

## Supporting Information

# Elucidation of the reaction mechanisms and diastereoselectivities of phosphine-catalyzed [4+2] annulations between allenolates and ketones or aldimines

Yan Qiao, Ke-Li Han\*

*State Key Laboratory of Molecular Reaction Dynamics*

*Dalian Institute of Chemical Physics*

*Chinese Academy of Science*

*NO.457, Zhongshan Road, Dalian 116023, P. R. China*

*klhan@dicp.ac.cn*

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## 1. The complete reference of Gaussian 09

Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J. and Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

## 2. Computed Energies of All Stationary Points

**Table S1.** For the reaction of 2-benzyl-2,3-butadienoate with trifluoromethyl ketone. The  $\delta G$ ,  $E+\delta E$ ,  $H$ , and  $G$  of stationary points for reaction pathways  $a_1(R,R,R)$ ,  $b_1(R,R,S)$ ,  $c_1(R,S,R)$ ,  $d_1(R,S,S)$  and their respective mirror image pathways  $d_1'(S,S,S)$ ,  $c_1'(S,S,R)$ ,  $b_1'(S,R,S)$ , and  $a_1'(S,R,R)$  at the M062x/6-31G(d,p) (B1) level and single-point energy at M062X/6-311++G(d,p) (B2) level in the  $CH_2Cl_2$ .

		$\delta G$	$E+\delta E$	$H$	$G$	$E(M062X/B2)$
<b>R1</b>		0.196565	-653.716465	-653.700984	-653.760006	-654.12384026
<b>PPh<sub>3</sub></b>		0.230047	-1035.708200	-1035.691485	-1035.754463	-1036.17043160
<b>TS1<sub>1</sub></b>		0.454815	-1689.418272	-1689.386679	-1689.481164	-1690.28696379
<b>M1<sub>1</sub></b>		0.456806	-1689.438176	-1689.406712	-1689.501852	-1690.30971320
<b>R2<sub>1</sub></b>		0.080126	-682.247550	-682.236920	-682.284117	-682.56675576
<b>TS2<sub>1</sub><sup>(R,R)</sup></b>	<b>TS2<sub>1</sub><sup>(S,S)</sup></b>	0.561312	-2371.692377	-2371.650562	-2371.769713	-2372.88031158
<b>M2<sub>1</sub><sup>(R,R)</sup></b>	<b>M2<sub>1</sub><sup>(S,S)</sup></b>	0.564871	-2371.701067	-2371.659493	-2371.777773	-2372.89415382
<b>TS3<sub>1</sub><sup>(R,R,R)</sup></b>	<b>TS3<sub>1</sub><sup>(S,S,S)</sup></b>	0.563198	-2371.689892	-2371.649078	-2371.762769	-2372.87512554
<b>M3<sub>1</sub><sup>(R,R,R)</sup></b>	<b>M3<sub>1</sub><sup>(S,S,S)</sup></b>	0.566172	-2371.721305	-2371.679780	-2371.796855	-2372.91250452
<b>TS4<sub>1</sub><sup>(R,R,R)</sup></b>	<b>TS4<sub>1</sub><sup>(S,S,S)</sup></b>	0.562303	-2371.659632	-2371.659632	-2371.775811	-2372.88971016
<b>M4<sub>1</sub><sup>(R,R,R)</sup></b>	<b>M4<sub>1</sub><sup>(S,S,S)</sup></b>	0.563983	-2371.698857	-2371.657205	-2371.775856	-2372.89277870
<b>M4<sub>1</sub><sup>'(R,R,R)</sup></b>	<b>M4<sub>1</sub><sup>'(S,S,S)</sup></b>	0.566640	-2371.700222	-2371.658854	-2371.774949	-2372.89778240
<b>TS5<sub>1</sub><sup>(R,R,R)</sup></b>	<b>TS5<sub>1</sub><sup>(S,S,S)</sup></b>	0.566217	-2371.684218	-2371.643330	-2371.759413	-2372.88039580
<b>M5<sub>1</sub><sup>(R,R,R)</sup></b>	<b>M5<sub>1</sub><sup>(S,S,S)</sup></b>	0.566744	-2371.712423	-2371.671393	-2371.788232	-2372.90369095
<b>TS6<sub>1</sub><sup>(R,R,R)</sup></b>	<b>TS6<sub>1</sub><sup>(S,S,S)</sup></b>	0.567135	-2371.710799	-2371.670188	-2371.785893	-2372.90193611
<b>P<sub>1</sub><sup>(R,R)</sup></b>	<b>P<sub>1</sub><sup>(S,S)</sup></b>	0.308731	-1336.028069	-1336.003609	-1336.083177	-1336.75406139
<b>TS3<sub>1</sub><sup>(R,R,S)</sup></b>	<b>TS3<sub>1</sub><sup>(S,S,R)</sup></b>	0.561472	-2371.692654	-2371.651657	-2371.766985	-2372.87660613
<b>M3<sub>1</sub><sup>(R,R,S)</sup></b>	<b>M3<sub>1</sub><sup>(S,S,R)</sup></b>	0.566186	-2371.721438	-2371.679770	-2371.796638	-2372.91099952
<b>TS4<sub>1</sub><sup>(R,R,S)</sup></b>	<b>TS4<sub>1</sub><sup>(S,S,R)</sup></b>	0.562745	-2371.695381	-2371.654382	2371.770332	-2372.88429514
<b>M4<sub>1</sub><sup>(R,R,S)</sup></b>	<b>M4<sub>1</sub><sup>(S,S,R)</sup></b>	0.563648	-2371.694031	-2371.652459	-2371.770338	-2372.88694590

<b>M4<sub>1</sub></b> <sup>(R,R,S)</sup>	<b>M4<sub>1</sub></b> <sup>(S,S,R)</sup>	0.564164	-2371.690954	-2371.649279	-2371.767547	-2372.88710762
<b>TS5<sub>1</sub></b> <sup>(R,R,S)</sup>	<b>TS5<sub>1</sub></b> <sup>(S,S,R)</sup>	0.564551	-2371.686725	-2371.686725	-2371.762192	-2372.87975092
<b>M5<sub>1</sub></b> <sup>(R,R,S)</sup>	<b>M5<sub>1</sub></b> <sup>(S,S,R)</sup>	0.566960	-2371.712207	-2371.671255	-2371.787453	-2372.90294802
<b>TS6<sub>1</sub></b> <sup>(R,R,S)</sup>	<b>TS6<sub>1</sub></b> <sup>(S,S,R)</sup>	0.566411	-2371.712655	-2371.672056	-2371.787655	-2372.90201211
<b>P<sub>1</sub></b> <sup>(R,S)</sup>	<b>P<sub>1</sub></b> <sup>(S,R)</sup>	0.309432	-1336.029521	-1336.005178	-1336.084524	-1336.75695149
<b>TS2<sub>1</sub></b> <sup>(R,S)</sup>	<b>TS2<sub>1</sub></b> <sup>(S,R)</sup>	0.566048	-2371.695952	-2371.654751	-2371.770005	-2372.88487012
<b>M2<sub>1</sub></b> <sup>(R,S)</sup>	<b>M2<sub>1</sub></b> <sup>(S,R)</sup>	0.567473	-2371.705921	-2371.664624	-2371.779968	-2372.89894452
<b>TS3<sub>1</sub></b> <sup>(R,S,R)</sup>	<b>TS3<sub>1</sub></b> <sup>(S,R,S)</sup>	0.562593	-2371.690419	-2371.649542	-2371.764039	-2372.87675399
<b>M3<sub>1</sub></b> <sup>(R,S,R)</sup>	<b>M3<sub>1</sub></b> <sup>(S,R,S)</sup>	0.566063	-2371.721107	-2371.679572	-2371.797020	-2372.91370622
<b>TS4<sub>1</sub></b> <sup>(R,S,R)</sup>	<b>TS4<sub>1</sub></b> <sup>(S,R,S)</sup>	0.564898	-2371.705119	-2371.664384	-2371.777955	-2372.89563452
<b>M4<sub>1</sub></b> <sup>(R,S,R)</sup>	<b>M4<sub>1</sub></b> <sup>(S,R,S)</sup>	0.566770	-2371.704170	-2371.662852	-2371.779036	-2372.90037071
<b>M4<sub>1</sub></b> <sup>(R,S,R)</sup>	<b>M4<sub>1</sub></b> <sup>(S,R,S)</sup>	0.565653	-2371.694565	-2371.653002	-2371.770677	-2372.89532907
<b>TS5<sub>1</sub></b> <sup>(R,S,R)</sup>	<b>TS5<sub>1</sub></b> <sup>(S,R,S)</sup>	0.566297	-2371.690916	-2371.650162	-2371.764858	-2372.88592990
<b>M5<sub>1</sub></b> <sup>(R,S,R)</sup>	<b>M5<sub>1</sub></b> <sup>(S,R,S)</sup>	0.571281	-2371.720751	-2371.680372	-2371.793315	-2372.91383238
<b>TS6<sub>1</sub></b> <sup>(R,S,R)</sup>	<b>TS6<sub>1</sub></b> <sup>(S,R,S)</sup>	0.569589	-2371.721922	-2371.681626	-2371.794950	-2372.91197612
<b>P<sub>1</sub></b> <sup>(S,R)</sup>	<b>P<sub>1</sub></b> <sup>(R,S)</sup>	0.309432	-1336.029521	-1336.005178	-1336.084524	-1336.75695149
<b>TS3<sub>1</sub></b> <sup>(R,S,S)</sup>	<b>TS3<sub>1</sub></b> <sup>(S,R,R)</sup>	0.562297	-2371.695667	-2371.654826	-2371.769509	-2372.88150951
<b>M3<sub>1</sub></b> <sup>(R,S,S)</sup>	<b>M3<sub>1</sub></b> <sup>(S,R,R)</sup>	0.568054	-2371.725109	-2371.683759	-2371.798710	-2372.91493416
<b>TS4<sub>1</sub></b> <sup>(R,S,S)</sup>	<b>TS4<sub>1</sub></b> <sup>(S,R,R)</sup>	0.560846	-2371.701597	-2371.660253	-2371.776993	-2372.88962841
<b>M4<sub>1</sub></b> <sup>(R,S,S)</sup>	<b>M4<sub>1</sub></b> <sup>(S,R,R)</sup>	0.565512	-2371.705728	-2371.664227	-2371.781484	-2372.89927729
<b>M4<sub>1</sub></b> <sup>(R,S,S)</sup>	<b>M4<sub>1</sub></b> <sup>(S,R,R)</sup>	0.564515	-2371.695108	-2371.653397	-2371.771338	-2372.89341863
<b>TS5<sub>1</sub></b> <sup>(R,S,S)</sup>	<b>TS5<sub>1</sub></b> <sup>(S,R,R)</sup>	0.565149	-2371.689593	-2371.648772	-2371.765120	-2372.88472095
<b>M5<sub>1</sub></b> <sup>(R,S,S)</sup>	<b>M5<sub>1</sub></b> <sup>(S,R,R)</sup>	0.568260	-2371.713413	-2371.672551	-2371.788040	-2372.90586024
<b>TS6<sub>1</sub></b> <sup>(R,S,S)</sup>	<b>TS6<sub>1</sub></b> <sup>(S,R,R)</sup>	0.566271	-2371.714144	-2371.673667	-2371.788938	-2372.90349100
<b>P<sub>1</sub></b> <sup>(S,S)</sup>	<b>P<sub>1</sub></b> <sup>(R,R)</sup>	0.308731	-1336.028069	-1336.003609	-1336.083177	-1336.75406139

**Table S2.** For the reaction of 2-benzyl-2,3-butadienoate with N-tosylbenzaldimine. The  $\delta G$ ,  $E+\delta E$ ,  $H$ , and  $G$  of stationary points for reaction pathways  $a_2$ (R,R,R),  $b_2$ (R,R,S),  $c_2$ (R,S,R),  $d_2$ (R,S,S) and their respective mirror image pathways  $d_2'$ (S,S,S),  $c_2'$ (S,S,R),  $b_2'$ (S,R,S), and  $a_2'$ (S,R,R.) at the M062x/6-31G(d,p) (B1) level and single-point energy at M062X/6-311++G(d,p) (B2) level in the  $CH_2Cl_2$ .

	$\delta G$	$E+\delta E$	$H$	$G$	$E(M062X/B2)$	
<b>R1</b>	0.196565	-653.716465	-653.700984	-653.760006	-654.12384026	
<b>PBu<sub>3</sub></b>	0.323461	-814.269343	-814.249671	-814.318338	-814.77590355	
<b>TS1<sub>2</sub></b>	0.548062	-1467.978271	-1467.943976	-1468.044557	-1468.89258947	
<b>M1<sub>2</sub></b>	0.551666	-1468.013299	-1467.979567	-1468.080014	-1468.93242185	
<b>R2<sub>2</sub></b>	0.197684	-1144.070711	-1144.053850	-1144.116800	-1144.52715258	
<b>TS2<sub>2</sub></b> <sup>(R,R)</sup>	<b>TS2<sub>2</sub></b> <sup>(S,S)</sup>	0.777957	-2612.091726	-2612.041713	-2612.177768	-2613.46769883
<b>M2<sub>2</sub></b> <sup>(R,R)</sup>	<b>M2<sub>2</sub></b> <sup>(S,S)</sup>	0.781548	-2612.117389	-2612.067337	-2612.203489	-2613.49687459
<b>TS3<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>TS3<sub>2</sub></b> <sup>(S,S,S)</sup>	0.773334	-2612.093503	-2612.043769	-2612.181374	-2613.46803919
<b>M3<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>M3<sub>2</sub></b> <sup>(S,S,S)</sup>	0.774746	-2612.111278	-2612.111278	-2612.201908	-2613.48835699
<b>TS4<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>TS4<sub>2</sub></b> <sup>(S,S,S)</sup>	0.772185	-2612.097253	-2612.046901	-2612.186111	-2613.47053059
<b>M4<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>M4<sub>2</sub></b> <sup>(S,S,S)</sup>	0.777256	-2612.110642	-2612.059996	-2612.199608	-2613.49172925

<b>M4<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>M4<sub>2</sub></b> <sup>(S,S,S)</sup>	0.782329	-2612.105867	-2612.055977	-2612.191626	-2613.48883315
<b>TS5<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>TS5<sub>2</sub></b> <sup>(S,S,S)</sup>	0.779384	-2612.090742	-2612.041084	-2612.177066	-2613.47028691
<b>M5<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>M5<sub>2</sub></b> <sup>(S,S,S)</sup>	0.786133	-2612.120320	-2612.120320	-2612.203552	-2613.50225508
<b>TS6<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>TS6<sub>2</sub></b> <sup>(S,S,S)</sup>	0.780249	-2612.109945	-2612.060423	-2612.196351	-2613.48796170
<b>P<sub>2</sub></b> <sup>(R,R)</sup>	<b>P<sub>2</sub></b> <sup>(S,S)</sup>	0.428827	-1797.860529	-1797.830110	-1797.923373	-1798.35219994
<b>TS3<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>TS3<sub>2</sub></b> <sup>(S,S,R)</sup>	0.776755	-2612.090931	-2612.090931	-2612.175878	-2613.46567721
<b>M3<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>M3<sub>2</sub></b> <sup>(S,S,R)</sup>	0.782293	-2612.110572	-2612.060667	-2612.195683	-2613.49118692
<b>TS4<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>TS4<sub>2</sub></b> <sup>(S,S,R)</sup>	0.774796	-2612.091797	-2612.041763	-2612.178760	-2613.46487972
<b>M4<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>M4<sub>2</sub></b> <sup>(S,S,R)</sup>	0.779794	-2612.111159	-2612.061010	-2612.198317	-2613.49193464
<b>M4<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>M4<sub>2</sub></b> <sup>(S,S,R)</sup>	0.781605	-2612.106056	-2612.056237	-2612.192033	-2613.48740574
<b>TS5<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>TS5<sub>2</sub></b> <sup>(S,S,R)</sup>	0.783325	-2612.084556	-2612.035681	-2612.168318	-2613.46421578
<b>M5<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>M5<sub>2</sub></b> <sup>(S,S,R)</sup>	0.785471	-2612.105823	-2612.056938	-2612.189443	-2613.48662517
<b>TS6<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>TS6<sub>2</sub></b> <sup>(S,S,R)</sup>	0.779927	-2612.090835	-2612.041275	-2612.176631	-2613.46672327
<b>P<sub>2</sub></b> <sup>(R,S)</sup>	<b>P<sub>2</sub></b> <sup>(S,R)</sup>	0.429811	-1797.858369	-1797.828071	-1797.920294	-1798.72582533
<b>TS2<sub>2</sub></b> <sup>(R,S)</sup>	<b>TS2<sub>2</sub></b> <sup>(S,R)</sup>	0.780791	-2612.092902	-2612.043215	-2612.176809	-2613.46922467
<b>M2<sub>2</sub></b> <sup>(R,S)</sup>	<b>M2<sub>2</sub></b> <sup>(S,R)</sup>	0.784039	-2612.114750	-2612.114750	-2612.198307	-2613.49435765
<b>TS3<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>TS3<sub>2</sub></b> <sup>(S,R,S)</sup>	0.775880	-2612.092848	-2612.043341	-2612.178834	-2613.46715662
<b>M3<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>M3<sub>2</sub></b> <sup>(S,R,S)</sup>	0.782931	-2612.112840	-2612.062907	-2612.197195	-2613.49218301
<b>TS4<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>TS4<sub>2</sub></b> <sup>(S,R,S)</sup>	0.775394	-2612.099517	-2612.049608	-2612.186022	-2613.47414381
<b>M4<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>M4<sub>2</sub></b> <sup>(S,R,S)</sup>	0.783685	-2612.118776	-2612.069221	-2612.203358	-2613.50018050
<b>M4<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>M4<sub>2</sub></b> <sup>(S,R,S)</sup>	0.781550	-2612.102134	-2612.051985	-2612.188160	-2613.48606310
<b>TS5<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>TS5<sub>2</sub></b> <sup>(S,R,S)</sup>	0.780052	-2612.087467	-2612.037781	-2612.173737	-2613.46790511
<b>M5<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>M5<sub>2</sub></b> <sup>(S,R,S)</sup>	0.783263	-2612.123190	-2612.073776	-2612.208260	-2613.50486075
<b>TS6<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>TS6<sub>2</sub></b> <sup>(S,R,S)</sup>	0.781733	-2612.115143	-2612.065880	-2612.200016	-2613.49308225
<b>P<sub>2</sub></b> <sup>(S,R)</sup>	<b>P<sub>2</sub></b> <sup>(R,S)</sup>	0.429811	-1797.858369	-1797.828071	-1797.920294	-1798.72582533
<b>TS3<sub>2</sub></b> <sup>(R,S,S)</sup>	<b>TS3<sub>2</sub></b> <sup>(S,R,R)</sup>	0.776202	-2612.091010	-2612.091010	-2612.177019	-2613.46614262
<b>M3<sub>2</sub></b> <sup>(R,S,S)</sup>	<b>M3<sub>2</sub></b> <sup>(S,R,R)</sup>	0.777015	-2612.111190	-2612.060747	-2612.200463	-2613.49037298
<b>TS4<sub>2</sub></b> <sup>(R,S,S)</sup>	<b>TS4<sub>2</sub></b> <sup>(S,R,R)</sup>	0.774117	-2612.093466	-2612.043529	-2612.181474	-2613.46808955
<b>M4<sub>2</sub></b> <sup>(R,S,S)</sup>	<b>M4<sub>2</sub></b> <sup>(S,R,R)</sup>	0.784291	-2612.116390	-2612.066891	-2612.199936	-2613.49773645
<b>M4<sub>2</sub></b> <sup>(R,S,S)</sup>	<b>M4<sub>2</sub></b> <sup>(S,R,R)</sup>	0.781454	-2612.106404	-2612.056458	-2612.192458	-2613.49031926
<b>TS5<sub>2</sub></b> <sup>(R,S,S)</sup>	<b>TS5<sub>2</sub></b> <sup>(S,R,R)</sup>	0.783001	-2612.092947	-2612.043835	-2612.176823	-2613.47456776
<b>M5<sub>2</sub></b> <sup>(R,S,S)</sup>	<b>M5<sub>2</sub></b> <sup>(S,R,R)</sup>	0.785073	-2612.108834	-2612.059802	-2612.192354	-2613.49041883
<b>TS6<sub>2</sub></b> <sup>(R,S,S)</sup>	<b>TS6<sub>2</sub></b> <sup>(S,R,R)</sup>	0.781169	-2612.100828	-2612.051525	-2612.185603	-2613.47742522
<b>P<sub>2</sub></b> <sup>(S,S)</sup>	<b>P<sub>2</sub></b> <sup>(R,R)</sup>	0.428827	-1797.860529	-1797.830110	-1797.923373	-1798.3521999

### 3. The computed NBO charge values of all stationary points

*Table S3.* The NBO charges on C1, C2, C3, C4, C5, O6, P, H1, and H2 atoms in all the stationary points for reaction of 2-benzyl-2,3-butadienoate with trifluoromethyl ketone at M06-2X/6-31G(d, p) level. (unit: e).

		C1	C2	C3	C4	C5	O6	P	H1	H2
<b>R1</b>		-0.489	-0.205	0.133	-0.504	—	—	—	0.270	0.267
<b>PPh<sub>3</sub></b>		—	—	—	—	—	—	0.924	—	—
<b>TS1<sub>1</sub></b>		-0.483	-0.303	0.003	-0.490	—	—	1.258	0.256	0.267
<b>M1<sub>1</sub></b>		-0.490	-0.327	-0.382	-0.505	—	—	1.755	0.236	0.283
<b>R2<sub>1</sub></b>		—	—	—	—	0.484	-0.502	—	—	—
<b>TS2<sub>1</sub><sup>(R,R)</sup></b>	<b>TS2<sub>1</sub><sup>(S,S)</sup></b>	-0.496	-0.206	-0.337	-0.614	0.384	-0.640	1.743	0.263	0.285
<b>M2<sub>1</sub><sup>(R,R)</sup></b>	<b>M2<sub>1</sub><sup>(S,S)</sup></b>	-0.513	-0.058	-0.302	-0.567	0.237	-0.882	1.737	0.298	0.288
<b>TS3<sub>1</sub><sup>(R,R,R)</sup></b>	<b>TS3<sub>1</sub><sup>(S,S,S)</sup></b>	-0.617	0.008	-0.452	-0.532	0.211	-0.867	1.740	0.434	0.263
<b>M3<sub>1</sub><sup>(R,R,R)</sup></b>	<b>M3<sub>1</sub><sup>(S,S,S)</sup></b>	-0.215	-0.148	-0.765	-0.483	0.199	-0.789	1.753	0.527	0.249
<b>TS4<sub>1</sub><sup>(R,R,R)</sup></b>	<b>TS4<sub>1</sub><sup>(S,S,S)</sup></b>	-0.174	-0.121	-0.736	-0.503	0.206	-0.861	1.757	0.421	0.263
<b>M4<sub>1</sub><sup>(R,R,R)</sup></b>	<b>M4<sub>1</sub><sup>(S,S,S)</sup></b>	-0.163	-0.126	-0.644	-0.515	0.221	-0.903	1.737	0.378	0.267
<b>M4<sub>1</sub><sup>′(R,R,R)</sup></b>	<b>M4<sub>1</sub><sup>′(S,S,S)</sup></b>	-0.167	-0.117	-0.590	-0.523	0.224	-0.897	1.754	0.336	0.267
<b>TS5<sub>1</sub><sup>(R,R,R)</sup></b>	<b>TS5<sub>1</sub><sup>(S,S,S)</sup></b>	-0.019	-0.283	-0.573	-0.510	0.223	-0.821	1.723	0.309	0.283
<b>M5<sub>1</sub><sup>(R,R,R)</sup></b>	<b>M5<sub>1</sub><sup>(S,S,S)</sup></b>	0.061	-0.417	-0.507	-0.504	0.207	-0.600	1.664	0.282	0.282
<b>TS6<sub>1</sub><sup>(R,R,R)</sup></b>	<b>TS6<sub>1</sub><sup>(S,S,S)</sup></b>	0.064	-0.364	-0.329	-0.525	0.206	-0.596	1.421	0.277	0.282
<b>P<sub>1</sub><sup>(R,R)</sup></b>	<b>P<sub>1</sub><sup>(S,S)</sup></b>	0.072	-0.174	-0.137	-0.541	0.199	-0.590	—	0.270	0.253
<b>TS3<sub>1</sub><sup>(R,R,S)</sup></b>	<b>TS3<sub>1</sub><sup>(S,S,R)</sup></b>	-0.609	0.027	-0.470	-0.528	0.210	-0.870	1.743	0.268	0.430
<b>M3<sub>1</sub><sup>(R,R,S)</sup></b>	<b>M3<sub>1</sub><sup>(S,S,R)</sup></b>	-0.290	-0.121	-0.738	-0.498	0.196	-0.772	1.740	0.242	0.521
<b>TS4<sub>1</sub><sup>(R,R,S)</sup></b>	<b>TS4<sub>1</sub><sup>(S,S,R)</sup></b>	-0.183	-0.107	-0.727	-0.502	0.206	-0.862	1.758	0.247	0.418
<b>M4<sub>1</sub><sup>(R,R,S)</sup></b>	<b>M4<sub>1</sub><sup>(S,S,R)</sup></b>	-0.171	-0.113	-0.643	-0.518	0.221	-0.895	1.738	0.251	0.376
<b>M4<sub>1</sub><sup>′(R,R,S)</sup></b>	<b>M4<sub>1</sub><sup>′(S,S,R)</sup></b>	-0.104	-0.196	-0.551	-0.519	0.236	-0.912	1.719	0.300	0.311
<b>TS5<sub>1</sub><sup>(R,R,S)</sup></b>	<b>TS5<sub>1</sub><sup>(S,S,R)</sup></b>	-0.031	-0.286	-0.547	-0.508	0.221	-0.800	1.705	0.262	0.308
<b>M5<sub>1</sub><sup>(R,R,S)</sup></b>	<b>M5<sub>1</sub><sup>(S,S,R)</sup></b>	0.079	-0.381	-0.482	-0.508	0.208	-0.607	1.637	0.206	0.284
<b>TS6<sub>1</sub><sup>(R,R,S)</sup></b>	<b>TS6<sub>1</sub><sup>(S,S,R)</sup></b>	0.081	-0.352	-0.357	-0.521	0.208	-0.602	1.464	0.209	0.281
<b>P<sub>1</sub><sup>(R,S)</sup></b>	<b>P<sub>1</sub><sup>(S,R)</sup></b>	0.076	-0.173	-0.129	-0.550	0.201	-0.591	—	0.243	0.270
<b>TS2<sub>1</sub><sup>(R,S)</sup></b>	<b>TS2<sub>1</sub><sup>(S,R)</sup></b>	-0.510	-0.199	-0.343	-0.601	0.380	-0.640	1.749	0.277	0.284
<b>M2<sub>1</sub><sup>(R,S)</sup></b>	<b>M2<sub>1</sub><sup>(S,R)</sup></b>	-0.524	-0.039	-0.322	-0.552	0.238	-0.892	1.735	0.314	0.274
<b>TS3<sub>1</sub><sup>(R,S,R)</sup></b>	<b>TS3<sub>1</sub><sup>(S,R,S)</sup></b>	-0.625	0.017	-0.450	-0.523	0.215	-0.860	1.739	0.443	0.259
<b>M3<sub>1</sub><sup>(R,S,R)</sup></b>	<b>M3<sub>1</sub><sup>(S,R,S)</sup></b>	-0.224	-0.126	-0.777	-0.491	0.195	-0.784	1.741	0.521	0.251
<b>TS4<sub>1</sub><sup>(R,S,R)</sup></b>	<b>TS4<sub>1</sub><sup>(S,R,S)</sup></b>	-0.175	-0.123	-0.732	-0.498	0.200	-0.857	1.753	0.424	0.263
<b>M4<sub>1</sub><sup>(R,S,R)</sup></b>	<b>M4<sub>1</sub><sup>(S,R,S)</sup></b>	-0.167	-0.125	-0.644	-0.510	0.222	-0.907	1.765	0.369	0.273
<b>M4<sub>1</sub><sup>′(R,S,R)</sup></b>	<b>M4<sub>1</sub><sup>′(S,R,S)</sup></b>	-0.182	-0.095	-0.607	-0.498	0.216	-0.896	1.735	0.333	0.265
<b>TS5<sub>1</sub><sup>(R,S,R)</sup></b>	<b>TS5<sub>1</sub><sup>(S,R,S)</sup></b>	-0.023	-0.282	-0.587	-0.515	0.217	-0.846	1.742	0.316	0.287
<b>M5<sub>1</sub><sup>(R,S,R)</sup></b>	<b>M5<sub>1</sub><sup>(S,R,S)</sup></b>	0.051	-0.456	-0.564	-0.508	0.204	-0.613	1.725	0.305	0.289
<b>TS6<sub>1</sub><sup>(R,S,R)</sup></b>	<b>TS6<sub>1</sub><sup>(S,R,S)</sup></b>	0.083	-0.348	-0.340	-0.516	0.205	-0.600	1.430	0.278	0.256
<b>P<sub>1</sub><sup>(S,R)</sup></b>	<b>P<sub>1</sub><sup>(R,S)</sup></b>	0.076	-0.173	-0.129	-0.550	0.201	-0.591	—	0.270	0.243
<b>TS3<sub>1</sub><sup>(R,S,S)</sup></b>	<b>TS3<sub>1</sub><sup>(S,R,R)</sup></b>	-0.610	0.026	-0.478	-0.517	0.214	-0.866	1.742	0.271	0.437
<b>M3<sub>1</sub><sup>(R,S,S)</sup></b>	<b>M3<sub>1</sub><sup>(S,R,R)</sup></b>	-0.358	-0.098	-0.696	-0.495	0.197	-0.780	1.735	0.243	0.527
<b>TS4<sub>1</sub><sup>(R,S,S)</sup></b>	<b>TS4<sub>1</sub><sup>(S,R,R)</sup></b>	-0.185	-0.101	0.746	-0.499	0.195	-0.863	1.773	0.245	0.421
<b>M4<sub>1</sub><sup>(R,S,S)</sup></b>	<b>M4<sub>1</sub><sup>(S,R,R)</sup></b>	-0.162	-0.120	-0.568	-0.515	0.213	-0.938	1.732	0.251	0.331
<b>M4<sub>1</sub><sup>′(R,S,S)</sup></b>	<b>M4<sub>1</sub><sup>′(S,R,R)</sup></b>	-0.106	-0.193	-0.568	-0.524	0.232	-0.900	1.732	0.287	0.312
<b>TS5<sub>1</sub><sup>(R,S,S)</sup></b>	<b>TS5<sub>1</sub><sup>(S,R,R)</sup></b>	-0.041	-0.300	-0.559	-0.512	0.217	-0.805	1.717	0.268	0.310

<b>M5<sub>1</sub></b> <sup>(R,S,S)</sup>	<b>M5<sub>1</sub></b> <sup>(S,R,R)</sup>	0.072	-0.397	-0.502	-0.506	0.207	-0.606	1.655	0.220	0.291
<b>TS6<sub>1</sub></b> <sup>(R,S,S)</sup>	<b>TS6<sub>1</sub></b> <sup>(S,R,R)</sup>	0.077	-0.352	-0.335	-0.519	0.205	-0.597	1.429	0.217	0.281
<b>P<sub>1</sub></b> <sup>(S,S)</sup>	<b>P<sub>1</sub></b> <sup>(R,R)</sup>	0.072	-0.174	-0.137	-0.541	0.199	-0.590	—	0.270	0.253

**Table S4.** The NBO charges on C1, C2, C3, C4, C5, N6, P, H1, and H2 atoms in all the stationary points for reaction of 2-benzyl-2,3-butadienoate with N-tosylbenzaldimine at M06-2X/6-31G(d, p) level. (unit: e).

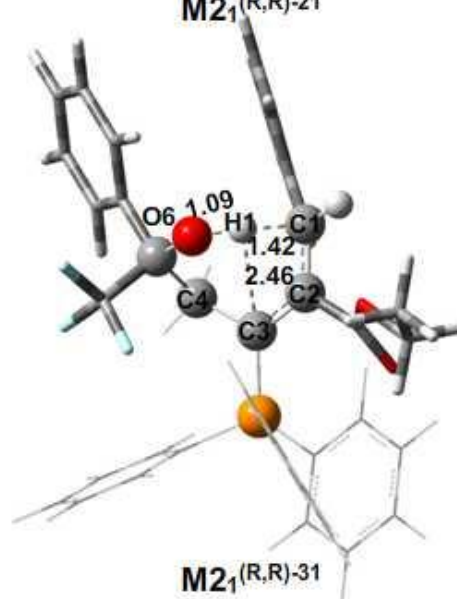
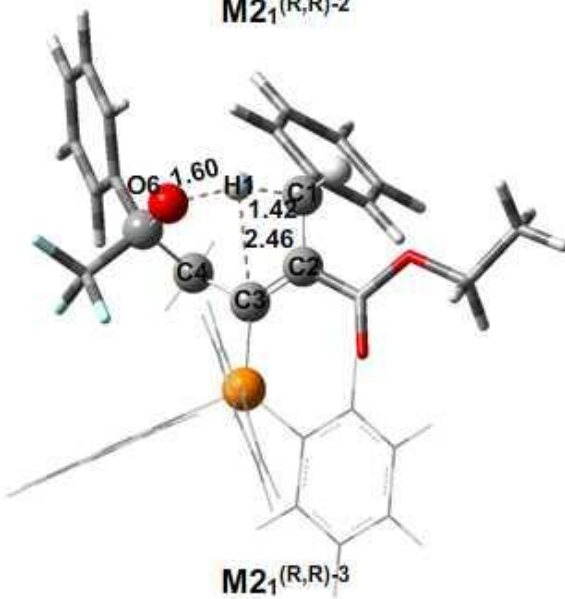
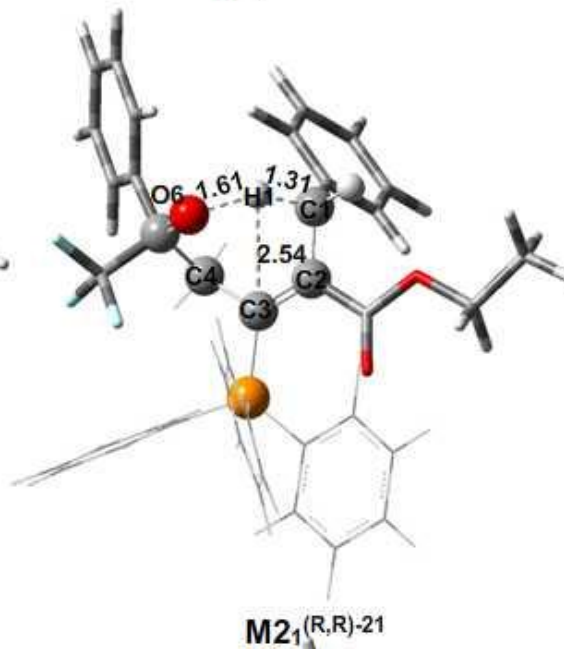
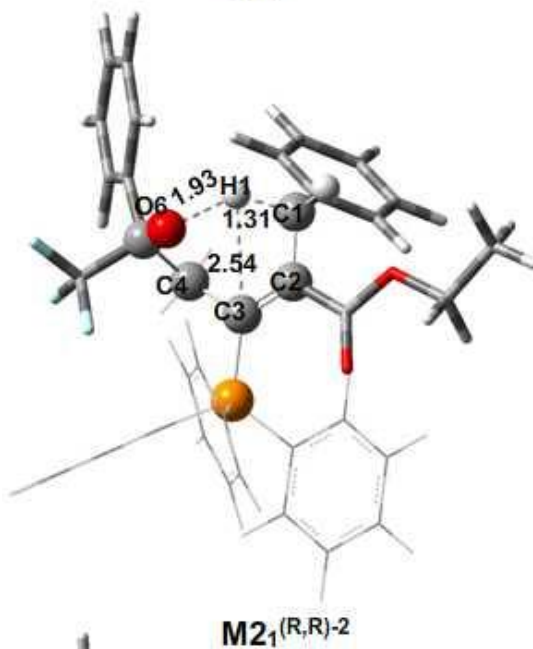
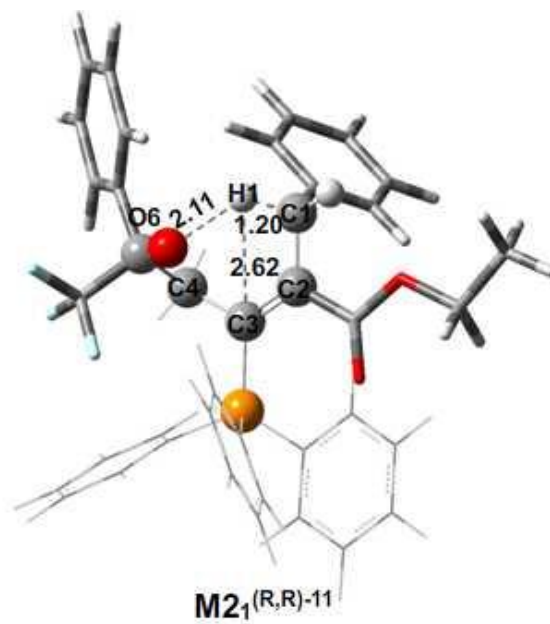
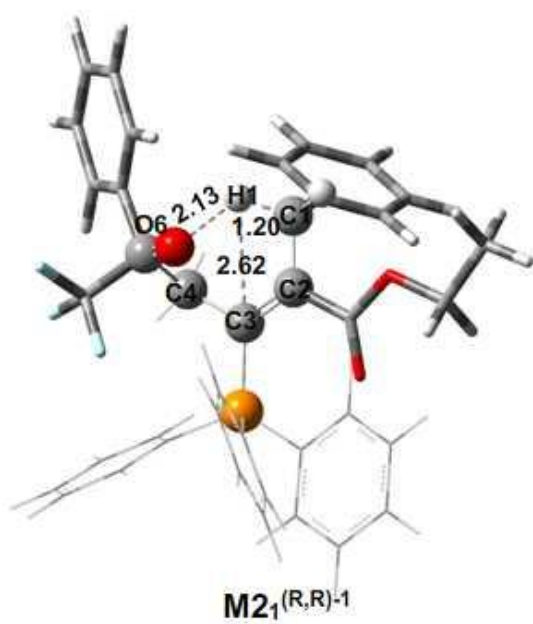
		C1	C2	C3	C4	C5	N6	P	H1	H2
<b>R1</b>		-0.489	-0.205	0.133	-0.504	—	—	—	0.270	0.267
<b>PBu<sub>3</sub></b>		—	—	—	—	—	—	0.883	—	—
<b>TS1<sub>2</sub></b>		-0.482	-0.282	0.076	-0.514	—	—	1.128	0.259	0.268
<b>M1<sub>2</sub></b>		-0.491	-0.313	-0.375	-0.515	—	—	1.752	0.236	0.284
<b>R2<sub>2</sub></b>		—	—	—	—	0.141	-0.716	—	—	—
<b>TS2<sub>2</sub></b> <sup>(R,R)</sup>	<b>TS2<sub>2</sub></b> <sup>(S,S)</sup>	-0.498	-0.233	-0.339	-0.573	0.090	-0.846	1.747	0.259	0.282
<b>M2<sub>2</sub></b> <sup>(R,R)</sup>	<b>M2<sub>2</sub></b> <sup>(S,S)</sup>	-0.519	-0.078	-0.285	-0.503	-0.057	-1.080	1.743	0.292	0.291
<b>TS3<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>TS3<sub>2</sub></b> <sup>(S,S,S)</sup>	-0.597	-0.035	-0.479	-0.485	-0.055	-1.027	1.742	0.426	0.277
<b>M3<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>M3<sub>2</sub></b> <sup>(S,S,S)</sup>	-0.237	-0.136	-0.770	-0.465	-0.070	-0.954	1.748	0.451	0.248
<b>TS4<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>TS4<sub>2</sub></b> <sup>(S,S,S)</sup>	-0.196	-0.125	-0.781	-0.462	-0.074	-1.049	1.779	0.428	0.264
<b>M4<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>M4<sub>2</sub></b> <sup>(S,S,S)</sup>	-0.143	-0.131	-0.604	-0.471	-0.076	-1.076	1.741	0.326	0.273
<b>M4<sub>2</sub>'</b> <sup>(R,R,R)</sup>	<b>M4<sub>2</sub>'</b> <sup>(S,S,S)</sup>	-0.125	-0.127	-0.582	-0.461	-0.075	-1.091	1.752	0.317	0.268
<b>TS5<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>TS5<sub>2</sub></b> <sup>(S,S,S)</sup>	-0.031	-0.315	-0.575	-0.465	-0.067	-0.966	1.733	0.294	0.291
<b>M5<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>M5<sub>2</sub></b> <sup>(S,S,S)</sup>	-0.094	-0.375	-0.571	-0.468	-0.065	-0.753	1.767	0.254	0.311
<b>TS6<sub>2</sub></b> <sup>(R,R,R)</sup>	<b>TS6<sub>2</sub></b> <sup>(S,S,S)</sup>	-0.097	-0.337	-0.267	-0.495	-0.061	-0.752	1.302	0.265	0.306
<b>P<sub>2</sub></b> <sup>(R,R)</sup>	<b>P<sub>2</sub></b> <sup>(S,S)</sup>	-0.104	-0.171	-0.138	-0.525	-0.080	-0.754	—	0.267	0.308
<b>TS3<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>TS3<sub>2</sub></b> <sup>(S,S,R)</sup>	-0.592	-0.003	-0.493	-0.477	-0.058	-1.033	1.733	0.272	0.433
<b>M3<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>M3<sub>2</sub></b> <sup>(S,S,R)</sup>	-0.330	-0.111	-0.715	-0.464	-0.066	-0.948	1.742	0.239	0.460
<b>TS4<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>TS4<sub>2</sub></b> <sup>(S,S,R)</sup>	-0.208	-0.109	-0.779	-0.466	-0.075	-1.042	1.780	0.245	0.425
<b>M4<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>M4<sub>2</sub></b> <sup>(S,S,R)</sup>	-0.156	-0.133	-0.597	-0.475	-0.072	-1.095	1.743	0.253	0.335
<b>M4<sub>2</sub>'</b> <sup>(R,R,S)</sup>	<b>M4<sub>2</sub>'</b> <sup>(S,S,R)</sup>	-0.091	-0.176	-0.582	-0.464	-0.074	-1.077	1.748	0.290	0.311
<b>TS5<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>TS5<sub>2</sub></b> <sup>(S,S,R)</sup>	-0.023	-0.328	-0.576	-0.475	-0.078	-0.942	1.757	0.256	0.288
<b>M5<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>M5<sub>2</sub></b> <sup>(S,S,R)</sup>	-0.075	-0.358	-0.565	-0.482	-0.068	-0.764	1.767	0.247	0.268
<b>TS6<sub>2</sub></b> <sup>(R,R,S)</sup>	<b>TS6<sub>2</sub></b> <sup>(S,S,R)</sup>	-0.087	-0.321	-0.214	-0.517	-0.069	-0.742	1.245	0.273	0.255
<b>P<sub>2</sub></b> <sup>(R,S)</sup>	<b>P<sub>2</sub></b> <sup>(S,R)</sup>	-0.090	-0.152	-0.141	-0.505	-0.070	-0.775	—	0.281	0.269
<b>TS2<sub>2</sub></b> <sup>(R,S)</sup>	<b>TS2<sub>2</sub></b> <sup>(S,R)</sup>	-0.495	-0.212	-0.343	-0.578	0.077	-0.870	1.747	0.278	0.273
<b>M2<sub>2</sub></b> <sup>(R,S)</sup>	<b>M2<sub>2</sub></b> <sup>(S,R)</sup>	-0.505	-0.056	-0.297	-0.505	-0.070	-1.105	1.731	0.303	0.275
<b>TS3<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>TS3<sub>2</sub></b> <sup>(S,R,S)</sup>	-0.596	-0.027	-0.467	-0.478	-0.065	-1.047	1.739	0.440	0.273
<b>M3<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>M3<sub>2</sub></b> <sup>(S,R,S)</sup>	-0.315	-0.124	-0.712	-0.464	-0.071	-0.960	1.759	0.460	0.261
<b>TS4<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>TS4<sub>2</sub></b> <sup>(S,R,S)</sup>	-0.195	-0.126	-0.780	-0.467	-0.089	-1.042	1.766	0.432	0.262
<b>M4<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>M4<sub>2</sub></b> <sup>(S,R,S)</sup>	-0.138	-0.141	-0.631	-0.469	-0.097	-1.088	1.730	0.354	0.270
<b>M4<sub>2</sub>'</b> <sup>(R,S,R)</sup>	<b>M4<sub>2</sub>'</b> <sup>(S,R,S)</sup>	-0.102	-0.162	-0.616	-0.465	-0.085	-1.069	1.735	0.321	0.270
<b>TS5<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>TS5<sub>2</sub></b> <sup>(S,R,S)</sup>	-0.024	-0.335	-0.597	-0.456	-0.074	-0.982	1.722	0.312	0.302
<b>M5<sub>2</sub></b> <sup>(R,S,R)</sup>	<b>M5<sub>2</sub></b> <sup>(S,R,S)</sup>	-0.097	-0.382	-0.556	-0.465	-0.057	-0.780	1.726	0.289	0.308

<b>TS6<sub>2</sub><sup>(R,S,R)</sup></b>	<b>TS6<sub>2</sub><sup>(S,R,S)</sup></b>	-0.085	-0.318	-0.309	-0.474	-0.062	-0.779	1.316	0.278	0.289
<b>P<sub>2</sub><sup>(S,R)</sup></b>	<b>P<sub>2</sub><sup>(R,S)</sup></b>	-0.090	-0.152	-0.141	-0.505	-0.070	-0.775	—	0.269	0.281
<b>TS3<sub>2</sub><sup>(R,S,S)</sup></b>	<b>TS3<sub>2</sub><sup>(S,R,R)</sup></b>	-0.593	-0.003	-0.494	-0.476	-0.067	-1.033	1.738	0.268	0.423
<b>M3<sub>2</sub><sup>(R,S,S)</sup></b>	<b>M3<sub>2</sub><sup>(S,R,R)</sup></b>	-0.333	-0.120	-0.708	-0.461	-0.073	-0.959	1.751	0.239	0.462
<b>TS4<sub>2</sub><sup>(R,S,S)</sup></b>	<b>TS4<sub>2</sub><sup>(S,R,R)</sup></b>	-0.209	-0.122	-0.763	-0.467	-0.087	-1.051	1.768	0.243	0.439
<b>M4<sub>2</sub><sup>(R,S,S)</sup></b>	<b>M4<sub>2</sub><sup>(S,R,R)</sup></b>	-0.151	-0.123	-0.625	-0.471	-0.091	-1.103	1.755	0.262	0.339
<b>M4<sub>2</sub>'<sup>(R,S,S)</sup></b>	<b>M4'<sup>(S,R,R)</sup></b>	-0.085	-0.169	-0.595	-0.475	-0.083	-1.071	1.752	0.264	0.321
<b>TS5<sub>2</sub><sup>(R,S,S)</sup></b>	<b>TS5<sub>2</sub><sup>(S,R,R)</sup></b>	-0.036	-0.335	-0.580	-0.474	-0.084	-0.929	1.744	0.246	0.305
<b>M5<sub>2</sub><sup>(R,S,S)</sup></b>	<b>M5<sub>2</sub><sup>(S,R,R)</sup></b>	-0.069	-0.372	-0.555	-0.483	-0.072	-0.754	1.728	0.214	0.287
<b>TS6<sub>2</sub><sup>(R,S,S)</sup></b>	<b>TS6<sub>2</sub><sup>(S,R,R)</sup></b>	-0.075	-0.306	-0.246	-0.505	-0.070	-0.756	1.247	0.231	0.271
<b>P<sub>2</sub><sup>(S,S)</sup></b>	<b>P<sub>2</sub><sup>(R,R)</sup></b>	-0.104	-0.171	-0.138	-0.525	-0.080	-0.754	—	0.308	0.267

#### 4. The detailed 1,3-H shift scan results.

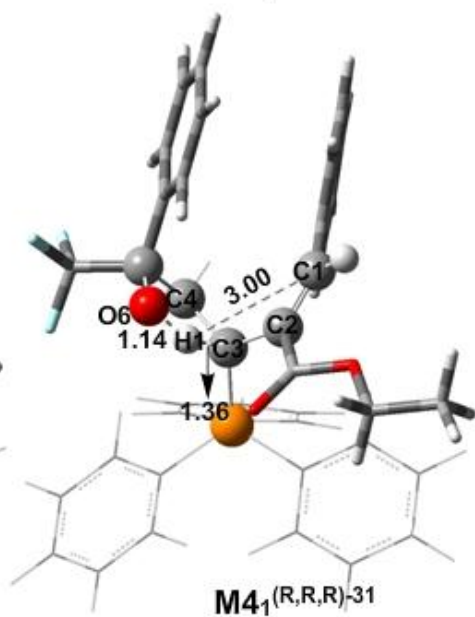
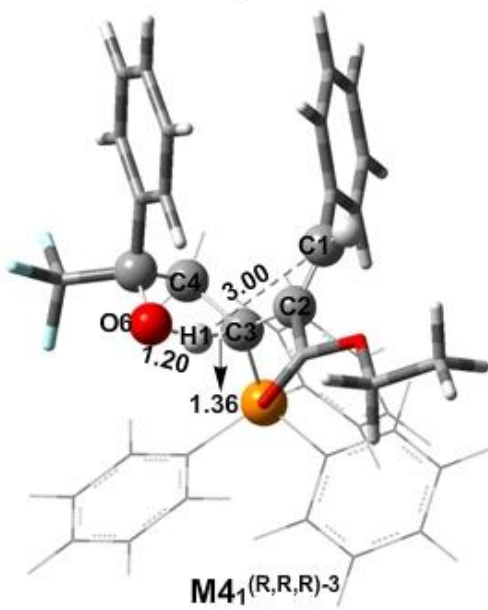
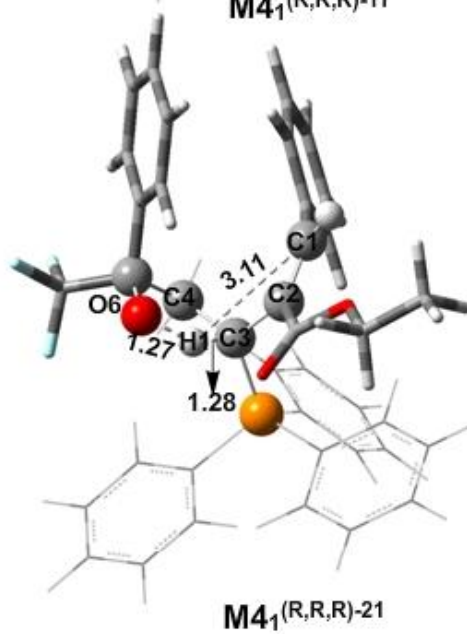
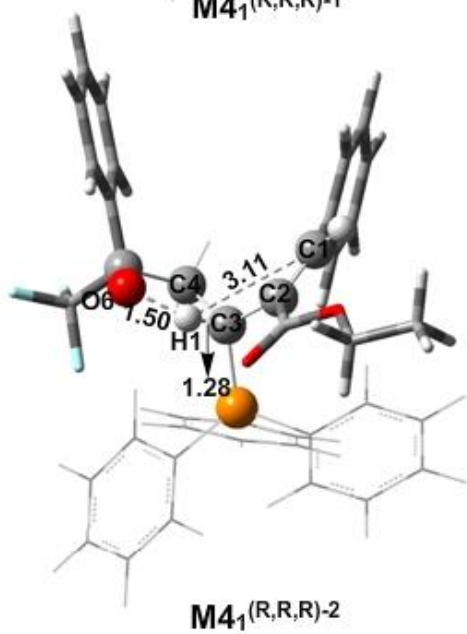
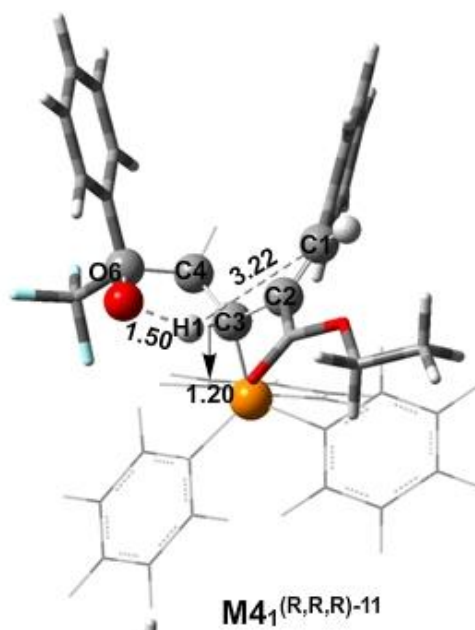
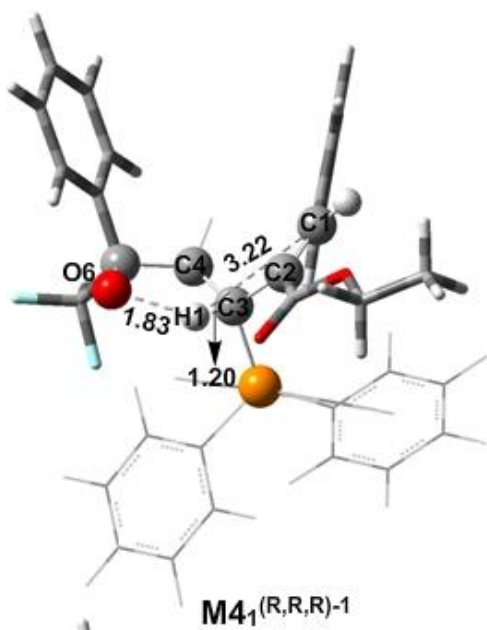
The 1,3-H shift of H1 transferring from C1 to C3 (**M2<sub>1</sub><sup>(R,R)</sup>** to **M4<sub>1</sub><sup>(R,R,R)</sup>**). During this process, the C1-H1 distance elongates from 1.09 Å in **M2<sub>1</sub><sup>(R,R)</sup>** to 3.33 Å in **M4<sub>1</sub><sup>(R,R,R)</sup>** (distance variation = 3.33-1.09=2.24 Å), while the H1-C3 distance shortens from 2.70 Å in **M2<sub>1</sub><sup>(R,R)</sup>** to 1.12 Å in **M4<sub>1</sub><sup>(R,R,R)</sup>** (distance variation = 2.70-1.12=1.58 Å) (Figure S1). Suppose the 1,3-H shift is completed using 20 steps, the C1-H1 will be elongated by 0.11 Å (2.24/20=0.11Å) every step, while the H1-C3 will be shortened by 0.08 Å (1.58/20=0.08Å) for each step. The distance variation is automatically adjusted in Gaussian 09 using the “addredundant and redundant” keywords. First, the C1-H1 and H1-C3 distances are altered from 1.09 and 2.70 Å in **M2<sub>1</sub><sup>(R,R)</sup>** to 1.20 (1.09+0.11) and 2.62 (2.70-0.08) Å in **M2<sub>1</sub><sup>(R,R)-1</sup>**. Then, fix the C1-H1 and H1-C3 distances at 1.20 and 2.62 Å and optimize the other parts of **M2<sub>1</sub><sup>(R,R)-1</sup>**, the optimized structure is **M2<sub>1</sub><sup>(R,R)-11</sup>** (Figure S1). During this process, we also monitored the H1-O6 distance variations, which is varied from 2.29 Å in **M2<sub>1</sub><sup>(R,R)</sup>** to 2.13 Å in **M2<sub>1</sub><sup>(R,R)-1</sup>**, and then to 2.11 Å in **M2<sub>1</sub><sup>(R,R)-11</sup>**. Next, we altered the C1-H1 and H1-C3 distances in **M2<sub>1</sub><sup>(R,R)-11</sup>** to 1.31 (1.20+0.11) and 2.54 (2.62-0.08) Å in **M2<sub>1</sub><sup>(R,R)-2</sup>**. Similarly, the two distances are fixed and the other parts of **M2<sub>1</sub><sup>(R,R)-2</sup>** are relaxed when optimization runs. The optimized structure is **M2<sub>1</sub><sup>(R,R)-21</sup>**. In the following, we repeated this procedure to **M2<sub>1</sub><sup>(R,R)-3</sup>** (in which the C1-H1 and H1-C3 distances are altered to 1.42 (1.31+0.11) and 2.46(2.54-0.08) Å), and obtained the optimized structure **M2<sub>1</sub><sup>(R,R)-31</sup>**. By now, the H1 has not transferred to C3. Unexpectedly, the distance of H1-O6 becomes 1.09 Å, which means the H1 has transferred to O6 rather than to C3. Therefore, the scan results further verified that H1 is preferred to be transferred to O6.

We also tried to scan the H-shift from C3 to C1 (**M4<sub>1</sub><sup>(R,R,R)</sup>** to **M2<sub>1</sub><sup>(R,R)</sup>**), the H1-C3 distance is elongated and simultaneously the H1-C1 distance is shortened. Similarly, H1 is transferred to O6 but not C1. (Figure S2)





**Figure S1.**  $\mathbf{M2}_1^{(R,R)-1}$ ,  $\mathbf{M2}_1^{(R,R)-2}$ , and  $\mathbf{M2}_1^{(R,R)-3}$  are the initial structures (in which the C1-H1 distance is gradually elongated and simultaneously the H1-C3 distance is gradually shortened).  $\mathbf{M2}_1^{(R,R)-11}$ ,  $\mathbf{M2}_1^{(R,R)-21}$ , and  $\mathbf{M2}_1^{(R,R)-31}$  are the corresponding optimized structures.



**Figure S2.**  $M4_1^{(R,R,R)-1}$ ,  $M4_1^{(R,R,R)-2}$ , and  $M4_1^{(R,R,R)-3}$  are the initial structures (in which the C3-H1 distance is gradually elongated and simultaneously the H1-C1 distance is gradually shortened).  $M4_1^{(R,R,R)-11}$ ,  $M4_1^{(R,R,R)-21}$ , and  $M4_1^{(R,R,R)-31}$  are the corresponding optimized structures.

## 5. Coordinates of all stationary points.

### 5.1 Coordinates of all stationary points for the reaction of 2-benzyl-2,3-butadienoate with trifluoromethyl ketone.

R1			
C	2.18122000	-1.87699700	0.13685100
C	1.43367800	-0.83524700	0.42762400
C	2.91262000	-2.91721900	-0.14002800
H	3.79662000	-3.15349200	0.44510100
H	2.65935100	-3.57141100	-0.96933600
C	1.76301500	0.46168600	-0.23683400
O	2.63354700	0.62946100	-1.06183300
O	0.95906600	1.43802900	0.19949700
C	1.13369800	2.72483300	-0.41648000
C	0.01562300	3.61054000	0.08563000
H	1.10416300	2.59922600	-1.50206500
H	2.12163900	3.11105000	-0.14849800
H	0.10307400	4.60541200	-0.35639900
H	-0.95433800	3.18852100	-0.18886800
H	0.05959700	3.70798700	1.17304700
C	0.24602000	-0.91221700	1.36913400
H	0.33515300	-0.12427100	2.12219100
H	0.28322800	-1.87449900	1.88721500
C	-1.07562500	-0.77164700	0.63978200
C	-1.90132000	0.33254800	0.85217400
C	-1.48334000	-1.75493700	-0.26482600
C	-3.11558700	0.45177500	0.17914400
H	-1.58246300	1.10794400	1.54377100
C	-2.69612700	-1.64083200	-0.93841100
H	-0.84066000	-2.61472500	-0.44137900
C	-3.51635700	-0.53550900	-0.71769800
H	-3.74731100	1.31704900	0.35569600
H	-3.00197500	-2.41458200	-1.63574600
H	-4.46209200	-0.44478000	-1.24241600
R2 <sub>1</sub>			
C	-0.74047600	0.80747300	-0.00006100

O	-1.05322400	1.97509200	-0.00016400
C	0.65676300	0.31559200	-0.00002100
C	0.98271900	-1.04631700	-0.00002300
C	1.67144200	1.28029800	0.00001700
C	2.31885500	-1.43167300	0.00001600
H	0.20820500	-1.80463200	-0.00006200
C	3.00224800	0.88916800	0.00005900
H	1.39423100	2.32906500	0.00001600
C	3.32540000	-0.46847500	0.00005800
H	2.57419300	-2.48566300	0.00001200
H	3.78832300	1.63655900	0.00009400
H	4.36606000	-0.77628700	0.00009100
C	-1.87795600	-0.23989600	0.00001100
F	-1.79670400	-1.02621800	-1.08225000
F	-3.06643300	0.34813300	-0.00008600
F	-1.79677300	-1.02600500	1.08242800
PPh <sub>3</sub>			
P	0.00054600	0.01401100	-1.26578900
C	1.63678500	-0.21093600	-0.44709500
C	2.73933400	0.40706900	-1.04969900
C	1.83210400	-0.94778100	0.72580500
C	4.00820500	0.30393700	-0.48627200
H	2.60259700	0.96992200	-1.97006800
C	3.10376000	-1.05918400	1.28446900
H	0.98865900	-1.43698700	1.20487600
C	4.19255500	-0.43267700	0.68185900
H	4.85267900	0.79022100	-0.96413600
H	3.24345000	-1.63513800	2.19404300
H	5.18198500	-0.52293800	1.11868800
C	-1.00214500	-1.29606100	-0.44093400
C	-1.80810000	-1.08005900	0.68108200
C	-0.93442800	-2.58389100	-0.98741100
C	-2.52735500	-2.13214100	1.24557500
H	-1.87497600	-0.08773600	1.11761300
C	-1.64357100	-3.63655400	-0.41692000
H	-0.32113900	-2.76334800	-1.86750500
C	-2.44487400	-3.41118300	0.70090800
H	-3.15094500	-1.95023900	2.11541000
H	-1.57669800	-4.62978000	-0.84949300
H	-3.00488500	-4.22867900	1.14371200
C	-0.63197500	1.53368700	-0.43439800
C	-1.76996300	2.12946300	-0.99224400
C	-0.05883500	2.10529600	0.70571400

C	-2.33460400	3.26242200	-0.41417900
H	-2.21726300	1.70091800	-1.88602800
C	-0.61741100	3.24706200	1.27771700
H	0.82516900	1.65702800	1.15005900
C	-1.75630600	3.82511200	0.72207400
H	-3.21959000	3.71040200	-0.85466900
H	-0.16276900	3.68324300	2.16169000
H	-2.18969100	4.71340500	1.17035700
TS1 <sub>1</sub>			
P	1.16442200	-0.05034300	-0.20370500
C	0.13694700	-0.64953300	1.17288800
C	-1.08346300	-0.00339100	1.39707300
C	0.48696200	-1.75535800	1.95457900
C	-1.94408000	-0.45894900	2.39368600
H	-1.35371800	0.87069000	0.81417400
C	-0.37418300	-2.20317600	2.95094000
H	1.42872900	-2.26733200	1.78329100
C	-1.59273200	-1.55943300	3.17128100
H	-2.88627300	0.05589800	2.55776400
H	-0.09307200	-3.05740700	3.55849800
H	-2.26286900	-1.91517300	3.94767000
C	1.53359400	1.68750800	0.23129000
C	1.44388200	2.16501500	1.54341700
C	1.89492700	2.56764500	-0.79524600
C	1.70699800	3.50424300	1.82014300
H	1.15949600	1.49265300	2.34699200
C	2.16451800	3.90428100	-0.51525200
H	1.94625800	2.20886500	-1.82026700
C	2.06694700	4.37467200	0.79331800
H	1.63163400	3.86744600	2.83997800
H	2.44104100	4.57849700	-1.31920000
H	2.26883700	5.41839900	1.01161400
C	2.74065000	-0.94768000	-0.11464900
C	2.74282600	-2.25743500	-0.61654200
C	3.92335600	-0.38354300	0.37295700
C	3.91889500	-3.00139000	-0.60162900
H	1.81686400	-2.67824200	-1.00437500
C	5.09876500	-1.13079500	0.37114800
H	3.92408500	0.63375900	0.75369100
C	5.09640800	-2.43785600	-0.11180100
H	3.91898800	-4.01805900	-0.98103900
H	6.01629200	-0.69292600	0.75083400
H	6.01410500	-3.01720000	-0.10995000

C	0.15919800	-0.45446400	-2.24403600
C	-1.17832300	-0.73722700	-2.11816800
C	1.15232400	-0.31802700	-3.11046500
H	2.13860800	0.05027100	-2.84822100
H	0.98395700	-0.61690100	-4.14250300
C	-2.23862500	0.26934800	-2.52576600
C	-1.48137600	-1.87746400	-1.29193500
O	-0.66025600	-2.70864100	-0.90807100
O	-2.78744500	-1.94655100	-0.92739700
C	-3.10670000	-2.94974000	0.03990900
C	-4.45752100	-2.59439200	0.62191900
H	-2.32792300	-2.96047700	0.80842600
H	-3.11763000	-3.93282900	-0.44467900
H	-4.75816800	-3.34068200	1.36156500
H	-4.40576100	-1.61826000	1.11259700
H	-5.22092100	-2.55209400	-0.15939500
C	-2.46837600	1.32749300	-1.46798500
C	-1.53154800	2.35232700	-1.30161200
C	-3.55021700	1.25925400	-0.58717500
C	-1.64986400	3.27147000	-0.26228800
H	-0.68374700	2.40981100	-1.98087600
C	-3.68547400	2.18899300	0.44335300
H	-4.27346200	0.45603700	-0.70002800
C	-2.73133300	3.19180100	0.61510400
H	-0.88905600	4.03685400	-0.13159100
H	-4.53167900	2.12397800	1.12128300
H	-2.82968000	3.90520800	1.42707100
H	-1.92634800	0.75160700	-3.45816800
H	-3.17360500	-0.26088700	-2.72658000
M1 <sub>1</sub>			
P	-1.17592300	-0.13469300	-0.07262100
C	-0.48713200	-0.04343100	1.59696800
C	0.72838700	-0.69326000	1.82706800
C	-1.15253900	0.61112100	2.63352200
C	1.27821700	-0.68032900	3.10681900
H	1.24705000	-1.19557900	1.01405300
C	-0.59726500	0.61365500	3.90872400
H	-2.08513300	1.13423500	2.44523700
C	0.61700000	-0.02977400	4.14575200
H	2.22657200	-1.17707100	3.28564000
H	-1.10910300	1.12572100	4.71662800
H	1.04846500	-0.02014700	5.14140400
C	-2.18219700	-1.65867500	-0.07984500

C	-1.99880100	-2.64957000	0.88832900
C	-3.13734600	-1.84420900	-1.08878400
C	-2.76287800	-3.81377000	0.84745600
H	-1.26537800	-2.51619500	1.67657800
C	-3.89194400	-3.01112500	-1.12878200
H	-3.29080900	-1.07627700	-1.84154700
C	-3.70674500	-3.99580600	-0.15885500
H	-2.61930200	-4.57619800	1.60551100
H	-4.62857500	-3.14922600	-1.91294200
H	-4.30165800	-4.90280200	-0.18722400
C	-2.39488400	1.13734800	-0.49023300
C	-2.12470400	2.05409400	-1.50915100
C	-3.63789100	1.13866600	0.14959400
C	-3.09879300	2.97441200	-1.87942300
H	-1.15446900	2.04160300	-1.99620300
C	-4.59835800	2.08056200	-0.20904500
H	-3.86608200	0.40086200	0.91428200
C	-4.32966600	2.99424100	-1.22484900
H	-2.89492100	3.68206000	-2.67598000
H	-5.55811400	2.08965000	0.29627500
H	-5.08358600	3.72001800	-1.51245700
C	0.17849200	-0.32931600	-1.27879500
C	1.23985300	0.63636800	-1.30031200
C	0.13348500	-1.48482100	-1.99637100
H	-0.66083100	-2.21053700	-1.90167300
H	0.92287800	-1.71528800	-2.70301000
C	2.49413700	0.28643000	-2.05935000
C	1.15937000	1.79080400	-0.50345900
O	0.16364700	2.16160000	0.15047000
O	2.30698200	2.54326900	-0.46155400
C	2.24272100	3.72043000	0.33940300
C	3.61216200	4.36576100	0.29625600
H	1.95669600	3.45409300	1.36197900
H	1.46993700	4.39171600	-0.05089600
H	3.61842100	5.27781900	0.89785600
H	4.36871200	3.68336300	0.69175900
H	3.88374200	4.62467900	-0.73009000
C	3.32237700	-0.79389600	-1.38296200
C	3.70898900	-1.95565900	-2.05145200
C	3.71164300	-0.63347000	-0.04762400
C	4.46050400	-2.93937900	-1.40742900
H	3.41650600	-2.09325800	-3.09042400
C	4.46398200	-1.60907200	0.59903000
H	3.40981700	0.26948900	0.47888400

C	4.83902900	-2.77005700	-0.07935800
H	4.74391800	-3.83969600	-1.94432700
H	4.76210200	-1.46462100	1.63369700
H	5.42081000	-3.53480000	0.42559700
H	2.25671500	-0.04037900	-3.08119100
H	3.10419100	1.18859200	-2.15649900
TS2 <sub>1</sub> <sup>(R,R)</sup>			
P	1.66797000	-0.28631000	-0.31972200
C	1.74157700	-1.85744600	-1.23894200
C	1.41251000	-1.86766000	-2.60229100
C	2.16814200	-3.03438300	-0.61972900
C	1.47885600	-3.05205800	-3.32438000
H	1.10235000	-0.94959700	-3.09590600
C	2.24256900	-4.21694400	-1.35299500
H	2.43508100	-3.03368600	0.43130100
C	1.89391200	-4.22811700	-2.69936400
H	1.21534200	-3.05572200	-4.37654400
H	2.57500700	-5.12786700	-0.86706700
H	1.94986100	-5.15067000	-3.26596600
C	2.52661900	-0.59730700	1.24467700
C	3.92140600	-0.58012100	1.30226600
C	1.76609200	-0.89441600	2.37964900
C	4.56157900	-0.87109500	2.50211300
H	4.51043700	-0.32689800	0.42635200
C	2.42136000	-1.18375700	3.57433200
H	0.68007100	-0.89533800	2.33540900
C	3.81285200	-1.17433300	3.63759200
H	5.64521500	-0.85407000	2.55024800
H	1.83847200	-1.41394500	4.45924700
H	4.31544600	-1.39916200	4.57247600
C	2.52957000	0.85782100	-1.43778900
C	1.97085500	2.09781800	-1.76017900
C	3.72124100	0.44759600	-2.04523400
C	2.61793500	2.92932100	-2.66724700
H	1.03052600	2.40360700	-1.31302500
C	4.37376300	1.29517100	-2.93525900
H	4.13255600	-0.53851300	-1.84666400
C	3.82339500	2.53578500	-3.24543800
H	2.17724900	3.88785700	-2.92146200
H	5.30262000	0.97667800	-3.39671600
H	4.32700600	3.19093800	-3.94883300
C	-0.07489000	0.23093200	-0.10389700
C	-0.41542500	1.30571800	0.71523300



C	-1.03058600	-0.56915200	-0.74486000
C	-1.95719100	-1.64169200	1.02482400
H	-0.73096700	-1.36240600	-1.41477100
H	-1.98048500	-0.10511900	-0.97723400
C	-1.86195900	1.74668900	0.80375700
H	-2.51121800	0.87745800	0.90064800
H	-1.99234600	2.33797400	1.71247900
C	0.60805900	2.12842200	1.33580400
O	1.81765900	2.01366500	1.15983100
O	0.11487700	3.09201600	2.14194600
C	1.08819500	3.94621200	2.75852000
C	0.32986800	4.97100100	3.57197700
H	1.69688600	4.41286800	1.97717000
H	1.75246700	3.33817800	3.37962300
H	1.03225400	5.65378000	4.05518000
H	-0.33606000	5.55506600	2.93051500
H	-0.26985400	4.48344000	4.34505200
C	-2.29667900	2.56639800	-0.39806700
C	-1.59551500	3.72280900	-0.75839000
C	-3.39799900	2.18664100	-1.16761800
C	-1.97977300	4.47551800	-1.86388700
H	-0.74640400	4.03869200	-0.15584900
C	-3.78606700	2.93726300	-2.27804700
H	-3.95621400	1.29235600	-0.89242500
C	-3.07687700	4.08184400	-2.63063300
H	-1.42589300	5.37146800	-2.12753600
H	-4.64209100	2.62545600	-2.86814200
H	-3.37603800	4.66647900	-3.49540800
C	-1.22318300	-2.97484900	0.79493100
C	-3.38494900	-1.59104300	0.53492500
C	-4.31717200	-0.97406200	1.37384100
C	-3.81349900	-2.11969000	-0.68807200
C	-5.65214800	-0.87207800	0.99504300
H	-3.97015200	-0.57419900	2.32071700
C	-5.14981200	-2.01942000	-1.06381100
H	-3.10290200	-2.59349900	-1.35646200
C	-6.07218400	-1.39276200	-0.22732100
H	-6.36531900	-0.38926000	1.65539800
H	-5.47055400	-2.42613500	-2.01728200
H	-7.11256300	-1.31397700	-0.52612200
O	-1.62286100	-1.03453700	2.05372200
F	0.04288100	-2.89899300	1.22401700
F	-1.82858900	-3.92949000	1.52969400
F	-1.18911900	-3.43598200	-0.46624800

M2<sub>1</sub>(R,R)

P	1.65649300	-0.42523400	-0.28920200
C	1.56968500	-2.00873800	-1.17722500
C	1.15591400	-2.00746000	-2.51690000
C	1.96820700	-3.20091900	-0.57152400
C	1.10918100	-3.19843400	-3.22920600
H	0.87140500	-1.07700600	-3.00242500
C	1.93434100	-4.38991900	-1.29701500
H	2.29323700	-3.20713900	0.46337500
C	1.49901800	-4.39060400	-2.61791800
H	0.77847300	-3.19594100	-4.26209600
H	2.24560300	-5.31493900	-0.82389800
H	1.46866400	-5.31950200	-3.17787300
C	2.47329500	-0.75147900	1.29111000
C	3.86566500	-0.75522700	1.39520000
C	1.66059600	-1.03683300	2.39488000
C	4.45705500	-1.06290700	2.61571300
H	4.48805100	-0.50233000	0.54292600
C	2.27253800	-1.34367700	3.60881600
H	0.57013700	-1.01635100	2.31277500
C	3.66069100	-1.35991900	3.72040600
H	5.53812200	-1.06283500	2.70435600
H	1.65612600	-1.56767300	4.47315300
H	4.12536800	-1.59790800	4.67185600
C	2.59383700	0.60194200	-1.46066600
C	2.10724200	1.83493900	-1.90072500
C	3.77466200	0.08023300	-2.00108600
C	2.81692600	2.55377700	-2.85701500
H	1.17260200	2.22778600	-1.51330100
C	4.49108400	0.81647200	-2.93933900
H	4.12802800	-0.90534500	-1.71019500
C	4.01293100	2.05276000	-3.36679500
H	2.43163900	3.50632600	-3.20457100
H	5.41266500	0.41509200	-3.34632700
H	4.56535200	2.61958200	-4.10886600
C	-0.02778600	0.22623800	-0.01119400
C	-0.26659300	1.36479700	0.68535600
C	-1.17617000	-0.60244700	-0.47213400
C	-1.92773500	-1.32938400	0.80080100
H	-0.89128400	-1.34747200	-1.21375200
H	-1.90634800	0.05705300	-0.94563400
C	-1.66944200	1.92331100	0.84441200
H	-2.36349600	1.10401900	1.01659900

H	-1.69517200	2.55228600	1.73604800
C	0.86061100	2.17222200	1.24275900
O	2.03553500	1.95136000	1.01884100
O	0.45438400	3.17924700	2.01254300
C	1.49610600	3.99610800	2.58473100
C	0.81749000	5.10106200	3.36051300
H	2.11969600	4.37950000	1.77260900
H	2.11934800	3.36190700	3.22068800
H	1.57204700	5.74532300	3.81668700
H	0.19486400	5.70874700	2.70006300
H	0.18935300	4.68655900	4.15177500
C	-2.07657500	2.73555000	-0.37048500
C	-1.32289800	3.84166100	-0.78096800
C	-3.21214100	2.38616900	-1.10624800
C	-1.69063800	4.57585600	-1.90416000
H	-0.45001400	4.14090100	-0.20480100
C	-3.58432400	3.12327600	-2.23043000
H	-3.80674400	1.52972500	-0.79073000
C	-2.82347200	4.21697700	-2.63405500
H	-1.09750100	5.43336400	-2.20653300
H	-4.46948800	2.83956900	-2.79109600
H	-3.11189200	4.78964100	-3.50957700
C	-1.48946500	-2.80940900	0.75554600
C	-3.44158800	-1.28652200	0.45774900
C	-4.30834600	-0.81117000	1.44017700
C	-3.96770300	-1.65712100	-0.78481300
C	-5.67410900	-0.69245300	1.18957900
H	-3.86640800	-0.52912400	2.39041800
C	-5.33287100	-1.54380500	-1.03741300
H	-3.31065500	-2.03242300	-1.56451300
C	-6.19081400	-1.05764700	-0.05130400
H	-6.33678100	-0.31435700	1.96271700
H	-5.72786200	-1.83333100	-2.00677300
H	-7.25399500	-0.96502600	-0.25072400
O	-1.62219200	-0.83314500	1.98338500
F	-0.19895500	-2.93776700	1.12882400
F	-2.20802600	-3.56034000	1.60577000
F	-1.58510600	-3.40784000	-0.45651000
TS3 <sub>1</sub> <sup>(R,R,R)</sup>			
P	-1.72068800	-0.56523800	0.29174700
C	-0.14240300	0.22539400	-0.04579300
C	1.12035300	-0.43292200	0.47421000
H	0.87930700	-1.24660900	1.16237200

C	-0.07004000	1.35233400	-0.80832500
C	1.20086900	1.93263300	-1.26714200
H	1.03802700	2.65908500	-2.06727600
H	1.64068400	0.78663900	-1.74573900
C	-1.31059700	1.95421100	-1.40633800
O	-2.09141400	1.36522400	-2.12121300
O	-1.44541700	3.22998300	-1.04931900
C	-2.66469000	3.86645200	-1.48268600
C	-2.71183300	5.22995100	-0.83407300
H	-2.65818800	3.92527100	-2.57461900
H	-3.50555000	3.23464300	-1.17818200
H	-3.62361000	5.74989900	-1.13615300
H	-1.85143300	5.83208100	-1.13397600
H	-2.71055600	5.13367500	0.25424800
C	2.18064400	2.46943800	-0.27086800
C	3.48824200	2.75510000	-0.69134700
C	1.86285000	2.71373400	1.07070000
C	4.43876100	3.25423200	0.19100200
H	3.75759000	2.56110300	-1.72653800
C	2.81811500	3.19571900	1.96454700
H	0.84937700	2.52125200	1.41655300
C	4.11144500	3.46914000	1.53053900
H	5.44570700	3.45605000	-0.16266600
H	2.54477900	3.36678400	3.00177900
H	4.85570800	3.84629200	2.22458100
C	-3.00711700	0.67333800	0.63044600
C	-4.30640700	0.51328900	0.14192900
C	-2.68398800	1.78829200	1.41387900
C	-5.28275900	1.45349900	0.45680200
H	-4.55434100	-0.32807400	-0.49627300
C	-3.66857800	2.72002500	1.73050700
H	-1.66811800	1.93371000	1.77127500
C	-4.96718000	2.55259100	1.25383000
H	-6.28894400	1.32961900	0.07159800
H	-3.41625000	3.57839900	2.34396900
H	-5.73134300	3.28391200	1.49582500
C	-2.21589200	-1.66403100	-1.05362400
C	-1.52661300	-1.62035600	-2.26815500
C	-3.26810500	-2.56809000	-0.85777500
C	-1.91942400	-2.46995500	-3.29829000
H	-0.66232500	-0.97042300	-2.38349400
C	-3.65665800	-3.40398800	-1.89828200
H	-3.77430200	-2.62715400	0.10262900
C	-2.98469400	-3.34875600	-3.11911900

H	-1.38364100	-2.44977500	-4.24107500
H	-4.47356200	-4.10244000	-1.75343500
H	-3.28496000	-4.00571900	-3.92905500
C	-1.59459600	-1.60642700	1.77653200
C	-1.07485700	-2.90329300	1.66260500
C	-1.97886300	-1.11439400	3.02720000
C	-0.93220100	-3.69112000	2.79936000
H	-0.77439000	-3.29187300	0.69476900
C	-1.83663700	-1.91273500	4.15859300
H	-2.39881200	-0.11911900	3.12480400
C	-1.31277900	-3.19755100	4.04606800
H	-0.52526700	-4.69232200	2.70852500
H	-2.14150100	-1.52940700	5.12629100
H	-1.20464200	-3.81741600	4.93006500
H	1.66288600	0.30574300	1.07021300
C	2.08599800	-0.97100100	-0.66279400
O	1.79387500	-0.51609800	-1.91883900
C	3.55044700	-0.71366200	-0.25706100
C	3.99978600	-0.81736300	1.06184200
C	4.46741600	-0.40067900	-1.25961900
C	5.33788300	-0.58741300	1.37404700
H	3.30693400	-1.08038100	1.85638700
C	5.80528100	-0.16965500	-0.95086500
H	4.09661400	-0.32581700	-2.27607300
C	6.24413700	-0.25828000	0.36818900
H	5.67207000	-0.66316700	2.40434800
H	6.50670600	0.08239200	-1.74098100
H	7.28609900	-0.07421100	0.61160900
C	1.91538900	-2.49579100	-0.70614400
F	0.65101300	-2.83970800	-1.03713300
F	2.72067300	-3.07117200	-1.60564500
F	2.15931500	-3.09449800	0.48114500
M3 <sub>1</sub> <sup>(R,R,R)</sup>			
P	-1.72796200	-0.33699900	0.39033600
C	-0.07492700	-0.01399500	0.04425900
C	0.91507000	-1.14002700	0.18503800
H	0.37384200	-2.06602100	0.40746300
C	0.31820400	1.32873400	-0.37082900
C	1.42002500	2.03373300	-0.00242300
H	1.64643600	2.92507300	-0.58327300
H	0.38632700	-0.33602100	-2.01599700
C	-0.51464300	1.93868300	-1.46403400
O	-1.08531600	1.27835900	-2.31578700

O	-0.59524900	3.26822400	-1.40734000
C	-1.43928200	3.89021300	-2.39273600
C	-1.54451300	5.35292600	-2.02675400
H	-0.99914200	3.73926300	-3.38293300
H	-2.41351500	3.39251400	-2.37375700
H	-2.18398200	5.86969100	-2.74591300
H	-0.56032500	5.82701900	-2.03320000
H	-1.98057000	5.46031500	-1.03033700
C	2.35933500	1.76781800	1.08740800
C	3.63122700	2.35891200	1.03474700
C	2.02374600	1.02295800	2.23154800
C	4.54890600	2.18498200	2.06261800
H	3.90098100	2.94739000	0.16177200
C	2.93967300	0.85802200	3.26557000
H	1.02978100	0.59068900	2.31113200
C	4.20942200	1.42732600	3.18242300
H	5.53353100	2.63674400	1.98769000
H	2.65893200	0.28253100	4.14253400
H	4.92526400	1.28822200	3.98635800
C	-2.61102200	1.25003300	0.51553800
C	-3.77060400	1.50682800	-0.22249000
C	-2.05783700	2.26477900	1.30910200
C	-4.38070300	2.75665700	-0.14869200
H	-4.18886500	0.74349200	-0.86953100
C	-2.67548800	3.50842600	1.38461200
H	-1.12640600	2.09250800	1.84116300
C	-3.83773900	3.75513300	0.65656300
H	-5.27753100	2.95099900	-0.72746000
H	-2.23942700	4.28810800	2.00004900
H	-4.31478000	4.72864800	0.71073700
C	-2.70379900	-1.41281200	-0.72498400
C	-2.16482200	-1.87132200	-1.92592600
C	-3.99254900	-1.81007200	-0.34079800
C	-2.91630000	-2.71313600	-2.74641900
H	-1.15583400	-1.59567600	-2.21033700
C	-4.74307000	-2.63578500	-1.16825300
H	-4.40648600	-1.47358400	0.60712700
C	-4.20272300	-3.08822500	-2.37323600
H	-2.49159700	-3.07562500	-3.67667200
H	-5.74331400	-2.93396900	-0.87220400
H	-4.78631800	-3.73989400	-3.01555600
C	-1.89997100	-1.23700000	1.98095200
C	-1.80012400	-2.63396700	1.98783700
C	-2.02267600	-0.55225100	3.19402800

C	-1.81021900	-3.33191600	3.19228700
H	-1.72453800	-3.18091900	1.05157400
C	-2.04621100	-1.25519700	4.39524700
H	-2.11610800	0.52862300	3.20796600
C	-1.93468600	-2.64398700	4.39660400
H	-1.72752300	-4.41367500	3.18709700
H	-2.15496700	-0.71644500	5.33071600
H	-1.94995400	-3.18942100	5.33450400
H	1.62477200	-1.00422800	1.01000900
C	1.76064100	-1.37101600	-1.11725700
O	1.10040500	-0.94459000	-2.28213400
C	3.15683100	-0.74925900	-1.02197600
C	4.01059900	-1.05089400	0.04438000
C	3.60117600	0.12061600	-2.01695600
C	5.28856400	-0.50445000	0.10305300
H	3.68350800	-1.71915600	0.83448600
C	4.87683900	0.67727700	-1.95094400
H	2.93650100	0.35669200	-2.83985600
C	5.72769900	0.36088200	-0.89537500
H	5.93622800	-0.74657300	0.93993100
H	5.20763400	1.35558300	-2.73174300
H	6.72251900	0.79279800	-0.84488400
C	1.89966800	-2.88350700	-1.31410200
F	0.70154000	-3.46043000	-1.50635200
F	2.65851400	-3.18722200	-2.37404200
F	2.44809500	-3.48161100	-0.24064800
TS4 <sub>1</sub> <sup>(R,R,R)</sup>			
P	1.23216100	0.84705300	0.42944300
C	2.86297400	0.09895200	0.13106800
C	3.83476700	0.79437200	-0.59365300
C	3.12098900	-1.20958900	0.56333600
C	5.05024700	0.18249000	-0.88937200
H	3.64034400	1.80279700	-0.94333200
C	4.33575600	-1.81560600	0.26139400
H	2.37262200	-1.76413700	1.12249400
C	5.29850000	-1.12191700	-0.46977800
H	5.79934800	0.72554100	-1.45533800
H	4.52590300	-2.83048900	0.59387300
H	6.24316300	-1.59926900	-0.70957900
C	1.02069000	1.00518400	2.23357900
C	1.91432500	0.41106400	3.13149200
C	-0.08838500	1.71005400	2.72723500
C	1.68266000	0.49107800	4.50244300

H	2.79573000	-0.10854900	2.77375300
C	-0.31104300	1.78521100	4.09782000
H	-0.76953600	2.21202400	2.04757400
C	0.56774900	1.16851900	4.98649900
H	2.38162000	0.02733800	5.19011800
H	0.38908800	1.22721000	6.05505200
C	1.28755300	2.52516400	-0.23950700
C	1.05408000	2.71928200	-1.60577700
C	1.63170200	3.60321000	0.58235300
C	1.15953000	4.00022900	-2.13838800
H	0.79261300	1.88074600	-2.24081000
C	1.72957700	4.88025200	0.03802500
H	1.81889600	3.45177700	1.64069500
C	1.49011900	5.07814000	-1.31975400
H	0.97531300	4.15659900	-3.19579000
H	1.99090200	5.71818700	0.67522300
H	1.56394700	6.07536900	-1.74155000
C	-0.05283300	-0.16328700	-0.36926800
C	0.44974000	-1.50255600	-0.82193600
C	-1.47437400	-0.08258800	0.18162200
C	-2.30633200	0.78045300	-0.88825900
H	-1.55921200	0.32405000	1.19287200
H	-1.90562900	-1.08239400	0.22158600
C	0.15860500	-2.72763000	-0.33840200
C	1.35686800	-1.41411800	-2.01543600
O	1.54383800	-0.38992000	-2.64141400
O	2.01152400	-2.54921600	-2.28097100
C	3.02699200	-2.45898500	-3.29553200
C	3.79412500	-3.76113700	-3.27480900
H	3.66741200	-1.60340700	-3.06007000
H	2.54929400	-2.27325300	-4.26174000
H	4.57954200	-3.73908300	-4.03358200
H	4.25845500	-3.91069600	-2.29687000
H	3.13344300	-4.60565200	-3.48329400
O	-1.53819600	1.04824800	-1.96612400
H	-0.36634500	0.45057100	-1.38078400
H	-1.17208500	2.33032100	4.46933900
C	-3.61937600	0.05479700	-1.22523900
C	-3.95860900	-0.11544500	-2.56578800
C	-4.48049900	-0.44138200	-0.24078000
C	-5.13499200	-0.77155400	-2.92290600
H	-3.27061500	0.27310800	-3.30848800
C	-5.65831300	-1.09461800	-0.59465100
H	-4.23094200	-0.31856400	0.80970200



C	-5.98956600	-1.26188100	-1.93828200
H	-5.38518700	-0.90104300	-3.97189500
H	-6.31727700	-1.47684600	0.17920100
H	-6.90600100	-1.77446500	-2.21414700
C	-0.53361500	-3.11154800	0.90161600
C	-1.20268700	-4.34292000	0.94436400
C	-0.48204800	-2.34023300	2.07211700
C	-1.83267700	-4.77280800	2.10718800
H	-1.23111000	-4.96097400	0.05129300
C	-1.09774100	-2.77558100	3.23931400
H	0.04949200	-1.39472600	2.07397800
C	-1.78218100	-3.98988800	3.25906500
H	-2.35709100	-5.72273600	2.11698700
H	-1.04069100	-2.16415100	4.13448000
H	-2.26648000	-4.32790200	4.16947200
H	0.50298800	-3.57060500	-0.93287100
C	-2.66887800	2.10965300	-0.21536500
F	-1.55346800	2.81603700	0.08179300
F	-3.42323500	2.89490500	-0.99575000
F	-3.33352500	1.97323700	0.95762400
M4 <sub>1</sub> <sup>(R,R,R)</sup>			
P	1.30243800	0.84071300	0.37055900
C	2.89049100	-0.01766000	0.15786400
C	3.87917400	0.53213900	-0.66349600
C	3.08364500	-1.28512500	0.72651000
C	5.05272000	-0.17560200	-0.90629400
H	3.72824100	1.49918400	-1.13053500
C	4.25737800	-1.98774600	0.47682200
H	2.31685000	-1.73496100	1.35099400
C	5.24109700	-1.43471800	-0.34112600
H	5.81378600	0.25490400	-1.54791000
H	4.39832600	-2.96869500	0.91748300
H	6.15343300	-1.98756300	-0.54013400
C	1.02534800	1.08866900	2.15213000
C	1.86778000	0.53640400	3.12317500
C	-0.06372100	1.88103300	2.54531300
C	1.59692600	0.73994300	4.47392100
H	2.73870400	-0.04195700	2.83886900
C	-0.32781400	2.07482900	3.89646900
H	-0.69713900	2.35478200	1.80273500
C	0.49551000	1.49766500	4.86151300
H	2.25496900	0.30903500	5.22062200
H	0.28636500	1.65148400	5.91496100

C	1.48051400	2.49024900	-0.34382000
C	0.81249000	2.86863000	-1.51060900
C	2.37451800	3.36597600	0.29070500
C	1.06279000	4.13252500	-2.04492000
H	0.04812900	2.22666200	-1.95237500
C	2.61591600	4.61817800	-0.25822400
H	2.88363100	3.06861400	1.20447000
C	1.96144900	4.99832100	-1.43091700
H	0.53957200	4.44029000	-2.94406400
H	3.30898300	5.29648800	0.22750300
H	2.14744100	5.97834900	-1.85870000
C	-0.02727500	-0.14959300	-0.46374400
C	0.45779300	-1.54789800	-0.77246700
C	-1.46195900	-0.01262000	0.05515600
C	-2.32196700	0.81984300	-1.01626800
H	-1.53429900	0.41344100	1.05943400
H	-1.89119900	-1.01066900	0.12853900
C	0.13601300	-2.71649400	-0.18547000
C	1.39373200	-1.57573700	-1.94609300
O	1.63625100	-0.59726800	-2.62308400
O	1.99061500	-2.75532700	-2.13457300
C	3.00340300	-2.78615000	-3.15625800
C	3.69368300	-4.12691700	-3.05482400
H	3.69289900	-1.95554900	-2.97893100
H	2.52852000	-2.63524300	-4.12976300
H	4.47296100	-4.20052800	-3.81649300
H	4.15584400	-4.24140300	-2.07109800
H	2.98241900	-4.94201800	-3.20590300
O	-1.65723100	1.07976100	-2.14645300
H	-0.12133100	0.34590500	-1.45997500
H	-1.17546200	2.68299500	4.19265600
C	-3.66241400	0.07590100	-1.24393300
C	-4.11952400	-0.05183400	-2.55381900
C	-4.43273100	-0.45897300	-0.20611200
C	-5.31834100	-0.70590200	-2.82987700
H	-3.49812600	0.36845400	-3.33714200
C	-5.63249000	-1.11278500	-0.47762300
H	-4.09632200	-0.36758900	0.82358100
C	-6.07968800	-1.23836300	-1.79186200
H	-5.66011400	-0.80117300	-3.85661700
H	-6.21806100	-1.52692300	0.33796700
H	-7.01375100	-1.74979000	-2.00361600
C	-0.62819500	-2.98987100	1.04107100
C	-1.35813200	-4.18440900	1.11773400

C	-0.60654400	-2.14533900	2.15902800
C	-2.08221300	-4.50282800	2.26114400
H	-1.36371800	-4.85782900	0.26537800
C	-1.31779500	-2.46939500	3.30862500
H	-0.02214300	-1.23159600	2.13717400
C	-2.06515700	-3.64514600	3.35949300
H	-2.65495100	-5.42356500	2.29761200
H	-1.28447200	-1.80325700	4.16486600
H	-2.62423700	-3.89674900	4.25473600
H	0.50398600	-3.60930900	-0.68572800
C	-2.69178400	2.15058000	-0.33437900
F	-1.58787500	2.90246400	-0.10033300
F	-3.50965900	2.90037500	-1.08497800
F	-3.29148200	2.01594800	0.87494000
M4 <sub>1</sub> <sup>(R,R,R)</sup>			
P	1.38545600	0.75922900	0.70035500
C	3.06568600	0.40748300	0.11993600
C	3.83893000	1.45917600	-0.38099900
C	3.55189300	-0.90800500	0.06032700
C	5.08464100	1.19685300	-0.94410300
H	3.46981800	2.47886600	-0.34351200
C	4.79863000	-1.15882200	-0.50070600
H	2.95423800	-1.73695200	0.42550500
C	5.56355700	-0.10811000	-1.00596300
H	5.67769600	2.01590600	-1.33571500
H	5.16961700	-2.17742000	-0.54618400
H	6.53404600	-0.30829200	-1.44788000
C	1.09851400	-0.00403300	2.31541600
C	2.09257800	-0.73590500	2.97094100
C	-0.14231500	0.20455100	2.93639000
C	1.83071600	-1.29271500	4.22081800
H	3.07218800	-0.86356100	2.52577900
C	-0.39434600	-0.35691400	4.18087200
H	-0.90461700	0.81091900	2.45857300
C	0.58774200	-1.11339600	4.81939600
H	2.60480000	-1.86056700	4.72538900
H	0.38646900	-1.55289400	5.79095400
C	1.21796400	2.54582000	0.91708300
C	0.72739300	3.35115400	-0.11719400
C	1.64045000	3.11934700	2.12205400
C	0.66134300	4.72966600	0.06243200
H	0.38500000	2.92026100	-1.05315100
C	1.57523300	4.49842200	2.28791100

H	2.01287600	2.49198500	2.92694500
C	1.08538500	5.30145000	1.25983500
H	0.27373200	5.35431200	-0.73473500
H	1.90249900	4.94351400	3.22119400
H	1.03023800	6.37663300	1.39418200
C	0.19140400	0.18703700	-0.58110200
C	0.57520100	-1.23267700	-0.94602600
C	-1.25503900	0.52454900	-0.20308400
C	-2.17547300	0.37558400	-1.47713200
H	-1.30309500	1.54411000	0.19903700
H	-1.61531900	-0.14626300	0.57438100
C	0.26908500	-2.38431800	-0.32718700
C	1.53336400	-1.27225000	-2.10494100
O	1.81832800	-0.30178200	-2.77435000
O	2.07761900	-2.47569300	-2.31189900
C	3.03989800	-2.54772900	-3.37785300
C	3.62260200	-3.94238800	-3.35763600
H	3.80086600	-1.77951700	-3.20981500
H	2.53545000	-2.32381500	-4.32189100
H	4.36448400	-4.04463900	-4.15250400
H	4.11046400	-4.14011800	-2.39987500
H	2.84200600	-4.69032500	-3.51266900
O	-1.77476700	-0.58649000	-2.30150500
H	0.47076400	0.78996400	-1.45132500
H	-1.35956300	-0.20485000	4.65133200
C	-3.64076200	0.22740800	-0.97346300
C	-4.43119000	-0.73836200	-1.59395700
C	-4.19209000	0.98135500	0.06697300
C	-5.74163800	-0.96427600	-1.17934100
H	-3.96565300	-1.30887800	-2.39168800
C	-5.50215800	0.75807200	0.48746000
H	-3.59991000	1.74984300	0.55658100
C	-6.28113900	-0.21695300	-0.13333400
H	-6.34362600	-1.72355400	-1.67072800
H	-5.91598800	1.34634300	1.30145200
H	-7.30112300	-0.39140300	0.19574600
C	-0.75345000	-2.62261600	0.71916900
C	-2.10181100	-2.45918000	0.38029100
C	-0.41333000	-3.09994700	1.98688100
C	-3.09554700	-2.72301000	1.31771800
H	-2.33502600	-2.09075700	-0.61732000
C	-1.41101400	-3.36757600	2.92140600
H	0.63240700	-3.23853000	2.25004600
C	-2.75149900	-3.17483300	2.59170400

H	-4.13679000	-2.56627700	1.04762500
H	-1.13836700	-3.71730900	3.91264700
H	-3.52512700	-3.37795700	3.32577500
H	0.76898600	-3.27628500	-0.69944400
C	-2.13062700	1.73485600	-2.22083000
F	-0.89840400	1.99503900	-2.72625300
F	-2.97594500	1.76483300	-3.26056300
F	-2.42991700	2.81214600	-1.44862600
TS5 <sub>1</sub> <sup>(R,R,R)</sup>			
P	-1.45090500	-1.10750400	-0.02551100
C	-3.08922600	-0.39198600	0.25203200
C	-4.17251100	-0.79427300	-0.53474500
C	-3.26632000	0.58132700	1.24626100
C	-5.42303000	-0.21586600	-0.33581700
H	-4.04436300	-1.54955900	-1.30270600
C	-4.51896100	1.15412200	1.43538400
H	-2.43133900	0.90827400	1.85666900
C	-5.59525800	0.75927300	0.64248500
H	-6.26121500	-0.52707200	-0.94955500
H	-4.65178700	1.91031200	2.20131900
H	-6.57050900	1.21107400	0.79070900
C	-1.00903600	-2.13591500	1.39655800
C	-1.86486200	-2.22874300	2.49924500
C	0.20350200	-2.83983500	1.39014500
C	-1.50146400	-3.00818700	3.59392200
H	-2.81014700	-1.69658000	2.50810400
C	0.55695600	-3.61727200	2.48758700
H	0.86431800	-2.79649300	0.53050900
C	-0.29225200	-3.69894700	3.58978600
H	-2.16788600	-3.07671800	4.44681500
H	-0.01208700	-4.30537700	4.44467600
C	-1.52599500	-2.15605800	-1.49707600
C	-1.67107000	-1.53289200	-2.74579400
C	-1.47466200	-3.54968700	-1.40652700
C	-1.74862500	-2.31059800	-3.89527500
H	-1.75231700	-0.45070500	-2.81973700
C	-1.54940400	-4.31825000	-2.56516600
H	-1.37552400	-4.03472000	-0.44102400
C	-1.68145300	-3.70048600	-3.80555300
H	-1.86304700	-1.83052600	-4.86086000
H	-1.50451700	-5.39954800	-2.49514100
H	-1.73680400	-4.30262900	-4.70637200
C	-0.22081200	0.23346200	-0.41481300

C	-0.45974300	1.57927300	0.21141100
C	1.23787000	-0.23136400	-0.36286200
C	2.26322600	0.86513800	-0.87044300
H	1.34846000	-1.12921300	-0.98067900
H	1.54391100	-0.48507700	0.65473700
C	0.43098600	2.13520100	1.08448900
C	-1.38014200	2.41615000	-0.56012700
O	-2.01170100	2.02717600	-1.53335200
O	-1.53023300	3.66026900	-0.06670500
C	-2.44819100	4.50279800	-0.77530300
C	-2.49712300	5.82617200	-0.04436400
H	-3.42653400	4.01302400	-0.80236300
H	-2.10422400	4.61859500	-1.80745800
H	-3.18464100	6.50636400	-0.55221900
H	-2.84317900	5.68568200	0.98238700
H	-1.50758000	6.28813700	-0.01824100
O	2.28794400	2.01458400	-0.17491300
H	-0.47586900	0.37390300	-1.47154300
H	1.49556100	-4.16014300	2.47915500
C	3.63974900	0.14381500	-0.87901400
C	4.61795700	0.62032800	-0.00871900
C	3.93435900	-0.96569800	-1.67930900
C	5.86435300	0.00301800	0.07136300
H	4.36535500	1.48787400	0.59028700
C	5.18278300	-1.57978600	-1.60791800
H	3.19376000	-1.34810200	-2.37546800
C	6.15235600	-1.09986900	-0.72886000
H	6.61448200	0.38616000	0.75735500
H	5.39932600	-2.43548100	-2.24080300
H	7.12402100	-1.58094100	-0.67106500
C	1.10570900	1.45727000	2.21651200
C	2.37206000	1.86486400	2.65794500
C	0.43563700	0.46692000	2.93706200
C	2.96326900	1.25976400	3.75812100
H	2.89041100	2.63155500	2.09458900
C	1.03104500	-0.15241200	4.03611300
H	-0.56955200	0.18193900	2.64874400
C	2.30014600	0.23917600	4.44574800
H	3.95032300	1.57670300	4.08039000
H	0.49406600	-0.93190100	4.56834400
H	2.77062200	-0.23717900	5.30001500
H	0.42152400	3.22079100	1.14936500
C	1.90006600	1.20023600	-2.33884300
F	0.85689600	2.04661500	-2.41102700

F	2.91428300	1.78961400	-2.99222200
F	1.54005900	0.11852900	-3.08345700
M5 <sub>1</sub> <sup>(R,R,R)</sup>			
P	-1.63334000	-0.91190900	0.33088900
C	-0.24057300	-0.15830100	-0.76035300
C	1.11415800	-0.81555300	-0.49752800
H	1.12244500	-1.86665500	-0.79813700
C	-0.15210900	1.31187300	-0.68213300
C	1.16056300	1.93899900	-0.37650200
H	1.14393500	2.94981200	-0.79295900
C	-1.17928600	1.97216400	-1.36716000
O	-2.17027000	1.41152800	-1.87902200
O	-1.06924800	3.34310900	-1.41509100
C	-2.15306400	4.02159600	-2.03964300
C	-1.87814500	5.50728300	-1.93240700
H	-2.23909800	3.70619700	-3.08529300
H	-3.08932300	3.74916700	-1.54045800
H	-2.68508200	6.07569900	-2.40140000
H	-0.93975000	5.76142700	-2.43171200
H	-1.80398300	5.80910700	-0.88452800
C	1.62253100	2.07355600	1.07389300
C	2.62840800	3.00230200	1.36549700
C	1.11777000	1.30529900	2.12070200
C	3.11961500	3.14792900	2.65880400
H	3.03097300	3.61383800	0.56079500
C	1.60418500	1.44074800	3.42013400
H	0.33397900	0.58185800	1.92516200
C	2.60884300	2.36364000	3.69347600
H	3.89872400	3.87625200	2.86195000
H	1.19393100	0.82154800	4.21282500
H	2.99016200	2.47612300	4.70327600
C	-2.86152700	0.31157400	0.85773000
C	-4.22088000	0.02571600	0.68954800
C	-2.46986800	1.52064800	1.44910700
C	-5.18033900	0.94816700	1.09228600
H	-4.53425000	-0.90971300	0.23804200
C	-3.43952600	2.43965800	1.84185400
H	-1.42126600	1.75832500	1.58068000
C	-4.79127700	2.15817100	1.66205800
H	-6.23215900	0.72076400	0.95606000
H	-3.13195000	3.37810200	2.29116100
H	-5.54136400	2.87878400	1.97169700
C	-2.49615600	-2.15619200	-0.65810000

C	-2.91072500	-1.76048400	-1.93906900
C	-2.78832800	-3.43830400	-0.18385000
C	-3.59939100	-2.66311100	-2.74285300
H	-2.71656000	-0.74397500	-2.27788400
C	-3.47716700	-4.33183100	-0.99946100
H	-2.48762400	-3.73891400	0.81449800
C	-3.87719200	-3.94691700	-2.27733200
H	-3.92318200	-2.36041100	-3.73287600
H	-3.70406900	-5.32729100	-0.63304800
H	-4.41398400	-4.64721700	-2.90902100
C	-0.98178300	-1.71534900	1.82337400
C	-0.15173500	-2.83797900	1.68962500
C	-1.25649100	-1.20791100	3.09811700
C	0.39778600	-3.43774700	2.81674500
H	0.05622100	-3.25492900	0.70827300
C	-0.69658800	-1.80972100	4.22232300
H	-1.90267200	-0.34386800	3.21621100
C	0.13070500	-2.92056300	4.08316800
H	1.03691300	-4.30684000	2.70490400
H	-0.91237900	-1.40881300	5.20701000
H	0.56573600	-3.38659900	4.96097400
H	1.38398600	-0.78219100	0.56112600
C	2.24766500	-0.09322600	-1.26290300
O	2.26936100	1.30300400	-1.09926700
C	3.58682500	-0.68165800	-0.80458200
C	3.91319400	-2.02030400	-1.04890800
C	4.47349500	0.11009800	-0.07550900
C	5.11146000	-2.55034600	-0.57961500
H	3.23919400	-2.65466800	-1.61444300
C	5.66990000	-0.42511000	0.39761300
H	4.21559400	1.14388600	0.12071100
C	5.99500900	-1.75467800	0.14610600
H	5.35257800	-3.58902800	-0.78241900
H	6.34866300	0.20303300	0.96608000
H	6.92820400	-2.16907500	0.51388500
C	2.08669000	-0.29630700	-2.78242200
F	1.05310000	0.39465400	-3.27635200
F	3.18067200	0.10704000	-3.43993500
F	1.87698400	-1.58876500	-3.10788200
H	-0.61791100	-0.47957200	-1.74091200
TS6 <sub>1</sub> <sup>(R,R,R)</sup>			
P	-1.70969500	-0.99701900	0.29211800
C	-0.23563300	-0.02846500	-0.95172400



C	1.07852700	-0.76616900	-0.76163300
H	1.04380000	-1.75274900	-1.23164200
C	-0.15885500	1.37144800	-0.73169700
C	1.15513400	1.95842600	-0.33945300
H	1.14264800	3.01735200	-0.61002400
C	-1.25444400	2.12746300	-1.22607100
O	-2.26117400	1.64299100	-1.75851500
O	-1.14754700	3.47588300	-1.03533700
C	-2.27519100	4.24344900	-1.45440700
C	-2.02257600	5.67801800	-1.04260200
H	-2.40089700	4.15057900	-2.53846400
H	-3.17784500	3.84001300	-0.98341000
H	-2.86059800	6.30981100	-1.34647500
H	-1.11215700	6.06012200	-1.51092300
H	-1.90934200	5.74935300	0.04218400
C	1.63398600	1.87411200	1.10758100
C	2.65629300	2.73656800	1.51824000
C	1.13525900	0.95989700	2.03396900
C	3.17103800	2.67579800	2.80884300
H	3.05387000	3.45971400	0.80959100
C	1.64402600	0.88946100	3.32963100
H	0.34000500	0.28200800	1.74580700
C	2.66701000	1.74733000	3.72049800
H	3.96461600	3.35378900	3.10727300
H	1.23660900	0.16065300	4.02450200
H	3.06814100	1.69780500	4.72767600
C	-2.89160000	0.24176300	0.88261500
C	-4.26114000	0.11700700	0.61933000
C	-2.41395600	1.38336800	1.54132700
C	-5.13804400	1.12662800	0.99747200
H	-4.64162700	-0.76367300	0.11243400
C	-3.29970600	2.39341400	1.91048500
H	-1.35861800	1.50128100	1.75872800
C	-4.65815600	2.27032300	1.63453900
H	-6.19812800	1.02048900	0.79240300
H	-2.92149000	3.27813600	2.41241200
H	-5.34440900	3.06055400	1.92165200
C	-2.61106100	-2.15247500	-0.76688500
C	-3.10141800	-1.63173400	-1.97516100
C	-2.79427000	-3.50379100	-0.45773900
C	-3.77464100	-2.46742600	-2.86078400
H	-2.97152900	-0.57289800	-2.19626700
C	-3.46318700	-4.33117400	-1.35519300
H	-2.42365300	-3.90709500	0.47938900

C	-3.95124700	-3.81553800	-2.55430200
H	-4.16032300	-2.06516900	-3.79159200
H	-3.60843500	-5.37894000	-1.11399100
H	-4.47337000	-4.46524400	-3.24919800
C	-1.06952200	-1.89546900	1.73448800
C	-0.14015600	-2.92625600	1.52790600
C	-1.40326900	-1.52078300	3.04155100
C	0.43445100	-3.57838400	2.61366900
H	0.13015900	-3.22440300	0.51800700
C	-0.81679700	-2.17187700	4.12365600
H	-2.11959600	-0.72386400	3.21400000
C	0.10103200	-3.19845100	3.91248300
H	1.14941200	-4.37630900	2.44435000
H	-1.08271800	-1.87763000	5.13361600
H	0.55745600	-3.70167900	4.75830200
H	1.30251000	-0.92530100	0.29517700
C	2.28048400	0.02089200	-1.35357900
O	2.21393100	1.41860800	-1.18665800
C	3.59477500	-0.52180700	-0.78438800
C	3.83836000	-1.89779500	-0.72213900
C	4.56945900	0.36113900	-0.32024700
C	5.03300400	-2.37924700	-0.19536000
H	3.09942400	-2.60277900	-1.08897600
C	5.76340200	-0.12259200	0.21010800
H	4.37848900	1.42601300	-0.36953000
C	5.99949500	-1.49269300	0.27455000
H	5.20752800	-3.44954600	-0.15208000
H	6.51001600	0.57622600	0.57406400
H	6.92984500	-1.86913700	0.68760000
C	2.28700800	-0.16088100	-2.87833200
F	1.16145400	0.30526100	-3.43636600
F	3.31361300	0.48578000	-3.44045400
F	2.39006900	-1.45713100	-3.22626400
H	-0.77950700	-0.31822600	-1.85399200
TS3 <sub>1</sub> <sup>(R,R,S)</sup>			
P	1.34853600	-1.21912400	-0.13226100
C	-0.02846900	-0.10927800	-0.40600600
C	-1.36657300	-0.67781100	-0.82948400
H	-1.27120100	-1.72279000	-1.13734100
C	0.08139900	1.22936100	-0.18246100
C	-1.09421600	2.11138400	-0.23080500
H	-1.75231200	1.42282000	0.62882200
C	1.38105900	1.82372100	0.28951300

O	1.93877400	1.51598200	1.32125800
O	1.83775500	2.72864000	-0.56711300
C	3.06119000	3.38324900	-0.18801600
C	3.39947200	4.36327500	-1.28671700
H	2.89757300	3.87907700	0.77399200
H	3.83374100	2.61873400	-0.05644900
H	4.31431400	4.90395000	-1.03281000
H	2.58955300	5.08605000	-1.41373700
H	3.55485700	3.83960700	-2.23271000
C	-0.92429600	3.55442200	0.09360700
C	-0.37551900	3.95563600	1.32229300
C	-1.33824300	4.55488300	-0.79251000
C	-0.20805900	5.30084800	1.63000200
H	-0.07601100	3.19757900	2.04343700
C	-1.19196600	5.90245900	-0.47920100
H	-1.77529500	4.26627400	-1.74567400
C	-0.61565900	6.28451800	0.73026300
H	0.22865200	5.58415600	2.58535000
H	-1.52049000	6.65959400	-1.18640700
H	-0.49373300	7.33614100	0.97313000
C	2.90201300	-0.48113200	-0.72239400
C	4.08548200	-0.60536500	0.00882700
C	2.89614600	0.21096900	-1.93798500
C	5.26537300	-0.05826600	-0.49253600
H	4.09057600	-1.10627400	0.97068000
C	4.07914500	0.75105100	-2.43300800
H	1.96780200	0.34636800	-2.48759600
C	5.26333000	0.61334900	-1.71229500
H	6.18312000	-0.15219000	0.07776900
H	4.07186800	1.28254700	-3.37984100
H	6.18520900	1.03951100	-2.09703300
C	1.48464800	-1.69335300	1.60342500
C	0.71623200	-1.02736800	2.56294000
C	2.33669600	-2.74457700	1.97022100
C	0.83413200	-1.39983600	3.89844600
H	0.00065800	-0.26614800	2.25614900
C	2.45154000	-3.09934600	3.30919300
H	2.90017800	-3.28673500	1.21370800
C	1.70317800	-2.42042500	4.27160000
H	0.23598700	-0.89376900	4.64824400
H	3.11470600	-3.90597200	3.59947300
H	1.78834900	-2.70188500	5.31716500
C	1.10362100	-2.75908100	-1.06544000
C	0.30107400	-3.76854400	-0.51434100

C	1.67558000	-2.93261800	-2.32874600
C	0.06610700	-4.93436700	-1.23307400
H	-0.14330300	-3.63964700	0.46818400
C	1.43912600	-4.10677100	-3.04073200
H	2.31306700	-2.16673700	-2.75798700
C	0.63387700	-5.10270600	-2.49563800
H	-0.56025100	-5.71033700	-0.80564700
H	1.88834600	-4.24057200	-4.01739800
H	0.45229500	-6.01631800	-3.05179600
H	-1.68741600	-0.13850900	-1.72761500
C	-2.50381200	-0.54126300	0.27104500
O	-2.19967400	0.30938800	1.29456700
C	-3.83273400	-0.19208500	-0.42962100
C	-4.24467000	-0.80155000	-1.61940100
C	-4.66092200	0.76069900	0.16393800
C	-5.45780000	-0.45127900	-2.20973900
H	-3.61909500	-1.55329200	-2.09384400
C	-5.87251000	1.11300200	-0.42635800
H	-4.32181400	1.21795000	1.08716100
C	-6.27526700	0.50725700	-1.61581100
H	-5.76416200	-0.92901700	-3.13660400
H	-6.50303100	1.86358800	0.04254400
H	-7.21862400	0.78115200	-2.07572500
C	-2.69015700	-1.92722600	0.90634800
F	-1.58162500	-2.31188800	1.57592700
F	-3.69851500	-1.94857000	1.78716600
F	-2.93525300	-2.90646300	0.00672400
H	-1.68574100	1.94715300	-1.13979600
M3 <sub>1</sub> <sup>(R,R,S)</sup>			
P	0.17683100	-1.65510500	-0.12442500
C	-0.07534400	0.06120900	-0.14439200
C	-1.39023000	0.60532300	-0.65210300
H	-1.96362300	-0.16086900	-1.18077500
C	1.01021000	1.00496600	0.06028200
C	0.91199500	2.35939900	-0.07201400
H	-0.81018000	1.22386000	1.58839800
C	2.33900700	0.42720800	0.45832000
O	2.50767900	-0.30162800	1.41594100
O	3.31377700	0.76776700	-0.38076800
C	4.61373700	0.23959600	-0.07053200
C	5.56573500	0.75724900	-1.12384500
H	4.89300500	0.57032300	0.93521400
H	4.54894300	-0.85393100	-0.06821700

H	6.57423700	0.38721200	-0.92600800
H	5.58538100	1.84978400	-1.11612400
H	5.25824400	0.41734000	-2.11565800
C	1.94915900	3.36553900	0.19217700
C	2.92570800	3.23338600	1.19538400
C	1.94719700	4.55341400	-0.55742500
C	3.88928100	4.21572100	1.39499400
H	2.91678300	2.36219200	1.84523400
C	2.90488700	5.54090500	-0.35303300
H	1.18641000	4.68932200	-1.32168300
C	3.89044500	5.37363300	0.61810200
H	4.63330300	4.08371300	2.17487800
H	2.88354100	6.44331200	-0.95654300
H	4.64029900	6.14144300	0.77825900
C	1.76014300	-2.13025800	-0.91443900
C	2.55824500	-3.18115800	-0.45230900
C	2.15623100	-1.40824200	-2.04602800
C	3.72495200	-3.51933700	-1.13372900
H	2.28203600	-3.72773200	0.44303900
C	3.32045900	-1.75278600	-2.72684900
H	1.56395400	-0.55967700	-2.37856400
C	4.10438800	-2.81049000	-2.27273000
H	4.34130200	-4.33465100	-0.76982300
H	3.61643800	-1.18802500	-3.60484500
H	5.01462500	-3.07703200	-2.80008400
C	0.10992800	-2.50900100	1.49123800
C	0.16674000	-1.76137900	2.66749700
C	-0.03310000	-3.90085800	1.55796000
C	0.09063400	-2.39825100	3.90265200
H	0.28360600	-0.68450000	2.60890500
C	-0.10454500	-4.53515600	2.79429300
H	-0.10039600	-4.48902100	0.64596600
C	-0.04386000	-3.78294400	3.96650000
H	0.13233300	-1.81204100	4.81451300
H	-0.21624100	-5.61323400	2.84189600
H	-0.10784200	-4.27762700	4.93038800
C	-1.12626000	-2.47756800	-1.10742500
C	-2.30268200	-2.92585500	-0.49852400
C	-0.97840500	-2.59725200	-2.49391200
C	-3.31986900	-3.48072100	-1.27065100
H	-2.43251500	-2.83114500	0.57353200
C	-1.99626200	-3.15565400	-3.25987500
H	-0.06857800	-2.26120000	-2.98021300
C	-3.16858100	-3.59688900	-2.64925800

H	-4.23193000	-3.81960200	-0.79063400
H	-1.87068100	-3.24878900	-4.33341400
H	-3.96222200	-4.03181500	-3.24811900
H	-1.18728500	1.38934200	-1.39220600
C	-2.33456400	1.23613200	0.42646600
O	-1.62886400	1.74245000	1.52988500
C	-3.18087100	2.34217900	-0.18536900
C	-3.93985100	2.09705300	-1.33504300
C	-3.18237400	3.62037000	0.37244300
C	-4.68950700	3.11621000	-1.91342000
H	-3.94784100	1.10801400	-1.78231700
C	-3.93255600	4.63997100	-0.21086700
H	-2.58819700	3.81046100	1.25828900
C	-4.68801400	4.39201400	-1.35312800
H	-5.27246800	2.91252600	-2.80594700
H	-3.92329500	5.63168600	0.23048300
H	-5.27004000	5.18767900	-1.80707400
C	-3.25698600	0.15821700	1.00784300
F	-2.53788600	-0.77886400	1.65906200
F	-4.12234300	0.66881700	1.89053300
F	-3.97524500	-0.48420700	0.06984100
H	-0.04638000	2.77344800	-0.37526700
TS4 <sub>1</sub> <sup>(R,R,S)</sup>			
P	0.61662700	-1.56907300	0.24840200
C	-0.92901300	-2.52053800	0.29105300
C	-1.23676500	-3.41415700	-0.73803000
C	-1.85115400	-2.29744500	1.32388000
C	-2.45132600	-4.09527200	-0.72273400
H	-0.53945400	-3.57037700	-1.55435700
C	-3.05354300	-2.99343100	1.34094900
H	-1.64049800	-1.56903200	2.10209600
C	-3.35340100	-3.89229800	0.31802000
H	-2.68880200	-4.78494400	-1.52564300
H	-3.76315600	-2.82249500	2.14321500
H	-4.29616700	-4.43002600	0.32987400
C	1.55579900	-1.96691600	1.76199600
C	0.99980000	-2.70636300	2.80995500
C	2.89504400	-1.55443600	1.84219400
C	1.76327200	-3.00173700	3.93737100
H	-0.01703000	-3.07485200	2.75110700
C	3.64735200	-1.84864400	2.97332000
H	3.35711000	-1.01494800	1.02179900
C	3.08180800	-2.56792100	4.02479500

H	1.32249600	-3.57892300	4.74308300
H	3.67308500	-2.80049800	4.90421900
C	1.61658200	-2.23994600	-1.10230600
C	1.77579200	-1.55724800	-2.31059000
C	2.16832200	-3.51755600	-0.92903900
C	2.48429800	-2.16654600	-3.34515600
H	1.39755800	-0.54710600	-2.43056400
C	2.86583000	-4.11624700	-1.97021100
H	2.05094000	-4.04248800	0.01556200
C	3.02117900	-3.43982700	-3.18012900
H	2.61972800	-1.63730000	-4.28221700
H	3.29072300	-5.10527100	-1.83709500
H	3.56851000	-3.90666900	-3.99268800
C	0.22011700	0.18984400	0.03776800
C	-1.25868000	0.46710400	0.04366400
C	1.15266400	1.18255600	0.72156200
C	1.87339800	1.97755100	-0.48187200
H	1.88172400	0.71876900	1.38960900
H	0.60080000	1.89898000	1.32960400
C	-1.88386200	1.28218900	0.91069900
C	-1.97956300	-0.15670500	-1.12155700
O	-1.46632900	-0.34764200	-2.20494100
O	-3.22323800	-0.52678900	-0.82300100
C	-4.02582200	-1.00950900	-1.91100200
C	-5.40864500	-1.25529500	-1.35120500
H	-3.56786300	-1.91987300	-2.30973600
H	-4.03069700	-0.25406500	-2.70384300
H	-6.07463500	-1.61269000	-2.13961800
H	-5.36806400	-2.00639900	-0.55819600
H	-5.81718600	-0.33005500	-0.93618000
O	1.34847000	1.60441500	-1.66902000
H	0.55542400	0.54228900	-1.07539000
H	4.68012100	-1.52154200	3.02715000
C	1.80736400	3.48915700	-0.22366600
C	1.36092200	4.31911800	-1.24995000
C	2.17873500	4.06131400	0.99721700
C	1.28250700	5.69770200	-1.06453300
H	1.07303600	3.84977100	-2.18407300
C	2.10481900	5.43933600	1.18402700
H	2.52780900	3.42803700	1.80827200
C	1.65612500	6.26264000	0.15260500
H	0.92998900	6.33292300	-1.87187900
H	2.39646600	5.87101000	2.13686100
H	1.59662300	7.33670900	0.29908600

C	3.34946500	1.56052100	-0.46840600
F	3.47148000	0.24060700	-0.74920800
F	4.07838600	2.21508000	-1.38161900
F	3.96782100	1.73875500	0.72262700
C	-3.25583800	1.81878200	0.81815000
C	-3.78930100	2.27556300	-0.39461000
C	-4.03272100	1.92399200	1.97694900
C	-5.08132300	2.78350400	-0.45218300
H	-3.17644000	2.24738300	-1.29192100
C	-5.32979500	2.42599600	1.91911900
H	-3.61949900	1.59502900	2.92671200
C	-5.85970600	2.85260000	0.70383300
H	-5.47895500	3.13743300	-1.39807000
H	-5.92450300	2.48760800	2.82492400
H	-6.86786200	3.25159200	0.65823200
H	-1.31556900	1.62966100	1.77185500
M4 <sub>1</sub> <sup>(R,R,S)</sup>			
P	0.28336000	-1.64849300	0.23331500
C	-1.42816400	-2.25028100	0.26843200
C	-1.92093000	-3.06434000	-0.75491400
C	-2.28962800	-1.80221500	1.28161800
C	-3.26094900	-3.44596800	-0.74958300
H	-1.26981700	-3.39194100	-1.55842600
C	-3.62225200	-2.19250000	1.28324400
H	-1.92718800	-1.13647400	2.05946300
C	-4.10751500	-3.01586000	0.26832200
H	-3.63978900	-4.07904400	-1.54478000
H	-4.28340700	-1.84416700	2.06919800
H	-5.14983500	-3.31854800	0.26947900
C	1.07866100	-2.12134100	1.80266600
C	0.37006800	-2.70283100	2.85866100
C	2.46722000	-1.95146000	1.91047000
C	1.03842500	-3.07341400	4.02341800
H	-0.69345500	-2.89113200	2.77994700
C	3.12401700	-2.31860200	3.07870500
H	3.03782700	-1.54493800	1.08268700
C	2.41003500	-2.87327200	4.13927600
H	0.48151300	-3.52650000	4.83641000
H	2.92647000	-3.16128100	5.04896100
C	1.17651600	-2.54012600	-1.05914300
C	1.72568100	-1.88895500	-2.16696400
C	1.29009400	-3.93123300	-0.91400400
C	2.37214600	-2.65236000	-3.13939300



H	1.71443400	-0.80179100	-2.24770800
C	1.93081600	-4.67621400	-1.89394200
H	0.87464500	-4.42776700	-0.04010300
C	2.46781600	-4.03379800	-3.01084300
H	2.80991500	-2.15582200	-3.99874500
H	2.01542300	-5.75212700	-1.78620200
H	2.97171600	-4.61464400	-3.77670200
C	0.25990100	0.16935000	-0.10797200
C	-1.15960900	0.69469700	-0.09805600
C	1.33375300	1.00267500	0.58938600
C	2.31462900	1.58922500	-0.55171000
H	1.88842900	0.45247300	1.35293500
H	0.87177000	1.84365800	1.10608200
C	-1.65942600	1.51187600	0.84195100
C	-1.94770000	0.22479000	-1.29014000
O	-1.43227600	-0.08405100	-2.34499600
O	-3.25084500	0.11379200	-1.04992100
C	-4.08054800	-0.22736900	-2.17278600
C	-5.51179200	-0.16063700	-1.69066900
H	-3.80192500	-1.22595700	-2.52311300
H	-3.88473600	0.48456000	-2.98058000
H	-6.19367700	-0.38365100	-2.51419000
H	-5.67947800	-0.88578200	-0.89065100
H	-5.73374300	0.83906700	-1.30784500
O	1.90223400	1.31266100	-1.79234800
H	0.58304300	0.26828400	-1.17583200
H	4.19667500	-2.17731300	3.15498700
C	2.51826200	3.09926000	-0.28400200
C	2.37389100	3.97506600	-1.35731600
C	2.83541900	3.62069800	0.97465000
C	2.53663400	5.34786900	-1.18316400
H	2.12261100	3.54032000	-2.31850000
C	3.00237000	4.99216200	1.15228100
H	2.95307500	2.95360800	1.82448500
C	2.85275800	5.86113900	0.07263300
H	2.41674000	6.01990200	-2.02818500
H	3.24721000	5.38355900	2.13537600
H	2.97990800	6.93047300	0.21169000
C	3.68201900	0.91481700	-0.33259800
F	3.61268700	-0.40941100	-0.61680600
F	4.63921800	1.42063200	-1.12186000
F	4.15402900	0.98416900	0.93725700
C	-2.95549800	2.21937100	0.83737900
C	-3.42333500	2.88511800	-0.30240400

C	-3.71410600	2.27161500	2.01131800
C	-4.63921200	3.55661600	-0.27790600
H	-2.81905100	2.88429500	-1.20544200
C	-4.93865400	2.93382500	2.03288800
H	-3.34674000	1.77835700	2.90747700
C	-5.40556100	3.57500900	0.88831800
H	-4.98723100	4.07307400	-1.16683300
H	-5.52449500	2.95427700	2.94613000
H	-6.35500800	4.10022700	0.90724800
H	-1.03604100	1.70798500	1.71373900
M4 <sub>1</sub> <sup>r(R,R,S)</sup>			
P	0.00563100	-1.80805300	0.32626100
C	0.22158000	-0.07086700	-0.35228500
C	1.52312100	0.54194300	0.18074800
H	2.31554100	-0.17987200	-0.04082900
C	-1.06376400	0.70992000	-0.22775000
C	-1.14919900	1.76505500	0.59979300
H	0.36107800	-0.27585400	-1.41704200
C	-2.07722600	0.27248300	-1.22633500
O	-1.81280300	-0.49271800	-2.13821300
O	-3.30022500	0.74567300	-1.01547500
C	-4.33352600	0.24904000	-1.88361400
C	-5.64520600	0.77629200	-1.34690900
H	-4.13399500	0.59122900	-2.90292000
H	-4.29261800	-0.84504200	-1.87471700
H	-6.46644700	0.45577100	-1.99167600
H	-5.63321700	1.86804600	-1.30787900
H	-5.82575000	0.39426700	-0.33837100
C	-2.20115900	2.78692500	0.78043400
C	-1.78044800	4.11739300	0.64406100
C	-3.52168000	2.51992300	1.15298300
C	-2.68167600	5.16015700	0.83307900
H	-0.74265400	4.29441200	0.37054800
C	-4.41353000	3.56738800	1.36403900
H	-3.84836500	1.49271200	1.27374600
C	-3.99983500	4.88772900	1.19574900
H	-2.35335000	6.18697700	0.70575100
H	-5.43659900	3.35074200	1.65620900
H	-4.70189300	5.70055800	1.35280300
C	-1.74447700	-2.28368100	0.36454500
C	-2.19102000	-3.36094600	-0.40663100
C	-2.66039200	-1.53871300	1.12235300
C	-3.54497000	-3.68303900	-0.42735400

H	-1.49166900	-3.94152700	-0.99863500
C	-4.01153200	-1.86818600	1.09485900
H	-2.32753700	-0.69499600	1.71893400
C	-4.45521000	-2.93591400	0.31630100
H	-3.88597700	-4.51757800	-1.03008100
H	-4.71544300	-1.28827800	1.68278100
H	-5.51061000	-3.18676000	0.29287300
C	0.88216800	-2.93311400	-0.78389000
C	0.73502500	-2.75314700	-2.16699300
C	1.63722200	-4.00053900	-0.28713700
C	1.36573500	-3.63019600	-3.04249000
H	0.10658000	-1.95613000	-2.55617700
C	2.26623100	-4.86935700	-1.17379300
H	1.73778100	-4.15475800	0.78208200
C	2.13580000	-4.68096600	-2.54724700
H	1.25326000	-3.49198800	-4.11218900
H	2.85743300	-5.69305800	-0.78891500
H	2.62953500	-5.35945000	-3.23508000
C	0.69638400	-1.98915900	1.99376800
C	2.08706200	-1.91172600	2.17205800
C	-0.12837700	-2.22522700	3.09845100
C	2.63459600	-2.04736000	3.44132700
H	2.74816100	-1.76457300	1.32455800
C	0.42943900	-2.35585000	4.36801000
H	-1.20072900	-2.32350900	2.97941000
C	1.80606300	-2.26230600	4.54149700
H	3.70970900	-1.98680600	3.56866500
H	-0.21833100	-2.53829700	5.21838600
H	2.23697800	-2.36640000	5.53162600
H	1.49530600	0.66766100	1.26822800
C	1.96394100	1.96237800	-0.37983400
O	1.29047500	2.99727800	0.11489800
C	3.49994700	2.04422800	-0.09173800
C	4.45119400	1.13192300	-0.56440900
C	3.93011500	3.09700200	0.71281700
C	5.79840500	1.27712300	-0.24027600
H	4.14844800	0.30568900	-1.20160700
C	5.27523500	3.24185600	1.04615500
H	3.16713600	3.78657400	1.05773500
C	6.21624800	2.33197900	0.56938800
H	6.52370100	0.56400000	-0.62143600
H	5.59131300	4.06821500	1.67673000
H	7.26594400	2.44306300	0.82398800
C	1.79901500	1.92734800	-1.91654600

F	0.50587500	2.00449800	-2.28596800
F	2.42756400	2.94949600	-2.51869900
F	2.27248000	0.78914200	-2.49905600
H	-0.22783500	2.01892500	1.11932200
TS5 <sub>1</sub> <sup>(R,R,S)</sup>			
P	0.31960800	1.96963200	0.27473000
C	-0.23982600	0.29477100	-0.37313700
C	-1.65497100	-0.09821600	0.05418900
H	-2.36648900	0.63625800	-0.33559200
C	0.78567900	-0.77188800	-0.12990900
C	0.50796300	-1.74710600	0.78689400
H	-0.25114900	0.49016400	-1.45100500
C	1.89486300	-0.72709800	-1.07693400
O	1.94392500	0.06491900	-2.01329300
O	2.93004000	-1.52793300	-0.77824500
C	4.09472500	-1.37974100	-1.59642600
C	5.15265400	-2.29236800	-1.01564300
H	3.84803200	-1.64217000	-2.62978200
H	4.40428000	-0.32912900	-1.58091400
H	6.06206300	-2.24743300	-1.61918000
H	4.79571900	-3.32520400	-0.99434100
H	5.39594800	-1.98983300	0.00610800
C	1.26340600	-3.01245300	0.91383800
C	1.24560600	-3.92298500	-0.14595000
C	1.98306200	-3.31082100	2.07081400
C	1.96771900	-5.10651700	-0.05958100
H	0.63419500	-3.67854300	-1.00838200
C	2.71693300	-4.49373700	2.15169600
H	1.98155300	-2.61159100	2.90324500
C	2.71278600	-5.39066600	1.08685800
H	1.94841600	-5.81383100	-0.88311800
H	3.28553200	-4.71722500	3.04901600
H	3.27761600	-6.31541500	1.15294000
C	2.12302800	1.99341600	0.41865900
C	2.88035200	2.87442200	-0.35926600
C	2.76423900	1.07158400	1.25907000
C	4.26979600	2.82192400	-0.30964400
H	2.39266800	3.59026400	-1.01224900
C	4.15415900	1.02137400	1.29572600
H	2.18618900	0.38298400	1.86632800
C	4.90620000	1.89125100	0.50826700
H	4.85398700	3.50467400	-0.91685300
H	4.64564700	0.29907800	1.93875700

H	5.99004000	1.84572600	0.53629300
C	-0.18490900	3.22006200	-0.92792000
C	0.09811800	2.96774400	-2.27881300
C	-0.80792100	4.41117400	-0.54527200
C	-0.25590800	3.90859200	-3.23901200
H	0.61660500	2.05583500	-2.56953300
C	-1.16193600	5.34295500	-1.51704200
H	-1.01745000	4.61180500	0.50047500
C	-0.89002700	5.09087000	-2.85942800
H	-0.03652300	3.71753900	-4.28378000
H	-1.64997200	6.26575200	-1.22274000
H	-1.16940100	5.81981400	-3.61312200
C	-0.40525500	2.37212600	1.88373600
C	-1.79978100	2.48516600	1.99463600
C	0.40016900	2.59189200	3.00586400
C	-2.37543800	2.79631300	3.22035600
H	-2.43644200	2.34471600	1.12677300
C	-0.18575300	2.90064700	4.23051300
H	1.47997400	2.53244900	2.92915200
C	-1.56945500	2.99788000	4.33980400
H	-3.45355800	2.88201100	3.29958400
H	0.44417700	3.06989100	5.09700200
H	-2.02251900	3.23753200	5.29607500
H	-1.76214900	-0.11100500	1.14359200
C	-2.09041500	-1.54102400	-0.42585600
O	-1.37246900	-2.55360300	0.09575200
C	-3.59850600	-1.64471400	-0.07227500
C	-4.58264200	-0.81793400	-0.62584300
C	-3.97577900	-2.59467900	0.87437400
C	-5.91471500	-0.94629700	-0.24019300
H	-4.31741900	-0.07641500	-1.37380500
C	-5.30675200	-2.71971100	1.26764200
H	-3.19509900	-3.22813500	1.28018800
C	-6.28216300	-1.89612500	0.71109000
H	-6.66748500	-0.30152400	-0.68412800
H	-5.58393700	-3.46498600	2.00781400
H	-7.32040200	-1.99369000	1.01312400
C	-1.96475800	-1.59629000	-1.96614000
F	-0.69019300	-1.77009200	-2.36100100
F	-2.66732700	-2.61045100	-2.49451200
F	-2.38803200	-0.46504100	-2.58971700
H	-0.13604900	-1.50441600	1.62601700

M5<sub>1</sub><sup>(R,R,S)</sup>

P	-1.93619800	-0.67637600	0.18965600
C	-0.21396500	-0.38048500	-0.68421100
C	0.78134400	-1.46979200	-0.27826700
H	0.52858300	-2.43887700	-0.71381300
C	0.31751100	0.96623100	-0.41291500
C	1.57723200	0.99172600	0.38210900
H	-0.52436600	-0.49948700	-1.72961200
C	-0.42089400	1.99681700	-1.00398900
O	-1.45562000	1.79089900	-1.67839200
O	-0.01653900	3.28142600	-0.76609400
C	-0.90125000	4.30184200	-1.21072600
C	-0.32259400	5.61738900	-0.73123000
H	-0.99005300	4.27543400	-2.30264600
H	-1.90200800	4.12951900	-0.79761000
H	-0.94051600	6.45433200	-1.06591800
H	0.69094200	5.74842400	-1.11941100
H	-0.27253700	5.63204900	0.36094900
C	2.21111400	2.34399300	0.59039100
C	3.00129500	2.90964400	-0.41012800
C	2.00320700	3.04288200	1.77662900
C	3.56250300	4.16954800	-0.23001700
H	3.16239200	2.35080800	-1.32697300
C	2.55509000	4.30998400	1.95584900
H	1.40638800	2.59337400	2.56740900
C	3.33567400	4.87640000	0.95115900
H	4.17739900	4.60453000	-1.01220000
H	2.38453300	4.84825700	2.88317600
H	3.77390700	5.85981500	1.09034800
C	-2.52149500	0.85149000	0.94520400
C	-3.78066000	1.36701200	0.62574200
C	-1.66800800	1.55841100	1.80131100
C	-4.18361400	2.58536300	1.15990200
H	-4.43683600	0.82619900	-0.04887900
C	-2.07527400	2.78466700	2.32381300
H	-0.69503200	1.15560400	2.06335000
C	-3.32787600	3.29796700	2.00026800
H	-5.16213700	2.98340500	0.91339100
H	-1.41033000	3.33660300	2.98007700
H	-3.64208600	4.25414100	2.40647600
C	-3.18011400	-1.28064800	-0.98005500
C	-3.25047900	-0.67798800	-2.24385600
C	-4.07498000	-2.29954000	-0.63190400
C	-4.20979800	-1.11325500	-3.15464500
H	-2.57690200	0.14106900	-2.48313800

C	-5.02889100	-2.72347800	-1.55108200
H	-4.03003000	-2.75914300	0.34998800
C	-5.09262800	-2.13488700	-2.81252300
H	-4.26856100	-0.64936300	-4.13361000
H	-5.72233100	-3.51247000	-1.28017000
H	-5.83635200	-2.47082600	-3.52795000
C	-1.79180000	-1.93296900	1.49490700
C	-1.50446700	-3.25573200	1.12399600
C	-1.92986600	-1.61086100	2.84761000
C	-1.35363700	-4.23653800	2.09598100
H	-1.41536300	-3.52295400	0.07406200
C	-1.77299900	-2.59888100	3.81798300
H	-2.16927100	-0.59654800	3.14775400
C	-1.48333900	-3.90737900	3.44515900
H	-1.13491600	-5.25711400	1.80093800
H	-1.88383300	-2.34178600	4.86594000
H	-1.36202500	-4.67381500	4.20330600
H	0.79770100	-1.60720900	0.80739900
C	2.22648800	-1.10763500	-0.68156500
O	2.61429900	0.17322200	-0.25000900
C	3.18237500	-2.15341900	-0.09624600
C	3.06111100	-3.50915700	-0.42002600
C	4.16505900	-1.75745000	0.81029300
C	3.91235200	-4.44850000	0.15445200
H	2.30808000	-3.84072600	-1.12726400
C	5.01420500	-2.70053000	1.38589600
H	4.25579900	-0.70664500	1.05728300
C	4.89166600	-4.04788100	1.06061400
H	3.80771700	-5.49658300	-0.10749600
H	5.77456400	-2.37706700	2.08984600
H	5.55436300	-4.78180600	1.50781500
C	2.38043600	-1.08557000	-2.21244400
F	1.73419300	-0.06030800	-2.77709700
F	3.66777900	-0.97990100	-2.56506800
F	1.89698000	-2.21018200	-2.77825600
H	1.42817100	0.54086200	1.38144900
TS6 <sub>1</sub> <sup>(R,R,S)</sup>			
P	-2.00859000	-0.64728000	0.17281100
C	-0.17625700	-0.35062900	-0.85812600
C	0.75006900	-1.49110500	-0.45947700
H	0.47049500	-2.43093900	-0.94072600
C	0.36117600	0.94655400	-0.56608000
C	1.61425500	0.93375400	0.25108300

H	-0.61633100	-0.45417400	-1.85254100
C	-0.39800000	2.02956500	-1.07179300
O	-1.43646100	1.87254900	-1.73782700
O	0.01636400	3.28055300	-0.73917700
C	-0.88015200	4.33898800	-1.06397000
C	-0.36087100	5.57842000	-0.36630400
H	-0.91903900	4.47461200	-2.15093800
H	-1.88774100	4.07522600	-0.72566600
H	-0.98352300	6.44323600	-0.60852200
H	0.66790600	5.78720600	-0.67229800
H	-0.37013100	5.42998700	0.71711800
C	2.27859700	2.26398100	0.49825200
C	3.02199700	2.87407500	-0.51272100
C	2.14918600	2.89658000	1.73173500
C	3.61110600	4.11466300	-0.29550000
H	3.12551400	2.36590400	-1.46665700
C	2.72848600	4.14584900	1.94869800
H	1.59452400	2.40840400	2.53017800
C	3.45826200	4.75844300	0.93340400
H	4.18767800	4.58563200	-1.08581800
H	2.61785600	4.63359900	2.91232700
H	3.91610300	5.72850300	1.10025200
C	-2.43143400	0.91532400	0.96308200
C	-3.62128300	1.59405500	0.67985400
C	-1.46599600	1.51171100	1.78327400
C	-3.84559500	2.85298900	1.22356400
H	-4.36095300	1.14301000	0.02555600
C	-1.69142300	2.78026200	2.31549400
H	-0.54803800	0.98230000	2.02080800
C	-2.87728700	3.45048100	2.03324900
H	-4.77271100	3.37399500	1.00908000
H	-0.93717300	3.24230300	2.94434400
H	-3.05053800	4.43969800	2.44520500
C	-3.36102400	-1.15434900	-0.92270800
C	-3.49367100	-0.48998100	-2.15093500
C	-4.23984700	-2.19087700	-0.58569700
C	-4.50563700	-0.86940600	-3.02950100
H	-2.81721400	0.32678700	-2.39209300
C	-5.24334500	-2.56293300	-1.47388400
H	-4.14344700	-2.70327700	0.36597300
C	-5.37492200	-1.90539000	-2.69574500
H	-4.61150100	-0.35587400	-3.97942900
H	-5.92404000	-3.36536500	-1.20957100
H	-6.15770800	-2.20072400	-3.38703500



C	-1.88641500	-1.91360100	1.47289700
C	-1.58010700	-3.22938600	1.09229400
C	-2.05673700	-1.61326600	2.82785300
C	-1.44972800	-4.22475000	2.05325400
H	-1.45806100	-3.48034100	0.04137300
C	-1.91864200	-2.61423100	3.78708600
H	-2.30550200	-0.60329100	3.13595800
C	-1.61441500	-3.91687900	3.40328700
H	-1.21654800	-5.23941400	1.74860800
H	-2.05612600	-2.37293200	4.83581300
H	-1.50695800	-4.69328700	4.15339300
H	0.71113800	-1.66696700	0.62031200
C	2.23171200	-1.18449000	-0.78350200
O	2.62611100	0.11232600	-0.40485900
C	3.12455600	-2.21816800	-0.08952300
C	2.95338800	-3.58940800	-0.30999100
C	4.09989500	-1.79210700	0.81185300
C	3.74875500	-4.51418300	0.35970000
H	2.20480200	-3.94480500	-1.01036900
C	4.89251500	-2.72067800	1.48346400
H	4.22915600	-0.72972700	0.98098200
C	4.72103200	-4.08337100	1.25983000
H	3.60590500	-5.57455900	0.17760100
H	5.64652100	-2.37397000	2.18312600
H	5.33891900	-4.80605700	1.78300600
C	2.47246700	-1.23835000	-2.29971100
F	1.81032200	-0.27611000	-2.95202500
F	3.77157400	-1.09280000	-2.58639200
F	2.07321400	-2.41200800	-2.82719300
H	1.44351900	0.46040100	1.23561500
TS2 <sub>1</sub> <sup>(R,S)</sup>			
P	0.14962400	-1.32076000	0.41324300
C	-0.39471800	0.36554100	-0.03680600
C	0.27492800	1.41611900	0.61193400
H	0.96606200	1.21223600	1.42066200
C	-1.42203800	0.56042900	-0.95580200
C	-2.03948500	1.93407900	-1.10414200
H	-2.65993000	1.94287400	-2.00287400
H	-1.25261800	2.67265700	-1.25843100
C	-2.02606000	-0.56107200	-1.65329000
O	-1.58529900	-1.70692000	-1.67515300
O	-3.16845800	-0.24864600	-2.30086400
C	-3.81009900	-1.33251000	-2.98611500

C	-5.07259800	-0.78081900	-3.61029100
H	-3.12340300	-1.73572100	-3.73620200
H	-4.02112600	-2.12913400	-2.26628300
H	-5.60032600	-1.57448900	-4.14379600
H	-4.83530400	0.01610900	-4.31870000
H	-5.73672700	-0.37735900	-2.84227300
C	-2.89068400	2.32704000	0.09028600
C	-2.65801100	3.52099400	0.77554700
C	-3.92712700	1.49484400	0.53002100
C	-3.43551600	3.87747500	1.87735500
H	-1.85373400	4.17296600	0.44242800
C	-4.70572500	1.84703400	1.62874400
H	-4.12026400	0.56476900	-0.00029500
C	-4.46045100	3.04073400	2.30831500
H	-3.23536600	4.80772100	2.40016100
H	-5.50838000	1.19172500	1.95442600
H	-5.06529500	3.31466900	3.16686400
C	-1.29645900	-2.26114100	0.97475100
C	-1.35795500	-3.64698300	0.82909200
C	-2.33963600	-1.56421500	1.59206500
C	-2.46826200	-4.33730300	1.30572900
H	-0.55989500	-4.18385800	0.32576700
C	-3.44746100	-2.26388400	2.06303400
H	-2.29633500	-0.48278800	1.69596600
C	-3.51207300	-3.64803900	1.92036700
H	-2.52196600	-5.41422800	1.18692200
H	-4.25973400	-1.72270500	2.53752700
H	-4.37832900	-4.19064500	2.28454700
C	1.14113900	-2.17518900	-0.83478200
C	1.19629200	-1.68460800	-2.14112900
C	1.88864800	-3.29988000	-0.46728600
C	1.98977300	-2.33315700	-3.08179100
H	0.64523000	-0.78569300	-2.40373200
C	2.67052500	-3.94860300	-1.41809100
H	1.87508800	-3.66104300	0.55748700
C	2.71914800	-3.46538000	-2.72415800
H	2.04305500	-1.94805900	-4.09482600
H	3.24564000	-4.82368500	-1.13594200
H	3.33388500	-3.96838200	-3.46365800
C	1.23376900	-1.22241500	1.87240500
C	2.60886100	-1.02791300	1.70334800
C	0.69585800	-1.31210000	3.16146800
C	3.43574300	-0.92989100	2.81847700
H	3.03736400	-0.95100600	0.70749300

C	1.52955000	-1.21178900	4.27045500
H	-0.36807200	-1.46750800	3.30541700
C	2.89919200	-1.02340100	4.10015500
H	4.50082000	-0.77923300	2.67732800
H	1.10757100	-1.28729900	5.26682600
H	3.54839700	-0.95193300	4.96675300
H	-0.26467300	2.35180100	0.70078200
C	1.54974000	2.17903600	-1.04283000
O	0.96082300	1.92091900	-2.10426500
C	2.86576600	1.51572400	-0.70592200
C	3.35370800	0.58177200	-1.62266200
C	3.64107400	1.83023900	0.41732400
C	4.56564200	-0.06771700	-1.40344200
H	2.76798100	0.38572300	-2.51230100
C	4.87126000	1.21102200	0.61531700
H	3.28959300	2.55376900	1.14318400
C	5.33214200	0.24867600	-0.28267300
H	4.91763800	-0.80658900	-2.11723200
H	5.46605900	1.47157100	1.48539200
H	6.28543200	-0.24240800	-0.11470300
C	1.45487500	3.65149900	-0.57694900
F	0.29558600	4.21375000	-0.94458100
F	1.57940800	3.86124800	0.74692300
F	2.43735300	4.35703200	-1.16670200
M2 <sub>1</sub> <sup>(R,S)</sup>			
P	-0.05748600	-1.32669000	-0.36018200
C	0.32843100	0.36855600	0.18716200
C	-0.54622700	1.48388000	-0.28537100
H	-1.04055100	1.24973800	-1.23036700
C	1.36577100	0.59839900	1.02186300
C	1.82348300	2.00064600	1.37776400
H	2.49582300	1.93999300	2.23896600
H	0.93887200	2.55946700	1.69019700
C	2.14672100	-0.53161500	1.61887200
O	1.65750800	-1.55310500	2.04997400
O	3.45845600	-0.29683400	1.60719900
C	4.29840800	-1.39811900	2.01086600
C	5.71907300	-1.02265400	1.65932800
H	4.16154300	-1.56443400	3.08279500
H	3.96425600	-2.29342500	1.47680300
H	6.39675600	-1.82281800	1.96470900
H	6.01474900	-0.10246200	2.16783300
H	5.81879500	-0.87692800	0.58037800

C	2.54193600	2.70909400	0.23808000
C	2.18176700	4.01212700	-0.11530900
C	3.58325900	2.08978900	-0.46369200
C	2.84539500	4.68239800	-1.14242300
H	1.36678500	4.49898000	0.41066400
C	4.24377000	2.75687000	-1.49165100
H	3.88430800	1.08227300	-0.19223600
C	3.87745100	4.05697500	-1.83544000
H	2.54882500	5.69369500	-1.40277200
H	5.05071200	2.26063100	-2.02243200
H	4.39252600	4.57667500	-2.63693500
C	1.50346700	-2.18508100	-0.72884300
C	1.66322400	-3.53953800	-0.43017100
C	2.55514700	-1.46286600	-1.30624200
C	2.86921600	-4.17143100	-0.71949300
H	0.86479600	-4.09437900	0.05095600
C	3.75953300	-2.10219000	-1.58869100
H	2.44814200	-0.40175700	-1.51723600
C	3.91671700	-3.45525900	-1.29590300
H	2.99372800	-5.22220600	-0.48147900
H	4.57299200	-1.53906200	-2.03466000
H	4.85767200	-3.95055200	-1.51131200
C	-1.07347100	-2.22869400	0.82378900
C	-1.29086200	-1.68414200	2.09126500
C	-1.65530200	-3.44866900	0.45262100
C	-2.07515900	-2.39051800	3.00043400
H	-0.90634200	-0.69337800	2.33351200
C	-2.43227500	-4.14265300	1.37203200
H	-1.51653300	-3.84810000	-0.54876600
C	-2.63500600	-3.61487200	2.64789700
H	-2.25797400	-1.97104800	3.98440700
H	-2.88275100	-5.08856300	1.09171100
H	-3.24391000	-4.15797500	3.36359800
C	-0.99413800	-1.27050500	-1.91110700
C	-2.39148000	-1.31169500	-1.87282000
C	-0.32583200	-1.16840200	-3.13783400
C	-3.11290800	-1.26224100	-3.06256700
H	-2.91772100	-1.37777100	-0.92387900
C	-1.05614800	-1.11162800	-4.31885600
H	0.75806700	-1.14431200	-3.17692300
C	-2.44915000	-1.16392100	-4.28142400
H	-4.19663900	-1.29356800	-3.02662700
H	-0.53729000	-1.03426700	-5.26808200
H	-3.01644300	-1.12790100	-5.20569300

H	0.08236800	2.36235600	-0.45778300
C	-1.63772700	1.84955400	0.87424400
O	-1.23910300	1.56190400	2.09930800
C	-2.99533300	1.20661100	0.46354000
C	-3.60131100	0.35905800	1.38818800
C	-3.64100800	1.43269200	-0.75796400
C	-4.79354600	-0.29797600	1.08967300
H	-3.09902400	0.23555500	2.34038500
C	-4.85260300	0.80920200	-1.04709400
H	-3.19852100	2.09647300	-1.49481500
C	-5.42572900	-0.07365000	-0.13226500
H	-5.23522800	-0.97525300	1.81544400
H	-5.34193200	0.99954000	-1.99817400
H	-6.36026700	-0.57425800	-0.36696000
C	-1.82145300	3.38105300	0.74903100
F	-0.73501300	4.04546400	1.19966200
F	-2.01687200	3.82597800	-0.51752400
F	-2.86031600	3.82324200	1.47416300
TS3 <sub>1</sub> (R,S,R)			
P	0.10854000	-1.48039200	0.32071300
C	-0.38555500	0.21952200	-0.01127700
C	0.42187500	1.36158300	0.58224000
H	1.03339900	1.02020600	1.42093000
C	-1.42433500	0.47917500	-0.85077500
C	-1.76077400	1.83872600	-1.31586500
H	-2.34380500	1.78710500	-2.24040100
H	-0.48197500	2.15700700	-1.61160700
C	-2.21556800	-0.63711600	-1.47317600
O	-1.76313200	-1.50365200	-2.18904600
O	-3.49929700	-0.54991100	-1.13023300
C	-4.33044400	-1.64632000	-1.56303200
C	-5.69102000	-1.44768400	-0.93717600
H	-4.36999500	-1.64535400	-2.65575400
H	-3.85848300	-2.57945300	-1.23696800
H	-6.35190300	-2.26778200	-1.22643600
H	-6.13628400	-0.50684100	-1.26768100
H	-5.60831400	-1.43395000	0.15216200
C	-2.41525000	2.79118300	-0.37314300
C	-2.76546400	4.06958000	-0.84124200
C	-2.72082200	2.49005200	0.96086300
C	-3.38100700	5.00044100	-0.01619600
H	-2.53839400	4.32648400	-1.87313000
C	-3.32655700	3.42808900	1.79666800

H	-2.49402900	1.49895400	1.34710700
C	-3.66187000	4.68875300	1.31638400
H	-3.63907500	5.97913800	-0.41061900
H	-3.54698100	3.16237400	2.82674000
H	-4.13688500	5.41785700	1.96473300
C	-1.35084400	-2.51881200	0.62920000
C	-1.42085400	-3.83018700	0.15024300
C	-2.40099600	-1.99214300	1.39025700
C	-2.52858700	-4.61640200	0.45422600
H	-0.62887100	-4.23290300	-0.47226400
C	-3.50078200	-2.78850400	1.69756900
H	-2.36750700	-0.96234900	1.73530600
C	-3.56395600	-4.09981600	1.23113600
H	-2.58404000	-5.63169000	0.07701300
H	-4.30832800	-2.37968000	2.29553400
H	-4.42485500	-4.71649200	1.46709900
C	1.11743600	-2.15631400	-1.01657800
C	1.21576000	-1.47184800	-2.22914100
C	1.81740100	-3.35394800	-0.81336100
C	2.00274600	-2.00326200	-3.24797300
H	0.71024400	-0.51846000	-2.35860200
C	2.59291000	-3.87849400	-1.83976100
H	1.76777600	-3.86745400	0.14346500
C	2.68196800	-3.20307600	-3.05730400
H	2.09149300	-1.47026200	-4.18889700
H	3.13165400	-4.80723000	-1.68717500
H	3.29314700	-3.61141400	-3.85572000
C	1.14017200	-1.54867900	1.80914600
C	2.52310200	-1.37893300	1.68200900
C	0.56384000	-1.71327200	3.07355000
C	3.32302200	-1.37320100	2.82082900
H	2.97645900	-1.24410500	0.70335500
C	1.37242300	-1.70813100	4.20513800
H	-0.50649600	-1.85627200	3.17977900
C	2.75006200	-1.53883200	4.07910500
H	4.39424300	-1.23575700	2.71755700
H	0.92542300	-1.84072100	5.18431600
H	3.37740700	-1.53765500	4.96428600
H	-0.28761500	2.08751100	0.99201500
C	1.33089800	2.08664800	-0.48397300
O	0.79408300	2.09227600	-1.74260500
C	2.74729200	1.48022600	-0.47308000
C	3.23033000	0.88924200	-1.63855100
C	3.56478400	1.48396500	0.66477500

C	4.47955600	0.27154700	-1.66286100
H	2.60178100	0.92281200	-2.52021100
C	4.82910100	0.90200200	0.63246100
H	3.21682300	1.93819600	1.58718500
C	5.28612800	0.27782400	-0.52736100
H	4.82452200	-0.20774700	-2.57450500
H	5.45316900	0.92516900	1.52097500
H	6.26452600	-0.19215400	-0.54680000
C	1.42969200	3.55216400	-0.02285300
F	0.24855000	4.17671900	-0.14862000
F	1.78667100	3.68739300	1.27607400
F	2.32206500	4.24529000	-0.74469300
M3 <sub>1</sub> <sup>(R,S,R)</sup>			
P	0.12979000	-1.07065400	-0.59539600
C	0.37787400	0.38400400	0.30649000
C	-0.67364800	1.46567500	0.32840300
H	-1.20262300	1.57262600	-0.62594000
C	1.70751200	0.65001000	0.85891100
C	2.44105800	1.78839400	0.74326000
H	3.32506300	1.85987900	1.37170400
H	-0.40525700	0.10087300	2.17600400
C	2.31183700	-0.43207700	1.70877100
O	1.66030300	-1.23707000	2.34912700
O	3.64598500	-0.46028500	1.66951800
C	4.27390700	-1.53072100	2.39549400
C	5.75336900	-1.46519000	2.09115500
H	4.06341800	-1.40938400	3.46220200
H	3.82919000	-2.47510200	2.06704300
H	6.27556500	-2.26833700	2.61575500
H	6.17313000	-0.50934300	2.41279400
H	5.92348800	-1.58054100	1.01781500
C	2.25499800	2.93329600	-0.15503900
C	1.51815700	2.87750800	-1.35278700
C	2.94454700	4.12292200	0.13475300
C	1.47842300	3.96729700	-2.21560000
H	0.98232700	1.96867800	-1.61045300
C	2.88924900	5.21773600	-0.71898900
H	3.53331300	4.17814900	1.04662500
C	2.15497700	5.14497400	-1.90168600
H	0.91099600	3.89625600	-3.13869400
H	3.42560000	6.12663100	-0.46515000
H	2.11256200	5.99667400	-2.57284700
C	1.76319200	-1.79807500	-0.95908600

C	2.03331100	-3.14392500	-0.69201300
C	2.78453000	-0.97223600	-1.45011700
C	3.30720600	-3.65824800	-0.92297800
H	1.25840200	-3.78892000	-0.29180600
C	4.05115700	-1.49371800	-1.68833100
H	2.59823500	0.08512300	-1.61718600
C	4.31441000	-2.83649500	-1.42236200
H	3.51127600	-4.70174700	-0.70744500
H	4.83534900	-0.84677700	-2.06685800
H	5.30645400	-3.24027200	-1.59826400
C	-0.85800700	-2.46432100	0.07795400
C	-0.92921300	-2.67472900	1.45690800
C	-1.48184700	-3.37021500	-0.79068600
C	-1.63946200	-3.76135300	1.96263800
H	-0.42327600	-1.99547200	2.13215800
C	-2.19325500	-4.45170400	-0.28135300
H	-1.41792400	-3.23074700	-1.86564100
C	-2.27860800	-4.64429100	1.09673300
H	-1.69433800	-3.91388200	3.03560700
H	-2.67972100	-5.14366900	-0.96091100
H	-2.83688100	-5.48660100	1.49300600
C	-0.72862200	-0.67880700	-2.16228200
C	-2.12700300	-0.62564500	-2.18848400
C	-0.00225600	-0.30109600	-3.29721700
C	-2.78677500	-0.19418900	-3.33685000
H	-2.70668600	-0.92787900	-1.31971700
C	-0.66746200	0.11977500	-4.44463200
H	1.08231800	-0.34496200	-3.29586300
C	-2.06009300	0.17699400	-4.46469100
H	-3.87130700	-0.15092700	-3.34113300
H	-0.09678600	0.39894600	-5.32404900
H	-2.57692600	0.50781300	-5.35978800
H	-0.17229700	2.41892700	0.51029800
C	-1.74585100	1.26703100	1.46572500
O	-1.23449200	0.49390700	2.51810800
C	-3.03793500	0.66977200	0.91331000
C	-3.48404900	-0.56971300	1.37050600
C	-3.76100400	1.31877800	-0.09525500
C	-4.60464600	-1.17443100	0.80172300
H	-2.93621300	-1.06171700	2.16416500
C	-4.89607100	0.72964400	-0.64232700
H	-3.43056400	2.28256700	-0.46800700
C	-5.31378400	-0.52791800	-0.20743200
H	-4.92105500	-2.15195800	1.15281200



H	-5.44504900	1.24670400	-1.42330700
H	-6.18776600	-0.99587600	-0.64920700
C	-2.02780100	2.63148600	2.09795700
F	-0.93094600	3.12578500	2.68913200
F	-2.41942600	3.54297000	1.18672400
F	-2.98709000	2.56396600	3.03061400
TS4 <sub>1</sub> <sup>(R,S,R)</sup>			
P	-0.33884000	-1.02016800	0.61802500
C	-0.31500600	0.30440900	-0.63445700
C	0.86654500	1.26998900	-0.59870400
H	1.31682300	1.43661900	0.38291700
C	-1.67438300	0.85174500	-0.94431300
C	-2.16735000	2.08187800	-0.69332000
H	-3.11713800	2.32531900	-1.16391900
H	0.13722400	-0.25758600	-1.63421300
C	-2.55066100	-0.11621200	-1.68435300
O	-2.14842100	-1.15829500	-2.16254300
O	-3.84180700	0.22928100	-1.69660500
C	-4.74553900	-0.76102700	-2.21785500
C	-6.14854600	-0.27506900	-1.93560200
H	-4.55690900	-0.88833800	-3.28765200
H	-4.53264600	-1.71093500	-1.71724400
H	-6.87353000	-0.99531100	-2.32092200
H	-6.32900800	0.68991400	-2.41466600
H	-6.30286800	-0.16708400	-0.85894000
C	-1.62437000	3.14805600	0.16364600
C	-1.90021600	4.48495400	-0.15523800
C	-0.92057000	2.87517900	1.34518200
C	-1.45068300	5.51845700	0.65971500
H	-2.46598200	4.70985200	-1.05507100
C	-0.48382600	3.90588100	2.16862600
H	-0.71919100	1.84689800	1.62734300
C	-0.74027600	5.23219300	1.82411600
H	-1.66252800	6.54824000	0.39091700
H	0.05481100	3.67005600	3.08120700
H	-0.39666500	6.03806600	2.46446600
C	-2.05175900	-1.54419800	0.93509900
C	-2.43305000	-2.86973500	0.70754100
C	-3.00688700	-0.60879100	1.35726100
C	-3.75815300	-3.25336300	0.89453600
H	-1.70385000	-3.59792900	0.36902600
C	-4.32898500	-0.99918000	1.54203900
H	-2.72912600	0.42733400	1.52762800

C	-4.70647300	-2.31981100	1.30541700
H	-4.04816200	-4.28220200	0.71049900
H	-5.06285500	-0.26894600	1.86605000
H	-5.74023900	-2.62012100	1.44266600
C	0.57337000	-2.48244300	0.06155400
C	0.44942000	-2.88774900	-1.27329500
C	1.33449400	-3.23701300	0.96048900
C	1.11011300	-4.03358900	-1.70358800
H	-0.15434300	-2.31016400	-1.96338400
C	2.00037600	-4.37505400	0.51599000
H	1.41763000	-2.93900000	2.00018100
C	1.89479400	-4.76797900	-0.81594500
H	1.02023800	-4.34657200	-2.73825100
H	2.60106400	-4.95227300	1.21072400
H	2.41872400	-5.65364000	-1.16129400
C	0.40133200	-0.51094900	2.20079200
C	1.79105500	-0.32921400	2.25468700
C	-0.37706600	-0.23621500	3.33049900
C	2.38536100	0.15277200	3.41574500
H	2.41426600	-0.57558800	1.39953300
C	0.22673200	0.24527600	4.48949500
H	-1.44886500	-0.39972500	3.31859400
C	1.60376800	0.44845100	4.53097600
H	3.46108300	0.29350800	3.44009000
H	-0.38274200	0.45717500	5.36139400
H	2.06832300	0.82700300	5.43556100
H	0.51678500	2.24194800	-0.95294000
C	1.93104100	0.67886800	-1.64447400
O	1.34018300	-0.26723400	-2.40841900
C	3.17014500	0.17451700	-0.88101000
C	3.50240300	-1.17580600	-0.97876400
C	3.92197900	0.99260800	-0.02694900
C	4.54017700	-1.71170600	-0.21632500
H	2.90784400	-1.79489500	-1.64139000
C	4.96666000	0.46267800	0.72539000
H	3.67808400	2.04607800	0.06868300
C	5.27249400	-0.89647100	0.64277000
H	4.76853700	-2.77127800	-0.28958700
H	5.53769600	1.10901100	1.38568100
H	6.07735000	-1.31236600	1.24111000
C	2.34122700	1.84452300	-2.55065700
F	1.30450200	2.27693900	-3.28808000
F	2.79163200	2.92839000	-1.87208300
F	3.31664500	1.50181300	-3.40816600

M4<sub>1</sub><sup>(R,S,R)</sup>

P	-0.91098200	1.28634900	0.20391700
C	-2.51762800	1.09818600	1.01506300
C	-2.68666500	1.61528200	2.30236600
C	-3.52781000	0.31991800	0.43210600
C	-3.85753000	1.34806600	3.00587000
H	-1.90359800	2.21138700	2.76046500
C	-4.69331800	0.05713500	1.14277400
H	-3.40299200	-0.09024800	-0.56530600
C	-4.85635600	0.56795800	2.43047000
H	-3.98447900	1.74790900	4.00580400
H	-5.47236500	-0.54796800	0.69098800
H	-5.76565000	0.35718300	2.98370700
C	-1.14992200	1.71855400	-1.53702800
C	-2.38252300	2.18387600	-2.00488500
C	-0.04099500	1.68571500	-2.39469700
C	-2.50768500	2.59564400	-3.33020100
H	-3.24074900	2.23653900	-1.34325300
C	-0.17443400	2.10417100	-3.71155300
H	0.92159600	1.33327500	-2.04139700
C	-1.40769300	2.55620500	-4.18070500
H	-3.46550600	2.95431500	-3.69114700
H	-1.50862500	2.87981100	-5.21156600
C	-0.02901500	2.65481200	0.98781200
C	0.98321200	2.41897400	1.92593700
C	-0.42502800	3.95914100	0.66298800
C	1.59367100	3.51548600	2.53521400
H	1.32663000	1.40314000	2.16164500
C	0.18931900	5.03718900	1.28724400
H	-1.20421400	4.13121200	-0.07513800
C	1.19967400	4.81339100	2.22313900
H	2.38640200	3.34651600	3.25664100
H	-0.11344200	6.04879700	1.03954600
H	1.68379400	5.65671900	2.70505500
C	0.01070000	-0.27285300	0.46332300
C	-0.90814700	-1.42783000	0.11592900
C	1.46259800	-0.23436000	-0.03571400
C	2.41265500	-0.85442600	1.06626900
H	1.79825100	0.80507800	-0.11098800
H	1.58215800	-0.68070900	-1.02090600
C	-1.21245200	-1.95788100	-1.08056000
C	-1.65791500	-1.93797000	1.32353000
O	-1.45892900	-1.54298600	2.45079400

O	-2.60207000	-2.83766400	1.02877900
C	-3.40535700	-3.27763000	2.13820400
C	-4.47580100	-4.18769900	1.58089600
H	-3.82816300	-2.39420700	2.62680400
H	-2.76030500	-3.78820400	2.85842000
H	-5.11313400	-4.54638600	2.39200000
H	-5.09868000	-3.65040100	0.86157000
H	-4.02934500	-5.05089300	1.08232800
O	2.06848300	-0.47022000	2.29765400
H	0.13576100	-0.28991700	1.56337600
C	3.85700600	-0.46901400	0.65725300
C	4.40087700	-0.71100300	-0.60909800
C	4.63538400	0.18701800	1.60838800
C	5.69843200	-0.30350700	-0.91172400
H	3.81605400	-1.22629100	-1.36613400
C	5.93322200	0.59595400	1.30914300
H	4.18057300	0.36051400	2.57781700
C	6.46980800	0.35135200	0.04693300
H	6.10883500	-0.49750000	-1.89849300
H	6.52835600	1.10526000	2.06186500
H	7.48105200	0.66772100	-0.19011100
C	2.31633900	-2.39196200	0.98977800
F	1.11427300	-2.84067700	1.40074200
F	3.23343000	-2.98891600	1.76641300
F	2.49063600	-2.90394800	-0.26094700
H	0.68321700	2.06715000	-4.37426900
C	-0.72466300	-1.62434800	-2.44143200
C	0.58182700	-1.89137300	-2.86033600
C	-1.64938100	-1.13562600	-3.37386200
C	0.97087500	-1.61672200	-4.17010900
H	1.28312200	-2.34076600	-2.16522800
C	-1.26039000	-0.86447400	-4.68024000
H	-2.67728800	-0.95864700	-3.06732500
C	0.05519600	-1.09615200	-5.07989900
H	1.98969100	-1.82644800	-4.48025200
H	-1.98327800	-0.46638300	-5.38528400
H	0.35984000	-0.88418600	-6.09979300
H	-1.97422800	-2.73497700	-1.06538000
M4 <sub>1</sub> <sup>r(R,S,R)</sup>			
P	-0.01161000	1.44945800	-0.17443400
C	-0.07588900	-0.36643900	0.22355600
C	0.30143600	-1.36742000	-0.88218000
H	0.71280400	-0.89967700	-1.77884400

C	-1.25926500	-0.80180700	1.05490600
C	-2.47996400	-1.23795800	0.68756800
H	-3.10315000	-1.58180800	1.50911700
H	0.75611600	-0.41639500	0.93294200
C	-0.95563400	-0.72215300	2.51737700
O	-0.08326000	-0.00376400	2.96995900
O	-1.74509900	-1.46838900	3.28746400
C	-1.51756200	-1.36390600	4.70478300
C	-2.47658600	-2.31534600	5.38269300
H	-0.47363400	-1.61548000	4.90848000
H	-1.68129500	-0.32577200	5.00850500
H	-2.34243000	-2.26288700	6.46533500
H	-2.29163200	-3.34168400	5.05883800
H	-3.51100100	-2.05414700	5.14804500
C	-3.14714300	-1.33168100	-0.61670900
C	-4.33366200	-2.08096500	-0.67846000
C	-2.71755000	-0.68441200	-1.78441500
C	-5.04786400	-2.19944300	-1.86410100
H	-4.68969000	-2.57876500	0.21916000
C	-3.43735300	-0.78951500	-2.96936200
H	-1.81555900	-0.08718100	-1.77793200
C	-4.60252300	-1.55165400	-3.01542500
H	-5.95632000	-2.79211200	-1.88840800
H	-3.08406200	-0.27004400	-3.85481700
H	-5.16340100	-1.63499700	-3.94053600
C	-1.21247400	2.34924500	0.83554200
C	-0.77242000	3.28642500	1.77472200
C	-2.58224000	2.08491600	0.69502600
C	-1.69982500	3.95680200	2.56727300
H	0.28672300	3.48871200	1.89354600
C	-3.50064300	2.76378200	1.48704200
H	-2.93729100	1.35968600	-0.03176300
C	-3.05965200	3.69675500	2.42442300
H	-1.35472600	4.68127000	3.29669000
H	-4.55976400	2.56045600	1.37310700
H	-3.77932200	4.22119800	3.04426300
C	1.64139800	2.06776900	0.22889800
C	2.29483400	1.61365600	1.38154900
C	2.21582600	3.07652500	-0.55553000
C	3.53034300	2.15323400	1.72405700
H	1.83988400	0.86357200	2.02079800
C	3.45176400	3.60652500	-0.20136400
H	1.70681500	3.44856200	-1.43824800
C	4.11110300	3.14126200	0.93359300

H	4.04145000	1.79029500	2.60920900
H	3.89716200	4.38259600	-0.81431300
H	5.07802500	3.55264200	1.20487800
C	-0.28465200	1.83417200	-1.92676600
C	0.67600400	1.40684400	-2.85570700
C	-1.41579400	2.52931000	-2.36447800
C	0.48416800	1.64560600	-4.21125900
H	1.58317100	0.91030000	-2.51986500
C	-1.59983200	2.76403400	-3.72469700
H	-2.15105300	2.89241600	-1.65524400
C	-0.65820100	2.31555100	-4.64678400
H	1.22865900	1.31072100	-4.92501700
H	-2.47981800	3.30265800	-4.05894000
H	-0.80733800	2.49845100	-5.70567500
H	-0.58050100	-1.93541200	-1.18405200
C	1.29739300	-2.36180700	-0.17939100
O	0.82503800	-2.77360400	0.99463700
C	2.69117000	-1.67028400	-0.07967000
C	3.31620000	-1.70205200	1.16596000
C	3.33231500	-1.00807300	-1.13336000
C	4.55395000	-1.09410600	1.36335600
H	2.78156400	-2.21392200	1.95994300
C	4.56245800	-0.38167300	-0.93652600
H	2.88474000	-0.99748600	-2.12425400
C	5.17899200	-0.42632900	0.31241100
H	5.02895500	-1.13259200	2.34010100
H	5.04374200	0.13508400	-1.76198700
H	6.13746100	0.06123000	0.46468300
C	1.45125400	-3.55378400	-1.14239600
F	0.29860800	-4.23428800	-1.28430600
F	1.82425600	-3.19531200	-2.40003900
F	2.36960100	-4.43539200	-0.71283900
TS5 <sub>1</sub> <sup>(R,S,R)</sup>			
P	-1.50780400	-0.83717300	0.37877100
C	0.18886200	-0.17160400	0.09628100
C	0.51458600	1.05906900	0.95461500
H	0.35375900	0.82071100	2.01271200
C	0.71153900	-0.01849200	-1.31054300
C	0.74583900	1.19520600	-1.91990700
H	1.44494000	1.31095200	-2.74419300
C	1.61341900	-1.10604400	-1.71894100
O	1.65886200	-2.19358100	-1.16680400
O	2.37435200	-0.81446200	-2.78900100

C	3.30882000	-1.82973000	-3.17798600
C	4.21892800	-1.22227200	-4.22224100
H	3.86316600	-2.15400500	-2.29264900
H	2.75679600	-2.69233800	-3.56549700
H	4.94630800	-1.96396400	-4.56018100
H	4.75971100	-0.36946000	-3.80400800
H	3.64502100	-0.88030800	-5.08678100
C	-0.35033000	2.20984200	-1.86125200
C	-0.21857400	3.49759400	-1.32789700
C	-1.55760400	1.85737500	-2.47836100
C	-1.28061300	4.39475600	-1.39740500
H	0.71214600	3.73269700	-0.82449000
C	-2.61207000	2.76351000	-2.55968100
H	-1.66990400	0.86644400	-2.91070600
C	-2.47697100	4.03703100	-2.01663900
H	-1.17079900	5.38423100	-0.96342800
H	-3.53940100	2.46742100	-3.04005000
H	-3.30097000	4.74237400	-2.06789400
C	-1.79704700	-2.29563400	-0.64760600
C	-2.30524700	-3.46346200	-0.06938800
C	-1.55360300	-2.23998700	-2.02612800
C	-2.56197000	-4.57330700	-0.86909500
H	-2.49884800	-3.50921900	0.99736100
C	-1.81261300	-3.35445800	-2.81566800
H	-1.15243100	-1.33717700	-2.47489100
C	-2.31510500	-4.51938000	-2.23807300
H	-2.95403100	-5.47926600	-0.42002300
H	-1.61946500	-3.31299400	-3.88199400
H	-2.51605400	-5.38705300	-2.85783000
C	-1.51067400	-1.36605500	2.11212200
C	-0.46464400	-2.18996700	2.55409900
C	-2.51568300	-0.97222700	2.99845500
C	-0.42267300	-2.59757000	3.88201700
H	0.30800000	-2.52851800	1.86759200
C	-2.46485600	-1.38707500	4.32749800
H	-3.33310200	-0.34446900	2.65969800
C	-1.41966700	-2.19201400	4.76931500
H	0.38785500	-3.23280300	4.22248000
H	-3.24399300	-1.07671600	5.01512500
H	-1.38169400	-2.50922400	5.80612700
C	-2.86585400	0.32610700	0.13038800
C	-2.86517500	1.54531700	0.82268000
C	-3.93010500	-0.00001900	-0.71599200
C	-3.92149900	2.43203400	0.65677500

H	-2.05907500	1.79433400	1.50471400
C	-4.98852400	0.89174600	-0.86680000
H	-3.93714600	-0.94337300	-1.25234200
C	-4.98270800	2.10534100	-0.18600900
H	-3.91504700	3.37744200	1.18813200
H	-5.81623800	0.63520100	-1.51921300
H	-5.80659100	2.80051200	-0.31038800
H	-0.11917100	1.90769700	0.69543600
C	1.99706300	1.55710400	0.70603900
O	2.16272300	2.25135400	-0.43583600
C	2.97488700	0.36571800	0.85401800
C	3.97947400	0.22298600	-0.10170300
C	2.88826100	-0.57573500	1.88590700
C	4.87767900	-0.84095600	-0.03598300
H	4.01758000	0.96125700	-0.89571000
C	3.77697500	-1.64635400	1.94828400
H	2.11926800	-0.47837100	2.64896600
C	4.77650000	-1.78234800	0.98631900
H	5.65864800	-0.93739700	-0.78591600
H	3.68974900	-2.37416800	2.74993000
H	5.47049800	-2.61581200	1.03467900
C	2.28679300	2.52539400	1.87021400
F	1.46052700	3.58906300	1.83530300
F	2.13216000	1.97828900	3.10220000
F	3.54029300	2.99967900	1.82352800
H	0.75837600	-1.01544100	0.50714600

M5<sub>1</sub><sup>(R,S,R)</sup>

P	1.62169600	-0.79381800	-0.22445800
C	-0.18874100	-0.37090600	-0.20329300
C	-0.56909600	0.56294600	-1.36281800
H	-0.44441000	0.08951600	-2.34076700
C	-0.77739300	0.11374600	1.08507200
C	-1.22719900	1.53582800	1.09769900
H	-1.86333700	1.67545500	1.97626800
C	-1.50662400	-0.87777500	1.77915100
O	-1.42179100	-2.10303700	1.61055600
O	-2.37413200	-0.38390500	2.73271600
C	-3.17697600	-1.35625800	3.38970400
C	-4.23989700	-0.61004400	4.16951100
H	-3.62310800	-2.02654400	2.64857600
H	-2.55290000	-1.97004400	4.05082000
H	-4.88105200	-1.31330200	4.70700700
H	-4.86284000	-0.02020100	3.49106300



H	-3.78590700	0.06925600	4.89551000
C	-0.12435100	2.58871100	1.17497000
C	-0.09553800	3.71446600	0.35045900
C	0.84856600	2.46329600	2.17235000
C	0.88548500	4.69306500	0.52059600
H	-0.84542600	3.82011300	-0.42474600
C	1.81825300	3.44239100	2.35105400
H	0.83476100	1.57916900	2.80493500
C	1.83859400	4.56649300	1.52482300
H	0.89616000	5.56100200	-0.13233500
H	2.56809000	3.32388200	3.12769900
H	2.60094700	5.32827100	1.65769900
C	1.94495700	-2.11252400	0.96895300
C	2.63638700	-3.26252000	0.57581200
C	1.53627500	-1.95238900	2.29920100
C	2.91405100	-4.25391900	1.51297000
H	2.95694900	-3.38750300	-0.45354900
C	1.82242800	-2.94688600	3.22679500
H	0.99154600	-1.05912600	2.58975200
C	2.50782600	-4.09621600	2.83499000
H	3.44853000	-5.14700900	1.20767900
H	1.50332400	-2.82703600	4.25656800
H	2.72520700	-4.87046600	3.56374400
C	2.00122800	-1.44254400	-1.87553300
C	1.09341200	-2.34310000	-2.45297100
C	3.16066500	-1.08269500	-2.56826200
C	1.34287500	-2.86552700	-3.71627600
H	0.19749600	-2.64823700	-1.91864600
C	3.40354000	-1.61236700	-3.83376300
H	3.87215000	-0.39284900	-2.12610000
C	2.49653200	-2.49830300	-4.40815300
H	0.63746300	-3.56058400	-4.15848500
H	4.30373700	-1.33046000	-4.36912500
H	2.68804900	-2.90691200	-5.39483700
C	2.76796200	0.56215900	0.11967000
C	2.79709500	1.67997500	-0.72633400
C	3.66446100	0.47259900	1.18831900
C	3.71742100	2.69474500	-0.49789100
H	2.12545600	1.75051700	-1.57637300
C	4.58458500	1.49436200	1.40823900
H	3.65303900	-0.39207600	1.84271800
C	4.61310200	2.60107000	0.56663400
H	3.73282100	3.56107900	-1.15019400
H	5.28087700	1.41892300	2.23660600

H	5.33136300	3.39601000	0.73951700
H	0.02509700	1.48114500	-1.35440100
C	-2.02727700	1.00147700	-1.12840900
O	-2.10495900	1.87667900	-0.03116900
C	-2.99538800	-0.17636900	-0.98496300
C	-3.98440800	-0.12782600	-0.00202800
C	-2.91802200	-1.29204200	-1.82177300
C	-4.86990800	-1.18886000	0.15728500
H	-4.02744400	0.73444300	0.65369000
C	-3.80282800	-2.35639200	-1.65862900
H	-2.16431700	-1.34042100	-2.60356000
C	-4.77838800	-2.30908500	-0.66693900
H	-5.63015200	-1.14270600	0.93171900
H	-3.72700700	-3.22317100	-2.30748500
H	-5.46462400	-3.13985200	-0.53741000
C	-2.48128100	1.85963100	-2.31088700
F	-1.68126000	2.92299300	-2.49262200
F	-2.46107200	1.15776500	-3.45713600
F	-3.72461500	2.31869200	-2.13983700
H	-0.61072100	-1.37042300	-0.38918600
TS6 <sub>1</sub> <sup>(R,S,R)</sup>			
P	1.51240200	-1.08698600	0.16353000
C	-0.52386700	-0.47340000	0.52387500
C	-1.38075600	-1.14711200	-0.53352800
H	-1.56335400	-2.19912300	-0.30137500
C	-0.68862200	0.93112300	0.62495000
C	-1.40455900	1.71711400	-0.44155600
H	-1.90051800	2.56736300	0.04491700
C	-0.10888000	1.53095800	1.77217700
O	0.46633700	0.91640700	2.67945900
O	-0.18992300	2.89532800	1.79049500
C	0.58174600	3.55338300	2.79465100
C	0.76842100	4.98863600	2.34903000
H	0.06176900	3.49515300	3.75782300
H	1.54126900	3.03888200	2.89892500
H	1.32263900	5.55105200	3.10446600
H	-0.19743000	5.47617900	2.19250100
H	1.33026200	5.01978600	1.41078100
C	-0.48502100	2.26703600	-1.51987900
C	-0.14581100	1.51278700	-2.64585800
C	0.11815400	3.51378400	-1.33080800
C	0.82742800	1.97010000	-3.53344500
H	-0.65970500	0.57554800	-2.83649900

C	1.08060600	3.97629900	-2.22435900
H	-0.15267800	4.10396000	-0.45994600
C	1.45294600	3.19685600	-3.31968600
H	1.09526200	1.36475000	-4.39426800
H	1.54396500	4.94576000	-2.06442000
H	2.21064800	3.55209700	-4.01070700
C	2.63376700	0.26603600	0.59094500
C	3.56460800	0.15017200	1.63036900
C	2.48367500	1.48847200	-0.07370800
C	4.32972900	1.24904900	2.00200000
H	3.68631000	-0.79272000	2.15287300
C	3.25061500	2.58769000	0.30913400
H	1.78486600	1.58651500	-0.89651700
C	4.16756800	2.47198300	1.34936200
H	5.05344100	1.15143500	2.80438800
H	3.12401000	3.53043600	-0.21410600
H	4.76185900	3.32971600	1.64803900
C	1.86528700	-2.46213800	1.28810200
C	1.49453400	-2.27837900	2.62974200
C	2.45022000	-3.66600600	0.88201700
C	1.71221200	-3.29893700	3.55073600
H	1.06672300	-1.32725300	2.94516700
C	2.65589100	-4.68226600	1.81065800
H	2.74933000	-3.80886800	-0.15153800
C	2.28578100	-4.50127300	3.14188100
H	1.43221300	-3.15355800	4.58884200
H	3.11151400	-5.61450500	1.49340100
H	2.44852100	-5.29607800	3.86249700
C	1.85633500	-1.62223800	-1.53645500
C	1.17193400	-2.74507400	-2.02843000
C	2.69673800	-0.90323400	-2.39281100
C	1.33900300	-3.14671300	-3.34862500
H	0.51329800	-3.31315200	-1.37573000
C	2.85120400	-1.30465900	-3.71723900
H	3.23102400	-0.03103900	-2.03104300
C	2.17571500	-2.42334700	-4.19728400
H	0.81059200	-4.02047600	-3.71499600
H	3.50541100	-0.73920400	-4.37277200
H	2.29940300	-2.73230700	-5.22992100
H	-0.91501800	-1.11447900	-1.52188600
C	-2.69250400	-0.35313300	-0.64049700
O	-2.42678700	0.94692800	-1.11184600
C	-3.52553200	-0.34532100	0.63858400
C	-4.28686100	0.78448900	0.94404900

C	-3.58414900	-1.45551800	1.48302600
C	-5.07424200	0.81347700	2.09129700
H	-4.25059200	1.63985200	0.27758900
C	-4.37143600	-1.42537500	2.63157600
H	-3.01499600	-2.35137200	1.25575100
C	-5.11599900	-0.29016200	2.94049900
H	-5.65533400	1.70032700	2.32320200
H	-4.40054800	-2.29168200	3.28451800
H	-5.72656200	-0.26652100	3.83729800
C	-3.53346500	-0.95726600	-1.76899000
F	-2.85987700	-0.98380800	-2.92978100
F	-3.87458900	-2.22318800	-1.47926600
F	-4.65953700	-0.26902300	-1.97622900
H	-0.53908900	-0.98415000	1.48940300
TS3 <sub>1</sub> <sup>(R,S,S)</sup>			
P	0.52704100	1.43538300	-0.13084700
C	-0.13370500	-0.15002300	-0.63607700
C	0.76940000	-1.15335800	-1.32895100
H	1.64508700	-0.66614600	-1.76416200
C	-1.41285000	-0.51111800	-0.33176900
C	-1.89366600	-1.88306800	-0.54669200
H	-0.91124500	-2.42754800	0.09429000
C	-2.34077200	0.45394900	0.35792500
O	-2.14884400	0.93972400	1.45131300
O	-3.40145400	0.71091600	-0.39812000
C	-4.36441100	1.61823200	0.17195400
C	-5.45476000	1.80790800	-0.85628200
H	-4.74000100	1.17762300	1.10040400
H	-3.85222400	2.55510400	0.41554800
H	-6.21571800	2.48754900	-0.46686100
H	-5.92702800	0.85151500	-1.09265800
H	-5.04357600	2.23449500	-1.77449700
C	-3.25921100	-2.23371800	-0.07024400
C	-3.62386100	-2.04682400	1.27266800
C	-4.21115500	-2.79151400	-0.93278200
C	-4.90026400	-2.36974300	1.72372300
H	-2.89277000	-1.64537200	1.97089100
C	-5.48321300	-3.13173500	-0.48081100
H	-3.94911900	-2.95160900	-1.97552000
C	-5.83888000	-2.91441700	0.84881800
H	-5.15734600	-2.20886500	2.76656700
H	-6.20196800	-3.56104300	-1.17259000
H	-6.83193100	-3.17415100	1.20108400

C	-0.67239600	2.76829400	-0.42813600
C	-0.81144600	3.82184300	0.47925300
C	-1.44753000	2.73716100	-1.59346500
C	-1.70967400	4.84973900	0.21053800
H	-0.23888700	3.83367500	1.40040400
C	-2.33958000	3.77324000	-1.85774200
H	-1.37235400	1.89851200	-2.28027900
C	-2.46962000	4.82878400	-0.95766200
H	-1.82072500	5.66276700	0.91960500
H	-2.93649500	3.74967800	-2.76319900
H	-3.17052100	5.63131600	-1.16233800
C	1.04225800	1.41809100	1.60374800
C	0.64962300	0.35996100	2.42527100
C	1.85074800	2.44828800	2.10402000
C	1.04952600	0.34972000	3.75972600
H	0.08055300	-0.46820800	2.01007200
C	2.24167900	2.42830400	3.43724400
H	2.18448700	3.25390300	1.45484900
C	1.83586000	1.38056800	4.26489900
H	0.75488200	-0.47556300	4.39944000
H	2.86657400	3.22406900	3.82773300
H	2.14583200	1.36516500	5.30485900
C	2.01341000	1.82429400	-1.09270700
C	3.25832900	1.38555400	-0.62903300
C	1.91647200	2.50973200	-2.30907500
C	4.40058100	1.63643600	-1.38332400
H	3.33991800	0.84613400	0.31147600
C	3.06374900	2.75412600	-3.05576300
H	0.95570700	2.86279700	-2.66945100
C	4.30481000	2.31974800	-2.59257400
H	5.36239600	1.28979200	-1.02068700
H	2.98844000	3.28893700	-3.99631400
H	5.19843000	2.51728900	-3.17553200
H	0.20425900	-1.57067900	-2.17125100
C	1.22359600	-2.32502700	-0.36788900
O	0.32689200	-2.60949600	0.62221700
H	-1.70404300	-2.22689700	-1.56817300
C	2.62063300	-2.00384000	0.20452800
C	2.75964900	-1.87669000	1.58513600
C	3.74736000	-1.80787000	-0.60302100
C	3.98054100	-1.51306500	2.15110600
H	1.88598400	-2.06577400	2.19693800
C	4.97823000	-1.48468300	-0.03822300
H	3.66975300	-1.90081000	-1.68162900

C	5.09680300	-1.31779100	1.34085200
H	4.05919500	-1.39106300	3.22767400
H	5.84367900	-1.34766400	-0.68013500
H	6.05228000	-1.04572000	1.77875900
C	1.34243600	-3.57641200	-1.25671700
F	1.89487100	-4.60773400	-0.60412100
F	2.07758000	-3.38165500	-2.37706600
F	0.13176400	-3.98412000	-1.68111300
M3 <sub>1</sub> <sup>(R,S,S)</sup>			
P	-0.54739200	-1.29138100	-0.17499700
C	0.19051600	0.23179200	-0.54199400
C	-0.63969200	1.32771800	-1.16515100
H	-1.48244800	0.91913800	-1.72821400
C	1.55555400	0.53124800	-0.19719900
C	2.20524900	1.71326400	-0.45201700
H	0.47778500	2.34436000	0.80633200
C	2.33881400	-0.54857000	0.50215300
O	2.03533200	-1.02793800	1.57526000
O	3.39414500	-0.94179500	-0.20538200
C	4.18709800	-1.98270100	0.39137600
C	5.30954300	-2.29341200	-0.57113200
H	4.55942000	-1.62333700	1.35628800
H	3.54011000	-2.84811200	0.57160800
H	5.94873000	-3.07535600	-0.15506800
H	5.91722900	-1.40321700	-0.74994700
H	4.90791400	-2.64284500	-1.52518300
C	3.57606100	2.08390500	-0.07671200
C	4.22265800	1.62575100	1.08553600
C	4.27785900	2.98846300	-0.89177700
C	5.52561700	2.00930000	1.38276500
H	3.69112600	0.98488900	1.78362500
C	5.57653500	3.38201500	-0.58854500
H	3.79242800	3.37487600	-1.78436100
C	6.21499500	2.88581100	0.54645700
H	5.99752700	1.63574000	2.28675000
H	6.09329800	4.07687000	-1.24387400
H	7.22940900	3.18878100	0.78447600
C	0.57675200	-2.69768600	-0.50782300
C	0.62922600	-3.81791800	0.32720500
C	1.38476400	-2.64850900	-1.64954200
C	1.45997800	-4.88796500	0.00657900
H	0.03765000	-3.85206500	1.23528800
C	2.20880400	-3.72449200	-1.97018000

H	1.38282100	-1.75806900	-2.27218700
C	2.24515200	-4.84583300	-1.14405300
H	1.49689100	-5.75277800	0.66049200
H	2.82629900	-3.68220400	-2.86149400
H	2.89064500	-5.68214800	-1.39215600
C	-1.19999600	-1.53152800	1.51678500
C	-0.82574600	-0.63087700	2.51355700
C	-2.08735200	-2.57400800	1.81479200
C	-1.32680500	-0.77617300	3.80565600
H	-0.16071400	0.18991200	2.26246700
C	-2.58581600	-2.71538100	3.10549200
H	-2.39964300	-3.26745800	1.03775100
C	-2.20424700	-1.81610000	4.10111600
H	-1.03669900	-0.07153000	4.57843600
H	-3.27453100	-3.52231100	3.33269000
H	-2.59759500	-1.92537800	5.10675400
C	-2.00361500	-1.55469000	-1.24449300
C	-3.27958700	-1.19462800	-0.80115200
C	-1.84071900	-2.08387600	-2.53040500
C	-4.38114500	-1.37231300	-1.63496100
H	-3.41925100	-0.77138400	0.19017100
C	-2.94421700	-2.25724900	-3.35822100
H	-0.85672000	-2.37258200	-2.88488200
C	-4.21640300	-1.90495600	-2.90977600
H	-5.36611800	-1.08516100	-1.28167900
H	-2.81107400	-2.67458300	-4.35065400
H	-5.07719700	-2.04642800	-3.55543200
H	-0.02102500	1.85590000	-1.90223500
C	-1.21894800	2.37834200	-0.14854500
O	-0.45376700	2.50585100	1.02457100
H	1.68039400	2.47508200	-1.02112600
C	-2.64916000	2.03407700	0.25821400
C	-2.93425300	1.68520800	1.57833300
C	-3.68571100	2.03161600	-0.68128200
C	-4.22457500	1.30820800	1.94836000
H	-2.13891500	1.70397100	2.31172900
C	-4.97967300	1.68737500	-0.30415800
H	-3.48607800	2.28987700	-1.71583300
C	-5.25298400	1.31136300	1.00987400
H	-4.42275300	1.01978300	2.97623100
H	-5.77306300	1.69587100	-1.04521200
H	-6.25985800	1.02705900	1.29874300
C	-1.19365600	3.76158600	-0.81454300
F	-1.82223200	4.68800700	-0.08434300

F	0.07439100	4.18160900	-0.97956700
F	-1.75727400	3.75789100	-2.03658700
TS4 <sub>1</sub> <sup>(R,S,S)</sup>			
P	0.27095900	1.44288300	-0.10314300
C	0.07723400	-0.34534900	0.11005600
C	1.05771000	-1.22077000	-0.66996100
H	1.64589100	-0.68596900	-1.41628200
C	-1.37246100	-0.73318400	0.05893100
C	-1.97614800	-1.35478700	-0.96825700
H	0.71606500	-0.58273600	1.19166700
C	-2.18982200	-0.26361200	1.21961200
O	-2.07370100	0.84468100	1.70680900
O	-3.04552200	-1.17816900	1.66378400
C	-4.04717200	-0.72439200	2.59044600
C	-5.08842400	-1.81769600	2.67396800
H	-3.57311900	-0.52067000	3.55486100
H	-4.46739000	0.21226100	2.21095200
H	-5.88576600	-1.52018900	3.35870400
H	-4.64499100	-2.74686200	3.03850600
H	-5.52052000	-1.99734400	1.68538400
C	-3.43539600	-1.54408600	-1.12049300
C	-3.96649200	-2.77715500	-1.50875300
C	-4.30546900	-0.46350100	-0.91831500
C	-5.34256400	-2.94109000	-1.64500500
H	-3.29746400	-3.61458000	-1.68551400
C	-5.67927700	-0.62586500	-1.05878500
H	-3.89170600	0.51115400	-0.66153800
C	-6.20236700	-1.86863700	-1.41561900
H	-5.74395800	-3.90758200	-1.93279100
H	-6.34185700	0.21900600	-0.89823100
H	-7.27432700	-1.99704600	-1.52681800
C	-1.13022400	2.12911600	-1.02148300
C	-2.02978000	3.03301200	-0.45352800
C	-1.36254200	1.61924100	-2.30587400
C	-3.14250600	3.44679200	-1.18348700
H	-1.87227400	3.39461300	0.55734000
C	-2.47432200	2.03577100	-3.02853500
H	-0.67842000	0.89043700	-2.73562800
C	-3.36297800	2.95208300	-2.46662900
H	-3.84071900	4.15144400	-0.74461500
H	-2.65128100	1.63911500	-4.02233700
H	-4.23426000	3.27272400	-3.02840200
C	0.51308400	2.36363100	1.44126000



C	0.57305600	1.72904200	2.68245000
C	0.73722000	3.74188600	1.34323800
C	0.84139100	2.48036000	3.82390300
H	0.41524900	0.65965900	2.76116100
C	0.99029900	4.48738700	2.48919700
H	0.71844200	4.23290300	0.37275300
C	1.04360900	3.85478100	3.73003000
H	0.89301200	1.98723600	4.78875300
H	1.15482800	5.55671800	2.41166100
H	1.25082100	4.43385700	4.62408900
C	1.79418400	1.80544400	-1.02281400
C	2.98388100	1.32777800	-0.45798500
C	1.81871700	2.52126200	-2.22087600
C	4.19047100	1.53284200	-1.11541700
H	2.95426900	0.76444000	0.47398200
C	3.03734500	2.74436600	-2.86041000
H	0.90198700	2.90814200	-2.65370700
C	4.21671400	2.24393300	-2.31537700
H	5.10342300	1.12397900	-0.69330500
H	3.05988400	3.30564500	-3.78844500
H	5.16008700	2.40807500	-2.82611300
H	0.53940800	-2.02584400	-1.19444900
C	2.04523700	-1.82501200	0.44250900
O	1.86203300	-1.15067000	1.61182700
H	-1.36419400	-1.69018700	-1.80421500
C	3.49844300	-1.83183400	-0.03618900
C	4.50227700	-1.47822300	0.86585200
C	3.85412200	-2.18359100	-1.34059300
C	5.83691400	-1.45103700	0.46741200
H	4.20657100	-1.20719200	1.87392000
C	5.18739100	-2.15488400	-1.74295500
H	3.08560800	-2.47431200	-2.05171600
C	6.18326000	-1.78539700	-0.84084100
H	6.60792500	-1.16756000	1.17790000
H	5.44863700	-2.42025200	-2.76288100
H	7.22209700	-1.76090500	-1.15515200
C	1.60885700	-3.27781800	0.66300700
F	2.35133500	-3.89601000	1.59363200
F	0.32876500	-3.33862000	1.07318300
F	1.68549300	-4.03281700	-0.45724100
M4 <sub>1</sub> <sup>(R,S,S)</sup>			
P	0.20957900	1.42961500	-0.11138200
C	0.08306400	-0.38566300	0.36758700

C	1.14436900	-1.27787700	-0.29351300
H	1.47779300	-0.88388500	-1.25776300
C	-1.34819500	-0.84675400	0.22318500
C	-1.81531400	-1.51961900	-0.84102400
H	0.33166600	-0.33722400	1.42855800
C	-2.20877000	-0.40287700	1.35914500
O	-2.01708200	0.64536600	1.94572200
O	-3.15426200	-1.27450600	1.68990800
C	-4.11454400	-0.83162800	2.66615800
C	-5.16481400	-1.91393600	2.76978200
H	-3.59900500	-0.65569200	3.61417800
H	-4.53611900	0.11990000	2.32656100
H	-5.93276400	-1.61685000	3.48724700
H	-4.71885100	-2.85251500	3.10575800
H	-5.63570700	-2.07752100	1.79714200
C	-3.22375000	-1.81656200	-1.16109600
C	-3.56729800	-3.04412400	-1.73579000
C	-4.22328500	-0.85403500	-0.96430500
C	-4.89206500	-3.32574300	-2.05815300
H	-2.79366900	-3.78565600	-1.91422900
C	-5.54340100	-1.13015000	-1.29759100
H	-3.95238300	0.12440800	-0.57210200
C	-5.88276300	-2.37181000	-1.83593700
H	-5.14944300	-4.28803500	-2.48861800
H	-6.30680800	-0.37332500	-1.14707000
H	-6.91407300	-2.58841300	-2.09534200
C	-1.34715300	1.89600500	-0.92807400
C	-2.33369800	2.64776200	-0.28522600
C	-1.58951700	1.38688200	-2.21237200
C	-3.53083000	2.92794800	-0.94347500
H	-2.17685000	3.00315700	0.72694400
C	-2.78713000	1.66430600	-2.86043400
H	-0.84006200	0.77868200	-2.71298400
C	-3.75482500	2.44507800	-2.22944900
H	-4.28864900	3.52145200	-0.44345400
H	-2.96421300	1.26765000	-3.85416000
H	-4.68880400	2.66390300	-2.73665700
C	0.48674900	2.50152700	1.32251400
C	0.98909200	1.99985000	2.52623600
C	0.26208200	3.87475400	1.16245200
C	1.21580100	2.87964300	3.58213300
H	1.27225000	0.95388100	2.60431900
C	0.49317400	4.74091200	2.22510200
H	-0.09278500	4.27063100	0.21460800

C	0.95995900	4.24072100	3.43928800
H	1.60590900	2.49610600	4.51896100
H	0.31149700	5.80317600	2.10239700
H	1.13905900	4.91695800	4.26900600
C	1.53896500	1.81775700	-1.29900100
C	2.84606900	1.41765100	-0.98947600
C	1.29498500	2.60569000	-2.43119300
C	3.88688700	1.75516400	-1.84880000
H	3.02274500	0.85051100	-0.07104200
C	2.34978600	2.94965200	-3.27232800
H	0.29801900	2.96257800	-2.66142900
C	3.64212400	2.51422400	-2.99102200
H	4.89284100	1.41877800	-1.61666100
H	2.15499300	3.55875800	-4.14863800
H	4.45865000	2.77641200	-3.65627300
H	0.70451500	-2.26015500	-0.49099900
C	2.38040800	-1.40009400	0.67746600
O	2.55129200	-0.30290200	1.43657500
H	-1.09123100	-1.83306000	-1.59330300
C	3.63050300	-1.79558700	-0.14268800
C	4.84438400	-1.19467400	0.18890200
C	3.60011300	-2.71755100	-1.19295400
C	6.00526700	-1.49194400	-0.52172900
H	4.83756700	-0.48284600	1.00813700
C	4.75850400	-3.01699800	-1.90721400
H	2.66771100	-3.20746100	-1.45994700
C	5.96490400	-2.40349400	-1.57513000
H	6.94257800	-1.01259000	-0.25384800
H	4.71857100	-3.72970900	-2.72567600
H	6.86640000	-2.63604900	-2.13362200
C	2.07547600	-2.58988100	1.61227600
F	3.07083300	-2.80963000	2.48274400
F	0.95953500	-2.36970000	2.34213600
F	1.86335100	-3.76077900	0.96374000
M4 <sub>1</sub> <sup>r(R,S,S)</sup>			
P	1.91628200	-0.74033500	0.07154400
C	0.44101200	0.38581900	-0.03015800
C	0.57269500	1.64914400	0.82840500
H	1.46008900	2.19355500	0.47923000
C	-0.86689000	-0.35885600	0.08786700
C	-1.53242800	-0.38307800	1.25419900
H	0.51341000	0.69925100	-1.07403800
C	-1.35540900	-0.84414100	-1.23185000

O	-0.63279800	-0.90918300	-2.21247600
O	-2.64649900	-1.15567400	-1.26183100
C	-3.17890300	-1.54193400	-2.53804600
C	-4.64388700	-1.84763200	-2.32076700
H	-3.02688800	-0.71553200	-3.23992100
H	-2.62363800	-2.41016600	-2.90526700
H	-5.10514800	-2.15613300	-3.26153700
H	-5.16586400	-0.96342800	-1.94696200
H	-4.76213100	-2.65099200	-1.58959600
C	-2.85376200	-0.94889300	1.58418700
C	-3.75280300	-0.11487900	2.25958700
C	-3.20896900	-2.27431900	1.31624200
C	-5.00338200	-0.59704600	2.63474400
H	-3.44679800	0.91195300	2.44674300
C	-4.45219200	-2.75762500	1.71021600
H	-2.50907800	-2.91952200	0.79202300
C	-5.35380600	-1.91899500	2.36524700
H	-5.70405000	0.05778000	3.14344600
H	-4.71965800	-3.78949200	1.50417100
H	-6.32512600	-2.29711600	2.66826500
C	1.45984900	-2.42765400	-0.39892300
C	2.01687300	-3.00820300	-1.54124000
C	0.51655800	-3.13736600	0.35958200
C	1.62119700	-4.28424400	-1.93283200
H	2.75115600	-2.46870500	-2.12946800
C	0.12809800	-4.41134900	-0.04013600
H	0.08439600	-2.70328000	1.25572400
C	0.67435100	-4.98175500	-1.18911300
H	2.05352800	-4.72887400	-2.82239600
H	-0.60001300	-4.95864100	0.54931800
H	0.36452600	-5.97401300	-1.49958800
C	3.11908800	-0.10788000	-1.12284200
C	2.66407800	0.22144800	-2.40894100
C	4.47255800	0.01923100	-0.79859400
C	3.56754000	0.69260700	-3.35473700
H	1.61843700	0.08412200	-2.67742400
C	5.36657500	0.49669400	-1.75332700
H	4.83005900	-0.24870900	0.19015300
C	4.91467700	0.83685200	-3.02518700
H	3.21830300	0.94700700	-4.34944600
H	6.41584900	0.60176700	-1.50031700
H	5.61433300	1.21156300	-3.76487400
C	2.68335000	-0.76822000	1.71054500
C	3.21174800	0.42277300	2.23333800

C	2.79501200	-1.95614600	2.44026900
C	3.82334300	0.42192700	3.48024400
H	3.16318600	1.34597600	1.66538000
C	3.40742100	-1.94634100	3.69071900
H	2.41859300	-2.88939900	2.03776500
C	3.91611100	-0.76109000	4.21227300
H	4.22906100	1.34553600	3.87782400
H	3.48881100	-2.87058600	4.25207000
H	4.39337900	-0.75813300	5.18660400
H	0.71480100	1.42125300	1.88804400
C	-0.72090000	2.58337100	0.78422700
O	-1.61428400	2.29546300	1.72850000
H	-1.07059800	0.15847200	2.07390900
C	-1.29370700	2.57624500	-0.66305200
C	-2.62668600	2.19824900	-0.81331500
C	-0.54051400	2.84636200	-1.81269700
C	-3.19870000	2.07703000	-2.07835100
H	-3.17499800	1.97537800	0.09742100
C	-1.10931200	2.73149800	-3.07973200
H	0.50280000	3.13854400	-1.72366900
C	-2.44114200	2.34272600	-3.21773600
H	-4.23643700	1.76878700	-2.17696100
H	-0.50971800	2.94113300	-3.96090400
H	-2.88286100	2.24562400	-4.20513100
C	-0.17847200	4.00451600	1.06356400
F	-1.15343500	4.92541700	1.01746900
F	0.37457600	4.07736800	2.28988300
F	0.78675800	4.43522800	0.20702900
TS5 <sub>1</sub> <sup>(R,S,S)</sup>			
P	-2.07883700	0.50986100	0.02482600
C	-0.46219100	-0.41741800	-0.05512000
C	-0.36535500	-1.63736500	0.86834500
H	-1.09573400	-2.39344100	0.55664200
C	0.75838500	0.45726000	0.01960600
C	1.43348500	0.50466100	1.21021000
H	-0.51146500	-0.79056800	-1.08210200
C	1.25608500	0.83806500	-1.29877800
O	0.57010100	0.78185900	-2.31518100
O	2.53031100	1.25008900	-1.32711800
C	3.06839400	1.57237700	-2.61207000
C	4.52588600	1.91578700	-2.39259400
H	2.94499600	0.70925900	-3.27448600
H	2.50782600	2.40950100	-3.04078800

H	4.99848400	2.18514500	-3.33996300
H	5.05569100	1.05977600	-1.96663200
H	4.62007400	2.75514800	-1.69907600
C	2.69165200	1.25170300	1.48401200
C	3.77979500	0.62717100	2.09833400
C	2.76273800	2.62086200	1.20098300
C	4.92531300	1.35962000	2.40553200
H	3.70881000	-0.43500700	2.30159900
C	3.90213200	3.35140700	1.51998600
H	1.92435500	3.10598700	0.70864800
C	4.99101900	2.72112800	2.12142500
H	5.77038300	0.86188700	2.87154800
H	3.94287000	4.41248000	1.29298600
H	5.88313900	3.28896700	2.36643100
C	-1.80855800	2.22884200	-0.45421400
C	-2.40624400	2.75387600	-1.60275100
C	-0.96511100	3.03118700	0.32799300
C	-2.15559000	4.07296100	-1.97101200
H	-3.06001200	2.13950500	-2.21269500
C	-0.72501400	4.34893800	-0.04491100
H	-0.50340100	2.63275500	1.22570000
C	-1.31492700	4.86753600	-1.19668400
H	-2.61816000	4.47690200	-2.86479700
H	-0.07761800	4.96958800	0.56573800
H	-1.12119200	5.89498700	-1.48669000
C	-3.20052900	-0.26036200	-1.16526800
C	-2.70490800	-0.54021400	-2.44782700
C	-4.53023700	-0.54589200	-0.84241900
C	-3.54470200	-1.11725000	-3.39425900
H	-1.67918400	-0.28546000	-2.70956300
C	-5.35937100	-1.12741000	-1.79746600
H	-4.91743400	-0.32061500	0.14604300
C	-4.86725900	-1.41537800	-3.06755800
H	-3.16524600	-1.33299000	-4.38711400
H	-6.38994500	-1.35440900	-1.54704400
H	-5.51726600	-1.86965500	-3.80808100
C	-2.85156000	0.46311500	1.66099900
C	-3.20187100	-0.78238300	2.20417100
C	-3.12603500	1.63446000	2.37371900
C	-3.80185700	-0.84909700	3.45561600
H	-3.02113000	-1.69726300	1.64798000
C	-3.72427900	1.55755100	3.62874200
H	-2.88609900	2.60503800	1.95431200
C	-4.05669100	0.32015000	4.17098400

H	-4.07048500	-1.81426400	3.87072700
H	-3.93401200	2.46899000	4.17765000
H	-4.52211800	0.26366400	5.14940100
H	-0.56873400	-1.38795800	1.91357400
C	1.10066100	-2.22687900	0.85029900
O	1.95506900	-1.52910600	1.63298500
H	0.85466100	0.28578500	2.10260000
C	1.59622900	-2.38971600	-0.60726500
C	2.86046900	-1.89325500	-0.92174500
C	0.83069600	-2.97586200	-1.62183700
C	3.35151200	-1.97061700	-2.22307400
H	3.42267200	-1.41726400	-0.12446700
C	1.31977600	-3.05514600	-2.92447100
H	-0.15831200	-3.36927600	-1.40081100
C	2.58288100	-2.55199600	-3.22989200
H	4.33626700	-1.57245400	-2.45368200
H	0.71114200	-3.50728200	-3.70193800
H	2.96296300	-2.61026000	-4.24526900
C	0.98770200	-3.63471000	1.46035900
F	2.17257800	-4.26034400	1.48780500
F	0.53446500	-3.58672900	2.72585000
F	0.13704600	-4.45116100	0.79247100
M5 <sub>1</sub> <sup>(R,S,S)</sup>			
P	2.03603100	0.50567900	-0.09252800
C	0.39168300	-0.46964700	0.17822600
C	0.29573100	-1.71375500	-0.70821400
H	1.02402000	-2.47794000	-0.42475900
C	-0.82473900	0.36239900	0.06176600
C	-1.71923900	-0.00054200	-1.07504300
H	0.54777900	-0.77748700	1.22067800
C	-1.06440800	1.16736000	1.18228400
O	-0.23035900	1.34421900	2.09612400
O	-2.28038400	1.79085000	1.24472800
C	-2.43999600	2.74635600	2.28545400
C	-3.82824300	3.33413100	2.12938900
H	-2.31350800	2.26455700	3.26080800
H	-1.66543200	3.51789300	2.20121500
H	-4.01023400	4.09440900	2.89310800
H	-4.58619400	2.55219000	2.22643400
H	-3.93748500	3.78909600	1.14126400
C	-2.98635800	0.81027000	-1.23987500
C	-4.24225700	0.29053300	-0.93605200
C	-2.89319900	2.11861300	-1.71926400

C	-5.38438900	1.07878000	-1.07996500
H	-4.32367400	-0.73440300	-0.59197200
C	-4.02862900	2.90481500	-1.86686600
H	-1.91552300	2.52691800	-1.96052600
C	-5.28314600	2.38760100	-1.54005100
H	-6.35730700	0.66308500	-0.83518700
H	-3.93775700	3.92176200	-2.23667800
H	-6.17305100	2.99911400	-1.65227600
C	1.68228700	2.27007200	-0.12628500
C	2.24621000	3.14432300	0.80612700
C	0.77261300	2.74517400	-1.07834200
C	1.90311500	4.49160900	0.78214900
H	2.94003200	2.77291600	1.55327500
C	0.43594900	4.09658700	-1.09753800
H	0.34456100	2.06643100	-1.81016700
C	0.99595800	4.96562400	-0.16479900
H	2.34053000	5.17114700	1.50550000
H	-0.26329300	4.46929600	-1.83902900
H	0.72855200	6.01729600	-0.17820000
C	3.18473400	0.15402500	1.26033300
C	2.67857800	0.20863000	2.56765800
C	4.53363600	-0.14370000	1.03623400
C	3.52863200	-0.04552600	3.64001700
H	1.63562900	0.47423600	2.72885600
C	5.37108700	-0.39770500	2.11806800
H	4.93123400	-0.17621700	0.02710000
C	4.86921700	-0.35240700	3.41719500
H	3.14078200	-0.00202700	4.65219900
H	6.41656400	-0.62861300	1.94386000
H	5.52625000	-0.55308300	4.25729400
C	2.86485700	0.06068600	-1.64564800
C	3.30705900	-1.26019100	-1.81422700
C	3.07279600	0.99234500	-2.66717500
C	3.93843600	-1.64099700	-2.99188800
H	3.17666400	-1.98861400	-1.01898700
C	3.70149400	0.60241800	-3.84748500
H	2.75551300	2.02188900	-2.54407200
C	4.13096000	-0.71061600	-4.01257000
H	4.28057400	-2.66314900	-3.11183600
H	3.85850600	1.33196400	-4.63455400
H	4.62136500	-1.01023600	-4.93283100
H	0.45511400	-1.48072400	-1.76612800
C	-1.12817400	-2.29077200	-0.54776200
O	-2.11888800	-1.40310400	-1.01153700



H	-1.16536000	0.09186500	-2.02761900
C	-1.39265400	-2.71156400	0.90210200
C	-2.39032900	-2.06656400	1.63442200
C	-0.61954600	-3.69393500	1.52977700
C	-2.61955300	-2.40431400	2.96584700
H	-2.96740600	-1.28048100	1.16182300
C	-0.85395500	-4.03397000	2.85985400
H	0.16778200	-4.20428500	0.98543900
C	-1.85596100	-3.39116200	3.58254000
H	-3.39615800	-1.88882000	3.52198500
H	-0.24762300	-4.80100100	3.33113400
H	-2.03547700	-3.65354000	4.62028100
C	-1.27470200	-3.48967700	-1.49199300
F	-2.47897200	-4.05872100	-1.38295600
F	-1.11738300	-3.11657500	-2.76974600
F	-0.35394700	-4.44228000	-1.25223300
TS6 <sub>1</sub> <sup>(R,S,S)</sup>			
P	-2.09137500	0.31576000	0.10069800
C	-0.20778100	-0.59524400	-0.42396700
C	-0.02166300	-1.78875000	0.49750200
H	-0.68422100	-2.61651400	0.23624600
C	0.85659600	0.35088400	-0.34490900
C	1.81769200	0.10343400	0.77936200
H	-0.53659000	-0.85130800	-1.43348300
C	0.82445200	1.38405600	-1.32004200
O	-0.05119400	1.46273200	-2.19485400
O	1.78128000	2.34043700	-1.21404000
C	1.60685800	3.49601900	-2.03031600
C	2.53575600	4.56022800	-1.48476000
H	1.83902500	3.25190700	-3.07347400
H	0.56045700	3.81412000	-1.98717200
H	2.46793600	5.47059500	-2.08578600
H	3.57122500	4.20928500	-1.49170200
H	2.26577900	4.79654400	-0.45149600
C	2.98156200	1.05462000	0.91613600
C	4.16718300	0.86171900	0.20907500
C	2.86596300	2.15855900	1.75987200
C	5.20804400	1.78020400	0.31931200
H	4.27533800	-0.01487200	-0.42071500
C	3.89987300	3.08394800	1.86527500
H	1.95823400	2.29373300	2.34303300
C	5.07469800	2.89924100	1.13909000
H	6.12824000	1.62021600	-0.23431700

H	3.79371000	3.94159000	2.52277100
H	5.88629600	3.61516600	1.22309500
C	-1.78419000	2.08688000	0.23082100
C	-2.44603800	3.02028200	-0.57418900
C	-0.75086800	2.50687200	1.07721400
C	-2.08062200	4.35967300	-0.52542700
H	-3.23680600	2.69698900	-1.24375700
C	-0.38113500	3.85076900	1.11378900
H	-0.24435900	1.78999800	1.71704800
C	-1.04181600	4.77437600	0.31059600
H	-2.60136800	5.08188400	-1.14536500
H	0.42576900	4.17099300	1.76552900
H	-0.75054900	5.81979500	0.33510400
C	-3.36008000	0.03125300	-1.16227000
C	-2.98146700	0.20350300	-2.50196500
C	-4.66277100	-0.37189500	-0.84678900
C	-3.91224700	-0.02106700	-3.51308600
H	-1.97006900	0.53027900	-2.73488500
C	-5.58123800	-0.59985000	-1.86669400
H	-4.96055800	-0.50340000	0.18853000
C	-5.20737600	-0.42592700	-3.19799300
H	-3.62200100	0.11725200	-4.54937500
H	-6.59168900	-0.90859700	-1.61997700
H	-5.92792400	-0.60436800	-3.98957500
C	-2.77092600	-0.25504400	1.68719400
C	-3.08912400	-1.61511500	1.82123600
C	-2.95136500	0.60279000	2.77687500
C	-3.58532600	-2.10373400	3.02427300
H	-2.96537600	-2.29218600	0.97942300
C	-3.44033500	0.10522700	3.98257300
H	-2.71909800	1.65858200	2.68426200
C	-3.75665300	-1.24438100	4.10875200
H	-3.83411200	-3.15564500	3.11548100
H	-3.57916200	0.77890600	4.82156100
H	-4.13844300	-1.62757800	5.04921900
H	-0.22520100	-1.52191500	1.54039400
C	1.44671500	-2.26576000	0.39877600
O	2.37784300	-1.23280000	0.64418700
H	1.28636800	0.11067200	1.74827400
C	1.70702100	-2.91535700	-0.96126000
C	2.53101500	-2.27710700	-1.88767500
C	1.07992500	-4.11259000	-1.32368000
C	2.73670300	-2.83034300	-3.15006500
H	2.99335800	-1.33563500	-1.61785900

C	1.29122700	-4.66660300	-2.58273800
H	0.42531400	-4.62290500	-0.62572200
C	2.12171800	-4.02819400	-3.50068700
H	3.37835800	-2.31900800	-3.86062000
H	0.80027800	-5.59795000	-2.84637900
H	2.28261700	-4.45977400	-4.48337400
C	1.70445800	-3.24982500	1.54824900
F	2.92005900	-3.79835500	1.47288900
F	1.61533300	-2.62325000	2.73079700
F	0.80791600	-4.25424900	1.57714600
$P_1^{(R,R)}$			
C	0.12390900	-1.58306400	-1.56714100
C	1.06229600	-1.02160600	-0.80494600
C	0.72826700	-0.00205500	0.26080600
H	0.90586600	-0.43892800	1.25305300
C	2.47211800	-1.46919000	-0.98006900
O	2.89204200	-2.08184200	-1.93735000
O	3.22297400	-1.13651800	0.07387600
C	4.61771700	-1.47980400	-0.00139300
C	5.29106300	-0.85333900	1.19881700
H	5.01912800	-1.09984000	-0.94446400
H	4.71042500	-2.56974000	-0.00864800
H	6.35954600	-1.07886200	1.18429800
H	5.15969200	0.23134700	1.18186200
H	4.86609000	-1.24295500	2.12678600
C	-1.33681700	-1.30334000	-1.40607400
C	-1.63796100	-0.52635300	-0.11600200
H	-1.89255300	-2.24711700	-1.42078000
H	-1.69688300	-0.71974300	-2.26108700
O	-0.63159000	0.42714900	0.15217200
C	1.55653200	1.26083100	0.12377900
C	2.41569800	1.66730300	1.14126600
C	1.45036000	2.02682800	-1.03752700
C	3.17001600	2.83012200	0.99954900
H	2.50182600	1.06451900	2.04154900
C	2.20067600	3.18981400	-1.18038800
H	0.77258000	1.70525800	-1.82408500
C	3.06335400	3.59236700	-0.16147300
H	3.83846500	3.14065100	1.79641900
H	2.11513100	3.78166100	-2.08613500
H	3.64974400	4.49896500	-0.27232100
H	0.42814500	-2.29520800	-2.32980400
C	-2.95517400	0.24000600	-0.19055100

C	-4.05656200	-0.30836800	-0.85156100
C	-3.08252300	1.47631200	0.44406700
C	-5.26522100	0.37963400	-0.89384500
H	-3.97901300	-1.27687800	-1.33558000
C	-4.29203200	2.16463800	0.39671000
H	-2.22892200	1.89868000	0.96044700
C	-5.38530700	1.62001200	-0.27166400
H	-6.11246900	-0.05559600	-1.41355300
H	-4.37896100	3.13007000	0.88476300
H	-6.32676600	2.15860100	-0.30740300
C	-1.74132700	-1.49361200	1.07811600
F	-1.84406600	-0.81951100	2.22748900
F	-0.67227000	-2.30119600	1.18454500
F	-2.81399400	-2.29018300	0.96377200
P <sub>1</sub> <sup>(R,S)</sup>			
C	-0.29387000	0.32578400	-2.16077200
C	-1.54015400	-0.47044800	-1.92840800
H	-2.39673200	-0.02503100	-2.43741900
C	0.64185600	0.45854700	-1.21814100
C	0.53340700	-0.21807800	0.13312300
H	0.42615900	0.55695600	0.90547400
C	1.79965300	1.35500300	-1.49377200
O	2.10679200	1.77509900	-2.58787400
O	2.45440800	1.66497600	-0.37108300
C	3.61994100	2.49457900	-0.51933500
C	4.28748900	2.56404200	0.83563900
H	3.30493100	3.47844700	-0.87896800
H	4.27006000	2.04969700	-1.27730400
H	5.17982900	3.19109900	0.77878600
H	3.60868000	2.99104200	1.57762900
H	4.58158400	1.56455300	1.16499700
C	1.74588500	-1.06695000	0.45967600
C	2.05042000	-2.17999200	-0.32518200
C	2.55961800	-0.74522600	1.54325200
C	3.16332500	-2.96154800	-0.02767300
H	1.40805400	-2.43169800	-1.16500400
C	3.67541700	-1.52381800	1.84091900
H	2.32308200	0.12657200	2.14726000
C	3.97850200	-2.63325700	1.05502100
H	3.39631900	-3.82656500	-0.64034000
H	4.30464700	-1.26534300	2.68670000
H	4.84675300	-3.24212600	1.28582500
H	-1.41853000	-1.47615900	-2.34600400

C	-1.77511600	-0.60185000	-0.42086700
O	-0.59026100	-1.09911300	0.17828400
C	-2.25489300	0.67114200	0.27468800
C	-2.10540100	0.75450100	1.66365300
C	-2.84183800	1.73565800	-0.40893600
C	-2.53336400	1.88245600	2.35451800
H	-1.64475300	-0.07224700	2.19523800
C	-3.27240100	2.86548800	0.28436500
H	-2.96571700	1.70315400	-1.48585900
C	-3.11939600	2.94224000	1.66520200
H	-2.40776000	1.93402600	3.43113100
H	-3.72582100	3.68739600	-0.25986700
H	-3.45203300	3.82443500	2.20259700
C	-2.79617800	-1.71829400	-0.18000600
F	-2.39578700	-2.87744500	-0.71812500
F	-3.96829700	-1.39367200	-0.74450500
F	-3.01275300	-1.94006400	1.11975500
H	-0.15213600	0.82484300	-3.11541100
TS2 <sub>1</sub> <sup>(S,R)</sup>			
P	0.14962400	-1.32076000	-0.41324300
C	-0.39471800	0.36554100	0.03680600
C	0.27492800	1.41611900	-0.61193400
H	0.96606200	1.21223600	-1.42066200
C	-1.42203800	0.56042900	0.95580200
C	-2.03948500	1.93407900	1.10414200
H	-2.65993000	1.94287400	2.00287400
H	-1.25261800	2.67265700	1.25843100
C	-2.02606000	-0.56107200	1.65329000
O	-1.58529900	-1.70692000	1.67515300
O	-3.16845800	-0.24864600	2.30086400
C	-3.81009900	-1.33251000	2.98611500
C	-5.07259800	-0.78081900	3.61029100
H	-3.12340300	-1.73572100	3.73620200
H	-4.02112600	-2.12913400	2.26628300
H	-5.60032600	-1.57448900	4.14379600
H	-4.83530400	0.01610900	4.31870000
H	-5.73672700	-0.37735900	2.84227300
C	-2.89068400	2.32704000	-0.09028600
C	-2.65801100	3.52099400	-0.77554700
C	-3.92712700	1.49484400	-0.53002100
C	-3.43551600	3.87747500	-1.87735500
H	-1.85373400	4.17296600	-0.44242800
C	-4.70572500	1.84703400	-1.62874400

H	-4.12026400	0.56476900	0.00029500
C	-4.46045100	3.04073400	-2.30831500
H	-3.23536600	4.80772100	-2.40016100
H	-5.50838000	1.19172500	-1.95442600
H	-5.06529500	3.31466900	-3.16686400
C	-1.29645900	-2.26114100	-0.97475100
C	-1.35795500	-3.64698300	-0.82909200
C	-2.33963600	-1.56421500	-1.59206500
C	-2.46826200	-4.33730300	-1.30572900
H	-0.55989500	-4.18385800	-0.32576700
C	-3.44746100	-2.26388400	-2.06303400
H	-2.29633500	-0.48278800	-1.69596600
C	-3.51207300	-3.64803900	-1.92036700
H	-2.52196600	-5.41422800	-1.18692200
H	-4.25973400	-1.72270500	-2.53752700
H	-4.37832900	-4.19064500	-2.28454700
C	1.14113900	-2.17518900	0.83478200
C	1.19629200	-1.68460800	2.14112900
C	1.88864800	-3.29988000	0.46728600
C	1.98977300	-2.33315700	3.08179100
H	0.64523000	-0.78569300	2.40373200
C	2.67052500	-3.94860300	1.41809100
H	1.87508800	-3.66104300	-0.55748700
C	2.71914800	-3.46538000	2.72415800
H	2.04305500	-1.94805900	4.09482600
H	3.24564000	-4.82368500	1.13594200
H	3.33388500	-3.96838200	3.46365800
C	1.23376900	-1.22241500	-1.87240500
C	2.60886100	-1.02791300	-1.70334800
C	0.69585800	-1.31210000	-3.16146800
C	3.43574300	-0.92989100	-2.81847700
H	3.03736400	-0.95100600	-0.70749300
C	1.52955000	-1.21178900	-4.27045500
H	-0.36807200	-1.46750800	-3.30541700
C	2.89919200	-1.02340100	-4.10015500
H	4.50082000	-0.77923300	-2.67732800
H	1.10757100	-1.28729900	-5.26682600
H	3.54839700	-0.95193300	-4.96675300
H	-0.26467300	2.35180100	-0.70078200
C	1.54974000	2.17903600	1.04283000
O	0.96082300	1.92091900	2.10426500
C	2.86576600	1.51572400	0.70592200
C	3.35370800	0.58177200	1.62266200
C	3.64107400	1.83023900	-0.41732400

C	4.56564200	-0.06771700	1.40344200
H	2.76798100	0.38572300	2.51230100
C	4.87126000	1.21102200	-0.61531700
H	3.28959300	2.55376900	-1.14318400
C	5.33214200	0.24867600	0.28267300
H	4.91763800	-0.80658900	2.11723200
H	5.46605900	1.47157100	-1.48539200
H	6.28543200	-0.24240800	0.11470300
C	1.45487500	3.65149900	0.57694900
F	0.29558600	4.21375000	0.94458100
F	1.57940800	3.86124800	-0.74692300
F	2.43735300	4.35703200	1.16670200
M2 <sub>1</sub> <sup>(S,R)</sup>			
P	-0.05748600	-1.32669000	0.36018200
C	0.32843100	0.36855600	-0.18716200
C	-0.54622700	1.48388000	0.28537100
H	-1.04055100	1.24973800	1.23036700
C	1.36577100	0.59839900	-1.02186300
C	1.82348300	2.00064600	-1.37776400
H	2.49582300	1.93999300	-2.23896600
H	0.93887200	2.55946700	-1.69019700
C	2.14672100	-0.53161500	-1.61887200
O	1.65750800	-1.55310500	-2.04997400
O	3.45845600	-0.29683400	-1.60719900
C	4.29840800	-1.39811900	-2.01086600
C	5.71907300	-1.02265400	-1.65932800
H	4.16154300	-1.56443400	-3.08279500
H	3.96425600	-2.29342500	-1.47680300
H	6.39675600	-1.82281800	-1.96470900
H	6.01474900	-0.10246200	-2.16783300
H	5.81879500	-0.87692800	-0.58037800
C	2.54193600	2.70909400	-0.23808000
C	2.18176700	4.01212700	0.11530900
C	3.58325900	2.08978900	0.46369200
C	2.84539500	4.68239800	1.14242300
H	1.36678500	4.49898000	-0.41066400
C	4.24377000	2.75687000	1.49165100
H	3.88430800	1.08227300	0.19223600
C	3.87745100	4.05697500	1.83544000
H	2.54882500	5.69369500	1.40277200
H	5.05071200	2.26063100	2.02243200
H	4.39252600	4.57667500	2.63693500
C	1.50346700	-2.18508100	0.72884300

C	1.66322400	-3.53953800	0.43017100
C	2.55514700	-1.46286600	1.30624200
C	2.86921600	-4.17143100	0.71949300
H	0.86479600	-4.09437900	-0.05095600
C	3.75953300	-2.10219000	1.58869100
H	2.44814200	-0.40175700	1.51723600
C	3.91671700	-3.45525900	1.29590300
H	2.99372800	-5.22220600	0.48147900
H	4.57299200	-1.53906200	2.03466000
H	4.85767200	-3.95055200	1.51131200
C	-1.07347100	-2.22869400	-0.82378900
C	-1.29086200	-1.68414200	-2.09126500
C	-1.65530200	-3.44866900	-0.45262100
C	-2.07515900	-2.39051800	-3.00043400
H	-0.90634200	-0.69337800	-2.33351200
C	-2.43227500	-4.14265300	-1.37203200
H	-1.51653300	-3.84810000	0.54876600
C	-2.63500600	-3.61487200	-2.64789700
H	-2.25797400	-1.97104800	-3.98440700
H	-2.88275100	-5.08856300	-1.09171100
H	-3.24391000	-4.15797500	-3.36359800
C	-0.99413800	-1.27050500	1.91110700
C	-2.39148000	-1.31169500	1.87282000
C	-0.32583200	-1.16840200	3.13783400
C	-3.11290800	-1.26224100	3.06256700
H	-2.91772100	-1.37777100	0.92387900
C	-1.05614800	-1.11162800	4.31885600
H	0.75806700	-1.14431200	3.17692300
C	-2.44915000	-1.16392100	4.28142400
H	-4.19663900	-1.29356800	3.02662700
H	-0.53729000	-1.03426700	5.26808200
H	-3.01644300	-1.12790100	5.20569300
H	0.08236800	2.36235600	0.45778300
C	-1.63772700	1.84955400	-0.87424400
O	-1.23910300	1.56190400	-2.09930800
C	-2.99533300	1.20661100	-0.46354000
C	-3.60131100	0.35905800	-1.38818800
C	-3.64100800	1.43269200	0.75796400
C	-4.79354600	-0.29797600	-1.08967300
H	-3.09902400	0.23555500	-2.34038500
C	-4.85260300	0.80920200	1.04709400
H	-3.19852100	2.09647300	1.49481500
C	-5.42572900	-0.07365000	0.13226500
H	-5.23522800	-0.97525300	-1.81544400



H	-5.34193200	0.99954000	1.99817400
H	-6.36026700	-0.57425800	0.36696000
C	-1.82145300	3.38105300	-0.74903100
F	-0.73501300	4.04546400	-1.19966200
F	-2.01687200	3.82597800	0.51752400
F	-2.86031600	3.82324200	-1.47416300
TS3 <sub>1</sub> <sup>(S,R,R)</sup>			
P	0.52704100	1.43538300	0.13084700
C	-0.13370500	-0.15002300	0.63607700
C	0.76940000	-1.15335800	1.32895100
H	1.64508700	-0.66614600	1.76416200
C	-1.41285000	-0.51111800	0.33176900
C	-1.89366600	-1.88306800	0.54669200
H	-0.91124500	-2.42754800	-0.09429000
C	-2.34077200	0.45394900	-0.35792500
O	-2.14884400	0.93972400	-1.45131300
O	-3.40145400	0.71091600	0.39812000
C	-4.36441100	1.61823200	-0.17195400
C	-5.45476000	1.80790800	0.85628200
H	-4.74000100	1.17762300	-1.10040400
H	-3.85222400	2.55510400	-0.41554800
H	-6.21571800	2.48754900	0.46686100
H	-5.92702800	0.85151500	1.09265800
H	-5.04357600	2.23449500	1.77449700
C	-3.25921100	-2.23371800	0.07024400
C	-3.62386100	-2.04682400	-1.27266800
C	-4.21115500	-2.79151400	0.93278200
C	-4.90026400	-2.36974300	-1.72372300
H	-2.89277000	-1.64537200	-1.97089100
C	-5.48321300	-3.13173500	0.48081100
H	-3.94911900	-2.95160900	1.97552000
C	-5.83888000	-2.91441700	-0.84881800
H	-5.15734600	-2.20886500	-2.76656700
H	-6.20196800	-3.56104300	1.17259000
H	-6.83193100	-3.17415100	-1.20108400
C	-0.67239600	2.76829400	0.42813600
C	-0.81144600	3.82184300	-0.47925300
C	-1.44753000	2.73716100	1.59346500
C	-1.70967400	4.84973900	-0.21053800
H	-0.23888700	3.83367500	-1.40040400
C	-2.33958000	3.77324000	1.85774200
H	-1.37235400	1.89851200	2.28027900

C	-2.46962000	4.82878400	0.95766200
H	-1.82072500	5.66276700	-0.91960500
H	-2.93649500	3.74967800	2.76319900
H	-3.17052100	5.63131600	1.16233800
C	1.04225800	1.41809100	-1.60374800
C	0.64962300	0.35996100	-2.42527100
C	1.85074800	2.44828800	-2.10402000
C	1.04952600	0.34972000	-3.75972600
H	0.08055300	-0.46820800	-2.01007200
C	2.24167900	2.42830400	-3.43724400
H	2.18448700	3.25390300	-1.45484900
C	1.83586000	1.38056800	-4.26489900
H	0.75488200	-0.47556300	-4.39944000
H	2.86657400	3.22406900	-3.82773300
H	2.14583200	1.36516500	-5.30485900
C	2.01341000	1.82429400	1.09270700
C	3.25832900	1.38555400	0.62903300
C	1.91647200	2.50973200	2.30907500
C	4.40058100	1.63643600	1.38332400
H	3.33991800	0.84613400	-0.31147600
C	3.06374900	2.75412600	3.05576300
H	0.95570700	2.86279700	2.66945100
C	4.30481000	2.31974800	2.59257400
H	5.36239600	1.28979200	1.02068700
H	2.98844000	3.28893700	3.99631400
H	5.19843000	2.51728900	3.17553200
H	0.20425900	-1.57067900	2.17125100
C	1.22359600	-2.32502700	0.36788900
O	0.32689200	-2.60949600	-0.62221700
H	-1.70404300	-2.22689700	1.56817300
C	2.62063300	-2.00384000	-0.20452800
C	2.75964900	-1.87669000	-1.58513600
C	3.74736000	-1.80787000	0.60302100
C	3.98054100	-1.51306500	-2.15110600
H	1.88598400	-2.06577400	-2.19693800
C	4.97823000	-1.48468300	0.03822300
H	3.66975300	-1.90081000	1.68162900
C	5.09680300	-1.31779100	-1.34085200
H	4.05919500	-1.39106300	-3.22767400
H	5.84367900	-1.34766400	0.68013500
H	6.05228000	-1.04572000	-1.77875900
C	1.34243600	-3.57641200	1.25671700
F	1.89487100	-4.60773400	0.60412100
F	2.07758000	-3.38165500	2.37706600

F	0.13176400	-3.98412000	1.68111300
M3 <sub>1</sub> (S,R,R)			
P	-0.54739200	-1.29138100	0.17499700
C	0.19051600	0.23179200	0.54199400
C	-0.63969200	1.32771800	1.16515100
H	-1.48244800	0.91913800	1.72821400
C	1.55555400	0.53124800	0.19719900
C	2.20524900	1.71326400	0.45201700
H	0.47778500	2.34436000	-0.80633200
C	2.33881400	-0.54857000	-0.50215300
O	2.03533200	-1.02793800	-1.57526000
O	3.39414500	-0.94179500	0.20538200
C	4.18709800	-1.98270100	-0.39137600
C	5.30954300	-2.29341200	0.57113200
H	4.55942000	-1.62333700	-1.35628800
H	3.54011000	-2.84811200	-0.57160800
H	5.94873000	-3.07535600	0.15506800
H	5.91722900	-1.40321700	0.74994700
H	4.90791400	-2.64284500	1.52518300
C	3.57606100	2.08390500	0.07671200
C	4.22265800	1.62575100	-1.08553600
C	4.27785900	2.98846300	0.89177700
C	5.52561700	2.00930000	-1.38276500
H	3.69112600	0.98488900	-1.78362500
C	5.57653500	3.38201500	0.58854500
H	3.79242800	3.37487600	1.78436100
C	6.21499500	2.88581100	-0.54645700
H	5.99752700	1.63574000	-2.28675000
H	6.09329800	4.07687000	1.24387400
H	7.22940900	3.18878100	-0.78447600
C	0.57675200	-2.69768600	0.50782300
C	0.62922600	-3.81791800	-0.32720500
C	1.38476400	-2.64850900	1.64954200
C	1.45997800	-4.88796500	-0.00657900
H	0.03765000	-3.85206500	-1.23528800
C	2.20880400	-3.72449200	1.97018000
H	1.38282100	-1.75806900	2.27218700
C	2.24515200	-4.84583300	1.14405300
H	1.49689100	-5.75277800	-0.66049200
H	2.82629900	-3.68220400	2.86149400
H	2.89064500	-5.68214800	1.39215600
C	-1.19999600	-1.53152800	-1.51678500

C	-0.82574600	-0.63087700	-2.51355700
C	-2.08735200	-2.57400800	-1.81479200
C	-1.32680500	-0.77617300	-3.80565600
H	-0.16071400	0.18991200	-2.26246700
C	-2.58581600	-2.71538100	-3.10549200
H	-2.39964300	-3.26745800	-1.03775100
C	-2.20424700	-1.81610000	-4.10111600
H	-1.03669900	-0.07153000	-4.57843600
H	-3.27453100	-3.52231100	-3.33269000
H	-2.59759500	-1.92537800	-5.10675400
C	-2.00361500	-1.55469000	1.24449300
C	-3.27958700	-1.19462800	0.80115200
C	-1.84071900	-2.08387600	2.53040500
C	-4.38114500	-1.37231300	1.63496100
H	-3.41925100	-0.77138400	-0.19017100
C	-2.94421700	-2.25724900	3.35822100
H	-0.85672000	-2.37258200	2.88488200
C	-4.21640300	-1.90495600	2.90977600
H	-5.36611800	-1.08516100	1.28167900
H	-2.81107400	-2.67458300	4.35065400
H	-5.07719700	-2.04642800	3.55543200
H	-0.02102500	1.85590000	1.90223500
C	-1.21894800	2.37834200	0.14854500
O	-0.45376700	2.50585100	-1.02457100
H	1.68039400	2.47508200	1.02112600
C	-2.64916000	2.03407700	-0.25821400
C	-2.93425300	1.68520800	-1.57833300
C	-3.68571100	2.03161600	0.68128200
C	-4.22457500	1.30820800	-1.94836000
H	-2.13891500	1.70397100	-2.31172900
C	-4.97967300	1.68737500	0.30415800
H	-3.48607800	2.28987700	1.71583300
C	-5.25298400	1.31136300	-1.00987400
H	-4.42275300	1.01978300	-2.97623100
H	-5.77306300	1.69587100	1.04521200
H	-6.25985800	1.02705900	-1.29874300
C	-1.19365600	3.76158600	0.81454300
F	-1.82223200	4.68800700	0.08434300
F	0.07439100	4.18160900	0.97956700
F	-1.75727400	3.75789100	2.03658700
TS4 <sub>1</sub> <sup>(S,R,R)</sup>			
P	0.27095900	1.44288300	0.10314300

C	0.07723400	-0.34534900	-0.11005600
C	1.05771000	-1.22077000	0.66996100
H	1.64589100	-0.68596900	1.41628200
C	-1.37246100	-0.73318400	-0.05893100
C	-1.97614800	-1.35478700	0.96825700
H	0.71606500	-0.58273600	-1.19166700
C	-2.18982200	-0.26361200	-1.21961200
O	-2.07370100	0.84468100	-1.70680900
O	-3.04552200	-1.17816900	-1.66378400
C	-4.04717200	-0.72439200	-2.59044600
C	-5.08842400	-1.81769600	-2.67396800
H	-3.57311900	-0.52067000	-3.55486100
H	-4.46739000	0.21226100	-2.21095200
H	-5.88576600	-1.52018900	-3.35870400
H	-4.64499100	-2.74686200	-3.03850600
H	-5.52052000	-1.99734400	-1.68538400
C	-3.43539600	-1.54408600	1.12049300
C	-3.96649200	-2.77715500	1.50875300
C	-4.30546900	-0.46350100	0.91831500
C	-5.34256400	-2.94109000	1.64500500
H	-3.29746400	-3.61458000	1.68551400
C	-5.67927700	-0.62586500	1.05878500
H	-3.89170600	0.51115400	0.66153800
C	-6.20236700	-1.86863700	1.41561900
H	-5.74395800	-3.90758200	1.93279100
H	-6.34185700	0.21900600	0.89823100
H	-7.27432700	-1.99704600	1.52681800
C	-1.13022400	2.12911600	1.02148300
C	-2.02978000	3.03301200	0.45352800
C	-1.36254200	1.61924100	2.30587400
C	-3.14250600	3.44679200	1.18348700
H	-1.87227400	3.39461300	-0.55734000
C	-2.47432200	2.03577100	3.02853500
H	-0.67842000	0.89043700	2.73562800
C	-3.36297800	2.95208300	2.46662900
H	-3.84071900	4.15144400	0.74461500
H	-2.65128100	1.63911500	4.02233700
H	-4.23426000	3.27272400	3.02840200
C	0.51308400	2.36363100	-1.44126000
C	0.57305600	1.72904200	-2.68245000
C	0.73722000	3.74188600	-1.34323800
C	0.84139100	2.48036000	-3.82390300
H	0.41524900	0.65965900	-2.76116100
C	0.99029900	4.48738700	-2.48919700

H	0.71844200	4.23290300	-0.37275300
C	1.04360900	3.85478100	-3.73003000
H	0.89301200	1.98723600	-4.78875300
H	1.15482800	5.55671800	-2.41166100
H	1.25082100	4.43385700	-4.62408900
C	1.79418400	1.80544400	1.02281400
C	2.98388100	1.32777800	0.45798500
C	1.81871700	2.52126200	2.22087600
C	4.19047100	1.53284200	1.11541700
H	2.95426900	0.76444000	-0.47398200
C	3.03734500	2.74436600	2.86041000
H	0.90198700	2.90814200	2.65370700
C	4.21671400	2.24393300	2.31537700
H	5.10342300	1.12397900	0.69330500
H	3.05988400	3.30564500	3.78844500
H	5.16008700	2.40807500	2.82611300
H	0.53940800	-2.02584400	1.19444900
C	2.04523700	-1.82501200	-0.44250900
O	1.86203300	-1.15067000	-1.61182700
H	-1.36419400	-1.69018700	1.80421500
C	3.49844300	-1.83183400	0.03618900
C	4.50227700	-1.47822300	-0.86585200
C	3.85412200	-2.18359100	1.34059300
C	5.83691400	-1.45103700	-0.46741200
H	4.20657100	-1.20719200	-1.87392000
C	5.18739100	-2.15488400	1.74295500
H	3.08560800	-2.47431200	2.05171600
C	6.18326000	-1.78539700	0.84084100
H	6.60792500	-1.16756000	-1.17790000
H	5.44863700	-2.42025200	2.76288100
H	7.22209700	-1.76090500	1.15515200
C	1.60885700	-3.27781800	-0.66300700
F	2.35133500	-3.89601000	-1.59363200
F	0.32876500	-3.33862000	-1.07318300
F	1.68549300	-4.03281700	0.45724100
M4 <sub>1</sub> <sup>(S,R,R)</sup>			
P	0.20957900	1.42961500	0.11138200
C	0.08306400	-0.38566300	-0.36758700
C	1.14436900	-1.27787700	0.29351300
H	1.47779300	-0.88388500	1.25776300
C	-1.34819500	-0.84675400	-0.22318500
C	-1.81531400	-1.51961900	0.84102400

H	0.33166600	-0.33722400	-1.42855800
C	-2.20877000	-0.40287700	-1.35914500
O	-2.01708200	0.64536600	-1.94572200
O	-3.15426200	-1.27450600	-1.68990800
C	-4.11454400	-0.83162800	-2.66615800
C	-5.16481400	-1.91393600	-2.76978200
H	-3.59900500	-0.65569200	-3.61417800
H	-4.53611900	0.11990000	-2.32656100
H	-5.93276400	-1.61685000	-3.48724700
H	-4.71885100	-2.85251500	-3.10575800
H	-5.63570700	-2.07752100	-1.79714200
C	-3.22375000	-1.81656200	1.16109600
C	-3.56729800	-3.04412400	1.73579000
C	-4.22328500	-0.85403500	0.96430500
C	-4.89206500	-3.32574300	2.05815300
H	-2.79366900	-3.78565600	1.91422900
C	-5.54340100	-1.13015000	1.29759100
H	-3.95238300	0.12440800	0.57210200
C	-5.88276300	-2.37181000	1.83593700
H	-5.14944300	-4.28803500	2.48861800
H	-6.30680800	-0.37332500	1.14707000
H	-6.91407300	-2.58841300	2.09534200
C	-1.34715300	1.89600500	0.92807400
C	-2.33369800	2.64776200	0.28522600
C	-1.58951700	1.38688200	2.21237200
C	-3.53083000	2.92794800	0.94347500
H	-2.17685000	3.00315700	-0.72694400
C	-2.78713000	1.66430600	2.86043400
H	-0.84006200	0.77868200	2.71298400
C	-3.75482500	2.44507800	2.22944900
H	-4.28864900	3.52145200	0.44345400
H	-2.96421300	1.26765000	3.85416000
H	-4.68880400	2.66390300	2.73665700
C	0.48674900	2.50152700	-1.32251400
C	0.98909200	1.99985000	-2.52623600
C	0.26208200	3.87475400	-1.16245200
C	1.21580100	2.87964300	-3.58213300
H	1.27225000	0.95388100	-2.60431900
C	0.49317400	4.74091200	-2.22510200
H	-0.09278500	4.27063100	-0.21460800
C	0.95995900	4.24072100	-3.43928800
H	1.60590900	2.49610600	-4.51896100
H	0.31149700	5.80317600	-2.10239700
H	1.13905900	4.91695800	-4.26900600

C	1.53896500	1.81775700	1.29900100
C	2.84606900	1.41765100	0.98947600
C	1.29498500	2.60569000	2.43119300
C	3.88688700	1.75516400	1.84880000
H	3.02274500	0.85051100	0.07104200
C	2.34978600	2.94965200	3.27232800
H	0.29801900	2.96257800	2.66142900
C	3.64212400	2.51422400	2.99102200
H	4.89284100	1.41877800	1.61666100
H	2.15499300	3.55875800	4.14863800
H	4.45865000	2.77641200	3.65627300
H	0.70451500	-2.26015500	0.49099900
C	2.38040800	-1.40009400	-0.67746600
O	2.55129200	-0.30290200	-1.43657500
H	-1.09123100	-1.83306000	1.59330300
C	3.63050300	-1.79558700	0.14268800
C	4.84438400	-1.19467400	-0.18890200
C	3.60011300	-2.71755100	1.19295400
C	6.00526700	-1.49194400	0.52172900
H	4.83756700	-0.48284600	-1.00813700
C	4.75850400	-3.01699800	1.90721400
H	2.66771100	-3.20746100	1.45994700
C	5.96490400	-2.40349400	1.57513000
H	6.94257800	-1.01259000	0.25384800
H	4.71857100	-3.72970900	2.72567600
H	6.86640000	-2.63604900	2.13362200
C	2.07547600	-2.58988100	-1.61227600
F	3.07083300	-2.80963000	-2.48274400
F	0.95953500	-2.36970000	-2.34213600
F	1.86335100	-3.76077900	-0.96374000
M4 <sub>1</sub> <sup>r(S,R,R)</sup>			
P	1.91628200	-0.74033500	-0.07154400
C	0.44101200	0.38581900	0.03015800
C	0.57269500	1.64914400	-0.82840500
H	1.46008900	2.19355500	-0.47923000
C	-0.86689000	-0.35885600	-0.08786700
C	-1.53242800	-0.38307800	-1.25419900
H	0.51341000	0.69925100	1.07403800
C	-1.35540900	-0.84414100	1.23185000
O	-0.63279800	-0.90918300	2.21247600
O	-2.64649900	-1.15567400	1.26183100
C	-3.17890300	-1.54193400	2.53804600



C	-4.64388700	-1.84763200	2.32076700
H	-3.02688800	-0.71553200	3.23992100
H	-2.62363800	-2.41016600	2.90526700
H	-5.10514800	-2.15613300	3.26153700
H	-5.16586400	-0.96342800	1.94696200
H	-4.76213100	-2.65099200	1.58959600
C	-2.85376200	-0.94889300	-1.58418700
C	-3.75280300	-0.11487900	-2.25958700
C	-3.20896900	-2.27431900	-1.31624200
C	-5.00338200	-0.59704600	-2.63474400
H	-3.44679800	0.91195300	-2.44674300
C	-4.45219200	-2.75762500	-1.71021600
H	-2.50907800	-2.91952200	-0.79202300
C	-5.35380600	-1.91899500	-2.36524700
H	-5.70405000	0.05778000	-3.14344600
H	-4.71965800	-3.78949200	-1.50417100
H	-6.32512600	-2.29711600	-2.66826500
C	1.45984900	-2.42765400	0.39892300
C	2.01687300	-3.00820300	1.54124000
C	0.51655800	-3.13736600	-0.35958200
C	1.62119700	-4.28424400	1.93283200
H	2.75115600	-2.46870500	2.12946800
C	0.12809800	-4.41134900	0.04013600
H	0.08439600	-2.70328000	-1.25572400
C	0.67435100	-4.98175500	1.18911300
H	2.05352800	-4.72887400	2.82239600
H	-0.60001300	-4.95864100	-0.54931800
H	0.36452600	-5.97401300	1.49958800
C	3.11908800	-0.10788000	1.12284200
C	2.66407800	0.22144800	2.40894100
C	4.47255800	0.01923100	0.79859400
C	3.56754000	0.69260700	3.35473700
H	1.61843700	0.08412200	2.67742400
C	5.36657500	0.49669400	1.75332700
H	4.83005900	-0.24870900	-0.19015300
C	4.91467700	0.83685200	3.02518700
H	3.21830300	0.94700700	4.34944600
H	6.41584900	0.60176700	1.50031700
H	5.61433300	1.21156300	3.76487400
C	2.68335000	-0.76822000	-1.71054500
C	3.21174800	0.42277300	-2.23333800
C	2.79501200	-1.95614600	-2.44026900
C	3.82334300	0.42192700	-3.48024400
H	3.16318600	1.34597600	-1.66538000

C	3.40742100	-1.94634100	-3.69071900
H	2.41859300	-2.88939900	-2.03776500
C	3.91611100	-0.76109000	-4.21227300
H	4.22906100	1.34553600	-3.87782400
H	3.48881100	-2.87058600	-4.25207000
H	4.39337900	-0.75813300	-5.18660400
H	0.71480100	1.42125300	-1.88804400
C	-0.72090000	2.58337100	-0.78422700
O	-1.61428400	2.29546300	-1.72850000
H	-1.07059800	0.15847200	-2.07390900
C	-1.29370700	2.57624500	0.66305200
C	-2.62668600	2.19824900	0.81331500
C	-0.54051400	2.84636200	1.81269700
C	-3.19870000	2.07703000	2.07835100
H	-3.17499800	1.97537800	-0.09742100
C	-1.10931200	2.73149800	3.07973200
H	0.50280000	3.13854400	1.72366900
C	-2.44114200	2.34272600	3.21773600
H	-4.23643700	1.76878700	2.17696100
H	-0.50971800	2.94113300	3.96090400
H	-2.88286100	2.24562400	4.20513100
C	-0.17847200	4.00451600	-1.06356400
F	-1.15343500	4.92541700	-1.01746900
F	0.37457600	4.07736800	-2.28988300
F	0.78675800	4.43522800	-0.20702900

TS5<sub>1</sub><sup>(S,R,R)</sup>

P	-2.07883700	0.50986100	-0.02482600
C	-0.46219100	-0.41741800	0.05512000
C	-0.36535500	-1.63736500	-0.86834500
H	-1.09573400	-2.39344100	-0.55664200
C	0.75838500	0.45726000	-0.01960600
C	1.43348500	0.50466100	-1.21021000
H	-0.51146500	-0.79056800	1.08210200
C	1.25608500	0.83806500	1.29877800
O	0.57010100	0.78185900	2.31518100
O	2.53031100	1.25008900	1.32711800
C	3.06839400	1.57237700	2.61207000
C	4.52588600	1.91578700	2.39259400
H	2.94499600	0.70925900	3.27448600
H	2.50782600	2.40950100	3.04078800
H	4.99848400	2.18514500	3.33996300
H	5.05569100	1.05977600	1.96663200

H	4.62007400	2.75514800	1.69907600
C	2.69165200	1.25170300	-1.48401200
C	3.77979500	0.62717100	-2.09833400
C	2.76273800	2.62086200	-1.20098300
C	4.92531300	1.35962000	-2.40553200
H	3.70881000	-0.43500700	-2.30159900
C	3.90213200	3.35140700	-1.51998600
H	1.92435500	3.10598700	-0.70864800
C	4.99101900	2.72112800	-2.12142500
H	5.77038300	0.86188700	-2.87154800
H	3.94287000	4.41248000	-1.29298600
H	5.88313900	3.28896700	-2.36643100
C	-1.80855800	2.22884200	0.45421400
C	-2.40624400	2.75387600	1.60275100
C	-0.96511100	3.03118700	-0.32799300
C	-2.15559000	4.07296100	1.97101200
H	-3.06001200	2.13950500	2.21269500
C	-0.72501400	4.34893800	0.04491100
H	-0.50340100	2.63275500	-1.22570000
C	-1.31492700	4.86753600	1.19668400
H	-2.61816000	4.47690200	2.86479700
H	-0.07761800	4.96958800	-0.56573800
H	-1.12119200	5.89498700	1.48669000
C	-3.20052900	-0.26036200	1.16526800
C	-2.70490800	-0.54021400	2.44782700
C	-4.53023700	-0.54589200	0.84241900
C	-3.54470200	-1.11725000	3.39425900
H	-1.67918400	-0.28546000	2.70956300
C	-5.35937100	-1.12741000	1.79746600
H	-4.91743400	-0.32061500	-0.14604300
C	-4.86725900	-1.41537800	3.06755800
H	-3.16524600	-1.33299000	4.38711400
H	-6.38994500	-1.35440900	1.54704400
H	-5.51726600	-1.86965500	3.80808100
C	-2.85156000	0.46311500	-1.66099900
C	-3.20187100	-0.78238300	-2.20417100
C	-3.12603500	1.63446000	-2.37371900
C	-3.80185700	-0.84909700	-3.45561600
H	-3.02113000	-1.69726300	-1.64798000
C	-3.72427900	1.55755100	-3.62874200
H	-2.88609900	2.60503800	-1.95431200
C	-4.05669100	0.32015000	-4.17098400
H	-4.07048500	-1.81426400	-3.87072700
H	-3.93401200	2.46899000	-4.17765000

H	-4.52211800	0.26366400	-5.14940100
H	-0.56873400	-1.38795800	-1.91357400
C	1.10066100	-2.22687900	-0.85029900
O	1.95506900	-1.52910600	-1.63298500
H	0.85466100	0.28578500	-2.10260000
C	1.59622900	-2.38971600	0.60726500
C	2.86046900	-1.89325500	0.92174500
C	0.83069600	-2.97586200	1.62183700
C	3.35151200	-1.97061700	2.22307400
H	3.42267200	-1.41726400	0.12446700
C	1.31977600	-3.05514600	2.92447100
H	-0.15831200	-3.36927600	1.40081100
C	2.58288100	-2.55199600	3.22989200
H	4.33626700	-1.57245400	2.45368200
H	0.71114200	-3.50728200	3.70193800
H	2.96296300	-2.61026000	4.24526900
C	0.98770200	-3.63471000	-1.46035900
F	2.17257800	-4.26034400	-1.48780500
F	0.53446500	-3.58672900	-2.72585000
F	0.13704600	-4.45116100	-0.79247100
M5 <sub>1</sub> (S,R,R)			
P	2.03603100	0.50567900	0.09252800
C	0.39168300	-0.46964700	-0.17822600
C	0.29573100	-1.71375500	0.70821400
H	1.02402000	-2.47794000	0.42475900
C	-0.82473900	0.36239900	-0.06176600
C	-1.71923900	-0.00054200	1.07504300
H	0.54777900	-0.77748700	-1.22067800
C	-1.06440800	1.16736000	-1.18228400
O	-0.23035900	1.34421900	-2.09612400
O	-2.28038400	1.79085000	-1.24472800
C	-2.43999600	2.74635600	-2.28545400
C	-3.82824300	3.33413100	-2.12938900
H	-2.31350800	2.26455700	-3.26080800
H	-1.66543200	3.51789300	-2.20121500
H	-4.01023400	4.09440900	-2.89310800
H	-4.58619400	2.55219000	-2.22643400
H	-3.93748500	3.78909600	-1.14126400
C	-2.98635800	0.81027000	1.23987500
C	-4.24225700	0.29053300	0.93605200
C	-2.89319900	2.11861300	1.71926400
C	-5.38438900	1.07878000	1.07996500

H	-4.32367400	-0.73440300	0.59197200
C	-4.02862900	2.90481500	1.86686600
H	-1.91552300	2.52691800	1.96052600
C	-5.28314600	2.38760100	1.54005100
H	-6.35730700	0.66308500	0.83518700
H	-3.93775700	3.92176200	2.23667800
H	-6.17305100	2.99911400	1.65227600
C	1.68228700	2.27007200	0.12628500
C	2.24621000	3.14432300	-0.80612700
C	0.77261300	2.74517400	1.07834200
C	1.90311500	4.49160900	-0.78214900
H	2.94003200	2.77291600	-1.55327500
C	0.43594900	4.09658700	1.09753800
H	0.34456100	2.06643100	1.81016700
C	0.99595800	4.96562400	0.16479900
H	2.34053000	5.17114700	-1.50550000
H	-0.26329300	4.46929600	1.83902900
H	0.72855200	6.01729600	0.17820000
C	3.18473400	0.15402500	-1.26033300
C	2.67857800	0.20863000	-2.56765800
C	4.53363600	-0.14370000	-1.03623400
C	3.52863200	-0.04552600	-3.64001700
H	1.63562900	0.47423600	-2.72885600
C	5.37108700	-0.39770500	-2.11806800
H	4.93123400	-0.17621700	-0.02710000
C	4.86921700	-0.35240700	-3.41719500
H	3.14078200	-0.00202700	-4.65219900
H	6.41656400	-0.62861300	-1.94386000
H	5.52625000	-0.55308300	-4.25729400
C	2.86485700	0.06068600	1.64564800
C	3.30705900	-1.26019100	1.81422700
C	3.07279600	0.99234500	2.66717500
C	3.93843600	-1.64099700	2.99188800
H	3.17666400	-1.98861400	1.01898700
C	3.70149400	0.60241800	3.84748500
H	2.75551300	2.02188900	2.54407200
C	4.13096000	-0.71061600	4.01257000
H	4.28057400	-2.66314900	3.11183600
H	3.85850600	1.33196400	4.63455400
H	4.62136500	-1.01023600	4.93283100
H	0.45511400	-1.48072400	1.76612800
C	-1.12817400	-2.29077200	0.54776200
O	-2.11888800	-1.40310400	1.01153700
H	-1.16536000	0.09186500	2.02761900

C	-1.39265400	-2.71156400	-0.90210200
C	-2.39032900	-2.06656400	-1.63442200
C	-0.61954600	-3.69393500	-1.52977700
C	-2.61955300	-2.40431400	-2.96584700
H	-2.96740600	-1.28048100	-1.16182300
C	-0.85395500	-4.03397000	-2.85985400
H	0.16778200	-4.20428500	-0.98543900
C	-1.85596100	-3.39116200	-3.58254000
H	-3.39615800	-1.88882000	-3.52198500
H	-0.24762300	-4.80100100	-3.33113400
H	-2.03547700	-3.65354000	-4.62028100
C	-1.27470200	-3.48967700	1.49199300
F	-2.47897200	-4.05872100	1.38295600
F	-1.11738300	-3.11657500	2.76974600
F	-0.35394700	-4.44228000	1.25223300
TS6 <sub>1</sub> <sup>(S,R,R)</sup>			
P	-2.09137500	0.31576000	-0.10069800
C	-0.20778100	-0.59524400	0.42396700
C	-0.02166300	-1.78875000	-0.49750200
H	-0.68422100	-2.61651400	-0.23624600
C	0.85659600	0.35088400	0.34490900
C	1.81769200	0.10343400	-0.77936200
H	-0.53659000	-0.85130800	1.43348300
C	0.82445200	1.38405600	1.32004200
O	-0.05119400	1.46273200	2.19485400
O	1.78128000	2.34043700	1.21404000
C	1.60685800	3.49601900	2.03031600
C	2.53575600	4.56022800	1.48476000
H	1.83902500	3.25190700	3.07347400
H	0.56045700	3.81412000	1.98717200
H	2.46793600	5.47059500	2.08578600
H	3.57122500	4.20928500	1.49170200
H	2.26577900	4.79654400	0.45149600
C	2.98156200	1.05462000	-0.91613600
C	4.16718300	0.86171900	-0.20907500
C	2.86596300	2.15855900	-1.75987200
C	5.20804400	1.78020400	-0.31931200
H	4.27533800	-0.01487200	0.42071500
C	3.89987300	3.08394800	-1.86527500
H	1.95823400	2.29373300	-2.34303300
C	5.07469800	2.89924100	-1.13909000
H	6.12824000	1.62021600	0.23431700

H	3.79371000	3.94159000	-2.52277100
H	5.88629600	3.61516600	-1.22309500
C	-1.78419000	2.08688000	-0.23082100
C	-2.44603800	3.02028200	0.57418900
C	-0.75086800	2.50687200	-1.07721400
C	-2.08062200	4.35967300	0.52542700
H	-3.23680600	2.69698900	1.24375700
C	-0.38113500	3.85076900	-1.11378900
H	-0.24435900	1.78999800	-1.71704800
C	-1.04181600	4.77437600	-0.31059600
H	-2.60136800	5.08188400	1.14536500
H	0.42576900	4.17099300	-1.76552900
H	-0.75054900	5.81979500	-0.33510400
C	-3.36008000	0.03125300	1.16227000
C	-2.98146700	0.20350300	2.50196500
C	-4.66277100	-0.37189500	0.84678900
C	-3.91224700	-0.02106700	3.51308600
H	-1.97006900	0.53027900	2.73488500
C	-5.58123800	-0.59985000	1.86669400
H	-4.96055800	-0.50340000	-0.18853000
C	-5.20737600	-0.42592700	3.19799300
H	-3.62200100	0.11725200	4.54937500
H	-6.59168900	-0.90859700	1.61997700
H	-5.92792400	-0.60436800	3.98957500
C	-2.77092600	-0.25504400	-1.68719400
C	-3.08912400	-1.61511500	-1.82123600
C	-2.95136500	0.60279000	-2.77687500
C	-3.58532600	-2.10373400	-3.02427300
H	-2.96537600	-2.29218600	-0.97942300
C	-3.44033500	0.10522700	-3.98257300
H	-2.71909800	1.65858200	-2.68426200
C	-3.75665300	-1.24438100	-4.10875200
H	-3.83411200	-3.15564500	-3.11548100
H	-3.57916200	0.77890600	-4.82156100
H	-4.13844300	-1.62757800	-5.04921900
H	-0.22520100	-1.52191500	-1.54039400
C	1.44671500	-2.26576000	-0.39877600
O	2.37784300	-1.23280000	-0.64418700
H	1.28636800	0.11067200	-1.74827400
C	1.70702100	-2.91535700	0.96126000
C	2.53101500	-2.27710700	1.88767500
C	1.07992500	-4.11259000	1.32368000
C	2.73670300	-2.83034300	3.15006500
H	2.99335800	-1.33563500	1.61785900

C	1.29122700	-4.66660300	2.58273800
H	0.42531400	-4.62290500	0.62572200
C	2.12171800	-4.02819400	3.50068700
H	3.37835800	-2.31900800	3.86062000
H	0.80027800	-5.59795000	2.84637900
H	2.28261700	-4.45977400	4.48337400
C	1.70445800	-3.24982500	-1.54824900
F	2.92005900	-3.79835500	-1.47288900
F	1.61533300	-2.62325000	-2.73079700
F	0.80791600	-4.25424900	-1.57714600
TS3 <sub>1</sub> <sup>(S,R,S)</sup>			
P	0.10854000	-1.48039200	-0.32071300
C	-0.38555500	0.21952200	0.01127700
C	0.42187500	1.36158300	-0.58224000
H	1.03339900	1.02020600	-1.42093000
C	-1.42433500	0.47917500	0.85077500
C	-1.76077400	1.83872600	1.31586500
H	-2.34380500	1.78710500	2.24040100
H	-0.48197500	2.15700700	1.61160700
C	-2.21556800	-0.63711600	1.47317600
O	-1.76313200	-1.50365200	2.18904600
O	-3.49929700	-0.54991100	1.13023300
C	-4.33044400	-1.64632000	1.56303200
C	-5.69102000	-1.44768400	0.93717600
H	-4.36999500	-1.64535400	2.65575400
H	-3.85848300	-2.57945300	1.23696800
H	-6.35190300	-2.26778200	1.22643600
H	-6.13628400	-0.50684100	1.26768100
H	-5.60831400	-1.43395000	-0.15216200
C	-2.41525000	2.79118300	0.37314300
C	-2.76546400	4.06958000	0.84124200
C	-2.72082200	2.49005200	-0.96086300
C	-3.38100700	5.00044100	0.01619600
H	-2.53839400	4.32648400	1.87313000
C	-3.32655700	3.42808900	-1.79666800
H	-2.49402900	1.49895400	-1.34710700
C	-3.66187000	4.68875300	-1.31638400
H	-3.63907500	5.97913800	0.41061900
H	-3.54698100	3.16237400	-2.82674000
H	-4.13688500	5.41785700	-1.96473300
C	-1.35084400	-2.51881200	-0.62920000
C	-1.42085400	-3.83018700	-0.15024300



C	-2.40099600	-1.99214300	-1.39025700
C	-2.52858700	-4.61640200	-0.45422600
H	-0.62887100	-4.23290300	0.47226400
C	-3.50078200	-2.78850400	-1.69756900
H	-2.36750700	-0.96234900	-1.73530600
C	-3.56395600	-4.09981600	-1.23113600
H	-2.58404000	-5.63169000	-0.07701300
H	-4.30832800	-2.37968000	-2.29553400
H	-4.42485500	-4.71649200	-1.46709900
C	1.11743600	-2.15631400	1.01657800
C	1.21576000	-1.47184800	2.22914100
C	1.81740100	-3.35394800	0.81336100
C	2.00274600	-2.00326200	3.24797300
H	0.71024400	-0.51846000	2.35860200
C	2.59291000	-3.87849400	1.83976100
H	1.76777600	-3.86745400	-0.14346500
C	2.68196800	-3.20307600	3.05730400
H	2.09149300	-1.47026200	4.18889700
H	3.13165400	-4.80723000	1.68717500
H	3.29314700	-3.61141400	3.85572000
C	1.14017200	-1.54867900	-1.80914600
C	2.52310200	-1.37893300	-1.68200900
C	0.56384000	-1.71327200	-3.07355000
C	3.32302200	-1.37320100	-2.82082900
H	2.97645900	-1.24410500	-0.70335500
C	1.37242300	-1.70813100	-4.20513800
H	-0.50649600	-1.85627200	-3.17977900
C	2.75006200	-1.53883200	-4.07910500
H	4.39424300	-1.23575700	-2.71755700
H	0.92542300	-1.84072100	-5.18431600
H	3.37740700	-1.53765500	-4.96428600
H	-0.28761500	2.08751100	-0.99201500
C	1.33089800	2.08664800	0.48397300
O	0.79408300	2.09227600	1.74260500
C	2.74729200	1.48022600	0.47308000
C	3.23033000	0.88924200	1.63855100
C	3.56478400	1.48396500	-0.66477500
C	4.47955600	0.27154700	1.66286100
H	2.60178100	0.92281200	2.52021100
C	4.82910100	0.90200200	-0.63246100
H	3.21682300	1.93819600	-1.58718500
C	5.28612800	0.27782400	0.52736100
H	4.82452200	-0.20774700	2.57450500
H	5.45316900	0.92516900	-1.52097500

H	6.26452600	-0.19215400	0.54680000
C	1.42969200	3.55216400	0.02285300
F	0.24855000	4.17671900	0.14862000
F	1.78667100	3.68739300	-1.27607400
F	2.32206500	4.24529000	0.74469300
M3 <sub>1</sub> <sup>(S,R,S)</sup>			
P	0.12979000	-1.07065400	0.59539600
C	0.37787400	0.38400400	-0.30649000
C	-0.67364800	1.46567500	-0.32840300
H	-1.20262300	1.57262600	0.62594000
C	1.70751200	0.65001000	-0.85891100
C	2.44105800	1.78839400	-0.74326000
H	3.32506300	1.85987900	-1.37170400
H	-0.40525700	0.10087300	-2.17600400
C	2.31183700	-0.43207700	-1.70877100
O	1.66030300	-1.23707000	-2.34912700
O	3.64598500	-0.46028500	-1.66951800
C	4.27390700	-1.53072100	-2.39549400
C	5.75336900	-1.46519000	-2.09115500
H	4.06341800	-1.40938400	-3.46220200
H	3.82919000	-2.47510200	-2.06704300
H	6.27556500	-2.26833700	-2.61575500
H	6.17313000	-0.50934300	-2.41279400
H	5.92348800	-1.58054100	-1.01781500
C	2.25499800	2.93329600	0.15503900
C	1.51815700	2.87750800	1.35278700
C	2.94454700	4.12292200	-0.13475300
C	1.47842300	3.96729700	2.21560000
H	0.98232700	1.96867800	1.61045300
C	2.88924900	5.21773600	0.71898900
H	3.53331300	4.17814900	-1.04662500
C	2.15497700	5.14497400	1.90168600
H	0.91099600	3.89625600	3.13869400
H	3.42560000	6.12663100	0.46515000
H	2.11256200	5.99667400	2.57284700
C	1.76319200	-1.79807500	0.95908600
C	2.03331100	-3.14392500	0.69201300
C	2.78453000	-0.97223600	1.45011700
C	3.30720600	-3.65824800	0.92297800
H	1.25840200	-3.78892000	0.29180600
C	4.05115700	-1.49371800	1.68833100
H	2.59823500	0.08512300	1.61718600

C	4.31441000	-2.83649500	1.42236200
H	3.51127600	-4.70174700	0.70744500
H	4.83534900	-0.84677700	2.06685800
H	5.30645400	-3.24027200	1.59826400
C	-0.85800700	-2.46432100	-0.07795400
C	-0.92921300	-2.67472900	-1.45690800
C	-1.48184700	-3.37021500	0.79068600
C	-1.63946200	-3.76135300	-1.96263800
H	-0.42327600	-1.99547200	-2.13215800
C	-2.19325500	-4.45170400	0.28135300
H	-1.41792400	-3.23074700	1.86564100
C	-2.27860800	-4.64429100	-1.09673300
H	-1.69433800	-3.91388200	-3.03560700
H	-2.67972100	-5.14366900	0.96091100
H	-2.83688100	-5.48660100	-1.49300600
C	-0.72862200	-0.67880700	2.16228200
C	-2.12700300	-0.62564500	2.18848400
C	-0.00225600	-0.30109600	3.29721700
C	-2.78677500	-0.19418900	3.33685000
H	-2.70668600	-0.92787900	1.31971700
C	-0.66746200	0.11977500	4.44463200
H	1.08231800	-0.34496200	3.29586300
C	-2.06009300	0.17699400	4.46469100
H	-3.87130700	-0.15092700	3.34113300
H	-0.09678600	0.39894600	5.32404900
H	-2.57692600	0.50781300	5.35978800
H	-0.17229700	2.41892700	-0.51029800
C	-1.74585100	1.26703100	-1.46572500
O	-1.23449200	0.49390700	-2.51810800
C	-3.03793500	0.66977200	-0.91331000
C	-3.48404900	-0.56971300	-1.37050600
C	-3.76100400	1.31877800	0.09525500
C	-4.60464600	-1.17443100	-0.80172300
H	-2.93621300	-1.06171700	-2.16416500
C	-4.89607100	0.72964400	0.64232700
H	-3.43056400	2.28256700	0.46800700
C	-5.31378400	-0.52791800	0.20743200
H	-4.92105500	-2.15195800	-1.15281200
H	-5.44504900	1.24670400	1.42330700
H	-6.18776600	-0.99587600	0.64920700
C	-2.02780100	2.63148600	-2.09795700
F	-0.93094600	3.12578500	-2.68913200
F	-2.41942600	3.54297000	-1.18672400
F	-2.98709000	2.56396600	-3.03061400

TS4<sub>1</sub><sup>(S,R,S)</sup>

P	-0.33884000	-1.02016800	-0.61802500
C	-0.31500600	0.30440900	0.63445700
C	0.86654500	1.26998900	0.59870400
H	1.31682300	1.43661900	-0.38291700
C	-1.67438300	0.85174500	0.94431300
C	-2.16735000	2.08187800	0.69332000
H	-3.11713800	2.32531900	1.16391900
H	0.13722400	-0.25758600	1.63421300
C	-2.55066100	-0.11621200	1.68435300
O	-2.14842100	-1.15829500	2.16254300
O	-3.84180700	0.22928100	1.69660500
C	-4.74553900	-0.76102700	2.21785500
C	-6.14854600	-0.27506900	1.93560200
H	-4.55690900	-0.88833800	3.28765200
H	-4.53264600	-1.71093500	1.71724400
H	-6.87353000	-0.99531100	2.32092200
H	-6.32900800	0.68991400	2.41466600
H	-6.30286800	-0.16708400	0.85894000
C	-1.62437000	3.14805600	-0.16364600
C	-1.90021600	4.48495400	0.15523800
C	-0.92057000	2.87517900	-1.34518200
C	-1.45068300	5.51845700	-0.65971500
H	-2.46598200	4.70985200	1.05507100
C	-0.48382600	3.90588100	-2.16862600
H	-0.71919100	1.84689800	-1.62734300
C	-0.74027600	5.23219300	-1.82411600
H	-1.66252800	6.54824000	-0.39091700
H	0.05481100	3.67005600	-3.08120700
H	-0.39666500	6.03806600	-2.46446600
C	-2.05175900	-1.54419800	-0.93509900
C	-2.43305000	-2.86973500	-0.70754100
C	-3.00688700	-0.60879100	-1.35726100
C	-3.75815300	-3.25336300	-0.89453600
H	-1.70385000	-3.59792900	-0.36902600
C	-4.32898500	-0.99918000	-1.54203900
H	-2.72912600	0.42733400	-1.52762800
C	-4.70647300	-2.31981100	-1.30541700
H	-4.04816200	-4.28220200	-0.71049900
H	-5.06285500	-0.26894600	-1.86605000
H	-5.74023900	-2.62012100	-1.44266600
C	0.57337000	-2.48244300	-0.06155400

C	0.44942000	-2.88774900	1.27329500
C	1.33449400	-3.23701300	-0.96048900
C	1.11011300	-4.03358900	1.70358800
H	-0.15434300	-2.31016400	1.96338400
C	2.00037600	-4.37505400	-0.51599000
H	1.41763000	-2.93900000	-2.00018100
C	1.89479400	-4.76797900	0.81594500
H	1.02023800	-4.34657200	2.73825100
H	2.60106400	-4.95227300	-1.21072400
H	2.41872400	-5.65364000	1.16129400
C	0.40133200	-0.51094900	-2.20079200
C	1.79105500	-0.32921400	-2.25468700
C	-0.37706600	-0.23621500	-3.33049900
C	2.38536100	0.15277200	-3.41574500
H	2.41426600	-0.57558800	-1.39953300
C	0.22673200	0.24527600	-4.48949500
H	-1.44886500	-0.39972500	-3.31859400
C	1.60376800	0.44845100	-4.53097600
H	3.46108300	0.29350800	-3.44009000
H	-0.38274200	0.45717500	-5.36139400
H	2.06832300	0.82700300	-5.43556100
H	0.51678500	2.24194800	0.95294000
C	1.93104100	0.67886800	1.64447400
O	1.34018300	-0.26723400	2.40841900
C	3.17014500	0.17451700	0.88101000
C	3.50240300	-1.17580600	0.97876400
C	3.92197900	0.99260800	0.02694900
C	4.54017700	-1.71170600	0.21632500
H	2.90784400	-1.79489500	1.64139000
C	4.96666000	0.46267800	-0.72539000
H	3.67808400	2.04607800	-0.06868300
C	5.27249400	-0.89647100	-0.64277000
H	4.76853700	-2.77127800	0.28958700
H	5.53769600	1.10901100	-1.38568100
H	6.07735000	-1.31236600	-1.24111000
C	2.34122700	1.84452300	2.55065700
F	1.30450200	2.27693900	3.28808000
F	2.79163200	2.92839000	1.87208300
F	3.31664500	1.50181300	3.40816600
M4 <sub>1</sub> <sup>(S,R,S)</sup>			
P	-0.91098200	1.28634900	-0.20391700
C	-2.51762800	1.09818600	-1.01506300

C	-2.68666500	1.61528200	-2.30236600
C	-3.52781000	0.31991800	-0.43210600
C	-3.85753000	1.34806600	-3.00587000
H	-1.90359800	2.21138700	-2.76046500
C	-4.69331800	0.05713500	-1.14277400
H	-3.40299200	-0.09024800	0.56530600
C	-4.85635600	0.56795800	-2.43047000
H	-3.98447900	1.74790900	-4.00580400
H	-5.47236500	-0.54796800	-0.69098800
H	-5.76565000	0.35718300	-2.98370700
C	-1.14992200	1.71855400	1.53702800
C	-2.38252300	2.18387600	2.00488500
C	-0.04099500	1.68571500	2.39469700
C	-2.50768500	2.59564400	3.33020100
H	-3.24074900	2.23653900	1.34325300
C	-0.17443400	2.10417100	3.71155300
H	0.92159600	1.33327500	2.04139700
C	-1.40769300	2.55620500	4.18070500
H	-3.46550600	2.95431500	3.69114700
H	-1.50862500	2.87981100	5.21156600
C	-0.02901500	2.65481200	-0.98781200
C	0.98321200	2.41897400	-1.92593700
C	-0.42502800	3.95914100	-0.66298800
C	1.59367100	3.51548600	-2.53521400
H	1.32663000	1.40314000	-2.16164500
C	0.18931900	5.03718900	-1.28724400
H	-1.20421400	4.13121200	0.07513800
C	1.19967400	4.81339100	-2.22313900
H	2.38640200	3.34651600	-3.25664100
H	-0.11344200	6.04879700	-1.03954600
H	1.68379400	5.65671900	-2.70505500
C	0.01070000	-0.27285300	-0.46332300
C	-0.90814700	-1.42783000	-0.11592900
C	1.46259800	-0.23436000	0.03571400
C	2.41265500	-0.85442600	-1.06626900
H	1.79825100	0.80507800	0.11098800
H	1.58215800	-0.68070900	1.02090600
C	-1.21245200	-1.95788100	1.08056000
C	-1.65791500	-1.93797000	-1.32353000
O	-1.45892900	-1.54298600	-2.45079400
O	-2.60207000	-2.83766400	-1.02877900
C	-3.40535700	-3.27763000	-2.13820400
C	-4.47580100	-4.18769900	-1.58089600
H	-3.82816300	-2.39420700	-2.62680400

H	-2.76030500	-3.78820400	-2.85842000
H	-5.11313400	-4.54638600	-2.39200000
H	-5.09868000	-3.65040100	-0.86157000
H	-4.02934500	-5.05089300	-1.08232800
O	2.06848300	-0.47022000	-2.29765400
H	0.13576100	-0.28991700	-1.56337600
C	3.85700600	-0.46901400	-0.65725300
C	4.40087700	-0.71100300	0.60909800
C	4.63538400	0.18701800	-1.60838800
C	5.69843200	-0.30350700	0.91172400
H	3.81605400	-1.22629100	1.36613400
C	5.93322200	0.59595400	-1.30914300
H	4.18057300	0.36051400	-2.57781700
C	6.46980800	0.35135200	-0.04693300
H	6.10883500	-0.49750000	1.89849300
H	6.52835600	1.10526000	-2.06186500
H	7.48105200	0.66772100	0.19011100
C	2.31633900	-2.39196200	-0.98977800
F	1.11427300	-2.84067700	-1.40074200
F	3.23343000	-2.98891600	-1.76641300
F	2.49063600	-2.90394800	0.26094700
H	0.68321700	2.06715000	4.37426900
C	-0.72466300	-1.62434800	2.44143200
C	0.58182700	-1.89137300	2.86033600
C	-1.64938100	-1.13562600	3.37386200
C	0.97087500	-1.61672200	4.17010900
H	1.28312200	-2.34076600	2.16522800
C	-1.26039000	-0.86447400	4.68024000
H	-2.67728800	-0.95864700	3.06732500
C	0.05519600	-1.09615200	5.07989900
H	1.98969100	-1.82644800	4.48025200
H	-1.98327800	-0.46638300	5.38528400
H	0.35984000	-0.88418600	6.09979300
H	-1.97422800	-2.73497700	1.06538000
M4 <sub>1</sub> <sup>r(S,R,S)</sup>			
P	-0.01161000	1.44945800	0.17443400
C	-0.07588900	-0.36643900	-0.22355600
C	0.30143600	-1.36742000	0.88218000
H	0.71280400	-0.89967700	1.77884400
C	-1.25926500	-0.80180700	-1.05490600
C	-2.47996400	-1.23795800	-0.68756800
H	-3.10315000	-1.58180800	-1.50911700

H	0.75611600	-0.41639500	-0.93294200
C	-0.95563400	-0.72215300	-2.51737700
O	-0.08326000	-0.00376400	-2.96995900
O	-1.74509900	-1.46838900	-3.28746400
C	-1.51756200	-1.36390600	-4.70478300
C	-2.47658600	-2.31534600	-5.38269300
H	-0.47363400	-1.61548000	-4.90848000
H	-1.68129500	-0.32577200	-5.00850500
H	-2.34243000	-2.26288700	-6.46533500
H	-2.29163200	-3.34168400	-5.05883800
H	-3.51100100	-2.05414700	-5.14804500
C	-3.14714300	-1.33168100	0.61670900
C	-4.33366200	-2.08096500	0.67846000
C	-2.71755000	-0.68441200	1.78441500
C	-5.04786400	-2.19944300	1.86410100
H	-4.68969000	-2.57876500	-0.21916000
C	-3.43735300	-0.78951500	2.96936200
H	-1.81555900	-0.08718100	1.77793200
C	-4.60252300	-1.55165400	3.01542500
H	-5.95632000	-2.79211200	1.88840800
H	-3.08406200	-0.27004400	3.85481700
H	-5.16340100	-1.63499700	3.94053600
C	-1.21247400	2.34924500	-0.83554200
C	-0.77242000	3.28642500	-1.77472200
C	-2.58224000	2.08491600	-0.69502600
C	-1.69982500	3.95680200	-2.56727300
H	0.28672300	3.48871200	-1.89354600
C	-3.50064300	2.76378200	-1.48704200
H	-2.93729100	1.35968600	0.03176300
C	-3.05965200	3.69675500	-2.42442300
H	-1.35472600	4.68127000	-3.29669000
H	-4.55976400	2.56045600	-1.37310700
H	-3.77932200	4.22119800	-3.04426300
C	1.64139800	2.06776900	-0.22889800
C	2.29483400	1.61365600	-1.38154900
C	2.21582600	3.07652500	0.55553000
C	3.53034300	2.15323400	-1.72405700
H	1.83988400	0.86357200	-2.02079800
C	3.45176400	3.60652500	0.20136400
H	1.70681500	3.44856200	1.43824800
C	4.11110300	3.14126200	-0.93359300
H	4.04145000	1.79029500	-2.60920900
H	3.89716200	4.38259600	0.81431300
H	5.07802500	3.55264200	-1.20487800



C	-0.28465200	1.83417200	1.92676600
C	0.67600400	1.40684400	2.85570700
C	-1.41579400	2.52931000	2.36447800
C	0.48416800	1.64560600	4.21125900
H	1.58317100	0.91030000	2.51986500
C	-1.59983200	2.76403400	3.72469700
H	-2.15105300	2.89241600	1.65524400
C	-0.65820100	2.31555100	4.64678400
H	1.22865900	1.31072100	4.92501700
H	-2.47981800	3.30265800	4.05894000
H	-0.80733800	2.49845100	5.70567500
H	-0.58050100	-1.93541200	1.18405200
C	1.29739300	-2.36180700	0.17939100
O	0.82503800	-2.77360400	-0.99463700
C	2.69117000	-1.67028400	0.07967000
C	3.31620000	-1.70205200	-1.16596000
C	3.33231500	-1.00807300	1.13336000
C	4.55395000	-1.09410600	-1.36335600
H	2.78156400	-2.21392200	-1.95994300
C	4.56245800	-0.38167300	0.93652600
H	2.88474000	-0.99748600	2.12425400
C	5.17899200	-0.42632900	-0.31241100
H	5.02895500	-1.13259200	-2.34010100
H	5.04374200	0.13508400	1.76198700
H	6.13746100	0.06123000	-0.46468300
C	1.45125400	-3.55378400	1.14239600
F	0.29860800	-4.23428800	1.28430600
F	1.82425600	-3.19531200	2.40003900
F	2.36960100	-4.43539200	0.71283900

TS5<sub>1</sub><sup>(S,R,S)</sup>

P	-1.50780400	-0.83717300	-0.37877100
C	0.18886200	-0.17160400	-0.09628100
C	0.51458600	1.05906900	-0.95461500
H	0.35375900	0.82071100	-2.01271200
C	0.71153900	-0.01849200	1.31054300
C	0.74583900	1.19520600	1.91990700
H	1.44494000	1.31095200	2.74419300
C	1.61341900	-1.10604400	1.71894100
O	1.65886200	-2.19358100	1.16680400
O	2.37435200	-0.81446200	2.78900100
C	3.30882000	-1.82973000	3.17798600
C	4.21892800	-1.22227200	4.22224100

H	3.86316600	-2.15400500	2.29264900
H	2.75679600	-2.69233800	3.56549700
H	4.94630800	-1.96396400	4.56018100
H	4.75971100	-0.36946000	3.80400800
H	3.64502100	-0.88030800	5.08678100
C	-0.35033000	2.20984200	1.86125200
C	-0.21857400	3.49759400	1.32789700
C	-1.55760400	1.85737500	2.47836100
C	-1.28061300	4.39475600	1.39740500
H	0.71214600	3.73269700	0.82449000
C	-2.61207000	2.76351000	2.55968100
H	-1.66990400	0.86644400	2.91070600
C	-2.47697100	4.03703100	2.01663900
H	-1.17079900	5.38423100	0.96342800
H	-3.53940100	2.46742100	3.04005000
H	-3.30097000	4.74237400	2.06789400
C	-1.79704700	-2.29563400	0.64760600
C	-2.30524700	-3.46346200	0.06938800
C	-1.55360300	-2.23998700	2.02612800
C	-2.56197000	-4.57330700	0.86909500
H	-2.49884800	-3.50921900	-0.99736100
C	-1.81261300	-3.35445800	2.81566800
H	-1.15243100	-1.33717700	2.47489100
C	-2.31510500	-4.51938000	2.23807300
H	-2.95403100	-5.47926600	0.42002300
H	-1.61946500	-3.31299400	3.88199400
H	-2.51605400	-5.38705300	2.85783000
C	-1.51067400	-1.36605500	-2.11212200
C	-0.46464400	-2.18996700	-2.55409900
C	-2.51568300	-0.97222700	-2.99845500
C	-0.42267300	-2.59757000	-3.88201700
H	0.30800000	-2.52851800	-1.86759200
C	-2.46485600	-1.38707500	-4.32749800
H	-3.33310200	-0.34446900	-2.65969800
C	-1.41966700	-2.19201400	-4.76931500
H	0.38785500	-3.23280300	-4.22248000
H	-3.24399300	-1.07671600	-5.01512500
H	-1.38169400	-2.50922400	-5.80612700
C	-2.86585400	0.32610700	-0.13038800
C	-2.86517500	1.54531700	-0.82268000
C	-3.93010500	-0.00001900	0.71599200
C	-3.92149900	2.43203400	-0.65677500
H	-2.05907500	1.79433400	-1.50471400
C	-4.98852400	0.89174600	0.86680000

H	-3.93714600	-0.94337300	1.25234200
C	-4.98270800	2.10534100	0.18600900
H	-3.91504700	3.37744200	-1.18813200
H	-5.81623800	0.63520100	1.51921300
H	-5.80659100	2.80051200	0.31038800
H	-0.11917100	1.90769700	-0.69543600
C	1.99706300	1.55710400	-0.70603900
O	2.16272300	2.25135400	0.43583600
C	2.97488700	0.36571800	-0.85401800
C	3.97947400	0.22298600	0.10170300
C	2.88826100	-0.57573500	-1.88590700
C	4.87767900	-0.84095600	0.03598300
H	4.01758000	0.96125700	0.89571000
C	3.77697500	-1.64635400	-1.94828400
H	2.11926800	-0.47837100	-2.64896600
C	4.77650000	-1.78234800	-0.98631900
H	5.65864800	-0.93739700	0.78591600
H	3.68974900	-2.37416800	-2.74993000
H	5.47049800	-2.61581200	-1.03467900
C	2.28679300	2.52539400	-1.87021400
F	1.46052700	3.58906300	-1.83530300
F	2.13216000	1.97828900	-3.10220000
F	3.54029300	2.99967900	-1.82352800
H	0.75837600	-1.01544100	-0.50714600

M5<sub>1</sub><sup>(S,R,S)</sup>

P	1.62169600	-0.79381800	0.22445800
C	-0.18874100	-0.37090600	0.20329300
C	-0.56909600	0.56294600	1.36281800
H	-0.44441000	0.08951600	2.34076700
C	-0.77739300	0.11374600	-1.08507200
C	-1.22719900	1.53582800	-1.09769900
H	-1.86333700	1.67545500	-1.97626800
C	-1.50662400	-0.87777500	-1.77915100
O	-1.42179100	-2.10303700	-1.61055600
O	-2.37413200	-0.38390500	-2.73271600
C	-3.17697600	-1.35625800	-3.38970400
C	-4.23989700	-0.61004400	-4.16951100
H	-3.62310800	-2.02654400	-2.64857600
H	-2.55290000	-1.97004400	-4.05082000
H	-4.88105200	-1.31330200	-4.70700700
H	-4.86284000	-0.02020100	-3.49106300
H	-3.78590700	0.06925600	-4.89551000

C	-0.12435100	2.58871100	-1.17497000
C	-0.09553800	3.71446600	-0.35045900
C	0.84856600	2.46329600	-2.17235000
C	0.88548500	4.69306500	-0.52059600
H	-0.84542600	3.82011300	0.42474600
C	1.81825300	3.44239100	-2.35105400
H	0.83476100	1.57916900	-2.80493500
C	1.83859400	4.56649300	-1.52482300
H	0.89616000	5.56100200	0.13233500
H	2.56809000	3.32388200	-3.12769900
H	2.60094700	5.32827100	-1.65769900
C	1.94495700	-2.11252400	-0.96895300
C	2.63638700	-3.26252000	-0.57581200
C	1.53627500	-1.95238900	-2.29920100
C	2.91405100	-4.25391900	-1.51297000
H	2.95694900	-3.38750300	0.45354900
C	1.82242800	-2.94688600	-3.22679500
H	0.99154600	-1.05912600	-2.58975200
C	2.50782600	-4.09621600	-2.83499000
H	3.44853000	-5.14700900	-1.20767900
H	1.50332400	-2.82703600	-4.25656800
H	2.72520700	-4.87046600	-3.56374400
C	2.00122800	-1.44254400	1.87553300
C	1.09341200	-2.34310000	2.45297100
C	3.16066500	-1.08269500	2.56826200
C	1.34287500	-2.86552700	3.71627600
H	0.19749600	-2.64823700	1.91864600
C	3.40354000	-1.61236700	3.83376300
H	3.87215000	-0.39284900	2.12610000
C	2.49653200	-2.49830300	4.40815300
H	0.63746300	-3.56058400	4.15848500
H	4.30373700	-1.33046000	4.36912500
H	2.68804900	-2.90691200	5.39483700
C	2.76796200	0.56215900	-0.11967000
C	2.79709500	1.67997500	0.72633400
C	3.66446100	0.47259900	-1.18831900
C	3.71742100	2.69474500	0.49789100
H	2.12545600	1.75051700	1.57637300
C	4.58458500	1.49436200	-1.40823900
H	3.65303900	-0.39207600	-1.84271800
C	4.61310200	2.60107000	-0.56663400
H	3.73282100	3.56107900	1.15019400
H	5.28087700	1.41892300	-2.23660600
H	5.33136300	3.39601000	-0.73951700

H	0.02509700	1.48114500	1.35440100
C	-2.02727700	1.00147700	1.12840900
O	-2.10495900	1.87667900	0.03116900
C	-2.99538800	-0.17636900	0.98496300
C	-3.98440800	-0.12782600	0.00202800
C	-2.91802200	-1.29204200	1.82177300
C	-4.86990800	-1.18886000	-0.15728500
H	-4.02744400	0.73444300	-0.65369000
C	-3.80282800	-2.35639200	1.65862900
H	-2.16431700	-1.34042100	2.60356000
C	-4.77838800	-2.30908500	0.66693900
H	-5.63015200	-1.14270600	-0.93171900
H	-3.72700700	-3.22317100	2.30748500
H	-5.46462400	-3.13985200	0.53741000
C	-2.48128100	1.85963100	2.31088700
F	-1.68126000	2.92299300	2.49262200
F	-2.46107200	1.15776500	3.45713600
F	-3.72461500	2.31869200	2.13983700
H	-0.61072100	-1.37042300	0.38918600
TS6 <sub>1</sub> <sup>(S,R,S)</sup>			
P	1.51240200	-1.08698600	-0.16353000
C	-0.52386700	-0.47340000	-0.52387500
C	-1.38075600	-1.14711200	0.53352800
H	-1.56335400	-2.19912300	0.30137500
C	-0.68862200	0.93112300	-0.62495000
C	-1.40455900	1.71711400	0.44155600
H	-1.90051800	2.56736300	-0.04491700
C	-0.10888000	1.53095800	-1.77217700
O	0.46633700	0.91640700	-2.67945900
O	-0.18992300	2.89532800	-1.79049500
C	0.58174600	3.55338300	-2.79465100
C	0.76842100	4.98863600	-2.34903000
H	0.06176900	3.49515300	-3.75782300
H	1.54126900	3.03888200	-2.89892500
H	1.32263900	5.55105200	-3.10446600
H	-0.19743000	5.47617900	-2.19250100
H	1.33026200	5.01978600	-1.41078100
C	-0.48502100	2.26703600	1.51987900
C	-0.14581100	1.51278700	2.64585800
C	0.11815400	3.51378400	1.33080800
C	0.82742800	1.97010000	3.53344500
H	-0.65970500	0.57554800	2.83649900

C	1.08060600	3.97629900	2.22435900
H	-0.15267800	4.10396000	0.45994600
C	1.45294600	3.19685600	3.31968600
H	1.09526200	1.36475000	4.39426800
H	1.54396500	4.94576000	2.06442000
H	2.21064800	3.55209700	4.01070700
C	2.63376700	0.26603600	-0.59094500
C	3.56460800	0.15017200	-1.63036900
C	2.48367500	1.48847200	0.07370800
C	4.32972900	1.24904900	-2.00200000
H	3.68631000	-0.79272000	-2.15287300
C	3.25061500	2.58769000	-0.30913400
H	1.78486600	1.58651500	0.89651700
C	4.16756800	2.47198300	-1.34936200
H	5.05344100	1.15143500	-2.80438800
H	3.12401000	3.53043600	0.21410600
H	4.76185900	3.32971600	-1.64803900
C	1.86528700	-2.46213800	-1.28810200
C	1.49453400	-2.27837900	-2.62974200
C	2.45022000	-3.66600600	-0.88201700
C	1.71221200	-3.29893700	-3.55073600
H	1.06672300	-1.32725300	-2.94516700
C	2.65589100	-4.68226600	-1.81065800
H	2.74933000	-3.80886800	0.15153800
C	2.28578100	-4.50127300	-3.14188100
H	1.43221300	-3.15355800	-4.58884200
H	3.11151400	-5.61450500	-1.49340100
H	2.44852100	-5.29607800	-3.86249700
C	1.85633500	-1.62223800	1.53645500
C	1.17193400	-2.74507400	2.02843000
C	2.69673800	-0.90323400	2.39281100
C	1.33900300	-3.14671300	3.34862500
H	0.51329800	-3.31315200	1.37573000
C	2.85120400	-1.30465900	3.71723900
H	3.23102400	-0.03103900	2.03104300
C	2.17571500	-2.42334700	4.19728400
H	0.81059200	-4.02047600	3.71499600
H	3.50541100	-0.73920400	4.37277200
H	2.29940300	-2.73230700	5.22992100
H	-0.91501800	-1.11447900	1.52188600
C	-2.69250400	-0.35313300	0.64049700
O	-2.42678700	0.94692800	1.11184600
C	-3.52553200	-0.34532100	-0.63858400
C	-4.28686100	0.78448900	-0.94404900

C	-3.58414900	-1.45551800	-1.48302600
C	-5.07424200	0.81347700	-2.09129700
H	-4.25059200	1.63985200	-0.27758900
C	-4.37143600	-1.42537500	-2.63157600
H	-3.01499600	-2.35137200	-1.25575100
C	-5.11599900	-0.29016200	-2.94049900
H	-5.65533400	1.70032700	-2.32320200
H	-4.40054800	-2.29168200	-3.28451800
H	-5.72656200	-0.26652100	-3.83729800
C	-3.53346500	-0.95726600	1.76899000
F	-2.85987700	-0.98380800	2.92978100
F	-3.87458900	-2.22318800	1.47926600
F	-4.65953700	-0.26902300	1.97622900
H	-0.53908900	-0.98415000	-1.48940300

TS2<sub>1</sub><sup>(S,S)</sup>

P	1.66797000	-0.28631000	0.31972200
C	1.74157700	-1.85744600	1.23894200
C	1.41251000	-1.86766000	2.60229100
C	2.16814200	-3.03438300	0.61972900
C	1.47885600	-3.05205800	3.32438000
H	1.10235000	-0.94959700	3.09590600
C	2.24256900	-4.21694400	1.35299500
H	2.43508100	-3.03368600	-0.43130100
C	1.89391200	-4.22811700	2.69936400
H	1.21534200	-3.05572200	4.37654400
H	2.57500700	-5.12786700	0.86706700
H	1.94986100	-5.15067000	3.26596600
C	2.52661900	-0.59730700	-1.24467700
C	3.92140600	-0.58012100	-1.30226600
C	1.76609200	-0.89441600	-2.37964900
C	4.56157900	-0.87109500	-2.50211300
H	4.51043700	-0.32689800	-0.42635200
C	2.42136000	-1.18375700	-3.57433200
H	0.68007100	-0.89533800	-2.33540900
C	3.81285200	-1.17433300	-3.63759200
H	5.64521500	-0.85407000	-2.55024800
H	1.83847200	-1.41394500	-4.45924700
H	4.31544600	-1.39916200	-4.57247600
C	2.52957000	0.85782100	1.43778900
C	1.97085500	2.09781800	1.76017900
C	3.72124100	0.44759600	2.04523400
C	2.61793500	2.92932100	2.66724700

H	1.03052600	2.40360700	1.31302500
C	4.37376300	1.29517100	2.93525900
H	4.13255600	-0.53851300	1.84666400
C	3.82339500	2.53578500	3.24543800
H	2.17724900	3.88785700	2.92146200
H	5.30262000	0.97667800	3.39671600
H	4.32700600	3.19093800	3.94883300
C	-0.07489000	0.23093200	0.10389700
C	-0.41542500	1.30571800	-0.71523300
C	-1.03058600	-0.56915200	0.74486000
C	-1.95719100	-1.64169200	-1.02482400
H	-0.73096700	-1.36240600	1.41477100
H	-1.98048500	-0.10511900	0.97723400
C	-1.86195900	1.74668900	-0.80375700
H	-2.51121800	0.87745800	-0.90064800
H	-1.99234600	2.33797400	-1.71247900
C	0.60805900	2.12842200	-1.33580400
O	1.81765900	2.01366500	-1.15983100
O	0.11487700	3.09201600	-2.14194600
C	1.08819500	3.94621200	-2.75852000
C	0.32986800	4.97100100	-3.57197700
H	1.69688600	4.41286800	-1.97717000
H	1.75246700	3.33817800	-3.37962300
H	1.03225400	5.65378000	-4.05518000
H	-0.33606000	5.55506600	-2.93051500
H	-0.26985400	4.48344000	-4.34505200
C	-2.29667900	2.56639800	0.39806700
C	-1.59551500	3.72280900	0.75839000
C	-3.39799900	2.18664100	1.16761800
C	-1.97977300	4.47551800	1.86388700
H	-0.74640400	4.03869200	0.15584900
C	-3.78606700	2.93726300	2.27804700
H	-3.95621400	1.29235600	0.89242500
C	-3.07687700	4.08184400	2.63063300
H	-1.42589300	5.37146800	2.12753600
H	-4.64209100	2.62545600	2.86814200
H	-3.37603800	4.66647900	3.49540800
C	-1.22318300	-2.97484900	-0.79493100
C	-3.38494900	-1.59104300	-0.53492500
C	-4.31717200	-0.97406200	-1.37384100
C	-3.81349900	-2.11969000	0.68807200
C	-5.65214800	-0.87207800	-0.99504300
H	-3.97015200	-0.57419900	-2.32071700
C	-5.14981200	-2.01942000	1.06381100



H	-3.10290200	-2.59349900	1.35646200
C	-6.07218400	-1.39276200	0.22732100
H	-6.36531900	-0.38926000	-1.65539800
H	-5.47055400	-2.42613500	2.01728200
H	-7.11256300	-1.31397700	0.52612200
O	-1.62286100	-1.03453700	-2.05372200
F	0.04288100	-2.89899300	-1.22401700
F	-1.82858900	-3.92949000	-1.52969400
F	-1.18911900	-3.43598200	0.46624800
M2 <sub>1</sub> <sup>(S,S)</sup>			
P	1.65649300	-0.42523400	0.28920200
C	1.56968500	-2.00873800	1.17722500
C	1.15591400	-2.00746000	2.51690000
C	1.96820700	-3.20091900	0.57152400
C	1.10918100	-3.19843400	3.22920600
H	0.87140500	-1.07700600	3.00242500
C	1.93434100	-4.38991900	1.29701500
H	2.29323700	-3.20713900	-0.46337500
C	1.49901800	-4.39060400	2.61791800
H	0.77847300	-3.19594100	4.26209600
H	2.24560300	-5.31493900	0.82389800
H	1.46866400	-5.31950200	3.17787300
C	2.47329500	-0.75147900	-1.29111000
C	3.86566500	-0.75522700	-1.39520000
C	1.66059600	-1.03683300	-2.39488000
C	4.45705500	-1.06290700	-2.61571300
H	4.48805100	-0.50233000	-0.54292600
C	2.27253800	-1.34367700	-3.60881600
H	0.57013700	-1.01635100	-2.31277500
C	3.66069100	-1.35991900	-3.72040600
H	5.53812200	-1.06283500	-2.70435600
H	1.65612600	-1.56767300	-4.47315300
H	4.12536800	-1.59790800	-4.67185600
C	2.59383700	0.60194200	1.46066600
C	2.10724200	1.83493900	1.90072500
C	3.77466200	0.08023300	2.00108600
C	2.81692600	2.55377700	2.85701500
H	1.17260200	2.22778600	1.51330100
C	4.49108400	0.81647200	2.93933900
H	4.12802800	-0.90534500	1.71019500
C	4.01293100	2.05276000	3.36679500
H	2.43163900	3.50632600	3.20457100

H	5.41266500	0.41509200	3.34632700
H	4.56535200	2.61958200	4.10886600
C	-0.02778600	0.22623800	0.01119400
C	-0.26659300	1.36479700	-0.68535600
C	-1.17617000	-0.60244700	0.47213400
C	-1.92773500	-1.32938400	-0.80080100
H	-0.89128400	-1.34747200	1.21375200
H	-1.90634800	0.05705300	0.94563400
C	-1.66944200	1.92331100	-0.84441200
H	-2.36349600	1.10401900	-1.01659900
H	-1.69517200	2.55228600	-1.73604800
C	0.86061100	2.17222200	-1.24275900
O	2.03553500	1.95136000	-1.01884100
O	0.45438400	3.17924700	-2.01254300
C	1.49610600	3.99610800	-2.58473100
C	0.81749000	5.10106200	-3.36051300
H	2.11969600	4.37950000	-1.77260900
H	2.11934800	3.36190700	-3.22068800
H	1.57204700	5.74532300	-3.81668700
H	0.19486400	5.70874700	-2.70006300
H	0.18935300	4.68655900	-4.15177500
C	-2.07657500	2.73555000	0.37048500
C	-1.32289800	3.84166100	0.78096800
C	-3.21214100	2.38616900	1.10624800
C	-1.69063800	4.57585600	1.90416000
H	-0.45001400	4.14090100	0.20480100
C	-3.58432400	3.12327600	2.23043000
H	-3.80674400	1.52972500	0.79073000
C	-2.82347200	4.21697700	2.63405500
H	-1.09750100	5.43336400	2.20653300
H	-4.46948800	2.83956900	2.79109600
H	-3.11189200	4.78964100	3.50957700
C	-1.48946500	-2.80940900	-0.75554600
C	-3.44158800	-1.28652200	-0.45774900
C	-4.30834600	-0.81117000	-1.44017700
C	-3.96770300	-1.65712100	0.78481300
C	-5.67410900	-0.69245300	-1.18957900
H	-3.86640800	-0.52912400	-2.39041800
C	-5.33287100	-1.54380500	1.03741300
H	-3.31065500	-2.03242300	1.56451300
C	-6.19081400	-1.05764700	0.05130400
H	-6.33678100	-0.31435700	-1.96271700
H	-5.72786200	-1.83333100	2.00677300
H	-7.25399500	-0.96502600	0.25072400

O	-1.62219200	-0.83314500	-1.98338500
F	-0.19895500	-2.93776700	-1.12882400
F	-2.20802600	-3.56034000	-1.60577000
F	-1.58510600	-3.40784000	0.45651000
TS3 <sub>1</sub> <sup>(S,S,R)</sup>			
P	1.34853600	-1.21912400	0.13226100
C	-0.02846900	-0.10927800	0.40600600
C	-1.36657300	-0.67781100	0.82948400
H	-1.27120100	-1.72279000	1.13734100
C	0.08139900	1.22936100	0.18246100
C	-1.09421600	2.11138400	0.23080500
H	-1.75231200	1.42282000	-0.62882200
C	1.38105900	1.82372100	-0.28951300
O	1.93877400	1.51598200	-1.32125800
O	1.83775500	2.72864000	0.56711300
C	3.06119000	3.38324900	0.18801600
C	3.39947200	4.36327500	1.28671700
H	2.89757300	3.87907700	-0.77399200
H	3.83374100	2.61873400	0.05644900
H	4.31431400	4.90395000	1.03281000
H	2.58955300	5.08605000	1.41373700
H	3.55485700	3.83960700	2.23271000
C	-0.92429600	3.55442200	-0.09360700
C	-0.37551900	3.95563600	-1.32229300
C	-1.33824300	4.55488300	0.79251000
C	-0.20805900	5.30084800	-1.63000200
H	-0.07601100	3.19757900	-2.04343700
C	-1.19196600	5.90245900	0.47920100
H	-1.77529500	4.26627400	1.74567400
C	-0.61565900	6.28451800	-0.73026300
H	0.22865200	5.58415600	-2.58535000
H	-1.52049000	6.65959400	1.18640700
H	-0.49373300	7.33614100	-0.97313000
C	2.90201300	-0.48113200	0.72239400
C	4.08548200	-0.60536500	-0.00882700
C	2.89614600	0.21096900	1.93798500
C	5.26537300	-0.05826600	0.49253600
H	4.09057600	-1.10627400	-0.97068000
C	4.07914500	0.75105100	2.43300800
H	1.96780200	0.34636800	2.48759600
C	5.26333000	0.61334900	1.71229500
H	6.18312000	-0.15219000	-0.07776900

H	4.07186800	1.28254700	3.37984100
H	6.18520900	1.03951100	2.09703300
C	1.48464800	-1.69335300	-1.60342500
C	0.71623200	-1.02736800	-2.56294000
C	2.33669600	-2.74457700	-1.97022100
C	0.83413200	-1.39983600	-3.89844600
H	0.00065800	-0.26614800	-2.25614900
C	2.45154000	-3.09934600	-3.30919300
H	2.90017800	-3.28673500	-1.21370800
C	1.70317800	-2.42042500	-4.27160000
H	0.23598700	-0.89376900	-4.64824400
H	3.11470600	-3.90597200	-3.59947300
H	1.78834900	-2.70188500	-5.31716500
C	1.10362100	-2.75908100	1.06544000
C	0.30107400	-3.76854400	0.51434100
C	1.67558000	-2.93261800	2.32874600
C	0.06610700	-4.93436700	1.23307400
H	-0.14330300	-3.63964700	-0.46818400
C	1.43912600	-4.10677100	3.04073200
H	2.31306700	-2.16673700	2.75798700
C	0.63387700	-5.10270600	2.49563800
H	-0.56025100	-5.71033700	0.80564700
H	1.88834600	-4.24057200	4.01739800
H	0.45229500	-6.01631800	3.05179600
H	-1.68741600	-0.13850900	1.72761500
C	-2.50381200	-0.54126300	-0.27104500
O	-2.19967400	0.30938800	-1.29456700
C	-3.83273400	-0.19208500	0.42962100
C	-4.24467000	-0.80155000	1.61940100
C	-4.66092200	0.76069900	-0.16393800
C	-5.45780000	-0.45127900	2.20973900
H	-3.61909500	-1.55329200	2.09384400
C	-5.87251000	1.11300200	0.42635800
H	-4.32181400	1.21795000	-1.08716100
C	-6.27526700	0.50725700	1.61581100
H	-5.76416200	-0.92901700	3.13660400
H	-6.50303100	1.86358800	-0.04254400
H	-7.21862400	0.78115200	2.07572500
C	-2.69015700	-1.92722600	-0.90634800
F	-1.58162500	-2.31188800	-1.57592700
F	-3.69851500	-1.94857000	-1.78716600
F	-2.93525300	-2.90646300	-0.00672400
H	-1.68574100	1.94715300	1.13979600

M3<sub>1</sub><sup>(S,S,R)</sup>

P	0.17683100	-1.65510500	0.12442500
C	-0.07534400	0.06120900	0.14439200
C	-1.39023000	0.60532300	0.65210300
H	-1.96362300	-0.16086900	1.18077500
C	1.01021000	1.00496600	-0.06028200
C	0.91199500	2.35939900	0.07201400
H	-0.81018000	1.22386000	-1.58839800
C	2.33900700	0.42720800	-0.45832000
O	2.50767900	-0.30162800	-1.41594100
O	3.31377700	0.76776700	0.38076800
C	4.61373700	0.23959600	0.07053200
C	5.56573500	0.75724900	1.12384500
H	4.89300500	0.57032300	-0.93521400
H	4.54894300	-0.85393100	0.06821700
H	6.57423700	0.38721200	0.92600800
H	5.58538100	1.84978400	1.11612400
H	5.25824400	0.41734000	2.11565800
C	1.94915900	3.36553900	-0.19217700
C	2.92570800	3.23338600	-1.19538400
C	1.94719700	4.55341400	0.55742500
C	3.88928100	4.21572100	-1.39499400
H	2.91678300	2.36219200	-1.84523400
C	2.90488700	5.54090500	0.35303300
H	1.18641000	4.68932200	1.32168300
C	3.89044500	5.37363300	-0.61810200
H	4.63330300	4.08371300	-2.17487800
H	2.88354100	6.44331200	0.95654300
H	4.64029900	6.14144300	-0.77825900
C	1.76014300	-2.13025800	0.91443900
C	2.55824500	-3.18115800	0.45230900
C	2.15623100	-1.40824200	2.04602800
C	3.72495200	-3.51933700	1.13372900
H	2.28203600	-3.72773200	-0.44303900
C	3.32045900	-1.75278600	2.72684900
H	1.56395400	-0.55967700	2.37856400
C	4.10438800	-2.81049000	2.27273000
H	4.34130200	-4.33465100	0.76982300
H	3.61643800	-1.18802500	3.60484500
H	5.01462500	-3.07703200	2.80008400
C	0.10992800	-2.50900100	-1.49123800
C	0.16674000	-1.76137900	-2.66749700
C	-0.03310000	-3.90085800	-1.55796000

C	0.09063400	-2.39825100	-3.90265200
H	0.28360600	-0.68450000	-2.60890500
C	-0.10454500	-4.53515600	-2.79429300
H	-0.10039600	-4.48902100	-0.64596600
C	-0.04386000	-3.78294400	-3.96650000
H	0.13233300	-1.81204100	-4.81451300
H	-0.21624100	-5.61323400	-2.84189600
H	-0.10784200	-4.27762700	-4.93038800
C	-1.12626000	-2.47756800	1.10742500
C	-2.30268200	-2.92585500	0.49852400
C	-0.97840500	-2.59725200	2.49391200
C	-3.31986900	-3.48072100	1.27065100
H	-2.43251500	-2.83114500	-0.57353200
C	-1.99626200	-3.15565400	3.25987500
H	-0.06857800	-2.26120000	2.98021300
C	-3.16858100	-3.59688900	2.64925800
H	-4.23193000	-3.81960200	0.79063400
H	-1.87068100	-3.24878900	4.33341400
H	-3.96222200	-4.03181500	3.24811900
H	-1.18728500	1.38934200	1.39220600
C	-2.33456400	1.23613200	-0.42646600
O	-1.62886400	1.74245000	-1.52988500
C	-3.18087100	2.34217900	0.18536900
C	-3.93985100	2.09705300	1.33504300
C	-3.18237400	3.62037000	-0.37244300
C	-4.68950700	3.11621000	1.91342000
H	-3.94784100	1.10801400	1.78231700
C	-3.93255600	4.63997100	0.21086700
H	-2.58819700	3.81046100	-1.25828900
C	-4.68801400	4.39201400	1.35312800
H	-5.27246800	2.91252600	2.80594700
H	-3.92329500	5.63168600	-0.23048300
H	-5.27004000	5.18767900	1.80707400
C	-3.25698600	0.15821700	-1.00784300
F	-2.53788600	-0.77886400	-1.65906200
F	-4.12234300	0.66881700	-1.89053300
F	-3.97524500	-0.48420700	-0.06984100
H	-0.04638000	2.77344800	0.37526700
TS4 <sub>1</sub> <sup>(S,S,R)</sup>			
P	0.61662700	-1.56907300	-0.24840200
C	-0.92901300	-2.52053800	-0.29105300
C	-1.23676500	-3.41415700	0.73803000

C	-1.85115400	-2.29744500	-1.32388000
C	-2.45132600	-4.09527200	0.72273400
H	-0.53945400	-3.57037700	1.55435700
C	-3.05354300	-2.99343100	-1.34094900
H	-1.64049800	-1.56903200	-2.10209600
C	-3.35340100	-3.89229800	-0.31802000
H	-2.68880200	-4.78494400	1.52564300
H	-3.76315600	-2.82249500	-2.14321500
H	-4.29616700	-4.43002600	-0.32987400
C	1.55579900	-1.96691600	-1.76199600
C	0.99980000	-2.70636300	-2.80995500
C	2.89504400	-1.55443600	-1.84219400
C	1.76327200	-3.00173700	-3.93737100
H	-0.01703000	-3.07485200	-2.75110700
C	3.64735200	-1.84864400	-2.97332000
H	3.35711000	-1.01494800	-1.02179900
C	3.08180800	-2.56792100	-4.02479500
H	1.32249600	-3.57892300	-4.74308300
H	3.67308500	-2.80049800	-4.90421900
C	1.61658200	-2.23994600	1.10230600
C	1.77579200	-1.55724800	2.31059000
C	2.16832200	-3.51755600	0.92903900
C	2.48429800	-2.16654600	3.34515600
H	1.39755800	-0.54710600	2.43056400
C	2.86583000	-4.11624700	1.97021100
H	2.05094000	-4.04248800	-0.01556200
C	3.02117900	-3.43982700	3.18012900
H	2.61972800	-1.63730000	4.28221700
H	3.29072300	-5.10527100	1.83709500
H	3.56851000	-3.90666900	3.99268800
C	0.22011700	0.18984400	-0.03776800
C	-1.25868000	0.46710400	-0.04366400
C	1.15266400	1.18255600	-0.72156200
C	1.87339800	1.97755100	0.48187200
H	1.88172400	0.71876900	-1.38960900
H	0.60080000	1.89898000	-1.32960400
C	-1.88386200	1.28218900	-0.91069900
C	-1.97956300	-0.15670500	1.12155700
O	-1.46632900	-0.34764200	2.20494100
O	-3.22323800	-0.52678900	0.82300100
C	-4.02582200	-1.00950900	1.91100200
C	-5.40864500	-1.25529500	1.35120500
H	-3.56786300	-1.91987300	2.30973600
H	-4.03069700	-0.25406500	2.70384300

H	-6.07463500	-1.61269000	2.13961800
H	-5.36806400	-2.00639900	0.55819600
H	-5.81718600	-0.33005500	0.93618000
O	1.34847000	1.60441500	1.66902000
H	0.55542400	0.54228900	1.07539000
H	4.68012100	-1.52154200	-3.02715000
C	1.80736400	3.48915700	0.22366600
C	1.36092200	4.31911800	1.24995000
C	2.17873500	4.06131400	-0.99721700
C	1.28250700	5.69770200	1.06453300
H	1.07303600	3.84977100	2.18407300
C	2.10481900	5.43933600	-1.18402700
H	2.52780900	3.42803700	-1.80827200
C	1.65612500	6.26264000	-0.15260500
H	0.92998900	6.33292300	1.87187900
H	2.39646600	5.87101000	-2.13686100
H	1.59662300	7.33670900	-0.29908600
C	3.34946500	1.56052100	0.46840600
F	3.47148000	0.24060700	0.74920800
F	4.07838600	2.21508000	1.38161900
F	3.96782100	1.73875500	-0.72262700
C	-3.25583800	1.81878200	-0.81815000
C	-3.78930100	2.27556300	0.39461000
C	-4.03272100	1.92399200	-1.97694900
C	-5.08132300	2.78350400	0.45218300
H	-3.17644000	2.24738300	1.29192100
C	-5.32979500	2.42599600	-1.91911900
H	-3.61949900	1.59502900	-2.92671200
C	-5.85970600	2.85260000	-0.70383300
H	-5.47895500	3.13743300	1.39807000
H	-5.92450300	2.48760800	-2.82492400
H	-6.86786200	3.25159200	-0.65823200
H	-1.31556900	1.62966100	-1.77185500
M4 <sub>1</sub> (S,S,R)			
P	0.28336000	-1.64849300	-0.23331500
C	-1.42816400	-2.25028100	-0.26843200
C	-1.92093000	-3.06434000	0.75491400
C	-2.28962800	-1.80221500	-1.28161800
C	-3.26094900	-3.44596800	0.74958300
H	-1.26981700	-3.39194100	1.55842600
C	-3.62225200	-2.19250000	-1.28324400
H	-1.92718800	-1.13647400	-2.05946300



C	-4.10751500	-3.01586000	-0.26832200
H	-3.63978900	-4.07904400	1.54478000
H	-4.28340700	-1.84416700	-2.06919800
H	-5.14983500	-3.31854800	-0.26947900
C	1.07866100	-2.12134100	-1.80266600
C	0.37006800	-2.70283100	-2.85866100
C	2.46722000	-1.95146000	-1.91047000
C	1.03842500	-3.07341400	-4.02341800
H	-0.69345500	-2.89113200	-2.77994700
C	3.12401700	-2.31860200	-3.07870500
H	3.03782700	-1.54493800	-1.08268700
C	2.41003500	-2.87327200	-4.13927600
H	0.48151300	-3.52650000	-4.83641000
H	2.92647000	-3.16128100	-5.04896100
C	1.17651600	-2.54012600	1.05914300
C	1.72568100	-1.88895500	2.16696400
C	1.29009400	-3.93123300	0.91400400
C	2.37214600	-2.65236000	3.13939300
H	1.71443400	-0.80179100	2.24770800
C	1.93081600	-4.67621400	1.89394200
H	0.87464500	-4.42776700	0.04010300
C	2.46781600	-4.03379800	3.01084300
H	2.80991500	-2.15582200	3.99874500
H	2.01542300	-5.75212700	1.78620200
H	2.97171600	-4.61464400	3.77670200
C	0.25990100	0.16935000	0.10797200
C	-1.15960900	0.69469700	0.09805600
C	1.33375300	1.00267500	-0.58938600
C	2.31462900	1.58922500	0.55171000
H	1.88842900	0.45247300	-1.35293500
H	0.87177000	1.84365800	-1.10608200
C	-1.65942600	1.51187600	-0.84195100
C	-1.94770000	0.22479000	1.29014000
O	-1.43227600	-0.08405100	2.34499600
O	-3.25084500	0.11379200	1.04992100
C	-4.08054800	-0.22736900	2.17278600
C	-5.51179200	-0.16063700	1.69066900
H	-3.80192500	-1.22595700	2.52311300
H	-3.88473600	0.48456000	2.98058000
H	-6.19367700	-0.38365100	2.51419000
H	-5.67947800	-0.88578200	0.89065100
H	-5.73374300	0.83906700	1.30784500
O	1.90223400	1.31266100	1.79234800
H	0.58304300	0.26828400	1.17583200

H	4.19667500	-2.17731300	-3.15498700
C	2.51826200	3.09926000	0.28400200
C	2.37389100	3.97506600	1.35731600
C	2.83541900	3.62069800	-0.97465000
C	2.53663400	5.34786900	1.18316400
H	2.12261100	3.54032000	2.31850000
C	3.00237000	4.99216200	-1.15228100
H	2.95307500	2.95360800	-1.82448500
C	2.85275800	5.86113900	-0.07263300
H	2.41674000	6.01990200	2.02818500
H	3.24721000	5.38355900	-2.13537600
H	2.97990800	6.93047300	-0.21169000
C	3.68201900	0.91481700	0.33259800
F	3.61268700	-0.40941100	0.61680600
F	4.63921800	1.42063200	1.12186000
F	4.15402900	0.98416900	-0.93725700
C	-2.95549800	2.21937100	-0.83737900
C	-3.42333500	2.88511800	0.30240400
C	-3.71410600	2.27161500	-2.01131800
C	-4.63921200	3.55661600	0.27790600
H	-2.81905100	2.88429500	1.20544200
C	-4.93865400	2.93382500	-2.03288800
H	-3.34674000	1.77835700	-2.90747700
C	-5.40556100	3.57500900	-0.88831800
H	-4.98723100	4.07307400	1.16683300
H	-5.52449500	2.95427700	-2.94613000
H	-6.35500800	4.10022700	-0.90724800
H	-1.03604100	1.70798500	-1.71373900
M4 <sub>1</sub> <sup>r(S,S,R)</sup>			
P	0.00563100	-1.80805300	-0.32626100
C	0.22158000	-0.07086700	0.35228500
C	1.52312100	0.54194300	-0.18074800
H	2.31554100	-0.17987200	0.04082900
C	-1.06376400	0.70992000	0.22775000
C	-1.14919900	1.76505500	-0.59979300
H	0.36107800	-0.27585400	1.41704200
C	-2.07722600	0.27248300	1.22633500
O	-1.81280300	-0.49271800	2.13821300
O	-3.30022500	0.74567300	1.01547500
C	-4.33352600	0.24904000	1.88361400
C	-5.64520600	0.77629200	1.34690900
H	-4.13399500	0.59122900	2.90292000

H	-4.29261800	-0.84504200	1.87471700
H	-6.46644700	0.45577100	1.99167600
H	-5.63321700	1.86804600	1.30787900
H	-5.82575000	0.39426700	0.33837100
C	-2.20115900	2.78692500	-0.78043400
C	-1.78044800	4.11739300	-0.64406100
C	-3.52168000	2.51992300	-1.15298300
C	-2.68167600	5.16015700	-0.83307900
H	-0.74265400	4.29441200	-0.37054800
C	-4.41353000	3.56738800	-1.36403900
H	-3.84836500	1.49271200	-1.27374600
C	-3.99983500	4.88772900	-1.19574900
H	-2.35335000	6.18697700	-0.70575100
H	-5.43659900	3.35074200	-1.65620900
H	-4.70189300	5.70055800	-1.35280300
C	-1.74447700	-2.28368100	-0.36454500
C	-2.19102000	-3.36094600	0.40663100
C	-2.66039200	-1.53871300	-1.12235300
C	-3.54497000	-3.68303900	0.42735400
H	-1.49166900	-3.94152700	0.99863500
C	-4.01153200	-1.86818600	-1.09485900
H	-2.32753700	-0.69499600	-1.71893400
C	-4.45521000	-2.93591400	-0.31630100
H	-3.88597700	-4.51757800	1.03008100
H	-4.71544300	-1.28827800	-1.68278100
H	-5.51061000	-3.18676000	-0.29287300
C	0.88216800	-2.93311400	0.78389000
C	0.73502500	-2.75314700	2.16699300
C	1.63722200	-4.00053900	0.28713700
C	1.36573500	-3.63019600	3.04249000
H	0.10658000	-1.95613000	2.55617700
C	2.26623100	-4.86935700	1.17379300
H	1.73778100	-4.15475800	-0.78208200
C	2.13580000	-4.68096600	2.54724700
H	1.25326000	-3.49198800	4.11218900
H	2.85743300	-5.69305800	0.78891500
H	2.62953500	-5.35945000	3.23508000
C	0.69638400	-1.98915900	-1.99376800
C	2.08706200	-1.91172600	-2.17205800
C	-0.12837700	-2.22522700	-3.09845100
C	2.63459600	-2.04736000	-3.44132700
H	2.74816100	-1.76457300	-1.32455800
C	0.42943900	-2.35585000	-4.36801000
H	-1.20072900	-2.32350900	-2.97941000

C	1.80606300	-2.26230600	-4.54149700
H	3.70970900	-1.98680600	-3.56866500
H	-0.21833100	-2.53829700	-5.21838600
H	2.23697800	-2.36640000	-5.53162600
H	1.49530600	0.66766100	-1.26822800
C	1.96394100	1.96237800	0.37983400
O	1.29047500	2.99727800	-0.11489800
C	3.49994700	2.04422800	0.09173800
C	4.45119400	1.13192300	0.56440900
C	3.93011500	3.09700200	-0.71281700
C	5.79840500	1.27712300	0.24027600
H	4.14844800	0.30568900	1.20160700
C	5.27523500	3.24185600	-1.04615500
H	3.16713600	3.78657400	-1.05773500
C	6.21624800	2.33197900	-0.56938800
H	6.52370100	0.56400000	0.62143600
H	5.59131300	4.06821500	-1.67673000
H	7.26594400	2.44306300	-0.82398800
C	1.79901500	1.92734800	1.91654600
F	0.50587500	2.00449800	2.28596800
F	2.42756400	2.94949600	2.51869900
F	2.27248000	0.78914200	2.49905600
H	-0.22783500	2.01892500	-1.11932200
TS5 <sub>1</sub> <sup>(S,S,R)</sup>			
P	0.31960800	1.96963200	-0.27473000
C	-0.23982600	0.29477100	0.37313700
C	-1.65497100	-0.09821600	-0.05418900
H	-2.36648900	0.63625800	0.33559200
C	0.78567900	-0.77188800	0.12990900
C	0.50796300	-1.74710600	-0.78689400
H	-0.25114900	0.49016400	1.45100500
C	1.89486300	-0.72709800	1.07693400
O	1.94392500	0.06491900	2.01329300
O	2.93004000	-1.52793300	0.77824500
C	4.09472500	-1.37974100	1.59642600
C	5.15265400	-2.29236800	1.01564300
H	3.84803200	-1.64217000	2.62978200
H	4.40428000	-0.32912900	1.58091400
H	6.06206300	-2.24743300	1.61918000
H	4.79571900	-3.32520400	0.99434100
H	5.39594800	-1.98983300	-0.00610800
C	1.26340600	-3.01245300	-0.91383800

C	1.24560600	-3.92298500	0.14595000
C	1.98306200	-3.31082100	-2.07081400
C	1.96771900	-5.10651700	0.05958100
H	0.63419500	-3.67854300	1.00838200
C	2.71693300	-4.49373700	-2.15169600
H	1.98155300	-2.61159100	-2.90324500
C	2.71278600	-5.39066600	-1.08685800
H	1.94841600	-5.81383100	0.88311800
H	3.28553200	-4.71722500	-3.04901600
H	3.27761600	-6.31541500	-1.15294000
C	2.12302800	1.99341600	-0.41865900
C	2.88035200	2.87442200	0.35926600
C	2.76423900	1.07158400	-1.25907000
C	4.26979600	2.82192400	0.30964400
H	2.39266800	3.59026400	1.01224900
C	4.15415900	1.02137400	-1.29572600
H	2.18618900	0.38298400	-1.86632800
C	4.90620000	1.89125100	-0.50826700
H	4.85398700	3.50467400	0.91685300
H	4.64564700	0.29907800	-1.93875700
H	5.99004000	1.84572600	-0.53629300
C	-0.18490900	3.22006200	0.92792000
C	0.09811800	2.96774400	2.27881300
C	-0.80792100	4.41117400	0.54527200
C	-0.25590800	3.90859200	3.23901200
H	0.61660500	2.05583500	2.56953300
C	-1.16193600	5.34295500	1.51704200
H	-1.01745000	4.61180500	-0.50047500
C	-0.89002700	5.09087000	2.85942800
H	-0.03652300	3.71753900	4.28378000
H	-1.64997200	6.26575200	1.22274000
H	-1.16940100	5.81981400	3.61312200
C	-0.40525500	2.37212600	-1.88373600
C	-1.79978100	2.48516600	-1.99463600
C	0.40016900	2.59189200	-3.00586400
C	-2.37543800	2.79631300	-3.22035600
H	-2.43644200	2.34471600	-1.12677300
C	-0.18575300	2.90064700	-4.23051300
H	1.47997400	2.53244900	-2.92915200
C	-1.56945500	2.99788000	-4.33980400
H	-3.45355800	2.88201100	-3.29958400
H	0.44417700	3.06989100	-5.09700200
H	-2.02251900	3.23753200	-5.29607500
H	-1.76214900	-0.11100500	-1.14359200

C	-2.09041500	-1.54102400	0.42585600
O	-1.37246900	-2.55360300	-0.09575200
C	-3.59850600	-1.64471400	0.07227500
C	-4.58264200	-0.81793400	0.62584300
C	-3.97577900	-2.59467900	-0.87437400
C	-5.91471500	-0.94629700	0.24019300
H	-4.31741900	-0.07641500	1.37380500
C	-5.30675200	-2.71971100	-1.26764200
H	-3.19509900	-3.22813500	-1.28018800
C	-6.28216300	-1.89612500	-0.71109000
H	-6.66748500	-0.30152400	0.68412800
H	-5.58393700	-3.46498600	-2.00781400
H	-7.32040200	-1.99369000	-1.01312400
C	-1.96475800	-1.59629000	1.96614000
F	-0.69019300	-1.77009200	2.36100100
F	-2.66732700	-2.61045100	2.49451200
F	-2.38803200	-0.46504100	2.58971700
H	-0.13604900	-1.50441600	-1.62601700

M5<sub>1</sub><sup>(S,S,R)</sup>

P	-1.93619800	-0.67637600	-0.18965600
C	-0.21396500	-0.38048500	0.68421100
C	0.78134400	-1.46979200	0.27826700
H	0.52858300	-2.43887700	0.71381300
C	0.31751100	0.96623100	0.41291500
C	1.57723200	0.99172600	-0.38210900
H	-0.52436600	-0.49948700	1.72961200
C	-0.42089400	1.99681700	1.00398900
O	-1.45562000	1.79089900	1.67839200
O	-0.01653900	3.28142600	0.76609400
C	-0.90125000	4.30184200	1.21072600
C	-0.32259400	5.61738900	0.73123000
H	-0.99005300	4.27543400	2.30264600
H	-1.90200800	4.12951900	0.79761000
H	-0.94051600	6.45433200	1.06591800
H	0.69094200	5.74842400	1.11941100
H	-0.27253700	5.63204900	-0.36094900
C	2.21111400	2.34399300	-0.59039100
C	3.00129500	2.90964400	0.41012800
C	2.00320700	3.04288200	-1.77662900
C	3.56250300	4.16954800	0.23001700
H	3.16239200	2.35080800	1.32697300
C	2.55509000	4.30998400	-1.95584900

H	1.40638800	2.59337400	-2.56740900
C	3.33567400	4.87640000	-0.95115900
H	4.17739900	4.60453000	1.01220000
H	2.38453300	4.84825700	-2.88317600
H	3.77390700	5.85981500	-1.09034800
C	-2.52149500	0.85149000	-0.94520400
C	-3.78066000	1.36701200	-0.62574200
C	-1.66800800	1.55841100	-1.80131100
C	-4.18361400	2.58536300	-1.15990200
H	-4.43683600	0.82619900	0.04887900
C	-2.07527400	2.78466700	-2.32381300
H	-0.69503200	1.15560400	-2.06335000
C	-3.32787600	3.29796700	-2.00026800
H	-5.16213700	2.98340500	-0.91339100
H	-1.41033000	3.33660300	-2.98007700
H	-3.64208600	4.25414100	-2.40647600
C	-3.18011400	-1.28064800	0.98005500
C	-3.25047900	-0.67798800	2.24385600
C	-4.07498000	-2.29954000	0.63190400
C	-4.20979800	-1.11325500	3.15464500
H	-2.57690200	0.14106900	2.48313800
C	-5.02889100	-2.72347800	1.55108200
H	-4.03003000	-2.75914300	-0.34998800
C	-5.09262800	-2.13488700	2.81252300
H	-4.26856100	-0.64936300	4.13361000
H	-5.72233100	-3.51247000	1.28017000
H	-5.83635200	-2.47082600	3.52795000
C	-1.79180000	-1.93296900	-1.49490700
C	-1.50446700	-3.25573200	-1.12399600
C	-1.92986600	-1.61086100	-2.84761000
C	-1.35363700	-4.23653800	-2.09598100
H	-1.41536300	-3.52295400	-0.07406200
C	-1.77299900	-2.59888100	-3.81798300
H	-2.16927100	-0.59654800	-3.14775400
C	-1.48333900	-3.90737900	-3.44515900
H	-1.13491600	-5.25711400	-1.80093800
H	-1.88383300	-2.34178600	-4.86594000
H	-1.36202500	-4.67381500	-4.20330600
H	0.79770100	-1.60720900	-0.80739900
C	2.22648800	-1.10763500	0.68156500
O	2.61429900	0.17322200	0.25000900
C	3.18237500	-2.15341900	0.09624600
C	3.06111100	-3.50915700	0.42002600
C	4.16505900	-1.75745000	-0.81029300

C	3.91235200	-4.44850000	-0.15445200
H	2.30808000	-3.84072600	1.12726400
C	5.01420500	-2.70053000	-1.38589600
H	4.25579900	-0.70664500	-1.05728300
C	4.89166600	-4.04788100	-1.06061400
H	3.80771700	-5.49658300	0.10749600
H	5.77456400	-2.37706700	-2.08984600
H	5.55436300	-4.78180600	-1.50781500
C	2.38043600	-1.08557000	2.21244400
F	1.73419300	-0.06030800	2.77709700
F	3.66777900	-0.97990100	2.56506800
F	1.89698000	-2.21018200	2.77825600
H	1.42817100	0.54086200	-1.38144900

TS6<sub>1</sub><sup>(S,S,R)</sup>

P	-2.00859000	-0.64728000	-0.17281100
C	-0.17625700	-0.35062900	0.85812600
C	0.75006900	-1.49110500	0.45947700
H	0.47049500	-2.43093900	0.94072600
C	0.36117600	0.94655400	0.56608000
C	1.61425500	0.93375400	-0.25108300
H	-0.61633100	-0.45417400	1.85254100
C	-0.39800000	2.02956500	1.07179300
O	-1.43646100	1.87254900	1.73782700
O	0.01636400	3.28055300	0.73917700
C	-0.88015200	4.33898800	1.06397000
C	-0.36087100	5.57842000	0.36630400
H	-0.91903900	4.47461200	2.15093800
H	-1.88774100	4.07522600	0.72566600
H	-0.98352300	6.44323600	0.60852200
H	0.66790600	5.78720600	0.67229800
H	-0.37013100	5.42998700	-0.71711800
C	2.27859700	2.26398100	-0.49825200
C	3.02199700	2.87407500	0.51272100
C	2.14918600	2.89658000	-1.73173500
C	3.61110600	4.11466300	0.29550000
H	3.12551400	2.36590400	1.46665700
C	2.72848600	4.14584900	-1.94869800
H	1.59452400	2.40840400	-2.53017800
C	3.45826200	4.75844300	-0.93340400
H	4.18767800	4.58563200	1.08581800
H	2.61785600	4.63359900	-2.91232700
H	3.91610300	5.72850300	-1.10025200



C	-2.43143400	0.91532400	-0.96308200
C	-3.62128300	1.59405500	-0.67985400
C	-1.46599600	1.51171100	-1.78327400
C	-3.84559500	2.85298900	-1.22356400
H	-4.36095300	1.14301000	-0.02555600
C	-1.69142300	2.78026200	-2.31549400
H	-0.54803800	0.98230000	-2.02080800
C	-2.87728700	3.45048100	-2.03324900
H	-4.77271100	3.37399500	-1.00908000
H	-0.93717300	3.24230300	-2.94434400
H	-3.05053800	4.43969800	-2.44520500
C	-3.36102400	-1.15434900	0.92270800
C	-3.49367100	-0.48998100	2.15093500
C	-4.23984700	-2.19087700	0.58569700
C	-4.50563700	-0.86940600	3.02950100
H	-2.81721400	0.32678700	2.39209300
C	-5.24334500	-2.56293300	1.47388400
H	-4.14344700	-2.70327700	-0.36597300
C	-5.37492200	-1.90539000	2.69574500
H	-4.61150100	-0.35587400	3.97942900
H	-5.92404000	-3.36536500	1.20957100
H	-6.15770800	-2.20072400	3.38703500
C	-1.88641500	-1.91360100	-1.47289700
C	-1.58010700	-3.22938600	-1.09229400
C	-2.05673700	-1.61326600	-2.82785300
C	-1.44972800	-4.22475000	-2.05325400
H	-1.45806100	-3.48034100	-0.04137300
C	-1.91864200	-2.61423100	-3.78708600
H	-2.30550200	-0.60329100	-3.13595800
C	-1.61441500	-3.91687900	-3.40328700
H	-1.21654800	-5.23941400	-1.74860800
H	-2.05612600	-2.37293200	-4.83581300
H	-1.50695800	-4.69328700	-4.15339300
H	0.71113800	-1.66696700	-0.62031200
C	2.23171200	-1.18449000	0.78350200
O	2.62611100	0.11232600	0.40485900
C	3.12455600	-2.21816800	0.08952300
C	2.95338800	-3.58940800	0.30999100
C	4.09989500	-1.79210700	-0.81185300
C	3.74875500	-4.51418300	-0.35970000
H	2.20480200	-3.94480500	1.01036900
C	4.89251500	-2.72067800	-1.48346400
H	4.22915600	-0.72972700	-0.98098200
C	4.72103200	-4.08337100	-1.25983000

H	3.60590500	-5.57455900	-0.17760100
H	5.64652100	-2.37397000	-2.18312600
H	5.33891900	-4.80605700	-1.78300600
C	2.47246700	-1.23835000	2.29971100
F	1.81032200	-0.27611000	2.95202500
F	3.77157400	-1.09280000	2.58639200
F	2.07321400	-2.41200800	2.82719300
H	1.44351900	0.46040100	-1.23561500

TS3<sub>1</sub><sup>(S,S,S)</sup>

P	-1.72068800	-0.56523800	-0.29174700
C	-0.14240300	0.22539400	0.04579300
C	1.12035300	-0.43292200	-0.47421000
H	0.87930700	-1.24660900	-1.16237200
C	-0.07004000	1.35233400	0.80832500
C	1.20086900	1.93263300	1.26714200
H	1.03802700	2.65908500	2.06727600
H	1.64068400	0.78663900	1.74573900
C	-1.31059700	1.95421100	1.40633800
O	-2.09141400	1.36522400	2.12121300
O	-1.44541700	3.22998300	1.04931900
C	-2.66469000	3.86645200	1.48268600
C	-2.71183300	5.22995100	0.83407300
H	-2.65818800	3.92527100	2.57461900
H	-3.50555000	3.23464300	1.17818200
H	-3.62361000	5.74989900	1.13615300
H	-1.85143300	5.83208100	1.13397600
H	-2.71055600	5.13367500	-0.25424800
C	2.18064400	2.46943800	0.27086800
C	3.48824200	2.75510000	0.69134700
C	1.86285000	2.71373400	-1.07070000
C	4.43876100	3.25423200	-0.19100200
H	3.75759000	2.56110300	1.72653800
C	2.81811500	3.19571900	-1.96454700
H	0.84937700	2.52125200	-1.41655300
C	4.11144500	3.46914000	-1.53053900
H	5.44570700	3.45605000	0.16266600
H	2.54477900	3.36678400	-3.00177900
H	4.85570800	3.84629200	-2.22458100
C	-3.00711700	0.67333800	-0.63044600
C	-4.30640700	0.51328900	-0.14192900
C	-2.68398800	1.78829200	-1.41387900
C	-5.28275900	1.45349900	-0.45680200

H	-4.55434100	-0.32807400	0.49627300
C	-3.66857800	2.72002500	-1.73050700
H	-1.66811800	1.93371000	-1.77127500
C	-4.96718000	2.55259100	-1.25383000
H	-6.28894400	1.32961900	-0.07159800
H	-3.41625000	3.57839900	-2.34396900
H	-5.73134300	3.28391200	-1.49582500
C	-2.21589200	-1.66403100	1.05362400
C	-1.52661300	-1.62035600	2.26815500
C	-3.26810500	-2.56809000	0.85777500
C	-1.91942400	-2.46995500	3.29829000
H	-0.66232500	-0.97042300	2.38349400
C	-3.65665800	-3.40398800	1.89828200
H	-3.77430200	-2.62715400	-0.10262900
C	-2.98469400	-3.34875600	3.11911900
H	-1.38364100	-2.44977500	4.24107500
H	-4.47356200	-4.10244000	1.75343500
H	-3.28496000	-4.00571900	3.92905500
C	-1.59459600	-1.60642700	-1.77653200
C	-1.07485700	-2.90329300	-1.66260500
C	-1.97886300	-1.11439400	-3.02720000
C	-0.93220100	-3.69112000	-2.79936000
H	-0.77439000	-3.29187300	-0.69476900
C	-1.83663700	-1.91273500	-4.15859300
H	-2.39881200	-0.11911900	-3.12480400
C	-1.31277900	-3.19755100	-4.04606800
H	-0.52526700	-4.69232200	-2.70852500
H	-2.14150100	-1.52940700	-5.12629100
H	-1.20464200	-3.81741600	-4.93006500
H	1.66288600	0.30574300	-1.07021300
C	2.08599800	-0.97100100	0.66279400
O	1.79387500	-0.51609800	1.91883900
C	3.55044700	-0.71366200	0.25706100
C	3.99978600	-0.81736300	-1.06184200
C	4.46741600	-0.40067900	1.25961900
C	5.33788300	-0.58741300	-1.37404700
H	3.30693400	-1.08038100	-1.85638700
C	5.80528100	-0.16965500	0.95086500
H	4.09661400	-0.32581700	2.27607300
C	6.24413700	-0.25828000	-0.36818900
H	5.67207000	-0.66316700	-2.40434800
H	6.50670600	0.08239200	1.74098100
H	7.28609900	-0.07421100	-0.61160900
C	1.91538900	-2.49579100	0.70614400

F	0.65101300	-2.83970800	1.03713300
F	2.72067300	-3.07117200	1.60564500
F	2.15931500	-3.09449800	-0.48114500
M3 <sub>1</sub> <sup>(S,S,S)</sup>			
P	-1.72796200	-0.33699900	-0.39033600
C	-0.07492700	-0.01399500	-0.04425900
C	0.91507000	-1.14002700	-0.18503800
H	0.37384200	-2.06602100	-0.40746300
C	0.31820400	1.32873400	0.37082900
C	1.42002500	2.03373300	0.00242300
H	1.64643600	2.92507300	0.58327300
H	0.38632700	-0.33602100	2.01599700
C	-0.51464300	1.93868300	1.46403400
O	-1.08531600	1.27835900	2.31578700
O	-0.59524900	3.26822400	1.40734000
C	-1.43928200	3.89021300	2.39273600
C	-1.54451300	5.35292600	2.02675400
H	-0.99914200	3.73926300	3.38293300
H	-2.41351500	3.39251400	2.37375700
H	-2.18398200	5.86969100	2.74591300
H	-0.56032500	5.82701900	2.03320000
H	-1.98057000	5.46031500	1.03033700
C	2.35933500	1.76781800	-1.08740800
C	3.63122700	2.35891200	-1.03474700
C	2.02374600	1.02295800	-2.23154800
C	4.54890600	2.18498200	-2.06261800
H	3.90098100	2.94739000	-0.16177200
C	2.93967300	0.85802200	-3.26557000
H	1.02978100	0.59068900	-2.31113200
C	4.20942200	1.42732600	-3.18242300
H	5.53353100	2.63674400	-1.98769000
H	2.65893200	0.28253100	-4.14253400
H	4.92526400	1.28822200	-3.98635800
C	-2.61102200	1.25003300	-0.51553800
C	-3.77060400	1.50682800	0.22249000
C	-2.05783700	2.26477900	-1.30910200
C	-4.38070300	2.75665700	0.14869200
H	-4.18886500	0.74349200	0.86953100
C	-2.67548800	3.50842600	-1.38461200
H	-1.12640600	2.09250800	-1.84116300
C	-3.83773900	3.75513300	-0.65656300
H	-5.27753100	2.95099900	0.72746000

H	-2.23942700	4.28810800	-2.00004900
H	-4.31478000	4.72864800	-0.71073700
C	-2.70379900	-1.41281200	0.72498400
C	-2.16482200	-1.87132200	1.92592600
C	-3.99254900	-1.81007200	0.34079800
C	-2.91630000	-2.71313600	2.74641900
H	-1.15583400	-1.59567600	2.21033700
C	-4.74307000	-2.63578500	1.16825300
H	-4.40648600	-1.47358400	-0.60712700
C	-4.20272300	-3.08822500	2.37323600
H	-2.49159700	-3.07562500	3.67667200
H	-5.74331400	-2.93396900	0.87220400
H	-4.78631800	-3.73989400	3.01555600
C	-1.89997100	-1.23700000	-1.98095200
C	-1.80012400	-2.63396700	-1.98783700
C	-2.02267600	-0.55225100	-3.19402800
C	-1.81021900	-3.33191600	-3.19228700
H	-1.72453800	-3.18091900	-1.05157400
C	-2.04621100	-1.25519700	-4.39524700
H	-2.11610800	0.52862300	-3.20796600
C	-1.93468600	-2.64398700	-4.39660400
H	-1.72752300	-4.41367500	-3.18709700
H	-2.15496700	-0.71644500	-5.33071600
H	-1.94995400	-3.18942100	-5.33450400
H	1.62477200	-1.00422800	-1.01000900
C	1.76064100	-1.37101600	1.11725700
O	1.10040500	-0.94459000	2.28213400
C	3.15683100	-0.74925900	1.02197600
C	4.01059900	-1.05089400	-0.04438000
C	3.60117600	0.12061600	2.01695600
C	5.28856400	-0.50445000	-0.10305300
H	3.68350800	-1.71915600	-0.83448600
C	4.87683900	0.67727700	1.95094400
H	2.93650100	0.35669200	2.83985600
C	5.72769900	0.36088200	0.89537500
H	5.93622800	-0.74657300	-0.93993100
H	5.20763400	1.35558300	2.73174300
H	6.72251900	0.79279800	0.84488400
C	1.89966800	-2.88350700	1.31410200
F	0.70154000	-3.46043000	1.50635200
F	2.65851400	-3.18722200	2.37404200
F	2.44809500	-3.48161100	0.24064800

TS4<sub>1</sub><sup>(S,S,S)</sup>

P	1.23216100	0.84705300	-0.42944300
C	2.86297400	0.09895200	-0.13106800
C	3.83476700	0.79437200	0.59365300
C	3.12098900	-1.20958900	-0.56333600
C	5.05024700	0.18249000	0.88937200
H	3.64034400	1.80279700	0.94333200
C	4.33575600	-1.81560600	-0.26139400
H	2.37262200	-1.76413700	-1.12249400
C	5.29850000	-1.12191700	0.46977800
H	5.79934800	0.72554100	1.45533800
H	4.52590300	-2.83048900	-0.59387300
H	6.24316300	-1.59926900	0.70957900
C	1.02069000	1.00518400	-2.23357900
C	1.91432500	0.41106400	-3.13149200
C	-0.08838500	1.71005400	-2.72723500
C	1.68266000	0.49107800	-4.50244300
H	2.79573000	-0.10854900	-2.77375300
C	-0.31104300	1.78521100	-4.09782000
H	-0.76953600	2.21202400	-2.04757400
C	0.56774900	1.16851900	-4.98649900
H	2.38162000	0.02733800	-5.19011800
H	0.38908800	1.22721000	-6.05505200
C	1.28755300	2.52516400	0.23950700
C	1.05408000	2.71928200	1.60577700
C	1.63170200	3.60321000	-0.58235300
C	1.15953000	4.00022900	2.13838800
H	0.79261300	1.88074600	2.24081000
C	1.72957700	4.88025200	-0.03802500
H	1.81889600	3.45177700	-1.64069500
C	1.49011900	5.07814000	1.31975400
H	0.97531300	4.15659900	3.19579000
H	1.99090200	5.71818700	-0.67522300
H	1.56394700	6.07536900	1.74155000
C	-0.05283300	-0.16328700	0.36926800
C	0.44974000	-1.50255600	0.82193600
C	-1.47437400	-0.08258800	-0.18162200
C	-2.30633200	0.78045300	0.88825900
H	-1.55921200	0.32405000	-1.19287200
H	-1.90562900	-1.08239400	-0.22158600
C	0.15860500	-2.72763000	0.33840200
C	1.35686800	-1.41411800	2.01543600
O	1.54383800	-0.38992000	2.64141400
O	2.01152400	-2.54921600	2.28097100

C	3.02699200	-2.45898500	3.29553200
C	3.79412500	-3.76113700	3.27480900
H	3.66741200	-1.60340700	3.06007000
H	2.54929400	-2.27325300	4.26174000
H	4.57954200	-3.73908300	4.03358200
H	4.25845500	-3.91069600	2.29687000
H	3.13344300	-4.60565200	3.48329400
O	-1.53819600	1.04824800	1.96612400
H	-0.36634500	0.45057100	1.38078400
H	-1.17208500	2.33032100	-4.46933900
C	-3.61937600	0.05479700	1.22523900
C	-3.95860900	-0.11544500	2.56578800
C	-4.48049900	-0.44138200	0.24078000
C	-5.13499200	-0.77155400	2.92290600
H	-3.27061500	0.27310800	3.30848800
C	-5.65831300	-1.09461800	0.59465100
H	-4.23094200	-0.31856400	-0.80970200
C	-5.98956600	-1.26188100	1.93828200
H	-5.38518700	-0.90104300	3.97189500
H	-6.31727700	-1.47684600	-0.17920100
H	-6.90600100	-1.77446500	2.21414700
C	-0.53361500	-3.11154800	-0.90161600
C	-1.20268700	-4.34292000	-0.94436400
C	-0.48204800	-2.34023300	-2.07211700
C	-1.83267700	-4.77280800	-2.10718800
H	-1.23111000	-4.96097400	-0.05129300
C	-1.09774100	-2.77558100	-3.23931400
H	0.04949200	-1.39472600	-2.07397800
C	-1.78218100	-3.98988800	-3.25906500
H	-2.35709100	-5.72273600	-2.11698700
H	-1.04069100	-2.16415100	-4.13448000
H	-2.26648000	-4.32790200	-4.16947200
H	0.50298800	-3.57060500	0.93287100
C	-2.66887800	2.10965300	0.21536500
F	-1.55346800	2.81603700	-0.08179300
F	-3.42323500	2.89490500	0.99575000
F	-3.33352500	1.97323700	-0.95762400
M4 <sub>1</sub> <sup>(S,S,S)</sup>			
P	1.30243800	0.84071300	-0.37055900
C	2.89049100	-0.01766000	-0.15786400
C	3.87917400	0.53213900	0.66349600
C	3.08364500	-1.28512500	-0.72651000

C	5.05272000	-0.17560200	0.90629400
H	3.72824100	1.49918400	1.13053500
C	4.25737800	-1.98774600	-0.47682200
H	2.31685000	-1.73496100	-1.35099400
C	5.24109700	-1.43471800	0.34112600
H	5.81378600	0.25490400	1.54791000
H	4.39832600	-2.96869500	-0.91748300
H	6.15343300	-1.98756300	0.54013400
C	1.02534800	1.08866900	-2.15213000
C	1.86778000	0.53640400	-3.12317500
C	-0.06372100	1.88103300	-2.54531300
C	1.59692600	0.73994300	-4.47392100
H	2.73870400	-0.04195700	-2.83886900
C	-0.32781400	2.07482900	-3.89646900
H	-0.69713900	2.35478200	-1.80273500
C	0.49551000	1.49766500	-4.86151300
H	2.25496900	0.30903500	-5.22062200
H	0.28636500	1.65148400	-5.91496100
C	1.48051400	2.49024900	0.34382000
C	0.81249000	2.86863000	1.51060900
C	2.37451800	3.36597600	-0.29070500
C	1.06279000	4.13252500	2.04492000
H	0.04812900	2.22666200	1.95237500
C	2.61591600	4.61817800	0.25822400
H	2.88363100	3.06861400	-1.20447000
C	1.96144900	4.99832100	1.43091700
H	0.53957200	4.44029000	2.94406400
H	3.30898300	5.29648800	-0.22750300
H	2.14744100	5.97834900	1.85870000
C	-0.02727500	-0.14959300	0.46374400
C	0.45779300	-1.54789800	0.77246700
C	-1.46195900	-0.01262000	-0.05515600
C	-2.32196700	0.81984300	1.01626800
H	-1.53429900	0.41344100	-1.05943400
H	-1.89119900	-1.01066900	-0.12853900
C	0.13601300	-2.71649400	0.18547000
C	1.39373200	-1.57573700	1.94609300
O	1.63625100	-0.59726800	2.62308400
O	1.99061500	-2.75532700	2.13457300
C	3.00340300	-2.78615000	3.15625800
C	3.69368300	-4.12691700	3.05482400
H	3.69289900	-1.95554900	2.97893100
H	2.52852000	-2.63524300	4.12976300
H	4.47296100	-4.20052800	3.81649300



H	4.15584400	-4.24140300	2.07109800
H	2.98241900	-4.94201800	3.20590300
O	-1.65723100	1.07976100	2.14645300
H	-0.12133100	0.34590500	1.45997500
H	-1.17546200	2.68299500	-4.19265600
C	-3.66241400	0.07590100	1.24393300
C	-4.11952400	-0.05183400	2.55381900
C	-4.43273100	-0.45897300	0.20611200
C	-5.31834100	-0.70590200	2.82987700
H	-3.49812600	0.36845400	3.33714200
C	-5.63249000	-1.11278500	0.47762300
H	-4.09632200	-0.36758900	-0.82358100
C	-6.07968800	-1.23836300	1.79186200
H	-5.66011400	-0.80117300	3.85661700
H	-6.21806100	-1.52692300	-0.33796700
H	-7.01375100	-1.74979000	2.00361600
C	-0.62819500	-2.98987100	-1.04107100
C	-1.35813200	-4.18440900	-1.11773400
C	-0.60654400	-2.14533900	-2.15902800
C	-2.08221300	-4.50282800	-2.26114400
H	-1.36371800	-4.85782900	-0.26537800
C	-1.31779500	-2.46939500	-3.30862500
H	-0.02214300	-1.23159600	-2.13717400
C	-2.06515700	-3.64514600	-3.35949300
H	-2.65495100	-5.42356500	-2.29761200
H	-1.28447200	-1.80325700	-4.16486600
H	-2.62423700	-3.89674900	-4.25473600
H	0.50398600	-3.60930900	0.68572800
C	-2.69178400	2.15058000	0.33437900
F	-1.58787500	2.90246400	0.10033300
F	-3.50965900	2.90037500	1.08497800
F	-3.29148200	2.01594800	-0.87494000

M4<sub>1</sub><sup>r(S,S,S)</sup>

P	1.38545600	0.75922900	-0.70035500
C	3.06568600	0.40748300	-0.11993600
C	3.83893000	1.45917600	0.38099900
C	3.55189300	-0.90800500	-0.06032700
C	5.08464100	1.19685300	0.94410300
H	3.46981800	2.47886600	0.34351200
C	4.79863000	-1.15882200	0.50070600
H	2.95423800	-1.73695200	-0.42550500
C	5.56355700	-0.10811000	1.00596300

H	5.67769600	2.01590600	1.33571500
H	5.16961700	-2.17742000	0.54618400
H	6.53404600	-0.30829200	1.44788000
C	1.09851400	-0.00403300	-2.31541600
C	2.09257800	-0.73590500	-2.97094100
C	-0.14231500	0.20455100	-2.93639000
C	1.83071600	-1.29271500	-4.22081800
H	3.07218800	-0.86356100	-2.52577900
C	-0.39434600	-0.35691400	-4.18087200
H	-0.90461700	0.81091900	-2.45857300
C	0.58774200	-1.11339600	-4.81939600
H	2.60480000	-1.86056700	-4.72538900
H	0.38646900	-1.55289400	-5.79095400
C	1.21796400	2.54582000	-0.91708300
C	0.72739300	3.35115400	0.11719400
C	1.64045000	3.11934700	-2.12205400
C	0.66134300	4.72966600	-0.06243200
H	0.38500000	2.92026100	1.05315100
C	1.57523300	4.49842200	-2.28791100
H	2.01287600	2.49198500	-2.92694500
C	1.08538500	5.30145000	-1.25983500
H	0.27373200	5.35431200	0.73473500
H	1.90249900	4.94351400	-3.22119400
H	1.03023800	6.37663300	-1.39418200
C	0.19140400	0.18703700	0.58110200
C	0.57520100	-1.23267700	0.94602600
C	-1.25503900	0.52454900	0.20308400
C	-2.17547300	0.37558400	1.47713200
H	-1.30309500	1.54411000	-0.19903700
H	-1.61531900	-0.14626300	-0.57438100
C	0.26908500	-2.38431800	0.32718700
C	1.53336400	-1.27225000	2.10494100
O	1.81832800	-0.30178200	2.77435000
O	2.07761900	-2.47569300	2.31189900
C	3.03989800	-2.54772900	3.37785300
C	3.62260200	-3.94238800	3.35763600
H	3.80086600	-1.77951700	3.20981500
H	2.53545000	-2.32381500	4.32189100
H	4.36448400	-4.04463900	4.15250400
H	4.11046400	-4.14011800	2.39987500
H	2.84200600	-4.69032500	3.51266900
O	-1.77476700	-0.58649000	2.30150500
H	0.47076400	0.78996400	1.45132500
H	-1.35956300	-0.20485000	-4.65133200

C	-3.64076200	0.22740800	0.97346300
C	-4.43119000	-0.73836200	1.59395700
C	-4.19209000	0.98135500	-0.06697300
C	-5.74163800	-0.96427600	1.17934100
H	-3.96565300	-1.30887800	2.39168800
C	-5.50215800	0.75807200	-0.48746000
H	-3.59991000	1.74984300	-0.55658100
C	-6.28113900	-0.21695300	0.13333400
H	-6.34362600	-1.72355400	1.67072800
H	-5.91598800	1.34634300	-1.30145200
H	-7.30112300	-0.39140300	-0.19574600
C	-0.75345000	-2.62261600	-0.71916900
C	-2.10181100	-2.45918000	-0.38029100
C	-0.41333000	-3.09994700	-1.98688100
C	-3.09554700	-2.72301000	-1.31771800
H	-2.33502600	-2.09075700	0.61732000
C	-1.41101400	-3.36757600	-2.92140600
H	0.63240700	-3.23853000	-2.25004600
C	-2.75149900	-3.17483300	-2.59170400
H	-4.13679000	-2.56627700	-1.04762500
H	-1.13836700	-3.71730900	-3.91264700
H	-3.52512700	-3.37795700	-3.32577500
H	0.76898600	-3.27628500	0.69944400
C	-2.13062700	1.73485600	2.22083000
F	-0.89840400	1.99503900	2.72625300
F	-2.97594500	1.76483300	3.26056300
F	-2.42991700	2.81214600	1.44862600

TS5<sub>1</sub><sup>(S,S,S)</sup>

P	-1.45090500	-1.10750400	0.02551100
C	-3.08922600	-0.39198600	-0.25203200
C	-4.17251100	-0.79427300	0.53474500
C	-3.26632000	0.58132700	-1.24626100
C	-5.42303000	-0.21586600	0.33581700
H	-4.04436300	-1.54955900	1.30270600
C	-4.51896100	1.15412200	-1.43538400
H	-2.43133900	0.90827400	-1.85666900
C	-5.59525800	0.75927300	-0.64248500
H	-6.26121500	-0.52707200	0.94955500
H	-4.65178700	1.91031200	-2.20131900
H	-6.57050900	1.21107400	-0.79070900
C	-1.00903600	-2.13591500	-1.39655800
C	-1.86486200	-2.22874300	-2.49924500

C	0.20350200	-2.83983500	-1.39014500
C	-1.50146400	-3.00818700	-3.59392200
H	-2.81014700	-1.69658000	-2.50810400
C	0.55695600	-3.61727200	-2.48758700
H	0.86431800	-2.79649300	-0.53050900
C	-0.29225200	-3.69894700	-3.58978600
H	-2.16788600	-3.07671800	-4.44681500
H	-0.01208700	-4.30537700	-4.44467600
C	-1.52599500	-2.15605800	1.49707600
C	-1.67107000	-1.53289200	2.74579400
C	-1.47466200	-3.54968700	1.40652700
C	-1.74862500	-2.31059800	3.89527500
H	-1.75231700	-0.45070500	2.81973700
C	-1.54940400	-4.31825000	2.56516600
H	-1.37552400	-4.03472000	0.44102400
C	-1.68145300	-3.70048600	3.80555300
H	-1.86304700	-1.83052600	4.86086000
H	-1.50451700	-5.39954800	2.49514100
H	-1.73680400	-4.30262900	4.70637200
C	-0.22081200	0.23346200	0.41481300
C	-0.45974300	1.57927300	-0.21141100
C	1.23787000	-0.23136400	0.36286200
C	2.26322600	0.86513800	0.87044300
H	1.34846000	-1.12921300	0.98067900
H	1.54391100	-0.48507700	-0.65473700
C	0.43098600	2.13520100	-1.08448900
C	-1.38014200	2.41615000	0.56012700
O	-2.01170100	2.02717600	1.53335200
O	-1.53023300	3.66026900	0.06670500
C	-2.44819100	4.50279800	0.77530300
C	-2.49712300	5.82617200	0.04436400
H	-3.42653400	4.01302400	0.80236300
H	-2.10422400	4.61859500	1.80745800
H	-3.18464100	6.50636400	0.55221900
H	-2.84317900	5.68568200	-0.98238700
H	-1.50758000	6.28813700	0.01824100
O	2.28794400	2.01458400	0.17491300
H	-0.47586900	0.37390300	1.47154300
H	1.49556100	-4.16014300	-2.47915500
C	3.63974900	0.14381500	0.87901400
C	4.61795700	0.62032800	0.00871900
C	3.93435900	-0.96569800	1.67930900
C	5.86435300	0.00301800	-0.07136300
H	4.36535500	1.48787400	-0.59028700

C	5.18278300	-1.57978600	1.60791800
H	3.19376000	-1.34810200	2.37546800
C	6.15235600	-1.09986900	0.72886000
H	6.61448200	0.38616000	-0.75735500
H	5.39932600	-2.43548100	2.24080300
H	7.12402100	-1.58094100	0.67106500
C	1.10570900	1.45727000	-2.21651200
C	2.37206000	1.86486400	-2.65794500
C	0.43563700	0.46692000	-2.93706200
C	2.96326900	1.25976400	-3.75812100
H	2.89041100	2.63155500	-2.09458900
C	1.03104500	-0.15241200	-4.03611300
H	-0.56955200	0.18193900	-2.64874400
C	2.30014600	0.23917600	-4.44574800
H	3.95032300	1.57670300	-4.08039000
H	0.49406600	-0.93190100	-4.56834400
H	2.77062200	-0.23717900	-5.30001500
H	0.42152400	3.22079100	-1.14936500
C	1.90006600	1.20023600	2.33884300
F	0.85689600	2.04661500	2.41102700
F	2.91428300	1.78961400	2.99222200
F	1.54005900	0.11852900	3.08345700

M5<sub>1</sub><sup>(S,S,S)</sup>

P	-1.63334000	-0.91190900	-0.33088900
C	-0.24057300	-0.15830100	0.76035300
C	1.11415800	-0.81555300	0.49752800
H	1.12244500	-1.86665500	0.79813700
C	-0.15210900	1.31187300	0.68213300
C	1.16056300	1.93899900	0.37650200
H	1.14393500	2.94981200	0.79295900
C	-1.17928600	1.97216400	1.36716000
O	-2.17027000	1.41152800	1.87902200
O	-1.06924800	3.34310900	1.41509100
C	-2.15306400	4.02159600	2.03964300
C	-1.87814500	5.50728300	1.93240700
H	-2.23909800	3.70619700	3.08529300
H	-3.08932300	3.74916700	1.54045800
H	-2.68508200	6.07569900	2.40140000
H	-0.93975000	5.76142700	2.43171200
H	-1.80398300	5.80910700	0.88452800
C	1.62253100	2.07355600	-1.07389300
C	2.62840800	3.00230200	-1.36549700

C	1.11777000	1.30529900	-2.12070200
C	3.11961500	3.14792900	-2.65880400
H	3.03097300	3.61383800	-0.56079500
C	1.60418500	1.44074800	-3.42013400
H	0.33397900	0.58185800	-1.92516200
C	2.60884300	2.36364000	-3.69347600
H	3.89872400	3.87625200	-2.86195000
H	1.19393100	0.82154800	-4.21282500
H	2.99016200	2.47612300	-4.70327600
C	-2.86152700	0.31157400	-0.85773000
C	-4.22088000	0.02571600	-0.68954800
C	-2.46986800	1.52064800	-1.44910700
C	-5.18033900	0.94816700	-1.09228600
H	-4.53425000	-0.90971300	-0.23804200
C	-3.43952600	2.43965800	-1.84185400
H	-1.42126600	1.75832500	-1.58068000
C	-4.79127700	2.15817100	-1.66205800
H	-6.23215900	0.72076400	-0.95606000
H	-3.13195000	3.37810200	-2.29116100
H	-5.54136400	2.87878400	-1.97169700
C	-2.49615600	-2.15619200	0.65810000
C	-2.91072500	-1.76048400	1.93906900
C	-2.78832800	-3.43830400	0.18385000
C	-3.59939100	-2.66311100	2.74285300
H	-2.71656000	-0.74397500	2.27788400
C	-3.47716700	-4.33183100	0.99946100
H	-2.48762400	-3.73891400	-0.81449800
C	-3.87719200	-3.94691700	2.27733200
H	-3.92318200	-2.36041100	3.73287600
H	-3.70406900	-5.32729100	0.63304800
H	-4.41398400	-4.64721700	2.90902100
C	-0.98178300	-1.71534900	-1.82337400
C	-0.15173500	-2.83797900	-1.68962500
C	-1.25649100	-1.20791100	-3.09811700
C	0.39778600	-3.43774700	-2.81674500
H	0.05622100	-3.25492900	-0.70827300
C	-0.69658800	-1.80972100	-4.22232300
H	-1.90267200	-0.34386800	-3.21621100
C	0.13070500	-2.92056300	-4.08316800
H	1.03691300	-4.30684000	-2.70490400
H	-0.91237900	-1.40881300	-5.20701000
H	0.56573600	-3.38659900	-4.96097400
H	1.38398600	-0.78219100	-0.56112600
C	2.24766500	-0.09322600	1.26290300

O	2.26936100	1.30300400	1.09926700
C	3.58682500	-0.68165800	0.80458200
C	3.91319400	-2.02030400	1.04890800
C	4.47349500	0.11009800	0.07550900
C	5.11146000	-2.55034600	0.57961500
H	3.23919400	-2.65466800	1.61444300
C	5.66990000	-0.42511000	-0.39761300
H	4.21559400	1.14388600	-0.12071100
C	5.99500900	-1.75467800	-0.14610600
H	5.35257800	-3.58902800	0.78241900
H	6.34866300	0.20303300	-0.96608000
H	6.92820400	-2.16907500	-0.51388500
C	2.08669000	-0.29630700	2.78242200
F	1.05310000	0.39465400	3.27635200
F	3.18067200	0.10704000	3.43993500
F	1.87698400	-1.58876500	3.10788200
H	-0.61791100	-0.47957200	1.74091200

TS6<sub>1</sub><sup>(S,S,S)</sup>

P	-1.70969500	-0.99701900	-0.29211800
C	-0.23563300	-0.02846500	0.95172400
C	1.07852700	-0.76616900	0.76163300
H	1.04380000	-1.75274900	1.23164200
C	-0.15885500	1.37144800	0.73169700
C	1.15513400	1.95842600	0.33945300
H	1.14264800	3.01735200	0.61002400
C	-1.25444400	2.12746300	1.22607100
O	-2.26117400	1.64299100	1.75851500
O	-1.14754700	3.47588300	1.03533700
C	-2.27519100	4.24344900	1.45440700
C	-2.02257600	5.67801800	1.04260200
H	-2.40089700	4.15057900	2.53846400
H	-3.17784500	3.84001300	0.98341000
H	-2.86059800	6.30981100	1.34647500
H	-1.11215700	6.06012200	1.51092300
H	-1.90934200	5.74935300	-0.04218400
C	1.63398600	1.87411200	-1.10758100
C	2.65629300	2.73656800	-1.51824000
C	1.13525900	0.95989700	-2.03396900
C	3.17103800	2.67579800	-2.80884300
H	3.05387000	3.45971400	-0.80959100
C	1.64402600	0.88946100	-3.32963100
H	0.34000500	0.28200800	-1.74580700

C	2.66701000	1.74733000	-3.72049800
H	3.96461600	3.35378900	-3.10727300
H	1.23660900	0.16065300	-4.02450200
H	3.06814100	1.69780500	-4.72767600
C	-2.89160000	0.24176300	-0.88261500
C	-4.26114000	0.11700700	-0.61933000
C	-2.41395600	1.38336800	-1.54132700
C	-5.13804400	1.12662800	-0.99747200
H	-4.64162700	-0.76367300	-0.11243400
C	-3.29970600	2.39341400	-1.91048500
H	-1.35861800	1.50128100	-1.75872800
C	-4.65815600	2.27032300	-1.63453900
H	-6.19812800	1.02048900	-0.79240300
H	-2.92149000	3.27813600	-2.41241200
H	-5.34440900	3.06055400	-1.92165200
C	-2.61106100	-2.15247500	0.76688500
C	-3.10141800	-1.63173400	1.97516100
C	-2.79427000	-3.50379100	0.45773900
C	-3.77464100	-2.46742600	2.86078400
H	-2.97152900	-0.57289800	2.19626700
C	-3.46318700	-4.33117400	1.35519300
H	-2.42365300	-3.90709500	-0.47938900
C	-3.95124700	-3.81553800	2.55430200
H	-4.16032300	-2.06516900	3.79159200
H	-3.60843500	-5.37894000	1.11399100
H	-4.47337000	-4.46524400	3.24919800
C	-1.06952200	-1.89546900	-1.73448800
C	-0.14015600	-2.92625600	-1.52790600
C	-1.40326900	-1.52078300	-3.04155100
C	0.43445100	-3.57838400	-2.61366900
H	0.13015900	-3.22440300	-0.51800700
C	-0.81679700	-2.17187700	-4.12365600
H	-2.11959600	-0.72386400	-3.21400000
C	0.10103200	-3.19845100	-3.91248300
H	1.14941200	-4.37630900	-2.44435000
H	-1.08271800	-1.87763000	-5.13361600
H	0.55745600	-3.70167900	-4.75830200
H	1.30251000	-0.92530100	-0.29517700
C	2.28048400	0.02089200	1.35357900
O	2.21393100	1.41860800	1.18665800
C	3.59477500	-0.52180700	0.78438800
C	3.83836000	-1.89779500	0.72213900
C	4.56945900	0.36113900	0.32024700
C	5.03300400	-2.37924700	0.19536000



H	3.09942400	-2.60277900	1.08897600
C	5.76340200	-0.12259200	-0.21010800
H	4.37848900	1.42601300	0.36953000
C	5.99949500	-1.49269300	-0.27455000
H	5.20752800	-3.44954600	0.15208000
H	6.51001600	0.57622600	-0.57406400
H	6.92984500	-1.86913700	-0.68760000
C	2.28700800	-0.16088100	2.87833200
F	1.16145400	0.30526100	3.43636600
F	3.31361300	0.48578000	3.44045400
F	2.39006900	-1.45713100	3.22626400
H	-0.77950700	-0.31822600	1.85399200
$P_1^{(S,R)}$			
C	-0.29387000	0.32578400	2.16077200
C	-1.54015400	-0.47044800	1.92840800
H	-2.39673200	-0.02503100	2.43741900
C	0.64185600	0.45854700	1.21814100
C	0.53340700	-0.21807800	-0.13312300
H	0.42615900	0.55695600	-0.90547400
C	1.79965300	1.35500300	1.49377200
O	2.10679200	1.77509900	2.58787400
O	2.45440800	1.66497600	0.37108300
C	3.61994100	2.49457900	0.51933500
C	4.28748900	2.56404200	-0.83563900
H	3.30493100	3.47844700	0.87896800
H	4.27006000	2.04969700	1.27730400
H	5.17982900	3.19109900	-0.77878600
H	3.60868000	2.99104200	-1.57762900
H	4.58158400	1.56455300	-1.16499700
C	1.74588500	-1.06695000	-0.45967600
C	2.05042000	-2.17999200	0.32518200
C	2.55961800	-0.74522600	-1.54325200
C	3.16332500	-2.96154800	0.02767300
H	1.40805400	-2.43169800	1.16500400
C	3.67541700	-1.52381800	-1.84091900
H	2.32308200	0.12657200	-2.14726000
C	3.97850200	-2.63325700	-1.05502100
H	3.39631900	-3.82656500	0.64034000
H	4.30464700	-1.26534300	-2.68670000
H	4.84675300	-3.24212600	-1.28582500
H	-1.41853000	-1.47615900	2.34600400
C	-1.77511600	-0.60185000	0.42086700

O	-0.59026100	-1.09911300	-0.17828400
C	-2.25489300	0.67114200	-0.27468800
C	-2.10540100	0.75450100	-1.66365300
C	-2.84183800	1.73565800	0.40893600
C	-2.53336400	1.88245600	-2.35451800
H	-1.64475300	-0.07224700	-2.19523800
C	-3.27240100	2.86548800	-0.28436500
H	-2.96571700	1.70315400	1.48585900
C	-3.11939600	2.94224000	-1.66520200
H	-2.40776000	1.93402600	-3.43113100
H	-3.72582100	3.68739600	0.25986700
H	-3.45203300	3.82443500	-2.20259700
C	-2.79617800	-1.71829400	0.18000600
F	-2.39578700	-2.87744500	0.71812500
F	-3.96829700	-1.39367200	0.74450500
F	-3.01275300	-1.94006400	-1.11975500
H	-0.15213600	0.82484300	3.11541100
$P_1^{(S,S)}$			
C	0.16117300	-1.58885700	1.56327100
C	1.08476400	-1.01324600	0.79359600
C	0.72758200	0.00726300	-0.26369700
H	0.89933600	-0.42302900	-1.25984100
C	2.50140900	-1.44548000	0.95135200
O	2.93866600	-2.05764600	1.90115500
O	3.23692200	-1.09945300	-0.10909300
C	4.63621700	-1.42711500	-0.05053300
C	5.28929500	-0.78753700	-1.25501900
H	5.04351400	-1.04688700	0.88990400
H	4.74139500	-2.51594200	-0.04938000
H	6.36037000	-1.00089700	-1.25312300
H	5.14578200	0.29548800	-1.23157000
H	4.85871300	-1.17775500	-2.18014500
C	-1.30430700	-1.32511500	1.41933700
C	-1.62828800	-0.54575400	0.13624900
H	-1.84907500	-2.27523900	1.43564400
H	-1.66166800	-0.74957100	2.28091800
O	-0.63580900	0.42039800	-0.13834100
C	1.54286400	1.27889600	-0.12973900
C	2.38623000	1.69979000	-1.15455500
C	1.44062200	2.03833400	1.03621900
C	3.12876500	2.87049700	-1.01557500
H	2.46941300	1.10213500	-2.05852700

C	2.17916600	3.20915700	1.17638600
H	0.77514200	1.70546000	1.82855500
C	3.02607200	3.62617800	0.15008600
H	3.78492900	3.19227000	-1.81817400
H	2.09675000	3.79585700	2.08576500
H	3.60327900	4.53890500	0.25881900
H	0.48177200	-2.30094200	2.31925700
C	-2.95324700	0.20515300	0.22863700
C	-4.04106800	-0.35877700	0.89895900
C	-3.10155200	1.44280000	-0.39877600
C	-5.25694600	0.31516600	0.95754300
H	-3.94724300	-1.32853200	1.37757500
C	-4.31822800	2.11703400	-0.33510900
H	-2.25848000	1.87724300	-0.92238500
C	-5.39790000	1.55691100	0.34250600
H	-6.09348300	-0.13208000	1.48435100
H	-4.42144100	3.08362200	-0.81767200
H	-6.34498200	2.08453700	0.39095400
C	-1.73362500	-1.50868400	-1.06119100
F	-1.85652500	-0.83057500	-2.20621900
F	-0.65666900	-2.30350400	-1.18296300
F	-2.79585100	-2.31797500	-0.93896900

## 5.2 Coordinates of all stationary points for the reaction of 2-benzyl-2,3-butadienoate with N-tosylbenzaldimine.

R2<sub>2</sub>

C	1.66369000	0.69456200	0.30741500
C	2.88491800	-0.09398700	0.13804300
C	3.89567200	0.03677200	1.09590000
C	3.05701400	-0.96028900	-0.94966700
C	5.07350000	-0.69199800	0.97067500
H	3.75477800	0.71206000	1.93518300
C	4.23255800	-1.68691800	-1.07030100
H	2.26441200	-1.04983400	-1.68535300
C	5.24022600	-1.55268400	-0.11124200
H	5.85728300	-0.58865500	1.71304500
H	4.37020100	-2.35964300	-1.91006700
H	6.15865800	-2.12224800	-0.21115000
N	0.69630700	0.63957100	-0.53221600
H	1.60826500	1.33855100	1.19237800
S	-0.61932500	1.65126800	-0.19403300
O	-0.82819300	2.44787400	-1.39833000

O	-0.44918800	2.33466600	1.08856100
C	-1.93337800	0.47907200	-0.04147500
C	-2.52767800	-0.01922400	-1.19628100
C	-2.34284300	0.07549100	1.22734800
C	-3.55712100	-0.94541600	-1.07018300
H	-2.19649100	0.32378100	-2.17088000
C	-3.37268300	-0.84983200	1.33069600
H	-1.86789200	0.49132800	2.10944700
C	-3.99167800	-1.37190300	0.18832600
H	-4.03336900	-1.34005300	-1.96240800
H	-3.70779500	-1.17136300	2.31256400
C	-5.11270500	-2.36726000	0.32646700
H	-5.45555900	-2.71792900	-0.64835300
H	-4.79203100	-3.23351400	0.91176100
H	-5.96331200	-1.91839800	0.84768800
PBu <sub>3</sub>			
P	-0.17779900	-0.91852700	-0.85005000
C	1.07052100	-1.95893400	0.06116900
C	2.50203900	-1.43402000	-0.04753800
H	1.01401000	-2.96862300	-0.36498500
H	0.77893200	-2.03697800	1.11741700
C	3.53022200	-2.39431500	0.55000100
H	2.75170600	-1.24516200	-1.10082400
H	2.57870900	-0.46646600	0.46643600
C	4.95515400	-1.85560600	0.45632200
H	3.27360100	-2.58864000	1.59887700
H	3.46230200	-3.35875300	0.03159100
H	5.67856700	-2.55649100	0.88075200
H	5.23401400	-1.67423100	-0.58655200
H	5.04939300	-0.90706000	0.99439600
C	-1.72151000	-1.64029300	-0.09899400
C	-3.00577500	-1.05826600	-0.68929100
H	-1.69997000	-1.49575800	0.98968200
H	-1.69114900	-2.72224500	-0.27895600
C	-4.26692100	-1.65118900	-0.06174000
H	-3.02097300	0.03215800	-0.55546400
H	-3.02166000	-1.23372600	-1.77271400
C	-5.54524800	-1.06911200	-0.65885000
H	-4.25552300	-2.74003000	-0.19618300
H	-4.24742600	-1.47320100	1.02068900
H	-6.43746200	-1.50473000	-0.20158700
H	-5.58603900	0.01459600	-0.50998800

H	-5.59279700	-1.25819700	-1.73590600
C	-0.07147200	0.66616000	0.13108500
C	0.81358100	1.72995400	-0.52156600
H	0.27763100	0.44050800	1.14855500
H	-1.09134300	1.05920200	0.22807200
C	0.91686100	3.00538300	0.31307100
H	1.82179000	1.33100200	-0.69511000
H	0.41071300	1.97421800	-1.51310100
C	1.78696200	4.06924800	-0.35070400
H	-0.09103700	3.40352600	0.48593300
H	1.32359200	2.75610600	1.30139500
H	1.84605900	4.97668100	0.25591800
H	2.80573000	3.69892300	-0.50301000
H	1.38448700	4.34522900	-1.33054100

TS1<sub>2</sub>

P	-1.44480200	0.22805600	0.34772800
C	-0.94396600	-0.27582500	-1.36268500
C	0.54346000	-0.09166000	-1.67870900
H	-1.20485600	-1.33859400	-1.44216200
H	-1.55696700	0.27239900	-2.09129100
C	0.84290500	-0.42540000	-3.14074300
H	1.14763300	-0.72865600	-1.01896300
H	0.86557400	0.93635700	-1.46778400
C	2.31147000	-0.23996500	-3.50696200
H	0.21956600	0.20926100	-3.78403200
H	0.53653500	-1.45975100	-3.34510200
H	2.49524700	-0.47901900	-4.55806200
H	2.95142400	-0.88166400	-2.89310500
H	2.62813200	0.79251300	-3.32791300
C	-3.02907800	-0.67895200	0.61441300
C	-4.13487900	-0.46910900	-0.41982600
H	-2.74093500	-1.73462000	0.67467300
H	-3.38274800	-0.39405600	1.61423800
C	-5.37004300	-1.32127700	-0.12620900
H	-3.75999900	-0.71428800	-1.42226300
H	-4.42990700	0.58752500	-0.44714600
C	-6.47942400	-1.11280300	-1.15350300
H	-5.74188200	-1.07964700	0.87735200
H	-5.07852700	-2.37843300	-0.10159500
H	-7.35618000	-1.72507200	-0.92707100
H	-6.13484100	-1.37706600	-2.15826200
H	-6.79747000	-0.06559100	-1.17608300

C	-2.02327100	1.98061100	0.14370500
C	-0.87637400	2.98600600	0.04346800
H	-2.66820800	2.04997600	-0.74191100
H	-2.65106000	2.21707400	1.01339500
C	-1.36044300	4.42716400	-0.10197000
H	-0.23362700	2.73602800	-0.81089400
H	-0.24189400	2.90175000	0.93520500
C	-0.20173500	5.41560500	-0.20133900
H	-1.99622200	4.68225600	0.75494900
H	-1.99506200	4.50637400	-0.99338200
H	-0.55650700	6.44343300	-0.31259000
H	0.43283200	5.18317000	-1.06286500
H	0.42524100	5.37184800	0.69548600
C	-0.18582600	-0.38700300	2.36663200
C	0.89720100	-1.15370900	2.07648300
C	-0.91711900	0.20872100	3.29206800
C	2.29545500	-0.64570600	2.38166100
H	2.96655100	-1.49816300	2.51531400
C	0.68738600	-2.26686300	1.17981800
O	-0.39941000	-2.60782300	0.72025200
O	1.83694800	-2.90659400	0.84901400
C	1.70771300	-4.02776500	-0.03325700
C	1.54371500	-3.58508300	-1.47514800
H	2.63033400	-4.59523300	0.10427500
H	0.85996000	-4.63927000	0.28565400
H	1.55205400	-4.45335000	-2.13939900
H	2.36146500	-2.91780800	-1.76345000
H	0.59598200	-3.05642300	-1.59752700
H	-0.82970100	-0.12744700	4.32258100
H	2.27104200	-0.09244300	3.32525400
C	2.82029900	0.25553400	1.28322500
C	2.36494300	1.57462700	1.19206000
C	3.71771000	-0.21203200	0.32137700
C	2.79468300	2.41074000	0.16557400
H	1.66650300	1.94246300	1.94037300
C	4.15664800	0.62407700	-0.70405400
H	4.06636800	-1.23992000	0.37775700
C	3.69585500	1.93633800	-0.78698800
H	2.42659200	3.43185600	0.11022800
H	4.85893900	0.24887300	-1.44266200
H	4.03834400	2.58524700	-1.58723900
H	-1.61173700	1.01498000	3.08143900

M1 <sub>2</sub>			
P	-1.48292600	0.60310500	0.43320300
C	-1.28876700	0.29202500	-1.36406000
C	0.17803700	0.27514300	-1.80301900
H	-1.74770800	-0.67169800	-1.58136400
H	-1.84769900	1.07717600	-1.88616200
C	0.32166000	0.02903800	-3.30261600
H	0.70028000	-0.51362500	-1.25290600
H	0.67508000	1.21670300	-1.53473200
C	1.78326500	-0.15563400	-3.70121100
H	-0.12153200	0.86418100	-3.85921900
H	-0.25122300	-0.86626800	-3.57637100
H	1.89217300	-0.30347000	-4.77864500
H	2.20921300	-1.02876700	-3.19431800
H	2.38060700	0.71600200	-3.41485100
C	-2.92585000	-0.22805900	1.18920600
C	-3.95743000	-0.71477200	0.17057700
H	-2.53714200	-1.06925600	1.76487400
H	-3.36903200	0.50022400	1.87880900
C	-5.19741600	-1.28797700	0.85526200
H	-3.49305400	-1.48765500	-0.45135600
H	-4.25899600	0.10466600	-0.49663500
C	-6.22539700	-1.79822000	-0.15074300
H	-5.64906200	-0.51777400	1.49226300
H	-4.89050200	-2.10310000	1.52148400
H	-7.10305500	-2.21268900	0.35137900
H	-5.79610200	-2.58250300	-0.78172800
H	-6.56308800	-0.98981600	-0.80679500
C	-1.94785900	2.37568400	0.50155400
C	-1.06362300	3.34382700	-0.29171300
H	-2.97495300	2.40851100	0.11392900
H	-2.01068800	2.66867200	1.55499800
C	-1.43620900	4.80044300	-0.01511500
H	-1.16626500	3.14527600	-1.36579700
H	-0.00775300	3.18604900	-0.04438400
C	-0.60361000	5.77468500	-0.84307900
H	-1.29783600	5.00672500	1.05352800
H	-2.50287900	4.94733000	-0.22463600
H	-0.86496800	6.81201400	-0.62001800
H	-0.76110600	5.60968900	-1.91342100
H	0.46359800	5.64422000	-0.63906400
C	0.03601500	0.35370800	1.41925100
C	0.66460700	-0.93934000	1.44111300
C	0.49203000	1.45739300	2.07046700

C	2.00658700	-1.06540100	2.11455600
H	2.22952800	-2.12655700	2.25518400
C	0.08717900	-2.00801900	0.74806100
O	-1.01488500	-1.98962800	0.15034800
O	0.83942400	-3.16099300	0.72629700
C	0.41182600	-4.15791400	-0.19850200
C	0.78717700	-3.77845200	-1.62225700
H	0.92378800	-5.07196400	0.11188200
H	-0.66690700	-4.30659000	-0.11025800
H	0.48571900	-4.56289600	-2.32206400
H	1.86837500	-3.63552100	-1.70882200
H	0.28064400	-2.84950000	-1.90082100
H	1.38941200	1.40500400	2.67654100
H	1.98526300	-0.61805100	3.11813500
C	3.13919500	-0.43238800	1.32232900
C	4.01704700	0.49000000	1.89249500
C	3.32093600	-0.78170300	-0.02072700
C	5.04897400	1.05644600	1.14314000
H	3.88991300	0.76987000	2.93633500
C	4.34970500	-0.22427600	-0.77218300
H	2.64084900	-1.50657100	-0.46444800
C	5.21789200	0.70209900	-0.19179300
H	5.71772000	1.77814300	1.60281600
H	4.47769600	-0.51127000	-1.81206100
H	6.01876300	1.14281300	-0.77730800
H	0.00467600	2.42065900	2.02886700
TS2 <sub>2</sub> <sup>(R,R)</sup>			
P	-0.03483000	1.93769900	0.95068600
C	-0.20122800	3.26697800	-0.30226300
C	0.59338300	3.01461700	-1.58576900
H	-1.26032200	3.36582800	-0.53836800
H	0.12886100	4.19104700	0.18633400
C	0.56811900	4.23608600	-2.50193100
H	0.16202900	2.15159600	-2.10513300
H	1.63252000	2.74405800	-1.35881100
C	1.22974200	3.95338700	-3.84728300
H	1.07014000	5.07381000	-2.00200500
H	-0.47259500	4.54645100	-2.65929600
H	1.23765700	4.84121900	-4.48452700
H	0.69548100	3.15848900	-4.37690700
H	2.26416100	3.62094900	-3.71326700
C	-1.49620300	1.85929500	2.04767800



C	-2.33183600	3.14012600	2.03543800
H	-2.09217700	1.00427400	1.73764000
H	-1.10678200	1.64396800	3.04766700
C	-3.45362200	3.07388900	3.07258200
H	-2.77230600	3.27431400	1.04117200
H	-1.70875000	4.02303400	2.23491600
C	-4.32722500	4.32492600	3.05595900
H	-3.01792100	2.93494900	4.06903800
H	-4.06722300	2.18645100	2.87424200
H	-5.12731000	4.26076100	3.79751000
H	-4.78812100	4.46519600	2.07340600
H	-3.73405800	5.21771200	3.27721100
C	1.28201800	2.53806100	2.07641700
C	2.51697800	3.18086700	1.43441200
H	0.78094600	3.27228200	2.72044400
H	1.56057100	1.70163600	2.72895400
C	3.59687900	3.47287900	2.47632900
H	2.23143300	4.11670200	0.93791200
H	2.93381200	2.53136000	0.65697200
C	4.81539700	4.15922600	1.86661400
H	3.89856900	2.52978100	2.94966400
H	3.17288100	4.09789100	3.27176400
H	5.58412300	4.34651400	2.62022100
H	4.53949900	5.11950400	1.42008000
H	5.25765600	3.53983700	1.08031200
C	0.55158900	0.38715300	0.16656200
C	-0.23260700	-0.31240600	-0.75503800
C	1.83735800	-0.02672500	0.51633800
C	0.36876000	-1.46080300	-1.54011100
H	-0.44551600	-2.06743600	-1.94589600
C	-1.54587300	0.17346200	-1.09792600
O	-2.08667600	1.17036600	-0.60832300
O	-2.16973500	-0.55439500	-2.04976900
C	-3.41445000	-0.03589800	-2.53203100
C	-3.17940300	1.07689400	-3.53800100
H	-3.91189400	-0.89312200	-2.99145600
H	-4.01204100	0.31068200	-1.68583400
H	-4.13407500	1.45586000	-3.91178900
H	-2.59805800	0.71069600	-4.38837300
H	-2.63996800	1.90189300	-3.06496300
H	2.37740800	-0.65370100	-0.18077600
C	1.27057000	-1.00737100	-2.67496500
C	2.58887800	-1.46019800	-2.76585800
C	0.79808700	-0.13419000	-3.66155100

C	3.41927100	-1.04957500	-3.80878000
H	2.96806900	-2.14383900	-2.00773300
C	1.62013300	0.27225700	-4.70800900
H	-0.22962500	0.21862900	-3.60733700
C	2.93716500	-0.18157400	-4.78366300
H	4.44261300	-1.40924700	-3.85702800
H	1.23308700	0.94182000	-5.47045000
H	3.57916800	0.13810200	-5.59829200
H	2.46285100	0.54353700	1.18872700
C	1.48364500	-1.85024100	1.84783000
H	1.42659900	-1.17115500	2.70084900
N	0.41539000	-2.51121900	1.44096400
S	-0.95826800	-2.20516900	2.27369700
O	-1.19218100	-3.30630000	3.22011200
O	-0.98038400	-0.85217900	2.85397000
C	-2.22790100	-2.31473000	1.03755700
C	-3.35367800	-1.50911400	1.17175200
C	-2.15238400	-3.28824700	0.04454000
C	-4.41637200	-1.68348200	0.29022700
H	-3.39853400	-0.76541900	1.96117800
C	-3.22114100	-3.44401100	-0.82935100
H	-1.26029200	-3.89944800	-0.04602900
C	-4.36925400	-2.65306200	-0.71450400
H	-5.29837000	-1.05550600	0.38462700
H	-3.16420100	-4.19285600	-1.61455300
C	-5.53923900	-2.85279700	-1.64233600
H	-6.25452100	-3.56331100	-1.21540900
H	-5.21513000	-3.25005100	-2.60731100
H	-6.07054000	-1.91308500	-1.81400900
C	2.82531300	-2.40041100	1.54593200
C	3.95140000	-1.84282300	2.15980500
C	2.98702200	-3.47912400	0.66989300
C	5.22070600	-2.34426600	1.89309400
H	3.82654600	-1.00991700	2.84808300
C	4.25813400	-3.97477100	0.39832600
H	2.10703500	-3.92485000	0.21596100
C	5.37822400	-3.40859600	1.00675600
H	6.08732400	-1.90544100	2.37692800
H	4.37526900	-4.81037300	-0.28448900
H	6.36839000	-3.79965000	0.79636900
H	0.93632400	-2.11074400	-0.87026900

M2<sub>2</sub><sup>(R,R)</sup>

P	0.11906800	1.97238300	-0.38954200
C	0.05765800	2.99349400	1.13065700
C	-0.95115600	2.47122400	2.16096600
H	1.06086900	3.00424600	1.55988400
H	-0.19160100	4.01350300	0.81601700
C	-1.02467500	3.37381100	3.39116000
H	-0.66026600	1.46042800	2.47330100
H	-1.95066900	2.38386700	1.71540100
C	-1.98724000	2.82060300	4.43858400
H	-1.33617600	4.38075600	3.08797600
H	-0.02071100	3.47330700	3.82139000
H	-2.01798600	3.45630800	5.32683100
H	-1.68500600	1.81470400	4.74863700
H	-3.00278100	2.75253900	4.03645700
C	1.66599500	2.23754300	-1.33219400
C	2.41849800	3.50149900	-0.91807400
H	2.29060500	1.35466900	-1.20566500
H	1.35850600	2.26691600	-2.38065900
C	3.62910500	3.73704100	-1.82193900
H	2.75531000	3.40231500	0.11974800
H	1.76051700	4.38012800	-0.96314500
C	4.41433100	4.98111300	-1.41763500
H	3.29178700	3.82883000	-2.86113100
H	4.27956900	2.85437700	-1.78238900
H	5.27566200	5.13715800	-2.07168900
H	4.78186600	4.89349300	-0.39063500
H	3.78414400	5.87422100	-1.47187200
C	-1.17481100	2.63117300	-1.50770000
C	-2.47565200	3.19841300	-0.93052600
H	-0.65242700	3.44075800	-2.03476000
H	-1.35273200	1.85137500	-2.25545800
C	-3.35426000	3.76853500	-2.04549000
H	-2.25585800	3.98989700	-0.20290200
H	-3.04956700	2.43585700	-0.39362500
C	-4.68418300	4.29594800	-1.51548400
H	-3.53493400	2.98575300	-2.79233600
H	-2.81054600	4.56958200	-2.56029600
H	-5.29601300	4.70807000	-2.32139800
H	-4.52574700	5.08553300	-0.77454000
H	-5.25535800	3.49569900	-1.03437600
C	-0.29036600	0.25057800	0.08753200
C	0.55010600	-0.57772100	0.74315100
C	-1.70385700	-0.18800300	-0.19747800
C	0.11062500	-1.94232200	1.24774100

H	0.99201500	-2.57831900	1.35044500
C	1.92512900	-0.12736500	1.11680200
O	2.28984500	1.03529900	1.09082000
O	2.70629600	-1.12422700	1.51438300
C	4.04780400	-0.77766500	1.91420500
C	4.06331200	-0.21393800	3.32185000
H	4.59526900	-1.71851500	1.84969500
H	4.45545400	-0.07150200	1.18698900
H	5.09301200	-0.00346700	3.62064200
H	3.64127000	-0.93440800	4.02680200
H	3.49244500	0.71570600	3.37067100
H	-2.01575300	-0.86387600	0.60123900
C	-0.59555200	-1.81813900	2.58677500
C	-1.88534100	-2.32402100	2.76455300
C	0.02719200	-1.17834000	3.66527400
C	-2.54274900	-2.18793600	3.98654100
H	-2.38065500	-2.82367700	1.93450500
C	-0.62707000	-1.03867900	4.88535300
H	1.03775200	-0.79201700	3.55309900
C	-1.91792500	-1.54110600	5.04891000
H	-3.54572200	-2.58559300	4.10449600
H	-0.12831600	-0.53968700	5.71062100
H	-2.42945800	-1.43033300	5.99951500
H	-2.39218700	0.65780500	-0.14857600
C	-1.92736300	-0.92005600	-1.57205600
H	-2.01070300	-0.13729800	-2.33794900
N	-0.88707800	-1.87689600	-1.87370000
S	0.26954400	-1.33318300	-2.78042100
O	0.33055700	-1.94431000	-4.12700100
O	0.33933900	0.16065300	-2.81421800
C	1.78917600	-1.86503100	-1.98773700
C	2.93149500	-1.08083600	-2.12309600
C	1.84733800	-3.07559200	-1.30194800
C	4.13049300	-1.50420900	-1.55440000
H	2.87602400	-0.14836000	-2.67627800
C	3.05276700	-3.49250700	-0.74650000
H	0.94499000	-3.66944800	-1.19352100
C	4.21126900	-2.71870700	-0.86734800
H	5.02000900	-0.88684400	-1.65468800
H	3.09604300	-4.43503600	-0.20663000
C	5.52249100	-3.19873900	-0.29936700
H	6.05540600	-3.81872500	-1.02778200
H	5.36813500	-3.80638100	0.59633900
H	6.17462800	-2.35993700	-0.04216800

C	-3.28996600	-1.58464900	-1.46791200
C	-4.44607500	-0.80426700	-1.55502600
C	-3.41616700	-2.95181700	-1.21905700
C	-5.70553700	-1.37547600	-1.39509600
H	-4.35787100	0.26173400	-1.76116800
C	-4.67587500	-3.52605100	-1.05545800
H	-2.51480900	-3.55476200	-1.17860100
C	-5.82353200	-2.74089700	-1.14143800
H	-6.59449000	-0.75702400	-1.47312400
H	-4.76166400	-4.59214900	-0.86747100
H	-6.80385300	-3.19030000	-1.01823700
H	-0.53750800	-2.40915800	0.50368000
TS3 <sub>2</sub> <sup>(R,R,R)</sup>			
P	1.16312800	0.89132800	-1.35190900
C	2.30234900	2.32617200	-1.17960500
C	1.76989100	3.46059600	-0.29969900
H	3.25590500	1.96143100	-0.79515700
H	2.47052400	2.69018700	-2.20012500
C	2.72534600	4.65310900	-0.29423200
H	1.63190700	3.10673900	0.72929500
H	0.78038900	3.78445900	-0.64597200
C	2.23839600	5.76960100	0.62452400
H	2.83879200	5.03134200	-1.31733300
H	3.71964900	4.31538000	0.02429000
H	2.92614200	6.61850000	0.61748300
H	2.15156200	5.41342800	1.65580300
H	1.25369800	6.13012300	0.31177000
C	2.04987100	-0.68100500	-1.66551200
C	3.51359800	-0.50918800	-2.08177700
H	1.97565900	-1.27630600	-0.75131600
H	1.47783700	-1.18989500	-2.45175700
C	4.07544300	-1.79926900	-2.67923700
H	4.09524200	-0.22044200	-1.19806300
H	3.62381200	0.30065600	-2.81569500
C	5.57752500	-1.71667700	-2.92990600
H	3.54853100	-2.01601600	-3.61628400
H	3.85271200	-2.63100400	-2.00157600
H	5.95782300	-2.64127900	-3.37115300
H	6.11918800	-1.54247200	-1.99459700
H	5.81645400	-0.89416700	-3.61140900
C	0.30098200	1.22948400	-2.92596200
C	-0.41970100	2.58041500	-2.99110000

H	1.07498800	1.16927900	-3.70156900
H	-0.38834200	0.40089700	-3.12218900
C	-1.35196000	2.66226700	-4.19970900
H	0.31973100	3.38938000	-3.04281700
H	-1.00192900	2.75238200	-2.07546100
C	-2.03010200	4.02373800	-4.31371300
H	-2.10931900	1.87241300	-4.11573800
H	-0.77935700	2.45000900	-5.11069800
H	-2.70278800	4.06018900	-5.17377400
H	-1.28864600	4.81985600	-4.43149000
H	-2.61736500	4.24268000	-3.41677000
C	-0.09052300	0.72608600	-0.06731400
C	0.20208700	0.72238300	1.27468000
C	-1.50522300	0.40662700	-0.54026500
C	-0.78626200	0.51146800	2.31673500
H	-0.33863400	0.29378900	3.28511400
C	1.65410300	0.74014500	1.67079100
O	2.56843900	0.51560200	0.89594200
O	1.84753300	1.03531900	2.94908800
C	3.22000000	1.15347000	3.38111600
C	3.79250800	2.49410200	2.96293100
H	3.17059300	1.05440500	4.46523600
H	3.79332800	0.32329900	2.96318400
H	4.80297100	2.60499600	3.36288400
H	3.17483200	3.30864500	3.34891600
H	3.84205500	2.56698300	1.87325600
H	-2.24635100	0.91927200	0.07982100
C	-1.98808000	1.37963800	2.46220900
C	-3.03997400	0.92773500	3.27589600
C	-2.13535700	2.62742200	1.84022100
C	-4.18101700	1.69570200	3.47390200
H	-2.94937600	-0.04902100	3.74570300
C	-3.28347100	3.39428400	2.02908100
H	-1.33685000	2.99834400	1.20005100
C	-4.31123200	2.93656500	2.84935300
H	-4.97740400	1.32107600	4.11016500
H	-3.37088300	4.35842000	1.53641800
H	-5.20470900	3.53464600	2.99702100
H	-1.68724900	0.75311400	-1.55817800
C	-1.80736300	-1.10514100	-0.49658900
H	-1.01222100	-1.62777400	-1.06216300
N	-1.80838600	-1.52037400	0.90927100
S	-1.42114500	-3.04192900	1.21640100
O	-1.62870200	-3.25560900	2.65339000

O	-2.04839800	-3.97303000	0.26902900
C	0.34481700	-3.19523600	0.94957400
C	0.84426700	-3.96204500	-0.09474200
C	1.20983100	-2.52732800	1.81876100
C	2.22590500	-4.06895900	-0.26433100
H	0.15401000	-4.48349600	-0.74958500
C	2.58052400	-2.63814700	1.63562400
H	0.80594700	-1.94500300	2.64414400
C	3.10969700	-3.41310500	0.59388100
H	2.62051300	-4.67785600	-1.07367100
H	3.25802500	-2.12493800	2.31328100
C	4.60273800	-3.52258700	0.42267200
H	4.86293500	-4.16864700	-0.41878800
H	5.06785900	-3.93114200	1.32454800
H	5.04597000	-2.53643700	0.24623200
C	-3.13047400	-1.36222600	-1.19785200
C	-3.15819000	-1.64210600	-2.56477400
C	-4.33523300	-1.23080700	-0.50560500
C	-4.37078400	-1.79299000	-3.23414800
H	-2.22123400	-1.75742400	-3.10674000
C	-5.54818100	-1.38050600	-1.17210300
H	-4.30389700	-1.02014800	0.55947400
C	-5.56995900	-1.66114800	-2.53767900
H	-4.37888900	-2.02125800	-4.29551000
H	-6.48065100	-1.28049800	-0.62498100
H	-6.51689800	-1.78258100	-3.05405700
H	-1.31820000	-0.63845900	1.74569800

M3<sub>2</sub><sup>(R,R,R)</sup>

P	0.04941000	-1.05679300	-1.45240700
C	-0.49714400	-2.80912100	-1.38410700
C	0.30301000	-3.75220000	-0.48148100
H	-1.55147400	-2.79667700	-1.08403400
H	-0.46925600	-3.16772300	-2.42121400
C	-0.09624800	-5.20931800	-0.70994600
H	0.13531000	-3.49751800	0.57071000
H	1.37903100	-3.62713100	-0.65335100
C	0.62611600	-6.15898800	0.24079700
H	0.11788900	-5.48490400	-1.75013200
H	-1.18198900	-5.30786800	-0.58047800
H	0.34609600	-7.19908600	0.05601200
H	0.38537400	-5.92371800	1.28244400
H	1.71113700	-6.07570500	0.12410700

C	-1.45712300	-0.16457600	-2.03800200
C	-2.03462300	-0.59426700	-3.38984800
H	-2.19495200	-0.31468600	-1.24350200
H	-1.22977500	0.90852500	-2.05712000
C	-3.36339100	0.11270400	-3.66201500
H	-2.19464800	-1.68017200	-3.41665200
H	-1.33536700	-0.35697200	-4.20025100
C	-3.95873500	-0.25827800	-5.01694700
H	-3.20443700	1.19748400	-3.60723600
H	-4.07083500	-0.13988200	-2.86147200
H	-4.90985200	0.25192700	-5.18827700
H	-4.13844100	-1.33605000	-5.08177700
H	-3.27874400	0.01602600	-5.82934800
C	1.21235700	-0.89723400	-2.86231900
C	2.49375300	-1.71703700	-2.72122600
H	0.66938200	-1.19190000	-3.76686500
H	1.44332800	0.17065300	-2.97129800
C	3.47021800	-1.46545800	-3.86922300
H	2.24336400	-2.78561200	-2.68493900
H	2.98341800	-1.47947600	-1.76925100
C	4.74490200	-2.29241800	-3.73050900
H	3.71993300	-0.39753200	-3.89683100
H	2.97733700	-1.69455900	-4.82196800
H	5.43792600	-2.09970200	-4.55310400
H	4.51613000	-3.36262100	-3.72562500
H	5.26051600	-2.05799400	-2.79366100
C	0.84957400	-0.51781800	-0.01368000
C	0.52778600	-1.03958800	1.30124100
C	1.70017600	0.73086100	-0.12536700
C	1.35404400	-1.14438400	2.38492100
H	0.88046300	-1.36186000	3.33774100
C	-0.91268500	-1.38431700	1.55812300
O	-1.83626800	-0.93597100	0.89878200
O	-1.10589900	-2.24342600	2.56509100
C	-2.46965000	-2.61467100	2.83751600
C	-2.93694900	-3.67762500	1.86154300
H	-2.45090400	-2.99216100	3.86064000
H	-3.09803600	-1.72109200	2.78942200
H	-3.93678800	-4.02340600	2.13654100
H	-2.25795300	-4.53487800	1.87815100
H	-2.97841500	-3.27205000	0.84786300
H	2.19234100	0.90946800	0.83450600
C	2.81135700	-1.03622600	2.45299000
C	3.41790600	-0.86148700	3.70964300



C	3.65470100	-1.19349700	1.33803300
C	4.80043600	-0.82122500	3.84620900
H	2.78547100	-0.75691200	4.58769100
C	5.03690900	-1.17047800	1.47723400
H	3.20415900	-1.35348400	0.36420100
C	5.61986600	-0.97332900	2.72891400
H	5.24054300	-0.67523800	4.82796300
H	5.66470300	-1.30361100	0.60077100
H	6.69965400	-0.94148800	2.83254900
H	2.50685900	0.66830000	-0.87184400
C	0.88572700	2.01566900	-0.45603700
H	0.54089400	1.96266700	-1.50056100
N	-0.26629800	2.02151600	0.45568400
S	-1.51101600	3.07867900	0.09949400
O	-1.32783600	4.30357600	0.87353300
O	-1.67811500	3.21589200	-1.35203900
C	-2.86799800	2.14505800	0.75537400
C	-3.81180500	1.61226200	-0.11622000
C	-2.91395600	1.89769800	2.12418800
C	-4.81267500	0.79824000	0.40019400
H	-3.74969500	1.83169300	-1.17729500
C	-3.92015500	1.07775200	2.62042900
H	-2.17274900	2.33347600	2.78693500
C	-4.87104800	0.50801200	1.76719900
H	-5.55772700	0.37606500	-0.26860600
H	-3.96750000	0.87309300	3.68619600
C	-5.92632300	-0.42379700	2.30154100
H	-6.89698300	-0.22832200	1.83930600
H	-6.03040700	-0.32854700	3.38418000
H	-5.66277900	-1.46369200	2.07878800
C	1.74782400	3.24836800	-0.31800200
C	2.46141800	3.70481600	-1.42760800
C	1.91605300	3.89034600	0.91111200
C	3.33374000	4.78435500	-1.31496400
H	2.32862500	3.21157700	-2.38824300
C	2.78371900	4.97283300	1.02351700
H	1.34859000	3.54585400	1.77003600
C	3.49585900	5.42209700	-0.08736500
H	3.88036300	5.13052800	-2.18653700
H	2.90253600	5.46928600	1.98152900
H	4.17042600	6.26758500	0.00236900
H	-0.64960600	1.06948300	0.51716400

TS4<sub>2</sub><sup>(R,R,R)</sup>

P	0.14995200	1.02303700	-1.42295600
C	0.76682800	2.74862900	-1.38670100
C	0.03818900	3.72977900	-0.46366200
H	1.82579700	2.69097200	-1.11571000
H	0.71382300	3.09741700	-2.42698100
C	0.58494800	5.14956200	-0.62270300
H	0.14915200	3.41685700	0.58029400
H	-1.03827000	3.73085100	-0.67504900
C	-0.09025900	6.13135900	0.33018900
H	0.44652700	5.47856500	-1.66082200
H	1.66742500	5.13979100	-0.44087500
H	0.31856800	7.13865000	0.21636600
H	0.05432500	5.82246400	1.37275800
H	-1.17045600	6.17923400	0.14349700
C	1.50039800	-0.00652700	-2.08705200
C	2.16039500	0.47864900	-3.37799800
H	2.23024400	-0.06287800	-1.27487300
H	1.09480600	-1.01975100	-2.21612700
C	3.33900100	-0.42361600	-3.74817400
H	2.51827500	1.51028400	-3.26609100
H	1.43970000	0.48059100	-4.20630100
C	3.99635100	-0.01116900	-5.06106000
H	2.98636000	-1.46139000	-3.81266500
H	4.07390800	-0.39394300	-2.93424600
H	4.84091800	-0.66024100	-5.30591800
H	4.36948200	1.01663300	-5.00440200
H	3.28146800	-0.06346000	-5.88852700
C	-1.14913500	0.96713800	-2.71468200
C	-2.30395300	1.95540800	-2.54309400
H	-0.64029300	1.14800900	-3.66832700
H	-1.51918800	-0.06284500	-2.75105300
C	-3.38900800	1.73557300	-3.59643800
H	-1.92537900	2.98205600	-2.62069200
H	-2.74807800	1.85199900	-1.54651700
C	-4.53757800	2.73140200	-3.45584800
H	-3.77097800	0.71067200	-3.50564900
H	-2.94362800	1.81708900	-4.59589500
H	-5.30590100	2.56256900	-4.21308000
H	-4.17872500	3.75944300	-3.56464900
H	-5.00870300	2.64347200	-2.47122900
C	-0.47056300	0.34033300	0.11282100
C	-0.16278100	1.01224600	1.40108700
C	-1.71844100	-0.53285900	-0.02037500

C	-0.99990100	1.31224200	2.41916600
H	-0.54516100	1.57049100	3.37289500
C	1.30303800	1.25723200	1.61038600
O	2.12449400	1.10895100	0.72384100
O	1.63222800	1.70171000	2.82609900
C	3.00671300	2.09147900	3.00904000
C	3.25017800	3.47070100	2.42648400
H	3.15422200	2.07545400	4.08990500
H	3.64774400	1.34000700	2.54225300
H	4.27664100	3.78382300	2.62766400
H	2.57027500	4.20005100	2.87416300
H	3.09748200	3.45835600	1.34576700
H	-2.17027300	-0.65036600	0.96865800
C	-2.47095900	1.35921600	2.38787500
C	-3.22077900	0.88257700	3.46940000
C	-3.14485900	1.94284000	1.30727400
C	-4.61130600	0.94894600	3.44880800
H	-2.70808300	0.44684400	4.32132200
C	-4.53235000	2.01741300	1.29071800
H	-2.55943500	2.35591900	0.49130200
C	-5.27055100	1.51172700	2.35927900
H	-5.18044400	0.56135600	4.28906400
H	-5.03770500	2.48072000	0.44701200
H	-6.35436300	1.56363700	2.34649200
H	-2.50804000	-0.16971900	-0.68698500
C	-1.24589500	-1.96603600	-0.45658700
H	-1.02562300	-1.96677200	-1.53910300
N	-0.03118000	-2.12383100	0.31999500
S	1.07641500	-3.19281600	-0.13682400
O	0.90886200	-4.49329300	0.53285100
O	1.24414200	-3.26589900	-1.60406900
C	2.52661100	-2.41332300	0.54339800
C	3.59898500	-2.11001900	-0.28723700
C	2.55622400	-2.09778900	1.89946300
C	4.70653700	-1.45985600	0.24775300
H	3.54755000	-2.36809000	-1.34051800
C	3.67312700	-1.45072000	2.41962100
H	1.70977400	-2.34412700	2.53286300
C	4.75773700	-1.11645000	1.60268000
H	5.54626800	-1.21089800	-0.39783100
H	3.70187300	-1.19851900	3.47652400
C	5.95494600	-0.39145600	2.15929100
H	6.87749500	-0.94246900	1.95591100
H	5.86820700	-0.25558100	3.23960900

H	6.05928800	0.59675500	1.69947600
C	-2.33818700	-2.98067700	-0.20300900
C	-3.41715900	-3.05496900	-1.08813800
C	-2.31997000	-3.81133900	0.91784300
C	-4.46544800	-3.94253000	-0.85562400
H	-3.43168400	-2.41922000	-1.97039800
C	-3.36821800	-4.69958100	1.14923700
H	-1.46608400	-3.76938400	1.58419800
C	-4.44430500	-4.76696300	0.26701600
H	-5.29492800	-3.99353100	-1.55417100
H	-3.34203600	-5.34685200	2.02054400
H	-5.25484800	-5.46422600	0.44634500
H	0.23764000	-0.82364400	0.27088500

M4<sub>2</sub><sup>(R,R,R)</sup>

P	0.30478600	0.64367900	-1.50899500
C	1.08282000	2.26359700	-1.85786600
C	0.62750500	3.49282900	-1.06416800
H	2.15900700	2.11161600	-1.73528100
H	0.89248700	2.42178800	-2.92799400
C	1.18186300	4.77553400	-1.68456000
H	0.97207200	3.42443300	-0.02749000
H	-0.46653300	3.55364100	-1.02772900
C	0.82324800	6.00728000	-0.85898600
H	0.79361400	4.87988900	-2.70487700
H	2.27204500	4.68821900	-1.77152600
H	1.21654000	6.91884100	-1.31479800
H	1.23582700	5.93017600	0.15185200
H	-0.26218100	6.11548200	-0.76978500
C	1.43951900	-0.64415600	-2.10174600
C	1.89958800	-0.51268300	-3.55455200
H	2.29190700	-0.59328500	-1.41406600
H	0.95185200	-1.61357900	-1.92507100
C	2.88407600	-1.63090000	-3.90196900
H	2.38260100	0.45854400	-3.71982900
H	1.04410800	-0.56532200	-4.23883600
C	3.36768000	-1.54770800	-5.34626700
H	2.40009200	-2.59815800	-3.72097100
H	3.73884000	-1.57772100	-3.21612800
H	4.07275100	-2.35057800	-5.57456400
H	3.86999400	-0.59390400	-5.53541000
H	2.52860000	-1.62839200	-6.04410300
C	-1.21194400	0.56305700	-2.52063900

C	-2.18000500	1.74234100	-2.38655700
H	-0.87233500	0.47143100	-3.55882100
H	-1.71410300	-0.37659600	-2.27103000
C	-3.49291300	1.46108300	-3.11812800
H	-1.72005200	2.65165400	-2.79343300
H	-2.40357900	1.94095200	-1.33148900
C	-4.45760200	2.63927200	-3.03352100
H	-3.95404200	0.56635400	-2.68093200
H	-3.27855500	1.22455000	-4.16718500
H	-5.39532900	2.42187000	-3.54996300
H	-4.02171800	3.53473800	-3.48694000
H	-4.69426500	2.87258000	-1.99078200
C	-0.06986100	0.21609800	0.26751000
C	0.41082800	1.21906800	1.29747900
C	-1.47101500	-0.38640000	0.45141600
C	-0.28844200	1.88090500	2.23324500
H	0.29646800	2.42237700	2.97407000
C	1.89964800	1.37307700	1.27126700
O	2.56913700	0.95739300	0.34280200
O	2.41035800	2.03187500	2.30730300
C	3.82402100	2.31437200	2.24595000
C	4.08813400	3.51072300	1.35267500
H	4.10655900	2.50994000	3.28081700
H	4.33891800	1.42040200	1.88854600
H	5.15144300	3.76086100	1.37432900
H	3.52037800	4.37862700	1.69694700
H	3.80867100	3.28666400	0.32004300
H	-1.72078300	-0.35406700	1.51469800
C	-1.75696500	1.98784000	2.37420400
C	-2.39208200	1.50899700	3.52521000
C	-2.51939700	2.61033500	1.38330600
C	-3.77439000	1.60169600	3.65091700
H	-1.80252100	1.04035100	4.30772200
C	-3.90127400	2.71614600	1.51664600
H	-2.01768400	3.03586200	0.51917200
C	-4.53250300	2.20079200	2.64573000
H	-4.26067700	1.20711100	4.53702300
H	-4.48191900	3.20593800	0.74143800
H	-5.61007800	2.27463400	2.74835100
H	-2.25051600	0.17957000	-0.06818500
C	-1.50661000	-1.88347800	0.05664200
H	-1.14336400	-2.00992400	-0.97640100
N	-0.70209500	-2.63594300	0.99905800
S	0.48617200	-3.50087300	0.46707000

O	0.57374300	-4.78743400	1.18623600
O	0.56324800	-3.60848900	-1.01572000
C	2.01487500	-2.65876500	0.93212100
C	3.13854400	-2.74973800	0.11317300
C	2.08453400	-1.96062400	2.13602700
C	4.33068100	-2.15257900	0.50992200
H	3.06484800	-3.27816000	-0.83272700
C	3.28620300	-1.37452700	2.52836100
H	1.19092700	-1.86960700	2.74789400
C	4.42709300	-1.47022300	1.72747300
H	5.20626300	-2.22237900	-0.13130200
H	3.33788600	-0.83289900	3.47020200
C	5.74139200	-0.87047700	2.15843800
H	6.49351600	-1.65119100	2.30710000
H	5.63911600	-0.31995500	3.09661900
H	6.13262600	-0.18620700	1.39888500
C	-2.96487000	-2.31971100	0.06861900
C	-3.70921900	-2.36233500	-1.11144600
C	-3.60180100	-2.61220000	1.27691700
C	-5.06676400	-2.68065100	-1.08844800
H	-3.22056900	-2.16515600	-2.06397300
C	-4.95629800	-2.92941400	1.30488100
H	-3.01237800	-2.60332400	2.18899900
C	-5.69473200	-2.96199900	0.12175000
H	-5.62924900	-2.71752200	-2.01643900
H	-5.43867200	-3.15604900	2.25099900
H	-6.75049200	-3.21333000	0.14342300
H	0.62248000	-0.62701000	0.40620500

M4<sub>2</sub>'<sup>(R,R,R)</sup>

P	1.06254900	1.35343900	-1.31733000
C	2.40045500	2.28770200	-0.48674700
C	2.13597200	2.90906400	0.89291500
H	3.27435800	1.63081900	-0.45696000
H	2.61770700	3.08649600	-1.20887900
C	3.14760100	4.01355100	1.19787300
H	2.20825700	2.14310200	1.67046100
H	1.12010300	3.31655300	0.95770400
C	2.92941500	4.61123700	2.58447100
H	3.06970400	4.79763900	0.43514000
H	4.16229000	3.60246000	1.12193700
H	3.66032900	5.39443500	2.79853700
H	3.02106100	3.84399200	3.35987800

H	1.93030100	5.05087300	2.66613000
C	1.81722000	0.45233700	-2.70569500
C	2.60290400	1.31354800	-3.69775200
H	2.45724300	-0.30533600	-2.23675800
H	0.99928200	-0.07786600	-3.21024200
C	3.21366700	0.46111100	-4.81053000
H	3.40468300	1.85025800	-3.17641000
H	1.94711900	2.07094400	-4.14395400
C	4.00633600	1.30250100	-5.80630400
H	2.41248000	-0.07756900	-5.32999500
H	3.86334600	-0.29978800	-4.36229400
H	4.43618900	0.68039700	-6.59477600
H	4.82586900	1.82845700	-5.30721700
H	3.36570100	2.05254700	-6.28003500
C	-0.08237300	2.59947300	-1.99724700
C	-0.88728600	3.38763800	-0.95041300
H	0.52382700	3.27762500	-2.60763800
H	-0.75258900	2.07761400	-2.68795700
C	-2.16671400	3.95950700	-1.56065200
H	-0.27073400	4.20396200	-0.55657500
H	-1.15288400	2.75650700	-0.09184700
C	-2.95881600	4.79309500	-0.55964100
H	-2.78340300	3.12690200	-1.92239400
H	-1.90818100	4.56402000	-2.43861900
H	-3.87046300	5.19184800	-1.01122400
H	-2.36425800	5.63790700	-0.19739600
H	-3.24395800	4.18754800	0.30623800
C	0.12903600	0.05064500	-0.35897000
C	0.50183400	0.10355300	1.10892200
C	-1.34096600	0.01686000	-0.80566000
C	-0.11428800	0.65966700	2.16547200
H	0.46691200	0.64943400	3.08596100
C	1.91292300	-0.37074000	1.30174200
O	2.66532400	-0.54799800	0.35816100
O	2.29538400	-0.49481700	2.57141100
C	3.70185100	-0.71513000	2.79897800
C	4.46716000	0.59102200	2.70994200
H	3.75123800	-1.14626000	3.79939600
H	4.06645100	-1.44179300	2.07121500
H	5.51923600	0.42033200	2.95011700
H	4.06509500	1.32358700	3.41465400
H	4.40991800	0.99920400	1.69673600
H	-1.95138600	0.72218700	-0.24162600
C	-1.40955000	1.36599900	2.29516600

C	-2.64162100	0.75642500	2.03344000
C	-1.38581000	2.67533500	2.79641200
C	-3.82430700	1.46714900	2.22296000
H	-2.64864700	-0.27615800	1.69251900
C	-2.56958600	3.38291900	2.97910100
H	-0.43225000	3.13820800	3.04102600
C	-3.79319300	2.77978100	2.68909900
H	-4.77392200	0.98545600	2.00947100
H	-2.53792600	4.40128900	3.35310800
H	-4.71807300	3.32888500	2.83519300
H	-1.40791700	0.32228800	-1.85477700
C	-1.94341600	-1.40459700	-0.73398600
H	-1.43818000	-1.99199800	-1.52035000
N	-1.75366400	-1.96979800	0.58405100
S	-1.35580500	-3.48722900	0.62569500
O	-1.66075400	-4.03768400	1.95925200
O	-1.83702500	-4.27372500	-0.53449100
C	0.43650400	-3.58954300	0.49496500
C	1.04559500	-3.58466100	-0.76085700
C	1.21709800	-3.61923300	1.64698100
C	2.43313300	-3.57697100	-0.85487600
H	0.42900400	-3.61294500	-1.65448200
C	2.60486800	-3.64361000	1.53916900
H	0.72991000	-3.64921700	2.61612300
C	3.23273200	-3.59802400	0.29241500
H	2.90651500	-3.56575200	-1.83381500
H	3.21073500	-3.69376500	2.44088800
C	4.73235200	-3.52171100	0.18379200
H	5.04383700	-2.47684100	0.06637100
H	5.10066100	-4.07420800	-0.68428900
H	5.21863200	-3.91723600	1.07889600
C	-3.41325200	-1.30098800	-1.14706200
C	-3.75245800	-0.93467400	-2.45400800
C	-4.43941700	-1.52497300	-0.22952900
C	-5.08302100	-0.78202100	-2.83232800
H	-2.96578500	-0.78131800	-3.19061300
C	-5.77377000	-1.36853500	-0.60299500
H	-4.17137500	-1.83992200	0.77412600
C	-6.10106600	-0.99261300	-1.90298000
H	-5.32675200	-0.50518300	-3.85369600
H	-6.56009200	-1.54801500	0.12433700
H	-7.13993600	-0.87464900	-2.19473700
H	0.60111800	-0.86408300	-0.74429600



TS5<sub>2</sub><sup>(R,R,R)</sup>

P	-1.90022600	-1.25374500	-0.87380800
C	-3.25789400	-1.15354000	0.35178100
C	-2.97327800	-1.35230100	1.84475700
H	-3.70349700	-0.16645400	0.18737700
H	-3.98057200	-1.90520800	0.00801400
C	-4.27568800	-1.35481700	2.64698700
H	-2.31514400	-0.55735000	2.21260500
H	-2.45621500	-2.30205600	2.01998400
C	-4.01879400	-1.49586500	4.14414800
H	-4.91451100	-2.17509300	2.29757400
H	-4.82453900	-0.42631700	2.44899400
H	-4.95396800	-1.49291800	4.70890100
H	-3.39857000	-0.67248000	4.51222600
H	-3.49420400	-2.43075300	4.36414900
C	-2.58855200	-0.57333700	-2.41906600
C	-3.87537500	-1.22747900	-2.92516200
H	-2.73977500	0.49258400	-2.20858400
H	-1.79191100	-0.64921800	-3.16975200
C	-4.35544100	-0.58074600	-4.22553700
H	-4.66483800	-1.13760000	-2.16948000
H	-3.71739500	-2.29894800	-3.09796600
C	-5.64475500	-1.21546400	-4.73771100
H	-3.56787500	-0.67082700	-4.98304700
H	-4.50738500	0.49190800	-4.05749300
H	-5.97554500	-0.74597100	-5.66712300
H	-6.44876900	-1.11157500	-4.00275000
H	-5.50368700	-2.28327800	-4.93120900
C	-1.52941600	-3.01048800	-1.22098100
C	-0.93007400	-3.85074600	-0.09047400
H	-2.48282000	-3.44651400	-1.54388700
H	-0.86896900	-3.02034200	-2.09587500
C	-0.71864800	-5.29990900	-0.52771800
H	-1.59147700	-3.83522300	0.78433300
H	0.02955600	-3.43142300	0.22775300
C	-0.09551900	-6.13943400	0.58340000
H	-0.07335300	-5.31576900	-1.41403000
H	-1.68032800	-5.73076500	-0.83146300
H	0.05292200	-7.17385100	0.26456300
H	-0.73607200	-6.14901800	1.47116100
H	0.87758600	-5.73327300	0.87731600
C	-0.38422100	-0.21927400	-0.54553700
C	-0.35452300	0.50841800	0.77385400

C	0.93757800	-0.89884800	-0.92410600
C	0.74009400	0.46389900	1.61448700
H	0.86104000	1.34150600	2.25211400
C	-1.35262200	1.55099300	0.87219800
O	-2.20982500	1.75061500	0.00906400
O	-1.36507900	2.20264700	2.05556200
C	-2.45849500	3.10240700	2.27136500
C	-3.70934700	2.33841600	2.66545900
H	-2.12294700	3.76234500	3.07411600
H	-2.62682300	3.69370700	1.36798700
H	-4.51733800	3.03295400	2.90908000
H	-3.51607400	1.70903300	3.53901500
H	-4.03377400	1.70683200	1.83465100
H	1.22698000	-1.66769200	-0.20385500
C	1.39561700	-0.74770400	2.17679700
C	2.69578800	-0.69167000	2.69725700
C	0.66572400	-1.92657400	2.31850200
C	3.25431100	-1.80648200	3.30840900
H	3.26089400	0.22832300	2.57824500
C	1.22825100	-3.05272200	2.91966900
H	-0.35897400	-1.95184600	1.96258100
C	2.52646400	-2.99528900	3.41426000
H	4.26523300	-1.75434800	3.70044400
H	0.64531700	-3.96548000	3.00646500
H	2.97036100	-3.86570800	3.88666100
H	0.84077800	-1.38741000	-1.90053700
C	2.09172700	0.12513400	-1.06246300
H	1.76961000	0.83770800	-1.83998100
N	2.37971600	0.78102700	0.21146500
S	2.90326600	2.27590300	0.12550600
O	3.38528600	2.66061500	1.46330900
O	3.81311500	2.49451200	-1.01593100
C	1.50169900	3.34489800	-0.20345100
C	1.01641600	3.47736300	-1.50656300
C	0.87527800	4.00546400	0.84735300
C	-0.12541600	4.23423400	-1.73948600
H	1.55073700	3.01733200	-2.33159300
C	-0.24831600	4.78725900	0.59452600
H	1.28073600	3.91461100	1.84970700
C	-0.78196700	4.88904900	-0.69143100
H	-0.50842000	4.33234500	-2.75185100
H	-0.72531200	5.31966400	1.41332500
C	-2.04683700	5.66578900	-0.94547000
H	-2.00873900	6.18675300	-1.90544000

H	-2.22653400	6.40162100	-0.15829100
H	-2.90730700	4.98799200	-0.97318900
C	3.30415900	-0.62054800	-1.60425400
C	3.53201700	-0.69733400	-2.97858500
C	4.16203700	-1.29746200	-0.73518500
C	4.60118300	-1.43577200	-3.48195500
H	2.87108200	-0.16528300	-3.65976300
C	5.22789100	-2.03992400	-1.23562200
H	3.98685200	-1.22102500	0.33499100
C	5.45179100	-2.11086600	-2.61016000
H	4.77359500	-1.47755900	-4.55311800
H	5.89051900	-2.56158600	-0.55137100
H	6.28812500	-2.68408900	-2.99802700
H	-0.54836700	0.57007700	-1.29766400

M5<sub>2</sub><sup>(R,R,R)</sup>

P	-1.94845600	0.97352400	0.77971200
C	-2.38608500	2.43514400	-0.22504300
C	-1.19570300	3.09892600	-0.91776900
H	-3.09688900	2.08648500	-0.97600000
H	-2.89113100	3.13263300	0.45551800
C	-1.55893600	4.44941000	-1.52780200
H	-0.85296100	2.42258400	-1.70538900
H	-0.35542200	3.22979200	-0.22110600
C	-0.37853700	5.05129700	-2.28514000
H	-1.88917900	5.13443200	-0.73685100
H	-2.41153400	4.31895300	-2.20607500
H	-0.63444500	6.01585300	-2.73035600
H	-0.05398700	4.38215600	-3.08945300
H	0.47386200	5.20483200	-1.61475000
C	-3.37232400	-0.15926000	0.91105900
C	-4.71661000	0.55087300	1.09470300
H	-3.36083000	-0.75694500	-0.00468900
H	-3.15744400	-0.82054200	1.76187100
C	-5.85400000	-0.44703100	1.31362900
H	-4.93769700	1.15635000	0.20787200
H	-4.68366200	1.24065200	1.94786800
C	-7.20200600	0.24521800	1.49156900
H	-5.62889400	-1.05757800	2.19708500
H	-5.89575800	-1.13435200	0.46048400
H	-8.00315300	-0.48121800	1.64754600
H	-7.45381200	0.84047900	0.60871200
H	-7.18394100	0.91783300	2.35469400

C	-1.73268500	1.61050900	2.48649100
C	-0.87625800	2.87342800	2.62872300
H	-2.74009600	1.81018500	2.87023200
H	-1.33079700	0.79117400	3.09483100
C	-0.68695900	3.25710400	4.09630200
H	-1.35463500	3.70536100	2.09658400
H	0.10771500	2.73419600	2.16656000
C	0.13048300	4.53504500	4.25716700
H	-0.19267500	2.42951300	4.61955700
H	-1.67083900	3.37958300	4.56508900
H	0.26316300	4.79143400	5.31095900
H	-0.36282400	5.37824800	3.76413200
H	1.12312300	4.42067700	3.81090100
C	-0.43753700	-0.03536000	0.37416100
C	-0.05850100	-0.14214800	-1.07577900
C	0.82535100	0.33167200	1.17047300
C	1.34879500	-0.60097800	-1.37049400
H	1.31691200	-1.26504800	-2.24020700
C	-1.05266700	-0.16492000	-2.02771700
O	-2.27657100	0.06451000	-1.82927900
O	-0.61518000	-0.45928000	-3.31131800
C	-1.50712600	-0.10173800	-4.36068100
C	-1.54458200	1.40555600	-4.55872500
H	-1.11680600	-0.60280100	-5.25018000
H	-2.50772700	-0.48735700	-4.14691400
H	-2.13757100	1.66735700	-5.43944600
H	-0.53033900	1.79367700	-4.69176200
H	-1.99352300	1.88119500	-3.68220900
H	1.28335900	1.22677600	0.73694900
C	2.41663200	0.44592900	-1.70701200
C	3.73199300	0.02285500	-1.92664400
C	2.11947000	1.79981600	-1.82342800
C	4.73215800	0.94088600	-2.22269700
H	3.96499000	-1.03508800	-1.83469800
C	3.12168700	2.72765100	-2.11375800
H	1.09652200	2.12185100	-1.67053700
C	4.43170400	2.30220200	-2.30743300
H	5.75044200	0.59853200	-2.38009900
H	2.87328700	3.78252100	-2.18851900
H	5.21414200	3.02143300	-2.52857600
H	0.63561400	0.52941500	2.22851900
C	1.79767700	-0.85890200	1.12370300
H	1.35832200	-1.63260000	1.76546100
N	1.89073700	-1.42395400	-0.24817900

S	1.70968900	-3.06557800	-0.36449900
O	2.07881100	-3.43952900	-1.72561600
O	2.41799900	-3.64661300	0.77315200
C	-0.01941500	-3.40496600	-0.14563900
C	-0.48891800	-3.78452400	1.11089200
C	-0.89358000	-3.14432600	-1.19874000
C	-1.86032700	-3.90022800	1.31081200
H	0.21762200	-3.99139800	1.90813500
C	-2.26166800	-3.24772100	-0.97446300
H	-0.51538100	-2.84485100	-2.17176000
C	-2.76148200	-3.62346600	0.27686500
H	-2.23791900	-4.20423900	2.28310900
H	-2.95186400	-3.02107400	-1.78166800
C	-4.24379600	-3.74397400	0.51018500
H	-4.81044200	-3.29480000	-0.30849400
H	-4.53499100	-3.25278500	1.44339300
H	-4.53874000	-4.79525600	0.58787700
C	3.16451900	-0.53395600	1.70482400
C	3.71652100	-1.40163200	2.64905200
C	3.88420300	0.60707000	1.33451100
C	4.96126900	-1.14200400	3.21687700
H	3.16771300	-2.29790800	2.92396700
C	5.13096500	0.86570300	1.89800500
H	3.48386200	1.29370700	0.59329000
C	5.67248400	-0.00540100	2.84190100
H	5.37467900	-1.82866400	3.94881500
H	5.68128100	1.75183200	1.59689900
H	6.64400800	0.19994500	3.28037100
H	-0.79379000	-1.00832500	0.78288200

TS6<sub>2</sub><sup>(R,R,R)</sup>

P	2.52407000	-0.01248300	-1.09840700
C	3.65013800	-1.38953900	-0.60371600
C	3.38881400	-1.98074400	0.78036400
H	3.51805400	-2.16785900	-1.36466600
H	4.68298300	-1.02478800	-0.68007800
C	4.37765700	-3.09199400	1.12730300
H	2.36882000	-2.38195200	0.80010200
H	3.44253100	-1.19601300	1.54480100
C	4.16816300	-3.62087900	2.54342100
H	5.40207200	-2.71380100	1.02007600
H	4.26950300	-3.90750300	0.40126900
H	4.86331800	-4.43128400	2.77691300

H	3.15022400	-4.00235500	2.66971700
H	4.31867900	-2.82557700	3.28061400
C	2.65809600	-0.00142700	-2.93438000
C	4.05733800	0.19192300	-3.52133400
H	2.23620000	-0.95911400	-3.26713200
H	1.98041600	0.77970100	-3.30316600
C	4.05802800	0.08634800	-5.04668300
H	4.74418100	-0.55828300	-3.10922600
H	4.45157500	1.17323600	-3.23051300
C	5.44816300	0.29784200	-5.63968100
H	3.36040700	0.82598500	-5.45807700
H	3.67380700	-0.89867900	-5.33798700
H	5.43419300	0.21396900	-6.72916700
H	6.15336400	-0.44475200	-5.25368400
H	5.83437600	1.28917800	-5.38294700
C	3.34884500	1.55437800	-0.58334000
C	3.34510400	1.83160300	0.92262400
H	4.38065000	1.53336300	-0.95692600
H	2.83172200	2.36343500	-1.11603000
C	4.06014000	3.14529000	1.24050000
H	3.84451500	1.01285900	1.45631400
H	2.31721500	1.86377900	1.31035700
C	4.06374200	3.46839000	2.73109000
H	3.57629700	3.95938200	0.68627900
H	5.09070900	3.08800100	0.86822000
H	4.62021600	4.38629700	2.93805200
H	4.52269600	2.65622100	3.30486300
H	3.04281700	3.59527500	3.10271400
C	0.28702000	-0.14235700	-0.91524400
C	-0.30859200	-0.89508600	0.10996100
C	-0.09340000	1.32430800	-0.88768700
C	-0.99603000	-0.16222700	1.22577600
H	-1.61510700	-0.88568200	1.76200900
C	-0.19041200	-2.30797700	0.03802000
O	0.44029300	-2.92033400	-0.83047500
O	-0.81309000	-2.97152300	1.06188700
C	-0.76476300	-4.39772600	1.01273000
C	0.54536300	-4.92371800	1.57110200
H	-1.61188200	-4.72947300	1.61916200
H	-0.91223300	-4.73060600	-0.01813700
H	0.53458000	-6.01640100	1.60772900
H	0.70155400	-4.54446100	2.58499700
H	1.37582300	-4.60246500	0.93730100
H	0.41813000	1.85389200	-0.07462900

C	-0.05647500	0.42625500	2.27837200
C	-0.27322000	1.66089400	2.89086200
C	1.02025600	-0.35585500	2.70515300
C	0.59784700	2.12333000	3.87776500
H	-1.13937800	2.24720600	2.60445400
C	1.88346400	0.09725100	3.69779900
H	1.16636900	-1.33411400	2.25733800
C	1.68163200	1.34694100	4.28104300
H	0.42224600	3.09090200	4.33871000
H	2.71569500	-0.52561700	4.01441300
H	2.35949500	1.71045800	5.04694200
H	0.15312600	1.83507800	-1.82272100
C	-1.60821200	1.45126000	-0.65091300
H	-2.10969100	0.85236400	-1.42688900
N	-1.92153000	0.89776500	0.69251200
S	-3.53640000	0.54382500	0.93174500
O	-3.67323700	0.14928700	2.32994400
O	-4.30632800	1.66592400	0.41054100
C	-3.89958100	-0.87027100	-0.08170500
C	-4.33511500	-0.67235100	-1.39055400
C	-3.69359900	-2.15296100	0.42338300
C	-4.54488500	-1.77877800	-2.20670300
H	-4.52767000	0.33351700	-1.75048900
C	-3.90756500	-3.24480500	-0.40769200
H	-3.37789900	-2.29388600	1.45136600
C	-4.32525200	-3.07509800	-1.73250000
H	-4.89122000	-1.63347400	-3.22565400
H	-3.75504600	-4.24834500	-0.02003000
C	-4.52200600	-4.27036700	-2.62644000
H	-5.01941500	-5.08307100	-2.09162800
H	-3.55571100	-4.64928600	-2.97417700
H	-5.11830400	-4.01562600	-3.50461100
C	-2.02191600	2.89929800	-0.81567900
C	-2.73714500	3.28372900	-1.94931800
C	-1.61533900	3.87623800	0.09437800
C	-3.05378700	4.62224600	-2.16802700
H	-3.05565600	2.52760400	-2.66309500
C	-1.93420700	5.21402200	-0.11902800
H	-1.04612800	3.58545300	0.97228900
C	-2.65509700	5.59122700	-1.25120300
H	-3.61717400	4.90619300	-3.05123800
H	-1.61657000	5.96429000	0.59833300
H	-2.90386000	6.63451700	-1.41686100
H	0.28605900	-0.61450400	-1.89903300

TS3<sub>2</sub><sup>(R,R,S)</sup>

P	0.25061000	1.99240000	-0.25015400
C	1.78221000	2.98107000	-0.06689300
C	2.34387900	3.04880300	1.35833600
H	2.52238300	2.58059600	-0.76567400
H	1.51333200	3.98609100	-0.41541700
C	3.43427200	4.11304800	1.47431500
H	2.74730200	2.07261900	1.64962700
H	1.54606400	3.27235700	2.07559300
C	4.03335900	4.16631500	2.87645300
H	3.00898100	5.09010600	1.21394000
H	4.22058600	3.91110900	0.73625000
H	4.81331800	4.92806100	2.94685700
H	4.47599100	3.20368900	3.15248300
H	3.26428500	4.40013900	3.61900200
C	0.06493800	1.54398900	-2.00999200
C	-0.09224200	2.74193100	-2.95272300
H	0.95290200	0.95412800	-2.25363900
H	-0.79381500	0.86288900	-2.08340200
C	-0.00930000	2.30266200	-4.41383100
H	0.68907300	3.48948900	-2.76099700
H	-1.05571100	3.23573400	-2.78238300
C	-0.20489900	3.46425300	-5.38261200
H	-0.76486200	1.52816500	-4.59493900
H	0.96518800	1.83002900	-4.58553900
H	-0.13688400	3.12800600	-6.42029200
H	0.55589200	4.23556100	-5.22791300
H	-1.18591700	3.92864100	-5.24305900
C	-1.11996100	3.13719300	0.12127800
C	-1.08523400	3.79341600	1.50738700
H	-1.08320000	3.90875100	-0.65473000
H	-2.05598200	2.58813200	-0.03663400
C	-2.43346900	4.42659100	1.85047800
H	-0.30234700	4.56164700	1.52432400
H	-0.82260000	3.06469000	2.28484100
C	-2.40992600	5.13615800	3.20028400
H	-3.20141200	3.64164500	1.85302700
H	-2.71135100	5.13264900	1.05868200
H	-3.38213200	5.57745900	3.43188400
H	-1.66509500	5.93785000	3.20683000
H	-2.15719100	4.43697600	4.00311700
C	0.10190600	0.57020800	0.83884700



C	1.08768700	-0.36291800	1.02317000
C	-1.26448900	0.35515800	1.47958100
C	0.85934800	-1.59390900	1.77139900
C	2.42395300	-0.14482000	0.36151400
O	2.57625100	0.11732700	-0.81618100
O	3.42118900	-0.27158000	1.22841400
C	4.75927700	-0.26726500	0.68793000
C	5.26540000	1.14517400	0.47791900
H	5.34916000	-0.80182200	1.43290700
H	4.75487300	-0.83678400	-0.24479800
H	6.30140300	1.11609800	0.13211900
H	5.23084000	1.70989100	1.41340200
H	4.66539900	1.66090900	-0.27589500
H	-1.14283700	-0.06857200	2.48336200
H	-1.79740500	1.29507800	1.62877900
C	-2.17501500	-0.58074700	0.66458700
H	-2.23569100	-0.17150100	-0.36284700
N	-1.56004900	-1.90806800	0.66028400
S	-1.94317300	-2.84901800	-0.57894600
O	-1.32119000	-4.15604400	-0.34219900
O	-3.38070800	-2.80778600	-0.88264700
C	-1.12923200	-2.16612400	-2.02177900
C	-1.85664600	-1.78173600	-3.14216700
C	0.25999900	-2.06921000	-2.00703300
C	-1.17506000	-1.32642700	-4.26984400
H	-2.93852000	-1.85991500	-3.12687200
C	0.92870300	-1.62212400	-3.13876600
H	0.80521900	-2.36813300	-1.11607800
C	0.22112200	-1.25949100	-4.29185900
H	-1.73599000	-1.03434100	-5.15396000
H	2.01292500	-1.54678300	-3.12639900
C	0.95126500	-0.84892800	-5.54414200
H	1.91050300	-0.38041700	-5.31012000
H	0.35869000	-0.14972200	-6.13979400
H	1.15653200	-1.72510900	-6.16799300
C	-3.57708800	-0.54022700	1.25221800
C	-4.46668500	0.45276100	0.83752500
C	-3.96491400	-1.41772000	2.26426200
C	-5.72346500	0.57360100	1.42488100
H	-4.17816100	1.12966600	0.03474700
C	-5.22139700	-1.29993100	2.85402600
H	-3.27596000	-2.19970900	2.56884900
C	-6.10300400	-0.30339000	2.43860400
H	-6.40812000	1.34484600	1.08569600

H	-5.51562100	-1.99052000	3.63852700
H	-7.08298800	-0.21518400	2.89677500
H	-0.31268300	-1.95181400	1.14057000
C	1.85815500	-2.68493000	1.85330600
C	1.95846700	-3.43611000	3.03529300
C	2.67617600	-3.07731200	0.77873100
C	2.83405100	-4.51118000	3.14567400
H	1.33608400	-3.16347400	3.88378500
C	3.56219800	-4.14372700	0.88971400
H	2.63106800	-2.54478800	-0.16905000
C	3.64943300	-4.87090800	2.07479100
H	2.88341200	-5.06677000	4.07754400
H	4.18070500	-4.41244400	0.03847300
H	4.33629200	-5.70649600	2.15923800
H	0.37905500	-1.40914300	2.73638600
M3 <sub>2</sub> <sup>(R,R,S)</sup>			
P	0.52667500	-1.70335200	-0.46550500
C	2.10398000	-2.64502700	-0.59392800
C	3.05629700	-2.14723600	-1.68422300
H	2.59398800	-2.62038700	0.38393900
H	1.81389700	-3.68727200	-0.78182700
C	4.20889500	-3.12380000	-1.91518800
H	3.45383100	-1.16400900	-1.40580800
H	2.51815000	-1.99640100	-2.62692100
C	5.20474100	-2.60332200	-2.94764000
H	3.80066300	-4.08765400	-2.24438700
H	4.72102100	-3.31501700	-0.96376600
H	6.01933600	-3.31339500	-3.10994500
H	5.64341600	-1.65361900	-2.62429100
H	4.71237100	-2.42816300	-3.90923500
C	-0.17965600	-2.13830700	1.17622300
C	0.02083500	-3.59456400	1.60786200
H	0.27682900	-1.45582900	1.89742700
H	-1.25013500	-1.88875700	1.12302000
C	-0.73198300	-3.90011800	2.90027700
H	1.08906300	-3.79080500	1.75799900
H	-0.31805100	-4.28817300	0.82700700
C	-0.51707200	-5.32882000	3.38812400
H	-1.80091300	-3.71612100	2.73655800
H	-0.41243900	-3.18647700	3.67039800
H	-1.06949700	-5.51873200	4.31255200
H	0.54245100	-5.52062000	3.58348200

H	-0.85537900	-6.05235000	2.63969400
C	-0.61009300	-2.54492300	-1.62986600
C	-0.10690600	-2.70025500	-3.06768900
H	-0.80637000	-3.53206300	-1.19711700
H	-1.56531400	-2.00798700	-1.60663900
C	-1.21994900	-3.17313100	-4.00236400
H	0.72010200	-3.42156400	-3.08865800
H	0.30021900	-1.75261200	-3.44165900
C	-0.72677800	-3.37693100	-5.43149000
H	-2.03080200	-2.43299200	-3.98919900
H	-1.64426400	-4.10737800	-3.61480200
H	-1.53522000	-3.70671600	-6.08847100
H	0.06542400	-4.13122500	-5.46677800
H	-0.32005900	-2.44609500	-5.83835500
C	0.58774100	-0.01175800	-0.86663400
C	1.54454300	0.90697900	-0.31139200
C	-0.51390200	0.52177700	-1.75655300
C	1.58426500	2.26446600	-0.52171500
C	2.60875100	0.31638100	0.57316000
O	2.39073000	-0.43829800	1.50274300
O	3.83675100	0.68925600	0.21186700
C	4.91073800	0.33492300	1.10231300
C	5.41756200	-1.06559400	0.82251600
H	5.67853400	1.08632200	0.91264500
H	4.55765600	0.43400800	2.13200100
H	6.27572100	-1.28480900	1.46257600
H	5.73277800	-1.15859800	-0.22054300
H	4.63696000	-1.80266800	1.02637100
H	-0.16317700	1.40435600	-2.30510600
H	-0.79649700	-0.18865100	-2.53830000
C	-1.83652000	0.90457500	-1.04789000
H	-2.22549700	-0.00023900	-0.54858400
N	-1.54128400	1.94281900	-0.05335800
S	-2.61189300	2.19830000	1.17821700
O	-2.04574800	3.28207900	1.97287700
O	-3.93504100	2.32174400	0.58165900
C	-2.64510900	0.74915700	2.21068700
C	-3.65500800	-0.19409200	2.03633400
C	-1.69643000	0.61379300	3.22245100
C	-3.72831400	-1.27194000	2.91370700
H	-4.39021600	-0.05751800	1.24995700
C	-1.78753800	-0.46755800	4.09051500
H	-0.92069300	1.36298600	3.34626300
C	-2.81650800	-1.40864700	3.96544600

H	-4.52343100	-2.00287100	2.79760700
H	-1.06340500	-0.57101800	4.89367500
C	-2.97454600	-2.51276200	4.97727100
H	-2.01354800	-2.79714800	5.41208800
H	-3.43162900	-3.39991500	4.53235700
H	-3.62303100	-2.18046700	5.79442500
C	-2.84589200	1.36657300	-2.07638200
C	-3.77802500	0.46295800	-2.58609500
C	-2.78587200	2.65693700	-2.60583800
C	-4.64064200	0.84031100	-3.61361100
H	-3.83716600	-0.54063800	-2.16900300
C	-3.64794500	3.03644300	-3.62941300
H	-2.06813900	3.36272100	-2.19745400
C	-4.57683600	2.12851500	-4.13774800
H	-5.36568000	0.13029800	-3.99883500
H	-3.59706600	4.04352500	-4.03138600
H	-5.24971100	2.42678500	-4.93528900
H	-0.58348500	1.92052500	0.30114700
C	2.44738600	3.25825700	0.12416400
C	2.78848700	4.42573700	-0.58008200
C	2.90857500	3.14679200	1.44893100
C	3.58868300	5.40981800	-0.01042600
H	2.42377200	4.54836300	-1.59665300
C	3.72040800	4.12274200	2.01494200
H	2.60233400	2.29730700	2.05512200
C	4.07117800	5.26026100	1.28848800
H	3.83975300	6.29638000	-0.58503300
H	4.06305500	4.00506100	3.03880600
H	4.69734300	6.02588400	1.73481300
H	0.87850600	2.69025400	-1.22994400

TS4<sub>2</sub><sup>(R,R,S)</sup>

P	-0.11165300	-0.38009200	1.83474500
C	1.42055700	-0.24496000	2.83676000
C	2.61228300	-1.08774500	2.37357700
H	1.69598300	0.81176100	2.86069500
H	1.11789500	-0.53321200	3.85223900
C	3.67097900	-1.21707500	3.46692100
H	3.05681600	-0.61329700	1.49348200
H	2.29364600	-2.08729300	2.05379400
C	4.89512800	-1.98974900	2.98481800
H	3.23048600	-1.71889200	4.33777500
H	3.96754800	-0.21556000	3.80186600

H	5.64864200	-2.07762700	3.77129900
H	5.35829800	-1.49080900	2.12736200
H	4.61723800	-3.00016200	2.66925700
C	-1.06769600	1.14321000	2.12060900
C	-1.24091000	1.57539700	3.57781200
H	-0.54356700	1.91598800	1.54670100
H	-2.04551200	0.99223600	1.64299900
C	-2.06597800	2.86015000	3.66892300
H	-0.26321100	1.74102700	4.04714700
H	-1.74204800	0.78980200	4.15690000
C	-2.26224600	3.32415200	5.10889500
H	-3.04030100	2.69034500	3.19353100
H	-1.56694400	3.64502300	3.08627000
H	-2.85242300	4.24270900	5.15372400
H	-1.29894300	3.51819800	5.59077900
H	-2.78227300	2.56093900	5.69611400
C	-1.04334400	-1.73637300	2.63944300
C	-0.24303600	-3.03380200	2.80208000
H	-1.36484100	-1.36766400	3.61966600
H	-1.95422200	-1.91266800	2.05765400
C	-1.13735900	-4.19589200	3.23268400
H	0.54806900	-2.88798000	3.54865900
H	0.26250800	-3.29568100	1.86307200
C	-0.34718100	-5.48167300	3.45438300
H	-1.90476300	-4.35603300	2.46475200
H	-1.66957000	-3.91933200	4.15085400
H	-1.00147600	-6.30396800	3.75350000
H	0.40473900	-5.34700300	4.23798300
H	0.17384600	-5.78115000	2.53975900
C	0.02444200	-0.71136300	0.07901500
C	1.36179200	-0.52377600	-0.55351800
C	-0.87129500	-1.83568800	-0.43849000
C	2.03221900	-1.48398900	-1.21990500
C	1.85157600	0.88983300	-0.43931100
O	1.66725000	1.56196500	0.56036900
O	2.43363300	1.36348000	-1.53734900
C	2.96919200	2.70053400	-1.45124300
C	4.32874600	2.69842300	-0.78031800
H	3.03235100	3.03461900	-2.48780700
H	2.25696900	3.32636600	-0.90950600
H	4.72087900	3.71785000	-0.74536400
H	5.03173800	2.07222400	-1.33399600
H	4.24744200	2.32636700	0.24438400
H	-0.48829000	-2.15799100	-1.41120900

H	-0.96717600	-2.73241900	0.18149700
C	-2.29461500	-1.23082400	-0.71442300
H	-2.84301300	-1.14209500	0.23886100
N	-1.97070600	0.08400800	-1.24155200
S	-3.07478700	1.25273500	-1.11224200
O	-3.92647800	1.34564700	-2.30748000
O	-3.80479600	1.21232800	0.17269000
C	-2.00308300	2.67326300	-1.07940500
C	-2.15412900	3.61576000	-0.07008900
C	-1.02988500	2.82500900	-2.06665300
C	-1.30691200	4.72141200	-0.04154000
H	-2.91443100	3.46724700	0.68997600
C	-0.19931200	3.93724600	-2.02817800
H	-0.91819700	2.07452300	-2.84278800
C	-0.32195600	4.89798800	-1.01598300
H	-1.41357200	5.45682200	0.75115900
H	0.55962500	4.06442700	-2.79548500
C	0.57796600	6.10587900	-1.00114000
H	0.64123200	6.54153500	-0.00199900
H	0.19758200	6.87653600	-1.67921100
H	1.58784600	5.84927200	-1.33256000
C	-3.08495200	-2.13730200	-1.62976600
C	-3.69690400	-3.27518300	-1.09763700
C	-3.16707100	-1.90023700	-3.00226700
C	-4.37578100	-4.16721800	-1.92274500
H	-3.64621800	-3.45832200	-0.02573000
C	-3.84817000	-2.79110700	-3.82869100
H	-2.70943900	-1.00274900	-3.40536700
C	-4.45209200	-3.92688600	-3.29341500
H	-4.84987500	-5.04550200	-1.49568600
H	-3.91289600	-2.59428600	-4.89447500
H	-4.98654500	-4.61680100	-3.93882400
C	3.36127900	-1.43066900	-1.85867400
C	4.44808300	-0.77124000	-1.26980100
C	3.57967800	-2.14047400	-3.04645400
C	5.70401700	-0.79230600	-1.86522800
H	4.31136500	-0.24670900	-0.32773400
C	4.83368700	-2.15632300	-3.64915700
H	2.75188300	-2.67594500	-3.50341000
C	5.90072700	-1.48016000	-3.06185500
H	6.53342000	-0.27895200	-1.38806900
H	4.97897100	-2.70132900	-4.57644600
H	6.88150800	-1.49919800	-3.52587700
H	1.55701600	-2.46289200	-1.26867600

H	-0.88511800	0.18184800	-0.56644900
M4 <sub>2</sub> <sup>(R,R,S)</sup>			
P	-0.00606600	-0.20462200	1.49054300
C	-1.23442700	-1.36804600	2.19294100
C	-2.72991000	-1.17577800	1.91096200
H	-0.92232500	-2.36633300	1.87177500
H	-1.04447100	-1.30019300	3.27309300
C	-3.59689700	-1.84249500	2.97764100
H	-2.95641400	-1.63927000	0.94782600
H	-3.00310100	-0.11834200	1.82457300
C	-5.07194800	-1.82161000	2.58638000
H	-3.45071800	-1.33185900	3.93718100
H	-3.26331600	-2.87766300	3.11922600
H	-5.69856700	-2.26317900	3.36470000
H	-5.23494000	-2.38838500	1.66269100
H	-5.41764900	-0.79700500	2.41362700
C	1.58734000	-1.07279300	1.56395600
C	1.97388000	-1.59109400	2.95244900
H	1.50019900	-1.89766200	0.84253100
H	2.36328800	-0.39657900	1.18186800
C	3.34493300	-2.26695500	2.91270800
H	1.22740600	-2.30482900	3.32170400
H	2.00768800	-0.76233900	3.67046500
C	3.78710300	-2.74890100	4.29078200
H	4.07432900	-1.55768100	2.50308100
H	3.30670900	-3.10854400	2.21094500
H	4.76683900	-3.23070400	4.24614000
H	3.07441200	-3.47230300	4.69914700
H	3.85501100	-1.91282700	4.99371700
C	0.02066500	1.24020700	2.60287000
C	-1.34503000	1.91934000	2.76939100
H	0.39476800	0.89412700	3.57242900
H	0.76525600	1.94173500	2.21247200
C	-1.21733700	3.26823500	3.47625200
H	-2.00902100	1.26791200	3.35027000
H	-1.82612100	2.06677400	1.79272800
C	-2.57362000	3.93222700	3.69253700
H	-0.57202700	3.92518400	2.88018400
H	-0.71184100	3.12212400	4.43815100
H	-2.46530500	4.89961200	4.18826900
H	-3.22045400	3.30493200	4.31315700
H	-3.08211800	4.09755000	2.73773900

C	-0.23945800	0.36615400	-0.26496900
C	-1.62533500	0.07309100	-0.80323000
C	0.25531200	1.80369100	-0.48702700
C	-2.55764900	1.03103400	-0.94847100
C	-1.77122100	-1.36468900	-1.18545400
O	-1.06510000	-2.22865000	-0.69565400
O	-2.68104700	-1.59370100	-2.12372200
C	-2.91168100	-2.97321400	-2.47875000
C	-3.79192700	-3.64830300	-1.44477300
H	-3.39926600	-2.92153600	-3.45214400
H	-1.94763800	-3.47553500	-2.58009600
H	-4.00194400	-4.67559500	-1.75186400
H	-4.74184100	-3.11648700	-1.34551400
H	-3.29082900	-3.67751900	-0.47333500
H	-0.07670900	2.09746800	-1.48925000
H	-0.18542000	2.51848500	0.21670200
C	1.79743100	1.91263900	-0.48312900
H	2.17908500	1.66712000	0.52336100
N	2.29356200	0.99889900	-1.48360000
S	3.67390900	0.30125600	-1.23270300
O	4.64011300	0.52327300	-2.33011600
O	4.23040200	0.52449900	0.12985000
C	3.32051000	-1.46100000	-1.29271500
C	4.13643200	-2.33522000	-0.58195200
C	2.24086000	-1.95149900	-2.02442400
C	3.86477400	-3.70129700	-0.59884700
H	4.95946300	-1.93955800	0.00508100
C	1.97611500	-3.31734200	-2.03057800
H	1.60374600	-1.25769100	-2.56446500
C	2.78267900	-4.21270300	-1.32022200
H	4.49681600	-4.38002400	-0.03148100
H	1.12177400	-3.69418000	-2.58710700
C	2.49803400	-5.69216700	-1.35234000
H	2.98156800	-6.20729600	-0.51949700
H	2.87056600	-6.13728200	-2.28071800
H	1.42384400	-5.88834300	-1.30410600
C	2.17511400	3.37494000	-0.72526100
C	1.90673400	4.33850100	0.25218300
C	2.77438200	3.77892200	-1.91726200
C	2.22030600	5.67770700	0.04287000
H	1.45866700	4.03622300	1.19786800
C	3.08854600	5.12053600	-2.13214700
H	3.00305500	3.02175900	-2.66020500
C	2.81072900	6.07405400	-1.15675400



H	2.01207100	6.41066800	0.81643100
H	3.55816700	5.42033400	-3.06434000
H	3.05954800	7.11735000	-1.32387100
C	-3.97086100	0.94519100	-1.36412100
C	-4.82803100	-0.06888500	-0.91995300
C	-4.49639900	1.97189300	-2.15767400
C	-6.16879400	-0.07225100	-1.28384800
H	-4.44606300	-0.85036200	-0.27262200
C	-5.83419700	1.95809200	-2.54021400
H	-3.84662200	2.77895700	-2.48455300
C	-6.67393000	0.93598000	-2.10389800
H	-6.82133200	-0.86075700	-0.92187700
H	-6.22245300	2.75147400	-3.17027400
H	-7.72029000	0.93092400	-2.39133300
H	-2.23990700	2.04493900	-0.70436200
H	0.47361200	-0.27137900	-0.80412700

M4<sub>2</sub><sup>(R,R,S)</sup>

P	0.57470400	2.24984300	0.17673300
C	1.66560800	2.34049900	1.63855100
C	1.08947500	1.73239700	2.93056500
H	2.59099000	1.83158200	1.35995000
H	1.90741800	3.40061000	1.77692900
C	2.21071800	1.34727600	3.89635700
H	0.49384100	0.83885400	2.70943000
H	0.41970600	2.44625800	3.41809000
C	1.67252200	0.71467200	5.17583800
H	2.80542800	2.23698200	4.13568200
H	2.89165800	0.64858800	3.39148200
H	2.48390900	0.44649700	5.85665800
H	1.10569300	-0.19496200	4.95124500
H	1.00423200	1.40350100	5.70128900
C	1.41465300	2.79752500	-1.35761000
C	2.73409900	3.53613200	-1.12347800
H	1.58286900	1.90645900	-1.96902400
H	0.69911500	3.44249400	-1.88116200
C	3.32232200	4.04385900	-2.43995300
H	3.44487500	2.85397600	-0.64289200
H	2.58650000	4.38616500	-0.44428600
C	4.66260900	4.74442700	-2.23746100
H	2.60903700	4.72959400	-2.91264100
H	3.44297900	3.19703000	-3.12648900
H	5.06661800	5.10898600	-3.18486100

H	5.39605500	4.06159800	-1.79805700
H	4.55734000	5.60079700	-1.56425900
C	-0.72957000	3.51072300	0.40357700
C	-1.48318800	3.53033100	1.74151600
H	-0.21951400	4.46819700	0.24112000
H	-1.42012200	3.39422800	-0.44129500
C	-2.85532900	4.18796800	1.59270700
H	-0.88982700	4.08148300	2.47959900
H	-1.61684500	2.51910100	2.14226600
C	-3.58798800	4.29966300	2.92552300
H	-3.45573900	3.59538100	0.88940400
H	-2.73402000	5.18101900	1.14337800
H	-4.57160900	4.75775400	2.79838300
H	-3.01981500	4.91001000	3.63413400
H	-3.73209100	3.31146500	3.37273300
C	-0.17599200	0.55377600	-0.09854500
C	0.66795200	-0.57672100	0.49271400
C	-1.67778300	0.53168800	0.26436300
C	0.11374600	-1.56845100	1.21179500
C	2.09463000	-0.56647600	0.06746800
O	2.61321600	0.41550400	-0.44380800
O	2.74197400	-1.70830900	0.24836400
C	4.15639100	-1.70935300	-0.02488400
C	4.91790000	-1.11106000	1.14178200
H	4.40086500	-2.76220000	-0.16963200
H	4.34217200	-1.16122400	-0.95188500
H	5.99275800	-1.18150900	0.95948900
H	4.68375200	-1.65065700	2.06282000
H	4.65895700	-0.05667000	1.26836000
H	-1.82506000	0.20212100	1.29906400
H	-2.08939400	1.54026200	0.21992100
C	-2.55462300	-0.31298000	-0.69138200
H	-2.42476400	0.13984300	-1.69069200
N	-2.17977000	-1.71162000	-0.65516900
S	-2.03263100	-2.39851500	-2.05731000
O	-1.80532000	-3.84347800	-1.86194900
O	-3.07326600	-2.02775700	-3.04417400
C	-0.51069000	-1.76675600	-2.77786700
C	-0.53227100	-0.64640300	-3.60480900
C	0.70822300	-2.30456500	-2.36266000
C	0.66670400	-0.02852600	-3.96539800
H	-1.48486600	-0.26357200	-3.95716900
C	1.89485300	-1.70478300	-2.76066700
H	0.71283000	-3.18278800	-1.72300100

C	1.89332100	-0.53518500	-3.53182000
H	0.64808000	0.86064100	-4.59067200
H	2.84423400	-2.13359000	-2.44907200
C	3.19038800	0.16537700	-3.83854600
H	3.05368500	0.95707400	-4.57915000
H	3.94167500	-0.53424200	-4.21585800
H	3.59120700	0.61513600	-2.92127000
C	-4.01224900	-0.07354100	-0.29942800
C	-4.61547800	1.16201300	-0.55715500
C	-4.74993400	-1.05348200	0.36251100
C	-5.92262500	1.41861100	-0.15341600
H	-4.05859700	1.92883900	-1.09451100
C	-6.05933000	-0.80107700	0.76903500
H	-4.28074800	-2.01580100	0.53721700
C	-6.64943400	0.43476000	0.51623600
H	-6.37692600	2.38145500	-0.36765000
H	-6.62186900	-1.57553400	1.28199700
H	-7.67035500	0.62905700	0.82979100
C	0.74841900	-2.73187800	1.86210700
C	1.76129500	-2.58736000	2.81564200
C	0.25223400	-4.00622100	1.57013300
C	2.28568600	-3.70421500	3.45539800
H	2.13136000	-1.59223500	3.05117100
C	0.79382200	-5.12525100	2.19810800
H	-0.54239700	-4.10982500	0.83440600
C	1.80751000	-4.97680700	3.14216500
H	3.06648700	-3.58257400	4.19960500
H	0.41718100	-6.11359600	1.95508100
H	2.22009800	-5.84913400	3.63874400
H	-0.96690100	-1.56192900	1.30135000
H	-0.09662500	0.46763800	-1.19465700
TS5 <sub>2</sub> <sup>(R,R,S)</sup>			
P	2.03790400	1.22695300	0.49358100
C	2.23157200	0.76701900	2.24561500
C	0.98938000	0.99888100	3.12421400
H	2.48030100	-0.29983000	2.21465000
H	3.10507000	1.30448900	2.63459500
C	1.00773800	0.06864600	4.33648300
H	0.07647300	0.80125700	2.55361800
H	0.94711000	2.03535000	3.46140000
C	-0.23860500	0.22338500	5.19967400
H	1.91049300	0.25853600	4.93317000

H	1.08888200	-0.96868400	3.98084300
H	-0.21476400	-0.44394800	6.06327000
H	-1.14084400	-0.00901500	4.62094500
H	-0.33567500	1.25060300	5.56739200
C	3.46511200	0.68567800	-0.51116200
C	4.78653900	0.62957700	0.25796400
H	3.20782700	-0.30582200	-0.90755800
H	3.52649800	1.39321200	-1.34926500
C	5.94626700	0.22263800	-0.65040700
H	4.69903200	-0.09414600	1.07543100
H	5.01125700	1.60504500	0.71551200
C	7.27893400	0.17466100	0.09885600
H	6.01113500	0.93120300	-1.49085900
H	5.72276300	-0.76455400	-1.08934600
H	8.09253000	-0.12227200	-0.56803000
H	7.23402500	-0.54375600	0.92416400
H	7.52730400	1.15780600	0.51695200
C	2.09059800	3.04815700	0.33139800
C	1.28041700	3.87129100	1.33724200
H	3.15095600	3.32010400	0.39541400
H	1.78173600	3.27214500	-0.70037200
C	1.19593900	5.33715100	0.91949700
H	1.75275900	3.79307500	2.32130900
H	0.26235700	3.47256000	1.44088900
C	0.43719500	6.18238400	1.93895000
H	0.69816200	5.39857300	-0.05910200
H	2.20804900	5.73160200	0.78296900
H	0.37232600	7.22323800	1.61968200
H	0.93824800	6.15513800	2.91397900
H	-0.57981400	5.80702500	2.07406600
C	0.48260200	0.52087000	-0.23518200
C	-0.02485000	-0.73316600	0.46512800
C	-0.62788400	1.57291900	-0.40022400
C	-1.40045200	-0.77792900	0.67317200
C	0.87715300	-1.84227100	0.52566700
O	2.10818600	-1.71786000	0.43437200
O	0.31484600	-3.05249500	0.71055400
C	1.20249700	-4.13213000	1.01553400
C	1.63404700	-4.08048800	2.47172000
H	0.62301700	-5.03661200	0.80533100
H	2.06382100	-4.09414800	0.34355500
H	2.27408300	-4.93606500	2.70566300
H	0.76450700	-4.10502400	3.12860500
H	2.19809500	-3.16518500	2.66379100

H	-1.00190700	1.87670600	0.58304400
H	-0.23133500	2.47924000	-0.86190900
C	-1.82865100	1.10608700	-1.29612400
H	-1.50482000	1.28850300	-2.33523400
N	-2.20821600	-0.29549300	-1.12454900
S	-2.14319100	-1.17494600	-2.46550000
O	-2.55726000	-2.54314600	-2.13159700
O	-2.83442800	-0.50670300	-3.57981700
C	-0.43341700	-1.27009800	-2.97693000
C	0.09714500	-0.29968500	-3.83464600
C	0.38871100	-2.24348600	-2.41996300
C	1.46272700	-0.28416700	-4.08449500
H	-0.57044900	0.41954600	-4.29817500
C	1.76026000	-2.21426700	-2.68083700
H	-0.04003000	-3.00044500	-1.77292000
C	2.31554000	-1.22512400	-3.50109700
H	1.87721000	0.46974000	-4.75157200
H	2.40709000	-2.95596200	-2.22804200
C	3.79753100	-1.17813700	-3.76305500
H	4.22404200	-0.22486900	-3.42821400
H	4.01118700	-1.27775600	-4.82886900
H	4.31904000	-1.98484100	-3.23619800
C	-2.99061000	2.05114200	-1.02389900
C	-2.92041600	3.38041000	-1.44716700
C	-4.10562400	1.63382400	-0.30002900
C	-3.94335500	4.27711100	-1.15159900
H	-2.06165600	3.71631200	-2.02506400
C	-5.13416900	2.52714700	-0.00365900
H	-4.16876500	0.58975000	0.00519500
C	-5.05669200	3.84980300	-0.42706800
H	-3.87832400	5.30348000	-1.49982000
H	-5.99841200	2.18569900	0.55803300
H	-5.85618400	4.54713400	-0.19601200
C	-2.16352600	-1.87867800	1.34735400
C	-1.72302000	-2.31008200	2.60410800
C	-3.37732800	-2.35656900	0.85382200
C	-2.47288000	-3.21110600	3.34899000
H	-0.78155000	-1.92896300	2.99098600
C	-4.12286800	-3.26882300	1.59911100
H	-3.71118800	-2.02992500	-0.12095300
C	-3.67821800	-3.70345600	2.84315600
H	-2.11103100	-3.53412700	4.32059100
H	-5.05935900	-3.64601300	1.20000200
H	-4.25985700	-4.41010800	3.42055300

H	-1.87136000	0.16668300	0.92622300
H	0.82715500	0.23855200	-1.24694000
M5 <sub>2</sub> <sup>(R,R,S)</sup>			
P	2.06557600	1.13953700	0.50567800
C	2.05303500	0.74820600	2.28253800
C	0.74200600	1.09097900	3.00879300
H	2.23324300	-0.33101300	2.31051800
H	2.90867700	1.25469300	2.74359100
C	0.62364700	0.31317900	4.31992500
H	-0.11269700	0.83053200	2.37392500
H	0.68411700	2.16374500	3.21721800
C	-0.69423100	0.59357700	5.03494100
H	1.46990200	0.56487000	4.97088000
H	0.70974600	-0.75973300	4.10127200
H	-0.76389400	0.03789100	5.97349000
H	-1.54297400	0.30253400	4.40695900
H	-0.79601100	1.65881600	5.26489400
C	3.55521000	0.51199400	-0.34328400
C	4.78913900	0.41258000	0.55409100
H	3.28463500	-0.47200900	-0.73448800
H	3.73542100	1.19913400	-1.18058900
C	6.01931200	-0.02690300	-0.23975300
H	4.59275000	-0.31327100	1.35230700
H	4.99911800	1.37644200	1.03804900
C	7.26291500	-0.14024300	0.63699500
H	6.19821500	0.69023200	-1.05065300
H	5.80847200	-0.99246000	-0.71587700
H	8.13312900	-0.45266100	0.05468800
H	7.11039200	-0.87305900	1.43504800
H	7.49826600	0.82060500	1.10536000
C	2.23138000	2.95462500	0.28212400
C	1.39813100	3.88137000	1.17086300
H	3.29781600	3.16607600	0.43244100
H	2.03208700	3.14832900	-0.77940500
C	1.50390900	5.33507100	0.70990400
H	1.75211600	3.80490600	2.20558600
H	0.34350000	3.58410000	1.17563900
C	0.72182100	6.28310300	1.61389300
H	1.13260600	5.41055800	-0.31962600
H	2.56035600	5.62881400	0.68329900
H	0.80106300	7.31664100	1.26844800
H	1.09711900	6.24096700	2.64092100

H	-0.33894900	6.01478000	1.63412300
C	0.56369800	0.46167100	-0.35515800
C	-0.06395900	-0.72456300	0.35401500
C	-0.48072300	1.55719300	-0.64125400
C	-1.56190100	-0.64268600	0.35533900
C	0.76511400	-1.80299800	0.61117800
O	2.02346800	-1.76603300	0.55203100
O	0.14573100	-2.99627400	0.92264700
C	0.97344400	-3.98767200	1.52037900
C	1.28138900	-3.65462700	2.97104300
H	0.40067000	-4.91554800	1.44776200
H	1.89732600	-4.09437600	0.94547500
H	1.87246100	-4.44990200	3.43400000
H	0.35402000	-3.53414300	3.53903100
H	1.85362500	-2.72393900	3.02214700
H	-0.83885700	1.99280900	0.29697300
H	-0.04915200	2.37913800	-1.22023700
C	-1.70788500	1.02382400	-1.43720100
H	-1.43138100	1.00909800	-2.49501600
N	-2.07003400	-0.35455000	-1.03194700
S	-1.91425500	-1.48417700	-2.25490700
O	-2.19488900	-2.78809100	-1.67237800
O	-2.73364000	-0.97212200	-3.35279100
C	-0.23710900	-1.50395000	-2.85272500
C	0.15209600	-0.61330500	-3.85123800
C	0.68053500	-2.36351000	-2.25427600
C	1.49449900	-0.55154500	-4.21603400
H	-0.58774900	0.00794900	-4.34568400
C	2.01710000	-2.27845500	-2.62149000
H	0.35188000	-3.06450400	-1.49415600
C	2.44544000	-1.36379800	-3.59196100
H	1.80647700	0.13836800	-4.99466500
H	2.74201800	-2.92338500	-2.13342100
C	3.90700900	-1.25417500	-3.93748700
H	4.44761200	-0.72574000	-3.14393800
H	4.05673800	-0.70511000	-4.86915900
H	4.36256900	-2.24233100	-4.03868000
C	-2.87510000	1.98233400	-1.27978300
C	-2.79603000	3.24450000	-1.87581300
C	-3.99825600	1.66178400	-0.51720300
C	-3.82027900	4.17149200	-1.71278300
H	-1.92985100	3.49949300	-2.48238800
C	-5.02298800	2.59240200	-0.34990900
H	-4.07699000	0.67567200	-0.06857300

C	-4.93792100	3.84791300	-0.94461000
H	-3.74855900	5.14415000	-2.18924900
H	-5.89311000	2.32978700	0.24350300
H	-5.73861600	4.56906600	-0.81673800
C	-2.40196500	-1.60701300	1.17446400
C	-1.97217800	-1.90847100	2.47205400
C	-3.66915000	-2.03252400	0.77847700
C	-2.77665900	-2.63327300	3.34270000
H	-0.98795700	-1.57302300	2.78693200
C	-4.47626800	-2.76624700	1.64948400
H	-4.02697900	-1.80214000	-0.21833500
C	-4.03618700	-3.07214600	2.93216100
H	-2.41843100	-2.85612900	4.34397200
H	-5.45492200	-3.09772700	1.31621200
H	-4.66526700	-3.64404400	3.60696100
H	-1.83689200	0.30908600	0.83988200
H	1.00818000	0.15461100	-1.32013700
TS6 <sub>2</sub> <sup>(R,R,S)</sup>			
P	2.36387400	1.04127200	0.04881600
C	2.78133700	1.20884400	1.83898900
C	1.56599100	1.56242800	2.70142600
H	3.16543900	0.22980800	2.14571400
H	3.58406200	1.94821100	1.96347900
C	1.92872200	1.73428700	4.17461700
H	0.82585200	0.76064300	2.60035400
H	1.08375500	2.47901000	2.33678600
C	0.69812200	1.97176900	5.04494900
H	2.63204100	2.57000300	4.27986900
H	2.46043300	0.83833600	4.52042900
H	0.96826500	2.12022900	6.09356500
H	0.01750100	1.11467800	4.99244100
H	0.14606300	2.85581900	4.71000700
C	3.59318800	-0.14898900	-0.62068900
C	5.07063800	0.16884900	-0.39437200
H	3.32037900	-1.10624800	-0.15439100
H	3.38321400	-0.25098800	-1.69526300
C	5.97937100	-0.95914400	-0.88412800
H	5.25731400	0.34292300	0.67313300
H	5.34022200	1.09601300	-0.91516900
C	7.45935900	-0.64072800	-0.69156800
H	5.77474200	-1.14946000	-1.94556900
H	5.72383900	-1.88149000	-0.34721500



H	8.09307700	-1.46236800	-1.03457600
H	7.68387800	-0.46028800	0.36425900
H	7.74029300	0.25738800	-1.25036200
C	2.80704400	2.66838500	-0.70673900
C	2.03760700	3.83744900	-0.08647000
H	3.88676500	2.83699600	-0.60703400
H	2.58601600	2.59459100	-1.77926200
C	2.31335300	5.16001800	-0.80035700
H	2.31455200	3.93692600	0.97137600
H	0.95821300	3.63258100	-0.10578900
C	1.57285300	6.32992200	-0.15872100
H	2.02173000	5.06622700	-1.85356200
H	3.39323900	5.35248600	-0.79271300
H	1.77767000	7.26743500	-0.68160200
H	1.87302300	6.45475700	0.88637800
H	0.49136600	6.16316300	-0.17697200
C	0.43606000	-0.11220100	-0.57383000
C	-0.37410500	-0.54058300	0.49065900
C	-0.22269900	0.78262500	-1.61229400
C	-1.80665200	-0.09133300	0.37791700
C	0.23423000	-1.45271400	1.40014500
O	1.45828800	-1.62546500	1.46188600
O	-0.61554800	-2.13940400	2.20647100
C	-0.01456500	-2.86472900	3.28257700
C	0.37736400	-1.92501300	4.40954200
H	-0.78036200	-3.57218600	3.60608900
H	0.85150300	-3.41770200	2.91035700
H	0.79838400	-2.48531200	5.24857100
H	-0.49994400	-1.37466200	4.76147400
H	1.12830200	-1.21194200	4.05590200
H	-0.29250100	1.79855000	-1.21266300
H	0.39315000	0.84190900	-2.51442100
C	-1.68434000	0.35149900	-2.01216800
H	-1.63548700	-0.23334900	-2.93213400
N	-2.32170000	-0.48734900	-0.97816900
S	-2.39023200	-2.11563600	-1.40062200
O	-2.85332100	-2.83936900	-0.22569700
O	-3.15776100	-2.15002800	-2.64363200
C	-0.75857600	-2.71372100	-1.80479200
C	-0.21594700	-2.45486800	-3.06075000
C	-0.02048700	-3.37643500	-0.82650600
C	1.10918500	-2.80513400	-3.31035400
H	-0.82081100	-2.00252000	-3.83966300
C	1.29745500	-3.71920900	-1.09215700

H	-0.47148800	-3.58378800	0.13874600
C	1.88851500	-3.41864800	-2.32669800
H	1.54127000	-2.59981100	-4.28536400
H	1.88495300	-4.21081100	-0.32206100
C	3.33662400	-3.74779000	-2.57316200
H	3.98127700	-3.12334700	-1.94497900
H	3.61186700	-3.57769300	-3.61581300
H	3.55061000	-4.79032600	-2.32321300
C	-2.52479000	1.58214600	-2.31645400
C	-2.10631200	2.43807000	-3.34111400
C	-3.68245100	1.89495500	-1.60501300
C	-2.82945700	3.58525500	-3.64762900
H	-1.21103700	2.19906900	-3.91019600
C	-4.40396100	3.05001600	-1.90776700
H	-4.02511000	1.22850100	-0.81926900
C	-3.98214300	3.89698700	-2.92718800
H	-2.49612700	4.23455900	-4.45096500
H	-5.30196400	3.28276700	-1.34424500
H	-4.54805600	4.79202900	-3.16413300
C	-2.77928600	-0.28362400	1.52590500
C	-2.35965700	0.09292600	2.80644000
C	-4.11151700	-0.64753500	1.34028100
C	-3.24010600	0.07953900	3.88041400
H	-1.32642700	0.39609000	2.95815400
C	-4.99788100	-0.66300000	2.41812500
H	-4.45804500	-0.93192100	0.35340600
C	-4.56800300	-0.30456600	3.69082100
H	-2.89027200	0.37244400	4.86620700
H	-6.02974800	-0.95832600	2.25502600
H	-5.25857800	-0.31884900	4.52793700
H	-1.79028200	1.00560600	0.26922000
H	1.15172100	-0.84571700	-0.94893000
TS2 <sub>2</sub> <sup>(R,S)</sup>			
P	1.41108200	0.61756400	1.04973300
C	3.17789900	0.98853800	0.75997000
C	3.49587000	2.38028900	0.20348800
H	3.58819600	0.19886200	0.11936600
H	3.65033000	0.86022200	1.74319500
C	4.95923500	2.48032900	-0.22689500
H	2.85073600	2.60893200	-0.65371900
H	3.28515000	3.14312400	0.96356400
C	5.31888600	3.87045600	-0.74110200

H	5.60234100	2.21519900	0.62138200
H	5.14884500	1.72929700	-1.00475600
H	6.36556000	3.92120000	-1.05089000
H	4.69959700	4.13985700	-1.60224400
H	5.15992700	4.62652200	0.03392900
C	1.44729000	-0.95620600	1.98268000
C	1.18819700	-0.82041900	3.48356200
H	2.44080900	-1.37996100	1.80599100
H	0.70784800	-1.60894300	1.51065500
C	1.31489700	-2.17386500	4.18260700
H	1.89864100	-0.11266800	3.93215500
H	0.18212600	-0.42062200	3.64024200
C	1.05495600	-2.07361600	5.68289200
H	0.60512800	-2.87559100	3.72675400
H	2.31636400	-2.58450900	4.00428100
H	1.14502600	-3.04846200	6.16841900
H	1.76940200	-1.39355300	6.15724200
H	0.04885300	-1.69020700	5.87881000
C	0.82807000	2.04907300	2.04131800
C	0.10180300	3.12082800	1.22219300
H	1.72311200	2.46864100	2.51606900
H	0.17263900	1.67004600	2.82582300
C	-0.27149600	4.32451700	2.08476700
H	0.72060100	3.45085900	0.37692600
H	-0.80718300	2.69674700	0.78019300
C	-1.07176300	5.35767700	1.29726000
H	-0.85673500	3.97981800	2.94689200
H	0.63979600	4.78086400	2.49111100
H	-1.34510100	6.21239100	1.92137000
H	-0.49567200	5.72950700	0.44391300
H	-1.99034700	4.91452100	0.89784600
C	0.57557100	0.48879600	-0.57892200
C	-0.80920300	0.35603300	-0.64711300
C	1.42772500	0.42233700	-1.68600900
C	-1.57570900	0.62776900	-1.92563700
H	-0.97191200	0.37085900	-2.79564300
C	-1.58282800	0.21388500	0.56614900
O	-1.11279500	0.08836200	1.69929800
O	-2.91133700	0.24824500	0.36247400
C	-3.73001300	0.36708200	1.53075700
C	-3.71062800	1.79664900	2.04300300
H	-3.38040300	-0.33723000	2.29007800
H	-4.72748200	0.06776000	1.20047000
H	-4.39750300	1.90732200	2.88592400

H	-2.70331300	2.06088900	2.37759600
H	-4.01016700	2.48745400	1.24985400
H	2.46717200	0.70797900	-1.61541400
C	-2.00726300	2.08207300	-1.98105700
C	-3.33791800	2.45098300	-1.77314800
C	-1.06357200	3.09159300	-2.20840300
C	-3.72022000	3.79254700	-1.79305600
H	-4.07596900	1.67569800	-1.58590500
C	-1.44065500	4.43033100	-2.23215200
H	-0.02144300	2.81892300	-2.36005100
C	-2.77338700	4.78675600	-2.02452200
H	-4.76040600	4.05861600	-1.62950800
H	-0.69435600	5.19873500	-2.41157500
H	-3.06876400	5.83129400	-2.04057000
H	0.99607600	0.52760100	-2.67468300
C	1.65394000	-1.82549300	-1.90231700
H	1.54656600	-1.64034000	-2.97293300
N	0.70005100	-2.45806300	-1.23397900
S	-0.59357700	-2.92407100	-2.11843100
O	-0.45907100	-4.35553000	-2.43444700
O	-0.85775400	-2.04512700	-3.26914500
C	-1.94944900	-2.77813900	-0.97823400
C	-3.21057200	-2.51443100	-1.49976300
C	-1.77396700	-3.03961700	0.37952300
C	-4.31095700	-2.50865700	-0.64596700
H	-3.32323300	-2.30794300	-2.55946800
C	-2.88042200	-3.01935000	1.21789000
H	-0.78120200	-3.24390100	0.76718900
C	-4.16404400	-2.76504100	0.71784600
H	-5.29823500	-2.29839800	-1.04790600
H	-2.74872000	-3.20679800	2.28053900
C	-5.35556500	-2.77847600	1.63980000
H	-5.13455400	-2.25716300	2.57548000
H	-6.22150900	-2.30152700	1.17527100
H	-5.63506500	-3.80536400	1.89616200
C	3.04785700	-1.90439700	-1.40282500
C	4.08385500	-1.27380800	-2.10582900
C	3.35630900	-2.62703200	-0.24712700
C	5.38876700	-1.31645200	-1.63043700
H	3.85455300	-0.73181800	-3.02028900
C	4.66348100	-2.66206700	0.23494700
H	2.55845500	-3.15806400	0.26139400
C	5.68057200	-1.99824300	-0.44680200
H	6.18025800	-0.81651600	-2.17972200

H	4.88857500	-3.21761400	1.14015500
H	6.69798300	-2.02452500	-0.07066100
H	-2.45638200	-0.01690300	-1.96900500
M2 <sub>2</sub> <sup>(R,S)</sup>			
P	0.83978800	0.35108400	1.22307000
C	2.42251000	1.25026900	1.38753900
C	2.36818100	2.76583200	1.16732100
H	3.15232700	0.78204100	0.72084400
H	2.75243900	1.03124200	2.41167200
C	3.77334000	3.36576300	1.12695300
H	1.84985000	3.00500700	0.22903100
H	1.79113100	3.24365400	1.96893500
C	3.74796900	4.87969100	0.94265800
H	4.29994900	3.10857700	2.05415700
H	4.33410200	2.89391500	0.31074600
H	4.75915800	5.29204600	0.90713800
H	3.24144800	5.15025600	0.01083300
H	3.21482000	5.36525900	1.76581500
C	1.16545500	-1.34839000	1.81199100
C	0.51402000	-1.71633700	3.14538200
H	2.25669700	-1.43666800	1.86888200
H	0.82790600	-2.00033200	1.00162500
C	0.89122000	-3.14285800	3.54571400
H	0.82359900	-1.02127100	3.93712900
H	-0.57384300	-1.64327200	3.04763500
C	0.19256700	-3.58631900	4.82733600
H	0.62673900	-3.82057500	2.72433400
H	1.97891800	-3.21179600	3.66681500
H	0.47488700	-4.60559500	5.10195500
H	0.45225400	-2.92814600	5.66228600
H	-0.89488800	-3.55868900	4.70546800
C	-0.27382700	1.30508100	2.33659700
C	-1.02827600	2.46478800	1.67223500
H	0.39373600	1.69437500	3.11533700
H	-0.96773300	0.61457200	2.81816100
C	-1.67802100	3.37935500	2.70860200
H	-0.35842800	3.05420300	1.03484200
H	-1.80908700	2.08893100	0.99996100
C	-2.44768700	4.51742700	2.04490000
H	-2.35233100	2.78795000	3.34114500
H	-0.90496700	3.78537800	3.37268300
H	-2.92885500	5.15923500	2.78702500

H	-1.77938300	5.13707800	1.43865400
H	-3.22224800	4.12776300	1.37567000
C	0.33660700	0.44722400	-0.53960300
C	-0.96509900	0.35819400	-0.89062600
C	1.44564100	0.66629300	-1.54409300
C	-1.54375100	0.83900800	-2.20409800
H	-0.81511500	0.72872500	-3.00512800
C	-1.95513300	-0.16290900	0.10388500
O	-1.63975500	-0.79383900	1.09532800
O	-3.21301400	0.12347600	-0.21620100
C	-4.22671400	-0.28805600	0.72201100
C	-4.30944600	0.70100300	1.86836700
H	-3.99300700	-1.29790800	1.06711400
H	-5.14675700	-0.30724700	0.13665500
H	-5.13662400	0.43564400	2.53065100
H	-3.38395700	0.68973500	2.45052900
H	-4.47799800	1.71198700	1.48653200
H	2.12286900	1.46628200	-1.23032200
C	-1.98968300	2.28518000	-2.04032700
C	-3.34150900	2.63109400	-2.06184300
C	-1.04274200	3.29463800	-1.83901600
C	-3.73934700	3.95662100	-1.89205100
H	-4.08621600	1.85371600	-2.20654300
C	-1.43453800	4.61831200	-1.66899400
H	0.01482500	3.03947800	-1.81258200
C	-2.78789500	4.95360100	-1.69394300
H	-4.79509700	4.20856100	-1.91281700
H	-0.68432200	5.38818900	-1.51633600
H	-3.09732300	5.98486900	-1.55694000
H	0.99873400	0.98267500	-2.48518500
C	2.27218800	-0.66154600	-1.83264700
H	2.44186900	-0.63171800	-2.91905100
N	1.57666100	-1.85630100	-1.40759100
S	0.58114000	-2.46734500	-2.45836500
O	1.05950500	-3.71384100	-3.10274900
O	0.04862500	-1.47118500	-3.42741000
C	-0.80730700	-2.97716700	-1.45125300
C	-2.09472000	-2.63749300	-1.84375200
C	-0.59911900	-3.72685800	-0.29265800
C	-3.17966400	-3.01928300	-1.05212900
H	-2.23589900	-2.07550100	-2.76174900
C	-1.68442800	-4.09364400	0.49075500
H	0.41123300	-4.00696500	-0.00764100
C	-2.99126900	-3.73958100	0.12636900

H	-4.18697500	-2.74302300	-1.35480300
H	-1.52297100	-4.66660700	1.40122300
C	-4.15593800	-4.13427900	0.99775200
H	-4.04166900	-3.72891400	2.00838000
H	-5.09972700	-3.76726000	0.58778000
H	-4.22611200	-5.22210500	1.09144700
C	3.65152800	-0.58954100	-1.19189800
C	4.50967100	0.46636400	-1.52351900
C	4.08678600	-1.53708000	-0.26570100
C	5.75419600	0.59519500	-0.91528300
H	4.19635400	1.19974100	-2.26422800
C	5.33172800	-1.40622700	0.35271900
H	3.42984600	-2.37032700	-0.04141900
C	6.16518000	-0.33695700	0.03814100
H	6.40356300	1.42257900	-1.18510700
H	5.65151500	-2.14680300	1.07988600
H	7.13261300	-0.23477500	0.51933300
H	-2.40248500	0.22186100	-2.47203800

TS3<sub>2</sub><sup>(R,S,R)</sup>

P	-2.39177000	-0.24496600	0.72631400
C	-2.09894800	-0.69419800	2.47206000
C	-1.60113300	0.44453500	3.36714700
H	-1.41583100	-1.55049100	2.48479500
H	-3.06226800	-1.07156000	2.83693600
C	-1.15777500	-0.06726100	4.73745200
H	-0.76320200	0.97167700	2.89108800
H	-2.40002100	1.18555600	3.49679200
C	-0.68194100	1.06169600	5.64618900
H	-1.99091900	-0.60289700	5.20793300
H	-0.35311600	-0.80054800	4.60042900
H	-0.36205800	0.67983100	6.61854600
H	0.16398500	1.59094000	5.19690000
H	-1.48061700	1.79017800	5.81549700
C	-3.12346700	-1.75382100	0.00433600
C	-4.63286100	-1.89031700	0.21106700
H	-2.58894200	-2.58769000	0.47516400
H	-2.87518500	-1.75549800	-1.05739000
C	-5.12140300	-3.25147900	-0.28676900
H	-4.89625300	-1.77849800	1.27143200
H	-5.15512300	-1.09535900	-0.33439300
C	-6.62835400	-3.42029500	-0.11966300
H	-4.84510800	-3.36316800	-1.34239500

H	-4.59036400	-4.04245400	0.25673700
H	-6.96295000	-4.39320400	-0.48765800
H	-6.91512500	-3.34196200	0.93377500
H	-7.17047000	-2.64642600	-0.67191100
C	-3.60954500	1.12948500	0.83655700
C	-3.00241800	2.53645600	0.85844300
H	-4.16164000	0.94634600	1.76646100
H	-4.31625700	1.03223600	0.01055700
C	-4.06665700	3.59523400	1.14479600
H	-2.20989400	2.60304800	1.61390800
H	-2.52275200	2.76089800	-0.10242100
C	-3.48582500	5.00572100	1.12507200
H	-4.86897400	3.51036900	0.40120600
H	-4.52481600	3.39213200	2.12040800
H	-4.25555800	5.75520300	1.32368700
H	-2.70328800	5.11593600	1.88197300
H	-3.03906300	5.23010800	0.15121300
C	-0.80528600	0.21599200	-0.01717100
C	-0.72579700	0.93496500	-1.18272500
C	0.45803100	-0.27347000	0.69292300
C	0.51184900	1.37634700	-1.81156400
H	1.23298900	0.18148300	-1.69805700
C	-1.99995900	1.17971900	-1.95273500
O	-2.99853000	0.48870800	-1.85993300
O	-1.92726900	2.24899000	-2.73585300
C	-3.11629700	2.58435000	-3.48243700
C	-4.12879600	3.28321300	-2.59623200
H	-3.52587500	1.67102800	-3.91853500
H	-2.75765600	3.23888000	-4.27682300
H	-4.97395400	3.62292800	-3.19955700
H	-4.50623800	2.60038000	-1.83106900
H	-3.67728400	4.15309400	-2.11119500
H	0.23325100	-0.60950300	1.70644500
C	1.43726700	2.33333000	-1.16353300
C	2.57831300	2.73527900	-1.88621700
C	1.28693100	2.84050900	0.13606300
C	3.53417700	3.57090000	-1.32602900
H	2.71750800	2.34932900	-2.89263600
C	2.25406400	3.67033500	0.70398700
H	0.39577000	2.58916100	0.70701000
C	3.38745400	4.03506100	-0.01652300
H	4.40758900	3.85124000	-1.90777800
H	2.11180400	4.03982200	1.71562800
H	4.13964400	4.67929800	0.42764400



H	1.17357400	0.54896500	0.79922700
C	1.18669400	-1.43145000	-0.02059100
H	2.01397100	-1.71029300	0.65397900
N	1.71401600	-0.94513000	-1.29280100
S	3.15621100	-1.46781600	-1.73810600
O	3.50983600	-0.75847300	-2.97543800
O	3.24218500	-2.93665200	-1.76238500
C	4.30724200	-0.95984300	-0.45711300
C	5.31936400	-1.82487000	-0.05669700
C	4.19607600	0.31136300	0.10720400
C	6.23187200	-1.40800100	0.91064400
H	5.37930100	-2.81539100	-0.49431900
C	5.11176100	0.71221900	1.07134700
H	3.39702000	0.97916100	-0.19982500
C	6.14426900	-0.13874600	1.48513600
H	7.02238700	-2.08303900	1.22666700
H	5.02085100	1.70379100	1.50796800
C	7.13121100	0.31674900	2.52845700
H	7.71292700	1.17346200	2.16453900
H	6.61406300	0.63688400	3.44196100
H	7.82937400	-0.48506600	2.79017900
C	0.29184000	-2.65711000	-0.15449500
C	0.00744400	-3.42414300	0.98071200
C	-0.26823700	-3.02963000	-1.37629600
C	-0.82555600	-4.53797300	0.90017800
H	0.46147700	-3.15755700	1.93423800
C	-1.10320200	-4.14295600	-1.46077800
H	-0.02679200	-2.44422700	-2.25772000
C	-1.38710000	-4.89854600	-0.32484800
H	-1.02882400	-5.12799100	1.78851600
H	-1.53107100	-4.42344500	-2.41855800
H	-2.03346600	-5.76789600	-0.39311200
H	0.37088600	1.62324600	-2.86214400

M3<sub>2</sub><sup>(R,S,R)</sup>

P	2.23063600	0.08776300	0.91585500
C	1.85706600	0.06534500	2.71923100
C	1.07623800	-1.15422600	3.20747800
H	1.32722900	0.99267500	2.96939400
H	2.82477300	0.12166600	3.23109400
C	0.84498700	-1.12565800	4.71778900
H	0.10770500	-1.20553400	2.69525700
H	1.61689200	-2.07150100	2.94239300

C	0.04637000	-2.33428400	5.19763500
H	1.81281000	-1.08914900	5.23257600
H	0.31691400	-0.20122300	4.98237000
H	-0.11490000	-2.30404800	6.27801600
H	-0.93398600	-2.37049300	4.71154600
H	0.56974900	-3.26587700	4.96085500
C	3.01684000	1.73058400	0.69412000
C	4.21924200	2.03866400	1.58936500
H	2.22371100	2.47060800	0.85544500
H	3.28770900	1.78556300	-0.36313000
C	4.79840300	3.41889400	1.27338700
H	3.92907400	2.01190900	2.64697400
H	5.00319200	1.28135900	1.45727500
C	5.99025800	3.76635900	2.16041600
H	5.09453300	3.44863100	0.21758400
H	4.00744900	4.17021400	1.39129800
H	6.39375400	4.75332800	1.92033400
H	5.70263900	3.76834900	3.21655600
H	6.79444400	3.03440400	2.03586100
C	3.59518300	-1.12637900	0.69482100
C	3.21208100	-2.57529200	0.37936700
H	4.16425800	-1.09398400	1.63237100
H	4.24893800	-0.72608600	-0.08683400
C	4.43656700	-3.49019900	0.40920700
H	2.46382900	-2.94124500	1.09282900
H	2.74200100	-2.64551300	-0.60796800
C	4.08546800	-4.93143500	0.05189000
H	5.18842900	-3.10577500	-0.29178200
H	4.89401800	-3.45166100	1.40550900
H	4.96919400	-5.57404300	0.06884600
H	3.35598400	-5.34112000	0.75729300
H	3.64557400	-4.98859300	-0.94907900
C	0.76997400	-0.26716200	0.03135600
C	0.79127800	-0.99171700	-1.20974500
C	-0.49740000	0.34725200	0.59413700
C	-0.18514200	-1.79397400	-1.75693000
H	-1.53326200	0.01644400	-1.69779700
C	2.01089300	-0.80363600	-2.07874100
O	2.83441900	0.07730800	-1.91530000
O	2.13886100	-1.72682300	-3.04024300
C	3.30491000	-1.62414900	-3.87589200
C	4.51097200	-2.22423900	-3.17864200
H	3.47150600	-0.57559700	-4.13100000
H	3.04610700	-2.18052700	-4.77742200

H	5.37561100	-2.21049400	-3.84659000
H	4.75685500	-1.64825600	-2.28299900
H	4.30969300	-3.26026300	-2.89199800
H	-0.29548500	0.77960200	1.58000500
C	-1.33547600	-2.41246300	-1.10784000
C	-2.40610600	-2.87061200	-1.90319700
C	-1.39251500	-2.67581200	0.27480400
C	-3.48956400	-3.53676200	-1.34381600
H	-2.37724800	-2.68967300	-2.97467400
C	-2.47499600	-3.34913000	0.83191200
H	-0.55364100	-2.37656300	0.89703900
C	-3.53406900	-3.77624100	0.03070500
H	-4.30444500	-3.86705400	-1.98037100
H	-2.48897300	-3.54596200	1.90023100
H	-4.38100400	-4.29292600	0.47084700
H	-1.30043900	-0.38817600	0.76070300
C	-1.14232600	1.50339800	-0.21624600
H	-1.95769200	1.88979300	0.41328500
N	-1.73655400	0.98434900	-1.45914600
S	-3.26965200	1.42145000	-1.84522000
O	-3.64304200	0.58705600	-2.98362800
O	-3.31787400	2.87498100	-1.95886700
C	-4.28643400	0.98701800	-0.44942600
C	-5.11608500	1.94546600	0.11903300
C	-4.24612400	-0.31910000	0.03958700
C	-5.92740600	1.58335600	1.19249100
H	-5.12081300	2.95541300	-0.27584300
C	-5.05636700	-0.65895800	1.11308300
H	-3.58920500	-1.06060900	-0.40719600
C	-5.90962200	0.28412600	1.70227700
H	-6.58247000	2.32461800	1.64055100
H	-5.02624700	-1.67505400	1.49772500
C	-6.78033100	-0.10805700	2.86669400
H	-6.16954900	-0.40112700	3.72571500
H	-7.42751900	0.71555000	3.17336100
H	-7.41052300	-0.96361300	2.60830700
C	-0.18540800	2.64404500	-0.48628500
C	-0.09230300	3.69922700	0.42295200
C	0.65826000	2.62868300	-1.59857900
C	0.83493900	4.72280700	0.22986900
H	-0.75098500	3.72096000	1.28853600
C	1.58072400	3.65161000	-1.79667100
H	0.58513700	1.80873200	-2.30626600
C	1.67527500	4.69925900	-0.88163800

H	0.89502700	5.54026100	0.94175500
H	2.23396800	3.62639300	-2.66350000
H	2.39735600	5.49498700	-1.03567400
H	-0.07535600	-2.04964900	-2.80535200
TS4 <sub>2</sub> <sup>(R,S,R)</sup>			
P	-1.69319300	0.91068100	-0.41326300
C	-2.69895100	0.85650700	1.11689500
C	-2.23810100	1.73936100	2.27735900
H	-2.77350000	-0.19029900	1.43224900
H	-3.70527600	1.16304100	0.80872100
C	-3.14397700	1.55861300	3.49561300
H	-1.21053000	1.49248000	2.56634000
H	-2.23973900	2.79478300	1.97513000
C	-2.69941200	2.41535600	4.67695600
H	-4.17504900	1.80856200	3.21774300
H	-3.14517400	0.49785800	3.77682900
H	-3.35432800	2.27365000	5.54007900
H	-1.67996200	2.15834800	4.98222800
H	-2.71159100	3.47802900	4.41547800
C	-2.63984100	-0.05384700	-1.65581500
C	-4.15549100	-0.10627000	-1.46249500
H	-2.21404200	-1.06209600	-1.64002400
H	-2.37415500	0.37766500	-2.62523700
C	-4.82246200	-0.93757300	-2.55800800
H	-4.39288400	-0.55661100	-0.49099900
H	-4.58326700	0.90566500	-1.46243800
C	-6.33330200	-1.03272200	-2.36797600
H	-4.59298900	-0.50162600	-3.53771200
H	-4.38241500	-1.94308100	-2.55476100
H	-6.79719500	-1.63383000	-3.15386400
H	-6.57496400	-1.49283100	-1.40434600
H	-6.79305800	-0.03950400	-2.38805100
C	-1.78800100	2.65843600	-0.97369000
C	-0.73757400	3.63840100	-0.43818400
H	-2.79278700	2.98705900	-0.67625700
H	-1.76670900	2.63810000	-2.06688000
C	-1.16825500	5.08814300	-0.65746900
H	-0.55072100	3.47024600	0.63002800
H	0.22050200	3.47384300	-0.94217500
C	-0.09807800	6.07717700	-0.20590100
H	-1.38930400	5.23819400	-1.72179400
H	-2.10423300	5.27320000	-0.11586600

H	-0.41901300	7.10999400	-0.36157800
H	0.12653200	5.94966400	0.85763000
H	0.83160900	5.92474500	-0.76320600
C	-0.03928600	0.24130100	-0.18392400
C	1.09376700	1.02442800	-0.74186500
C	0.19554800	-0.65988400	1.02570400
C	2.25291500	1.40833000	-0.15765000
H	-0.09283300	-0.90520500	-0.95409500
C	0.94442500	1.31412100	-2.20634800
O	-0.05837100	1.02309800	-2.83410200
O	1.97476200	1.96309700	-2.75790900
C	1.80386300	2.39268400	-4.12214900
C	0.98006600	3.66557700	-4.17153300
H	1.33690400	1.58775200	-4.69227800
H	2.81839000	2.55567600	-4.48698100
H	0.90904900	4.02524300	-5.20074900
H	-0.03147600	3.47996100	-3.80125100
H	1.44513800	4.44478000	-3.56208400
H	-0.25447000	-0.33143800	1.96712700
C	2.62008700	1.44536700	1.26323000
C	3.96295900	1.28493200	1.63164000
C	1.68569100	1.73690700	2.26540000
C	4.34932700	1.36097300	2.96595500
H	4.70403700	1.09828500	0.85880100
C	2.06946500	1.82460600	3.59759100
H	0.65465000	1.91266000	1.97857400
C	3.40276800	1.62459500	3.95468000
H	5.39290400	1.22597400	3.23383100
H	1.32916200	2.05531400	4.35779800
H	3.70456100	1.68831300	4.99504400
H	1.27562100	-0.70784300	1.18778700
C	-0.27572300	-2.13012500	0.67424900
H	0.43483300	-2.81734500	1.15230600
N	-0.22966400	-2.21105200	-0.77922600
S	0.83138400	-3.22778000	-1.43209400
O	0.81408200	-3.00409400	-2.88134400
O	0.62865400	-4.59909100	-0.94323700
C	2.44765300	-2.73683300	-0.84787100
C	3.00814700	-3.36003800	0.26619400
C	3.09194800	-1.66856700	-1.46354200
C	4.21914100	-2.89648800	0.76715000
H	2.50166900	-4.20755800	0.71668300
C	4.30894100	-1.22207000	-0.95676000
H	2.64834900	-1.20101900	-2.33805900

C	4.88385800	-1.82113200	0.16695400
H	4.66129900	-3.37889600	1.63469300
H	4.81849800	-0.39381000	-1.44278100
C	6.18895600	-1.32949300	0.73571000
H	6.62854500	-0.55010000	0.10916100
H	6.03696700	-0.91665400	1.73851100
H	6.91099800	-2.14595400	0.82411100
C	-1.65487800	-2.44527400	1.23231800
C	-1.88102800	-2.31487900	2.60889500
C	-2.71585200	-2.83527900	0.41597500
C	-3.14717100	-2.52051500	3.14708200
H	-1.05779900	-2.03981700	3.26465800
C	-3.98959900	-3.03641200	0.95208600
H	-2.53172400	-2.98174300	-0.64328500
C	-4.21333600	-2.86609800	2.31480500
H	-3.30455700	-2.40882900	4.21565600
H	-4.80651300	-3.32761200	0.29769300
H	-5.20425500	-3.01538200	2.73126500
H	3.03144400	1.76365100	-0.82722200
M4 <sub>2</sub> <sup>(R,S,R)</sup>			
P	1.26408800	0.62864700	1.13603800
C	2.72143700	1.32792600	0.27194700
C	2.54872400	2.36783300	-0.83820000
H	3.30572400	0.48277800	-0.10586000
H	3.29783600	1.76591700	1.09902900
C	3.89911000	2.98525000	-1.20438400
H	2.12622700	1.89085000	-1.72900400
H	1.86350300	3.16835300	-0.53950500
C	3.79818300	3.87585600	-2.43845100
H	4.27306000	3.56140200	-0.34948400
H	4.62144900	2.17973600	-1.38221500
H	4.75743100	4.34404300	-2.67177300
H	3.48678500	3.29160600	-3.31072700
H	3.06166500	4.67191600	-2.28826100
C	1.85477800	-0.78371600	2.12432300
C	3.26235000	-0.64388100	2.70373500
H	1.77486000	-1.65668100	1.46494900
H	1.10021200	-0.91616700	2.90848600
C	3.64570200	-1.87932900	3.51866300
H	3.98868300	-0.51944000	1.89148500
H	3.33381300	0.24917500	3.33912000
C	5.05807000	-1.77628500	4.08618000

H	2.92233700	-2.01693100	4.33072000
H	3.56512700	-2.76496700	2.87624100
H	5.32072000	-2.66712900	4.66157100
H	5.79310300	-1.66530900	3.28270400
H	5.15149000	-0.90882100	4.74707500
C	0.70536600	1.90078500	2.32000700
C	0.26844400	3.24640800	1.72927500
H	1.54582100	2.03684300	3.01206000
H	-0.10050900	1.44375900	2.90022900
C	-0.55345800	4.05058000	2.73686000
H	1.14997700	3.82550600	1.43258700
H	-0.33915500	3.09456100	0.82859100
C	-0.94877600	5.41918300	2.19214700
H	-1.45254400	3.47577200	2.99243400
H	0.02000300	4.16431800	3.66469800
H	-1.54960000	5.97541300	2.91545400
H	-0.06279500	6.01732700	1.95849700
H	-1.53498600	5.31703600	1.27346800
C	-0.13790000	-0.05690800	0.11960100
C	-1.48403500	0.58381500	0.40901000
C	0.17510600	-0.40142000	-1.34814900
C	-2.28513000	1.29677600	-0.40579500
H	-0.21552700	-1.04758300	0.59536000
C	-2.02953900	0.18696400	1.74779800
O	-1.38980800	-0.46989200	2.54971100
O	-3.26079800	0.63742700	1.99776300
C	-3.83011600	0.27812400	3.27225400
C	-3.36959400	1.23223100	4.35588000
H	-3.55088300	-0.75184200	3.50360200
H	-4.90831900	0.33561900	3.11366200
H	-3.85451500	0.97738800	5.30128800
H	-2.28805200	1.15978300	4.49392600
H	-3.63145900	2.26131200	4.09907300
H	0.68097600	0.40343700	-1.88150300
C	-2.00710700	1.87778700	-1.72665200
C	-3.01873600	1.88491400	-2.69585800
C	-0.78575400	2.48884900	-2.02352400
C	-2.78811600	2.44010200	-3.94976500
H	-3.98386800	1.44336500	-2.46164500
C	-0.55665400	3.05899900	-3.27037700
H	-0.01704400	2.52668800	-1.26041700
C	-1.55628600	3.02544600	-4.24108500
H	-3.57288700	2.42450000	-4.69893400
H	0.39813700	3.53265400	-3.47917100

H	-1.38220500	3.46588700	-5.21728800
H	-0.79694900	-0.52338900	-1.83405300
C	0.96827100	-1.74240700	-1.51907900
H	0.70906200	-2.09706900	-2.52933400
N	0.63254700	-2.72581000	-0.51029600
S	-0.51255800	-3.74178900	-0.87517900
O	-0.55459700	-4.79619200	0.15314800
O	-0.48426400	-4.20241300	-2.28271200
C	-2.09861400	-2.89940400	-0.73297000
C	-2.67920500	-2.30560700	-1.84931500
C	-2.70456800	-2.77758500	0.51765900
C	-3.84733700	-1.55804800	-1.70760300
H	-2.21574700	-2.43660700	-2.82272600
C	-3.88213800	-2.05023500	0.64228000
H	-2.25334600	-3.26235900	1.37806100
C	-4.45750000	-1.40852300	-0.46062800
H	-4.29467000	-1.09298300	-2.58233700
H	-4.36511500	-1.96896400	1.61351600
C	-5.69167600	-0.56447500	-0.28327400
H	-6.49241300	-1.12886500	0.20333800
H	-5.47058400	0.29990300	0.35360000
H	-6.06639200	-0.19657600	-1.24117400
C	2.47382200	-1.49197300	-1.54433700
C	3.01269600	-0.62283100	-2.50266700
C	3.34584900	-2.11374100	-0.64942300
C	4.37440600	-0.33959600	-2.53025200
H	2.35750200	-0.16630600	-3.24216600
C	4.71152400	-1.82216700	-0.66400300
H	2.93706300	-2.83602200	0.04927200
C	5.22938700	-0.92414000	-1.59403100
H	4.77029100	0.33840000	-3.28096900
H	5.37110500	-2.30493900	0.05191400
H	6.29036400	-0.69585800	-1.60531500
H	-3.29318600	1.47438500	-0.03785800
M4 <sub>2</sub> <sup>(R,S,R)</sup>			
P	1.64484800	1.52753600	-0.55797600
C	0.48280400	2.79748600	-1.19078100
C	-0.80992300	3.13750900	-0.44449100
H	0.24935200	2.47915800	-2.21457000
H	1.10397700	3.69813700	-1.28244300
C	-1.59613100	4.23382300	-1.16352800
H	-1.45161900	2.25342400	-0.36097900



H	-0.58369000	3.47513600	0.57398500
C	-2.81613800	4.65039900	-0.34725700
H	-0.94885500	5.10059500	-1.34257000
H	-1.90793600	3.86269600	-2.14750600
H	-3.43620200	5.37059300	-0.88683000
H	-3.43650700	3.77776400	-0.11576900
H	-2.51192400	5.10730200	0.60000700
C	2.81923600	1.26432900	-1.92974800
C	3.47726000	2.51796600	-2.50990200
H	2.25781300	0.72934400	-2.70736200
H	3.56328600	0.56207100	-1.53509900
C	4.49915600	2.15432400	-3.58825500
H	2.71788800	3.17778900	-2.94561400
H	3.98050100	3.08753200	-1.71895000
C	5.15528000	3.38990400	-4.19697800
H	5.26330000	1.50083000	-3.15152100
H	4.00062900	1.57192100	-4.37221000
H	5.88297400	3.11257900	-4.96323900
H	4.40809800	4.04051700	-4.66150300
H	5.67728800	3.97195500	-3.43140600
C	2.63166300	2.14614300	0.84442900
C	1.91076100	2.51128000	2.14461800
H	3.16758200	3.01931200	0.45249800
H	3.37709500	1.36177100	1.02137600
C	2.89967100	3.05437200	3.17712800
H	1.13715100	3.26540800	1.95671700
H	1.41216600	1.62865200	2.55696700
C	2.21241300	3.40236900	4.49385700
H	3.68182300	2.30507600	3.34939800
H	3.39898400	3.94090100	2.76826000
H	2.92833500	3.78699100	5.22390200
H	1.44245700	4.16492800	4.34254600
H	1.72935300	2.52072500	4.92577300
C	0.93571800	-0.16355900	-0.28041000
C	1.18456400	-0.79897800	1.07446600
C	-0.42857900	-0.39178000	-0.95222800
C	0.37805700	-0.94658400	2.14341600
C	2.54955700	-1.41066200	1.13494900
O	3.45344500	-1.04255600	0.40246000
O	2.69750800	-2.35768800	2.05762200
C	4.00862500	-2.94919300	2.16245300
C	4.93640800	-2.06780600	2.97526100
H	4.39228000	-3.12026100	1.15400500
H	3.83272300	-3.90833300	2.65066000

H	5.90496300	-2.56007500	3.09084400
H	5.09226500	-1.11087800	2.47291200
H	4.51907000	-1.88723900	3.96849000
H	-0.40299000	0.11619700	-1.92628000
C	-0.89057900	-0.29308100	2.47986100
C	-1.18461400	0.99710400	2.03482900
C	-1.77010900	-0.90575300	3.38364300
C	-2.32285600	1.66885800	2.46341000
H	-0.48414500	1.49025900	1.37444100
C	-2.91997400	-0.24613800	3.80371700
H	-1.55010000	-1.90471400	3.74804200
C	-3.19596700	1.04595900	3.35282800
H	-2.52248500	2.67652900	2.10787800
H	-3.59859300	-0.73497300	4.49474100
H	-4.08642700	1.56326200	3.69549900
H	-1.25990600	0.02731800	-0.38052300
C	-0.75562400	-1.90943700	-1.18684500
H	-1.34415000	-1.93165500	-2.11881200
N	-1.49022800	-2.45636300	-0.05856300
S	-2.99271300	-2.75949100	-0.38738300
O	-3.67743600	-3.22813300	0.83300000
O	-3.21802500	-3.59293300	-1.59476500
C	-3.77301700	-1.19202000	-0.81716800
C	-4.06408400	-0.88345800	-2.14354300
C	-3.98071700	-0.24482400	0.18178000
C	-4.57623600	0.37057200	-2.46456600
H	-3.90316900	-1.63903400	-2.90546000
C	-4.50292100	1.00317300	-0.14764000
H	-3.74361500	-0.49390400	1.21257600
C	-4.80799700	1.33016000	-1.47420300
H	-4.81422000	0.60630100	-3.49904900
H	-4.68802700	1.73004400	0.64056500
C	-5.37942000	2.67656800	-1.84078400
H	-5.72915100	3.21482600	-0.95663100
H	-4.62858600	3.30191200	-2.33643100
H	-6.21969000	2.56830100	-2.53187900
C	0.51386500	-2.69622900	-1.48338300
C	1.20702200	-2.47729900	-2.67971500
C	1.05615600	-3.57583200	-0.54590400
C	2.42528800	-3.10523800	-2.92500900
H	0.78627900	-1.80337000	-3.42457000
C	2.27433400	-4.21016600	-0.79060400
H	0.50522500	-3.74541800	0.37348400
C	2.96614500	-3.97233500	-1.97549100

H	2.94938300	-2.92386000	-3.85844200
H	2.68261700	-4.89373900	-0.05114200
H	3.91521600	-4.46425900	-2.16390400
H	0.75326600	-1.61418300	2.91608900
H	1.64242200	-0.69989800	-0.92306100

TS5<sub>2</sub><sup>(R,S,R)</sup>

P	2.54148800	0.83368800	-0.75354600
C	2.22851500	2.22032000	-1.91069000
C	1.14181200	3.25324300	-1.60155400
H	2.02598000	1.74231200	-2.87759800
H	3.19958100	2.72214800	-2.01086600
C	1.11557900	4.35816900	-2.65773100
H	0.15934300	2.77022700	-1.57016500
H	1.30919700	3.70673200	-0.61746700
C	0.02683700	5.38719800	-2.36913200
H	2.09566200	4.84874000	-2.69323800
H	0.95397800	3.90810200	-3.64440300
H	0.00435900	6.16789700	-3.13306000
H	-0.95954400	4.91308100	-2.34178700
H	0.19375300	5.86955000	-1.40062500
C	3.70305500	-0.25637600	-1.64374800
C	4.98276000	0.39822000	-2.16551800
H	3.13021100	-0.70280200	-2.46755100
H	3.91952900	-1.06202900	-0.93143300
C	5.92051700	-0.63576700	-2.79116200
H	4.74029100	1.16067300	-2.91546600
H	5.50961800	0.90873000	-1.34983300
C	7.20060600	-0.00013600	-3.32480000
H	6.16418800	-1.39689100	-2.04087700
H	5.39375400	-1.15352000	-3.60145600
H	7.85957000	-0.74933300	-3.76991500
H	6.97517500	0.74827600	-4.09073400
H	7.75198200	0.49879900	-2.52193800
C	3.41939900	1.38096900	0.74820200
C	2.68184800	2.29466700	1.73044700
H	4.33918900	1.86213900	0.39412700
H	3.70487100	0.44249400	1.23981300
C	3.56569100	2.62763600	2.93256800
H	2.38097700	3.22663300	1.23696100
H	1.77162200	1.79785800	2.08068900
C	2.85115500	3.53886800	3.92599500
H	3.85939800	1.69337000	3.42681200

H	4.49120200	3.10298400	2.58521500
H	3.48610400	3.76642700	4.78558400
H	2.57086100	4.48562300	3.45383100
H	1.93562600	3.06777400	4.29654700
C	1.10659700	-0.28301200	-0.36318700
C	0.81815000	-0.53632600	1.09806500
C	-0.15180400	-0.13454400	-1.22818300
C	-0.41608500	-0.27937400	1.68502700
C	1.71709700	-1.50811200	1.67888500
O	2.79539500	-1.82355600	1.17050300
O	1.31396800	-2.03038700	2.85903700
C	2.22196200	-2.93832700	3.49635300
C	3.32507600	-2.18900100	4.22094300
H	2.63216400	-3.62014800	2.74784200
H	1.60164700	-3.50370700	4.19403800
H	3.96634400	-2.89260200	4.75810700
H	3.93721400	-1.63566500	3.50556200
H	2.89916800	-1.48795800	4.94299900
H	0.13147900	-0.12490000	-2.28723800
C	-1.15088300	1.00987700	1.70951400
C	-0.69324700	2.14769700	1.04218000
C	-2.31235800	1.11715800	2.48618500
C	-1.40170300	3.34485600	1.08384600
H	0.23498400	2.09527600	0.48776400
C	-3.01829000	2.31385000	2.54199900
H	-2.67865600	0.23789400	3.00577700
C	-2.57459500	3.42894900	1.83117200
H	-1.03145500	4.21108600	0.54188400
H	-3.92377100	2.37496000	3.13719100
H	-3.13152500	4.35951400	1.87028900
H	-0.70381000	0.78552900	-1.02511400
C	-1.11858200	-1.33024000	-0.99268900
H	-1.90454600	-1.21881900	-1.75795100
N	-1.69147000	-1.23838200	0.34317700
S	-3.15034900	-1.81184400	0.55211900
O	-3.46344200	-1.74246500	1.99083100
O	-3.38272200	-3.11841300	-0.09286300
C	-4.28425000	-0.69603200	-0.28936900
C	-5.52226900	-1.17775400	-0.71324700
C	-3.94900200	0.64089400	-0.47781300
C	-6.42673900	-0.31155400	-1.31448000
H	-5.76034100	-2.22795300	-0.57823900
C	-4.86378200	1.49890300	-1.08479600
H	-2.97973700	1.00704700	-0.15118300

C	-6.11203200	1.03909500	-1.50822400
H	-7.39230300	-0.68583700	-1.64465800
H	-4.60113800	2.54371100	-1.22949400
C	-7.09671100	1.96147500	-2.17912400
H	-7.18355900	1.72833100	-3.24513000
H	-8.09303000	1.85645400	-1.74123700
H	-6.78857400	3.00497900	-2.08695700
C	-0.39417700	-2.64447900	-1.27062000
C	-0.03496000	-2.97159900	-2.58126600
C	-0.01546900	-3.49935700	-0.23540800
C	0.69475300	-4.12582000	-2.85349300
H	-0.33846600	-2.32024300	-3.39880500
C	0.72098600	-4.65159900	-0.50394800
H	-0.30492100	-3.24730200	0.78083300
C	1.07943100	-4.96873400	-1.81208700
H	0.95902800	-4.36957700	-3.87806300
H	1.01225600	-5.30515500	0.31294100
H	1.64904300	-5.86865900	-2.02134300
H	-0.63434000	-0.89386600	2.55561200
H	1.56901200	-1.22036300	-0.70430100

M5<sub>2</sub><sup>(R,S,R)</sup>

P	-2.54774000	0.03369100	-0.69544100
C	-2.50797600	-0.99656500	-2.20577500
C	-1.41825000	-2.08535500	-2.22898200
H	-2.42583800	-0.33106000	-3.07156200
H	-3.50058700	-1.46165500	-2.26498400
C	-1.86142600	-3.29076000	-3.05848300
H	-0.49672800	-1.67951100	-2.65727200
H	-1.14828900	-2.41363800	-1.21427500
C	-0.77805000	-4.35898400	-3.15742800
H	-2.76827800	-3.71996100	-2.61244800
H	-2.14460400	-2.94799500	-4.06137500
H	-1.11311600	-5.21005800	-3.75556100
H	0.12733000	-3.95384600	-3.62060500
H	-0.50365300	-4.72430400	-2.16318800
C	-3.97917900	1.15222700	-0.80810000
C	-5.35716200	0.49091000	-0.75747900
H	-3.85333400	1.73204700	-1.73147900
H	-3.84466000	1.83837000	0.03676400
C	-6.47677300	1.51853000	-0.92837300
H	-5.45060300	-0.27438200	-1.53876200
H	-5.48256400	-0.01865500	0.20581300

C	-7.86076100	0.88289100	-0.83772800
H	-6.36958600	2.29332700	-0.16018900
H	-6.35766600	2.01959600	-1.89646000
H	-8.64888500	1.62827600	-0.96844600
H	-7.99021700	0.11685900	-1.60852700
H	-8.00672600	0.40543200	0.13600000
C	-2.75972100	-1.09875300	0.71262400
C	-3.56414300	-2.37669800	0.46280700
H	-3.19307000	-0.48438400	1.50872700
H	-1.74186600	-1.34200900	1.03945800
C	-3.59798400	-3.23457200	1.72842200
H	-4.58959400	-2.14438800	0.15080500
H	-3.11479500	-2.96400800	-0.34698700
C	-4.36273800	-4.53870100	1.52405700
H	-2.56545300	-3.44790400	2.03387400
H	-4.05098900	-2.65707800	2.54343300
H	-4.37100200	-5.14240800	2.43479000
H	-5.40152500	-4.34127900	1.24167600
H	-3.90740700	-5.13591100	0.72771600
C	-1.04663300	1.13955000	-0.47201000
C	-0.30298700	0.87542800	0.78990400
C	-0.10498100	1.13276800	-1.68285200
C	1.10382300	0.37623300	0.70049800
C	-0.96750200	1.17806900	1.96491400
O	-2.16512600	1.54985100	2.03753800
O	-0.21869300	1.02312200	3.12523400
C	-0.95505800	1.06094700	4.34129800
C	-1.65675200	-0.26295300	4.59813100
H	-1.67962700	1.87813000	4.30840900
H	-0.21797600	1.26973800	5.12126300
H	-2.19738200	-0.23784000	5.54861000
H	-2.37312800	-0.46015300	3.79588700
H	-0.93219000	-1.08170000	4.63448200
H	-0.57599900	1.59558100	-2.55570300
C	1.18999300	-1.12449400	0.38959600
C	0.66858000	-2.00712000	1.34385200
C	1.75714100	-1.65440000	-0.76784800
C	0.70743200	-3.38281400	1.14306300
H	0.23250800	-1.59165100	2.25155700
C	1.80757600	-3.03407400	-0.97027400
H	2.18318300	-0.98254200	-1.50711200
C	1.28178300	-3.90303300	-0.01856900
H	0.30338700	-4.05182300	1.89716300
H	2.25933400	-3.42828100	-1.87640900

H	1.32234000	-4.97656200	-0.17547500
H	0.18305400	0.11559400	-1.95711300
C	1.18164100	1.91238900	-1.34875700
H	1.82321800	1.89033600	-2.23598300
N	1.88280800	1.18110000	-0.28147200
S	3.42428200	1.62192800	0.10735100
O	3.48561200	2.11525900	1.48322200
O	3.90258300	2.47093400	-0.98248600
C	4.31942600	0.09028900	0.07152400
C	4.84028100	-0.35548800	-1.14184100
C	4.38024400	-0.69271600	1.21773900
C	5.40736900	-1.62026100	-1.20225900
H	4.79175100	0.28140500	-2.01924700
C	4.94580300	-1.96211600	1.13633400
H	3.98250600	-0.31701600	2.15507900
C	5.45141500	-2.44691600	-0.07157500
H	5.81726700	-1.98110300	-2.14176400
H	4.98839900	-2.58586300	2.02393200
C	6.02319500	-3.83584500	-0.17410500
H	7.02394700	-3.81670500	-0.62125500
H	6.08773200	-4.31341000	0.80826100
H	5.38844500	-4.46135900	-0.81610000
C	0.87354700	3.37045500	-1.03561700
C	0.57081000	4.22132700	-2.10187000
C	0.84627700	3.87670800	0.26472800
C	0.23775800	5.55366000	-1.87879300
H	0.60536600	3.83636700	-3.11909500
C	0.51451700	5.21218300	0.48853000
H	1.08291600	3.22381100	1.09918800
C	0.20693900	6.05286500	-0.57790900
H	0.00891700	6.20220300	-2.71869700
H	0.49743400	5.59565100	1.50390600
H	-0.04888100	7.09213500	-0.39755400
H	1.55635000	0.53335800	1.68547500
H	-1.53104900	2.12611200	-0.41076300
TS6 <sub>2</sub> <sup>(R,S,R)</sup>			
P	-2.40636000	0.15723200	-0.95715300
C	-2.63861100	-1.09954200	-2.30086100
C	-1.41396200	-1.96361300	-2.60404700
H	-2.93338400	-0.53413900	-3.19310500
H	-3.49021900	-1.73639400	-2.02998500
C	-1.71230300	-3.06532600	-3.61884700

H	-0.60124500	-1.33432200	-2.98811000
H	-1.04282300	-2.42135400	-1.68015600
C	-0.47092900	-3.89294400	-3.94163000
H	-2.50154500	-3.71498400	-3.22058700
H	-2.11150300	-2.61645200	-4.53651100
H	-0.69568000	-4.69454100	-4.64943400
H	0.31182900	-3.26586100	-4.38016300
H	-0.06080000	-4.34966800	-3.03455100
C	-3.87305200	1.24850000	-1.12490500
C	-5.22913800	0.54463200	-1.05685400
H	-3.76745400	1.79255600	-2.07234100
H	-3.76827500	1.97931300	-0.31381100
C	-6.39401600	1.53199000	-1.13433400
H	-5.32001600	-0.18192200	-1.87444700
H	-5.30372800	-0.02556000	-0.12088700
C	-7.74967000	0.83688300	-1.04819300
H	-6.29728400	2.26359900	-0.32324600
H	-6.32335500	2.09666300	-2.07207800
H	-8.57115800	1.55469000	-1.11385600
H	-7.86971100	0.11255700	-1.85993200
H	-7.85031100	0.29638100	-0.10181700
C	-2.62073500	-0.68049700	0.66574600
C	-3.06872200	-2.14041700	0.65674400
H	-3.31930700	-0.05107000	1.23065200
H	-1.65552100	-0.59230600	1.18244500
C	-3.12642200	-2.70246300	2.07681100
H	-4.05368500	-2.24344900	0.18209100
H	-2.36715500	-2.74336700	0.06568500
C	-3.42779200	-4.19768500	2.09711700
H	-2.16326500	-2.51324000	2.56739200
H	-3.88492400	-2.15444800	2.65012900
H	-3.48722000	-4.58094000	3.11901300
H	-4.37864600	-4.41563800	1.60014200
H	-2.64201100	-4.75328000	1.57432900
C	-0.75359400	1.59812200	-0.66955600
C	-0.21014400	1.51434800	0.63029800
C	0.22949000	1.43752800	-1.82225800
C	1.12432000	0.86401400	0.89914000
C	-1.04854600	1.90500200	1.71096900
O	-2.22894300	2.25900300	1.60724900
O	-0.43923000	1.82611400	2.93362600
C	-1.29191700	1.94034600	4.07314900
C	-2.03823800	0.63929300	4.31586200
H	-1.98669000	2.77106100	3.93053700



H	-0.62305100	2.17335600	4.90460000
H	-2.61888900	0.69578400	5.24051800
H	-2.72086400	0.44144600	3.48570200
H	-1.33296200	-0.19374000	4.39267700
H	-0.11188500	1.99280100	-2.69962100
C	0.96178200	-0.61481400	1.22956800
C	0.98125500	-1.02683000	2.56275300
C	0.71854100	-1.56348600	0.23200000
C	0.76075000	-2.36318400	2.89592200
H	1.16605600	-0.28996200	3.33978300
C	0.50343700	-2.89820300	0.56101500
H	0.74573500	-1.25547500	-0.80994200
C	0.51958000	-3.30319200	1.89662700
H	0.78360600	-2.67016500	3.93737500
H	0.34049200	-3.63091300	-0.22588000
H	0.35386000	-4.34520400	2.15287200
H	0.33510300	0.39346900	-2.12349600
C	1.62451800	1.91417900	-1.39244400
H	2.31716500	1.69425800	-2.20961400
N	2.03060900	1.06859900	-0.26059800
S	3.63901700	0.76172900	-0.02007100
O	3.99066300	1.09661000	1.35841700
O	4.35985800	1.38898100	-1.12525400
C	3.78857000	-0.99928300	-0.19273000
C	3.61323700	-1.55580300	-1.45583400
C	3.96287200	-1.79396100	0.93491000
C	3.58736500	-2.93957200	-1.58217900
H	3.48655800	-0.91463500	-2.32366000
C	3.93318400	-3.17527600	0.78980500
H	4.08767700	-1.33081000	1.90744000
C	3.72982400	-3.76504600	-0.46211400
H	3.44438100	-3.38666200	-2.56178300
H	4.04857500	-3.80802000	1.66547600
C	3.62922400	-5.26188800	-0.58475200
H	4.43431200	-5.75839300	-0.03718000
H	2.68149900	-5.61092200	-0.16057300
H	3.67051100	-5.58107700	-1.62792000
C	1.69147200	3.41060700	-1.11676800
C	1.34104000	4.30277600	-2.13431400
C	2.11447500	3.92415000	0.10917000
C	1.39972200	5.67794400	-1.92850900
H	1.02665800	3.92115400	-3.10270500
C	2.17478300	5.30070000	0.31732900
H	2.40947100	3.24666700	0.90528600

C	1.81407900	6.18241700	-0.69757200
H	1.12435100	6.35498600	-2.73110200
H	2.50633600	5.68261800	1.27774900
H	1.86025700	7.25415900	-0.53348900
H	1.56473600	1.34631100	1.77786800
H	-1.46088200	2.42065200	-0.78487100
TS3 <sub>2</sub> <sup>(R,S,S)</sup>			
P	-2.44083300	-0.13776500	0.46306200
C	-2.85103400	-1.37614800	1.73902900
C	-2.44272100	-1.02019000	3.17298100
H	-2.40611600	-2.32367300	1.41813900
H	-3.93635800	-1.51588100	1.67747000
C	-2.48270100	-2.24858900	4.08208900
H	-1.43345600	-0.58791300	3.19653400
H	-3.12051600	-0.25291400	3.56588500
C	-2.14123800	-1.90674100	5.52891200
H	-3.47857300	-2.70445600	4.02766800
H	-1.77652500	-2.99597500	3.69776600
H	-2.15818700	-2.79727300	6.16152200
H	-1.14360700	-1.46243000	5.59885100
H	-2.85686000	-1.18774200	5.93890500
C	-3.18203300	-0.79213400	-1.06917700
C	-4.70463300	-0.65182900	-1.15230700
H	-2.89405600	-1.84891500	-1.10301800
H	-2.68942800	-0.28137900	-1.89997500
C	-5.24318300	-1.36414800	-2.39381000
H	-5.18417500	-1.07865100	-0.26177000
H	-4.98642900	0.40710600	-1.18883800
C	-6.75907700	-1.24407700	-2.51620100
H	-4.75976800	-0.94388600	-3.28392400
H	-4.95028400	-2.42048000	-2.35178100
H	-7.12672400	-1.75729600	-3.40801900
H	-7.25660700	-1.68297600	-1.64573600
H	-7.06337900	-0.19493700	-2.58165200
C	-3.34403700	1.37484800	0.97205700
C	-2.62677300	2.27799900	1.98198800
H	-4.28149400	0.99842100	1.40147900
H	-3.60446500	1.93343600	0.06966300
C	-3.58527100	3.32034600	2.55755300
H	-2.19930300	1.68697500	2.79953000
H	-1.78350900	2.78542600	1.50116500
C	-2.88121400	4.28503800	3.50676600

H	-4.05051600	3.87654400	1.73409300
H	-4.40001000	2.80740500	3.08308500
H	-3.57846200	5.02088100	3.91420900
H	-2.42966400	3.74635900	4.34552000
H	-2.08055200	4.82678000	2.99277900
C	-0.64923900	0.02189300	0.38108100
C	-0.01791700	1.12984800	-0.12431900
C	0.19547700	-1.13571300	0.91513700
C	1.43241200	1.24978200	-0.14774400
C	-0.85256200	2.20165300	-0.77923400
O	-1.79551400	1.97168300	-1.51177300
O	-0.44387400	3.42207600	-0.45606400
C	-1.05585300	4.52366600	-1.15638600
C	-2.37029500	4.91773800	-0.51343200
H	-1.18820600	4.23709600	-2.20250400
H	-0.31820300	5.32420200	-1.09158800
H	-2.77486900	5.80201000	-1.01164600
H	-3.09916200	4.10861400	-0.60381800
H	-2.22516900	5.15472800	0.54431300
H	-0.38229100	-1.77441100	1.58648100
C	2.11731500	2.31602500	-0.90711400
C	1.79826800	2.57706500	-2.25086800
C	3.16926600	3.04611300	-0.33541200
C	2.47117900	3.55611200	-2.97343500
H	1.01647100	1.99270800	-2.73419300
C	3.85886900	4.01172500	-1.06401600
H	3.44088100	2.85183400	0.69994400
C	3.50757000	4.28098400	-2.38483500
H	2.19873200	3.74173100	-4.00828800
H	4.66865000	4.56166600	-0.59334200
H	4.04020000	5.03723400	-2.95210300
H	1.01526700	-0.73360600	1.52300700
C	0.80373000	-2.03934900	-0.18142200
H	1.41548200	-2.78394400	0.35292900
N	1.62206800	-1.23889900	-1.09839900
S	3.08153400	-1.81715400	-1.42931400
O	3.64042800	-1.00782000	-2.51685400
O	3.06372400	-3.27991900	-1.58173200
C	4.08529400	-1.48244900	0.01218300
C	4.29948100	-2.46977600	0.96735900
C	4.56193500	-0.18557500	0.20737200
C	4.99681700	-2.15139300	2.13200400
H	3.93534800	-3.47640800	0.78871700
C	5.25424900	0.11603700	1.37232100

H	4.39108700	0.57348500	-0.55109300
C	5.48082100	-0.86065200	2.35150500
H	5.16922700	-2.92018800	2.88001200
H	5.63148500	1.12414000	1.52601800
C	6.25164300	-0.51950000	3.60031800
H	5.90322300	0.42333100	4.03029400
H	6.15038500	-1.30176900	4.35524700
H	7.31688200	-0.40216000	3.37755800
C	-0.27659200	-2.81506700	-0.92930500
C	-1.02216400	-3.78901000	-0.25489300
C	-0.54719000	-2.57861600	-2.27730600
C	-2.03091600	-4.49568800	-0.90525400
H	-0.79929400	-4.01107300	0.78807800
C	-1.55120800	-3.28945300	-2.93414700
H	0.04303700	-1.83478200	-2.80092400
C	-2.30037900	-4.24465100	-2.25119500
H	-2.59524300	-5.25092500	-0.36710400
H	-1.75113100	-3.09214700	-3.98293900
H	-3.08203000	-4.79678500	-2.76342800
H	1.65282700	0.04080400	-0.74108500
H	1.89422800	1.04038200	0.82213200
M3 <sub>2</sub> <sup>(R,S,S)</sup>			
P	-2.35147600	0.08332300	0.44482900
C	-2.94067600	-0.98483600	1.81353900
C	-2.49528100	-0.57163700	3.21793700
H	-2.62509900	-2.00774000	1.58378000
H	-4.03477400	-0.98627900	1.74482400
C	-2.74258400	-1.67895000	4.24196800
H	-1.42951400	-0.30743800	3.21667600
H	-3.03897600	0.33133700	3.52273200
C	-2.34677900	-1.25768000	5.65396300
H	-3.80158200	-1.96368400	4.21885900
H	-2.17497200	-2.57041900	3.94496400
H	-2.51995900	-2.06080700	6.37434900
H	-1.28672500	-0.98876000	5.69650400
H	-2.92459500	-0.38569600	5.97552500
C	-3.27857700	-0.58563700	-0.99349600
C	-4.76533200	-0.23048400	-1.06797500
H	-3.15490400	-1.67383200	-0.93500300
H	-2.74799300	-0.24316600	-1.88594500
C	-5.45369000	-0.98422500	-2.20697100
H	-5.27266700	-0.47414800	-0.12471000

H	-4.88999900	0.84829900	-1.22094500
C	-6.93575600	-0.64052700	-2.32103300
H	-4.94131900	-0.75170500	-3.14862000
H	-5.32746400	-2.06224400	-2.04598100
H	-7.41116600	-1.18684300	-3.13954500
H	-7.46664700	-0.89025900	-1.39692400
H	-7.07440600	0.42930300	-2.50576600
C	-3.08983600	1.73059400	0.80073500
C	-2.29183500	2.63390500	1.74589500
H	-4.07752400	1.51380100	1.22905100
H	-3.26434700	2.23229800	-0.15514900
C	-3.12740400	3.82838000	2.20614400
H	-1.94928300	2.07071400	2.62123400
H	-1.38547600	2.99371000	1.24674700
C	-2.31856900	4.80383000	3.05591500
H	-3.53274900	4.34648800	1.32781400
H	-3.99252000	3.46410000	2.77429700
H	-2.92572000	5.65407900	3.37640000
H	-1.92840300	4.31045600	3.95164000
H	-1.46291500	5.19245800	2.49387400
C	-0.60929000	0.04416800	0.37311300
C	0.17095900	1.12633100	-0.15824100
C	0.09598900	-1.18784500	0.91243900
C	1.52663900	1.28946800	0.01834400
C	-0.55513800	2.13741400	-1.00956100
O	-1.46397500	1.86207400	-1.76991700
O	-0.12307300	3.38468800	-0.81597700
C	-0.65102800	4.40291100	-1.68303500
C	-1.93501100	4.97722300	-1.11826000
H	-0.80503300	3.97678300	-2.67693800
H	0.13782700	5.15549700	-1.73183300
H	-2.27673700	5.80865900	-1.73965100
H	-2.72026600	4.21717700	-1.09830500
H	-1.77234300	5.34843600	-0.10246200
H	-0.52073700	-1.71371800	1.64745500
C	2.44390700	2.17379400	-0.70574900
C	2.31791500	2.44885300	-2.07943700
C	3.55961800	2.70871900	-0.03820800
C	3.23657700	3.25658200	-2.73997600
H	1.50011500	1.99987900	-2.63960300
C	4.48859000	3.50313800	-0.70174600
H	3.68725000	2.49528700	1.02029300
C	4.32920500	3.78962000	-2.05680900
H	3.11202300	3.45051300	-3.80118600

H	5.33865400	3.90427300	-0.15737600
H	5.05371900	4.40740400	-2.57714500
H	1.00453300	-0.90934200	1.46178700
C	0.50731100	-2.23983900	-0.15129000
H	1.10835200	-3.00200700	0.36317700
N	1.34054700	-1.62717300	-1.19434400
S	2.86350400	-2.18256600	-1.45608300
O	3.38252800	-1.40515100	-2.57537900
O	2.77729400	-3.63704500	-1.52974700
C	3.83920400	-1.78467000	-0.02671600
C	3.91792100	-2.69074000	1.02882300
C	4.47435400	-0.54679100	0.03302100
C	4.63519700	-2.33722500	2.16638000
H	3.44852900	-3.66544000	0.94325200
C	5.18871000	-0.21299300	1.17812100
H	4.41310500	0.14070000	-0.80513300
C	5.27406000	-1.09620700	2.25965000
H	4.71083000	-3.04033700	2.99072000
H	5.69360900	0.74802500	1.22793900
C	6.02571400	-0.71472600	3.50739400
H	5.35001300	-0.25012500	4.23286400
H	6.46922200	-1.59161100	3.98407800
H	6.81984800	0.00182500	3.28778800
C	-0.68436400	-2.95391900	-0.77207300
C	-1.49127100	-3.76141900	0.03794900
C	-1.00137700	-2.83300500	-2.12473900
C	-2.60746400	-4.40827600	-0.48487900
H	-1.23752900	-3.89525200	1.08834300
C	-2.11312000	-3.48741400	-2.65392500
H	-0.37069000	-2.22222600	-2.76071300
C	-2.92457900	-4.26944300	-1.83647000
H	-3.22260600	-5.02918000	0.15880500
H	-2.34797200	-3.37850700	-3.70825100
H	-3.79208300	-4.77506900	-2.24864800
H	1.29247300	-0.60996000	-1.24994900
H	2.02020600	0.64054400	0.73903300
TS4 <sub>2</sub> <sup>(R,S,S)</sup>			
P	-1.70388300	1.23071700	-0.16165000
C	-2.88982100	1.05438700	1.21838600
C	-2.44319900	1.68490300	2.54250600
H	-3.09709100	-0.01366600	1.34296700
H	-3.82433200	1.51649000	0.88181600

C	-3.30549000	1.19448200	3.70554100
H	-1.38938000	1.45584900	2.75009900
H	-2.51642900	2.77733000	2.47209900
C	-2.91651700	1.84672000	5.02831800
H	-4.35943400	1.39956900	3.48122100
H	-3.21203800	0.10347700	3.77920100
H	-3.54005200	1.48460500	5.84930000
H	-1.87279900	1.63070300	5.27698400
H	-3.02847400	2.93409600	4.97454100
C	-2.54412300	0.63411600	-1.67416500
C	-4.06384300	0.79575400	-1.70663400
H	-2.26441300	-0.41953400	-1.77171700
H	-2.06178400	1.16037600	-2.50425700
C	-4.65063000	0.24293400	-3.00516000
H	-4.51200100	0.25424500	-0.86433500
H	-4.34543600	1.85199800	-1.59804200
C	-6.17021000	0.37093400	-3.05034000
H	-4.20263000	0.76500300	-3.85898400
H	-4.36265700	-0.81185700	-3.10017400
H	-6.57637200	-0.03196000	-3.98133000
H	-6.63099900	-0.17200900	-2.21875500
H	-6.47655000	1.41905100	-2.97488300
C	-1.51403800	3.04381600	-0.37535500
C	-0.51851200	3.77582700	0.53455000
H	-2.52679400	3.43593900	-0.21155900
H	-1.27596500	3.22089200	-1.42808600
C	-0.79032200	5.28033300	0.53743700
H	-0.56630900	3.39444900	1.56041400
H	0.50580200	3.60011900	0.19247000
C	0.25445600	6.05089400	1.33846300
H	-0.80987300	5.64334900	-0.49822600
H	-1.79059200	5.46416800	0.94920800
H	0.04211500	7.12269600	1.34276900
H	0.28019500	5.70724800	2.37719000
H	1.25405000	5.90599500	0.91607400
C	-0.19778200	0.29113300	0.13679000
C	1.09932900	0.98991900	-0.05374600
C	-0.30846000	-0.81495100	1.18794100
C	2.14634900	0.87846400	0.79714500
H	-0.23491800	-0.68408900	-0.83028800
C	1.18792200	1.73864300	-1.35212400
O	0.42303500	1.55187300	-2.27977600
O	2.12531700	2.68782100	-1.35889500
C	2.28331400	3.44981900	-2.56926900

C	1.34088700	4.63732500	-2.57308000
H	2.11005700	2.79651600	-3.42645500
H	3.32775400	3.76530700	-2.55750400
H	1.52572600	5.25670200	-3.45405500
H	0.30091000	4.30196700	-2.60255400
H	1.49430600	5.24993900	-1.68019300
H	-0.88733500	-0.56780500	2.08247800
H	0.70170400	-1.06598800	1.51892100
C	-0.87672900	-2.12913000	0.50180200
H	-0.33090000	-2.97377900	0.94542100
N	-0.57751300	-1.96245200	-0.90932600
S	0.28497800	-3.10151800	-1.63791800
O	0.70721700	-2.56535600	-2.93668200
O	-0.40766100	-4.39838600	-1.63395400
C	1.75596600	-3.33808700	-0.64490500
C	1.98242400	-4.54858300	-0.00044400
C	2.64140700	-2.27188600	-0.49029200
C	3.11091100	-4.69099600	0.80397400
H	1.27503000	-5.36019900	-0.13253300
C	3.76179900	-2.42596400	0.31652100
H	2.44795500	-1.32787500	-0.99257300
C	4.01218500	-3.63760300	0.97332900
H	3.29085200	-5.63456000	1.31170000
H	4.45123000	-1.59399700	0.44034600
C	5.24335400	-3.80205800	1.82537300
H	5.50073100	-2.86726900	2.32927500
H	5.10167200	-4.57755200	2.58118500
H	6.10155800	-4.09054200	1.20987300
C	-2.35463400	-2.34631000	0.78354000
C	-2.79150000	-2.43869700	2.11119300
C	-3.29941100	-2.43257200	-0.23793000
C	-4.14501300	-2.55481700	2.41075300
H	-2.06384600	-2.40657500	2.91978300
C	-4.65908400	-2.54511100	0.05914200
H	-2.95461600	-2.41837500	-1.26684500
C	-5.08764400	-2.59120900	1.38233000
H	-4.46582700	-2.61372600	3.44639500
H	-5.38193400	-2.59906700	-0.75018300
H	-6.14494000	-2.67128500	1.61329300
C	3.58053600	1.15351700	0.60310500
C	4.34752700	1.50285700	1.72331800
C	4.24330900	0.96903900	-0.62090000
C	5.72016400	1.70659200	1.61972400
H	3.85524500	1.61993600	2.68508300



C	5.61503900	1.16461600	-0.72448600
H	3.68348900	0.65098300	-1.49556200
C	6.35965400	1.54047300	0.39398100
H	6.29112600	1.98630700	2.49930800
H	6.10734700	1.00942700	-1.67919700
H	7.43150800	1.68821600	0.31139900
H	1.92684300	0.44471500	1.77065700

M4<sub>2</sub><sup>(R,S,S)</sup>

P	-1.06963000	-1.20306100	0.79484600
C	-2.00526900	-2.28689600	-0.33293400
C	-1.16711100	-3.06650400	-1.35575200
H	-2.74457500	-1.65514800	-0.83355000
H	-2.56311800	-2.98199800	0.30697200
C	-2.03386700	-3.58898800	-2.49912000
H	-0.36529900	-2.43824800	-1.77107000
H	-0.67366100	-3.91119300	-0.86144300
C	-1.23359700	-4.42255300	-3.49391900
H	-2.85729900	-4.18467400	-2.08153000
H	-2.49956900	-2.73699300	-3.01043000
H	-1.86382000	-4.78001900	-4.31181800
H	-0.41800600	-3.83326400	-3.92902100
H	-0.78912000	-5.29541200	-3.00413600
C	-2.22793900	-0.42893700	1.96962900
C	-3.42795800	-1.28886200	2.36413900
H	-2.54223400	0.50468900	1.48716200
H	-1.62427000	-0.14580100	2.83938900
C	-4.36606900	-0.53252300	3.30602600
H	-3.98966300	-1.56972300	1.46342400
H	-3.09902800	-2.21938700	2.84535000
C	-5.58531100	-1.36900100	3.68478200
H	-3.81712900	-0.23439200	4.20595600
H	-4.68678300	0.39491400	2.81493500
H	-6.25566400	-0.81529900	4.34851200
H	-6.15466000	-1.65255400	2.79215500
H	-5.28536500	-2.28918500	4.19584700
C	0.03099200	-2.30379100	1.76907200
C	1.28942300	-2.89605500	1.11682400
H	-0.64407700	-3.12182700	2.06342700
H	0.28883900	-1.75927900	2.68314000
C	1.79666900	-4.12087500	1.87830400
H	1.10350600	-3.16956000	0.07366400
H	2.09457000	-2.15492200	1.09020800

C	3.06080000	-4.68803100	1.23505000
H	1.99786600	-3.84257300	2.92149000
H	1.01182500	-4.88733100	1.90370800
H	3.43689800	-5.55007100	1.79274600
H	2.86135300	-5.00932500	0.20660000
H	3.85214500	-3.93206700	1.19812100
C	-0.25670700	0.19728800	-0.10826700
C	1.24491100	0.00939000	-0.13835400
C	-0.89479400	0.56412200	-1.46153000
C	1.87848600	-0.47103400	-1.21912600
H	-0.46908700	1.04094700	0.56115000
C	1.85529700	0.25759800	1.20883100
O	1.16041400	0.42715400	2.19510400
O	3.18211200	0.20068000	1.24829500
C	3.78990200	0.27344600	2.55456700
C	3.66548100	-1.04975500	3.28448600
H	3.32321100	1.08947200	3.11347600
H	4.83316300	0.52126000	2.35024200
H	4.20415300	-0.99503000	4.23572900
H	2.62013200	-1.27809200	3.49758900
H	4.09872900	-1.85727000	2.68954700
H	-1.09437900	-0.31026100	-2.08878900
H	-0.12895800	1.15080700	-1.98053000
C	-2.17210000	1.47199200	-1.36276500
H	-2.16269000	2.05976600	-2.29558700
N	-2.15506100	2.33724300	-0.20355400
S	-1.50337200	3.75265300	-0.39162900
O	-1.91526500	4.62219200	0.72439700
O	-1.66837500	4.31538900	-1.75215100
C	0.28550000	3.62114000	-0.19962800
C	1.11944300	3.62333300	-1.31441100
C	0.83090900	3.48720400	1.07827700
C	2.49963700	3.50663200	-1.14670100
H	0.68160700	3.74338000	-2.30036600
C	2.20697600	3.38405300	1.23200400
H	0.17319600	3.48687600	1.94431000
C	3.06244400	3.39377100	0.12529800
H	3.14747000	3.52061000	-2.01966000
H	2.62775400	3.29984200	2.23321300
C	4.55327100	3.30115300	0.32295000
H	4.82534400	2.33832700	0.77054500
H	5.08774300	3.39398100	-0.62649700
H	4.90961500	4.08720600	0.99294100
C	-3.46287600	0.65960500	-1.40562700

C	-3.73796000	-0.15251800	-2.51324300
C	-4.39873100	0.70565100	-0.37032200
C	-4.88224900	-0.94389400	-2.55823500
H	-3.04403700	-0.16712500	-3.35190600
C	-5.54287200	-0.09248100	-0.40819200
H	-4.21826600	1.38930800	0.45050800
C	-5.78382000	-0.93056600	-1.49317600
H	-5.07229500	-1.56981800	-3.42508400
H	-6.25328800	-0.04801100	0.41304100
H	-6.67324200	-1.55164900	-1.51932600
C	3.30638700	-0.79682000	-1.42855800
C	3.64953100	-2.10279000	-1.79050200
C	4.30991800	0.17235700	-1.33602900
C	4.98155000	-2.44600600	-2.00923500
H	2.86831700	-2.85430600	-1.89538200
C	5.63657200	-0.16616000	-1.57375600
H	4.03227600	1.18784600	-1.07787900
C	5.97828000	-1.47715700	-1.90030300
H	5.23729400	-3.46747900	-2.26939200
H	6.40760600	0.59586500	-1.50064300
H	7.01522000	-1.74181200	-2.08020200
H	1.24359200	-0.71377500	-2.07108800

M4<sub>2</sub><sup>r(R,S,S)</sup>

P	-2.19970400	-0.80390800	-0.88349800
C	-1.58218700	-1.24742000	-2.53906300
C	-0.26596500	-2.03284300	-2.55684600
H	-1.48876200	-0.31418400	-3.10471100
H	-2.37248000	-1.83308700	-3.02174200
C	0.31304800	-2.11405400	-3.96856700
H	0.48070500	-1.57168500	-1.89387700
H	-0.44503500	-3.04660500	-2.17877100
C	1.46856900	-3.10577400	-4.03887900
H	-0.47643500	-2.40673700	-4.67127700
H	0.64824900	-1.11344800	-4.26887300
H	1.96510800	-3.07778600	-5.01252900
H	2.21444800	-2.87729800	-3.27197000
H	1.11448700	-4.12677400	-3.86717400
C	-3.87930600	-0.12637100	-1.05776500
C	-4.91107700	-1.05722000	-1.69885600
H	-3.77852700	0.80569700	-1.62872700
H	-4.17853400	0.15202900	-0.03934100
C	-6.29186300	-0.40218000	-1.75139100

H	-4.60213700	-1.32343000	-2.71644700
H	-4.97884500	-1.99206100	-1.12919800
C	-7.33468400	-1.31617900	-2.38752500
H	-6.59947900	-0.13398200	-0.73394900
H	-6.22271100	0.53564500	-2.31509900
H	-8.31514600	-0.83518700	-2.41817800
H	-7.05411600	-1.57415700	-3.41328300
H	-7.43371300	-2.24820800	-1.82278700
C	-2.33320800	-2.34044900	0.10371500
C	-1.06354900	-2.97806200	0.69429600
H	-2.80239200	-3.04741500	-0.59387600
H	-3.06388000	-2.13570000	0.89342000
C	-1.30662400	-4.43641900	1.07953100
H	-0.22694500	-2.92369000	-0.01021000
H	-0.73949500	-2.43644600	1.58650600
C	-0.05796200	-5.06379300	1.69302900
H	-2.14128000	-4.48787900	1.79011400
H	-1.61423800	-5.00356000	0.19254500
H	-0.23691800	-6.10021200	1.98834100
H	0.77229900	-5.05301900	0.97963900
H	0.26271400	-4.50842600	2.58036700
C	-1.20512700	0.57774100	-0.15500200
C	-0.33880700	0.10306900	0.98906400
C	-0.53510200	1.42702400	-1.24393300
C	0.96290100	-0.17339200	0.82618700
C	-1.14414100	-0.13380000	2.22154300
O	-2.36255100	-0.05975700	2.21009900
O	-0.44439100	-0.49106500	3.29197100
C	-1.19899300	-0.85091300	4.46762500
C	-1.75556500	-2.25607800	4.34051100
H	-1.99158900	-0.11498000	4.61528200
H	-0.47613300	-0.77622900	5.28029400
H	-2.26372500	-2.53759100	5.26589100
H	-2.47724000	-2.31113000	3.52136700
H	-0.94915500	-2.97145800	4.15782100
H	-1.28693000	1.63441300	-2.01656300
C	1.96441900	-0.64209000	1.80582900
C	2.35022500	0.14804300	2.89221300
C	2.61597600	-1.85689700	1.57282700
C	3.36111500	-0.28397900	3.74432600
H	1.86087000	1.10381500	3.05048900
C	3.61147200	-2.29869600	2.43984900
H	2.34462600	-2.45252500	0.70392200
C	3.98816300	-1.51025500	3.52500400

H	3.66240500	0.33859500	4.58049200
H	4.10145300	-3.25029300	2.25975000
H	4.77427600	-1.84585600	4.19368400
H	0.28531200	0.89236800	-1.73770100
C	-0.01139500	2.81132200	-0.73674300
H	0.10105000	3.41840200	-1.64766600
N	1.22999500	2.75170900	0.00535800
S	2.55370600	3.01273200	-0.78766200
O	3.59567100	3.49486200	0.13927600
O	2.37956200	3.80128200	-2.03262500
C	3.21710600	1.43917700	-1.36804000
C	2.89512600	0.95893600	-2.63491800
C	4.00702900	0.67026400	-0.51365700
C	3.38069800	-0.28080200	-3.05170800
H	2.29639400	1.57397000	-3.30048900
C	4.48548000	-0.56388500	-0.93785500
H	4.25207800	1.05203500	0.47275500
C	4.18909500	-1.05514300	-2.21399700
H	3.15281300	-0.63983500	-4.05295500
H	5.10924000	-1.15444100	-0.27116200
C	4.76064600	-2.37541900	-2.66564600
H	5.84332300	-2.40035400	-2.51352600
H	4.33478000	-3.20748300	-2.09423100
H	4.56003500	-2.55563700	-3.72412000
C	-1.10952300	3.44860000	0.10227000
C	-2.25993800	3.94680600	-0.51638500
C	-1.03986200	3.45450000	1.49657900
C	-3.32113600	4.43734500	0.24041600
H	-2.32104100	3.95737900	-1.60299400
C	-2.10213700	3.94033800	2.25678700
H	-0.13593900	3.07653600	1.96403700
C	-3.24658600	4.43132200	1.63235400
H	-4.20367600	4.83000800	-0.25559700
H	-2.03492600	3.93753700	3.34066900
H	-4.07269800	4.81202100	2.22464900
H	-1.99732500	1.18934000	0.29071100
H	1.36676800	-0.04489300	-0.17902200

TS5<sub>2</sub><sup>(R,S,S)</sup>

P	-2.41456200	-0.98764800	-0.46535000
C	-1.97232500	-2.23955300	-1.71827000
C	-0.72500700	-3.06592700	-1.38468700
H	-1.84692700	-1.70382300	-2.66654700

H	-2.83623900	-2.90266100	-1.83846700
C	-0.26275400	-3.90023600	-2.57826700
H	0.10596800	-2.41933800	-1.06664800
H	-0.94876800	-3.72746100	-0.53869400
C	0.82930500	-4.88701500	-2.17979200
H	-1.11934800	-4.43686900	-3.00362300
H	0.10355900	-3.22275900	-3.36002800
H	1.24190100	-5.40489700	-3.04968300
H	1.64821600	-4.36432600	-1.67665000
H	0.43945400	-5.64071500	-1.48896000
C	-4.10909800	-0.41960000	-0.81045700
C	-5.20880900	-1.47135900	-0.64943300
H	-4.09737600	-0.01534200	-1.83048400
H	-4.26216400	0.42235200	-0.12423800
C	-6.58117700	-0.90747300	-1.01860900
H	-5.00024200	-2.34448000	-1.28015900
H	-5.23368500	-1.82702100	0.38736200
C	-7.69085600	-1.94015200	-0.84405300
H	-6.78698200	-0.02823500	-0.39688800
H	-6.55693100	-0.55697000	-2.05726200
H	-8.66432300	-1.52527500	-1.11610500
H	-7.51019700	-2.81692700	-1.47370100
H	-7.74762300	-2.28006700	0.19453300
C	-2.45723300	-1.80280000	1.17317200
C	-1.13972300	-2.09361700	1.91048900
H	-2.99210700	-2.74345200	0.98224800
H	-3.10539500	-1.17425300	1.79250400
C	-1.34235000	-3.13642600	3.00847000
H	-0.36606800	-2.44386300	1.21747600
H	-0.75199500	-1.17536900	2.35870100
C	-0.04892100	-3.39906000	3.77479800
H	-2.12108700	-2.78517200	3.69748300
H	-1.71343800	-4.06970000	2.56647800
H	-0.19833100	-4.12805200	4.57480900
H	0.72638400	-3.78726900	3.10572700
H	0.33261600	-2.47533100	4.22250700
C	-1.32074000	0.50282200	-0.61086100
C	-0.50647300	0.76033700	0.62604400
C	-0.46454200	0.55105000	-1.88362200
C	0.86084900	0.52464900	0.55254700
C	-1.28257300	1.25386200	1.72551900
O	-2.51987100	1.25257800	1.70842900
O	-0.59365500	1.64741600	2.81807100
C	-1.35597300	1.84646900	4.01322600

C	-1.68767700	0.51349400	4.66038700
H	-2.26046500	2.41222300	3.78083500
H	-0.71028900	2.44784600	4.65573700
H	-2.19696900	0.66669200	5.61525100
H	-2.34320200	-0.06934800	4.00699200
H	-0.77002000	-0.05432100	4.84071000
H	-1.11160200	0.57524300	-2.76784500
C	1.79498500	0.67043700	1.70131800
C	2.27353200	1.90764900	2.13023700
C	2.19564600	-0.49051200	2.36789500
C	3.12826700	1.98328600	3.22453000
H	1.98983000	2.79613400	1.57745100
C	3.03947100	-0.41471400	3.47359500
H	1.84733800	-1.45861900	2.01403600
C	3.50792100	0.82494700	3.90294700
H	3.50401500	2.94856800	3.54892700
H	3.33812400	-1.32233100	3.98928600
H	4.17427800	0.88814400	4.75753800
H	0.18073000	-0.32977100	-1.98583400
C	0.42640000	1.82802100	-1.90520000
H	0.87830000	1.86347000	-2.90373000
N	1.48589400	1.81566000	-0.88978800
S	2.99473100	1.67832200	-1.42509700
O	3.90413800	2.28554400	-0.44729700
O	3.12532000	2.11417800	-2.82900300
C	3.40657300	-0.06544800	-1.43513300
C	2.97644400	-0.86515000	-2.49184500
C	4.10542500	-0.61926600	-0.36564900
C	3.26396200	-2.22776800	-2.48043700
H	2.45221500	-0.41449900	-3.33015000
C	4.38540200	-1.98176700	-0.36686700
H	4.42797300	0.02250900	0.44769400
C	3.97846300	-2.80284500	-1.42365600
H	2.94958200	-2.85112500	-3.31397200
H	4.94066300	-2.41508700	0.46127900
C	4.32846900	-4.26913400	-1.42111600
H	5.40761900	-4.40784700	-1.31021900
H	3.84655100	-4.78724200	-0.58580200
H	4.01398800	-4.75469700	-2.34740700
C	-0.45613900	3.06363100	-1.77605700
C	-1.24931300	3.44941300	-2.86102300
C	-0.53892700	3.79422700	-0.59003700
C	-2.11210000	4.53739300	-2.76447900
H	-1.18284000	2.89572000	-3.79555200

C	-1.40581300	4.88118000	-0.48871400
H	0.08317500	3.49884300	0.24857900
C	-2.19535500	5.25605700	-1.57315600
H	-2.71447300	4.82729500	-3.61994300
H	-1.46121700	5.43894300	0.44123000
H	-2.86648400	6.10544700	-1.49408600
H	-2.06650800	1.30575800	-0.68871700
H	1.16140400	-0.29105600	-0.10777500

M5<sub>2</sub><sup>(R,S,S)</sup>

P	2.53929200	0.17046600	-0.43519300
C	2.72213400	1.70393500	-1.42874900
C	1.95413000	2.94606900	-0.96832700
H	2.46273700	1.45266300	-2.46362200
H	3.79629300	1.92841100	-1.42724200
C	2.27848400	4.14196400	-1.86463400
H	0.86970900	2.76821500	-0.97468800
H	2.22473700	3.19167800	0.06648800
C	1.53777700	5.40322000	-1.43688100
H	3.36114300	4.31649000	-1.84550800
H	2.02135600	3.89324300	-2.90140000
H	1.79487900	6.25403500	-2.07253400
H	0.45714000	5.24788000	-1.49809300
H	1.77931100	5.66856400	-0.40236800
C	4.00399200	-0.81899800	-0.88541000
C	5.32159100	-0.34450400	-0.26841800
H	4.05940300	-0.79824400	-1.98169400
H	3.76703300	-1.83832900	-0.56860100
C	6.50270400	-1.17882300	-0.76522900
H	5.50684900	0.71231200	-0.50206000
H	5.26366400	-0.42016400	0.82393900
C	7.82221100	-0.74096700	-0.13685400
H	6.31274500	-2.23464900	-0.53935700
H	6.56466100	-1.09942300	-1.85727700
H	8.65574400	-1.34714100	-0.49990800
H	8.03894800	0.30557300	-0.37283300
H	7.78551800	-0.83719800	0.95260400
C	2.66767100	0.67695000	1.31374700
C	1.38204700	1.17336600	1.99279800
H	3.43342600	1.46459900	1.32485800
H	3.06633700	-0.19273400	1.84185400
C	1.70162400	1.96910700	3.25722300
H	0.78690500	1.79884700	1.31332400



H	0.75748300	0.31244100	2.25118000
C	0.43933300	2.33831500	4.03063400
H	2.36606600	1.37344400	3.89627200
H	2.25933000	2.87503600	2.98721300
H	0.66795900	2.96128400	4.89886600
H	-0.26109700	2.88990600	3.39327200
H	-0.07152000	1.43781100	4.38764100
C	1.01458900	-0.80801400	-0.92761400
C	0.16837900	-1.27417200	0.21588900
C	0.17522800	-0.09320600	-1.98850500
C	-1.17356000	-0.61239800	0.38109600
C	0.88555600	-2.04617600	1.12677600
O	2.11993500	-2.27027300	1.00088600
O	0.22062900	-2.56781600	2.21021100
C	1.02281300	-3.01781600	3.29280400
C	1.47112300	-1.84992300	4.15689300
H	1.88189600	-3.57910100	2.91844700
H	0.37781000	-3.69176100	3.86310000
H	1.99769200	-2.20095800	5.04882500
H	2.14686500	-1.20254700	3.59016900
H	0.60215700	-1.26134300	4.46814600
H	0.69704300	-0.02655200	-2.94746200
C	-1.98841900	-1.15325900	1.53704800
C	-2.60046000	-2.40402500	1.45841300
C	-2.08864500	-0.41725600	2.71300800
C	-3.29172600	-2.91480800	2.54837900
H	-2.51263900	-2.97435300	0.53786500
C	-2.77248000	-0.93106500	3.81539800
H	-1.61775400	0.56229700	2.77280800
C	-3.37514100	-2.18209900	3.73495400
H	-3.76411800	-3.89019600	2.48003100
H	-2.83695900	-0.35012900	4.73084300
H	-3.91312900	-2.58489400	4.58758500
H	-0.06577000	0.93393600	-1.68969300
C	-1.15813900	-0.83008200	-2.15722100
H	-1.71692700	-0.32575000	-2.94990200
N	-1.95781000	-0.70254500	-0.91636300
S	-3.31141300	0.26396100	-1.03177300
O	-4.20717400	-0.07100900	0.06599900
O	-3.79680300	0.15273800	-2.40649800
C	-2.80464300	1.95295000	-0.77457500
C	-2.43052100	2.73374600	-1.86378500
C	-2.80305100	2.47121400	0.52075300
C	-2.06609000	4.06116000	-1.64887900

H	-2.46307300	2.31973000	-2.86675100
C	-2.42712800	3.79340700	0.71665900
H	-3.12100200	1.84655500	1.35009600
C	-2.06604600	4.60985000	-0.36278300
H	-1.80127100	4.68567100	-2.49752700
H	-2.43952900	4.21058600	1.71994700
C	-1.71760000	6.05579700	-0.12536500
H	-2.53318500	6.56497800	0.39549200
H	-0.82412900	6.14283600	0.50056100
H	-1.52920200	6.58099500	-1.06381400
C	-1.04203400	-2.29098000	-2.57686700
C	0.03351600	-2.74674700	-3.34374700
C	-2.07815000	-3.18264000	-2.28629400
C	0.08674700	-4.06845900	-3.78348300
H	0.84275900	-2.07358800	-3.61036600
C	-2.02843000	-4.50143600	-2.72705300
H	-2.92626500	-2.83163000	-1.70766400
C	-0.94161900	-4.95276900	-3.47332500
H	0.93658000	-4.40319400	-4.37007400
H	-2.84263700	-5.17813900	-2.48685800
H	-0.89964300	-5.98249000	-3.81328400
H	1.50431400	-1.67897500	-1.38777300
H	-1.02802500	0.46924200	0.57209800

TS6<sub>2</sub><sup>(R,S,S)</sup>

P	2.64690500	-0.32574900	-0.51702100
C	3.36439100	1.09416000	-1.45844000
C	2.81692700	2.46737400	-1.06742800
H	3.16682300	0.89710700	-2.51961400
H	4.45383700	1.08669000	-1.32775000
C	3.42867500	3.57163300	-1.92997100
H	1.72088800	2.49089900	-1.16027600
H	3.04337800	2.66950000	-0.01191800
C	2.92394000	4.95849000	-1.55039500
H	4.52083300	3.53145600	-1.83540800
H	3.20138200	3.36871400	-2.98370000
H	3.37508200	5.73559100	-2.17265000
H	1.83843700	5.01525300	-1.67203700
H	3.15434000	5.18686400	-0.50454000
C	3.77878700	-1.72077700	-0.91432300
C	5.24059100	-1.57317200	-0.49038600
H	3.70986200	-1.87313600	-1.99993000
H	3.32296500	-2.59483300	-0.43497000

C	6.07286400	-2.79873500	-0.87066700
H	5.68699600	-0.68444900	-0.95359500
H	5.30005900	-1.42373600	0.59517100
C	7.53309900	-2.65924700	-0.45032800
H	5.63317400	-3.68929100	-0.40559800
H	6.01059300	-2.95201500	-1.95508800
H	8.11579300	-3.54069300	-0.72947800
H	7.99353800	-1.78709400	-0.92522200
H	7.61614500	-2.53063600	0.63346300
C	2.96363600	0.06189300	1.25786700
C	1.80514500	0.77127000	1.97431400
H	3.87853000	0.66697400	1.32002100
H	3.16587000	-0.89979500	1.74255800
C	2.24246800	1.33989900	3.32343600
H	1.40179100	1.58498300	1.35416900
H	0.98018900	0.06454000	2.13090900
C	1.08589200	1.96722000	4.09576200
H	2.69421500	0.53715400	3.92066400
H	3.03143600	2.08487000	3.15850500
H	1.42719700	2.42791400	5.02624000
H	0.59067900	2.74094300	3.49785900
H	0.33505900	1.21208500	4.35139500
C	0.58663100	-1.23737700	-0.97529200
C	-0.22606500	-1.36251800	0.16017800
C	0.02376700	-0.39300500	-2.09649700
C	-1.30792000	-0.31583100	0.34024500
C	0.31282000	-2.23944300	1.16519300
O	1.42520700	-2.77054700	1.06170500
O	-0.44492100	-2.43794800	2.26872500
C	0.17488300	-3.10461700	3.36847300
C	1.06942000	-2.14749300	4.13709500
H	0.73716200	-3.96904400	3.00857200
H	-0.65741200	-3.44715300	3.98723400
H	1.47369900	-2.62960500	5.03106700
H	1.90331700	-1.82737900	3.50612200
H	0.49781800	-1.26500200	4.44192000
H	0.52384500	-0.58650400	-3.04905900
C	-2.20142700	-0.54324700	1.54064200
C	-3.16108900	-1.55477500	1.53446000
C	-2.01160000	0.21694000	2.68924900
C	-3.90826200	-1.81186400	2.67597200
H	-3.30432500	-2.13984800	0.62948300
C	-2.75383800	-0.04373000	3.84116200
H	-1.26553000	1.00944300	2.68728600

C	-3.70161000	-1.06210400	3.83647300
H	-4.65236000	-2.60270700	2.66856500
H	-2.59215500	0.55031900	4.73596700
H	-4.28431300	-1.26963400	4.72854200
H	0.14746100	0.67501800	-1.88316700
C	-1.48485200	-0.65174800	-2.18833800
H	-1.89072400	-0.02524400	-2.98608000
N	-2.12474900	-0.21120900	-0.92648700
S	-3.15517600	1.09672900	-1.03743000
O	-4.10794900	1.02428400	0.06091700
O	-3.65631400	1.12006000	-2.40999800
C	-2.19699700	2.57516900	-0.78067600
C	-1.60916800	3.21490600	-1.86749200
C	-2.07602500	3.08342400	0.51244800
C	-0.90601200	4.39778500	-1.65070100
H	-1.73615500	2.81589700	-2.86902100
C	-1.35964600	4.25603700	0.71038900
H	-2.56552600	2.57533300	1.33744500
C	-0.77799800	4.93677900	-0.36641800
H	-0.47274700	4.92337600	-2.49710200
H	-1.27334000	4.66918100	1.71158600
C	-0.05653800	6.23715700	-0.12833300
H	-0.68070700	6.92016900	0.45403700
H	0.86533300	6.07120800	0.43767600
H	0.20629100	6.72674100	-1.06819900
C	-1.87867200	-2.08922400	-2.50894300
C	-1.00929500	-2.96708500	-3.15979300
C	-3.17453000	-2.52550000	-2.21920800
C	-1.41880800	-4.25672500	-3.49504400
H	0.00066000	-2.65737100	-3.41020300
C	-3.58566500	-3.81223700	-2.55341300
H	-3.86081200	-1.84798800	-1.72011000
C	-2.70687700	-4.68589400	-3.19046500
H	-0.72417800	-4.92690500	-3.99175100
H	-4.59527600	-4.13214100	-2.31506200
H	-3.02362100	-5.69138400	-3.44794700
H	1.12107000	-2.14091200	-1.26424800
H	-0.80852100	0.66376200	0.48125300
$P_2^{(R,R)}$			
S	1.48402900	-1.28187600	1.52075800
O	1.19977900	-0.52624700	2.73665500
O	1.59825400	-2.73486900	1.56691800

O	-0.41039700	3.29617200	-1.82586500
O	-0.71815900	3.08652200	0.39529100
N	0.25705800	-0.94017200	0.46118000
C	3.88249400	-1.52370700	0.21129000
H	3.69397600	-2.59165200	0.23914400
C	5.00855000	-1.00364600	-0.41563500
H	5.71882000	-1.67837600	-0.88472100
C	5.24407600	0.37548400	-0.44906500
C	4.33010000	1.22992600	0.17609500
H	4.50897400	2.30081600	0.16953000
C	3.20025600	0.72954000	0.81221200
H	2.50405800	1.39995300	1.30752500
C	2.98595800	-0.64717300	0.81813900
C	0.26000000	-1.63895700	-0.84417900
H	0.80301000	-2.57563400	-0.68658500
C	0.98923400	-0.79524300	-1.89273200
H	0.83035500	-1.20468100	-2.89422600
H	2.07233100	-0.84569500	-1.72123400
C	0.56566200	0.63923300	-1.83237700
H	0.78057700	1.28454200	-2.68063200
C	-0.03904900	1.17568000	-0.76804400
C	-0.35099900	0.40576700	0.49497200
H	0.10505900	0.93721600	1.33533300
C	-1.84122600	0.30101700	0.82288900
C	-2.19611000	-0.20683100	2.07415300
H	-1.40913500	-0.49970800	2.76566000
C	-3.53403000	-0.35255700	2.42174000
H	-3.79939600	-0.75020900	3.39644400
C	-4.53308900	0.01260900	1.51968300
H	-5.57859000	-0.10387600	1.78712800
C	-4.18343100	0.52517400	0.27418800
H	-4.95462400	0.80507200	-0.43691900
C	-2.84107300	0.67219800	-0.07220400
H	-2.57936300	1.05116100	-1.05727300
C	-1.18040500	-1.99445800	-1.19740500
C	-1.90858800	-2.74987800	-0.27306100
H	-1.42424100	-3.05287900	0.65219400
C	-3.23744600	-3.07272000	-0.51084300
H	-3.79356200	-3.64737300	0.22308100
C	-3.85762800	-2.65130400	-1.68834100
H	-4.89793200	-2.89800300	-1.87556100
C	-3.13684300	-1.91235000	-2.61838300
H	-3.61056800	-1.57869600	-3.53628400
C	-1.80270100	-1.58338000	-2.37338700

H	-1.26843600	-0.98272200	-3.10235800
C	-0.40194900	2.62094100	-0.81902900
C	6.45763300	0.92111500	-1.15320900
H	6.61577800	1.97417700	-0.91366900
H	7.35458400	0.36231000	-0.87412800
H	6.34214500	0.83409900	-2.23815000
C	-1.21863800	4.43560600	0.45749700
H	-1.08438300	4.72887300	1.49906000
H	-0.60164400	5.07055300	-0.18140000
C	-2.67806700	4.47432600	0.04666100
H	-2.78644900	4.18625400	-1.00151000
H	-3.26392300	3.78924200	0.66424300
H	-3.07325200	5.48535200	0.17115600
$P_2^{(R,S)}$			
C	-1.87825200	0.32772400	-2.11310700
C	-1.55854400	0.97594300	-0.99185500
C	-1.50550200	-1.10609500	-2.32600700
C	-0.69206800	0.39588100	0.10593100
C	-2.01141100	2.38846500	-0.83484700
O	-2.46071300	3.07030100	-1.73006900
O	-1.87148600	2.81021700	0.42707700
C	-2.12328700	4.20615300	0.67248300
C	-0.92957900	5.03700900	0.24082000
H	-3.03242100	4.49944600	0.14369500
H	-2.29244400	4.26936900	1.74794300
H	-1.09747500	6.08763200	0.48989100
H	-0.78191600	4.95528900	-0.83829000
H	-0.02471000	4.69347000	0.74876800
H	-2.24969600	-1.60314900	-2.95068300
C	0.60041100	1.20378500	0.19366900
C	0.95223400	1.85293100	1.37393300
C	1.44050900	1.29115500	-0.91779800
C	2.14069800	2.57868300	1.44831100
H	0.29549400	1.78081600	2.23653900
C	2.63044800	2.00562300	-0.84353700
H	1.16587300	0.77318300	-1.83402600
C	2.98120900	2.65349500	0.34116800
H	2.41047000	3.07980100	2.37266500
H	3.28699200	2.05436300	-1.70687800
H	3.91137100	3.21009100	0.40046900
H	-0.55155800	-1.17258000	-2.86391800
C	-1.36147500	-1.81585300	-0.97540600

H	-0.89452300	-2.78935600	-1.14174400
N	-0.39854300	-1.02533900	-0.18755000
S	0.56328800	-1.82219600	0.91866400
O	0.36837700	-1.23021900	2.24054700
O	0.31989600	-3.24969500	0.72684800
C	2.22448500	-1.46834700	0.40480300
C	2.63216600	-1.87059000	-0.86485000
C	3.07584400	-0.78646000	1.26333000
C	3.91770200	-1.55758700	-1.28296900
H	1.94924300	-2.40625600	-1.51835200
C	4.36099500	-0.48333200	0.82622600
H	2.72330400	-0.47811000	2.24118500
C	4.79402400	-0.85104300	-0.44935700
H	4.24836500	-1.85946400	-2.27244900
H	5.03203200	0.06388300	1.48229100
C	6.16364600	-0.45731000	-0.93467000
H	6.12928800	0.53580600	-1.39578500
H	6.53730600	-1.15825000	-1.68405000
H	6.87836600	-0.41355400	-0.11001700
C	-2.69796800	-2.04516900	-0.27019800
C	-3.78190800	-2.56947200	-0.98352300
C	-2.85883100	-1.80277300	1.09544600
C	-4.99672900	-2.82316100	-0.35479400
H	-3.68169200	-2.79908900	-2.03990600
C	-4.07669600	-2.05296000	1.72633400
H	-2.03089600	-1.42468200	1.68676900
C	-5.15197300	-2.55876700	1.00428200
H	-5.82291100	-3.23053900	-0.92900600
H	-4.17890400	-1.85217400	2.78805100
H	-6.10037100	-2.75192000	1.49488200
H	-1.21569200	0.49036500	1.06492400
H	-2.44173400	0.85885500	-2.87504500
TS2 <sub>2</sub> <sup>(S,R)</sup>			
P	1.41108200	0.61756400	-1.04973300
C	3.17789900	0.98853800	-0.75997000
C	3.49587000	2.38028900	-0.20348800
H	3.58819600	0.19886200	-0.11936600
H	3.65033000	0.86022200	-1.74319500
C	4.95923500	2.48032900	0.22689500
H	2.85073600	2.60893200	0.65371900
H	3.28515000	3.14312400	-0.96356400
C	5.31888600	3.87045600	0.74110200

H	5.60234100	2.21519900	-0.62138200
H	5.14884500	1.72929700	1.00475600
H	6.36556000	3.92120000	1.05089000
H	4.69959700	4.13985700	1.60224400
H	5.15992700	4.62652200	-0.03392900
C	1.44729000	-0.95620600	-1.98268000
C	1.18819700	-0.82041900	-3.48356200
H	2.44080900	-1.37996100	-1.80599100
H	0.70784800	-1.60894300	-1.51065500
C	1.31489700	-2.17386500	-4.18260700
H	1.89864100	-0.11266800	-3.93215500
H	0.18212600	-0.42062200	-3.64024200
C	1.05495600	-2.07361600	-5.68289200
H	0.60512800	-2.87559100	-3.72675400
H	2.31636400	-2.58450900	-4.00428100
H	1.14502600	-3.04846200	-6.16841900
H	1.76940200	-1.39355300	-6.15724200
H	0.04885300	-1.69020700	-5.87881000
C	0.82807000	2.04907300	-2.04131800
C	0.10180300	3.12082800	-1.22219300
H	1.72311200	2.46864100	-2.51606900
H	0.17263900	1.67004600	-2.82582300
C	-0.27149600	4.32451700	-2.08476700
H	0.72060100	3.45085900	-0.37692600
H	-0.80718300	2.69674700	-0.78019300
C	-1.07176300	5.35767700	-1.29726000
H	-0.85673500	3.97981800	-2.94689200
H	0.63979600	4.78086400	-2.49111100
H	-1.34510100	6.21239100	-1.92137000
H	-0.49567200	5.72950700	-0.44391300
H	-1.99034700	4.91452100	-0.89784600
C	0.57557100	0.48879600	0.57892200
C	-0.80920300	0.35603300	0.64711300
C	1.42772500	0.42233700	1.68600900
C	-1.57570900	0.62776900	1.92563700
H	-0.97191200	0.37085900	2.79564300
C	-1.58282800	0.21388500	-0.56614900
O	-1.11279500	0.08836200	-1.69929800
O	-2.91133700	0.24824500	-0.36247400
C	-3.73001300	0.36708200	-1.53075700
C	-3.71062800	1.79664900	-2.04300300
H	-3.38040300	-0.33723000	-2.29007800
H	-4.72748200	0.06776000	-1.20047000
H	-4.39750300	1.90732200	-2.88592400



H	-2.70331300	2.06088900	-2.37759600
H	-4.01016700	2.48745400	-1.24985400
H	2.46717200	0.70797900	1.61541400
C	-2.00726300	2.08207300	1.98105700
C	-3.33791800	2.45098300	1.77314800
C	-1.06357200	3.09159300	2.20840300
C	-3.72022000	3.79254700	1.79305600
H	-4.07596900	1.67569800	1.58590500
C	-1.44065500	4.43033100	2.23215200
H	-0.02144300	2.81892300	2.36005100
C	-2.77338700	4.78675600	2.02452200
H	-4.76040600	4.05861600	1.62950800
H	-0.69435600	5.19873500	2.41157500
H	-3.06876400	5.83129400	2.04057000
H	0.99607600	0.52760100	2.67468300
C	1.65394000	-1.82549300	1.90231700
H	1.54656600	-1.64034000	2.97293300
N	0.70005100	-2.45806300	1.23397900
S	-0.59357700	-2.92407100	2.11843100
O	-0.45907100	-4.35553000	2.43444700
O	-0.85775400	-2.04512700	3.26914500
C	-1.94944900	-2.77813900	0.97823400
C	-3.21057200	-2.51443100	1.49976300
C	-1.77396700	-3.03961700	-0.37952300
C	-4.31095700	-2.50865700	0.64596700
H	-3.32323300	-2.30794300	2.55946800
C	-2.88042200	-3.01935000	-1.21789000
H	-0.78120200	-3.24390100	-0.76718900
C	-4.16404400	-2.76504100	-0.71784600
H	-5.29823500	-2.29839800	1.04790600
H	-2.74872000	-3.20679800	-2.28053900
C	-5.35556500	-2.77847600	-1.63980000
H	-5.13455400	-2.25716300	-2.57548000
H	-6.22150900	-2.30152700	-1.17527100
H	-5.63506500	-3.80536400	-1.89616200
C	3.04785700	-1.90439700	1.40282500
C	4.08385500	-1.27380800	2.10582900
C	3.35630900	-2.62703200	0.24712700
C	5.38876700	-1.31645200	1.63043700
H	3.85455300	-0.73181800	3.02028900
C	4.66348100	-2.66206700	-0.23494700
H	2.55845500	-3.15806400	-0.26139400
C	5.68057200	-1.99824300	0.44680200
H	6.18025800	-0.81651600	2.17972200

H	4.88857500	-3.21761400	-1.14015500
H	6.69798300	-2.02452500	0.07066100
H	-2.45638200	-0.01690300	1.96900500
M2 <sub>2</sub> <sup>(S,R)</sup>			
P	0.83978800	0.35108400	-1.22307000
C	2.42251000	1.25026900	-1.38753900
C	2.36818100	2.76583200	-1.16732100
H	3.15232700	0.78204100	-0.72084400
H	2.75243900	1.03124200	-2.41167200
C	3.77334000	3.36576300	-1.12695300
H	1.84985000	3.00500700	-0.22903100
H	1.79113100	3.24365400	-1.96893500
C	3.74796900	4.87969100	-0.94265800
H	4.29994900	3.10857700	-2.05415700
H	4.33410200	2.89391500	-0.31074600
H	4.75915800	5.29204600	-0.90713800
H	3.24144800	5.15025600	-0.01083300
H	3.21482000	5.36525900	-1.76581500
C	1.16545500	-1.34839000	-1.81199100
C	0.51402000	-1.71633700	-3.14538200
H	2.25669700	-1.43666800	-1.86888200
H	0.82790600	-2.00033200	-1.00162500
C	0.89122000	-3.14285800	-3.54571400
H	0.82359900	-1.02127100	-3.93712900
H	-0.57384300	-1.64327200	-3.04763500
C	0.19256700	-3.58631900	-4.82733600
H	0.62673900	-3.82057500	-2.72433400
H	1.97891800	-3.21179600	-3.66681500
H	0.47488700	-4.60559500	-5.10195500
H	0.45225400	-2.92814600	-5.66228600
H	-0.89488800	-3.55868900	-4.70546800
C	-0.27382700	1.30508100	-2.33659700
C	-1.02827600	2.46478800	-1.67223500
H	0.39373600	1.69437500	-3.11533700
H	-0.96773300	0.61457200	-2.81816100
C	-1.67802100	3.37935500	-2.70860200
H	-0.35842800	3.05420300	-1.03484200
H	-1.80908700	2.08893100	-0.99996100
C	-2.44768700	4.51742700	-2.04490000
H	-2.35233100	2.78795000	-3.34114500
H	-0.90496700	3.78537800	-3.37268300
H	-2.92885500	5.15923500	-2.78702500

H	-1.77938300	5.13707800	-1.43865400
H	-3.22224800	4.12776300	-1.37567000
C	0.33660700	0.44722400	0.53960300
C	-0.96509900	0.35819400	0.89062600
C	1.44564100	0.66629300	1.54409300
C	-1.54375100	0.83900800	2.20409800
H	-0.81511500	0.72872500	3.00512800
C	-1.95513300	-0.16290900	-0.10388500
O	-1.63975500	-0.79383900	-1.09532800
O	-3.21301400	0.12347600	0.21620100
C	-4.22671400	-0.28805600	-0.72201100
C	-4.30944600	0.70100300	-1.86836700
H	-3.99300700	-1.29790800	-1.06711400
H	-5.14675700	-0.30724700	-0.13665500
H	-5.13662400	0.43564400	-2.53065100
H	-3.38395700	0.68973500	-2.45052900
H	-4.47799800	1.71198700	-1.48653200
H	2.12286900	1.46628200	1.23032200
C	-1.98968300	2.28518000	2.04032700
C	-3.34150900	2.63109400	2.06184300
C	-1.04274200	3.29463800	1.83901600
C	-3.73934700	3.95662100	1.89205100
H	-4.08621600	1.85371600	2.20654300
C	-1.43453800	4.61831200	1.66899400
H	0.01482500	3.03947800	1.81258200
C	-2.78789500	4.95360100	1.69394300
H	-4.79509700	4.20856100	1.91281700
H	-0.68432200	5.38818900	1.51633600
H	-3.09732300	5.98486900	1.55694000
H	0.99873400	0.98267500	2.48518500
C	2.27218800	-0.66154600	1.83264700
H	2.44186900	-0.63171800	2.91905100
N	1.57666100	-1.85630100	1.40759100
S	0.58114000	-2.46734500	2.45836500
O	1.05950500	-3.71384100	3.10274900
O	0.04862500	-1.47118500	3.42741000
C	-0.80730700	-2.97716700	1.45125300
C	-2.09472000	-2.63749300	1.84375200
C	-0.59911900	-3.72685800	0.29265800
C	-3.17966400	-3.01928300	1.05212900
H	-2.23589900	-2.07550100	2.76174900
C	-1.68442800	-4.09364400	-0.49075500
H	0.41123300	-4.00696500	0.00764100
C	-2.99126900	-3.73958100	-0.12636900

H	-4.18697500	-2.74302300	1.35480300
H	-1.52297100	-4.66660700	-1.40122300
C	-4.15593800	-4.13427900	-0.99775200
H	-4.04166900	-3.72891400	-2.00838000
H	-5.09972700	-3.76726000	-0.58778000
H	-4.22611200	-5.22210500	-1.09144700
C	3.65152800	-0.58954100	1.19189800
C	4.50967100	0.46636400	1.52351900
C	4.08678600	-1.53708000	0.26570100
C	5.75419600	0.59519500	0.91528300
H	4.19635400	1.19974100	2.26422800
C	5.33172800	-1.40622700	-0.35271900
H	3.42984600	-2.37032700	0.04141900
C	6.16518000	-0.33695700	-0.03814100
H	6.40356300	1.42257900	1.18510700
H	5.65151500	-2.14680300	-1.07988600
H	7.13261300	-0.23477500	-0.51933300
H	-2.40248500	0.22186100	2.47203800

TS3<sub>2</sub><sup>(S,R,R)</sup>

P	-2.44083300	-0.13776500	-0.46306200
C	-2.85103400	-1.37614800	-1.73902900
C	-2.44272100	-1.02019000	-3.17298100
H	-2.40611600	-2.32367300	-1.41813900
H	-3.93635800	-1.51588100	-1.67747000
C	-2.48270100	-2.24858900	-4.08208900
H	-1.43345600	-0.58791300	-3.19653400
H	-3.12051600	-0.25291400	-3.56588500
C	-2.14123800	-1.90674100	-5.52891200
H	-3.47857300	-2.70445600	-4.02766800
H	-1.77652500	-2.99597500	-3.69776600
H	-2.15818700	-2.79727300	-6.16152200
H	-1.14360700	-1.46243000	-5.59885100
H	-2.85686000	-1.18774200	-5.93890500
C	-3.18203300	-0.79213400	1.06917700
C	-4.70463300	-0.65182900	1.15230700
H	-2.89405600	-1.84891500	1.10301800
H	-2.68942800	-0.28137900	1.89997500
C	-5.24318300	-1.36414800	2.39381000
H	-5.18417500	-1.07865100	0.26177000
H	-4.98642900	0.40710600	1.18883800
C	-6.75907700	-1.24407700	2.51620100
H	-4.75976800	-0.94388600	3.28392400

H	-4.95028400	-2.42048000	2.35178100
H	-7.12672400	-1.75729600	3.40801900
H	-7.25660700	-1.68297600	1.64573600
H	-7.06337900	-0.19493700	2.58165200
C	-3.34403700	1.37484800	-0.97205700
C	-2.62677300	2.27799900	-1.98198800
H	-4.28149400	0.99842100	-1.40147900
H	-3.60446500	1.93343600	-0.06966300
C	-3.58527100	3.32034600	-2.55755300
H	-2.19930300	1.68697500	-2.79953000
H	-1.78350900	2.78542600	-1.50116500
C	-2.88121400	4.28503800	-3.50676600
H	-4.05051600	3.87654400	-1.73409300
H	-4.40001000	2.80740500	-3.08308500
H	-3.57846200	5.02088100	-3.91420900
H	-2.42966400	3.74635900	-4.34552000
H	-2.08055200	4.82678000	-2.99277900
C	-0.64923900	0.02189300	-0.38108100
C	-0.01791700	1.12984800	0.12431900
C	0.19547700	-1.13571300	-0.91513700
C	1.43241200	1.24978200	0.14774400
C	-0.85256200	2.20165300	0.77923400
O	-1.79551400	1.97168300	1.51177300
O	-0.44387400	3.42207600	0.45606400
C	-1.05585300	4.52366600	1.15638600
C	-2.37029500	4.91773800	0.51343200
H	-1.18820600	4.23709600	2.20250400
H	-0.31820300	5.32420200	1.09158800
H	-2.77486900	5.80201000	1.01164600
H	-3.09916200	4.10861400	0.60381800
H	-2.22516900	5.15472800	-0.54431300
H	-0.38229100	-1.77441100	-1.58648100
C	2.11731500	2.31602500	0.90711400
C	1.79826800	2.57706500	2.25086800
C	3.16926600	3.04611300	0.33541200
C	2.47117900	3.55611200	2.97343500
H	1.01647100	1.99270800	2.73419300
C	3.85886900	4.01172500	1.06401600
H	3.44088100	2.85183400	-0.69994400
C	3.50757000	4.28098400	2.38483500
H	2.19873200	3.74173100	4.00828800
H	4.66865000	4.56166600	0.59334200
H	4.04020000	5.03723400	2.95210300
H	1.01526700	-0.73360600	-1.52300700

C	0.80373000	-2.03934900	0.18142200
H	1.41548200	-2.78394400	-0.35292900
N	1.62206800	-1.23889900	1.09839900
S	3.08153400	-1.81715400	1.42931400
O	3.64042800	-1.00782000	2.51685400
O	3.06372400	-3.27991900	1.58173200
C	4.08529400	-1.48244900	-0.01218300
C	4.29948100	-2.46977600	-0.96735900
C	4.56193500	-0.18557500	-0.20737200
C	4.99681700	-2.15139300	-2.13200400
H	3.93534800	-3.47640800	-0.78871700
C	5.25424900	0.11603700	-1.37232100
H	4.39108700	0.57348500	0.55109300
C	5.48082100	-0.86065200	-2.35150500
H	5.16922700	-2.92018800	-2.88001200
H	5.63148500	1.12414000	-1.52601800
C	6.25164300	-0.51950000	-3.60031800
H	5.90322300	0.42333100	-4.03029400
H	6.15038500	-1.30176900	-4.35524700
H	7.31688200	-0.40216000	-3.37755800
C	-0.27659200	-2.81506700	0.92930500
C	-1.02216400	-3.78901000	0.25489300
C	-0.54719000	-2.57861600	2.27730600
C	-2.03091600	-4.49568800	0.90525400
H	-0.79929400	-4.01107300	-0.78807800
C	-1.55120800	-3.28945300	2.93414700
H	0.04303700	-1.83478200	2.80092400
C	-2.30037900	-4.24465100	2.25119500
H	-2.59524300	-5.25092500	0.36710400
H	-1.75113100	-3.09214700	3.98293900
H	-3.08203000	-4.79678500	2.76342800
H	1.65282700	0.04080400	0.74108500
H	1.89422800	1.04038200	-0.82213200

M3<sub>2</sub><sup>(S,R,R)</sup>

P	-2.35147600	0.08332300	-0.44482900
C	-2.94067600	-0.98483600	-1.81353900
C	-2.49528100	-0.57163700	-3.21793700
H	-2.62509900	-2.00774000	-1.58378000
H	-4.03477400	-0.98627900	-1.74482400
C	-2.74258400	-1.67895000	-4.24196800
H	-1.42951400	-0.30743800	-3.21667600
H	-3.03897600	0.33133700	-3.52273200

C	-2.34677900	-1.25768000	-5.65396300
H	-3.80158200	-1.96368400	-4.21885900
H	-2.17497200	-2.57041900	-3.94496400
H	-2.51995900	-2.06080700	-6.37434900
H	-1.28672500	-0.98876000	-5.69650400
H	-2.92459500	-0.38569600	-5.97552500
C	-3.27857700	-0.58563700	0.99349600
C	-4.76533200	-0.23048400	1.06797500
H	-3.15490400	-1.67383200	0.93500300
H	-2.74799300	-0.24316600	1.88594500
C	-5.45369000	-0.98422500	2.20697100
H	-5.27266700	-0.47414800	0.12471000
H	-4.88999900	0.84829900	1.22094500
C	-6.93575600	-0.64052700	2.32103300
H	-4.94131900	-0.75170500	3.14862000
H	-5.32746400	-2.06224400	2.04598100
H	-7.41116600	-1.18684300	3.13954500
H	-7.46664700	-0.89025900	1.39692400
H	-7.07440600	0.42930300	2.50576600
C	-3.08983600	1.73059400	-0.80073500
C	-2.29183500	2.63390500	-1.74589500
H	-4.07752400	1.51380100	-1.22905100
H	-3.26434700	2.23229800	0.15514900
C	-3.12740400	3.82838000	-2.20614400
H	-1.94928300	2.07071400	-2.62123400
H	-1.38547600	2.99371000	-1.24674700
C	-2.31856900	4.80383000	-3.05591500
H	-3.53274900	4.34648800	-1.32781400
H	-3.99252000	3.46410000	-2.77429700
H	-2.92572000	5.65407900	-3.37640000
H	-1.92840300	4.31045600	-3.95164000
H	-1.46291500	5.19245800	-2.49387400
C	-0.60929000	0.04416800	-0.37311300
C	0.17095900	1.12633100	0.15824100
C	0.09598900	-1.18784500	-0.91243900
C	1.52663900	1.28946800	-0.01834400
C	-0.55513800	2.13741400	1.00956100
O	-1.46397500	1.86207400	1.76991700
O	-0.12307300	3.38468800	0.81597700
C	-0.65102800	4.40291100	1.68303500
C	-1.93501100	4.97722300	1.11826000
H	-0.80503300	3.97678300	2.67693800
H	0.13782700	5.15549700	1.73183300
H	-2.27673700	5.80865900	1.73965100

H	-2.72026600	4.21717700	1.09830500
H	-1.77234300	5.34843600	0.10246200
H	-0.52073700	-1.71371800	-1.64745500
C	2.44390700	2.17379400	0.70574900
C	2.31791500	2.44885300	2.07943700
C	3.55961800	2.70871900	0.03820800
C	3.23657700	3.25658200	2.73997600
H	1.50011500	1.99987900	2.63960300
C	4.48859000	3.50313800	0.70174600
H	3.68725000	2.49528700	-1.02029300
C	4.32920500	3.78962000	2.05680900
H	3.11202300	3.45051300	3.80118600
H	5.33865400	3.90427300	0.15737600
H	5.05371900	4.40740400	2.57714500
H	1.00453300	-0.90934200	-1.46178700
C	0.50731100	-2.23983900	0.15129000
H	1.10835200	-3.00200700	-0.36317700
N	1.34054700	-1.62717300	1.19434400
S	2.86350400	-2.18256600	1.45608300
O	3.38252800	-1.40515100	2.57537900
O	2.77729400	-3.63704500	1.52974700
C	3.83920400	-1.78467000	0.02671600
C	3.91792100	-2.69074000	-1.02882300
C	4.47435400	-0.54679100	-0.03302100
C	4.63519700	-2.33722500	-2.16638000
H	3.44852900	-3.66544000	-0.94325200
C	5.18871000	-0.21299300	-1.17812100
H	4.41310500	0.14070000	0.80513300
C	5.27406000	-1.09620700	-2.25965000
H	4.71083000	-3.04033700	-2.99072000
H	5.69360900	0.74802500	-1.22793900
C	6.02571400	-0.71472600	-3.50739400
H	5.35001300	-0.25012500	-4.23286400
H	6.46922200	-1.59161100	-3.98407800
H	6.81984800	0.00182500	-3.28778800
C	-0.68436400	-2.95391900	0.77207300
C	-1.49127100	-3.76141900	-0.03794900
C	-1.00137700	-2.83300500	2.12473900
C	-2.60746400	-4.40827600	0.48487900
H	-1.23752900	-3.89525200	-1.08834300
C	-2.11312000	-3.48741400	2.65392500
H	-0.37069000	-2.22222600	2.76071300
C	-2.92457900	-4.26944300	1.83647000
H	-3.22260600	-5.02918000	-0.15880500



H	-2.34797200	-3.37850700	3.70825100
H	-3.79208300	-4.77506900	2.24864800
H	1.29247300	-0.60996000	1.24994900
H	2.02020600	0.64054400	-0.73903300
TS4 <sub>2</sub> <sup>(S,R,R)</sup>			
P	-1.70388300	1.23071700	0.16165000
C	-2.88982100	1.05438700	-1.21838600
C	-2.44319900	1.68490300	-2.54250600
H	-3.09709100	-0.01366600	-1.34296700
H	-3.82433200	1.51649000	-0.88181600
C	-3.30549000	1.19448200	-3.70554100
H	-1.38938000	1.45584900	-2.75009900
H	-2.51642900	2.77733000	-2.47209900
C	-2.91651700	1.84672000	-5.02831800
H	-4.35943400	1.39956900	-3.48122100
H	-3.21203800	0.10347700	-3.77920100
H	-3.54005200	1.48460500	-5.84930000
H	-1.87279900	1.63070300	-5.27698400
H	-3.02847400	2.93409600	-4.97454100
C	-2.54412300	0.63411600	1.67416500
C	-4.06384300	0.79575400	1.70663400
H	-2.26441300	-0.41953400	1.77171700
H	-2.06178400	1.16037600	2.50425700
C	-4.65063000	0.24293400	3.00516000
H	-4.51200100	0.25424500	0.86433500
H	-4.34543600	1.85199800	1.59804200
C	-6.17021000	0.37093400	3.05034000
H	-4.20263000	0.76500300	3.85898400
H	-4.36265700	-0.81185700	3.10017400
H	-6.57637200	-0.03196000	3.98133000
H	-6.63099900	-0.17200900	2.21875500
H	-6.47655000	1.41905100	2.97488300
C	-1.51403800	3.04381600	0.37535500
C	-0.51851200	3.77582700	-0.53455000
H	-2.52679400	3.43593900	0.21155900
H	-1.27596500	3.22089200	1.42808600
C	-0.79032200	5.28033300	-0.53743700
H	-0.56630900	3.39444900	-1.56041400
H	0.50580200	3.60011900	-0.19247000
C	0.25445600	6.05089400	-1.33846300
H	-0.80987300	5.64334900	0.49822600
H	-1.79059200	5.46416800	-0.94920800

H	0.04211500	7.12269600	-1.34276900
H	0.28019500	5.70724800	-2.37719000
H	1.25405000	5.90599500	-0.91607400
C	-0.19778200	0.29113300	-0.13679000
C	1.09932900	0.98991900	0.05374600
C	-0.30846000	-0.81495100	-1.18794100
C	2.14634900	0.87846400	-0.79714500
H	-0.23491800	-0.68408900	0.83028800
C	1.18792200	1.73864300	1.35212400
O	0.42303500	1.55187300	2.27977600
O	2.12531700	2.68782100	1.35889500
C	2.28331400	3.44981900	2.56926900
C	1.34088700	4.63732500	2.57308000
H	2.11005700	2.79651600	3.42645500
H	3.32775400	3.76530700	2.55750400
H	1.52572600	5.25670200	3.45405500
H	0.30091000	4.30196700	2.60255400
H	1.49430600	5.24993900	1.68019300
H	-0.88733500	-0.56780500	-2.08247800
H	0.70170400	-1.06598800	-1.51892100
C	-0.87672900	-2.12913000	-0.50180200
H	-0.33090000	-2.97377900	-0.94542100
N	-0.57751300	-1.96245200	0.90932600
S	0.28497800	-3.10151800	1.63791800
O	0.70721700	-2.56535600	2.93668200
O	-0.40766100	-4.39838600	1.63395400
C	1.75596600	-3.33808700	0.64490500
C	1.98242400	-4.54858300	0.00044400
C	2.64140700	-2.27188600	0.49029200
C	3.11091100	-4.69099600	-0.80397400
H	1.27503000	-5.36019900	0.13253300
C	3.76179900	-2.42596400	-0.31652100
H	2.44795500	-1.32787500	0.99257300
C	4.01218500	-3.63760300	-0.97332900
H	3.29085200	-5.63456000	-1.31170000
H	4.45123000	-1.59399700	-0.44034600
C	5.24335400	-3.80205800	-1.82537300
H	5.50073100	-2.86726900	-2.32927500
H	5.10167200	-4.57755200	-2.58118500
H	6.10155800	-4.09054200	-1.20987300
C	-2.35463400	-2.34631000	-0.78354000
C	-2.79150000	-2.43869700	-2.11119300
C	-3.29941100	-2.43257200	0.23793000
C	-4.14501300	-2.55481700	-2.41075300

H	-2.06384600	-2.40657500	-2.91978300
C	-4.65908400	-2.54511100	-0.05914200
H	-2.95461600	-2.41837500	1.26684500
C	-5.08764400	-2.59120900	-1.38233000
H	-4.46582700	-2.61372600	-3.44639500
H	-5.38193400	-2.59906700	0.75018300
H	-6.14494000	-2.67128500	-1.61329300
C	3.58053600	1.15351700	-0.60310500
C	4.34752700	1.50285700	-1.72331800
C	4.24330900	0.96903900	0.62090000
C	5.72016400	1.70659200	-1.61972400
H	3.85524500	1.61993600	-2.68508300
C	5.61503900	1.16461600	0.72448600
H	3.68348900	0.65098300	1.49556200
C	6.35965400	1.54047300	-0.39398100
H	6.29112600	1.98630700	-2.49930800
H	6.10734700	1.00942700	1.67919700
H	7.43150800	1.68821600	-0.31139900
H	1.92684300	0.44471500	-1.77065700

M4<sub>2</sub><sup>(S,R,R)</sup>

P	-1.06963000	-1.20306100	-0.79484600
C	-2.00526900	-2.28689600	0.33293400
C	-1.16711100	-3.06650400	1.35575200
H	-2.74457500	-1.65514800	0.83355000
H	-2.56311800	-2.98199800	-0.30697200
C	-2.03386700	-3.58898800	2.49912000
H	-0.36529900	-2.43824800	1.77107000
H	-0.67366100	-3.91119300	0.86144300
C	-1.23359700	-4.42255300	3.49391900
H	-2.85729900	-4.18467400	2.08153000
H	-2.49956900	-2.73699300	3.01043000
H	-1.86382000	-4.78001900	4.31181800
H	-0.41800600	-3.83326400	3.92902100
H	-0.78912000	-5.29541200	3.00413600
C	-2.22793900	-0.42893700	-1.96962900
C	-3.42795800	-1.28886200	-2.36413900
H	-2.54223400	0.50468900	-1.48716200
H	-1.62427000	-0.14580100	-2.83938900
C	-4.36606900	-0.53252300	-3.30602600
H	-3.98966300	-1.56972300	-1.46342400
H	-3.09902800	-2.21938700	-2.84535000
C	-5.58531100	-1.36900100	-3.68478200

H	-3.81712900	-0.23439200	-4.20595600
H	-4.68678300	0.39491400	-2.81493500
H	-6.25566400	-0.81529900	-4.34851200
H	-6.15466000	-1.65255400	-2.79215500
H	-5.28536500	-2.28918500	-4.19584700
C	0.03099200	-2.30379100	-1.76907200
C	1.28942300	-2.89605500	-1.11682400
H	-0.64407700	-3.12182700	-2.06342700
H	0.28883900	-1.75927900	-2.68314000
C	1.79666900	-4.12087500	-1.87830400
H	1.10350600	-3.16956000	-0.07366400
H	2.09457000	-2.15492200	-1.09020800
C	3.06080000	-4.68803100	-1.23505000
H	1.99786600	-3.84257300	-2.92149000
H	1.01182500	-4.88733100	-1.90370800
H	3.43689800	-5.55007100	-1.79274600
H	2.86135300	-5.00932500	-0.20660000
H	3.85214500	-3.93206700	-1.19812100
C	-0.25670700	0.19728800	0.10826700
C	1.24491100	0.00939000	0.13835400
C	-0.89479400	0.56412200	1.46153000
C	1.87848600	-0.47103400	1.21912600
H	-0.46908700	1.04094700	-0.56115000
C	1.85529700	0.25759800	-1.20883100
O	1.16041400	0.42715400	-2.19510400
O	3.18211200	0.20068000	-1.24829500
C	3.78990200	0.27344600	-2.55456700
C	3.66548100	-1.04975500	-3.28448600
H	3.32321100	1.08947200	-3.11347600
H	4.83316300	0.52126000	-2.35024200
H	4.20415300	-0.99503000	-4.23572900
H	2.62013200	-1.27809200	-3.49758900
H	4.09872900	-1.85727000	-2.68954700
H	-1.09437900	-0.31026100	2.08878900
H	-0.12895800	1.15080700	1.98053000
C	-2.17210000	1.47199200	1.36276500
H	-2.16269000	2.05976600	2.29558700
N	-2.15506100	2.33724300	0.20355400
S	-1.50337200	3.75265300	0.39162900
O	-1.91526500	4.62219200	-0.72439700
O	-1.66837500	4.31538900	1.75215100
C	0.28550000	3.62114000	0.19962800
C	1.11944300	3.62333300	1.31441100
C	0.83090900	3.48720400	-1.07827700

C	2.49963700	3.50663200	1.14670100
H	0.68160700	3.74338000	2.30036600
C	2.20697600	3.38405300	-1.23200400
H	0.17319600	3.48687600	-1.94431000
C	3.06244400	3.39377100	-0.12529800
H	3.14747000	3.52061000	2.01966000
H	2.62775400	3.29984200	-2.23321300
C	4.55327100	3.30115300	-0.32295000
H	4.82534400	2.33832700	-0.77054500
H	5.08774300	3.39398100	0.62649700
H	4.90961500	4.08720600	-0.99294100
C	-3.46287600	0.65960500	1.40562700
C	-3.73796000	-0.15251800	2.51324300
C	-4.39873100	0.70565100	0.37032200
C	-4.88224900	-0.94389400	2.55823500
H	-3.04403700	-0.16712500	3.35190600
C	-5.54287200	-0.09248100	0.40819200
H	-4.21826600	1.38930800	-0.45050800
C	-5.78382000	-0.93056600	1.49317600
H	-5.07229500	-1.56981800	3.42508400
H	-6.25328800	-0.04801100	-0.41304100
H	-6.67324200	-1.55164900	1.51932600
C	3.30638700	-0.79682000	1.42855800
C	3.64953100	-2.10279000	1.79050200
C	4.30991800	0.17235700	1.33602900
C	4.98155000	-2.44600600	2.00923500
H	2.86831700	-2.85430600	1.89538200
C	5.63657200	-0.16616000	1.57375600
H	4.03227600	1.18784600	1.07787900
C	5.97828000	-1.47715700	1.90030300
H	5.23729400	-3.46747900	2.26939200
H	6.40760600	0.59586500	1.50064300
H	7.01522000	-1.74181200	2.08020200
H	1.24359200	-0.71377500	2.07108800
M4 <sub>2</sub> <sup>(S,R,R)</sup>			
P	-2.19970400	-0.80390800	0.88349800
C	-1.58218700	-1.24742000	2.53906300
C	-0.26596500	-2.03284300	2.55684600
H	-1.48876200	-0.31418400	3.10471100
H	-2.37248000	-1.83308700	3.02174200
C	0.31304800	-2.11405400	3.96856700
H	0.48070500	-1.57168500	1.89387700

H	-0.44503500	-3.04660500	2.17877100
C	1.46856900	-3.10577400	4.03887900
H	-0.47643500	-2.40673700	4.67127700
H	0.64824900	-1.11344800	4.26887300
H	1.96510800	-3.07778600	5.01252900
H	2.21444800	-2.87729800	3.27197000
H	1.11448700	-4.12677400	3.86717400
C	-3.87930600	-0.12637100	1.05776500
C	-4.91107700	-1.05722000	1.69885600
H	-3.77852700	0.80569700	1.62872700
H	-4.17853400	0.15202900	0.03934100
C	-6.29186300	-0.40218000	1.75139100
H	-4.60213700	-1.32343000	2.71644700
H	-4.97884500	-1.99206100	1.12919800
C	-7.33468400	-1.31617900	2.38752500
H	-6.59947900	-0.13398200	0.73394900
H	-6.22271100	0.53564500	2.31509900
H	-8.31514600	-0.83518700	2.41817800
H	-7.05411600	-1.57415700	3.41328300
H	-7.43371300	-2.24820800	1.82278700
C	-2.33320800	-2.34044900	-0.10371500
C	-1.06354900	-2.97806200	-0.69429600
H	-2.80239200	-3.04741500	0.59387600
H	-3.06388000	-2.13570000	-0.89342000
C	-1.30662400	-4.43641900	-1.07953100
H	-0.22694500	-2.92369000	0.01021000
H	-0.73949500	-2.43644600	-1.58650600
C	-0.05796200	-5.06379300	-1.69302900
H	-2.14128000	-4.48787900	-1.79011400
H	-1.61423800	-5.00356000	-0.19254500
H	-0.23691800	-6.10021200	-1.98834100
H	0.77229900	-5.05301900	-0.97963900
H	0.26271400	-4.50842600	-2.58036700
C	-1.20512700	0.57774100	0.15500200
C	-0.33880700	0.10306900	-0.98906400
C	-0.53510200	1.42702400	1.24393300
C	0.96290100	-0.17339200	-0.82618700
C	-1.14414100	-0.13380000	-2.22154300
O	-2.36255100	-0.05975700	-2.21009900
O	-0.44439100	-0.49106500	-3.29197100
C	-1.19899300	-0.85091300	-4.46762500
C	-1.75556500	-2.25607800	-4.34051100
H	-1.99158900	-0.11498000	-4.61528200
H	-0.47613300	-0.77622900	-5.28029400

H	-2.26372500	-2.53759100	-5.26589100
H	-2.47724000	-2.31113000	-3.52136700
H	-0.94915500	-2.97145800	-4.15782100
H	-1.28693000	1.63441300	2.01656300
C	1.96441900	-0.64209000	-1.80582900
C	2.35022500	0.14804300	-2.89221300
C	2.61597600	-1.85689700	-1.57282700
C	3.36111500	-0.28397900	-3.74432600
H	1.86087000	1.10381500	-3.05048900
C	3.61147200	-2.29869600	-2.43984900
H	2.34462600	-2.45252500	-0.70392200
C	3.98816300	-1.51025500	-3.52500400
H	3.66240500	0.33859500	-4.58049200
H	4.10145300	-3.25029300	-2.25975000
H	4.77427600	-1.84585600	-4.19368400
H	0.28531200	0.89236800	1.73770100
C	-0.01139500	2.81132200	0.73674300
H	0.10105000	3.41840200	1.64766600
N	1.22999500	2.75170900	-0.00535800
S	2.55370600	3.01273200	0.78766200
O	3.59567100	3.49486200	-0.13927600
O	2.37956200	3.80128200	2.03262500
C	3.21710600	1.43917700	1.36804000
C	2.89512600	0.95893600	2.63491800
C	4.00702900	0.67026400	0.51365700
C	3.38069800	-0.28080200	3.05170800
H	2.29639400	1.57397000	3.30048900
C	4.48548000	-0.56388500	0.93785500
H	4.25207800	1.05203500	-0.47275500
C	4.18909500	-1.05514300	2.21399700
H	3.15281300	-0.63983500	4.05295500
H	5.10924000	-1.15444100	0.27116200
C	4.76064600	-2.37541900	2.66564600
H	5.84332300	-2.40035400	2.51352600
H	4.33478000	-3.20748300	2.09423100
H	4.56003500	-2.55563700	3.72412000
C	-1.10952300	3.44860000	-0.10227000
C	-2.25993800	3.94680600	0.51638500
C	-1.03986200	3.45450000	-1.49657900
C	-3.32113600	4.43734500	-0.24041600
H	-2.32104100	3.95737900	1.60299400
C	-2.10213700	3.94033800	-2.25678700
H	-0.13593900	3.07653600	-1.96403700
C	-3.24658600	4.43132200	-1.63235400

H	-4.20367600	4.83000800	0.25559700
H	-2.03492600	3.93753700	-3.34066900
H	-4.07269800	4.81202100	-2.22464900
H	-1.99732500	1.18934000	-0.29071100
H	1.36676800	-0.04489300	0.17902200
TS5 <sub>2</sub> <sup>(S,R,R)</sup>			
P	-2.41456200	-0.98764800	0.46535000
C	-1.97232500	-2.23955300	1.71827000
C	-0.72500700	-3.06592700	1.38468700
H	-1.84692700	-1.70382300	2.66654700
H	-2.83623900	-2.90266100	1.83846700
C	-0.26275400	-3.90023600	2.57826700
H	0.10596800	-2.41933800	1.06664800
H	-0.94876800	-3.72746100	0.53869400
C	0.82930500	-4.88701500	2.17979200
H	-1.11934800	-4.43686900	3.00362300
H	0.10355900	-3.22275900	3.36002800
H	1.24190100	-5.40489700	3.04968300
H	1.64821600	-4.36432600	1.67665000
H	0.43945400	-5.64071500	1.48896000
C	-4.10909800	-0.41960000	0.81045700
C	-5.20880900	-1.47135900	0.64943300
H	-4.09737600	-0.01534200	1.83048400
H	-4.26216400	0.42235200	0.12423800
C	-6.58117700	-0.90747300	1.01860900
H	-5.00024200	-2.34448000	1.28015900
H	-5.23368500	-1.82702100	-0.38736200
C	-7.69085600	-1.94015200	0.84405300
H	-6.78698200	-0.02823500	0.39688800
H	-6.55693100	-0.55697000	2.05726200
H	-8.66432300	-1.52527500	1.11610500
H	-7.51019700	-2.81692700	1.47370100
H	-7.74762300	-2.28006700	-0.19453300
C	-2.45723300	-1.80280000	-1.17317200
C	-1.13972300	-2.09361700	-1.91048900
H	-2.99210700	-2.74345200	-0.98224800
H	-3.10539500	-1.17425300	-1.79250400
C	-1.34235000	-3.13642600	-3.00847000
H	-0.36606800	-2.44386300	-1.21747600
H	-0.75199500	-1.17536900	-2.35870100
C	-0.04892100	-3.39906000	-3.77479800
H	-2.12108700	-2.78517200	-3.69748300



H	-1.71343800	-4.06970000	-2.56647800
H	-0.19833100	-4.12805200	-4.57480900
H	0.72638400	-3.78726900	-3.10572700
H	0.33261600	-2.47533100	-4.22250700
C	-1.32074000	0.50282200	0.61086100
C	-0.50647300	0.76033700	-0.62604400
C	-0.46454200	0.55105000	1.88362200
C	0.86084900	0.52464900	-0.55254700
C	-1.28257300	1.25386200	-1.72551900
O	-2.51987100	1.25257800	-1.70842900
O	-0.59365500	1.64741600	-2.81807100
C	-1.35597300	1.84646900	-4.01322600
C	-1.68767700	0.51349400	-4.66038700
H	-2.26046500	2.41222300	-3.78083500
H	-0.71028900	2.44784600	-4.65573700
H	-2.19696900	0.66669200	-5.61525100
H	-2.34320200	-0.06934800	-4.00699200
H	-0.77002000	-0.05432100	-4.84071000
H	-1.11160200	0.57524300	2.76784500
C	1.79498500	0.67043700	-1.70131800
C	2.27353200	1.90764900	-2.13023700
C	2.19564600	-0.49051200	-2.36789500
C	3.12826700	1.98328600	-3.22453000
H	1.98983000	2.79613400	-1.57745100
C	3.03947100	-0.41471400	-3.47359500
H	1.84733800	-1.45861900	-2.01403600
C	3.50792100	0.82494700	-3.90294700
H	3.50401500	2.94856800	-3.54892700
H	3.33812400	-1.32233100	-3.98928600
H	4.17427800	0.88814400	-4.75753800
H	0.18073000	-0.32977100	1.98583400
C	0.42640000	1.82802100	1.90520000
H	0.87830000	1.86347000	2.90373000
N	1.48589400	1.81566000	0.88978800
S	2.99473100	1.67832200	1.42509700
O	3.90413800	2.28554400	0.44729700
O	3.12532000	2.11417800	2.82900300
C	3.40657300	-0.06544800	1.43513300
C	2.97644400	-0.86515000	2.49184500
C	4.10542500	-0.61926600	0.36564900
C	3.26396200	-2.22776800	2.48043700
H	2.45221500	-0.41449900	3.33015000
C	4.38540200	-1.98176700	0.36686700
H	4.42797300	0.02250900	-0.44769400

C	3.97846300	-2.80284500	1.42365600
H	2.94958200	-2.85112500	3.31397200
H	4.94066300	-2.41508700	-0.46127900
C	4.32846900	-4.26913400	1.42111600
H	5.40761900	-4.40784700	1.31021900
H	3.84655100	-4.78724200	0.58580200
H	4.01398800	-4.75469700	2.34740700
C	-0.45613900	3.06363100	1.77605700
C	-1.24931300	3.44941300	2.86102300
C	-0.53892700	3.79422700	0.59003700
C	-2.11210000	4.53739300	2.76447900
H	-1.18284000	2.89572000	3.79555200
C	-1.40581300	4.88118000	0.48871400
H	0.08317500	3.49884300	-0.24857900
C	-2.19535500	5.25605700	1.57315600
H	-2.71447300	4.82729500	3.61994300
H	-1.46121700	5.43894300	-0.44123000
H	-2.86648400	6.10544700	1.49408600
H	-2.06650800	1.30575800	0.68871700
H	1.16140400	-0.29105600	0.10777500

M5<sub>2</sub><sup>(S,R,R)</sup>

P	2.53929200	0.17046600	0.43519300
C	2.72213400	1.70393500	1.42874900
C	1.95413000	2.94606900	0.96832700
H	2.46273700	1.45266300	2.46362200
H	3.79629300	1.92841100	1.42724200
C	2.27848400	4.14196400	1.86463400
H	0.86970900	2.76821500	0.97468800
H	2.22473700	3.19167800	-0.06648800
C	1.53777700	5.40322000	1.43688100
H	3.36114300	4.31649000	1.84550800
H	2.02135600	3.89324300	2.90140000
H	1.79487900	6.25403500	2.07253400
H	0.45714000	5.24788000	1.49809300
H	1.77931100	5.66856400	0.40236800
C	4.00399200	-0.81899800	0.88541000
C	5.32159100	-0.34450400	0.26841800
H	4.05940300	-0.79824400	1.98169400
H	3.76703300	-1.83832900	0.56860100
C	6.50270400	-1.17882300	0.76522900
H	5.50684900	0.71231200	0.50206000
H	5.26366400	-0.42016400	-0.82393900

C	7.82221100	-0.74096700	0.13685400
H	6.31274500	-2.23464900	0.53935700
H	6.56466100	-1.09942300	1.85727700
H	8.65574400	-1.34714100	0.49990800
H	8.03894800	0.30557300	0.37283300
H	7.78551800	-0.83719800	-0.95260400
C	2.66767100	0.67695000	-1.31374700
C	1.38204700	1.17336600	-1.99279800
H	3.43342600	1.46459900	-1.32485800
H	3.06633700	-0.19273400	-1.84185400
C	1.70162400	1.96910700	-3.25722300
H	0.78690500	1.79884700	-1.31332400
H	0.75748300	0.31244100	-2.25118000
C	0.43933300	2.33831500	-4.03063400
H	2.36606600	1.37344400	-3.89627200
H	2.25933000	2.87503600	-2.98721300
H	0.66795900	2.96128400	-4.89886600
H	-0.26109700	2.88990600	-3.39327200
H	-0.07152000	1.43781100	-4.38764100
C	1.01458900	-0.80801400	0.92761400
C	0.16837900	-1.27417200	-0.21588900
C	0.17522800	-0.09320600	1.98850500
C	-1.17356000	-0.61239800	-0.38109600
C	0.88555600	-2.04617600	-1.12677600
O	2.11993500	-2.27027300	-1.00088600
O	0.22062900	-2.56781600	-2.21021100
C	1.02281300	-3.01781600	-3.29280400
C	1.47112300	-1.84992300	-4.15689300
H	1.88189600	-3.57910100	-2.91844700
H	0.37781000	-3.69176100	-3.86310000
H	1.99769200	-2.20095800	-5.04882500
H	2.14686500	-1.20254700	-3.59016900
H	0.60215700	-1.26134300	-4.46814600
H	0.69704300	-0.02655200	2.94746200
C	-1.98841900	-1.15325900	-1.53704800
C	-2.60046000	-2.40402500	-1.45841300
C	-2.08864500	-0.41725600	-2.71300800
C	-3.29172600	-2.91480800	-2.54837900
H	-2.51263900	-2.97435300	-0.53786500
C	-2.77248000	-0.93106500	-3.81539800
H	-1.61775400	0.56229700	-2.77280800
C	-3.37514100	-2.18209900	-3.73495400
H	-3.76411800	-3.89019600	-2.48003100
H	-2.83695900	-0.35012900	-4.73084300

H	-3.91312900	-2.58489400	-4.58758500
H	-0.06577000	0.93393600	1.68969300
C	-1.15813900	-0.83008200	2.15722100
H	-1.71692700	-0.32575000	2.94990200
N	-1.95781000	-0.70254500	0.91636300
S	-3.31141300	0.26396100	1.03177300
O	-4.20717400	-0.07100900	-0.06599900
O	-3.79680300	0.15273800	2.40649800
C	-2.80464300	1.95295000	0.77457500
C	-2.43052100	2.73374600	1.86378500
C	-2.80305100	2.47121400	-0.52075300
C	-2.06609000	4.06116000	1.64887900
H	-2.46307300	2.31973000	2.86675100
C	-2.42712800	3.79340700	-0.71665900
H	-3.12100200	1.84655500	-1.35009600
C	-2.06604600	4.60985000	0.36278300
H	-1.80127100	4.68567100	2.49752700
H	-2.43952900	4.21058600	-1.71994700
C	-1.71760000	6.05579700	0.12536500
H	-2.53318500	6.56497800	-0.39549200
H	-0.82412900	6.14283600	-0.50056100
H	-1.52920200	6.58099500	1.06381400
C	-1.04203400	-2.29098000	2.57686700
C	0.03351600	-2.74674700	3.34374700
C	-2.07815000	-3.18264000	2.28629400
C	0.08674700	-4.06845900	3.78348300
H	0.84275900	-2.07358800	3.61036600
C	-2.02843000	-4.50143600	2.72705300
H	-2.92626500	-2.83163000	1.70766400
C	-0.94161900	-4.95276900	3.47332500
H	0.93658000	-4.40319400	4.37007400
H	-2.84263700	-5.17813900	2.48685800
H	-0.89964300	-5.98249000	3.81328400
H	1.50431400	-1.67897500	1.38777300
H	-1.02802500	0.46924200	-0.57209800
TS6 <sub>2</sub> <sup>(S,R,R)</sup>			
P	2.64690500	-0.32574900	0.51702100
C	3.36439100	1.09416000	1.45844000
C	2.81692700	2.46737400	1.06742800
H	3.16682300	0.89710700	2.51961400
H	4.45383700	1.08669000	1.32775000
C	3.42867500	3.57163300	1.92997100

H	1.72088800	2.49089900	1.16027600
H	3.04337800	2.66950000	0.01191800
C	2.92394000	4.95849000	1.55039500
H	4.52083300	3.53145600	1.83540800
H	3.20138200	3.36871400	2.98370000
H	3.37508200	5.73559100	2.17265000
H	1.83843700	5.01525300	1.67203700
H	3.15434000	5.18686400	0.50454000
C	3.77878700	-1.72077700	0.91432300
C	5.24059100	-1.57317200	0.49038600
H	3.70986200	-1.87313600	1.99993000
H	3.32296500	-2.59483300	0.43497000
C	6.07286400	-2.79873500	0.87066700
H	5.68699600	-0.68444900	0.95359500
H	5.30005900	-1.42373600	-0.59517100
C	7.53309900	-2.65924700	0.45032800
H	5.63317400	-3.68929100	0.40559800
H	6.01059300	-2.95201500	1.95508800
H	8.11579300	-3.54069300	0.72947800
H	7.99353800	-1.78709400	0.92522200
H	7.61614500	-2.53063600	-0.63346300
C	2.96363600	0.06189300	-1.25786700
C	1.80514500	0.77127000	-1.97431400
H	3.87853000	0.66697400	-1.32002100
H	3.16587000	-0.89979500	-1.74255800
C	2.24246800	1.33989900	-3.32343600
H	1.40179100	1.58498300	-1.35416900
H	0.98018900	0.06454000	-2.13090900
C	1.08589200	1.96722000	-4.09576200
H	2.69421500	0.53715400	-3.92066400
H	3.03143600	2.08487000	-3.15850500
H	1.42719700	2.42791400	-5.02624000
H	0.59067900	2.74094300	-3.49785900
H	0.33505900	1.21208500	-4.35139500
C	0.58663100	-1.23737700	0.97529200
C	-0.22606500	-1.36251800	-0.16017800
C	0.02376700	-0.39300500	2.09649700
C	-1.30792000	-0.31583100	-0.34024500
C	0.31282000	-2.23944300	-1.16519300
O	1.42520700	-2.77054700	-1.06170500
O	-0.44492100	-2.43794800	-2.26872500
C	0.17488300	-3.10461700	-3.36847300
C	1.06942000	-2.14749300	-4.13709500
H	0.73716200	-3.96904400	-3.00857200

H	-0.65741200	-3.44715300	-3.98723400
H	1.47369900	-2.62960500	-5.03106700
H	1.90331700	-1.82737900	-3.50612200
H	0.49781800	-1.26500200	-4.44192000
H	0.52384500	-0.58650400	3.04905900
C	-2.20142700	-0.54324700	-1.54064200
C	-3.16108900	-1.55477500	-1.53446000
C	-2.01160000	0.21694000	-2.68924900
C	-3.90826200	-1.81186400	-2.67597200
H	-3.30432500	-2.13984800	-0.62948300
C	-2.75383800	-0.04373000	-3.84116200
H	-1.26553000	1.00944300	-2.68728600
C	-3.70161000	-1.06210400	-3.83647300
H	-4.65236000	-2.60270700	-2.66856500
H	-2.59215500	0.55031900	-4.73596700
H	-4.28431300	-1.26963400	-4.72854200
H	0.14746100	0.67501800	1.88316700
C	-1.48485200	-0.65174800	2.18833800
H	-1.89072400	-0.02524400	2.98608000
N	-2.12474900	-0.21120900	0.92648700
S	-3.15517600	1.09672900	1.03743000
O	-4.10794900	1.02428400	-0.06091700
O	-3.65631400	1.12006000	2.40999800
C	-2.19699700	2.57516900	0.78067600
C	-1.60916800	3.21490600	1.86749200
C	-2.07602500	3.08342400	-0.51244800
C	-0.90601200	4.39778500	1.65070100
H	-1.73615500	2.81589700	2.86902100
C	-1.35964600	4.25603700	-0.71038900
H	-2.56552600	2.57533300	-1.33744500
C	-0.77799800	4.93677900	0.36641800
H	-0.47274700	4.92337600	2.49710200
H	-1.27334000	4.66918100	-1.71158600
C	-0.05653800	6.23715700	0.12833300
H	-0.68070700	6.92016900	-0.45403700
H	0.86533300	6.07120800	-0.43767600
H	0.20629100	6.72674100	1.06819900
C	-1.87867200	-2.08922400	2.50894300
C	-1.00929500	-2.96708500	3.15979300
C	-3.17453000	-2.52550000	2.21920800
C	-1.41880800	-4.25672500	3.49504400
H	0.00066000	-2.65737100	3.41020300
C	-3.58566500	-3.81223700	2.55341300
H	-3.86081200	-1.84798800	1.72011000

C	-2.70687700	-4.68589400	3.19046500
H	-0.72417800	-4.92690500	3.99175100
H	-4.59527600	-4.13214100	2.31506200
H	-3.02362100	-5.69138400	3.44794700
H	1.12107000	-2.14091200	1.26424800
H	-0.80852100	0.66376200	-0.48125300

TS3<sub>2</sub><sup>(S,R,S)</sup>

P	-2.39177000	-0.24496600	-0.72631400
C	-2.09894800	-0.69419800	-2.47206000
C	-1.60113300	0.44453500	-3.36714700
H	-1.41583100	-1.55049100	-2.48479500
H	-3.06226800	-1.07156000	-2.83693600
C	-1.15777500	-0.06726100	-4.73745200
H	-0.76320200	0.97167700	-2.89108800
H	-2.40002100	1.18555600	-3.49679200
C	-0.68194100	1.06169600	-5.64618900
H	-1.99091900	-0.60289700	-5.20793300
H	-0.35311600	-0.80054800	-4.60042900
H	-0.36205800	0.67983100	-6.61854600
H	0.16398500	1.59094000	-5.19690000
H	-1.48061700	1.79017800	-5.81549700
C	-3.12346700	-1.75382100	-0.00433600
C	-4.63286100	-1.89031700	-0.21106700
H	-2.58894200	-2.58769000	-0.47516400
H	-2.87518500	-1.75549800	1.05739000
C	-5.12140300	-3.25147900	0.28676900
H	-4.89625300	-1.77849800	-1.27143200
H	-5.15512300	-1.09535900	0.33439300
C	-6.62835400	-3.42029500	0.11966300
H	-4.84510800	-3.36316800	1.34239500
H	-4.59036400	-4.04245400	-0.25673700
H	-6.96295000	-4.39320400	0.48765800
H	-6.91512500	-3.34196200	-0.93377500
H	-7.17047000	-2.64642600	0.67191100
C	-3.60954500	1.12948500	-0.83655700
C	-3.00241800	2.53645600	-0.85844300
H	-4.16164000	0.94634600	-1.76646100
H	-4.31625700	1.03223600	-0.01055700
C	-4.06665700	3.59523400	-1.14479600
H	-2.20989400	2.60304800	-1.61390800
H	-2.52275200	2.76089800	0.10242100
C	-3.48582500	5.00572100	-1.12507200

H	-4.86897400	3.51036900	-0.40120600
H	-4.52481600	3.39213200	-2.12040800
H	-4.25555800	5.75520300	-1.32368700
H	-2.70328800	5.11593600	-1.88197300
H	-3.03906300	5.23010800	-0.15121300
C	-0.80528600	0.21599200	0.01717100
C	-0.72579700	0.93496500	1.18272500
C	0.45803100	-0.27347000	-0.69292300
C	0.51184900	1.37634700	1.81156400
H	1.23298900	0.18148300	1.69805700
C	-1.99995900	1.17971900	1.95273500
O	-2.99853000	0.48870800	1.85993300
O	-1.92726900	2.24899000	2.73585300
C	-3.11629700	2.58435000	3.48243700
C	-4.12879600	3.28321300	2.59623200
H	-3.52587500	1.67102800	3.91853500
H	-2.75765600	3.23888000	4.27682300
H	-4.97395400	3.62292800	3.19955700
H	-4.50623800	2.60038000	1.83106900
H	-3.67728400	4.15309400	2.11119500
H	0.23325100	-0.60950300	-1.70644500
C	1.43726700	2.33333000	1.16353300
C	2.57831300	2.73527900	1.88621700
C	1.28693100	2.84050900	-0.13606300
C	3.53417700	3.57090000	1.32602900
H	2.71750800	2.34932900	2.89263600
C	2.25406400	3.67033500	-0.70398700
H	0.39577000	2.58916100	-0.70701000
C	3.38745400	4.03506100	0.01652300
H	4.40758900	3.85124000	1.90777800
H	2.11180400	4.03982200	-1.71562800
H	4.13964400	4.67929800	-0.42764400
H	1.17357400	0.54896500	-0.79922700
C	1.18669400	-1.43145000	0.02059100
H	2.01397100	-1.71029300	-0.65397900
N	1.71401600	-0.94513000	1.29280100
S	3.15621100	-1.46781600	1.73810600
O	3.50983600	-0.75847300	2.97543800
O	3.24218500	-2.93665200	1.76238500
C	4.30724200	-0.95984300	0.45711300
C	5.31936400	-1.82487000	0.05669700
C	4.19607600	0.31136300	-0.10720400
C	6.23187200	-1.40800100	-0.91064400
H	5.37930100	-2.81539100	0.49431900



C	5.11176100	0.71221900	-1.07134700
H	3.39702000	0.97916100	0.19982500
C	6.14426900	-0.13874600	-1.48513600
H	7.02238700	-2.08303900	-1.22666700
H	5.02085100	1.70379100	-1.50796800
C	7.13121100	0.31674900	-2.52845700
H	7.71292700	1.17346200	-2.16453900
H	6.61406300	0.63688400	-3.44196100
H	7.82937400	-0.48506600	-2.79017900
C	0.29184000	-2.65711000	0.15449500
C	0.00744400	-3.42414300	-0.98071200
C	-0.26823700	-3.02963000	1.37629600
C	-0.82555600	-4.53797300	-0.90017800
H	0.46147700	-3.15755700	-1.93423800
C	-1.10320200	-4.14295600	1.46077800
H	-0.02679200	-2.44422700	2.25772000
C	-1.38710000	-4.89854600	0.32484800
H	-1.02882400	-5.12799100	-1.78851600
H	-1.53107100	-4.42344500	2.41855800
H	-2.03346600	-5.76789600	0.39311200
H	0.37088600	1.62324600	2.86214400
M3 <sub>2</sub> <sup>(S,R,S)</sup>			
P	2.23063600	0.08776300	-0.91585500
C	1.85706600	0.06534500	-2.71923100
C	1.07623800	-1.15422600	-3.20747800
H	1.32722900	0.99267500	-2.96939400
H	2.82477300	0.12166600	-3.23109400
C	0.84498700	-1.12565800	-4.71778900
H	0.10770500	-1.20553400	-2.69525700
H	1.61689200	-2.07150100	-2.94239300
C	0.04637000	-2.33428400	-5.19763500
H	1.81281000	-1.08914900	-5.23257600
H	0.31691400	-0.20122300	-4.98237000
H	-0.11490000	-2.30404800	-6.27801600
H	-0.93398600	-2.37049300	-4.71154600
H	0.56974900	-3.26587700	-4.96085500
C	3.01684000	1.73058400	-0.69412000
C	4.21924200	2.03866400	-1.58936500
H	2.22371100	2.47060800	-0.85544500
H	3.28770900	1.78556300	0.36313000
C	4.79840300	3.41889400	-1.27338700
H	3.92907400	2.01190900	-2.64697400

H	5.00319200	1.28135900	-1.45727500
C	5.99025800	3.76635900	-2.16041600
H	5.09453300	3.44863100	-0.21758400
H	4.00744900	4.17021400	-1.39129800
H	6.39375400	4.75332800	-1.92033400
H	5.70263900	3.76834900	-3.21655600
H	6.79444400	3.03440400	-2.03586100
C	3.59518300	-1.12637900	-0.69482100
C	3.21208100	-2.57529200	-0.37936700
H	4.16425800	-1.09398400	-1.63237100
H	4.24893800	-0.72608600	0.08683400
C	4.43656700	-3.49019900	-0.40920700
H	2.46382900	-2.94124500	-1.09282900
H	2.74200100	-2.64551300	0.60796800
C	4.08546800	-4.93143500	-0.05189000
H	5.18842900	-3.10577500	0.29178200
H	4.89401800	-3.45166100	-1.40550900
H	4.96919400	-5.57404300	-0.06884600
H	3.35598400	-5.34112000	-0.75729300
H	3.64557400	-4.98859300	0.94907900
C	0.76997400	-0.26716200	-0.03135600
C	0.79127800	-0.99171700	1.20974500
C	-0.49740000	0.34725200	-0.59413700
C	-0.18514200	-1.79397400	1.75693000
H	-1.53326200	0.01644400	1.69779700
C	2.01089300	-0.80363600	2.07874100
O	2.83441900	0.07730800	1.91530000
O	2.13886100	-1.72682300	3.04024300
C	3.30491000	-1.62414900	3.87589200
C	4.51097200	-2.22423900	3.17864200
H	3.47150600	-0.57559700	4.13100000
H	3.04610700	-2.18052700	4.77742200
H	5.37561100	-2.21049400	3.84659000
H	4.75685500	-1.64825600	2.28299900
H	4.30969300	-3.26026300	2.89199800
H	-0.29548500	0.77960200	-1.58000500
C	-1.33547600	-2.41246300	1.10784000
C	-2.40610600	-2.87061200	1.90319700
C	-1.39251500	-2.67581200	-0.27480400
C	-3.48956400	-3.53676200	1.34381600
H	-2.37724800	-2.68967300	2.97467400
C	-2.47499600	-3.34913000	-0.83191200
H	-0.55364100	-2.37656300	-0.89703900
C	-3.53406900	-3.77624100	-0.03070500

H	-4.30444500	-3.86705400	1.98037100
H	-2.48897300	-3.54596200	-1.90023100
H	-4.38100400	-4.29292600	-0.47084700
H	-1.30043900	-0.38817600	-0.76070300
C	-1.14232600	1.50339800	0.21624600
H	-1.95769200	1.88979300	-0.41328500
N	-1.73655400	0.98434900	1.45914600
S	-3.26965200	1.42145000	1.84522000
O	-3.64304200	0.58705600	2.98362800
O	-3.31787400	2.87498100	1.95886700
C	-4.28643400	0.98701800	0.44942600
C	-5.11608500	1.94546600	-0.11903300
C	-4.24612400	-0.31910000	-0.03958700
C	-5.92740600	1.58335600	-1.19249100
H	-5.12081300	2.95541300	0.27584300
C	-5.05636700	-0.65895800	-1.11308300
H	-3.58920500	-1.06060900	0.40719600
C	-5.90962200	0.28412600	-1.70227700
H	-6.58247000	2.32461800	-1.64055100
H	-5.02624700	-1.67505400	-1.49772500
C	-6.78033100	-0.10805700	-2.86669400
H	-6.16954900	-0.40112700	-3.72571500
H	-7.42751900	0.71555000	-3.17336100
H	-7.41052300	-0.96361300	-2.60830700
C	-0.18540800	2.64404500	0.48628500
C	-0.09230300	3.69922700	-0.42295200
C	0.65826000	2.62868300	1.59857900
C	0.83493900	4.72280700	-0.22986900
H	-0.75098500	3.72096000	-1.28853600
C	1.58072400	3.65161000	1.79667100
H	0.58513700	1.80873200	2.30626600
C	1.67527500	4.69925900	0.88163800
H	0.89502700	5.54026100	-0.94175500
H	2.23396800	3.62639300	2.66350000
H	2.39735600	5.49498700	1.03567400
H	-0.07535600	-2.04964900	2.80535200
TS4 <sub>2</sub> <sup>(S,R,S)</sup>			
P	-1.69319300	0.91068100	0.41326300
C	-2.69895100	0.85650700	-1.11689500
C	-2.23810100	1.73936100	-2.27735900
H	-2.77350000	-0.19029900	-1.43224900
H	-3.70527600	1.16304100	-0.80872100

C	-3.14397700	1.55861300	-3.49561300
H	-1.21053000	1.49248000	-2.56634000
H	-2.23973900	2.79478300	-1.97513000
C	-2.69941200	2.41535600	-4.67695600
H	-4.17504900	1.80856200	-3.21774300
H	-3.14517400	0.49785800	-3.77682900
H	-3.35432800	2.27365000	-5.54007900
H	-1.67996200	2.15834800	-4.98222800
H	-2.71159100	3.47802900	-4.41547800
C	-2.63984100	-0.05384700	1.65581500
C	-4.15549100	-0.10627000	1.46249500
H	-2.21404200	-1.06209600	1.64002400
H	-2.37415500	0.37766500	2.62523700
C	-4.82246200	-0.93757300	2.55800800
H	-4.39288400	-0.55661100	0.49099900
H	-4.58326700	0.90566500	1.46243800
C	-6.33330200	-1.03272200	2.36797600
H	-4.59298900	-0.50162600	3.53771200
H	-4.38241500	-1.94308100	2.55476100
H	-6.79719500	-1.63383000	3.15386400
H	-6.57496400	-1.49283100	1.40434600
H	-6.79305800	-0.03950400	2.38805100
C	-1.78800100	2.65843600	0.97369000
C	-0.73757400	3.63840100	0.43818400
H	-2.79278700	2.98705900	0.67625700
H	-1.76670900	2.63810000	2.06688000
C	-1.16825500	5.08814300	0.65746900
H	-0.55072100	3.47024600	-0.63002800
H	0.22050200	3.47384300	0.94217500
C	-0.09807800	6.07717700	0.20590100
H	-1.38930400	5.23819400	1.72179400
H	-2.10423300	5.27320000	0.11586600
H	-0.41901300	7.10999400	0.36157800
H	0.12653200	5.94966400	-0.85763000
H	0.83160900	5.92474500	0.76320600
C	-0.03928600	0.24130100	0.18392400
C	1.09376700	1.02442800	0.74186500
C	0.19554800	-0.65988400	-1.02570400
C	2.25291500	1.40833000	0.15765000
H	-0.09283300	-0.90520500	0.95409500
C	0.94442500	1.31412100	2.20634800
O	-0.05837100	1.02309800	2.83410200
O	1.97476200	1.96309700	2.75790900
C	1.80386300	2.39268400	4.12214900

C	0.98006600	3.66557700	4.17153300
H	1.33690400	1.58775200	4.69227800
H	2.81839000	2.55567600	4.48698100
H	0.90904900	4.02524300	5.20074900
H	-0.03147600	3.47996100	3.80125100
H	1.44513800	4.44478000	3.56208400
H	-0.25447000	-0.33143800	-1.96712700
C	2.62008700	1.44536700	-1.26323000
C	3.96295900	1.28493200	-1.63164000
C	1.68569100	1.73690700	-2.26540000
C	4.34932700	1.36097300	-2.96595500
H	4.70403700	1.09828500	-0.85880100
C	2.06946500	1.82460600	-3.59759100
H	0.65465000	1.91266000	-1.97857400
C	3.40276800	1.62459500	-3.95468000
H	5.39290400	1.22597400	-3.23383100
H	1.32916200	2.05531400	-4.35779800
H	3.70456100	1.68831300	-4.99504400
H	1.27562100	-0.70784300	-1.18778700
C	-0.27572300	-2.13012500	-0.67424900
H	0.43483300	-2.81734500	-1.15230600
N	-0.22966400	-2.21105200	0.77922600
S	0.83138400	-3.22778000	1.43209400
O	0.81408200	-3.00409400	2.88134400
O	0.62865400	-4.59909100	0.94323700
C	2.44765300	-2.73683300	0.84787100
C	3.00814700	-3.36003800	-0.26619400
C	3.09194800	-1.66856700	1.46354200
C	4.21914100	-2.89648800	-0.76715000
H	2.50166900	-4.20755800	-0.71668300
C	4.30894100	-1.22207000	0.95676000
H	2.64834900	-1.20101900	2.33805900
C	4.88385800	-1.82113200	-0.16695400
H	4.66129900	-3.37889600	-1.63469300
H	4.81849800	-0.39381000	1.44278100
C	6.18895600	-1.32949300	-0.73571000
H	6.62854500	-0.55010000	-0.10916100
H	6.03696700	-0.91665400	-1.73851100
H	6.91099800	-2.14595400	-0.82411100
C	-1.65487800	-2.44527400	-1.23231800
C	-1.88102800	-2.31487900	-2.60889500
C	-2.71585200	-2.83527900	-0.41597500
C	-3.14717100	-2.52051500	-3.14708200
H	-1.05779900	-2.03981700	-3.26465800

C	-3.98959900	-3.03641200	-0.95208600
H	-2.53172400	-2.98174300	0.64328500
C	-4.21333600	-2.86609800	-2.31480500
H	-3.30455700	-2.40882900	-4.21565600
H	-4.80651300	-3.32761200	-0.29769300
H	-5.20425500	-3.01538200	-2.73126500
H	3.03144400	1.76365100	0.82722200
M4 <sub>2</sub> <sup>(S,R,S)</sup>			
P	1.26408800	0.62864700	-1.13603800
C	2.72143700	1.32792600	-0.27194700
C	2.54872400	2.36783300	0.83820000
H	3.30572400	0.48277800	0.10586000
H	3.29783600	1.76591700	-1.09902900
C	3.89911000	2.98525000	1.20438400
H	2.12622700	1.89085000	1.72900400
H	1.86350300	3.16835300	0.53950500
C	3.79818300	3.87585600	2.43845100
H	4.27306000	3.56140200	0.34948400
H	4.62144900	2.17973600	1.38221500
H	4.75743100	4.34404300	2.67177300
H	3.48678500	3.29160600	3.31072700
H	3.06166500	4.67191600	2.28826100
C	1.85477800	-0.78371600	-2.12432300
C	3.26235000	-0.64388100	-2.70373500
H	1.77486000	-1.65668100	-1.46494900
H	1.10021200	-0.91616700	-2.90848600
C	3.64570200	-1.87932900	-3.51866300
H	3.98868300	-0.51944000	-1.89148500
H	3.33381300	0.24917500	-3.33912000
C	5.05807000	-1.77628500	-4.08618000
H	2.92233700	-2.01693100	-4.33072000
H	3.56512700	-2.76496700	-2.87624100
H	5.32072000	-2.66712900	-4.66157100
H	5.79310300	-1.66530900	-3.28270400
H	5.15149000	-0.90882100	-4.74707500
C	0.70536600	1.90078500	-2.32000700
C	0.26844400	3.24640800	-1.72927500
H	1.54582100	2.03684300	-3.01206000
H	-0.10050900	1.44375900	-2.90022900
C	-0.55345800	4.05058000	-2.73686000
H	1.14997700	3.82550600	-1.43258700
H	-0.33915500	3.09456100	-0.82859100

C	-0.94877600	5.41918300	-2.19214700
H	-1.45254400	3.47577200	-2.99243400
H	0.02000300	4.16431800	-3.66469800
H	-1.54960000	5.97541300	-2.91545400
H	-0.06279500	6.01732700	-1.95849700
H	-1.53498600	5.31703600	-1.27346800
C	-0.13790000	-0.05690800	-0.11960100
C	-1.48403500	0.58381500	-0.40901000
C	0.17510600	-0.40142000	1.34814900
C	-2.28513000	1.29677600	0.40579500
H	-0.21552700	-1.04758300	-0.59536000
C	-2.02953900	0.18696400	-1.74779800
O	-1.38980800	-0.46989200	-2.54971100
O	-3.26079800	0.63742700	-1.99776300
C	-3.83011600	0.27812400	-3.27225400
C	-3.36959400	1.23223100	-4.35588000
H	-3.55088300	-0.75184200	-3.50360200
H	-4.90831900	0.33561900	-3.11366200
H	-3.85451500	0.97738800	-5.30128800
H	-2.28805200	1.15978300	-4.49392600
H	-3.63145900	2.26131200	-4.09907300
H	0.68097600	0.40343700	1.88150300
C	-2.00710700	1.87778700	1.72665200
C	-3.01873600	1.88491400	2.69585800
C	-0.78575400	2.48884900	2.02352400
C	-2.78811600	2.44010200	3.94976500
H	-3.98386800	1.44336500	2.46164500
C	-0.55665400	3.05899900	3.27037700
H	-0.01704400	2.52668800	1.26041700
C	-1.55628600	3.02544600	4.24108500
H	-3.57288700	2.42450000	4.69893400
H	0.39813700	3.53265400	3.47917100
H	-1.38220500	3.46588700	5.21728800
H	-0.79694900	-0.52338900	1.83405300
C	0.96827100	-1.74240700	1.51907900
H	0.70906200	-2.09706900	2.52933400
N	0.63254700	-2.72581000	0.51029600
S	-0.51255800	-3.74178900	0.87517900
O	-0.55459700	-4.79619200	-0.15314800
O	-0.48426400	-4.20241300	2.28271200
C	-2.09861400	-2.89940400	0.73297000
C	-2.67920500	-2.30560700	1.84931500
C	-2.70456800	-2.77758500	-0.51765900
C	-3.84733700	-1.55804800	1.70760300

H	-2.21574700	-2.43660700	2.82272600
C	-3.88213800	-2.05023500	-0.64228000
H	-2.25334600	-3.26235900	-1.37806100
C	-4.45750000	-1.40852300	0.46062800
H	-4.29467000	-1.09298300	2.58233700
H	-4.36511500	-1.96896400	-1.61351600
C	-5.69167600	-0.56447500	0.28327400
H	-6.49241300	-1.12886500	-0.20333800
H	-5.47058400	0.29990300	-0.35360000
H	-6.06639200	-0.19657600	1.24117400
C	2.47382200	-1.49197300	1.54433700
C	3.01269600	-0.62283100	2.50266700
C	3.34584900	-2.11374100	0.64942300
C	4.37440600	-0.33959600	2.53025200
H	2.35750200	-0.16630600	3.24216600
C	4.71152400	-1.82216700	0.66400300
H	2.93706300	-2.83602200	-0.04927200
C	5.22938700	-0.92414000	1.59403100
H	4.77029100	0.33840000	3.28096900
H	5.37110500	-2.30493900	-0.05191400
H	6.29036400	-0.69585800	1.60531500
H	-3.29318600	1.47438500	0.03785800
M4 <sub>2</sub> <sup>r(S,R,S)</sup>			
P	1.64484800	1.52753600	0.55797600
C	0.48280400	2.79748600	1.19078100
C	-0.80992300	3.13750900	0.44449100
H	0.24935200	2.47915800	2.21457000
H	1.10397700	3.69813700	1.28244300
C	-1.59613100	4.23382300	1.16352800
H	-1.45161900	2.25342400	0.36097900
H	-0.58369000	3.47513600	-0.57398500
C	-2.81613800	4.65039900	0.34725700
H	-0.94885500	5.10059500	1.34257000
H	-1.90793600	3.86269600	2.14750600
H	-3.43620200	5.37059300	0.88683000
H	-3.43650700	3.77776400	0.11576900
H	-2.51192400	5.10730200	-0.60000700
C	2.81923600	1.26432900	1.92974800
C	3.47726000	2.51796600	2.50990200
H	2.25781300	0.72934400	2.70736200
H	3.56328600	0.56207100	1.53509900
C	4.49915600	2.15432400	3.58825500



H	2.71788800	3.17778900	2.94561400
H	3.98050100	3.08753200	1.71895000
C	5.15528000	3.38990400	4.19697800
H	5.26330000	1.50083000	3.15152100
H	4.00062900	1.57192100	4.37221000
H	5.88297400	3.11257900	4.96323900
H	4.40809800	4.04051700	4.66150300
H	5.67728800	3.97195500	3.43140600
C	2.63166300	2.14614300	-0.84442900
C	1.91076100	2.51128000	-2.14461800
H	3.16758200	3.01931200	-0.45249800
H	3.37709500	1.36177100	-1.02137600
C	2.89967100	3.05437200	-3.17712800
H	1.13715100	3.26540800	-1.95671700
H	1.41216600	1.62865200	-2.55696700
C	2.21241300	3.40236900	-4.49385700
H	3.68182300	2.30507600	-3.34939800
H	3.39898400	3.94090100	-2.76826000
H	2.92833500	3.78699100	-5.22390200
H	1.44245700	4.16492800	-4.34254600
H	1.72935300	2.52072500	-4.92577300
C	0.93571800	-0.16355900	0.28041000
C	1.18456400	-0.79897800	-1.07446600
C	-0.42857900	-0.39178000	0.95222800
C	0.37805700	-0.94658400	-2.14341600
C	2.54955700	-1.41066200	-1.13494900
O	3.45344500	-1.04255600	-0.40246000
O	2.69750800	-2.35768800	-2.05762200
C	4.00862500	-2.94919300	-2.16245300
C	4.93640800	-2.06780600	-2.97526100
H	4.39228000	-3.12026100	-1.15400500
H	3.83272300	-3.90833300	-2.65066000
H	5.90496300	-2.56007500	-3.09084400
H	5.09226500	-1.11087800	-2.47291200
H	4.51907000	-1.88723900	-3.96849000
H	-0.40299000	0.11619700	1.92628000
C	-0.89057900	-0.29308100	-2.47986100
C	-1.18461400	0.99710400	-2.03482900
C	-1.77010900	-0.90575300	-3.38364300
C	-2.32285600	1.66885800	-2.46341000
H	-0.48414500	1.49025900	-1.37444100
C	-2.91997400	-0.24613800	-3.80371700
H	-1.55010000	-1.90471400	-3.74804200
C	-3.19596700	1.04595900	-3.35282800

H	-2.52248500	2.67652900	-2.10787800
H	-3.59859300	-0.73497300	-4.49474100
H	-4.08642700	1.56326200	-3.69549900
H	-1.25990600	0.02731800	0.38052300
C	-0.75562400	-1.90943700	1.18684500
H	-1.34415000	-1.93165500	2.11881200
N	-1.49022800	-2.45636300	0.05856300
S	-2.99271300	-2.75949100	0.38738300
O	-3.67743600	-3.22813300	-0.83300000
O	-3.21802500	-3.59293300	1.59476500
C	-3.77301700	-1.19202000	0.81716800
C	-4.06408400	-0.88345800	2.14354300
C	-3.98071700	-0.24482400	-0.18178000
C	-4.57623600	0.37057200	2.46456600
H	-3.90316900	-1.63903400	2.90546000
C	-4.50292100	1.00317300	0.14764000
H	-3.74361500	-0.49390400	-1.21257600
C	-4.80799700	1.33016000	1.47420300
H	-4.81422000	0.60630100	3.49904900
H	-4.68802700	1.73004400	-0.64056500
C	-5.37942000	2.67656800	1.84078400
H	-5.72915100	3.21482600	0.95663100
H	-4.62858600	3.30191200	2.33643100
H	-6.21969000	2.56830100	2.53187900
C	0.51386500	-2.69622900	1.48338300
C	1.20702200	-2.47729900	2.67971500
C	1.05615600	-3.57583200	0.54590400
C	2.42528800	-3.10523800	2.92500900
H	0.78627900	-1.80337000	3.42457000
C	2.27433400	-4.21016600	0.79060400
H	0.50522500	-3.74541800	-0.37348400
C	2.96614500	-3.97233500	1.97549100
H	2.94938300	-2.92386000	3.85844200
H	2.68261700	-4.89373900	0.05114200
H	3.91521600	-4.46425900	2.16390400
H	0.75326600	-1.61418300	-2.91608900
H	1.64242200	-0.69989800	0.92306100
TS5 <sub>2</sub> <sup>(S,R,S)</sup>			
P	2.54148800	0.83368800	0.75354600
C	2.22851500	2.22032000	1.91069000
C	1.14181200	3.25324300	1.60155400
H	2.02598000	1.74231200	2.87759800

H	3.19958100	2.72214800	2.01086600
C	1.11557900	4.35816900	2.65773100
H	0.15934300	2.77022700	1.57016500
H	1.30919700	3.70673200	0.61746700
C	0.02683700	5.38719800	2.36913200
H	2.09566200	4.84874000	2.69323800
H	0.95397800	3.90810200	3.64440300
H	0.00435900	6.16789700	3.13306000
H	-0.95954400	4.91308100	2.34178700
H	0.19375300	5.86955000	1.40062500
C	3.70305500	-0.25637600	1.64374800
C	4.98276000	0.39822000	2.16551800
H	3.13021100	-0.70280200	2.46755100
H	3.91952900	-1.06202900	0.93143300
C	5.92051700	-0.63576700	2.79116200
H	4.74029100	1.16067300	2.91546600
H	5.50961800	0.90873000	1.34983300
C	7.20060600	-0.00013600	3.32480000
H	6.16418800	-1.39689100	2.04087700
H	5.39375400	-1.15352000	3.60145600
H	7.85957000	-0.74933300	3.76991500
H	6.97517500	0.74827600	4.09073400
H	7.75198200	0.49879900	2.52193800
C	3.41939900	1.38096900	-0.74820200
C	2.68184800	2.29466700	-1.73044700
H	4.33918900	1.86213900	-0.39412700
H	3.70487100	0.44249400	-1.23981300
C	3.56569100	2.62763600	-2.93256800
H	2.38097700	3.22663300	-1.23696100
H	1.77162200	1.79785800	-2.08068900
C	2.85115500	3.53886800	-3.92599500
H	3.85939800	1.69337000	-3.42681200
H	4.49120200	3.10298400	-2.58521500
H	3.48610400	3.76642700	-4.78558400
H	2.57086100	4.48562300	-3.45383100
H	1.93562600	3.06777400	-4.29654700
C	1.10659700	-0.28301200	0.36318700
C	0.81815000	-0.53632600	-1.09806500
C	-0.15180400	-0.13454400	1.22818300
C	-0.41608500	-0.27937400	-1.68502700
C	1.71709700	-1.50811200	-1.67888500
O	2.79539500	-1.82355600	-1.17050300
O	1.31396800	-2.03038700	-2.85903700
C	2.22196200	-2.93832700	-3.49635300

C	3.32507600	-2.18900100	-4.22094300
H	2.63216400	-3.62014800	-2.74784200
H	1.60164700	-3.50370700	-4.19403800
H	3.96634400	-2.89260200	-4.75810700
H	3.93721400	-1.63566500	-3.50556200
H	2.89916800	-1.48795800	-4.94299900
H	0.13147900	-0.12490000	2.28723800
C	-1.15088300	1.00987700	-1.70951400
C	-0.69324700	2.14769700	-1.04218000
C	-2.31235800	1.11715800	-2.48618500
C	-1.40170300	3.34485600	-1.08384600
H	0.23498400	2.09527600	-0.48776400
C	-3.01829000	2.31385000	-2.54199900
H	-2.67865600	0.23789400	-3.00577700
C	-2.57459500	3.42894900	-1.83117200
H	-1.03145500	4.21108600	-0.54188400
H	-3.92377100	2.37496000	-3.13719100
H	-3.13152500	4.35951400	-1.87028900
H	-0.70381000	0.78552900	1.02511400
C	-1.11858200	-1.33024000	0.99268900
H	-1.90454600	-1.21881900	1.75795100
N	-1.69147000	-1.23838200	-0.34317700
S	-3.15034900	-1.81184400	-0.55211900
O	-3.46344200	-1.74246500	-1.99083100
O	-3.38272200	-3.11841300	0.09286300
C	-4.28425000	-0.69603200	0.28936900
C	-5.52226900	-1.17775400	0.71324700
C	-3.94900200	0.64089400	0.47781300
C	-6.42673900	-0.31155400	1.31448000
H	-5.76034100	-2.22795300	0.57823900
C	-4.86378200	1.49890300	1.08479600
H	-2.97973700	1.00704700	0.15118300
C	-6.11203200	1.03909500	1.50822400
H	-7.39230300	-0.68583700	1.64465800
H	-4.60113800	2.54371100	1.22949400
C	-7.09671100	1.96147500	2.17912400
H	-7.18355900	1.72833100	3.24513000
H	-8.09303000	1.85645400	1.74123700
H	-6.78857400	3.00497900	2.08695700
C	-0.39417700	-2.64447900	1.27062000
C	-0.03496000	-2.97159900	2.58126600
C	-0.01546900	-3.49935700	0.23540800
C	0.69475300	-4.12582000	2.85349300
H	-0.33846600	-2.32024300	3.39880500

C	0.72098600	-4.65159900	0.50394800
H	-0.30492100	-3.24730200	-0.78083300
C	1.07943100	-4.96873400	1.81208700
H	0.95902800	-4.36957700	3.87806300
H	1.01225600	-5.30515500	-0.31294100
H	1.64904300	-5.86865900	2.02134300
H	-0.63434000	-0.89386600	-2.55561200
H	1.56901200	-1.22036300	0.70430100

M5<sub>2</sub><sup>(S,R,S)</sup>

P	-2.54774000	0.03369100	0.69544100
C	-2.50797600	-0.99656500	2.20577500
C	-1.41825000	-2.08535500	2.22898200
H	-2.42583800	-0.33106000	3.07156200
H	-3.50058700	-1.46165500	2.26498400
C	-1.86142600	-3.29076000	3.05848300
H	-0.49672800	-1.67951100	2.65727200
H	-1.14828900	-2.41363800	1.21427500
C	-0.77805000	-4.35898400	3.15742800
H	-2.76827800	-3.71996100	2.61244800
H	-2.14460400	-2.94799500	4.06137500
H	-1.11311600	-5.21005800	3.75556100
H	0.12733000	-3.95384600	3.62060500
H	-0.50365300	-4.72430400	2.16318800
C	-3.97917900	1.15222700	0.80810000
C	-5.35716200	0.49091000	0.75747900
H	-3.85333400	1.73204700	1.73147900
H	-3.84466000	1.83837000	-0.03676400
C	-6.47677300	1.51853000	0.92837300
H	-5.45060300	-0.27438200	1.53876200
H	-5.48256400	-0.01865500	-0.20581300
C	-7.86076100	0.88289100	0.83772800
H	-6.36958600	2.29332700	0.16018900
H	-6.35766600	2.01959600	1.89646000
H	-8.64888500	1.62827600	0.96844600
H	-7.99021700	0.11685900	1.60852700
H	-8.00672600	0.40543200	-0.13600000
C	-2.75972100	-1.09875300	-0.71262400
C	-3.56414300	-2.37669800	-0.46280700
H	-3.19307000	-0.48438400	-1.50872700
H	-1.74186600	-1.34200900	-1.03945800
C	-3.59798400	-3.23457200	-1.72842200
H	-4.58959400	-2.14438800	-0.15080500

H	-3.11479500	-2.96400800	0.34698700
C	-4.36273800	-4.53870100	-1.52405700
H	-2.56545300	-3.44790400	-2.03387400
H	-4.05098900	-2.65707800	-2.54343300
H	-4.37100200	-5.14240800	-2.43479000
H	-5.40152500	-4.34127900	-1.24167600
H	-3.90740700	-5.13591100	-0.72771600
C	-1.04663300	1.13955000	0.47201000
C	-0.30298700	0.87542800	-0.78990400
C	-0.10498100	1.13276800	1.68285200
C	1.10382300	0.37623300	-0.70049800
C	-0.96750200	1.17806900	-1.96491400
O	-2.16512600	1.54985100	-2.03753800
O	-0.21869300	1.02312200	-3.12523400
C	-0.95505800	1.06094700	-4.34129800
C	-1.65675200	-0.26295300	-4.59813100
H	-1.67962700	1.87813000	-4.30840900
H	-0.21797600	1.26973800	-5.12126300
H	-2.19738200	-0.23784000	-5.54861000
H	-2.37312800	-0.46015300	-3.79588700
H	-0.93219000	-1.08170000	-4.63448200
H	-0.57599900	1.59558100	2.55570300
C	1.18999300	-1.12449400	-0.38959600
C	0.66858000	-2.00712000	-1.34385200
C	1.75714100	-1.65440000	0.76784800
C	0.70743200	-3.38281400	-1.14306300
H	0.23250800	-1.59165100	-2.25155700
C	1.80757600	-3.03407400	0.97027400
H	2.18318300	-0.98254200	1.50711200
C	1.28178300	-3.90303300	0.01856900
H	0.30338700	-4.05182300	-1.89716300
H	2.25933400	-3.42828100	1.87640900
H	1.32234000	-4.97656200	0.17547500
H	0.18305400	0.11559400	1.95711300
C	1.18164100	1.91238900	1.34875700
H	1.82321800	1.89033600	2.23598300
N	1.88280800	1.18110000	0.28147200
S	3.42428200	1.62192800	-0.10735100
O	3.48561200	2.11525900	-1.48322200
O	3.90258300	2.47093400	0.98248600
C	4.31942600	0.09028900	-0.07152400
C	4.84028100	-0.35548800	1.14184100
C	4.38024400	-0.69271600	-1.21773900
C	5.40736900	-1.62026100	1.20225900

H	4.79175100	0.28140500	2.01924700
C	4.94580300	-1.96211600	-1.13633400
H	3.98250600	-0.31701600	-2.15507900
C	5.45141500	-2.44691600	0.07157500
H	5.81726700	-1.98110300	2.14176400
H	4.98839900	-2.58586300	-2.02393200
C	6.02319500	-3.83584500	0.17410500
H	7.02394700	-3.81670500	0.62125500
H	6.08773200	-4.31341000	-0.80826100
H	5.38844500	-4.46135900	0.81610000
C	0.87354700	3.37045500	1.03561700
C	0.57081000	4.22132700	2.10187000
C	0.84627700	3.87670800	-0.26472800
C	0.23775800	5.55366000	1.87879300
H	0.60536600	3.83636700	3.11909500
C	0.51451700	5.21218300	-0.48853000
H	1.08291600	3.22381100	-1.09918800
C	0.20693900	6.05286500	0.57790900
H	0.00891700	6.20220300	2.71869700
H	0.49743400	5.59565100	-1.50390600
H	-0.04888100	7.09213500	0.39755400
H	1.55635000	0.53335800	-1.68547500
H	-1.53104900	2.12611200	0.41076300
TS6 <sub>2</sub> <sup>(S,R,S)</sup>			
P	-2.40636000	0.15723200	0.95715300
C	-2.63861100	-1.09954200	2.30086100
C	-1.41396200	-1.96361300	2.60404700
H	-2.93338400	-0.53413900	3.19310500
H	-3.49021900	-1.73639400	2.02998500
C	-1.71230300	-3.06532600	3.61884700
H	-0.60124500	-1.33432200	2.98811000
H	-1.04282300	-2.42135400	1.68015600
C	-0.47092900	-3.89294400	3.94163000
H	-2.50154500	-3.71498400	3.22058700
H	-2.11150300	-2.61645200	4.53651100
H	-0.69568000	-4.69454100	4.64943400
H	0.31182900	-3.26586100	4.38016300
H	-0.06080000	-4.34966800	3.03455100
C	-3.87305200	1.24850000	1.12490500
C	-5.22913800	0.54463200	1.05685400
H	-3.76745400	1.79255600	2.07234100
H	-3.76827500	1.97931300	0.31381100

C	-6.39401600	1.53199000	1.13433400
H	-5.32001600	-0.18192200	1.87444700
H	-5.30372800	-0.02556000	0.12088700
C	-7.74967000	0.83688300	1.04819300
H	-6.29728400	2.26359900	0.32324600
H	-6.32335500	2.09666300	2.07207800
H	-8.57115800	1.55469000	1.11385600
H	-7.86971100	0.11255700	1.85993200
H	-7.85031100	0.29638100	0.10181700
C	-2.62073500	-0.68049700	-0.66574600
C	-3.06872200	-2.14041700	-0.65674400
H	-3.31930700	-0.05107000	-1.23065200
H	-1.65552100	-0.59230600	-1.18244500
C	-3.12642200	-2.70246300	-2.07681100
H	-4.05368500	-2.24344900	-0.18209100
H	-2.36715500	-2.74336700	-0.06568500
C	-3.42779200	-4.19768500	-2.09711700
H	-2.16326500	-2.51324000	-2.56739200
H	-3.88492400	-2.15444800	-2.65012900
H	-3.48722000	-4.58094000	-3.11901300
H	-4.37864600	-4.41563800	-1.60014200
H	-2.64201100	-4.75328000	-1.57432900
C	-0.75359400	1.59812200	0.66955600
C	-0.21014400	1.51434800	-0.63029800
C	0.22949000	1.43752800	1.82225800
C	1.12432000	0.86401400	-0.89914000
C	-1.04854600	1.90500200	-1.71096900
O	-2.22894300	2.25900300	-1.60724900
O	-0.43923000	1.82611400	-2.93362600
C	-1.29191700	1.94034600	-4.07314900
C	-2.03823800	0.63929300	-4.31586200
H	-1.98669000	2.77106100	-3.93053700
H	-0.62305100	2.17335600	-4.90460000
H	-2.61888900	0.69578400	-5.24051800
H	-2.72086400	0.44144600	-3.48570200
H	-1.33296200	-0.19374000	-4.39267700
H	-0.11188500	1.99280100	2.69962100
C	0.96178200	-0.61481400	-1.22956800
C	0.98125500	-1.02683000	-2.56275300
C	0.71854100	-1.56348600	-0.23200000
C	0.76075000	-2.36318400	-2.89592200
H	1.16605600	-0.28996200	-3.33978300
C	0.50343700	-2.89820300	-0.56101500
H	0.74573500	-1.25547500	0.80994200



C	0.51958000	-3.30319200	-1.89662700
H	0.78360600	-2.67016500	-3.93737500
H	0.34049200	-3.63091300	0.22588000
H	0.35386000	-4.34520400	-2.15287200
H	0.33510300	0.39346900	2.12349600
C	1.62451800	1.91417900	1.39244400
H	2.31716500	1.69425800	2.20961400
N	2.03060900	1.06859900	0.26059800
S	3.63901700	0.76172900	0.02007100
O	3.99066300	1.09661000	-1.35841700
O	4.35985800	1.38898100	1.12525400
C	3.78857000	-0.99928300	0.19273000
C	3.61323700	-1.55580300	1.45583400
C	3.96287200	-1.79396100	-0.93491000
C	3.58736500	-2.93957200	1.58217900
H	3.48655800	-0.91463500	2.32366000
C	3.93318400	-3.17527600	-0.78980500
H	4.08767700	-1.33081000	-1.90744000
C	3.72982400	-3.76504600	0.46211400
H	3.44438100	-3.38666200	2.56178300
H	4.04857500	-3.80802000	-1.66547600
C	3.62922400	-5.26188800	0.58475200
H	4.43431200	-5.75839300	0.03718000
H	2.68149900	-5.61092200	0.16057300
H	3.67051100	-5.58107700	1.62792000
C	1.69147200	3.41060700	1.11676800
C	1.34104000	4.30277600	2.13431400
C	2.11447500	3.92415000	-0.10917000
C	1.39972200	5.67794400	1.92850900
H	1.02665800	3.92115400	3.10270500
C	2.17478300	5.30070000	-0.31732900
H	2.40947100	3.24666700	-0.90528600
C	1.81407900	6.18241700	0.69757200
H	1.12435100	6.35498600	2.73110200
H	2.50633600	5.68261800	-1.27774900
H	1.86025700	7.25415900	0.53348900
H	1.56473600	1.34631100	-1.77786800
H	-1.46088200	2.42065200	0.78487100
TS2 <sub>2</sub> <sup>(S,S)</sup>			
P	-0.03483000	1.93769900	-0.95068600
C	-0.20122800	3.26697800	0.30226300
C	0.59338300	3.01461700	1.58576900

H	-1.26032200	3.36582800	0.53836800
H	0.12886100	4.19104700	-0.18633400
C	0.56811900	4.23608600	2.50193100
H	0.16202900	2.15159600	2.10513300
H	1.63252000	2.74405800	1.35881100
C	1.22974200	3.95338700	3.84728300
H	1.07014000	5.07381000	2.00200500
H	-0.47259500	4.54645100	2.65929600
H	1.23765700	4.84121900	4.48452700
H	0.69548100	3.15848900	4.37690700
H	2.26416100	3.62094900	3.71326700
C	-1.49620300	1.85929500	-2.04767800
C	-2.33183600	3.14012600	-2.03543800
H	-2.09217700	1.00427400	-1.73764000
H	-1.10678200	1.64396800	-3.04766700
C	-3.45362200	3.07388900	-3.07258200
H	-2.77230600	3.27431400	-1.04117200
H	-1.70875000	4.02303400	-2.23491600
C	-4.32722500	4.32492600	-3.05595900
H	-3.01792100	2.93494900	-4.06903800
H	-4.06722300	2.18645100	-2.87424200
H	-5.12731000	4.26076100	-3.79751000
H	-4.78812100	4.46519600	-2.07340600
H	-3.73405800	5.21771200	-3.27721100
C	1.28201800	2.53806100	-2.07641700
C	2.51697800	3.18086700	-1.43441200
H	0.78094600	3.27228200	-2.72044400
H	1.56057100	1.70163600	-2.72895400
C	3.59687900	3.47287900	-2.47632900
H	2.23143300	4.11670200	-0.93791200
H	2.93381200	2.53136000	-0.65697200
C	4.81539700	4.15922600	-1.86661400
H	3.89856900	2.52978100	-2.94966400
H	3.17288100	4.09789100	-3.27176400
H	5.58412300	4.34651400	-2.62022100
H	4.53949900	5.11950400	-1.42008000
H	5.25765600	3.53983700	-1.08031200
C	0.55158900	0.38715300	-0.16656200
C	-0.23260700	-0.31240600	0.75503800
C	1.83735800	-0.02672500	-0.51633800
C	0.36876000	-1.46080300	1.54011100
H	-0.44551600	-2.06743600	1.94589600
C	-1.54587300	0.17346200	1.09792600
O	-2.08667600	1.17036600	0.60832300

O	-2.16973500	-0.55439500	2.04976900
C	-3.41445000	-0.03589800	2.53203100
C	-3.17940300	1.07689400	3.53800100
H	-3.91189400	-0.89312200	2.99145600
H	-4.01204100	0.31068200	1.68583400
H	-4.13407500	1.45586000	3.91178900
H	-2.59805800	0.71069600	4.38837300
H	-2.63996800	1.90189300	3.06496300
H	2.37740800	-0.65370100	0.18077600
C	1.27057000	-1.00737100	2.67496500
C	2.58887800	-1.46019800	2.76585800
C	0.79808700	-0.13419000	3.66155100
C	3.41927100	-1.04957500	3.80878000
H	2.96806900	-2.14383900	2.00773300
C	1.62013300	0.27225700	4.70800900
H	-0.22962500	0.21862900	3.60733700
C	2.93716500	-0.18157400	4.78366300
H	4.44261300	-1.40924700	3.85702800
H	1.23308700	0.94182000	5.47045000
H	3.57916800	0.13810200	5.59829200
H	2.46285100	0.54353700	-1.18872700
C	1.48364500	-1.85024100	-1.84783000
H	1.42659900	-1.17115500	-2.70084900
N	0.41539000	-2.51121900	-1.44096400
S	-0.95826800	-2.20516900	-2.27369700
O	-1.19218100	-3.30630000	-3.22011200
O	-0.98038400	-0.85217900	-2.85397000
C	-2.22790100	-2.31473000	-1.03755700
C	-3.35367800	-1.50911400	-1.17175200
C	-2.15238400	-3.28824700	-0.04454000
C	-4.41637200	-1.68348200	-0.29022700
H	-3.39853400	-0.76541900	-1.96117800
C	-3.22114100	-3.44401100	0.82935100
H	-1.26029200	-3.89944800	0.04602900
C	-4.36925400	-2.65306200	0.71450400
H	-5.29837000	-1.05550600	-0.38462700
H	-3.16420100	-4.19285600	1.61455300
C	-5.53923900	-2.85279700	1.64233600
H	-6.25452100	-3.56331100	1.21540900
H	-5.21513000	-3.25005100	2.60731100
H	-6.07054000	-1.91308500	1.81400900
C	2.82531300	-2.40041100	-1.54593200
C	3.95140000	-1.84282300	-2.15980500
C	2.98702200	-3.47912400	-0.66989300

C	5.22070600	-2.34426600	-1.89309400
H	3.82654600	-1.00991700	-2.84808300
C	4.25813400	-3.97477100	-0.39832600
H	2.10703500	-3.92485000	-0.21596100
C	5.37822400	-3.40859600	-1.00675600
H	6.08732400	-1.90544100	-2.37692800
H	4.37526900	-4.81037300	0.28448900
H	6.36839000	-3.79965000	-0.79636900
H	0.93632400	-2.11074400	0.87026900
M2 <sub>2</sub> <sup>(S,S)</sup>			
P	0.11906800	1.97238300	0.38954200
C	0.05765800	2.99349400	-1.13065700
C	-0.95115600	2.47122400	-2.16096600
H	1.06086900	3.00424600	-1.55988400
H	-0.19160100	4.01350300	-0.81601700
C	-1.02467500	3.37381100	-3.39116000
H	-0.66026600	1.46042800	-2.47330100
H	-1.95066900	2.38386700	-1.71540100
C	-1.98724000	2.82060300	-4.43858400
H	-1.33617600	4.38075600	-3.08797600
H	-0.02071100	3.47330700	-3.82139000
H	-2.01798600	3.45630800	-5.32683100
H	-1.68500600	1.81470400	-4.74863700
H	-3.00278100	2.75253900	-4.03645700
C	1.66599500	2.23754300	1.33219400
C	2.41849800	3.50149900	0.91807400
H	2.29060500	1.35466900	1.20566500
H	1.35850600	2.26691600	2.38065900
C	3.62910500	3.73704100	1.82193900
H	2.75531000	3.40231500	-0.11974800
H	1.76051700	4.38012800	0.96314500
C	4.41433100	4.98111300	1.41763500
H	3.29178700	3.82883000	2.86113100
H	4.27956900	2.85437700	1.78238900
H	5.27566200	5.13715800	2.07168900
H	4.78186600	4.89349300	0.39063500
H	3.78414400	5.87422100	1.47187200
C	-1.17481100	2.63117300	1.50770000
C	-2.47565200	3.19841300	0.93052600
H	-0.65242700	3.44075800	2.03476000
H	-1.35273200	1.85137500	2.25545800
C	-3.35426000	3.76853500	2.04549000

H	-2.25585800	3.98989700	0.20290200
H	-3.04956700	2.43585700	0.39362500
C	-4.68418300	4.29594800	1.51548400
H	-3.53493400	2.98575300	2.79233600
H	-2.81054600	4.56958200	2.56029600
H	-5.29601300	4.70807000	2.32139800
H	-4.52574700	5.08553300	0.77454000
H	-5.25535800	3.49569900	1.03437600
C	-0.29036600	0.25057800	-0.08753200
C	0.55010600	-0.57772100	-0.74315100
C	-1.70385700	-0.18800300	0.19747800
C	0.11062500	-1.94232200	-1.24774100
H	0.99201500	-2.57831900	-1.35044500
C	1.92512900	-0.12736500	-1.11680200
O	2.28984500	1.03529900	-1.09082000
O	2.70629600	-1.12422700	-1.51438300
C	4.04780400	-0.77766500	-1.91420500
C	4.06331200	-0.21393800	-3.32185000
H	4.59526900	-1.71851500	-1.84969500
H	4.45545400	-0.07150200	-1.18698900
H	5.09301200	-0.00346700	-3.62064200
H	3.64127000	-0.93440800	-4.02680200
H	3.49244500	0.71570600	-3.37067100
H	-2.01575300	-0.86387600	-0.60123900
C	-0.59555200	-1.81813900	-2.58677500
C	-1.88534100	-2.32402100	-2.76455300
C	0.02719200	-1.17834000	-3.66527400
C	-2.54274900	-2.18793600	-3.98654100
H	-2.38065500	-2.82367700	-1.93450500
C	-0.62707000	-1.03867900	-4.88535300
H	1.03775200	-0.79201700	-3.55309900
C	-1.91792500	-1.54110600	-5.04891000
H	-3.54572200	-2.58559300	-4.10449600
H	-0.12831600	-0.53968700	-5.71062100
H	-2.42945800	-1.43033300	-5.99951500
H	-2.39218700	0.65780500	0.14857600
C	-1.92736300	-0.92005600	1.57205600
H	-2.01070300	-0.13729800	2.33794900
N	-0.88707800	-1.87689600	1.87370000
S	0.26954400	-1.33318300	2.78042100
O	0.33055700	-1.94431000	4.12700100
O	0.33933900	0.16065300	2.81421800
C	1.78917600	-1.86503100	1.98773700
C	2.93149500	-1.08083600	2.12309600

C	1.84733800	-3.07559200	1.30194800
C	4.13049300	-1.50420900	1.55440000
H	2.87602400	-0.14836000	2.67627800
C	3.05276700	-3.49250700	0.74650000
H	0.94499000	-3.66944800	1.19352100
C	4.21126900	-2.71870700	0.86734800
H	5.02000900	-0.88684400	1.65468800
H	3.09604300	-4.43503600	0.20663000
C	5.52249100	-3.19873900	0.29936700
H	6.05540600	-3.81872500	1.02778200
H	5.36813500	-3.80638100	-0.59633900
H	6.17462800	-2.35993700	0.04216800
C	-3.28996600	-1.58464900	1.46791200
C	-4.44607500	-0.80426700	1.55502600
C	-3.41616700	-2.95181700	1.21905700
C	-5.70553700	-1.37547600	1.39509600
H	-4.35787100	0.26173400	1.76116800
C	-4.67587500	-3.52605100	1.05545800
H	-2.51480900	-3.55476200	1.17860100
C	-5.82353200	-2.74089700	1.14143800
H	-6.59449000	-0.75702400	1.47312400
H	-4.76166400	-4.59214900	0.86747100
H	-6.80385300	-3.19030000	1.01823700
H	-0.53750800	-2.40915800	-0.50368000
TS <sub>3</sub> <sup>(S,S,R)</sup>			
P	0.25061000	1.99240000	0.25015400
C	1.78221000	2.98107000	0.06689300
C	2.34387900	3.04880300	-1.35833600
H	2.52238300	2.58059600	0.76567400
H	1.51333200	3.98609100	0.41541700
C	3.43427200	4.11304800	-1.47431500
H	2.74730200	2.07261900	-1.64962700
H	1.54606400	3.27235700	-2.07559300
C	4.03335900	4.16631500	-2.87645300
H	3.00898100	5.09010600	-1.21394000
H	4.22058600	3.91110900	-0.73625000
H	4.81331800	4.92806100	-2.94685700
H	4.47599100	3.20368900	-3.15248300
H	3.26428500	4.40013900	-3.61900200
C	0.06493800	1.54398900	2.00999200
C	-0.09224200	2.74193100	2.95272300
H	0.95290200	0.95412800	2.25363900

H	-0.79381500	0.86288900	2.08340200
C	-0.00930000	2.30266200	4.41383100
H	0.68907300	3.48948900	2.76099700
H	-1.05571100	3.23573400	2.78238300
C	-0.20489900	3.46425300	5.38261200
H	-0.76486200	1.52816500	4.59493900
H	0.96518800	1.83002900	4.58553900
H	-0.13688400	3.12800600	6.42029200
H	0.55589200	4.23556100	5.22791300
H	-1.18591700	3.92864100	5.24305900
C	-1.11996100	3.13719300	-0.12127800
C	-1.08523400	3.79341600	-1.50738700
H	-1.08320000	3.90875100	0.65473000
H	-2.05598200	2.58813200	0.03663400
C	-2.43346900	4.42659100	-1.85047800
H	-0.30234700	4.56164700	-1.52432400
H	-0.82260000	3.06469000	-2.28484100
C	-2.40992600	5.13615800	-3.20028400
H	-3.20141200	3.64164500	-1.85302700
H	-2.71135100	5.13264900	-1.05868200
H	-3.38213200	5.57745900	-3.43188400
H	-1.66509500	5.93785000	-3.20683000
H	-2.15719100	4.43697600	-4.00311700
C	0.10190600	0.57020800	-0.83884700
C	1.08768700	-0.36291800	-1.02317000
C	-1.26448900	0.35515800	-1.47958100
C	0.85934800	-1.59390900	-1.77139900
C	2.42395300	-0.14482000	-0.36151400
O	2.57625100	0.11732700	0.81618100
O	3.42118900	-0.27158000	-1.22841400
C	4.75927700	-0.26726500	-0.68793000
C	5.26540000	1.14517400	-0.47791900
H	5.34916000	-0.80182200	-1.43290700
H	4.75487300	-0.83678400	0.24479800
H	6.30140300	1.11609800	-0.13211900
H	5.23084000	1.70989100	-1.41340200
H	4.66539900	1.66090900	0.27589500
H	-1.14283700	-0.06857200	-2.48336200
H	-1.79740500	1.29507800	-1.62877900
C	-2.17501500	-0.58074700	-0.66458700
H	-2.23569100	-0.17150100	0.36284700
N	-1.56004900	-1.90806800	-0.66028400
S	-1.94317300	-2.84901800	0.57894600
O	-1.32119000	-4.15604400	0.34219900

O	-3.38070800	-2.80778600	0.88264700
C	-1.12923200	-2.16612400	2.02177900
C	-1.85664600	-1.78173600	3.14216700
C	0.25999900	-2.06921000	2.00703300
C	-1.17506000	-1.32642700	4.26984400
H	-2.93852000	-1.85991500	3.12687200
C	0.92870300	-1.62212400	3.13876600
H	0.80521900	-2.36813300	1.11607800
C	0.22112200	-1.25949100	4.29185900
H	-1.73599000	-1.03434100	5.15396000
H	2.01292500	-1.54678300	3.12639900
C	0.95126500	-0.84892800	5.54414200
H	1.91050300	-0.38041700	5.31012000
H	0.35869000	-0.14972200	6.13979400
H	1.15653200	-1.72510900	6.16799300
C	-3.57708800	-0.54022700	-1.25221800
C	-4.46668500	0.45276100	-0.83752500
C	-3.96491400	-1.41772000	-2.26426200
C	-5.72346500	0.57360100	-1.42488100
H	-4.17816100	1.12966600	-0.03474700
C	-5.22139700	-1.29993100	-2.85402600
H	-3.27596000	-2.19970900	-2.56884900
C	-6.10300400	-0.30339000	-2.43860400
H	-6.40812000	1.34484600	-1.08569600
H	-5.51562100	-1.99052000	-3.63852700
H	-7.08298800	-0.21518400	-2.89677500
H	-0.31268300	-1.95181400	-1.14057000
C	1.85815500	-2.68493000	-1.85330600
C	1.95846700	-3.43611000	-3.03529300
C	2.67617600	-3.07731200	-0.77873100
C	2.83405100	-4.51118000	-3.14567400
H	1.33608400	-3.16347400	-3.88378500
C	3.56219800	-4.14372700	-0.88971400
H	2.63106800	-2.54478800	0.16905000
C	3.64943300	-4.87090800	-2.07479100
H	2.88341200	-5.06677000	-4.07754400
H	4.18070500	-4.41244400	-0.03847300
H	4.33629200	-5.70649600	-2.15923800
H	0.37905500	-1.40914300	-2.73638600
M3 <sub>2</sub> <sup>(S,S,R)</sup>			
P	0.52667500	-1.70335200	0.46550500
C	2.10398000	-2.64502700	0.59392800



C	3.05629700	-2.14723600	1.68422300
H	2.59398800	-2.62038700	-0.38393900
H	1.81389700	-3.68727200	0.78182700
C	4.20889500	-3.12380000	1.91518800
H	3.45383100	-1.16400900	1.40580800
H	2.51815000	-1.99640100	2.62692100
C	5.20474100	-2.60332200	2.94764000
H	3.80066300	-4.08765400	2.24438700
H	4.72102100	-3.31501700	0.96376600
H	6.01933600	-3.31339500	3.10994500
H	5.64341600	-1.65361900	2.62429100
H	4.71237100	-2.42816300	3.90923500
C	-0.17965600	-2.13830700	-1.17622300
C	0.02083500	-3.59456400	-1.60786200
H	0.27682900	-1.45582900	-1.89742700
H	-1.25013500	-1.88875700	-1.12302000
C	-0.73198300	-3.90011800	-2.90027700
H	1.08906300	-3.79080500	-1.75799900
H	-0.31805100	-4.28817300	-0.82700700
C	-0.51707200	-5.32882000	-3.38812400
H	-1.80091300	-3.71612100	-2.73655800
H	-0.41243900	-3.18647700	-3.67039800
H	-1.06949700	-5.51873200	-4.31255200
H	0.54245100	-5.52062000	-3.58348200
H	-0.85537900	-6.05235000	-2.63969400
C	-0.61009300	-2.54492300	1.62986600
C	-0.10690600	-2.70025500	3.06768900
H	-0.80637000	-3.53206300	1.19711700
H	-1.56531400	-2.00798700	1.60663900
C	-1.21994900	-3.17313100	4.00236400
H	0.72010200	-3.42156400	3.08865800
H	0.30021900	-1.75261200	3.44165900
C	-0.72677800	-3.37693100	5.43149000
H	-2.03080200	-2.43299200	3.98919900
H	-1.64426400	-4.10737800	3.61480200
H	-1.53522000	-3.70671600	6.08847100
H	0.06542400	-4.13122500	5.46677800
H	-0.32005900	-2.44609500	5.83835500
C	0.58774100	-0.01175800	0.86663400
C	1.54454300	0.90697900	0.31139200
C	-0.51390200	0.52177700	1.75655300
C	1.58426500	2.26446600	0.52171500
C	2.60875100	0.31638100	-0.57316000
O	2.39073000	-0.43829800	-1.50274300

O	3.83675100	0.68925600	-0.21186700
C	4.91073800	0.33492300	-1.10231300
C	5.41756200	-1.06559400	-0.82251600
H	5.67853400	1.08632200	-0.91264500
H	4.55765600	0.43400800	-2.13200100
H	6.27572100	-1.28480900	-1.46257600
H	5.73277800	-1.15859800	0.22054300
H	4.63696000	-1.80266800	-1.02637100
H	-0.16317700	1.40435600	2.30510600
H	-0.79649700	-0.18865100	2.53830000
C	-1.83652000	0.90457500	1.04789000
H	-2.22549700	-0.00023900	0.54858400
N	-1.54128400	1.94281900	0.05335800
S	-2.61189300	2.19830000	-1.17821700
O	-2.04574800	3.28207900	-1.97287700
O	-3.93504100	2.32174400	-0.58165900
C	-2.64510900	0.74915700	-2.21068700
C	-3.65500800	-0.19409200	-2.03633400
C	-1.69643000	0.61379300	-3.22245100
C	-3.72831400	-1.27194000	-2.91370700
H	-4.39021600	-0.05751800	-1.24995700
C	-1.78753800	-0.46755800	-4.09051500
H	-0.92069300	1.36298600	-3.34626300
C	-2.81650800	-1.40864700	-3.96544600
H	-4.52343100	-2.00287100	-2.79760700
H	-1.06340500	-0.57101800	-4.89367500
C	-2.97454600	-2.51276200	-4.97727100
H	-2.01354800	-2.79714800	-5.41208800
H	-3.43162900	-3.39991500	-4.53235700
H	-3.62303100	-2.18046700	-5.79442500
C	-2.84589200	1.36657300	2.07638200
C	-3.77802500	0.46295800	2.58609500
C	-2.78587200	2.65693700	2.60583800
C	-4.64064200	0.84031100	3.61361100
H	-3.83716600	-0.54063800	2.16900300
C	-3.64794500	3.03644300	3.62941300
H	-2.06813900	3.36272100	2.19745400
C	-4.57683600	2.12851500	4.13774800
H	-5.36568000	0.13029800	3.99883500
H	-3.59706600	4.04352500	4.03138600
H	-5.24971100	2.42678500	4.93528900
H	-0.58348500	1.92052500	-0.30114700
C	2.44738600	3.25825700	-0.12416400
C	2.78848700	4.42573700	0.58008200

C	2.90857500	3.14679200	-1.44893100
C	3.58868300	5.40981800	0.01042600
H	2.42377200	4.54836300	1.59665300
C	3.72040800	4.12274200	-2.01494200
H	2.60233400	2.29730700	-2.05512200
C	4.07117800	5.26026100	-1.28848800
H	3.83975300	6.29638000	0.58503300
H	4.06305500	4.00506100	-3.03880600
H	4.69734300	6.02588400	-1.73481300
H	0.87850600	2.69025400	1.22994400

TS4<sub>2</sub><sup>(S,S,R)</sup>

P	-0.11165300	-0.38009200	-1.83474500
C	1.42055700	-0.24496000	-2.83676000
C	2.61228300	-1.08774500	-2.37357700
H	1.69598300	0.81176100	-2.86069500
H	1.11789500	-0.53321200	-3.85223900
C	3.67097900	-1.21707500	-3.46692100
H	3.05681600	-0.61329700	-1.49348200
H	2.29364600	-2.08729300	-2.05379400
C	4.89512800	-1.98974900	-2.98481800
H	3.23048600	-1.71889200	-4.33777500
H	3.96754800	-0.21556000	-3.80186600
H	5.64864200	-2.07762700	-3.77129900
H	5.35829800	-1.49080900	-2.12736200
H	4.61723800	-3.00016200	-2.66925700
C	-1.06769600	1.14321000	-2.12060900
C	-1.24091000	1.57539700	-3.57781200
H	-0.54356700	1.91598800	-1.54670100
H	-2.04551200	0.99223600	-1.64299900
C	-2.06597800	2.86015000	-3.66892300
H	-0.26321100	1.74102700	-4.04714700
H	-1.74204800	0.78980200	-4.15690000
C	-2.26224600	3.32415200	-5.10889500
H	-3.04030100	2.69034500	-3.19353100
H	-1.56694400	3.64502300	-3.08627000
H	-2.85242300	4.24270900	-5.15372400
H	-1.29894300	3.51819800	-5.59077900
H	-2.78227300	2.56093900	-5.69611400
C	-1.04334400	-1.73637300	-2.63944300
C	-0.24303600	-3.03380200	-2.80208000
H	-1.36484100	-1.36766400	-3.61966600
H	-1.95422200	-1.91266800	-2.05765400

C	-1.13735900	-4.19589200	-3.23268400
H	0.54806900	-2.88798000	-3.54865900
H	0.26250800	-3.29568100	-1.86307200
C	-0.34718100	-5.48167300	-3.45438300
H	-1.90476300	-4.35603300	-2.46475200
H	-1.66957000	-3.91933200	-4.15085400
H	-1.00147600	-6.30396800	-3.75350000
H	0.40473900	-5.34700300	-4.23798300
H	0.17384600	-5.78115000	-2.53975900
C	0.02444200	-0.71136300	-0.07901500
C	1.36179200	-0.52377600	0.55351800
C	-0.87129500	-1.83568800	0.43849000
C	2.03221900	-1.48398900	1.21990500
C	1.85157600	0.88983300	0.43931100
O	1.66725000	1.56196500	-0.56036900
O	2.43363300	1.36348000	1.53734900
C	2.96919200	2.70053400	1.45124300
C	4.32874600	2.69842300	0.78031800
H	3.03235100	3.03461900	2.48780700
H	2.25696900	3.32636600	0.90950600
H	4.72087900	3.71785000	0.74536400
H	5.03173800	2.07222400	1.33399600
H	4.24744200	2.32636700	-0.24438400
H	-0.48829000	-2.15799100	1.41120900
H	-0.96717600	-2.73241900	-0.18149700
C	-2.29461500	-1.23082400	0.71442300
H	-2.84301300	-1.14209500	-0.23886100
N	-1.97070600	0.08400800	1.24155200
S	-3.07478700	1.25273500	1.11224200
O	-3.92647800	1.34564700	2.30748000
O	-3.80479600	1.21232800	-0.17269000
C	-2.00308300	2.67326300	1.07940500
C	-2.15412900	3.61576000	0.07008900
C	-1.02988500	2.82500900	2.06665300
C	-1.30691200	4.72141200	0.04154000
H	-2.91443100	3.46724700	-0.68997600
C	-0.19931200	3.93724600	2.02817800
H	-0.91819700	2.07452300	2.84278800
C	-0.32195600	4.89798800	1.01598300
H	-1.41357200	5.45682200	-0.75115900
H	0.55962500	4.06442700	2.79548500
C	0.57796600	6.10587900	1.00114000
H	0.64123200	6.54153500	0.00199900
H	0.19758200	6.87653600	1.67921100

H	1.58784600	5.84927200	1.33256000
C	-3.08495200	-2.13730200	1.62976600
C	-3.69690400	-3.27518300	1.09763700
C	-3.16707100	-1.90023700	3.00226700
C	-4.37578100	-4.16721800	1.92274500
H	-3.64621800	-3.45832200	0.02573000
C	-3.84817000	-2.79110700	3.82869100
H	-2.70943900	-1.00274900	3.40536700
C	-4.45209200	-3.92688600	3.29341500
H	-4.84987500	-5.04550200	1.49568600
H	-3.91289600	-2.59428600	4.89447500
H	-4.98654500	-4.61680100	3.93882400
C	3.36127900	-1.43066900	1.85867400
C	4.44808300	-0.77124000	1.26980100
C	3.57967800	-2.14047400	3.04645400
C	5.70401700	-0.79230600	1.86522800
H	4.31136500	-0.24670900	0.32773400
C	4.83368700	-2.15632300	3.64915700
H	2.75188300	-2.67594500	3.50341000
C	5.90072700	-1.48016000	3.06185500
H	6.53342000	-0.27895200	1.38806900
H	4.97897100	-2.70132900	4.57644600
H	6.88150800	-1.49919800	3.52587700
H	1.55701600	-2.46289200	1.26867600
H	-0.88511800	0.18184800	0.56644900

M4<sub>2</sub><sup>(S,S,R)</sup>

P	-0.00606600	-0.20462200	-1.49054300
C	-1.23442700	-1.36804600	-2.19294100
C	-2.72991000	-1.17577800	-1.91096200
H	-0.92232500	-2.36633300	-1.87177500
H	-1.04447100	-1.30019300	-3.27309300
C	-3.59689700	-1.84249500	-2.97764100
H	-2.95641400	-1.63927000	-0.94782600
H	-3.00310100	-0.11834200	-1.82457300
C	-5.07194800	-1.82161000	-2.58638000
H	-3.45071800	-1.33185900	-3.93718100
H	-3.26331600	-2.87766300	-3.11922600
H	-5.69856700	-2.26317900	-3.36470000
H	-5.23494000	-2.38838500	-1.66269100
H	-5.41764900	-0.79700500	-2.41362700
C	1.58734000	-1.07279300	-1.56395600
C	1.97388000	-1.59109400	-2.95244900

H	1.50019900	-1.89766200	-0.84253100
H	2.36328800	-0.39657900	-1.18186800
C	3.34493300	-2.26695500	-2.91270800
H	1.22740600	-2.30482900	-3.32170400
H	2.00768800	-0.76233900	-3.67046500
C	3.78710300	-2.74890100	-4.29078200
H	4.07432900	-1.55768100	-2.50308100
H	3.30670900	-3.10854400	-2.21094500
H	4.76683900	-3.23070400	-4.24614000
H	3.07441200	-3.47230300	-4.69914700
H	3.85501100	-1.91282700	-4.99371700
C	0.02066500	1.24020700	-2.60287000
C	-1.34503000	1.91934000	-2.76939100
H	0.39476800	0.89412700	-3.57242900
H	0.76525600	1.94173500	-2.21247200
C	-1.21733700	3.26823500	-3.47625200
H	-2.00902100	1.26791200	-3.35027000
H	-1.82612100	2.06677400	-1.79272800
C	-2.57362000	3.93222700	-3.69253700
H	-0.57202700	3.92518400	-2.88018400
H	-0.71184100	3.12212400	-4.43815100
H	-2.46530500	4.89961200	-4.18826900
H	-3.22045400	3.30493200	-4.31315700
H	-3.08211800	4.09755000	-2.73773900
C	-0.23945800	0.36615400	0.26496900
C	-1.62533500	0.07309100	0.80323000
C	0.25531200	1.80369100	0.48702700
C	-2.55764900	1.03103400	0.94847100
C	-1.77122100	-1.36468900	1.18545400
O	-1.06510000	-2.22865000	0.69565400
O	-2.68104700	-1.59370100	2.12372200
C	-2.91168100	-2.97321400	2.47875000
C	-3.79192700	-3.64830300	1.44477300
H	-3.39926600	-2.92153600	3.45214400
H	-1.94763800	-3.47553500	2.58009600
H	-4.00194400	-4.67559500	1.75186400
H	-4.74184100	-3.11648700	1.34551400
H	-3.29082900	-3.67751900	0.47333500
H	-0.07670900	2.09746800	1.48925000
H	-0.18542000	2.51848500	-0.21670200
C	1.79743100	1.91263900	0.48312900
H	2.17908500	1.66712000	-0.52336100
N	2.29356200	0.99889900	1.48360000
S	3.67390900	0.30125600	1.23270300

O	4.64011300	0.52327300	2.33011600
O	4.23040200	0.52449900	-0.12985000
C	3.32051000	-1.46100000	1.29271500
C	4.13643200	-2.33522000	0.58195200
C	2.24086000	-1.95149900	2.02442400
C	3.86477400	-3.70129700	0.59884700
H	4.95946300	-1.93955800	-0.00508100
C	1.97611500	-3.31734200	2.03057800
H	1.60374600	-1.25769100	2.56446500
C	2.78267900	-4.21270300	1.32022200
H	4.49681600	-4.38002400	0.03148100
H	1.12177400	-3.69418000	2.58710700
C	2.49803400	-5.69216700	1.35234000
H	2.98156800	-6.20729600	0.51949700
H	2.87056600	-6.13728200	2.28071800
H	1.42384400	-5.88834300	1.30410600
C	2.17511400	3.37494000	0.72526100
C	1.90673400	4.33850100	-0.25218300
C	2.77438200	3.77892200	1.91726200
C	2.22030600	5.67770700	-0.04287000
H	1.45866700	4.03622300	-1.19786800
C	3.08854600	5.12053600	2.13214700
H	3.00305500	3.02175900	2.66020500
C	2.81072900	6.07405400	1.15675400
H	2.01207100	6.41066800	-0.81643100
H	3.55816700	5.42033400	3.06434000
H	3.05954800	7.11735000	1.32387100
C	-3.97086100	0.94519100	1.36412100
C	-4.82803100	-0.06888500	0.91995300
C	-4.49639900	1.97189300	2.15767400
C	-6.16879400	-0.07225100	1.28384800
H	-4.44606300	-0.85036200	0.27262200
C	-5.83419700	1.95809200	2.54021400
H	-3.84662200	2.77895700	2.48455300
C	-6.67393000	0.93598000	2.10389800
H	-6.82133200	-0.86075700	0.92187700
H	-6.22245300	2.75147400	3.17027400
H	-7.72029000	0.93092400	2.39133300
H	-2.23990700	2.04493900	0.70436200
H	0.47361200	-0.27137900	0.80412700

M4<sub>2</sub><sup>r(S,S,R)</sup>

P	0.57470400	2.24984300	-0.17673300
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C	1.66560800	2.34049900	-1.63855100
C	1.08947500	1.73239700	-2.93056500
H	2.59099000	1.83158200	-1.35995000
H	1.90741800	3.40061000	-1.77692900
C	2.21071800	1.34727600	-3.89635700
H	0.49384100	0.83885400	-2.70943000
H	0.41970600	2.44625800	-3.41809000
C	1.67252200	0.71467200	-5.17583800
H	2.80542800	2.23698200	-4.13568200
H	2.89165800	0.64858800	-3.39148200
H	2.48390900	0.44649700	-5.85665800
H	1.10569300	-0.19496200	-4.95124500
H	1.00423200	1.40350100	-5.70128900
C	1.41465300	2.79752500	1.35761000
C	2.73409900	3.53613200	1.12347800
H	1.58286900	1.90645900	1.96902400
H	0.69911500	3.44249400	1.88116200
C	3.32232200	4.04385900	2.43995300
H	3.44487500	2.85397600	0.64289200
H	2.58650000	4.38616500	0.44428600
C	4.66260900	4.74442700	2.23746100
H	2.60903700	4.72959400	2.91264100
H	3.44297900	3.19703000	3.12648900
H	5.06661800	5.10898600	3.18486100
H	5.39605500	4.06159800	1.79805700
H	4.55734000	5.60079700	1.56425900
C	-0.72957000	3.51072300	-0.40357700
C	-1.48318800	3.53033100	-1.74151600
H	-0.21951400	4.46819700	-0.24112000
H	-1.42012200	3.39422800	0.44129500
C	-2.85532900	4.18796800	-1.59270700
H	-0.88982700	4.08148300	-2.47959900
H	-1.61684500	2.51910100	-2.14226600
C	-3.58798800	4.29966300	-2.92552300
H	-3.45573900	3.59538100	-0.88940400
H	-2.73402000	5.18101900	-1.14337800
H	-4.57160900	4.75775400	-2.79838300
H	-3.01981500	4.91001000	-3.63413400
H	-3.73209100	3.31146500	-3.37273300
C	-0.17599200	0.55377600	0.09854500
C	0.66795200	-0.57672100	-0.49271400
C	-1.67778300	0.53168800	-0.26436300
C	0.11374600	-1.56845100	-1.21179500
C	2.09463000	-0.56647600	-0.06746800



O	2.61321600	0.41550400	0.44380800
O	2.74197400	-1.70830900	-0.24836400
C	4.15639100	-1.70935300	0.02488400
C	4.91790000	-1.11106000	-1.14178200
H	4.40086500	-2.76220000	0.16963200
H	4.34217200	-1.16122400	0.95188500
H	5.99275800	-1.18150900	-0.95948900
H	4.68375200	-1.65065700	-2.06282000
H	4.65895700	-0.05667000	-1.26836000
H	-1.82506000	0.20212100	-1.29906400
H	-2.08939400	1.54026200	-0.21992100
C	-2.55462300	-0.31298000	0.69138200
H	-2.42476400	0.13984300	1.69069200
N	-2.17977000	-1.71162000	0.65516900
S	-2.03263100	-2.39851500	2.05731000
O	-1.80532000	-3.84347800	1.86194900
O	-3.07326600	-2.02775700	3.04417400
C	-0.51069000	-1.76675600	2.77786700
C	-0.53227100	-0.64640300	3.60480900
C	0.70822300	-2.30456500	2.36266000
C	0.66670400	-0.02852600	3.96539800
H	-1.48486600	-0.26357200	3.95716900
C	1.89485300	-1.70478300	2.76066700
H	0.71283000	-3.18278800	1.72300100
C	1.89332100	-0.53518500	3.53182000
H	0.64808000	0.86064100	4.59067200
H	2.84423400	-2.13359000	2.44907200
C	3.19038800	0.16537700	3.83854600
H	3.05368500	0.95707400	4.57915000
H	3.94167500	-0.53424200	4.21585800
H	3.59120700	0.61513600	2.92127000
C	-4.01224900	-0.07354100	0.29942800
C	-4.61547800	1.16201300	0.55715500
C	-4.74993400	-1.05348200	-0.36251100
C	-5.92262500	1.41861100	0.15341600
H	-4.05859700	1.92883900	1.09451100
C	-6.05933000	-0.80107700	-0.76903500
H	-4.28074800	-2.01580100	-0.53721700
C	-6.64943400	0.43476000	-0.51623600
H	-6.37692600	2.38145500	0.36765000
H	-6.62186900	-1.57553400	-1.28199700
H	-7.67035500	0.62905700	-0.82979100
C	0.74841900	-2.73187800	-1.86210700
C	1.76129500	-2.58736000	-2.81564200

C	0.25223400	-4.00622100	-1.57013300
C	2.28568600	-3.70421500	-3.45539800
H	2.13136000	-1.59223500	-3.05117100
C	0.79382200	-5.12525100	-2.19810800
H	-0.54239700	-4.10982500	-0.83440600
C	1.80751000	-4.97680700	-3.14216500
H	3.06648700	-3.58257400	-4.19960500
H	0.41718100	-6.11359600	-1.95508100
H	2.22009800	-5.84913400	-3.63874400
H	-0.96690100	-1.56192900	-1.30135000
H	-0.09662500	0.46763800	1.19465700

TS5<sub>2</sub> (S,S,R)

P	2.03790400	1.22695300	-0.49358100
C	2.23157200	0.76701900	-2.24561500
C	0.98938000	0.99888100	-3.12421400
H	2.48030100	-0.29983000	-2.21465000
H	3.10507000	1.30448900	-2.63459500
C	1.00773800	0.06864600	-4.33648300
H	0.07647300	0.80125700	-2.55361800
H	0.94711000	2.03535000	-3.46140000
C	-0.23860500	0.22338500	-5.19967400
H	1.91049300	0.25853600	-4.93317000
H	1.08888200	-0.96868400	-3.98084300
H	-0.21476400	-0.44394800	-6.06327000
H	-1.14084400	-0.00901500	-4.62094500
H	-0.33567500	1.25060300	-5.56739200
C	3.46511200	0.68567800	0.51116200
C	4.78653900	0.62957700	-0.25796400
H	3.20782700	-0.30582200	0.90755800
H	3.52649800	1.39321200	1.34926500
C	5.94626700	0.22263800	0.65040700
H	4.69903200	-0.09414600	-1.07543100
H	5.01125700	1.60504500	-0.71551200
C	7.27893400	0.17466100	-0.09885600
H	6.01113500	0.93120300	1.49085900
H	5.72276300	-0.76455400	1.08934600
H	8.09253000	-0.12227200	0.56803000
H	7.23402500	-0.54375600	-0.92416400
H	7.52730400	1.15780600	-0.51695200
C	2.09059800	3.04815700	-0.33139800
C	1.28041700	3.87129100	-1.33724200
H	3.15095600	3.32010400	-0.39541400

H	1.78173600	3.27214500	0.70037200
C	1.19593900	5.33715100	-0.91949700
H	1.75275900	3.79307500	-2.32130900
H	0.26235700	3.47256000	-1.44088900
C	0.43719500	6.18238400	-1.93895000
H	0.69816200	5.39857300	0.05910200
H	2.20804900	5.73160200	-0.78296900
H	0.37232600	7.22323800	-1.61968200
H	0.93824800	6.15513800	-2.91397900
H	-0.57981400	5.80702500	-2.07406600
C	0.48260200	0.52087000	0.23518200
C	-0.02485000	-0.73316600	-0.46512800
C	-0.62788400	1.57291900	0.40022400
C	-1.40045200	-0.77792900	-0.67317200
C	0.87715300	-1.84227100	-0.52566700
O	2.10818600	-1.71786000	-0.43437200
O	0.31484600	-3.05249500	-0.71055400
C	1.20249700	-4.13213000	-1.01553400
C	1.63404700	-4.08048800	-2.47172000
H	0.62301700	-5.03661200	-0.80533100
H	2.06382100	-4.09414800	-0.34355500
H	2.27408300	-4.93606500	-2.70566300
H	0.76450700	-4.10502400	-3.12860500
H	2.19809500	-3.16518500	-2.66379100
H	-1.00190700	1.87670600	-0.58304400
H	-0.23133500	2.47924000	0.86190900
C	-1.82865100	1.10608700	1.29612400
H	-1.50482000	1.28850300	2.33523400
N	-2.20821600	-0.29549300	1.12454900
S	-2.14319100	-1.17494600	2.46550000
O	-2.55726000	-2.54314600	2.13159700
O	-2.83442800	-0.50670300	3.57981700
C	-0.43341700	-1.27009800	2.97693000
C	0.09714500	-0.29968500	3.83464600
C	0.38871100	-2.24348600	2.41996300
C	1.46272700	-0.28416700	4.08449500
H	-0.57044900	0.41954600	4.29817500
C	1.76026000	-2.21426700	2.68083700
H	-0.04003000	-3.00044500	1.77292000
C	2.31554000	-1.22512400	3.50109700
H	1.87721000	0.46974000	4.75157200
H	2.40709000	-2.95596200	2.22804200
C	3.79753100	-1.17813700	3.76305500
H	4.22404200	-0.22486900	3.42821400

H	4.01118700	-1.27775600	4.82886900
H	4.31904000	-1.98484100	3.23619800
C	-2.99061000	2.05114200	1.02389900
C	-2.92041600	3.38041000	1.44716700
C	-4.10562400	1.63382400	0.30002900
C	-3.94335500	4.27711100	1.15159900
H	-2.06165600	3.71631200	2.02506400
C	-5.13416900	2.52714700	0.00365900
H	-4.16876500	0.58975000	-0.00519500
C	-5.05669200	3.84980300	0.42706800
H	-3.87832400	5.30348000	1.49982000
H	-5.99841200	2.18569900	-0.55803300
H	-5.85618400	4.54713400	0.19601200
C	-2.16352600	-1.87867800	-1.34735400
C	-1.72302000	-2.31008200	-2.60410800
C	-3.37732800	-2.35656900	-0.85382200
C	-2.47288000	-3.21110600	-3.34899000
H	-0.78155000	-1.92896300	-2.99098600
C	-4.12286800	-3.26882300	-1.59911100
H	-3.71118800	-2.02992500	0.12095300
C	-3.67821800	-3.70345600	-2.84315600
H	-2.11103100	-3.53412700	-4.32059100
H	-5.05935900	-3.64601300	-1.20000200
H	-4.25985700	-4.41010800	-3.42055300
H	-1.87136000	0.16668300	-0.92622300
H	0.82715500	0.23855200	1.24694000

M5<sub>2</sub><sup>(S,S,R)</sup>

P	2.06557600	1.13953700	-0.50567800
C	2.05303500	0.74820600	-2.28253800
C	0.74200600	1.09097900	-3.00879300
H	2.23324300	-0.33101300	-2.31051800
H	2.90867700	1.25469300	-2.74359100
C	0.62364700	0.31317900	-4.31992500
H	-0.11269700	0.83053200	-2.37392500
H	0.68411700	2.16374500	-3.21721800
C	-0.69423100	0.59357700	-5.03494100
H	1.46990200	0.56487000	-4.97088000
H	0.70974600	-0.75973300	-4.10127200
H	-0.76389400	0.03789100	-5.97349000
H	-1.54297400	0.30253400	-4.40695900
H	-0.79601100	1.65881600	-5.26489400
C	3.55521000	0.51199400	0.34328400

C	4.78913900	0.41258000	-0.55409100
H	3.28463500	-0.47200900	0.73448800
H	3.73542100	1.19913400	1.18058900
C	6.01931200	-0.02690300	0.23975300
H	4.59275000	-0.31327100	-1.35230700
H	4.99911800	1.37644200	-1.03804900
C	7.26291500	-0.14024300	-0.63699500
H	6.19821500	0.69023200	1.05065300
H	5.80847200	-0.99246000	0.71587700
H	8.13312900	-0.45266100	-0.05468800
H	7.11039200	-0.87305900	-1.43504800
H	7.49826600	0.82060500	-1.10536000
C	2.23138000	2.95462500	-0.28212400
C	1.39813100	3.88137000	-1.17086300
H	3.29781600	3.16607600	-0.43244100
H	2.03208700	3.14832900	0.77940500
C	1.50390900	5.33507100	-0.70990400
H	1.75211600	3.80490600	-2.20558600
H	0.34350000	3.58410000	-1.17563900
C	0.72182100	6.28310300	-1.61389300
H	1.13260600	5.41055800	0.31962600
H	2.56035600	5.62881400	-0.68329900
H	0.80106300	7.31664100	-1.26844800
H	1.09711900	6.24096700	-2.64092100
H	-0.33894900	6.01478000	-1.63412300
C	0.56369800	0.46167100	0.35515800
C	-0.06395900	-0.72456300	-0.35401500
C	-0.48072300	1.55719300	0.64125400
C	-1.56190100	-0.64268600	-0.35533900
C	0.76511400	-1.80299800	-0.61117800
O	2.02346800	-1.76603300	-0.55203100
O	0.14573100	-2.99627400	-0.92264700
C	0.97344400	-3.98767200	-1.52037900
C	1.28138900	-3.65462700	-2.97104300
H	0.40067000	-4.91554800	-1.44776200
H	1.89732600	-4.09437600	-0.94547500
H	1.87246100	-4.44990200	-3.43400000
H	0.35402000	-3.53414300	-3.53903100
H	1.85362500	-2.72393900	-3.02214700
H	-0.83885700	1.99280900	-0.29697300
H	-0.04915200	2.37913800	1.22023700
C	-1.70788500	1.02382400	1.43720100
H	-1.43138100	1.00909800	2.49501600
N	-2.07003400	-0.35455000	1.03194700

S	-1.91425500	-1.48417700	2.25490700
O	-2.19488900	-2.78809100	1.67237800
O	-2.73364000	-0.97212200	3.35279100
C	-0.23710900	-1.50395000	2.85272500
C	0.15209600	-0.61330500	3.85123800
C	0.68053500	-2.36351000	2.25427600
C	1.49449900	-0.55154500	4.21603400
H	-0.58774900	0.00794900	4.34568400
C	2.01710000	-2.27845500	2.62149000
H	0.35188000	-3.06450400	1.49415600
C	2.44544000	-1.36379800	3.59196100
H	1.80647700	0.13836800	4.99466500
H	2.74201800	-2.92338500	2.13342100
C	3.90700900	-1.25417500	3.93748700
H	4.44761200	-0.72574000	3.14393800
H	4.05673800	-0.70511000	4.86915900
H	4.36256900	-2.24233100	4.03868000
C	-2.87510000	1.98233400	1.27978300
C	-2.79603000	3.24450000	1.87581300
C	-3.99825600	1.66178400	0.51720300
C	-3.82027900	4.17149200	1.71278300
H	-1.92985100	3.49949300	2.48238800
C	-5.02298800	2.59240200	0.34990900
H	-4.07699000	0.67567200	0.06857300
C	-4.93792100	3.84791300	0.94461000
H	-3.74855900	5.14415000	2.18924900
H	-5.89311000	2.32978700	-0.24350300
H	-5.73861600	4.56906600	0.81673800
C	-2.40196500	-1.60701300	-1.17446400
C	-1.97217800	-1.90847100	-2.47205400
C	-3.66915000	-2.03252400	-0.77847700
C	-2.77665900	-2.63327300	-3.34270000
H	-0.98795700	-1.57302300	-2.78693200
C	-4.47626800	-2.76624700	-1.64948400
H	-4.02697900	-1.80214000	0.21833500
C	-4.03618700	-3.07214600	-2.93216100
H	-2.41843100	-2.85612900	-4.34397200
H	-5.45492200	-3.09772700	-1.31621200
H	-4.66526700	-3.64404400	-3.60696100
H	-1.83689200	0.30908600	-0.83988200
H	1.00818000	0.15461100	1.32013700

TS6<sub>2</sub> (S,S,R)

P	2.36387400	1.04127200	-0.04881600
C	2.78133700	1.20884400	-1.83898900
C	1.56599100	1.56242800	-2.70142600
H	3.16543900	0.22980800	-2.14571400
H	3.58406200	1.94821100	-1.96347900
C	1.92872200	1.73428700	-4.17461700
H	0.82585200	0.76064300	-2.60035400
H	1.08375500	2.47901000	-2.33678600
C	0.69812200	1.97176900	-5.04494900
H	2.63204100	2.57000300	-4.27986900
H	2.46043300	0.83833600	-4.52042900
H	0.96826500	2.12022900	-6.09356500
H	0.01750100	1.11467800	-4.99244100
H	0.14606300	2.85581900	-4.71000700
C	3.59318800	-0.14898900	0.62068900
C	5.07063800	0.16884900	0.39437200
H	3.32037900	-1.10624800	0.15439100
H	3.38321400	-0.25098800	1.69526300
C	5.97937100	-0.95914400	0.88412800
H	5.25731400	0.34292300	-0.67313300
H	5.34022200	1.09601300	0.91516900
C	7.45935900	-0.64072800	0.69156800
H	5.77474200	-1.14946000	1.94556900
H	5.72383900	-1.88149000	0.34721500
H	8.09307700	-1.46236800	1.03457600
H	7.68387800	-0.46028800	-0.36425900
H	7.74029300	0.25738800	1.25036200
C	2.80704400	2.66838500	0.70673900
C	2.03760700	3.83744900	0.08647000
H	3.88676500	2.83699600	0.60703400
H	2.58601600	2.59459100	1.77926200
C	2.31335300	5.16001800	0.80035700
H	2.31455200	3.93692600	-0.97137600
H	0.95821300	3.63258100	0.10578900
C	1.57285300	6.32992200	0.15872100
H	2.02173000	5.06622700	1.85356200
H	3.39323900	5.35248600	0.79271300
H	1.77767000	7.26743500	0.68160200
H	1.87302300	6.45475700	-0.88637800
H	0.49136600	6.16316300	0.17697200
C	0.43606000	-0.11220100	0.57383000
C	-0.37410500	-0.54058300	-0.49065900
C	-0.22269900	0.78262500	1.61229400
C	-1.80665200	-0.09133300	-0.37791700

C	0.23423000	-1.45271400	-1.40014500
O	1.45828800	-1.62546500	-1.46188600
O	-0.61554800	-2.13940400	-2.20647100
C	-0.01456500	-2.86472900	-3.28257700
C	0.37736400	-1.92501300	-4.40954200
H	-0.78036200	-3.57218600	-3.60608900
H	0.85150300	-3.41770200	-2.91035700
H	0.79838400	-2.48531200	-5.24857100
H	-0.49994400	-1.37466200	-4.76147400
H	1.12830200	-1.21194200	-4.05590200
H	-0.29250100	1.79855000	1.21266300
H	0.39315000	0.84190900	2.51442100
C	-1.68434000	0.35149900	2.01216800
H	-1.63548700	-0.23334900	2.93213400
N	-2.32170000	-0.48734900	0.97816900
S	-2.39023200	-2.11563600	1.40062200
O	-2.85332100	-2.83936900	0.22569700
O	-3.15776100	-2.15002800	2.64363200
C	-0.75857600	-2.71372100	1.80479200
C	-0.21594700	-2.45486800	3.06075000
C	-0.02048700	-3.37643500	0.82650600
C	1.10918500	-2.80513400	3.31035400
H	-0.82081100	-2.00252000	3.83966300
C	1.29745500	-3.71920900	1.09215700
H	-0.47148800	-3.58378800	-0.13874600
C	1.88851500	-3.41864800	2.32669800
H	1.54127000	-2.59981100	4.28536400
H	1.88495300	-4.21081100	0.32206100
C	3.33662400	-3.74779000	2.57316200
H	3.98127700	-3.12334700	1.94497900
H	3.61186700	-3.57769300	3.61581300
H	3.55061000	-4.79032600	2.32321300
C	-2.52479000	1.58214600	2.31645400
C	-2.10631200	2.43807000	3.34111400
C	-3.68245100	1.89495500	1.60501300
C	-2.82945700	3.58525500	3.64762900
H	-1.21103700	2.19906900	3.91019600
C	-4.40396100	3.05001600	1.90776700
H	-4.02511000	1.22850100	0.81926900
C	-3.98214300	3.89698700	2.92718800
H	-2.49612700	4.23455900	4.45096500
H	-5.30196400	3.28276700	1.34424500
H	-4.54805600	4.79202900	3.16413300
C	-2.77928600	-0.28362400	-1.52590500



C	-2.35965700	0.09292600	-2.80644000
C	-4.11151700	-0.64753500	-1.34028100
C	-3.24010600	0.07953900	-3.88041400
H	-1.32642700	0.39609000	-2.95815400
C	-4.99788100	-0.66300000	-2.41812500
H	-4.45804500	-0.93192100	-0.35340600
C	-4.56800300	-0.30456600	-3.69082100
H	-2.89027200	0.37244400	-4.86620700
H	-6.02974800	-0.95832600	-2.25502600
H	-5.25857800	-0.31884900	-4.52793700
H	-1.79028200	1.00560600	-0.26922000
H	1.15172100	-0.84571700	0.94893000
TS3 <sub>2</sub> (S,S,S)			
P	1.16312800	0.89132800	1.35190900
C	2.30234900	2.32617200	1.17960500
C	1.76989100	3.46059600	0.29969900
H	3.25590500	1.96143100	0.79515700
H	2.47052400	2.69018700	2.20012500
C	2.72534600	4.65310900	0.29423200
H	1.63190700	3.10673900	-0.72929500
H	0.78038900	3.78445900	0.64597200
C	2.23839600	5.76960100	-0.62452400
H	2.83879200	5.03134200	1.31733300
H	3.71964900	4.31538000	-0.02429000
H	2.92614200	6.61850000	-0.61748300
H	2.15156200	5.41342800	-1.65580300
H	1.25369800	6.13012300	-0.31177000
C	2.04987100	-0.68100500	1.66551200
C	3.51359800	-0.50918800	2.08177700
H	1.97565900	-1.27630600	0.75131600
H	1.47783700	-1.18989500	2.45175700
C	4.07544300	-1.79926900	2.67923700
H	4.09524200	-0.22044200	1.19806300
H	3.62381200	0.30065600	2.81569500
C	5.57752500	-1.71667700	2.92990600
H	3.54853100	-2.01601600	3.61628400
H	3.85271200	-2.63100400	2.00157600
H	5.95782300	-2.64127900	3.37115300
H	6.11918800	-1.54247200	1.99459700
H	5.81645400	-0.89416700	3.61140900
C	0.30098200	1.22948400	2.92596200
C	-0.41970100	2.58041500	2.99110000

H	1.07498800	1.16927900	3.70156900
H	-0.38834200	0.40089700	3.12218900
C	-1.35196000	2.66226700	4.19970900
H	0.31973100	3.38938000	3.04281700
H	-1.00192900	2.75238200	2.07546100
C	-2.03010200	4.02373800	4.31371300
H	-2.10931900	1.87241300	4.11573800
H	-0.77935700	2.45000900	5.11069800
H	-2.70278800	4.06018900	5.17377400
H	-1.28864600	4.81985600	4.43149000
H	-2.61736500	4.24268000	3.41677000
C	-0.09052300	0.72608600	0.06731400
C	0.20208700	0.72238300	-1.27468000
C	-1.50522300	0.40662700	0.54026500
C	-0.78626200	0.51146800	-2.31673500
H	-0.33863400	0.29378900	-3.28511400
C	1.65410300	0.74014500	-1.67079100
O	2.56843900	0.51560200	-0.89594200
O	1.84753300	1.03531900	-2.94908800
C	3.22000000	1.15347000	-3.38111600
C	3.79250800	2.49410200	-2.96293100
H	3.17059300	1.05440500	-4.46523600
H	3.79332800	0.32329900	-2.96318400
H	4.80297100	2.60499600	-3.36288400
H	3.17483200	3.30864500	-3.34891600
H	3.84205500	2.56698300	-1.87325600
H	-2.24635100	0.91927200	-0.07982100
C	-1.98808000	1.37963800	-2.46220900
C	-3.03997400	0.92773500	-3.27589600
C	-2.13535700	2.62742200	-1.84022100
C	-4.18101700	1.69570200	-3.47390200
H	-2.94937600	-0.04902100	-3.74570300
C	-3.28347100	3.39428400	-2.02908100
H	-1.33685000	2.99834400	-1.20005100
C	-4.31123200	2.93656500	-2.84935300
H	-4.97740400	1.32107600	-4.11016500
H	-3.37088300	4.35842000	-1.53641800
H	-5.20470900	3.53464600	-2.99702100
H	-1.68724900	0.75311400	1.55817800
C	-1.80736300	-1.10514100	0.49658900
H	-1.01222100	-1.62777400	1.06216300
N	-1.80838600	-1.52037400	-0.90927100
S	-1.42114500	-3.04192900	-1.21640100
O	-1.62870200	-3.25560900	-2.65339000

O	-2.04839800	-3.97303000	-0.26902900
C	0.34481700	-3.19523600	-0.94957400
C	0.84426700	-3.96204500	0.09474200
C	1.20983100	-2.52732800	-1.81876100
C	2.22590500	-4.06895900	0.26433100
H	0.15401000	-4.48349600	0.74958500
C	2.58052400	-2.63814700	-1.63562400
H	0.80594700	-1.94500300	-2.64414400
C	3.10969700	-3.41310500	-0.59388100
H	2.62051300	-4.67785600	1.07367100
H	3.25802500	-2.12493800	-2.31328100
C	4.60273800	-3.52258700	-0.42267200
H	4.86293500	-4.16864700	0.41878800
H	5.06785900	-3.93114200	-1.32454800
H	5.04597000	-2.53643700	-0.24623200
C	-3.13047400	-1.36222600	1.19785200
C	-3.15819000	-1.64210600	2.56477400
C	-4.33523300	-1.23080700	0.50560500
C	-4.37078400	-1.79299000	3.23414800
H	-2.22123400	-1.75742400	3.10674000
C	-5.54818100	-1.38050600	1.17210300
H	-4.30389700	-1.02014800	-0.55947400
C	-5.56995900	-1.66114800	2.53767900
H	-4.37888900	-2.02125800	4.29551000
H	-6.48065100	-1.28049800	0.62498100
H	-6.51689800	-1.78258100	3.05405700
H	-1.31820000	-0.63845900	-1.74569800
M3 <sub>2</sub> <sup>(S,S,S)</sup>			
P	0.04941000	-1.05679300	1.45240700
C	-0.49714400	-2.80912100	1.38410700
C	0.30301000	-3.75220000	0.48148100
H	-1.55147400	-2.79667700	1.08403400
H	-0.46925600	-3.16772300	2.42121400
C	-0.09624800	-5.20931800	0.70994600
H	0.13531000	-3.49751800	-0.57071000
H	1.37903100	-3.62713100	0.65335100
C	0.62611600	-6.15898800	-0.24079700
H	0.11788900	-5.48490400	1.75013200
H	-1.18198900	-5.30786800	0.58047800
H	0.34609600	-7.19908600	-0.05601200
H	0.38537400	-5.92371800	-1.28244400
H	1.71113700	-6.07570500	-0.12410700

C	-1.45712300	-0.16457600	2.03800200
C	-2.03462300	-0.59426700	3.38984800
H	-2.19495200	-0.31468600	1.24350200
H	-1.22977500	0.90852500	2.05712000
C	-3.36339100	0.11270400	3.66201500
H	-2.19464800	-1.68017200	3.41665200
H	-1.33536700	-0.35697200	4.20025100
C	-3.95873500	-0.25827800	5.01694700
H	-3.20443700	1.19748400	3.60723600
H	-4.07083500	-0.13988200	2.86147200
H	-4.90985200	0.25192700	5.18827700
H	-4.13844100	-1.33605000	5.08177700
H	-3.27874400	0.01602600	5.82934800
C	1.21235700	-0.89723400	2.86231900
C	2.49375300	-1.71703700	2.72122600
H	0.66938200	-1.19190000	3.76686500
H	1.44332800	0.17065300	2.97129800
C	3.47021800	-1.46545800	3.86922300
H	2.24336400	-2.78561200	2.68493900
H	2.98341800	-1.47947600	1.76925100
C	4.74490200	-2.29241800	3.73050900
H	3.71993300	-0.39753200	3.89683100
H	2.97733700	-1.69455900	4.82196800
H	5.43792600	-2.09970200	4.55310400
H	4.51613000	-3.36262100	3.72562500
H	5.26051600	-2.05799400	2.79366100
C	0.84957400	-0.51781800	0.01368000
C	0.52778600	-1.03958800	-1.30124100
C	1.70017600	0.73086100	0.12536700
C	1.35404400	-1.14438400	-2.38492100
H	0.88046300	-1.36186000	-3.33774100
C	-0.91268500	-1.38431700	-1.55812300
O	-1.83626800	-0.93597100	-0.89878200
O	-1.10589900	-2.24342600	-2.56509100
C	-2.46965000	-2.61467100	-2.83751600
C	-2.93694900	-3.67762500	-1.86154300
H	-2.45090400	-2.99216100	-3.86064000
H	-3.09803600	-1.72109200	-2.78942200
H	-3.93678800	-4.02340600	-2.13654100
H	-2.25795300	-4.53487800	-1.87815100
H	-2.97841500	-3.27205000	-0.84786300
H	2.19234100	0.90946800	-0.83450600
C	2.81135700	-1.03622600	-2.45299000
C	3.41790600	-0.86148700	-3.70964300

C	3.65470100	-1.19349700	-1.33803300
C	4.80043600	-0.82122500	-3.84620900
H	2.78547100	-0.75691200	-4.58769100
C	5.03690900	-1.17047800	-1.47723400
H	3.20415900	-1.35348400	-0.36420100
C	5.61986600	-0.97332900	-2.72891400
H	5.24054300	-0.67523800	-4.82796300
H	5.66470300	-1.30361100	-0.60077100
H	6.69965400	-0.94148800	-2.83254900
H	2.50685900	0.66830000	0.87184400
C	0.88572700	2.01566900	0.45603700
H	0.54089400	1.96266700	1.50056100
N	-0.26629800	2.02151600	-0.45568400
S	-1.51101600	3.07867900	-0.09949400
O	-1.32783600	4.30357600	-0.87353300
O	-1.67811500	3.21589200	1.35203900
C	-2.86799800	2.14505800	-0.75537400
C	-3.81180500	1.61226200	0.11622000
C	-2.91395600	1.89769800	-2.12418800
C	-4.81267500	0.79824000	-0.40019400
H	-3.74969500	1.83169300	1.17729500
C	-3.92015500	1.07775200	-2.62042900
H	-2.17274900	2.33347600	-2.78693500
C	-4.87104800	0.50801200	-1.76719900
H	-5.55772700	0.37606500	0.26860600
H	-3.96750000	0.87309300	-3.68619600
C	-5.92632300	-0.42379700	-2.30154100
H	-6.89698300	-0.22832200	-1.83930600
H	-6.03040700	-0.32854700	-3.38418000
H	-5.66277900	-1.46369200	-2.07878800
C	1.74782400	3.24836800	0.31800200
C	2.46141800	3.70481600	1.42760800
C	1.91605300	3.89034600	-0.91111200
C	3.33374000	4.78435500	1.31496400
H	2.32862500	3.21157700	2.38824300
C	2.78371900	4.97283300	-1.02351700
H	1.34859000	3.54585400	-1.77003600
C	3.49585900	5.42209700	0.08736500
H	3.88036300	5.13052800	2.18653700
H	2.90253600	5.46928600	-1.98152900
H	4.17042600	6.26758500	-0.00236900
H	-0.64960600	1.06948300	-0.51716400

TS4<sub>2</sub><sup>(S,S,S)</sup>

P	0.14995200	1.02303700	1.42295600
C	0.76682800	2.74862900	1.38670100
C	0.03818900	3.72977900	0.46366200
H	1.82579700	2.69097200	1.11571000
H	0.71382300	3.09741700	2.42698100
C	0.58494800	5.14956200	0.62270300
H	0.14915200	3.41685700	-0.58029400
H	-1.03827000	3.73085100	0.67504900
C	-0.09025900	6.13135900	-0.33018900
H	0.44652700	5.47856500	1.66082200
H	1.66742500	5.13979100	0.44087500
H	0.31856800	7.13865000	-0.21636600
H	0.05432500	5.82246400	-1.37275800
H	-1.17045600	6.17923400	-0.14349700
C	1.50039800	-0.00652700	2.08705200
C	2.16039500	0.47864900	3.37799800
H	2.23024400	-0.06287800	1.27487300
H	1.09480600	-1.01975100	2.21612700
C	3.33900100	-0.42361600	3.74817400
H	2.51827500	1.51028400	3.26609100
H	1.43970000	0.48059100	4.20630100
C	3.99635100	-0.01116900	5.06106000
H	2.98636000	-1.46139000	3.81266500
H	4.07390800	-0.39394300	2.93424600
H	4.84091800	-0.66024100	5.30591800
H	4.36948200	1.01663300	5.00440200
H	3.28146800	-0.06346000	5.88852700
C	-1.14913500	0.96713800	2.71468200
C	-2.30395300	1.95540800	2.54309400
H	-0.64029300	1.14800900	3.66832700
H	-1.51918800	-0.06284500	2.75105300
C	-3.38900800	1.73557300	3.59643800
H	-1.92537900	2.98205600	2.62069200
H	-2.74807800	1.85199900	1.54651700
C	-4.53757800	2.73140200	3.45584800
H	-3.77097800	0.71067200	3.50564900
H	-2.94362800	1.81708900	4.59589500
H	-5.30590100	2.56256900	4.21308000
H	-4.17872500	3.75944300	3.56464900
H	-5.00870300	2.64347200	2.47122900
C	-0.47056300	0.34033300	-0.11282100
C	-0.16278100	1.01224600	-1.40108700
C	-1.71844100	-0.53285900	0.02037500

C	-0.99990100	1.31224200	-2.41916600
H	-0.54516100	1.57049100	-3.37289500
C	1.30303800	1.25723200	-1.61038600
O	2.12449400	1.10895100	-0.72384100
O	1.63222800	1.70171000	-2.82609900
C	3.00671300	2.09147900	-3.00904000
C	3.25017800	3.47070100	-2.42648400
H	3.15422200	2.07545400	-4.08990500
H	3.64774400	1.34000700	-2.54225300
H	4.27664100	3.78382300	-2.62766400
H	2.57027500	4.20005100	-2.87416300
H	3.09748200	3.45835600	-1.34576700
H	-2.17027300	-0.65036600	-0.96865800
C	-2.47095900	1.35921600	-2.38787500
C	-3.22077900	0.88257700	-3.46940000
C	-3.14485900	1.94284000	-1.30727400
C	-4.61130600	0.94894600	-3.44880800
H	-2.70808300	0.44684400	-4.32132200
C	-4.53235000	2.01741300	-1.29071800
H	-2.55943500	2.35591900	-0.49130200
C	-5.27055100	1.51172700	-2.35927900
H	-5.18044400	0.56135600	-4.28906400
H	-5.03770500	2.48072000	-0.44701200
H	-6.35436300	1.56363700	-2.34649200
H	-2.50804000	-0.16971900	0.68698500
C	-1.24589500	-1.96603600	0.45658700
H	-1.02562300	-1.96677200	1.53910300
N	-0.03118000	-2.12383100	-0.31999500
S	1.07641500	-3.19281600	0.13682400
O	0.90886200	-4.49329300	-0.53285100
O	1.24414200	-3.26589900	1.60406900
C	2.52661100	-2.41332300	-0.54339800
C	3.59898500	-2.11001900	0.28723700
C	2.55622400	-2.09778900	-1.89946300
C	4.70653700	-1.45985600	-0.24775300
H	3.54755000	-2.36809000	1.34051800
C	3.67312700	-1.45072000	-2.41962100
H	1.70977400	-2.34412700	-2.53286300
C	4.75773700	-1.11645000	-1.60268000
H	5.54626800	-1.21089800	0.39783100
H	3.70187300	-1.19851900	-3.47652400
C	5.95494600	-0.39145600	-2.15929100
H	6.87749500	-0.94246900	-1.95591100
H	5.86820700	-0.25558100	-3.23960900

H	6.05928800	0.59675500	-1.69947600
C	-2.33818700	-2.98067700	0.20300900
C	-3.41715900	-3.05496900	1.08813800
C	-2.31997000	-3.81133900	-0.91784300
C	-4.46544800	-3.94253000	0.85562400
H	-3.43168400	-2.41922000	1.97039800
C	-3.36821800	-4.69958100	-1.14923700
H	-1.46608400	-3.76938400	-1.58419800
C	-4.44430500	-4.76696300	-0.26701600
H	-5.29492800	-3.99353100	1.55417100
H	-3.34203600	-5.34685200	-2.02054400
H	-5.25484800	-5.46422600	-0.44634500
H	0.23764000	-0.82364400	-0.27088500
M4 <sub>2</sub> (S,S,S)			
P	0.30478600	0.64367900	1.50899500
C	1.08282000	2.26359700	1.85786600
C	0.62750500	3.49282900	1.06416800
H	2.15900700	2.11161600	1.73528100
H	0.89248700	2.42178800	2.92799400
C	1.18186300	4.77553400	1.68456000
H	0.97207200	3.42443300	0.02749000
H	-0.46653300	3.55364100	1.02772900
C	0.82324800	6.00728000	0.85898600
H	0.79361400	4.87988900	2.70487700
H	2.27204500	4.68821900	1.77152600
H	1.21654000	6.91884100	1.31479800
H	1.23582700	5.93017600	-0.15185200
H	-0.26218100	6.11548200	0.76978500
C	1.43951900	-0.64415600	2.10174600
C	1.89958800	-0.51268300	3.55455200
H	2.29190700	-0.59328500	1.41406600
H	0.95185200	-1.61357900	1.92507100
C	2.88407600	-1.63090000	3.90196900
H	2.38260100	0.45854400	3.71982900
H	1.04410800	-0.56532200	4.23883600
C	3.36768000	-1.54770800	5.34626700
H	2.40009200	-2.59815800	3.72097100
H	3.73884000	-1.57772100	3.21612800
H	4.07275100	-2.35057800	5.57456400
H	3.86999400	-0.59390400	5.53541000
H	2.52860000	-1.62839200	6.04410300
C	-1.21194400	0.56305700	2.52063900



C	-2.18000500	1.74234100	2.38655700
H	-0.87233500	0.47143100	3.55882100
H	-1.71410300	-0.37659600	2.27103000
C	-3.49291300	1.46108300	3.11812800
H	-1.72005200	2.65165400	2.79343300
H	-2.40357900	1.94095200	1.33148900
C	-4.45760200	2.63927200	3.03352100
H	-3.95404200	0.56635400	2.68093200
H	-3.27855500	1.22455000	4.16718500
H	-5.39532900	2.42187000	3.54996300
H	-4.02171800	3.53473800	3.48694000
H	-4.69426500	2.87258000	1.99078200
C	-0.06986100	0.21609800	-0.26751000
C	0.41082800	1.21906800	-1.29747900
C	-1.47101500	-0.38640000	-0.45141600
C	-0.28844200	1.88090500	-2.23324500
H	0.29646800	2.42237700	-2.97407000
C	1.89964800	1.37307700	-1.27126700
O	2.56913700	0.95739300	-0.34280200
O	2.41035800	2.03187500	-2.30730300
C	3.82402100	2.31437200	-2.24595000
C	4.08813400	3.51072300	-1.35267500
H	4.10655900	2.50994000	-3.28081700
H	4.33891800	1.42040200	-1.88854600
H	5.15144300	3.76086100	-1.37432900
H	3.52037800	4.37862700	-1.69694700
H	3.80867100	3.28666400	-0.32004300
H	-1.72078300	-0.35406700	-1.51469800
C	-1.75696500	1.98784000	-2.37420400
C	-2.39208200	1.50899700	-3.52521000
C	-2.51939700	2.61033500	-1.38330600
C	-3.77439000	1.60169600	-3.65091700
H	-1.80252100	1.04035100	-4.30772200
C	-3.90127400	2.71614600	-1.51664600
H	-2.01768400	3.03586200	-0.51917200
C	-4.53250300	2.20079200	-2.64573000
H	-4.26067700	1.20711100	-4.53702300
H	-4.48191900	3.20593800	-0.74143800
H	-5.61007800	2.27463400	-2.74835100
H	-2.25051600	0.17957000	0.06818500
C	-1.50661000	-1.88347800	-0.05664200
H	-1.14336400	-2.00992400	0.97640100
N	-0.70209500	-2.63594300	-0.99905800
S	0.48617200	-3.50087300	-0.46707000

O	0.57374300	-4.78743400	-1.18623600
O	0.56324800	-3.60848900	1.01572000
C	2.01487500	-2.65876500	-0.93212100
C	3.13854400	-2.74973800	-0.11317300
C	2.08453400	-1.96062400	-2.13602700
C	4.33068100	-2.15257900	-0.50992200
H	3.06484800	-3.27816000	0.83272700
C	3.28620300	-1.37452700	-2.52836100
H	1.19092700	-1.86960700	-2.74789400
C	4.42709300	-1.47022300	-1.72747300
H	5.20626300	-2.22237900	0.13130200
H	3.33788600	-0.83289900	-3.47020200
C	5.74139200	-0.87047700	-2.15843800
H	6.49351600	-1.65119100	-2.30710000
H	5.63911600	-0.31995500	-3.09661900
H	6.13262600	-0.18620700	-1.39888500
C	-2.96487000	-2.31971100	-0.06861900
C	-3.70921900	-2.36233500	1.11144600
C	-3.60180100	-2.61220000	-1.27691700
C	-5.06676400	-2.68065100	1.08844800
H	-3.22056900	-2.16515600	2.06397300
C	-4.95629800	-2.92941400	-1.30488100
H	-3.01237800	-2.60332400	-2.18899900
C	-5.69473200	-2.96199900	-0.12175000
H	-5.62924900	-2.71752200	2.01643900
H	-5.43867200	-3.15604900	-2.25099900
H	-6.75049200	-3.21333000	-0.14342300
H	0.62248000	-0.62701000	-0.40620500
M4 <sub>2</sub> <sup>r(S,S,S)</sup>			
P	1.06254900	1.35343900	1.31733000
C	2.40045500	2.28770200	0.48674700
C	2.13597200	2.90906400	-0.89291500
H	3.27435800	1.63081900	0.45696000
H	2.61770700	3.08649600	1.20887900
C	3.14760100	4.01355100	-1.19787300
H	2.20825700	2.14310200	-1.67046100
H	1.12010300	3.31655300	-0.95770400
C	2.92941500	4.61123700	-2.58447100
H	3.06970400	4.79763900	-0.43514000
H	4.16229000	3.60246000	-1.12193700
H	3.66032900	5.39443500	-2.79853700
H	3.02106100	3.84399200	-3.35987800

H	1.93030100	5.05087300	-2.66613000
C	1.81722000	0.45233700	2.70569500
C	2.60290400	1.31354800	3.69775200
H	2.45724300	-0.30533600	2.23675800
H	0.99928200	-0.07786600	3.21024200
C	3.21366700	0.46111100	4.81053000
H	3.40468300	1.85025800	3.17641000
H	1.94711900	2.07094400	4.14395400
C	4.00633600	1.30250100	5.80630400
H	2.41248000	-0.07756900	5.32999500
H	3.86334600	-0.29978800	4.36229400
H	4.43618900	0.68039700	6.59477600
H	4.82586900	1.82845700	5.30721700
H	3.36570100	2.05254700	6.28003500
C	-0.08237300	2.59947300	1.99724700
C	-0.88728600	3.38763800	0.95041300
H	0.52382700	3.27762500	2.60763800
H	-0.75258900	2.07761400	2.68795700
C	-2.16671400	3.95950700	1.56065200
H	-0.27073400	4.20396200	0.55657500
H	-1.15288400	2.75650700	0.09184700
C	-2.95881600	4.79309500	0.55964100
H	-2.78340300	3.12690200	1.92239400
H	-1.90818100	4.56402000	2.43861900
H	-3.87046300	5.19184800	1.01122400
H	-2.36425800	5.63790700	0.19739600
H	-3.24395800	4.18754800	-0.30623800
C	0.12903600	0.05064500	0.35897000
C	0.50183400	0.10355300	-1.10892200
C	-1.34096600	0.01686000	0.80566000
C	-0.11428800	0.65966700	-2.16547200
H	0.46691200	0.64943400	-3.08596100
C	1.91292300	-0.37074000	-1.30174200
O	2.66532400	-0.54799800	-0.35816100
O	2.29538400	-0.49481700	-2.57141100
C	3.70185100	-0.71513000	-2.79897800
C	4.46716000	0.59102200	-2.70994200
H	3.75123800	-1.14626000	-3.79939600
H	4.06645100	-1.44179300	-2.07121500
H	5.51923600	0.42033200	-2.95011700
H	4.06509500	1.32358700	-3.41465400
H	4.40991800	0.99920400	-1.69673600
H	-1.95138600	0.72218700	0.24162600
C	-1.40955000	1.36599900	-2.29516600

C	-2.64162100	0.75642500	-2.03344000
C	-1.38581000	2.67533500	-2.79641200
C	-3.82430700	1.46714900	-2.22296000
H	-2.64864700	-0.27615800	-1.69251900
C	-2.56958600	3.38291900	-2.97910100
H	-0.43225000	3.13820800	-3.04102600
C	-3.79319300	2.77978100	-2.68909900
H	-4.77392200	0.98545600	-2.00947100
H	-2.53792600	4.40128900	-3.35310800
H	-4.71807300	3.32888500	-2.83519300
H	-1.40791700	0.32228800	1.85477700
C	-1.94341600	-1.40459700	0.73398600
H	-1.43818000	-1.99199800	1.52035000
N	-1.75366400	-1.96979800	-0.58405100
S	-1.35580500	-3.48722900	-0.62569500
O	-1.66075400	-4.03768400	-1.95925200
O	-1.83702500	-4.27372500	0.53449100
C	0.43650400	-3.58954300	-0.49496500
C	1.04559500	-3.58466100	0.76085700
C	1.21709800	-3.61923300	-1.64698100
C	2.43313300	-3.57697100	0.85487600
H	0.42900400	-3.61294500	1.65448200
C	2.60486800	-3.64361000	-1.53916900
H	0.72991000	-3.64921700	-2.61612300
C	3.23273200	-3.59802400	-0.29241500
H	2.90651500	-3.56575200	1.83381500
H	3.21073500	-3.69376500	-2.44088800
C	4.73235200	-3.52171100	-0.18379200
H	5.04383700	-2.47684100	-0.06637100
H	5.10066100	-4.07420800	0.68428900
H	5.21863200	-3.91723600	-1.07889600
C	-3.41325200	-1.30098800	1.14706200
C	-3.75245800	-0.93467400	2.45400800
C	-4.43941700	-1.52497300	0.22952900
C	-5.08302100	-0.78202100	2.83232800
H	-2.96578500	-0.78131800	3.19061300
C	-5.77377000	-1.36853500	0.60299500
H	-4.17137500	-1.83992200	-0.77412600
C	-6.10106600	-0.99261300	1.90298000
H	-5.32675200	-0.50518300	3.85369600
H	-6.56009200	-1.54801500	-0.12433700
H	-7.13993600	-0.87464900	2.19473700
H	0.60111800	-0.86408300	0.74429600

TS5<sub>2</sub> (S,S,S)

P	-1.90022600	-1.25374500	0.87380800
C	-3.25789400	-1.15354000	-0.35178100
C	-2.97327800	-1.35230100	-1.84475700
H	-3.70349700	-0.16645400	-0.18737700
H	-3.98057200	-1.90520800	-0.00801400
C	-4.27568800	-1.35481700	-2.64698700
H	-2.31514400	-0.55735000	-2.21260500
H	-2.45621500	-2.30205600	-2.01998400
C	-4.01879400	-1.49586500	-4.14414800
H	-4.91451100	-2.17509300	-2.29757400
H	-4.82453900	-0.42631700	-2.44899400
H	-4.95396800	-1.49291800	-4.70890100
H	-3.39857000	-0.67248000	-4.51222600
H	-3.49420400	-2.43075300	-4.36414900
C	-2.58855200	-0.57333700	2.41906600
C	-3.87537500	-1.22747900	2.92516200
H	-2.73977500	0.49258400	2.20858400
H	-1.79191100	-0.64921800	3.16975200
C	-4.35544100	-0.58074600	4.22553700
H	-4.66483800	-1.13760000	2.16948000
H	-3.71739500	-2.29894800	3.09796600
C	-5.64475500	-1.21546400	4.73771100
H	-3.56787500	-0.67082700	4.98304700
H	-4.50738500	0.49190800	4.05749300
H	-5.97554500	-0.74597100	5.66712300
H	-6.44876900	-1.11157500	4.00275000
H	-5.50368700	-2.28327800	4.93120900
C	-1.52941600	-3.01048800	1.22098100
C	-0.93007400	-3.85074600	0.09047400
H	-2.48282000	-3.44651400	1.54388700
H	-0.86896900	-3.02034200	2.09587500
C	-0.71864800	-5.29990900	0.52771800
H	-1.59147700	-3.83522300	-0.78433300
H	0.02955600	-3.43142300	-0.22775300
C	-0.09551900	-6.13943400	-0.58340000
H	-0.07335300	-5.31576900	1.41403000
H	-1.68032800	-5.73076500	0.83146300
H	0.05292200	-7.17385100	-0.26456300
H	-0.73607200	-6.14901800	-1.47116100
H	0.87758600	-5.73327300	-0.87731600
C	-0.38422100	-0.21927400	0.54553700
C	-0.35452300	0.50841800	-0.77385400

C	0.93757800	-0.89884800	0.92410600
C	0.74009400	0.46389900	-1.61448700
H	0.86104000	1.34150600	-2.25211400
C	-1.35262200	1.55099300	-0.87219800
O	-2.20982500	1.75061500	-0.00906400
O	-1.36507900	2.20264700	-2.05556200
C	-2.45849500	3.10240700	-2.27136500
C	-3.70934700	2.33841600	-2.66545900
H	-2.12294700	3.76234500	-3.07411600
H	-2.62682300	3.69370700	-1.36798700
H	-4.51733800	3.03295400	-2.90908000
H	-3.51607400	1.70903300	-3.53901500
H	-4.03377400	1.70683200	-1.83465100
H	1.22698000	-1.66769200	0.20385500
C	1.39561700	-0.74770400	-2.17679700
C	2.69578800	-0.69167000	-2.69725700
C	0.66572400	-1.92657400	-2.31850200
C	3.25431100	-1.80648200	-3.30840900
H	3.26089400	0.22832300	-2.57824500
C	1.22825100	-3.05272200	-2.91966900
H	-0.35897400	-1.95184600	-1.96258100
C	2.52646400	-2.99528900	-3.41426000
H	4.26523300	-1.75434800	-3.70044400
H	0.64531700	-3.96548000	-3.00646500
H	2.97036100	-3.86570800	-3.88666100
H	0.84077800	-1.38741000	1.90053700
C	2.09172700	0.12513400	1.06246300
H	1.76961000	0.83770800	1.83998100
N	2.37971600	0.78102700	-0.21146500
S	2.90326600	2.27590300	-0.12550600
O	3.38528600	2.66061500	-1.46330900
O	3.81311500	2.49451200	1.01593100
C	1.50169900	3.34489800	0.20345100
C	1.01641600	3.47736300	1.50656300
C	0.87527800	4.00546400	-0.84735300
C	-0.12541600	4.23423400	1.73948600
H	1.55073700	3.01733200	2.33159300
C	-0.24831600	4.78725900	-0.59452600
H	1.28073600	3.91461100	-1.84970700
C	-0.78196700	4.88904900	0.69143100
H	-0.50842000	4.33234500	2.75185100
H	-0.72531200	5.31966400	-1.41332500
C	-2.04683700	5.66578900	0.94547000
H	-2.00873900	6.18675300	1.90544000

H	-2.22653400	6.40162100	0.15829100
H	-2.90730700	4.98799200	0.97318900
C	3.30415900	-0.62054800	1.60425400
C	3.53201700	-0.69733400	2.97858500
C	4.16203700	-1.29746200	0.73518500
C	4.60118300	-1.43577200	3.48195500
H	2.87108200	-0.16528300	3.65976300
C	5.22789100	-2.03992400	1.23562200
H	3.98685200	-1.22102500	-0.33499100
C	5.45179100	-2.11086600	2.61016000
H	4.77359500	-1.47755900	4.55311800
H	5.89051900	-2.56158600	0.55137100
H	6.28812500	-2.68408900	2.99802700
H	-0.54836700	0.57007700	1.29766400

M5<sub>2</sub><sup>(S,S,S)</sup>

P	-1.94845600	0.97352400	-0.77971200
C	-2.38608500	2.43514400	0.22504300
C	-1.19570300	3.09892600	0.91776900
H	-3.09688900	2.08648500	0.97600000
H	-2.89113100	3.13263300	-0.45551800
C	-1.55893600	4.44941000	1.52780200
H	-0.85296100	2.42258400	1.70538900
H	-0.35542200	3.22979200	0.22110600
C	-0.37853700	5.05129700	2.28514000
H	-1.88917900	5.13443200	0.73685100
H	-2.41153400	4.31895300	2.20607500
H	-0.63444500	6.01585300	2.73035600
H	-0.05398700	4.38215600	3.08945300
H	0.47386200	5.20483200	1.61475000
C	-3.37232400	-0.15926000	-0.91105900
C	-4.71661000	0.55087300	-1.09470300
H	-3.36083000	-0.75694500	0.00468900
H	-3.15744400	-0.82054200	-1.76187100
C	-5.85400000	-0.44703100	-1.31362900
H	-4.93769700	1.15635000	-0.20787200
H	-4.68366200	1.24065200	-1.94786800
C	-7.20200600	0.24521800	-1.49156900
H	-5.62889400	-1.05757800	-2.19708500
H	-5.89575800	-1.13435200	-0.46048400
H	-8.00315300	-0.48121800	-1.64754600
H	-7.45381200	0.84047900	-0.60871200
H	-7.18394100	0.91783300	-2.35469400

C	-1.73268500	1.61050900	-2.48649100
C	-0.87625800	2.87342800	-2.62872300
H	-2.74009600	1.81018500	-2.87023200
H	-1.33079700	0.79117400	-3.09483100
C	-0.68695900	3.25710400	-4.09630200
H	-1.35463500	3.70536100	-2.09658400
H	0.10771500	2.73419600	-2.16656000
C	0.13048300	4.53504500	-4.25716700
H	-0.19267500	2.42951300	-4.61955700
H	-1.67083900	3.37958300	-4.56508900
H	0.26316300	4.79143400	-5.31095900
H	-0.36282400	5.37824800	-3.76413200
H	1.12312300	4.42067700	-3.81090100
C	-0.43753700	-0.03536000	-0.37416100
C	-0.05850100	-0.14214800	1.07577900
C	0.82535100	0.33167200	-1.17047300
C	1.34879500	-0.60097800	1.37049400
H	1.31691200	-1.26504800	2.24020700
C	-1.05266700	-0.16492000	2.02771700
O	-2.27657100	0.06451000	1.82927900
O	-0.61518000	-0.45928000	3.31131800
C	-1.50712600	-0.10173800	4.36068100
C	-1.54458200	1.40555600	4.55872500
H	-1.11680600	-0.60280100	5.25018000
H	-2.50772700	-0.48735700	4.14691400
H	-2.13757100	1.66735700	5.43944600
H	-0.53033900	1.79367700	4.69176200
H	-1.99352300	1.88119500	3.68220900
H	1.28335900	1.22677600	-0.73694900
C	2.41663200	0.44592900	1.70701200
C	3.73199300	0.02285500	1.92664400
C	2.11947000	1.79981600	1.82342800
C	4.73215800	0.94088600	2.22269700
H	3.96499000	-1.03508800	1.83469800
C	3.12168700	2.72765100	2.11375800
H	1.09652200	2.12185100	1.67053700
C	4.43170400	2.30220200	2.30743300
H	5.75044200	0.59853200	2.38009900
H	2.87328700	3.78252100	2.18851900
H	5.21414200	3.02143300	2.52857600
H	0.63561400	0.52941500	-2.22851900
C	1.79767700	-0.85890200	-1.12370300
H	1.35832200	-1.63260000	-1.76546100
N	1.89073700	-1.42395400	0.24817900



S	1.70968900	-3.06557800	0.36449900
O	2.07881100	-3.43952900	1.72561600
O	2.41799900	-3.64661300	-0.77315200
C	-0.01941500	-3.40496600	0.14563900
C	-0.48891800	-3.78452400	-1.11089200
C	-0.89358000	-3.14432600	1.19874000
C	-1.86032700	-3.90022800	-1.31081200
H	0.21762200	-3.99139800	-1.90813500
C	-2.26166800	-3.24772100	0.97446300
H	-0.51538100	-2.84485100	2.17176000
C	-2.76148200	-3.62346600	-0.27686500
H	-2.23791900	-4.20423900	-2.28310900
H	-2.95186400	-3.02107400	1.78166800
C	-4.24379600	-3.74397400	-0.51018500
H	-4.81044200	-3.29480000	0.30849400
H	-4.53499100	-3.25278500	-1.44339300
H	-4.53874000	-4.79525600	-0.58787700
C	3.16451900	-0.53395600	-1.70482400
C	3.71652100	-1.40163200	-2.64905200
C	3.88420300	0.60707000	-1.33451100
C	4.96126900	-1.14200400	-3.21687700
H	3.16771300	-2.29790800	-2.92396700
C	5.13096500	0.86570300	-1.89800500
H	3.48386200	1.29370700	-0.59329000
C	5.67248400	-0.00540100	-2.84190100
H	5.37467900	-1.82866400	-3.94881500
H	5.68128100	1.75183200	-1.59689900
H	6.64400800	0.19994500	-3.28037100
H	-0.79379000	-1.00832500	-0.78288200

TS6<sub>2</sub> (S,S,S)

P	2.52407000	-0.01248300	1.09840700
C	3.65013800	-1.38953900	0.60371600
C	3.38881400	-1.98074400	-0.78036400
H	3.51805400	-2.16785900	1.36466600
H	4.68298300	-1.02478800	0.68007800
C	4.37765700	-3.09199400	-1.12730300
H	2.36882000	-2.38195200	-0.80010200
H	3.44253100	-1.19601300	-1.54480100
C	4.16816300	-3.62087900	-2.54342100
H	5.40207200	-2.71380100	-1.02007600
H	4.26950300	-3.90750300	-0.40126900
H	4.86331800	-4.43128400	-2.77691300

H	3.15022400	-4.00235500	-2.66971700
H	4.31867900	-2.82557700	-3.28061400
C	2.65809600	-0.00142700	2.93438000
C	4.05733800	0.19192300	3.52133400
H	2.23620000	-0.95911400	3.26713200
H	1.98041600	0.77970100	3.30316600
C	4.05802800	0.08634800	5.04668300
H	4.74418100	-0.55828300	3.10922600
H	4.45157500	1.17323600	3.23051300
C	5.44816300	0.29784200	5.63968100
H	3.36040700	0.82598500	5.45807700
H	3.67380700	-0.89867900	5.33798700
H	5.43419300	0.21396900	6.72916700
H	6.15336400	-0.44475200	5.25368400
H	5.83437600	1.28917800	5.38294700
C	3.34884500	1.55437800	0.58334000
C	3.34510400	1.83160300	-0.92262400
H	4.38065000	1.53336300	0.95692600
H	2.83172200	2.36343500	1.11603000
C	4.06014000	3.14529000	-1.24050000
H	3.84451500	1.01285900	-1.45631400
H	2.31721500	1.86377900	-1.31035700
C	4.06374200	3.46839000	-2.73109000
H	3.57629700	3.95938200	-0.68627900
H	5.09070900	3.08800100	-0.86822000
H	4.62021600	4.38629700	-2.93805200
H	4.52269600	2.65622100	-3.30486300
H	3.04281700	3.59527500	-3.10271400
C	0.28702000	-0.14235700	0.91524400
C	-0.30859200	-0.89508600	-0.10996100
C	-0.09340000	1.32430800	0.88768700
C	-0.99603000	-0.16222700	-1.22577600
H	-1.61510700	-0.88568200	-1.76200900
C	-0.19041200	-2.30797700	-0.03802000
O	0.44029300	-2.92033400	0.83047500
O	-0.81309000	-2.97152300	-1.06188700
C	-0.76476300	-4.39772600	-1.01273000
C	0.54536300	-4.92371800	-1.57110200
H	-1.61188200	-4.72947300	-1.61916200
H	-0.91223300	-4.73060600	0.01813700
H	0.53458000	-6.01640100	-1.60772900
H	0.70155400	-4.54446100	-2.58499700
H	1.37582300	-4.60246500	-0.93730100
H	0.41813000	1.85389200	0.07462900

C	-0.05647500	0.42625500	-2.27837200
C	-0.27322000	1.66089400	-2.89086200
C	1.02025600	-0.35585500	-2.70515300
C	0.59784700	2.12333000	-3.87776500
H	-1.13937800	2.24720600	-2.60445400
C	1.88346400	0.09725100	-3.69779900
H	1.16636900	-1.33411400	-2.25733800
C	1.68163200	1.34694100	-4.28104300
H	0.42224600	3.09090200	-4.33871000
H	2.71569500	-0.52561700	-4.01441300
H	2.35949500	1.71045800	-5.04694200
H	0.15312600	1.83507800	1.82272100
C	-1.60821200	1.45126000	0.65091300
H	-2.10969100	0.85236400	1.42688900
N	-1.92153000	0.89776500	-0.69251200
S	-3.53640000	0.54382500	-0.93174500
O	-3.67323700	0.14928700	-2.32994400
O	-4.30632800	1.66592400	-0.41054100
C	-3.89958100	-0.87027100	0.08170500
C	-4.33511500	-0.67235100	1.39055400
C	-3.69359900	-2.15296100	-0.42338300
C	-4.54488500	-1.77877800	2.20670300
H	-4.52767000	0.33351700	1.75048900
C	-3.90756500	-3.24480500	0.40769200
H	-3.37789900	-2.29388600	-1.45136600
C	-4.32525200	-3.07509800	1.73250000
H	-4.89122000	-1.63347400	3.22565400
H	-3.75504600	-4.24834500	0.02003000
C	-4.52200600	-4.27036700	2.62644000
H	-5.01941500	-5.08307100	2.09162800
H	-3.55571100	-4.64928600	2.97417700
H	-5.11830400	-4.01562600	3.50461100
C	-2.02191600	2.89929800	0.81567900
C	-2.73714500	3.28372900	1.94931800
C	-1.61533900	3.87623800	-0.09437800
C	-3.05378700	4.62224600	2.16802700
H	-3.05565600	2.52760400	2.66309500
C	-1.93420700	5.21402200	0.11902800
H	-1.04612800	3.58545300	-0.97228900
C	-2.65509700	5.59122700	1.25120300
H	-3.61717400	4.90619300	3.05123800
H	-1.61657000	5.96429000	-0.59833300
H	-2.90386000	6.63451700	1.41686100
H	0.28605900	-0.61450400	1.89903300

$P_2^{(S,R)}$			
C	-1.87825200	0.32772400	2.11310700
C	-1.55854400	0.97594300	0.99185500
C	-1.50550200	-1.10609500	2.32600700
C	-0.69206800	0.39588100	-0.10593100
C	-2.01141100	2.38846500	0.83484700
O	-2.46071300	3.07030100	1.73006900
O	-1.87148600	2.81021700	-0.42707700
C	-2.12328700	4.20615300	-0.67248300
C	-0.92957900	5.03700900	-0.24082000
H	-3.03242100	4.49944600	-0.14369500
H	-2.29244400	4.26936900	-1.74794300
H	-1.09747500	6.08763200	-0.48989100
H	-0.78191600	4.95528900	0.83829000
H	-0.02471000	4.69347000	-0.74876800
H	-2.24969600	-1.60314900	2.95068300
C	0.60041100	1.20378500	-0.19366900
C	0.95223400	1.85293100	-1.37393300
C	1.44050900	1.29115500	0.91779800
C	2.14069800	2.57868300	-1.44831100
H	0.29549400	1.78081600	-2.23653900
C	2.63044800	2.00562300	0.84353700
H	1.16587300	0.77318300	1.83402600
C	2.98120900	2.65349500	-0.34116800
H	2.41047000	3.07980100	-2.37266500
H	3.28699200	2.05436300	1.70687800
H	3.91137100	3.21009100	-0.40046900
H	-0.55155800	-1.17258000	2.86391800
C	-1.36147500	-1.81585300	0.97540600
H	-0.89452300	-2.78935600	1.14174400
N	-0.39854300	-1.02533900	0.18755000
S	0.56328800	-1.82219600	-0.91866400
O	0.36837700	-1.23021900	-2.24054700
O	0.31989600	-3.24969500	-0.72684800
C	2.22448500	-1.46834700	-0.40480300
C	2.63216600	-1.87059000	0.86485000
C	3.07584400	-0.78646000	-1.26333000
C	3.91770200	-1.55758700	1.28296900
H	1.94924300	-2.40625600	1.51835200
C	4.36099500	-0.48333200	-0.82622600
H	2.72330400	-0.47811000	-2.24118500
C	4.79402400	-0.85104300	0.44935700

H	4.24836500	-1.85946400	2.27244900
H	5.03203200	0.06388300	-1.48229100
C	6.16364600	-0.45731000	0.93467000
H	6.12928800	0.53580600	1.39578500
H	6.53730600	-1.15825000	1.68405000
H	6.87836600	-0.41355400	0.11001700
C	-2.69796800	-2.04516900	0.27019800
C	-3.78190800	-2.56947200	0.98352300
C	-2.85883100	-1.80277300	-1.09544600
C	-4.99672900	-2.82316100	0.35479400
H	-3.68169200	-2.79908900	2.03990600
C	-4.07669600	-2.05296000	-1.72633400
H	-2.03089600	-1.42468200	-1.68676900
C	-5.15197300	-2.55876700	-1.00428200
H	-5.82291100	-3.23053900	0.92900600
H	-4.17890400	-1.85217400	-2.78805100
H	-6.10037100	-2.75192000	-1.49488200
H	-1.21569200	0.49036500	-1.06492400
H	-2.44173400	0.85885500	2.87504500
P <sub>2</sub> <sup>(S,S)</sup>			
S	1.48402900	-1.28187600	-1.52075800
O	1.19977900	-0.52624700	-2.73665500
O	1.59825400	-2.73486900	-1.56691800
O	-0.41039700	3.29617200	1.82586500
O	-0.71815900	3.08652200	-0.39529100
N	0.25705800	-0.94017200	-0.46118000
C	3.88249400	-1.52370700	-0.21129000
H	3.69397600	-2.59165200	-0.23914400
C	5.00855000	-1.00364600	0.41563500
H	5.71882000	-1.67837600	0.88472100
C	5.24407600	0.37548400	0.44906500
C	4.33010000	1.22992600	-0.17609500
H	4.50897400	2.30081600	-0.16953000
C	3.20025600	0.72954000	-0.81221200
H	2.50405800	1.39995300	-1.30752500
C	2.98595800	-0.64717300	-0.81813900
C	0.26000000	-1.63895700	0.84417900
H	0.80301000	-2.57563400	0.68658500
C	0.98923400	-0.79524300	1.89273200
H	0.83035500	-1.20468100	2.89422600
H	2.07233100	-0.84569500	1.72123400
C	0.56566200	0.63923300	1.83237700

H	0.78057700	1.28454200	2.68063200
C	-0.03904900	1.17568000	0.76804400
C	-0.35099900	0.40576700	-0.49497200
H	0.10505900	0.93721600	-1.33533300
C	-1.84122600	0.30101700	-0.82288900
C	-2.19611000	-0.20683100	-2.07415300
H	-1.40913500	-0.49970800	-2.76566000
C	-3.53403000	-0.35255700	-2.42174000
H	-3.79939600	-0.75020900	-3.39644400
C	-4.53308900	0.01260900	-1.51968300
H	-5.57859000	-0.10387600	-1.78712800
C	-4.18343100	0.52517400	-0.27418800
H	-4.95462400	0.80507200	0.43691900
C	-2.84107300	0.67219800	0.07220400
H	-2.57936300	1.05116100	1.05727300
C	-1.18040500	-1.99445800	1.19740500
C	-1.90858800	-2.74987800	0.27306100
H	-1.42424100	-3.05287900	-0.65219400
C	-3.23744600	-3.07272000	0.51084300
H	-3.79356200	-3.64737300	-0.22308100
C	-3.85762800	-2.65130400	1.68834100
H	-4.89793200	-2.89800300	1.87556100
C	-3.13684300	-1.91235000	2.61838300
H	-3.61056800	-1.57869600	3.53628400
C	-1.80270100	-1.58338000	2.37338700
H	-1.26843600	-0.98272200	3.10235800
C	-0.40194900	2.62094100	0.81902900
C	6.45763300	0.92111500	1.15320900
H	6.61577800	1.97417700	0.91366900
H	7.35458400	0.36231000	0.87412800
H	6.34214500	0.83409900	2.23815000
C	-1.21863800	4.43560600	-0.45749700
H	-1.08438300	4.72887300	-1.49906000
H	-0.60164400	5.07055300	0.18140000
C	-2.67806700	4.47432600	-0.04666100
H	-2.78644900	4.18625400	1.00151000
H	-3.26392300	3.78924200	-0.66424300
H	-3.07325200	5.48535200	-0.17115600

