2.130761	-2.661411
C	3.323846	-0.705235	3.792861	H	-1.552625	-1.103669	-1.695442
H	1.321655	-0.343592	3.101921	C	-4.030408	-3.244248	-2.649258
C	4.416519	-1.58752	3.801383	H	-4.585225	-5.041102	-1.566209
H	5.160898	-3.485378	3.066844	H	-3.268374	-1.415745	-3.472705
H	3.415565	0.241008	4.319299	O	2.048174	-1.971571	-1.076244
O	2.098539	-1.878936	-1.343155	O	2.912645	-4.213238	-0.135316
O	2.787222	-4.337713	-1.038182	O	1.573125	-4.324183	-2.159222
O	0.798511	-3.856753	-2.501875	C	3.987395	-3.415223	0.360709
C	3.681712	-4.311484	-2.15825	C	5.214648	-3.661508	-0.501657
C	3.665183	-5.68066	-2.81698	H	3.698839	-2.326929	0.318214
H	3.326878	-3.526117	-2.884106	H	6.091793	-3.131067	-0.059176
H	4.400457	-5.697237	-3.655847	H	5.433645	-4.753958	-0.558171
H	3.938366	-6.468981	-2.076355	H	5.055507	-3.276089	-1.537086

H	2.648525	-5.905502	-3.219393	C	0.373125	-4.1945	-2.917435
C	-0.231731	-3.002405	-3.006319	C	-0.202416	-5.587626	-3.119316
C	-1.537437	-3.779898	-3.022618	H	-0.364025	-3.549479	-2.355215
H	-0.322972	-2.086679	-2.352302	H	-1.091591	-5.531062	-3.790204
H	-2.362398	-3.106393	-3.35972	H	0.565793	-6.251521	-3.583242
H	-1.462223	-4.646378	-3.721506	H	-0.508807	-6.033085	-2.143616
H	-1.781869	-4.170456	-2.005089	H	1.339831	-1.208932	-1.042349
H	1.392825	-1.150287	-1.174254	C	-6.923326	0.466268	-0.929986
C	5.182223	2.592945	2.298667	C	-4.309624	-1.481734	2.927481
C	5.726688	0.494516	-2.250267	C	6.540097	-0.004409	-2.033062
C	-6.579179	-1.747304	2.612864	C	5.113885	0.468569	2.771369
C	-5.496307	-1.647995	-2.308936	F	-7.386558	-0.801623	-1.187628
F	6.273611	1.846314	2.669521	F	-6.676241	0.994781	-2.173095
F	4.28478	2.415698	3.323648	F	-8.036275	1.144612	-0.492876
F	5.602664	3.893551	2.447162	F	-3.982696	-1.002017	4.171815
F	6.902871	1.109518	-2.612049	F	-5.414212	-2.26903	3.151628
F	6.130133	-0.728639	-1.770606	F	-3.31491	-2.386496	2.643605
F	5.118987	0.208416	-3.446674	F	6.889586	-1.314315	-1.808712
F	-6.737094	-0.949466	3.718499	F	7.745826	0.652299	-2.112396
F	-5.919426	-2.85717	3.086695	F	6.069425	0.006359	-3.322434
F	-7.845807	-2.204546	2.340503	F	6.021843	1.28025	3.40811
F	-6.402216	-0.990218	-3.105378	F	5.585255	-0.802577	3.00377
F	-5.917969	-2.956106	-2.332763	F	3.985415	0.552351	3.54884
F	-4.339295	-1.655639	-3.048316	H	2.113133	-4.0284	5.521418
O	5.505885	-1.177763	4.510405	O	-4.91657	-3.323977	-3.680815
C	6.644359	-2.023247	4.542311	C	-5.842624	-4.399777	-3.693088
H	7.057498	-2.182708	3.537382	H	-6.485055	-4.38863	-2.802803
H	7.383185	-1.506258	5.157267	H	-6.457149	-4.253896	-4.583075
H	6.411915	-2.996391	4.995277	H	-5.333384	-5.370557	-3.759512
C	5.069835	-3.967605	-1.647676	C	0.703852	-3.549927	-4.253937
H	5.360168	-4.658927	-0.821676	H	1.496232	-4.139137	-4.774121
H	5.805998	-4.064831	-2.480518	H	-0.211127	-3.521674	-4.891284
H	5.096957	-2.918627	-1.264984	H	1.077901	-2.508536	-4.106813
C	0.155162	-2.579205	-4.41466	C	4.251811	-3.831327	1.798291
H	1.088822	-1.96848	-4.392143	H	4.649864	-4.87291	1.833259
H	0.330654	-3.476134	-5.054473	H	5.000785	-3.135659	2.248634
H	-0.668086	-1.968525	-4.854938	H	3.310816	-3.793237	2.400807
<i>(R)</i> -TS4-5				<i>(S)</i> -TS4-5			
C	-0.475636	-3.583983	-1.155351	C	0.480856	-3.419133	1.109011
P	-1.295692	-3.309566	1.245735	P	2.361285	-2.94941	-0.627233

C	3.820978	6.187333	-3.175199	C	0.37642	6.686541	-3.942248
C	4.41046	4.980961	-2.891596	C	1.417784	5.911555	-3.49718
C	3.81959	4.089632	-1.953209	C	1.22977	4.990816	-2.428963
C	2.619965	4.461128	-1.294432	C	-0.04058	4.888957	-1.807413
C	2.031842	5.718065	-1.613499	C	-1.101935	5.702176	-2.297445
C	2.615453	6.555908	-2.531256	C	-0.898666	6.574476	-3.337893
H	5.388247	2.599292	-2.12938	H	3.292009	4.311595	-2.430468
H	4.2724	6.876819	-3.903734	H	0.516695	7.395639	-4.771272
H	5.345507	4.678833	-3.387083	H	2.41324	5.982223	-3.961098
C	4.418604	2.838006	-1.663107	C	2.296709	4.174151	-1.977479
C	2.024142	3.558364	-0.362611	C	-0.22628	3.957037	-0.74188
H	1.092908	6.00113	-1.111129	H	-2.094406	5.610211	-1.827991
H	2.151025	7.522319	-2.778728	H	-1.725841	7.19355	-3.716366
C	2.553676	2.271653	-0.22272	C	0.802699	3.06313	-0.425422
C	3.818466	1.93781	-0.807931	C	2.109086	3.230176	-0.989944
C	0.827629	3.927283	0.402248	C	-1.500469	3.863822	-0.02052
C	0.841361	5.053042	1.280522	C	-2.037361	4.991552	0.670821
C	-0.303883	3.105623	0.351517	C	-2.141053	2.623192	0.07747
C	2.006922	5.845921	1.485315	C	-1.364155	6.24618	0.72195
C	-0.332007	5.384057	2.004407	C	-3.270955	4.863476	1.358375
C	-1.497795	3.468488	1.049904	C	-3.38268	2.500499	0.777332
C	1.990821	6.915823	2.345096	C	-1.908001	7.312635	1.39332
H	2.92835	5.579769	0.943413	H	-0.391299	6.343906	0.214118
C	-0.326586	6.504759	2.88113	C	-3.821123	5.988036	2.034965
C	-1.494856	4.587847	1.853902	C	-3.930081	3.609279	1.385091
C	0.809659	7.255567	3.04744	C	-3.15542	7.187447	2.051005
H	2.897598	7.51932	2.50123	H	-1.378751	8.276668	1.430611
H	-1.250982	6.749921	3.425822	H	-4.787149	5.870736	2.548964
H	-2.406006	4.878326	2.401668	H	-4.890441	3.5307	1.919751
H	0.819228	8.12027	3.727093	H	-3.575483	8.058269	2.575333
O	-0.34905	2.000508	-0.473844	O	-1.663973	1.521934	-0.603419
O	1.956047	1.327112	0.587787	O	0.636264	2.075201	0.52658
P	0.517633	0.643253	0.022443	P	-0.315513	0.752259	0.056534
O	-0.072323	0.007286	1.258604	O	-0.664727	0.039143	1.3406
O	0.705976	-0.170715	-1.229432	O	0.276636	-0.03208	-1.081929
H	-0.148403	-1.578578	-1.593928	H	-0.682805	-1.703119	1.039722
N	-0.78241	-2.399526	-1.711174	N	-0.55938	-2.682737	0.704585
C	-2.74387	2.705735	0.916377	C	-4.085439	1.21776	0.884754
C	-2.996029	1.583076	1.718149	C	-3.724986	0.301362	1.88241
C	-3.724715	3.158901	0.026229	C	-5.15093	0.924049	0.025771
C	-4.250892	0.973035	1.668896	C	-4.45829	-0.877797	2.037235
H	-2.203324	1.174838	2.374406	H	-2.851331	0.498053	2.531791
C	-4.961882	2.512756	-0.037412	C	-5.862218	-0.268376	0.182831
H	-3.527243	4.029536	-0.620628	H	-5.429802	1.631528	-0.773116
C	-5.238668	1.426105	0.790657	C	-5.532956	-1.16996	1.196035

H	-6.223514	0.930532	0.761421	H	-6.115284	-2.097599	1.329715
C	4.509493	0.696226	-0.463627	C	3.253747	2.459657	-0.505506
C	5.180491	-0.038228	-1.449216	C	4.182161	1.928223	-1.41215
C	4.555708	0.260354	0.871287	C	3.463327	2.297542	0.871831
C	5.904279	-1.181473	-1.098591	C	5.314387	1.262322	-0.939791
H	5.135738	0.277104	-2.505011	H	4.010807	2.021497	-2.498032
C	5.287194	-0.878898	1.205133	C	4.601501	1.6304	1.328104
H	3.998185	0.817909	1.647309	H	2.716681	2.686055	1.587693
C	5.973073	-1.60442	0.227738	C	5.532794	1.106784	0.429665
H	6.553673	-2.50001	0.505822	H	6.421079	0.563632	0.794764
H	-1.234045	-4.34719	-1.282729	H	0.496899	-4.426743	0.715294
C	0.906762	-4.03124	-0.993532	C	1.19005	-3.164963	2.357972
C	1.120694	-5.363027	-0.60192	C	2.015354	-4.189013	2.856634
C	2.039215	-3.242095	-1.272352	C	1.08714	-1.979272	3.114565
C	2.383353	-5.923028	-0.496542	C	2.70445	-4.079736	4.054203
C	3.314448	-3.790936	-1.177863	C	1.774296	-1.855012	4.317634
H	1.915586	-2.202077	-1.556319	H	0.479445	-1.156104	2.750114
C	3.488438	-5.125507	-0.795904	C	2.577532	-2.899782	4.788707
H	2.482251	-6.958666	-0.189666	H	3.322132	-4.906287	4.388565
H	4.180888	-3.177004	-1.412993	H	1.688873	-0.935197	4.887772
H	4.486935	-5.547995	-0.728787	O	2.438186	-1.459751	-1.222496
C	-2.083705	-2.126179	-2.118962	O	3.928034	-3.209904	-0.14473
O	-1.871543	-1.826333	1.439026	O	2.309446	-4.00804	-1.876629
O	-2.558118	-4.284581	1.549767	C	4.306082	-2.280507	0.859797
O	-0.31351	-3.654947	2.536404	C	5.776718	-2.468261	1.146691
C	-3.380216	-3.980047	2.673211	H	3.679428	-2.481094	1.772288
C	-3.212496	-5.031519	3.747009	H	4.096934	-1.238092	0.492558
H	-4.437596	-3.982231	2.282362	H	6.075386	-1.790631	1.9834
H	-3.138603	-2.951815	3.056582	H	5.98881	-3.525762	1.431394
H	-3.952821	-4.845774	4.561205	H	6.380416	-2.218518	0.239867
H	-3.383977	-6.049563	3.323067	C	3.224221	-3.7873	-2.945447
H	-2.183165	-4.999566	4.178683	C	2.460809	-3.498291	-4.219251
C	0.857874	-2.847111	2.49318	H	3.816113	-4.739458	-3.054586
C	1.764806	-3.277252	3.620196	H	3.916774	-2.943551	-2.686085
H	0.552784	-1.768882	2.595309	H	3.168416	-3.494532	-5.082009
H	1.35263	-2.999019	1.493906	H	1.682392	-4.280796	-4.387811
H	2.71956	-2.697517	3.568126	H	1.954799	-2.5049	-4.162169
H	1.27408	-3.087174	4.604315	H	1.574269	-0.917937	-1.163158
H	1.992427	-4.367145	3.546343	C	-6.997765	-0.596421	-0.778591
H	-1.180328	-1.077085	1.316593	C	-4.058537	-1.853273	3.137312
C	-6.008749	3.02054	-1.019563	C	6.33966	0.709302	-1.922923
C	-4.590754	-0.187508	2.597669	C	4.845534	1.494388	2.825376
C	6.628027	-1.957405	-2.191847	F	-7.967532	-1.419993	-0.261471
C	5.364356	-1.347433	2.654082	F	-6.590097	-1.240063	-1.924275
F	-7.274811	2.524554	-0.827622	F	-7.69067	0.496425	-1.238127

F	-5.733812	2.729161	-2.335697	F	-3.853129	-1.27082	4.363776
F	-6.176151	4.384342	-1.012371	F	-4.970018	-2.850332	3.386166
F	-3.597474	-0.556638	3.466812	F	-2.887166	-2.530481	2.889081
F	-5.669431	0.066136	3.416124	F	6.923281	-0.471357	-1.531268
F	-4.941667	-1.348543	1.953229	F	7.406413	1.5491	-2.144204
F	5.821686	-2.315495	-3.246777	F	5.854041	0.450254	-3.180052
F	7.185758	-3.144965	-1.784318	F	5.505924	2.559423	3.388519
F	7.666323	-1.276103	-2.777099	F	5.604534	0.405009	3.184451
F	4.410495	-0.818733	3.486353	F	3.70694	1.367552	3.583618
F	6.556291	-1.057495	3.273025	H	3.111753	-2.795976	5.728855
F	5.228738	-2.707187	2.809764	C	-1.289767	-3.065316	-0.420691
N	-3.020987	-3.017528	-2.140821	S	-2.684817	-2.116067	-0.938886
S	-2.505456	-0.492684	-2.654545	N	-1.001693	-4.118007	-1.114677
C	-4.136656	-1.092625	-2.941222	C	-2.90627	-3.281329	-2.236289
C	-5.248543	-0.397903	-3.418082	C	-1.895946	-4.26919	-2.161839
C	-4.20517	-2.464679	-2.601916	C	-3.889497	-3.304914	-3.225909
C	-6.438774	-1.107797	-3.552042	C	-1.836676	-5.307118	-3.114043
H	-5.196273	0.660054	-3.662251	C	-3.83202	-4.339263	-4.155778
C	-5.414088	-3.176979	-2.736403	H	-4.671267	-2.550692	-3.265828
C	-6.515013	-2.469735	-3.217032	C	-2.821456	-5.314503	-4.100508
H	-7.325193	-0.597014	-3.918141	H	-4.581287	-4.391732	-4.940876
H	-7.462548	-2.990271	-3.331904	H	-2.805214	-6.101258	-4.850626
C	-5.484734	-4.635759	-2.366553	C	-0.742601	-6.340049	-3.044452
H	-4.806473	-5.235303	-2.985335	H	0.244248	-5.863619	-3.021414
H	-5.180574	-4.794685	-1.325517	H	-0.821245	-6.93942	-2.129167
H	-6.499659	-5.023755	-2.495306	H	-0.788329	-7.018676	-3.901764
F	0.042998	-6.118441	-0.306687	F	2.142763	-5.319597	2.133441

(R)-2-component-int1

C	-2.023714	5.824729	3.416283
C	-2.878901	4.800009	3.097058
C	-2.553832	3.882749	2.059094
C	-1.347327	4.044995	1.331989
C	-0.47606	5.110422	1.69724
C	-0.805264	5.974773	2.712073
H	-4.368318	2.714088	2.304648
H	-2.269862	6.533691	4.220696
H	-3.826747	4.66509	3.640066
C	-3.418191	2.80183	1.752599
C	-1.027254	3.123533	0.287313
H	0.475014	5.22554	1.15297
H	-0.123164	6.792055	2.991375
C	-1.851388	2.01256	0.082368
C	-3.090369	1.873537	0.787742
C	0.203794	3.275472	-0.49829

(S)- 2-component-int1

C	-2.022485	5.824962	3.416487
C	-2.877921	4.800519	3.097043
C	-2.552982	3.88328	2.059018
C	-1.346344	4.045274	1.332077
C	-0.474821	5.110414	1.697554
C	-0.803906	5.974742	2.712445
H	-4.36781	2.715083	2.304248
H	-2.268532	6.533903	4.220951
H	-3.825872	4.665805	3.639919
C	-3.417598	2.802625	1.752315
C	-1.026407	3.123844	0.287332
H	0.47635	5.225325	1.15341
H	-0.121611	6.791803	2.991921
C	-1.850824	2.013121	0.082174
C	-3.089911	1.874334	0.787409
C	0.204748	3.275534	-0.498153

C	0.469383	4.454796	-1.258152	C	0.470721	4.454885	-1.257842
C	1.097418	2.202254	-0.572759	C	1.098066	2.202067	-0.572719
C	-0.466425	5.523677	-1.353272	C	-0.464765	5.524057	-1.352859
C	1.690434	4.559689	-1.972453	C	1.691834	4.559516	-1.972074
C	2.345209	2.323512	-1.260992	C	2.345892	2.323027	-1.260941
C	-0.187053	6.640058	-2.10202	C	-0.18502	6.640466	-2.101426
H	-1.424907	5.433978	-0.817309	H	-1.423306	5.434563	-0.816969
C	1.961204	5.733093	-2.730194	C	1.962997	5.732954	-2.729623
C	2.62255	3.490458	-1.937645	C	2.623613	3.489986	-1.937413
C	1.043072	6.751203	-2.79332	C	1.045175	6.75135	-2.792642
H	-0.918255	7.45921	-2.176215	H	-0.915975	7.459846	-2.175539
H	2.918459	5.801238	-3.269289	H	2.920299	5.80089	-3.268661
H	3.577345	3.605547	-2.475967	H	3.578448	3.604851	-2.475712
H	1.247465	7.657527	-3.382537	H	1.249871	7.657702	-3.381709
O	0.845119	1.031582	0.124281	O	0.84544	1.031391	0.124194
O	-1.582631	1.0671	-0.891953	O	-1.582202	1.067716	-0.892239
P	-0.283914	0.024929	-0.642008	P	-0.283858	0.025112	-0.642196
O	0.156093	-0.576578	-1.928462	O	0.156006	-0.576545	-1.928629
O	-0.716078	-0.92756	0.549864	O	-0.716487	-0.927224	0.549619
H	-0.1835	-1.828547	0.649177	H	-0.184075	-1.828293	0.649369
N	0.610683	-3.127173	0.977367	N	0.60958	-3.126957	0.978303
C	3.332202	1.238088	-1.243913	C	3.332495	1.237243	-1.244103
C	3.235677	0.160984	-2.13611	C	3.235692	0.160518	-2.136721
C	4.399475	1.298778	-0.338845	C	4.399687	1.29722	-0.338887
C	4.215999	-0.834085	-2.122411	C	4.215711	-0.834858	-2.123361
H	2.383716	0.083189	-2.839615	H	2.383743	0.083251	-2.840294
C	5.369629	0.294712	-0.338381	C	5.369495	0.292829	-0.33872
H	4.471219	2.133733	0.378067	H	4.471624	2.131887	0.378344
C	5.287159	-0.775793	-1.229343	C	5.286782	-0.777279	-1.230148
H	6.05787	-1.564986	-1.227735	H	6.057253	-1.566704	-1.228767
C	-4.020278	0.783631	0.491159	C	-4.020013	0.784636	0.490673
C	-4.614329	0.068711	1.540404	C	-4.614407	0.069869	1.539832
C	-4.356559	0.470758	-0.834079	C	-4.356082	0.471756	-0.834616
C	-5.544605	-0.934639	1.262913	C	-5.544788	-0.933342	1.2622
H	-4.340315	0.289398	2.585825	H	-4.340569	0.290559	2.585298
C	-5.289837	-0.53368	-1.094679	C	-5.289439	-0.532575	-1.09536
H	-3.875165	1.017028	-1.665413	H	-3.874456	1.017922	-1.665885
C	-5.8924	-1.241642	-0.052751	C	-5.892334	-1.240383	-0.053523
H	-6.631508	-2.032123	-0.267284	H	-6.631504	-2.030776	-0.268165
C	0.533893	-4.260088	0.346878	C	0.531899	-4.260517	0.349078
H	1.226319	-5.07554	0.59767	H	1.223585	-5.076263	0.600961
C	-0.434203	-4.590967	-0.707535	C	-0.43627	-4.591892	-0.705121
C	-0.261845	-5.805375	-1.374128	C	-0.265553	-5.807922	-1.369184
C	-1.541455	-3.753017	-1.085035	C	-1.541922	-3.752874	-1.084954
C	-1.131396	-6.19625	-2.394171	C	-1.135224	-6.199456	-2.38887

H	0.576206	-6.467567	-1.10355	H	0.571248	-6.47096	-1.096812
C	-2.390433	-4.157399	-2.10276	C	-2.391048	-4.157947	-2.102282
H	-1.708865	-2.812855	-0.569263	H	-1.708027	-2.811339	-0.571283
C	-2.190588	-5.374703	-2.761897	C	-2.192885	-5.376931	-2.758815
H	-0.969603	-7.155557	-2.907787	H	-0.974746	-7.160081	-2.900433
H	-3.22984	-3.508711	-2.404032	H	-3.229233	-3.508485	-2.405299
H	-2.872137	-5.676504	-3.571412	H	-2.874535	-5.67928	-3.568041
C	1.574201	-2.917229	1.992557	C	1.57332	-2.916694	1.993229
C	2.651323	-3.775174	2.259974	C	2.650031	-3.774993	2.261174
C	1.441944	-1.730651	2.797995	C	1.441814	-1.729397	2.797729
C	3.56122	-3.503936	3.281703	C	3.560207	-3.503433	3.282568
H	2.822153	-4.6836	1.660703	H	2.820325	-4.683957	1.662566
C	2.338292	-1.466878	3.812837	C	2.33843	-1.465308	3.812253
H	0.622753	-1.045935	2.590162	H	0.622981	-1.044389	2.589458
C	3.404406	-2.357511	4.061767	C	3.404098	-2.356315	4.061754
H	4.394257	-4.199343	3.456823	H	4.39291	-4.199134	3.458112
H	2.238644	-0.56382	4.433827	H	2.239348	-0.561704	4.432539
C	6.54297	0.373927	0.630237	C	6.542798	0.371109	0.630019
C	4.11649	-2.013646	-3.08414	C	4.115989	-2.013897	-3.08571
C	-6.202605	-1.690238	2.411765	C	-6.203164	-1.688762	2.410955
C	-5.653876	-0.878392	-2.534484	C	-5.653158	-0.877355	-2.53523
F	6.289574	1.076967	1.782347	F	6.290559	1.076086	1.781194
F	7.660746	0.98005	0.107683	F	7.661817	0.974427	0.10688
F	6.999828	-0.844639	1.071264	F	6.997266	-0.84777	1.072659
F	5.333494	-2.509143	-3.491869	F	5.332913	-2.509733	-3.493268
F	3.473818	-3.110231	-2.562908	F	3.472626	-3.110461	-2.565304
F	3.454535	-1.746904	-4.255151	F	3.454583	-1.746224	-4.256823
F	-6.579657	-2.975167	2.10743	F	-6.580345	-2.973655	2.106626
F	-7.354632	-1.102952	2.878431	F	-7.355208	-1.101268	2.877319
F	-5.41751	-1.821793	3.530929	F	-5.418346	-1.820358	3.530309
F	-6.962164	-1.259611	-2.711187	F	-6.961419	-1.258535	-2.71222
F	-4.929318	-1.92257	-3.058687	F	-4.928513	-1.92159	-3.059204
F	-5.474626	0.143937	-3.432244	F	-5.473659	0.144915	-3.433008
O	4.230131	-1.995196	5.10369	O	4.230153	-1.993613	5.10328
C	5.358501	-2.832813	5.334502	C	5.358059	-2.831698	5.334663
H	6.014657	-2.869249	4.431386	H	6.014132	-2.8692	4.431529
H	5.883716	-2.329515	6.185652	H	5.883619	-2.328041	6.185389
H	5.030897	-3.860438	5.625055	H	5.029891	-3.858911	5.62603