

Supporting Information

Theoretical Study on Copper-Catalyzed Asymmetric Alkene Trifluoromethyl-arylation Cross-coupling Reaction: Origin of Regio- and Stereo-selectivity

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1. The calculated Free energy profiles for Paths I using *N*-methyl-acrylamide **1b** as substrate.

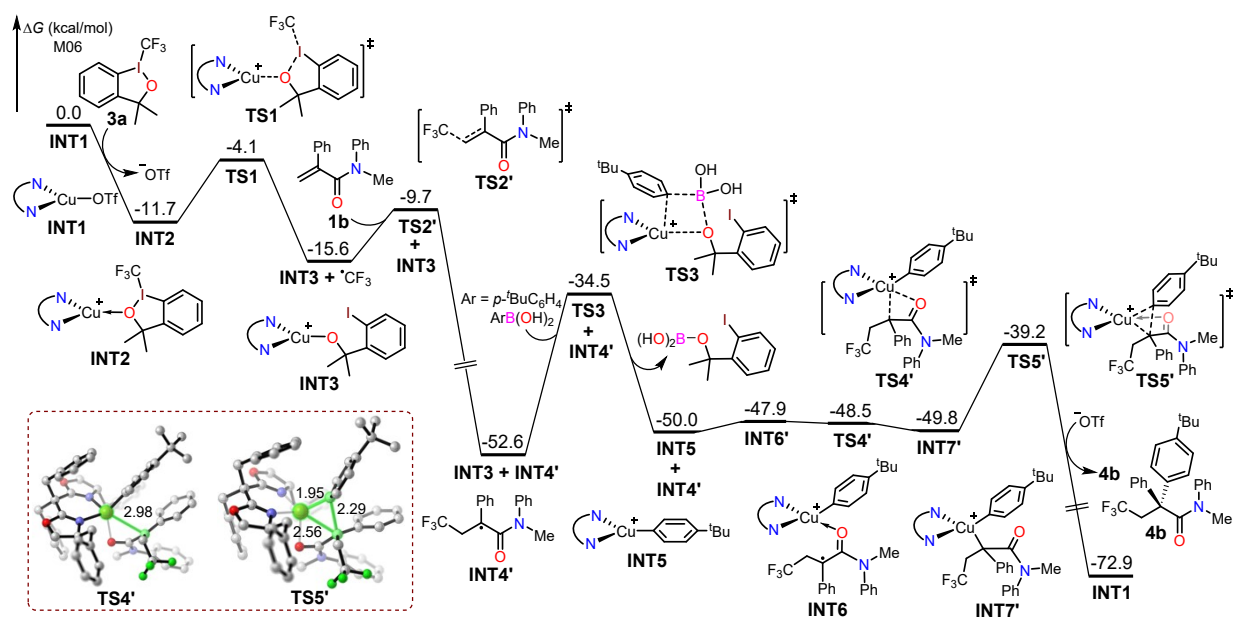


Figure S1. Free energy profiles and structural information for Paths I using *N*-methyl-acrylamide **1b** as substrate. Key bond distances are in angstroms.

2. The calculated Free energy profiles for Paths I using ketone **1c** as substrate.

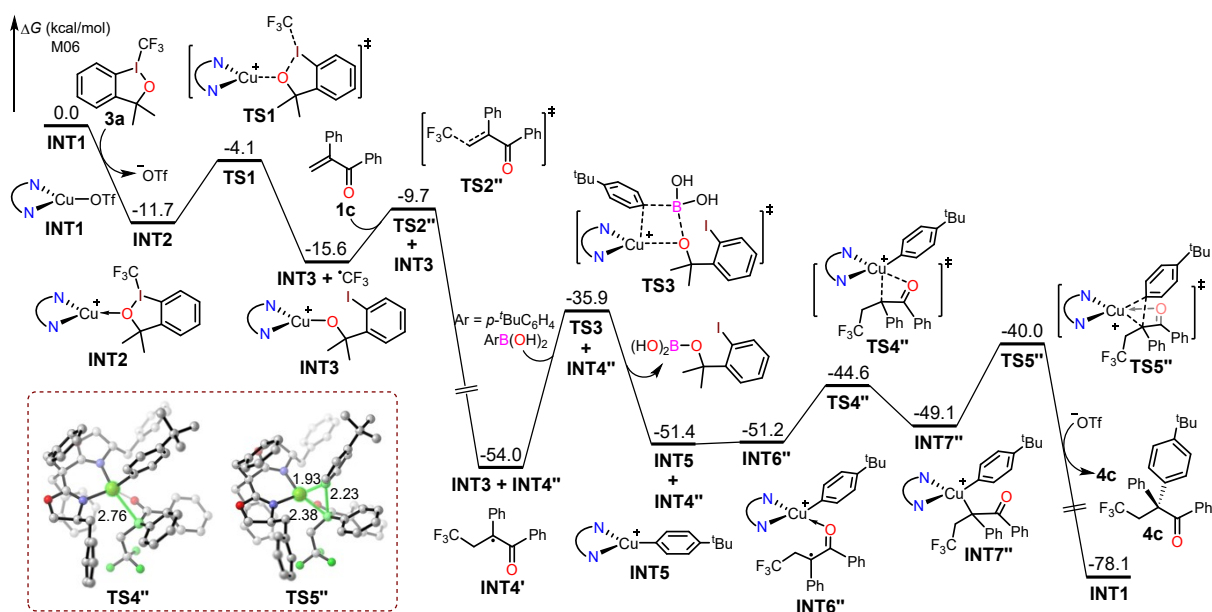


Figure S2. Free energy profiles and structural information for Paths I using ketone **1c** as substrate. Key bond distances are in angstroms.

3. The calculated structure information and free energy of two conformations for INT4 and INT4'.

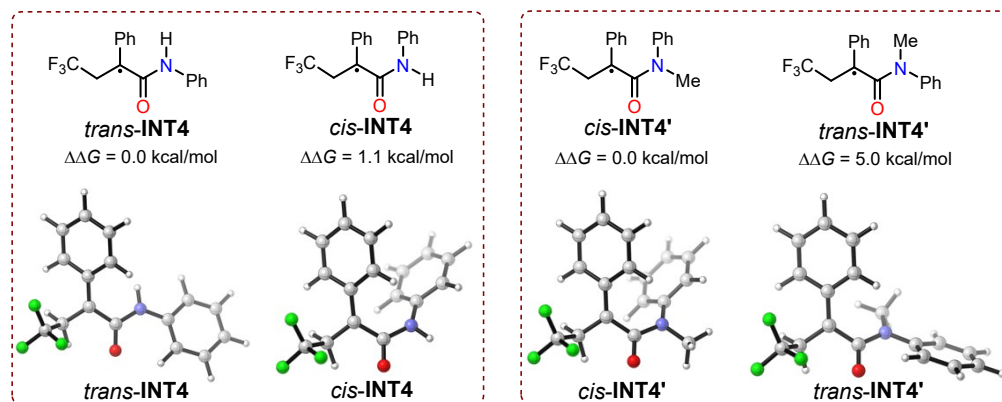


Figure S3. The calculated structure information and free energy of two conformations for INT4 and INT4'.

4. The calculated free energy profiles for neutral pathway.

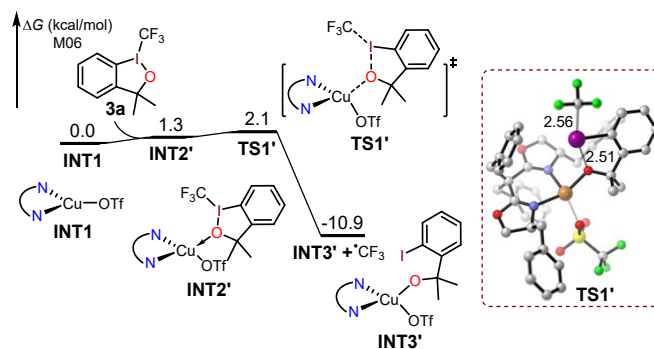


Figure S4. Free energy profiles for neutral pathway.

As depicted in Figure S4, we also examined the neutral pathway for the Cu-catalyzed asymmetric alkene trifluoromethyl-arylation cross-coupling reaction. The calculated results revealed that the free energy of **TS1'** is 6.2 kcal/mol higher than that of **TS1**, indicating that this neutral pathway is unfavorable.

5. The calculated free energy profiles for the pathway involving coordination of the methanol.

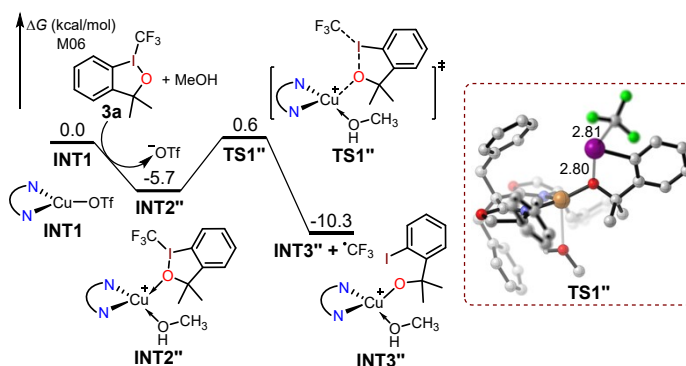


Figure S5. Free energy profiles for the pathway involving coordination of the methanol.

As depicted in Figure S5, we also examined the pathway involving coordination of the methanol. The calculated results revealed that the free energy of **TS1''** is 4.7 kcal/mol higher than that of **TS1**, indicating that this pathway is also unfavorable.

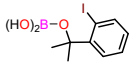
6. Complete reference for Gaussian 16

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-

Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

7. M06-L absolute calculation energies, enthalpies, and free energies.

Table S1. M06-L absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{(\text{elec-M06-L})}^1$	$H_{(\text{corr-M06-L P})}^2$	$G_{(\text{corr-M06-L})}^3$	$E_{(\text{solv-M06-L})}^4$	IF ⁵
INT1	-2771.600405	0.687292	0.560326	-2772.248421	-
3a	-772.990264	0.196582	0.137192	-773.2369394	-
·OTf	-961.439967	0.03562	-0.004819	-961.725638	-
INT2	-2583.050593	0.848779	0.703338	-2583.779400	-
TS1	-2583.035819	0.847659	0.700845	-2583.764817	-56.2
INT3	-2245.517826	0.830507	0.694535	-2246.146347	-
·CF3	-337.5130629	0.016544	-0.014566	-337.6158581	-
TS2	-1046.823693	0.275388	0.206404	-1047.127871	-38.7
1a	-709.303519	0.257798	0.201158	-709.504483	-
INT4	-1046.897806	0.278048	0.211492	-1047.204045	-
TS3	-2810.968021	1.083092	0.920847	-2811.762687	-184.1
ArB(OH) ₂	-565.427306	0.251680	0.200018	-565.6189899	-
INT5	-2198.817557	0.865898	0.738379	-2199.43391	-
	-612.129471	0.219589	0.162228	-612.3333265	-
INT6	-3245.765066	1.143900	0.972680	-3246.663421	-
TS4	-3245.761880	1.143487	0.975661	-3246.659529	-5.7
INT7	-3245.773140	1.144290	0.974915	-3246.67024	-
TS5	-3245.761285	1.144474	0.979344	-3246.655524	-140.3
4a	-1435.773089	0.494624	0.406169	-1436.186253	-

TS6	-3245.737934	1.142488	0.974544	-3246.627995	-233.2
TS7	-3337.008311	0.940662	0.788555	-3337.822386	-172.3
INT8	-2199.007293	0.864710	0.735559	-2199.572791	-
TfOB(OH) ₂	-1137.969259	0.07577	0.024355	-1138.239638	-
TS8	-2972.009904	1.059383	0.891921	-2972.810457	-147.9
INT9	-2634.524568	1.043025	0.882398	-2635.212144	-
INT6-R	-3245.765228	1.143483	0.971803	-3246.660295	-
TS4-R	-3245.763992	1.143088	0.976794	-3246.658072	-55.9
INT7-R	-3245.773751	1.144672	0.976855	-3246.667743	-
TS5-R	-3245.761656	1.143811	0.97672	-3246.652347	-122.2
4a-R	-1435.773089	0.494624	0.406169	-1436.186253	-
TS9	-1046.855244	0.274544	0.209509	-1047.166244	-540.1
INT10	-1046.873315	0.276352	0.212042	-1047.183157	-
TS9'	-1086.160779	0.304070	0.235529	-1086.479221	-545.1
INT10'	-1086.180098	0.305980	0.238246	-1086.497406	-
INT11	-3245.770026	1.144503	0.972746	-3246.664909	-
TS10	-3245.748251	1.142097	0.973608	-3246.645489	-316.7
6a	-1435.738120	0.493092	0.400569	-1436.150899	-
INT4''	-991.533340	0.258708	0.194678	-991.819476	-
INT11''	-3190.412933	1.125545	0.951581	-3191.290813	-
TS10''	-3190.398820	1.123798	0.958126	-3191.277002	-243.3
6c	-1380.389664	0.474953	0.387732	-1380.778344	-
TS2'	-1086.116865	0.303262	0.228987	-1086.434878	-80.6
1b	-748.596276	0.286047	0.225354	-748.810162	-
INT4'	-1086.190572	0.306243	0.234619	-1086.508776	-
INT6'	-3285.060133	1.172739	0.999177	-3285.965550	-
TS4'	-3285.058037	1.171412	0.996319	-3285.963626	-85.7
INT7'	-3285.068915	1.173372	1.002481	-3285.971897	-
TS5'	-3285.053491	1.172128	1.001814	-3285.954272	-192.3
4b	-1475.058427	0.522796	0.432412	-1475.480959	-

TS2''	-991.455749	0.255927	0.188021	-991.742104	-38.2
1c	-653.935315	0.238565	0.184056	-654.117147	-
INT6''	-3190.393601	1.124933	0.951767	-3191.271756	-
TS4''	-3190.392106	1.124698	0.958629	-3191.268037	-66.4
INT7''	-3190.400676	1.125972	0.960054	-3191.276710	-
TS5''	-3190.390189	1.125375	0.960556	-3191.262585	-149.1
4c	-1380.401126	0.475222	0.389271	-1380.794432	-
INT2'	-3544.631538	0.886469	0.724992	-3545.510785	-
TS1'	-3544.628751	0.885054	0.72249	-3545.506932	-91.4
INT3'	-3207.121146	0.868749	0.715309	-3207.890034	-
INT2''	-2698.769089	0.906221	0.751904	-2699.537096	-
MeOH	-115.6914875	0.055841	0.028761	-115.7474487	-
TS1''	-2698.753053	0.905745	0.749968	-2699.525092	-71.7
INT3''	-2361.236360	0.888814	0.743914	-2361.90604	-

¹The electronic energy calculated by M06-L in methanol solvent. ²The thermal correction to enthalpy calculated by M06-L in methanol solvent. ³The thermal correction to Gibbs free energy calculated by M06-L in methanol solvent. ⁴The electronic energy calculated by M06-L in methanol solvent. ⁵The M06-L calculated imaginary frequencies for the transition states.

8. M06-L geometries for all the optimized compounds and transition states. The S**2 values of radicals.

INT1				H	-6.80291100	2.76266300	-0.99805800
C	-3.15160200	-0.75496000	1.71092300	H	-8.54482700	1.01367000	-0.70584000
C	-2.64687500	0.03544700	0.49731900	C	0.19903500	-2.14054600	1.45674900
C	-1.02865200	-1.29722900	1.24098800	C	-0.24349900	-3.63339000	1.38086400
H	-4.03460900	-1.36947500	1.50027100	H	-0.83087200	-3.84571000	2.28164200
H	-2.72107200	1.11847300	0.64344100	H	0.66600400	-4.24406800	1.43206000
H	-3.34279000	-0.14142300	2.59783900	C	0.79131900	-1.85359800	2.87997600
O	-2.05870700	-1.65524600	2.03628000	H	-0.05595400	-1.78392300	3.57444600
N	-1.22478300	-0.33300700	0.42093900	H	1.37790500	-2.73349600	3.17195500
C	-3.32480700	-0.33734900	-0.82421600	C	-1.04991700	-3.95092100	0.15058000
H	-2.78613700	0.19256700	-1.61961400	C	-2.43085600	-4.15349600	0.24018300
H	-3.19023000	-1.41735300	-0.99147800	C	-0.44938000	-4.00131900	-1.11273000
C	-4.78064000	0.02725500	-0.82522700	C	-3.19314500	-4.39728700	-0.89952200
C	-5.76909400	-0.94760500	-0.66301300	H	-2.90824200	-4.11571500	1.21925700
C	-5.16867700	1.36773000	-0.94150100	C	-1.21004300	-4.23341900	-2.25475100
C	-7.11728900	-0.59841600	-0.61991500	H	0.63033300	-3.87190700	-1.20136900
H	-5.47232800	-1.99566000	-0.58410200	C	-2.58549200	-4.42954900	-2.15206300
C	-6.51437300	1.71751000	-0.89862800	H	-4.26540100	-4.56406200	-0.80814500
H	-4.40109000	2.13032900	-1.07871200	H	-0.72570100	-4.26777000	-3.22885500
C	-7.49233700	0.73695500	-0.73633000	H	-3.17975500	-4.61267400	-3.04502400
H	-7.87511000	-1.37117100	-0.49950800	C	1.66161700	-0.62717600	2.92128200
				C	3.04599100	-0.75961400	3.06756600

C	1.13102300	0.65320100	2.72082200
C	3.88012600	0.35536900	3.02538700
H	3.47037400	-1.75355900	3.21520500
C	1.96315400	1.76811400	2.65570000
H	0.05486100	0.78543400	2.61172200
C	3.34063000	1.62178700	2.80987900
H	4.95416300	0.23295600	3.16058500
H	1.53134900	2.75062000	2.47952100
H	3.99029700	2.49362900	2.76155700
C	3.42185900	-2.20348200	-0.19876700
C	2.77400000	-1.05572700	-0.98536000
C	1.30753900	-1.88250200	0.47192100
H	4.21594900	-1.85911200	0.47788400
H	2.65495300	-1.31619900	-2.04795300
H	3.80371100	-3.02324400	-0.81272400
O	2.34950800	-2.73009600	0.62216600
N	1.43343400	-0.94378800	-0.39177800
C	3.51491500	0.27634700	-0.86998200
H	2.93628100	1.03892500	-1.41117100
H	3.51208400	0.57490900	0.18865200
C	4.92166500	0.18053700	-1.38748900
C	6.00617000	0.13745600	-0.50640600
C	5.17394400	0.08420200	-2.76082900
C	7.30898400	0.00307200	-0.98070100
H	5.81888800	0.22613000	0.56539600
C	6.47323000	-0.05018300	-3.23866700
H	4.33969800	0.13095100	-3.46214200
C	7.54532300	-0.09332800	-2.34899900
H	8.14137000	-0.02135700	-0.27935200
H	6.65149300	-0.11476800	-4.31068100
H	8.56239000	-0.19485800	-2.72295200
Cu	0.23825100	0.67725600	-0.52791700
S	-0.73648300	3.35878900	-1.14281800
O	-1.96294900	2.55771300	-1.26880400
O	-0.59899500	4.57150100	-1.93204500
O	0.51998100	2.50733900	-1.12677400
C	-0.79124400	3.93271100	0.60941300
F	-0.92691600	2.87242900	1.44348800
F	-1.82942700	4.74540300	0.81230000
F	0.33106900	4.57477900	0.95126500

3a

C	2.27360400	-0.96890700	0.09264200
C	0.51470100	0.81684600	-0.12629500
C	0.01051900	2.10282600	-0.20023100
C	0.92273200	3.15595200	-0.13812800
C	2.28173800	2.89373900	0.00801100
C	2.74164000	1.58260400	0.08039200
C	1.85411200	0.50531300	0.00098700
H	-1.04824600	2.30411100	-0.31914100
H	0.56066100	4.17940900	-0.20956300
H	2.99074100	3.71763300	0.06115000
H	3.80692500	1.38711400	0.19707100
I	-0.71508900	-0.97396200	-0.18702300
O	1.30800100	-1.75922800	-0.52201000
C	3.58392200	-1.21358400	-0.65453700
H	4.42982600	-0.68249500	-0.20056500
H	3.80604400	-2.28527400	-0.63233800
H	3.49124900	-0.90586300	-1.70109300
C	2.43352500	-1.32841500	1.57898400
H	2.70467900	-2.38642200	1.66850700
H	3.20606000	-0.72371200	2.07184100
H	1.49246100	-1.17388400	2.12274200

C	-2.61362700	0.32791000	0.15525800
F	-3.61592100	-0.55286800	0.33791900
F	-2.94972100	1.11135900	-0.88908800
F	-2.54790200	1.11011800	1.24530000

-OTf

S	-0.92002800	0.00001100	-0.00002900
O	-1.22827300	-0.61092300	1.30469300
O	-1.22890100	1.43529200	-0.12324200
O	-1.22726800	-0.82460100	-1.18165500
C	0.92551600	0.00008100	0.00025100
F	1.43123300	0.53351000	-1.13272900
F	1.43067500	-1.24847300	0.10497400
F	1.43174500	0.71509600	1.02782000

INT2

C	-1.49355900	-3.40056200	1.80454400
C	-1.59710300	-2.26851900	0.76814700
C	0.53670100	-2.59902000	1.29288000
H	-1.80714000	-4.37553700	1.41075200
H	-2.14820400	-1.40364500	1.17026800
H	-2.01420500	-3.21165300	2.74705600
O	-0.07283200	-3.48951300	2.10142800
N	-0.20573600	-1.86517600	0.55790500
C	-2.22381000	-2.67064600	-0.56752800
H	-2.00059600	-1.86104700	-1.27626200
H	-1.71100400	-3.57176700	-0.93517800
C	-3.70485400	-2.88484500	-0.45960900
C	-4.25370500	-4.16654600	-0.37481800
C	-4.56245900	-1.78046000	-0.39627800
C	-5.62777700	-4.34395800	-0.22919100
H	-3.59565600	-5.03505400	-0.44005000
C	-5.93479800	-1.95346000	-0.25165700
H	-4.13914300	-0.77544800	-0.47409800
C	-6.47035500	-3.23772000	-0.16578700
H	-6.04142600	-5.34881000	-0.17105900
H	-6.59109000	-1.08600300	-0.21186300
H	-7.54400900	-3.37492300	-0.05591900
C	2.03569700	-2.61542200	1.39963200
C	2.51073800	-4.08135700	1.14874900
H	2.18229800	-4.67943800	2.00628000
H	3.60691000	-4.08017600	1.15104700
C	2.43111400	-2.16956800	2.84445300
H	1.90541400	-2.83477000	3.53998600
H	3.50534400	-2.35093000	2.96414600
C	1.95641100	-4.64838000	-0.12991900
C	0.85127500	-5.50569500	-0.10485400
C	2.48581900	-4.27735200	-1.37087000
C	0.28031700	-5.96883800	-1.28757500
H	0.44425100	-5.81743600	0.85694200
C	1.91474700	-4.73434200	-2.55508200
H	3.36921600	-3.63753100	-1.40871000
C	0.80500000	-5.57616300	-2.51661600
H	-0.57165400	-6.64599900	-1.24854800
H	2.34587600	-4.44445500	-3.51146000
H	0.36246700	-5.93880800	-3.44196800
C	2.09821200	-0.72780800	3.11165600
C	3.07242600	0.26666700	2.97344800
C	0.79451500	-0.34261000	3.44567300
C	2.75430000	1.61031600	3.15577300
H	4.09680900	-0.02264500	2.73248900
C	0.47250100	0.99998000	3.62923400
H	0.02977800	-1.10814100	3.58722700

C	1.45134700	1.98252500	3.47715700	H	-3.38588900	1.70190600	-1.34219100
H	3.52915100	2.36934300	3.06038800	H	-4.67796400	0.62393500	-0.82203100
H	-0.53784100	1.27800600	3.92815500	C	-5.06950400	2.70652000	-0.44283100
H	1.20563800	3.03014000	3.63626000	C	-6.44338000	2.50462900	-0.28183600
C	4.65055100	-0.83197700	-0.39697600	C	-4.58158400	4.01758300	-0.45450300
C	3.43522500	-0.12514100	-1.00716200	C	-7.31115800	3.58454800	-0.13714900
C	2.74512600	-1.69348500	0.43611100	H	-6.83445200	1.48533000	-0.28735500
H	5.32126300	-0.16222300	0.15256700	C	-5.44480100	5.09872700	-0.31130700
H	3.40505300	-0.24937300	-2.09855100	H	-3.51264800	4.19060500	-0.59117600
H	5.23854300	-1.41512300	-1.11165200	C	-6.81246900	4.88406000	-0.15019300
O	4.08086000	-1.76463000	0.55727700	H	-8.37888800	3.41039300	-0.01989400
N	2.28957900	-0.85078000	-0.42651800	H	-5.05120400	6.11310900	-0.33042500
C	3.33298000	1.36362900	-0.66451300	H	-7.48829600	5.72950800	-0.04098300
H	2.36555300	1.72374900	-1.04970700	C	-2.65156500	-2.33866200	1.18124600
H	3.28519700	1.45953500	0.43007000	C	-3.93233700	-3.15282600	0.82462100
C	4.47723300	2.15925300	-1.22198100	H	-4.59819000	-3.10501300	1.69373900
C	5.53005400	2.56954600	-0.39884000	H	-3.62720600	-4.19964900	0.70837100
C	4.53481100	2.46528600	-2.58609200	C	-2.15024500	-2.75822700	2.60562400
C	6.61436600	3.26983700	-0.92200600	H	-2.85821700	-2.34125500	3.33300400
H	5.49061600	2.34666500	0.66956500	H	-2.22996600	-3.85024100	2.66622300
C	5.61546700	3.16503700	-3.11248000	C	-4.64364700	-2.64574000	-0.40197600
H	3.71563000	2.15959600	-3.23979800	C	-5.87105900	-1.98519700	-0.28542500
C	6.65911500	3.56770200	-2.28094800	C	-4.08242200	-2.79232100	-1.67629600
H	7.42262000	3.58680000	-0.26605900	C	-6.52290300	-1.48625200	-1.41117600
H	5.64243500	3.40168800	-4.17428800	H	-6.32129000	-1.87108400	0.70092500
H	7.50322200	4.11711200	-2.69204600	C	-4.72430000	-2.28199400	-2.80081700
Cu	0.45347900	-0.32952300	-0.71400500	H	-3.14487700	-3.33779200	-1.79479800
C	-1.36259900	1.29159300	-2.35439900	C	-5.94615900	-1.62491500	-2.67111800
C	-2.78048100	2.82677100	-0.90786900	H	-7.48858700	-0.99504100	-1.30445500
C	-3.80154700	3.72442400	-0.64683000	H	-4.27758800	-2.41247400	-3.78450400
C	-4.60940400	4.11219800	-1.71467100	H	-6.45329900	-1.23547500	-3.55118100
C	-4.37206600	3.60382700	-2.98701100	C	-0.73634200	-2.32715900	2.87924900
C	-3.33968300	2.69741100	-3.19922000	C	0.29531300	-3.27109400	2.87685000
C	-2.51424000	2.27459600	-2.15118600	C	-0.40653000	-0.97683700	3.05625100
H	-3.99597600	4.11333600	0.34594300	C	1.62129600	-2.88221100	3.05655200
H	-5.42532700	4.80841600	-1.53647600	H	0.04950200	-4.32565500	2.74701400
H	-5.00018200	3.90857400	-3.82062400	C	0.91985400	-0.58099900	3.21097900
H	-3.16703200	2.30194000	-4.19836600	H	-1.19611700	-0.22465400	3.09404700
I	-1.42978700	2.15322900	0.66235000	C	1.93722900	-1.53459700	3.21299800
O	-1.15807100	0.63262400	-1.11693700	H	2.40752600	-3.63499600	3.08208800
C	-1.70954600	0.21632600	-3.37987800	H	1.15713300	0.47355100	3.34093000
H	-1.80012100	0.61966800	-4.39472200	H	2.97171300	-1.22753100	3.35862700
H	-0.90482700	-0.52940300	-3.39218500	C	-0.09335200	-4.10060300	-0.70898900
H	-2.64517100	-0.29038000	-3.11837900	C	0.24667700	-2.66267700	-1.12067800
C	-0.11130300	2.05872600	-2.78792600	C	-1.54313700	-2.66218000	0.21937900
H	0.71928600	1.34924100	-2.91622400	H	0.66440200	-4.55194300	-0.05598900
H	-0.26434600	2.59179800	-3.73401300	H	0.08527200	-2.50530300	-2.19801600
H	0.18562700	2.79642500	-2.03048000	H	-0.30457500	-4.77876200	-1.53846600
C	-2.07204000	3.85511300	2.07889700	O	-1.31573500	-3.97339100	0.07140600
F	-1.23691800	3.80435300	3.12105900	N	-0.74735100	-1.85901100	-0.39016200
F	-3.31895800	3.68830100	2.52516500	C	1.65373300	-2.20318600	-0.75052400
F	-1.97304400	5.04581300	1.49686500	H	1.71512600	-1.12896900	-0.98498700
				H	1.76427200	-2.29059000	0.34156000
				C	2.72914700	-2.97052900	-1.46271400
				C	3.44983100	-3.97119300	-0.80485300
				C	3.00356900	-2.72060000	-2.81194500
				C	4.42182300	-4.70798600	-1.47753500
				H	3.25304000	-4.16380000	0.25150500
				C	3.97390000	-3.45397900	-3.48656000
				H	2.45453700	-1.93487500	-3.33461600
				C	4.68422900	-4.45117200	-2.82021100
				H	4.97817800	-5.48044000	-0.95043200
				H	4.18106400	-3.24434200	-4.53403500
TS1	S**2 = 1.04						
C	-4.29896400	0.81836300	1.89945300				
C	-3.38273400	1.27271400	0.76178800				
C	-3.03216900	-0.88365900	1.18898200				
H	-5.36109700	1.00899100	1.71830300				
H	-2.78520800	2.14948800	1.04254300				
H	-4.02026000	1.20702900	2.88490700				
O	-4.11130900	-0.62385300	1.93761700				
N	-2.49073900	0.11164400	0.57840100				
C	-4.13095800	1.53936600	-0.55101300				

H	5.44517900	-5.02319600	-3.34662900
Cu	-0.55246600	0.08693500	-0.01240400
C	0.82837000	2.31118400	-1.05610500
C	3.11280600	2.96831200	-0.08002400
C	4.12656300	3.87449300	0.20536800
C	3.99536500	5.19428700	-0.21638400
C	2.85687200	5.57940300	-0.91168800
C	1.85214100	4.65321100	-1.16886000
C	1.94073600	3.31846200	-0.75307800
H	5.00872100	3.56801100	0.75951300
H	4.78387300	5.90932400	0.00599300
H	2.74111700	6.60644000	-1.24997700
H	0.96455200	4.98059500	-1.70474000
I	3.41800100	0.94977700	0.58779600
O	0.67187900	1.47162100	0.06940800
C	-0.51746500	3.00247700	-1.29230900
H	-0.52926100	3.61318900	-2.20191400
H	-1.28533400	2.22617700	-1.41324800
H	-0.79052600	3.63041200	-0.43674800
C	1.19832700	1.49875600	-2.30410200
H	0.41622700	0.74846300	-2.49977800
H	1.29172400	2.13581800	-3.19193300
H	2.15019200	0.97092100	-2.16661800
C	6.23669900	1.23762000	0.36431200
F	6.69309100	0.00096100	0.38080300
F	6.72285400	1.93681500	1.37820000
F	6.49085800	1.83218300	-0.78561300

INT3 S**2 = 0.75

C	0.94747100	-3.87417400	-0.71106900
C	1.10108100	-2.39338200	-1.08191000
C	-0.69565700	-2.67197400	0.23288000
H	1.75290400	-4.24275500	-0.06445400
H	0.93844000	-2.23134300	-2.15799200
H	0.82709000	-4.55024000	-1.56002800
O	-0.28629200	-3.92977200	0.06477700
N	-0.01074000	-1.75469500	-0.35385300
C	2.42853900	-1.76486300	-0.66938200
H	2.37088900	-0.68761000	-0.88706700
H	2.52577900	-1.85462200	0.42324900
C	3.60281700	-2.38855000	-1.36634900
C	4.40318700	-3.33026600	-0.71356600
C	3.89282100	-2.06528400	-2.69630700
C	5.46809800	-3.93924500	-1.37310500
H	4.19707500	-3.57435300	0.33031500
C	4.95624100	-2.67062000	-3.35757000
H	3.28415700	-1.32051800	-3.21282200
C	5.74479500	-3.61135800	-2.69730300
H	6.08659900	-4.66530200	-0.84939800
H	5.17574800	-2.40298500	-4.38914800
H	6.57896700	-4.08182300	-3.21320100
C	-1.85046000	-2.51905200	1.18209000
C	-1.31008300	-2.86220500	2.61417500
H	-1.24048500	-3.95487100	2.67579600
H	-2.07820800	-2.54697600	3.33194100
C	-2.99597800	-3.50687700	0.80484600
H	-2.54219600	-4.49919700	0.69682400
H	-3.67643700	-3.55516900	1.66247400
C	0.02851200	-2.24075200	2.89988400
C	1.17695100	-3.03748000	2.92106200
C	0.17204000	-0.85562500	3.06203400
C	2.43645800	-2.47052800	3.10805100
H	1.07692200	-4.11726500	2.80389200

C	1.43182700	-0.28230200	3.21821500
H	-0.71258600	-0.21673700	3.09021900
C	2.56766400	-1.09073900	3.24265100
H	3.31658000	-3.10990100	3.15180600
H	1.52712600	0.79614100	3.32992300
H	3.54979300	-0.64317200	3.38158200
C	-3.74937300	-3.10563200	-0.43612000
C	-5.05712900	-2.61760200	-0.34392700
C	-3.15233600	-3.18123700	-1.70047300
C	-5.75196300	-2.21901800	-1.48393000
H	-5.53597300	-2.56193500	0.63394500
C	-3.83890700	-2.76960400	-2.83902300
H	-2.14876500	-3.59733200	-1.80115300
C	-5.14092300	-2.28482400	-2.73366900
H	-6.77785000	-1.86535400	-1.39659300
H	-3.36289700	-2.84484800	-3.81464600
H	-5.68220800	-1.97440200	-3.62464700
C	-3.94237600	0.37642000	1.85685300
C	-3.07185500	0.96000600	0.74321000
C	-2.43548000	-1.13528000	1.18403500
H	-5.01568600	0.41906400	1.65005900
H	-2.61243300	1.91113600	1.04032900
H	-3.74177700	0.79068600	2.85040300
O	-3.55834800	-1.02877200	1.89504500
N	-2.02081800	-0.06728900	0.59280100
C	-3.81245200	1.11873500	-0.59096600
H	-3.07873100	1.40271000	-1.35825400
H	-4.20324500	0.13217200	-0.88270200
C	-4.92353800	2.12545300	-0.50413600
C	-6.25283800	1.70915600	-0.38591000
C	-4.64579000	3.49639400	-0.49148100
C	-7.28241500	2.63868000	-0.25958700
H	-6.47904800	0.64132400	-0.41069000
C	-5.67127700	4.42772700	-0.36615000
H	-3.61394400	3.83650400	-0.59517800
C	-6.99249000	4.00011300	-0.24780600
H	-8.31272400	2.29888000	-0.17610500
H	-5.44076800	5.49116100	-0.36585600
H	-7.79494800	4.72829000	-0.15248800
Cu	-0.13371900	0.17303000	0.01784400
C	0.98701900	2.59012700	-0.99276100
C	3.16471500	3.52080900	0.04688300
C	4.00764700	4.58041500	0.37419700
C	3.64010800	5.88661600	0.06988400
C	2.42856100	6.12274700	-0.56477900
C	1.59762800	5.05513100	-0.88239500
C	1.92963300	3.72527900	-0.58608800
H	4.95623600	4.38513100	0.86715200
H	4.30489700	6.70732700	0.32961000
H	2.12295900	7.13617000	-0.81448100
H	0.65306900	5.26808600	-1.37594700
I	3.93079100	1.58702400	0.57286700
O	0.86189600	1.68509700	0.08834200
C	-0.43111000	3.08439600	-1.30361500
H	-0.46425500	3.72098900	-2.19385600
H	-1.06495400	2.21025800	-1.50542200
H	-0.85234100	3.63543600	-0.45534000
C	1.52973700	1.86431400	-2.23097600
H	0.86417000	1.02694100	-2.49272700
H	1.58335000	2.54179500	-3.09092900
H	2.53379900	1.46552500	-2.04935500

CF3 S**2 = 0.75

C	-0.00024500	0.00000100	0.33568600
F	0.58248400	-1.11729000	-0.07461500
F	0.67697000	1.06276800	-0.07459800
F	-1.25929100	0.05452100	-0.07457800

TS2 S**2 = 0.75

C	1.90503800	-0.90258400	1.72079900
H	1.53526500	-1.82392900	2.16327600
H	2.96587900	-0.67559500	1.80413700
C	1.03546000	-0.03526800	1.16822600
C	1.48042800	1.24238500	0.57627000
C	2.63872900	1.28993000	-0.21459700
C	0.78784400	2.44279200	0.81041100
C	3.09055900	2.49083300	-0.74876600
H	3.17496300	0.36599000	-0.42308300
C	1.24240800	3.64390500	0.27539000
H	-0.10026200	2.43455200	1.44193700
C	2.39377500	3.67257000	-0.50785000
H	3.98722400	2.50169500	-1.36574500
H	0.69697100	4.56357900	0.47964200
H	2.74600900	4.61221400	-0.92900600
C	-0.39973000	-0.48515700	1.12788700
O	-0.80147500	-1.42819100	1.79894100
N	-1.18567100	0.21247700	0.24022400
H	-0.72085200	0.93878500	-0.29075300
C	-2.55317100	0.06545000	-0.03314900
C	-3.11679700	0.97368800	-0.94059800
C	-3.36217400	-0.91752000	0.55143600
C	-4.46519300	0.90609500	-1.26027400
H	-2.48562500	1.73951300	-1.39332100
C	-4.71234600	-0.96960700	0.21945600
H	-2.92820600	-1.61928600	1.25274000
C	-5.27447600	-0.06798300	-0.68033200
H	-4.88384600	1.62070200	-1.96650600
H	-5.33417600	-1.73630700	0.67878800
H	-6.33245900	-0.12321800	-0.92808400
C	2.29353400	-2.42247600	-0.55693000
F	2.16505200	-3.73678400	-0.65053800
F	3.54793400	-2.05936200	-0.82151900
F	1.45226500	-1.80638900	-1.37698800

1a

C	1.92437400	2.73921100	-0.17174100
H	1.28444500	3.61725800	-0.19643400
H	2.99895000	2.87582200	-0.27062400
C	1.38314600	1.52496800	0.00556800
C	2.21656200	0.30356600	0.03740500
C	2.04899600	-0.67452700	1.03132000
C	3.23121100	0.11725600	-0.91242200
C	2.87560300	-1.79287300	1.07593800
H	1.27806600	-0.53990800	1.78994500
C	4.05491700	-1.00163900	-0.86855400
H	3.35758200	0.86084800	-1.69853900
C	3.88016300	-1.96132100	0.12602700
H	2.73738800	-2.53293700	1.86215500
H	4.83270300	-1.12927500	-1.61934500
H	4.52273000	-2.83903100	0.15917000
C	-0.11603300	1.47822200	0.13904000
O	-0.77840500	2.48403500	0.35925000
N	-0.66267800	0.23016000	-0.05920800
H	-0.00973100	-0.51358700	-0.27431000
C	-2.01370400	-0.14685900	-0.07793700
C	-2.29402400	-1.49192400	-0.35712800

C	-3.07031600	0.74106900	0.16427900
C	-3.60507100	-1.94492800	-0.40008400
H	-1.47143100	-2.18370900	-0.54323100
C	-4.37810300	0.26895200	0.11674200
H	-2.85577300	1.78023600	0.38048500
C	-4.65889900	-1.06527500	-0.16402400
H	-3.80158100	-2.99271400	-0.62037700
H	-5.19240000	0.96730900	0.30332800
H	-5.68790100	-1.41709800	-0.19834900

INT4 S**2 = 0.75

C	-1.84003200	-1.34498600	-0.94943700
H	-1.26635300	-2.21753700	-1.27377700
H	-2.45117100	-1.00287100	-1.79401700
C	-0.89906500	-0.28985800	-0.46024800
C	-1.35066800	1.05116200	-0.19011900
C	-0.69256700	1.89753500	0.74050200
C	-2.50588100	1.57513300	-0.82329700
C	-1.14169300	3.18527500	0.98763700
H	0.14659100	1.50897600	1.31325500
C	-2.94162500	2.86592100	-0.57861700
H	-3.05732700	0.95752000	-1.52844800
C	-2.26100400	3.68557000	0.32317300
H	-0.62342600	3.79935500	1.72201100
H	-3.82432600	3.23918500	-1.09465700
H	-2.61029100	4.69751600	0.51794200
C	0.47270900	-0.78600400	-0.22644100
O	0.69408500	-1.98255100	-0.04307000
N	1.47249600	0.16641500	-0.30001300
H	1.18206100	1.09469600	-0.58066500
C	2.85490800	-0.00251700	-0.15564100
C	3.66472800	1.11053900	-0.42743500
C	3.45037900	-1.20414900	0.25439200
C	5.04340500	1.02780100	-0.29733100
H	3.20162000	2.04562600	-0.74529900
C	4.83400000	-1.26745500	0.37935900
H	2.82838800	-2.06603800	0.46183900
C	5.63945600	-0.16480600	0.10715400
H	5.65375700	1.90223000	-0.51551400
H	5.28707900	-2.20465100	0.69834800
H	6.72041300	-0.23251700	0.20935500
C	-2.79953600	-1.83408400	0.11479000
F	-3.55651900	-2.84478300	-0.35929900
F	-3.64385700	-0.86012400	0.51816400
F	-2.15654100	-2.27914400	1.20376100

TS3 S**2 = 0.75

C	-3.85668900	-0.63886600	1.87686000
C	-2.87447400	-0.89680000	0.72952700
C	-1.99510600	0.58352600	2.16597700
H	-4.12950600	-1.53894200	2.43693000
H	-3.31170600	-0.63410400	-0.24461900
H	-4.76813300	-0.11193200	1.57638000
O	-3.13083900	0.23786400	2.78070500
N	-1.77743700	0.04867900	1.01424600
C	-2.33491800	-2.33128900	0.68597300
H	-1.68391600	-2.41733200	-0.19569800
H	-1.69400000	-2.49152000	1.56564800
C	-3.43962700	-3.34880900	0.64440900
C	-3.67309500	-4.20013100	1.72764700
C	-4.29448900	-3.41871700	-0.46051200
C	-4.72928400	-5.10844300	1.70508100
H	-3.01276200	-4.15512700	2.59585000

C	-5.35310400	-4.32025700	-0.48460800
H	-4.11978400	-2.75707500	-1.31022600
C	-5.57258000	-5.16877000	0.59923100
H	-4.89285500	-5.76955100	2.55363600
H	-6.00837100	-4.36417000	-1.35299900
H	-6.39845300	-5.87651400	0.58037700
C	-1.17082100	1.55145100	2.96922000
C	-0.81734500	0.88912400	4.33804300
H	-1.76489700	0.64133300	4.83049400
H	-0.32730000	1.65950300	4.94464800
C	-2.03375300	2.82813900	3.23202200
H	-2.91235100	2.50651300	3.80309700
H	-1.44384100	3.48427200	3.88207000
C	0.06112700	-0.32418400	4.21182200
C	-0.48891200	-1.58741200	3.96595500
C	1.45146100	-0.20944000	4.31690400
C	0.32895200	-2.70600800	3.82370300
H	-1.57442000	-1.69746600	3.91730500
C	2.27122700	-1.32723300	4.18544700
H	1.88902800	0.76567500	4.53527700
C	1.71185600	-2.57791700	3.93360300
H	-0.11526500	-3.68436600	3.64646200
H	3.35004800	-1.22303300	4.28562400
H	2.35198300	-3.45217100	3.83128800
C	-2.43982900	3.54498600	1.97462100
C	-1.65053500	4.57617200	1.45555300
C	-3.59788800	3.17584400	1.28068600
C	-1.99812300	5.21274300	0.26650700
H	-0.75960700	4.89202300	2.00177000
C	-3.95258300	3.81521000	0.09644100
H	-4.24407900	2.40122600	1.69522600
C	-3.14888000	4.83035100	-0.41890100
H	-1.37407800	6.01803400	-0.11834800
H	-4.87003900	3.53223800	-0.41725600
H	-3.42980900	5.33634600	-1.34051200
C	2.05297800	3.06635800	2.24664300
C	1.76401100	2.45115800	0.87762700
C	0.10183600	1.97195600	2.29304900
H	2.24771900	4.14256100	2.22066100
H	2.58265200	1.80606600	0.53536400
H	2.85146000	2.56246800	2.80218700
O	0.81825500	2.85792000	2.99477000
N	0.57327100	1.62029900	1.15115100
C	1.43594600	3.46824200	-0.21942600
H	1.13714100	2.90538100	-1.11408100
H	0.56609700	4.05592600	0.10492400
C	2.60243000	4.36284400	-0.52168100
C	2.65823300	5.66844200	-0.02518800
C	3.67903400	3.88543300	-1.27706800
C	3.76226300	6.48044000	-0.27526400
H	1.81577700	6.05724000	0.55185700
C	4.78385900	4.69210000	-1.52693200
H	3.63597000	2.87278400	-1.68089200
C	4.82870300	5.99184200	-1.02486200
H	3.78721800	7.49701300	0.11222300
H	5.61179600	4.30813300	-2.12045000
H	5.69149200	6.62422000	-1.22295400
Cu	-0.21517800	0.33727700	-0.19334600
C	2.16636300	-1.27810900	-0.73450000
C	4.50095500	-2.29142900	-1.29686300
C	5.75824400	-2.17922600	-1.89394300
C	6.11134500	-1.03296900	-2.59400600
C	5.19811600	0.00801900	-2.68942300

C	3.94837900	-0.11332400	-2.09804600
C	3.55006100	-1.26167500	-1.39473500
H	6.46846600	-2.99662400	-1.80475700
H	7.09521400	-0.96308100	-3.05255400
H	5.44993200	0.92091900	-3.22653800
H	3.24525800	0.70821500	-2.19188600
I	4.24549300	-4.14097100	-0.22416400
O	1.46437900	-0.05597900	-1.15194400
C	1.29776700	-2.49595300	-1.05801700
H	1.49153300	-3.31675600	-0.36417900
H	0.24585200	-2.20883600	-0.92647400
H	1.42625900	-2.84865300	-2.08229300
C	2.30205400	-1.13738100	0.77762700
H	1.31478400	-1.16516300	1.26628200
H	2.88627000	-1.96503800	1.18997200
H	2.80197100	-0.20165500	1.05079500
C	-3.18710300	1.29980400	-2.48873700
C	-1.86232300	1.26558900	-2.05619900
C	-1.10424600	0.07733500	-2.06375900
C	-1.75079500	-1.07701900	-2.54426600
C	-3.05367900	-1.03181800	-3.02282000
C	-3.81538400	0.14923600	-2.98072200
H	-3.72482800	2.24497400	-2.45240000
H	-1.40982800	2.19963600	-1.70514500
H	-1.19859100	-2.01601300	-2.60229000
H	-3.49509300	-1.93917300	-3.43746900
B	0.84166200	0.14249700	-2.48196300
O	1.04169100	1.49689900	-2.82950400
H	0.46427900	1.77817300	-3.54890300
O	1.06444900	-0.90234100	-3.37596400
H	1.10237500	-0.58640800	-4.28558900
C	-5.25950600	0.13894600	-3.47081400
C	-6.03802400	-0.96552900	-2.74182300
H	-6.01119000	-0.82734200	-1.65184300
H	-7.08922300	-0.95932900	-3.05443900
H	-5.63967300	-1.96323300	-2.96279700
C	-5.27096700	-0.15041300	-4.97858100
H	-6.30170200	-0.18362200	-5.35247500
H	-4.73539200	0.62629100	-5.53753800
H	-4.80192200	-1.11402900	-5.21083900
C	-5.96400800	1.47097300	-3.21878900
H	-7.00293100	1.41435600	-3.56242900
H	-5.98467100	1.72453700	-2.15055500
H	-5.48875800	2.29956900	-3.75783000

ArB(OH)₂

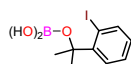
C	0.37038200	-1.19605100	-0.03020400
C	-1.01928300	-1.19504900	-0.01593300
C	-1.75157800	0.00000000	-0.01059800
C	-1.01928300	1.19505000	-0.01595400
C	0.37038100	1.19605200	-0.03022400
C	1.10037700	0.00000000	-0.04279400
H	0.89400900	-2.15053900	-0.03447000
H	-1.55560400	-2.14378900	-0.01123600
H	-1.55560500	2.14378900	-0.01127300
H	0.89400800	2.15054000	-0.03450700
B	-3.30316100	0.00000000	0.00062100
O	-3.94721500	-1.21471600	0.00550000
H	-4.90902800	-1.15364400	0.01284000
O	-3.94721500	1.21471500	0.00547900
H	-4.90902900	1.15364400	0.01282100
C	2.62834500	0.00000000	-0.00149300
C	3.21069600	1.23825700	-0.69064300

H	2.96041400	2.16643000	-0.16461500
H	4.30555900	1.17149800	-0.71611000
H	2.85466400	1.33014700	-1.72434700
C	3.21069400	-1.23824700	-0.69066200
H	4.30555800	-1.17149000	-0.71612600
H	2.96041000	-2.16642800	-0.16465000
H	2.85466400	-1.33011900	-1.72436800
C	3.06943900	-0.00001100	1.46955800
H	4.16530800	-0.00001200	1.54697000
H	2.69244600	0.88578900	1.99591200
H	2.69244600	-0.88581900	1.99589900

INT5 S**2 = 0.75

C	-2.01836200	-2.62426400	1.47770600
C	-1.95497600	-1.32738600	0.65768300
C	0.11404300	-2.14096300	0.96745200
H	-2.52938600	-3.44025600	0.95324600
H	-2.30384200	-0.46042300	1.23682300
H	-2.44170000	-2.51667900	2.47917300
O	-0.62625900	-3.02558200	1.63836000
N	-0.51190600	-1.16067300	0.42100600
C	-2.72778000	-1.38657800	-0.65825400
H	-2.47712200	-0.48576600	-1.23576500
H	-2.37257600	-2.25351000	-1.23509200
C	-4.20672300	-1.46545800	-0.40963400
C	-4.89856900	-2.67040700	-0.55021600
C	-4.90487300	-0.33113500	0.02177400
C	-6.26091100	-2.74545900	-0.26898000
H	-4.36464300	-3.55576600	-0.90121200
C	-6.26464300	-0.40431900	0.30462500
H	-4.37241700	0.61821600	0.12596900
C	-6.94523300	-1.61252900	0.16079300
H	-6.78825900	-3.68959700	-0.39092100
H	-6.79870300	0.48499900	0.63503400
H	-8.00972700	-1.66791400	0.37872700
C	1.58065400	-2.46432900	0.96402800
C	1.73743100	-3.91155900	0.39943400
H	1.35686100	-4.59871900	1.16345400
H	2.81014800	-4.10898200	0.29017000
C	2.11163400	-2.39411200	2.43476300
H	1.49791300	-3.08114500	3.02955700
H	3.13463400	-2.78787300	2.42894600
C	0.99393600	-4.10346800	-0.89501300
C	-0.23120400	-4.77795200	-0.90877300
C	1.47033900	-3.55678400	-2.09212400
C	-0.96776500	-4.89629400	-2.08467900
H	-0.60159200	-5.22329500	0.01467100
C	0.73373400	-3.66838500	-3.26789300
H	2.44251300	-3.06000300	-2.11070200
C	-0.49079900	-4.33329400	-3.26572000
H	-1.91087500	-5.44052800	-2.08072000
H	1.12393100	-3.24952300	-4.19336400
H	-1.06263400	-4.42599400	-4.18656600
C	2.07091800	-0.99685200	2.98707900
C	3.20235300	-0.17599900	2.93410200
C	0.88011700	-0.46278800	3.49390000
C	3.14479500	1.14682500	3.36650700
H	4.14237800	-0.58673000	2.56090200
C	0.81861100	0.86030100	3.92194400
H	-0.00448900	-1.09797100	3.56951500
C	1.94961500	1.67145300	3.85207900
H	4.03872900	1.76783700	3.33412500
H	-0.11086100	1.25556000	4.32787000

H	1.90428400	2.70309500	4.19366600
C	4.39819200	-0.80459700	-0.63068600
C	3.29854200	0.19986300	-1.00218800
C	2.41361200	-1.51316800	0.14920200
H	5.15722000	-0.39274100	0.04356000
H	3.17538700	0.26440300	-2.09215400
H	4.89536500	-1.27117100	-1.48446300
O	3.70082300	-1.85730100	0.09048100
N	2.08068100	-0.41468600	-0.43534300
C	3.50445900	1.60525200	-0.43049300
H	2.64652700	2.22808400	-0.72926000
H	3.47551400	1.53512100	0.66644900
C	4.79815700	2.21415900	-0.89117700
C	5.91891800	2.21522700	-0.05529200
C	4.92128100	2.74093400	-2.18093800
C	7.13644600	2.72766200	-0.49614000
H	5.82902600	1.82261900	0.96008100
C	6.13502800	3.25664700	-2.62321100
H	4.05214200	2.75950700	-2.84025500
C	7.24605000	3.24844900	-1.78222500
H	7.99791000	2.72671000	0.16849200
H	6.21385800	3.67154800	-3.62599100
H	8.19449400	3.65341400	-2.12811000
Cu	0.32604700	0.47099000	-0.34840900
C	-2.67052900	3.11738600	-1.60793700
C	-1.65268600	2.16218200	-1.59714700
C	-1.13089000	1.68956000	-0.38880100
C	-1.71250500	2.13427900	0.80599300
C	-2.73436800	3.07702400	0.78700000
C	-3.24010500	3.58681900	-0.41992100
H	-3.03089700	3.48318500	-2.56704100
H	-1.26864800	1.80151500	-2.55268300
H	-1.35560200	1.75919600	1.76805100
H	-3.15498100	3.41714100	1.73362600
C	-4.40883200	4.56871000	-0.39595900
C	-4.06490600	5.76237900	0.50429900
H	-3.17966400	6.29605700	0.13783700
H	-4.90093000	6.47198200	0.52393400
H	-3.86896400	5.45974500	1.53946600
C	-5.64161100	3.84433600	0.16574800
H	-6.49613000	4.53001300	0.22388900
H	-5.92955800	3.00191700	-0.47656100
H	-5.46030800	3.45213600	1.17500800
C	-4.74851600	5.09547300	-1.78906400
H	-5.57241800	5.81522800	-1.72338100
H	-3.89735400	5.61165300	-2.25043100
H	-5.07034400	4.29452000	-2.46598600



C	0.78390000	1.43286000	0.31533700
C	-1.38561200	0.05518300	-0.07963600
C	-2.75444100	-0.00599700	-0.34129400
C	-3.49848500	1.15618200	-0.50516500
C	-2.86428000	2.38604900	-0.40366400
C	-1.49868100	2.43466400	-0.15330800
C	-0.71266500	1.28495800	0.01003100
H	-3.24200800	-0.97455100	-0.41848100
H	-4.56565700	1.09039700	-0.70882600
H	-3.42333100	3.31204100	-0.52483400
H	-1.02023600	3.40824700	-0.08930500
I	-0.48368600	-1.87986100	0.17822300
O	1.43880500	0.51883600	-0.57005400

C	1.31598500	2.83230100	0.01867800	H	-1.04131800	-1.41732200	-5.20639500
H	0.90099700	3.58274600	0.70034300	H	3.17074500	-2.26972200	-5.14887800
H	2.40077000	2.82778700	0.15671800	H	1.26605300	-0.90166700	-5.97171900
H	1.09523800	3.13078800	-1.01200200	C	-3.21227600	-3.19757800	-1.12009100
C	1.03503900	1.09922900	1.78765600	C	-2.67935200	-1.93208800	-0.44083600
H	2.08874200	1.24559500	2.04130500	C	-0.98631300	-3.32199100	-0.86291000
H	0.42862400	1.75788300	2.42042600	H	-3.58823300	-3.02147600	-2.13609400
H	0.76150900	0.06522700	2.01900500	H	-3.00670900	-1.89527200	0.60760400
B	2.74981500	0.16750900	-0.55926100	H	-3.96839000	-3.74127600	-0.54847000
O	3.64313300	0.76591600	0.31002200	O	-2.04821000	-4.05757200	-1.22711000
H	4.53950300	0.42267900	0.23625000	N	-1.22066400	-2.13693500	-0.42406600
O	3.08963300	-0.79796600	-1.47542000	C	-3.00314000	-0.62432900	-1.14181300
H	4.02501300	-1.02059700	-1.47833900	H	-2.34648000	0.15529200	-0.71086900

INT6 S**2 = 2.00

C	3.75510800	-2.92358500	-0.78392000	C	-4.43115300	-0.15653500	-1.07600000
C	3.04650800	-1.59381900	-0.49910600	C	-4.81990600	0.92094800	-1.88071100
C	1.53100200	-3.21399100	-0.75750100	C	-5.38033700	-0.72529300	-0.22116300
H	4.47118400	-3.21942700	-0.01063600	C	-6.11590500	1.41706800	-1.83198400
H	3.28141200	-0.83440600	-1.25726900	H	-4.08411400	1.38221200	-2.54201600
H	4.23824300	-2.97178700	-1.76505600	C	-6.68238300	-0.22770100	-0.16817800
O	2.68119400	-3.90581300	-0.78720400	H	-5.11497100	-1.57150600	0.41430500
N	1.62362100	-1.94139900	-0.63268500	C	-7.05356200	0.84385600	-0.97306400
C	3.31705000	-1.03532000	0.89750000	H	-6.39687000	2.25703900	-2.46497200
H	2.57421900	-0.24978200	1.10027000	H	-7.40786000	-0.68694600	0.50026000
H	3.11667300	-1.82737400	1.63486900	H	-8.07075600	1.22812800	-0.93697600
C	4.71381400	-0.50869700	1.06687000	Cu	0.12822200	-0.59940600	-0.27936000
C	5.58079500	-1.07131700	2.00723000	C	1.91613400	3.09026600	-1.31108000
C	5.16740500	0.57153200	0.29977200	C	1.66985600	1.83750900	-0.74373300
C	6.86487300	-0.56224900	2.19095900	C	0.63899900	1.02730700	-1.21117300
H	5.23830700	-1.91194000	2.61276500	C	-0.11358200	1.47672500	-2.30120800
C	6.44952300	1.08018300	0.47834600	C	0.12373900	2.73622700	-2.85162800
H	4.50093100	1.03340900	-0.43138200	C	1.14068700	3.57242900	-2.36860900
C	7.30139100	0.51665200	1.42717800	H	2.72607000	3.69040100	-0.89977700
H	7.52419800	-1.01028300	2.93174000	H	2.28280900	1.52869800	0.10339900
H	6.78377800	1.92512300	-0.12108200	H	-0.91264600	0.86420900	-0.72370100
H	8.30351900	0.91626200	1.56792100	H	-0.50301300	3.07178900	-3.67987700
C	0.31141300	-4.08061600	-0.92805900	C	1.35155300	4.95552200	-2.98170200
C	0.26096900	-5.13281900	0.23246800	C	0.09070000	5.79767400	-2.74471600
H	1.22767900	-5.64989600	0.24720300	H	-0.10588500	5.91482200	-1.66961400
H	-0.50581000	-5.87131400	-0.03094100	H	0.20614800	6.80052300	-3.17497700
C	0.43991800	-4.78190900	-2.31509400	H	-0.79471400	5.33990900	-3.20440800
H	1.28654900	-5.47518000	-2.25502100	C	1.59603100	4.82456400	-4.49004900
H	-0.46515600	-5.37859000	-2.47372700	H	1.73744100	5.81380600	-4.94298500
C	-0.04949000	-4.47161200	1.54662600	H	2.49334100	4.22865100	-4.69613400
C	0.94652100	-3.78582700	2.24878600	H	0.75304600	4.34575900	-5.00224200
C	-1.36618600	-4.40085900	2.01366200	C	2.53991300	5.68676900	-2.35848500
C	0.63247400	-3.01902700	3.36705700	H	2.66049300	6.67064000	-2.82648400
H	1.98179500	-3.85939800	1.91027500	H	2.40202500	5.85112700	-1.28135400
C	-1.68436500	-3.63800500	3.13457200	H	3.47888100	5.13733700	-2.49962200
H	-2.14853500	-4.94842700	1.48521800	C	-2.56306200	0.11857200	2.27938600
C	-0.68680400	-2.93341900	3.80677500	H	-1.93739500	-0.76812600	2.10567100
H	1.41969200	-2.48606900	3.89813900	H	-3.55120700	-0.06059500	1.83740700
H	-2.71312600	-3.59377200	3.48889500	C	-1.89822700	1.32280000	1.69031000
H	-0.93608700	-2.33087200	4.67718600	C	-2.63270900	2.37075100	1.04592000
C	0.65034500	-3.77389300	-3.41290200	C	-4.03111700	2.50930400	1.24017900
C	-0.41712900	-3.01633200	-3.90876100	C	-2.00237000	3.26058100	0.13212800
C	1.93903400	-3.49445800	-3.87787700	C	-4.74830000	3.49356500	0.58272300
C	-0.19816600	-1.98997200	-4.82303400	H	-4.54439700	1.85654000	1.94177700
H	-1.43351600	-3.24983800	-3.58975200	C	-2.73730300	4.22652200	-0.53510800
C	2.16170500	-2.46791000	-4.79196800	H	-0.93985300	3.14781800	-0.09008400
H	2.77389300	-4.09690200	-3.51834700	C	-4.10997500	4.35697100	-0.30997300
C	1.09422300	-1.70451800	-5.25809100	H	-5.81744900	3.58591100	0.76184500
				H	-2.23690300	4.87873000	-1.24851300

H	-4.67954600	5.12258500	-0.83283800	C	3.33201800	-2.31609000	3.69666200
C	-0.43454600	1.32759400	1.83045900	C	0.94288300	-2.16088300	3.90198300
O	0.23862100	0.27742300	1.67332200	C	3.47356800	-1.12943100	4.41189100
N	0.12533200	2.50581100	2.19589200	H	4.21557500	-2.84928700	3.34607100
H	-0.51717600	3.28644900	2.27296900	C	1.07864300	-0.97006400	4.60992700
C	1.49392700	2.81708600	2.35323900	H	-0.05323100	-2.57146000	3.73424300
C	1.90382900	4.10933700	2.01393500	C	2.34519900	-0.44424600	4.85729200
C	2.41900200	1.88523200	2.83249500	H	4.46916500	-0.74439400	4.62794200
C	3.24378700	4.46141700	2.12316200	H	0.19187100	-0.45291800	4.97165400
H	1.17314300	4.82351600	1.63127800	H	2.45174600	0.48466300	5.41421400
C	3.75845000	2.24918500	2.93015700	C	4.39976100	-1.62353400	0.46278200
H	2.08808600	0.89273800	3.12278700	C	3.35557400	-0.66186800	-0.10596300
C	4.17738100	3.52847200	2.56957700	C	2.35133700	-2.50742800	0.63520400
H	3.55833700	5.46623900	1.84803800	H	4.82617800	-1.27679700	1.41439300
H	4.48351200	1.52240400	3.29166900	H	3.46918500	-0.58497900	-1.19626700
H	5.22866500	3.79739400	2.64520800	H	5.20669600	-1.88514000	-0.22491000
C	-2.73221700	0.21219300	3.78107800	O	3.64725800	-2.82934300	0.74084300
F	-3.29560800	-0.90777300	4.27214900	N	2.07396400	-1.34339400	0.16209700
F	-3.50983900	1.25052500	4.13859700	C	3.36323100	0.72141200	0.53358800
F	-1.54125700	0.37266500	4.39470600	H	2.52518100	1.30442500	0.11067800
				H	3.13689200	0.59627800	1.60411300
TS4	S**2 = 0.44			C	4.66618100	1.45154400	0.36070900
C	-2.10829500	-3.73212400	1.80454300	C	5.36629400	1.92341600	1.47381100
C	-2.05389700	-2.36272100	1.11727800	C	5.20993800	1.66963900	-0.91091400
C	-0.00755800	-3.26306300	1.16752600	C	6.56916000	2.60916700	1.32327300
H	-2.80751900	-4.43134300	1.33574600	H	4.95536800	1.75393400	2.47021400
H	-2.39382600	-1.55604200	1.78111500	C	6.41153900	2.35286700	-1.06659200
H	-2.30400800	-3.69478800	2.88127800	H	4.68871600	1.29929900	-1.79680100
O	-0.76762300	-4.26821700	1.63165100	C	7.09363000	2.82711700	0.05254800
N	-0.61049800	-2.16806000	0.87861400	H	7.09867700	2.97184500	2.20194400
C	-2.83733200	-2.31836300	-0.19361700	H	6.81853400	2.51359200	-2.06296500
H	-2.52739700	-1.42489000	-0.75013600	H	8.03376700	3.36101900	-0.06735400
H	-2.52910000	-3.17336100	-0.81345000	Cu	0.27350200	-0.42581100	0.27199600
C	-4.32688200	-2.34249100	0.01047700	C	-2.89698600	2.12435700	1.39451000
C	-5.10988600	-3.34928200	-0.56080500	C	-2.14622600	1.08883800	0.83249800
C	-4.96512200	-1.34132500	0.75338400	C	-0.80159400	0.91537800	1.15205100
C	-6.49503100	-3.35243400	-0.40901700	C	-0.23347900	1.76986900	2.10342400
H	-4.62619100	-4.13529100	-1.14276800	C	-0.98246500	2.81084600	2.65184800
C	-6.34709500	-1.34280400	0.90951800	C	-2.32694900	3.01601800	2.30823800
H	-4.37433000	-0.54007600	1.20125700	H	-3.93883800	2.22724800	1.09350000
C	-7.11746400	-2.34710900	0.32579900	H	-2.62732700	0.44552700	0.09519600
H	-7.08753500	-4.14333100	-0.86479900	H	0.80662900	1.65217500	2.41471400
H	-6.82622900	-0.55200500	1.48430500	H	-0.50177600	3.48034400	3.36716700
H	-8.19870400	-2.34777000	0.44719500	C	-3.10109000	4.18693800	2.91064000
C	1.45108900	-3.62359800	1.08795800	C	-2.44997900	5.49758000	2.44843700
C	1.61595600	-4.78451900	0.04733500	H	-2.48709900	5.58801600	1.35358300
H	0.92575500	-5.58844900	0.32900900	H	-2.97474900	6.36305100	2.87224800
H	2.63668700	-5.17140700	0.14987800	H	-1.39940000	5.56121900	2.75982600
C	1.92414100	-4.04486500	2.51865400	C	-3.05332600	4.11033400	4.44167600
H	1.20439000	-4.77276900	2.90917600	H	-3.60083200	4.95166600	4.88432800
H	2.88658200	-4.55684600	2.41339900	H	-3.51013900	3.18255700	4.80694600
C	1.36649900	-4.27517700	-1.34655500	H	-2.02635200	4.14957800	4.82355200
C	0.06175500	-4.10327300	-1.81791900	C	-4.56435400	4.19746000	2.47031100
C	2.42745600	-3.81494400	-2.13447900	H	-5.08627600	5.04526700	2.92891400
C	-0.18363000	-3.45259500	-3.02343800	H	-4.66481000	4.30153000	1.38177000
H	-0.77078800	-4.48592000	-1.22477300	H	-5.09054400	3.28362800	2.77311400
C	2.18752200	-3.17034700	-3.34526000	C	1.58722200	0.66904000	-2.60910000
H	3.45159500	-3.95902800	-1.78668400	H	1.38779300	-0.38168100	-2.35429100
C	0.87952100	-2.97312200	-3.78551800	H	2.61186900	0.90745800	-2.31003300
H	-1.20762200	-3.31376800	-3.36651300	C	0.58581900	1.55715600	-1.93406700
H	3.02306300	-2.81994900	-3.94884400	C	0.92000700	2.87283800	-1.47251600
H	0.69161300	-2.45686900	-4.72476800	C	2.18240500	3.44985300	-1.77619700
C	2.06585100	-2.84246500	3.41717700	C	0.04849800	3.62218600	-0.63366600

C	2.54809800	4.68713800	-1.27702800	H	0.35095400	2.88696000	-0.79301700
H	2.86898400	2.93073200	-2.43906400	C	3.06912100	3.55969200	-2.71799100
C	0.42488100	4.86126300	-0.14389300	H	3.97532100	2.17315600	-4.09434300
H	-0.90173000	3.19456800	-0.31588100	H	1.95701200	4.69673900	-1.26182300
C	1.67238800	5.40390900	-0.45876200	H	3.79580500	4.34755600	-2.90350200
H	3.52273200	5.09912800	-1.53029900	C	-1.25134800	0.67281100	-2.24279200
H	-0.25443700	5.40128900	0.51288400	O	-2.03340100	-0.28018600	-2.23462600
H	1.96284100	6.37489900	-0.06365100	N	-1.63311800	1.95657100	-2.48683100
C	-0.78468200	0.99231600	-1.97849800	H	-0.89385700	2.64692700	-2.52374700
O	-0.95831700	-0.22494500	-1.77580600	C	-2.93358200	2.49058600	-2.38606700
N	-1.78441200	1.85241300	-2.30067500	C	-3.03070800	3.85367600	-2.07990300
H	-1.50762800	2.81742800	-2.43974800	C	-4.09546900	1.72258200	-2.52489100
C	-3.17647500	1.62094600	-2.24828700	C	-4.27432700	4.44354300	-1.89737600
C	-3.99526800	2.71236600	-1.93971700	H	-2.12098900	4.44487200	-1.96212000
C	-3.73899500	0.35974300	-2.46806900	C	-5.33412000	2.32718500	-2.32876600
C	-5.36879900	2.53825500	-1.82225600	H	-4.02251800	0.67111700	-2.77638000
H	-3.54647200	3.69110200	-1.76241500	C	-5.43494700	3.68003900	-2.01292000
C	-5.11464500	0.19836000	-2.33398000	H	-4.33522700	5.50381300	-1.65837300
H	-3.10424400	-0.47684600	-2.74004400	H	-6.23481500	1.72619000	-2.43834300
C	-5.93230100	1.27717000	-2.00567700	H	-6.41009600	4.14001500	-1.86933700
H	-5.99783500	3.39124900	-1.57576900	C	0.28817200	-1.23722600	-3.94368900
H	-5.55019300	-0.78756200	-2.48534300	F	1.38299900	-1.77305900	-4.53529200
H	-7.00546400	1.13522800	-1.89916300	F	-0.00102700	-0.10299500	-4.61201300
C	1.53417900	0.75434400	-4.12188800	F	-0.72209900	-2.08984600	-4.13727700
F	2.41882500	-0.09565400	-4.67493100	C	4.45755000	-1.27670100	0.19734800
F	1.82695200	1.99265100	-4.56291600	C	3.32151000	-0.34106400	-0.22023100
F	0.31249400	0.43854300	-4.59172300	C	2.49594900	-2.01908900	0.98706800

INT7

Cu	0.20798400	-0.30097000	0.00189200	H	5.25207300	-0.78174600	0.76422900
C	-3.08187500	2.17004200	1.09192300	H	3.28625900	-0.20123200	-1.30902200
C	-2.34967500	1.18121300	0.42769300	H	4.89831000	-1.84854200	-0.62687800
C	-0.98136900	1.09473700	0.61179500	O	3.81414500	-2.22552900	1.08696300
C	-0.33491500	1.97834000	1.47720100	N	2.10787500	-1.06584100	0.21413400
C	-1.08091400	2.95881700	2.13257800	C	3.34422000	1.00645200	0.48420600
C	-2.46333500	3.08885800	1.94205600	H	2.39480600	1.51572500	0.25895100
H	-4.15206900	2.22707300	0.89848200	H	3.32481000	0.81953600	1.57045600
H	-2.86694800	0.52281200	-0.26877600	C	4.49057700	1.91510300	0.13489500
H	0.74001900	1.92132500	1.66093600	C	4.61661500	3.12669200	0.82513700
H	-0.55693900	3.64586400	2.79906400	C	5.42270100	1.61949900	-0.86252800
C	-3.21928300	4.22904700	2.62045300	C	5.63373000	4.02247500	0.51828600
C	-2.65527700	5.56282700	2.11079200	H	3.89622200	3.36508900	1.61050700
H	-2.77237400	5.65029000	1.02273400	C	6.44764900	2.51281900	-1.17058900
H	-3.18237400	6.40532100	2.57558700	H	5.34785000	0.69094600	-1.43054800
H	-1.58858500	5.67094400	2.34308200	C	6.55470500	3.71735300	-0.48359700
C	-3.02610400	4.14279400	4.13978500	H	5.71290100	4.96029000	1.06474200
H	-3.55196400	4.96574000	4.63931600	H	7.16387300	2.26327500	-1.95120000
H	-3.42200400	3.20071100	4.53879100	H	7.35479500	4.41465800	-0.72246500
H	-1.96873500	4.20925400	4.42430700	C	1.70353100	-2.95380100	1.85315600
C	-4.71571900	4.18908000	2.31489200	C	2.24568600	-2.81375700	3.31487900
H	-5.22070400	5.01908500	2.82229700	H	3.23843200	-3.27661400	3.33882300
H	-4.91755200	4.28799200	1.24040700	H	1.59199400	-3.41292300	3.95996400
H	-5.18131100	3.25910400	2.66473000	C	1.92316100	-4.41025400	1.33261000
C	0.57084300	-0.98230800	-2.45438500	H	2.99334800	-4.62706600	1.43131800
H	-0.01376400	-1.74070400	-1.91352700	H	1.38638200	-5.08620300	2.00789300
H	1.62574300	-1.20554500	-2.27684900	C	2.32871600	-1.38303300	3.77801400
C	0.21491700	0.42152300	-1.96079800	C	3.56727300	-0.73493100	3.84759500
C	1.20996300	1.49451700	-2.20641300	C	1.17700200	-0.65428100	4.10003100
C	2.26567700	1.31648200	-3.12107600	C	3.65392100	0.60646600	4.21421900
C	1.12279000	2.74033800	-1.54936000	H	4.47315700	-1.29503800	3.61525200
C	3.17489900	2.33773400	-3.37558700	C	1.25845900	0.68802800	4.45942800
H	2.36329200	0.38056500	-3.66755500	H	0.20339000	-1.14616900	4.08993000
C	2.03780300	3.75463000	-1.80060400	C	2.49725600	1.32499700	4.50907100
				H	4.62771500	1.09062700	4.26817000
				H	0.35085000	1.23489500	4.70904200

H	2.56213100	2.37263400	4.79741100	C	-0.21952700	1.89504200	0.40452300
C	1.46916900	-4.57593400	-0.09149000	C	-0.13356200	2.53440500	1.75695500
C	0.15273000	-4.94212000	-0.38975300	C	1.05226600	3.12446400	2.22436100
C	2.33985700	-4.29197000	-1.15023700	C	-1.22415500	2.49956900	2.65022800
C	-0.28740600	-5.00806800	-1.71007500	C	1.14467700	3.65561200	3.50724100
H	-0.52988400	-5.19189300	0.42493100	H	1.93223200	3.19658900	1.59024100
C	1.90478400	-4.35954100	-2.47094800	C	-1.13805700	3.04319700	3.92386500
H	3.37783300	-4.03620400	-0.93072400	H	-2.14000500	1.98535800	2.36202000
C	0.58629000	-4.71150000	-2.75391800	C	0.05042600	3.62380300	4.36384200
H	-1.31448300	-5.29949800	-1.92459000	H	2.08349400	4.10151000	3.82920000
H	2.59553600	-4.14278700	-3.28369100	H	-2.00101500	2.99356500	4.58496600
H	0.24365400	-4.75988400	-3.78485000	H	0.12250000	4.03986700	5.36616900
C	-1.84948000	-3.07902300	2.59775600	C	-1.48513900	1.95438900	-0.42752400
C	-1.87234200	-1.98168200	1.53092500	O	-1.55488100	1.19936900	-1.40423700
C	0.22969600	-2.67140600	1.86079900	N	-2.43533400	2.85811000	-0.09936000
H	-2.48315100	-3.93916100	2.35939800	H	-2.27310200	3.41641700	0.73122800
H	-2.32135600	-1.05332100	1.90795900	C	-3.69449300	3.00522400	-0.73119500
H	-2.07727000	-2.73248700	3.61078800	C	-4.78441800	3.36436900	0.06537900
O	-0.46726100	-3.53730200	2.60515800	C	-3.85822400	2.81099200	-2.10540000
N	-0.43713200	-1.73997800	1.27755700	C	-6.04130600	3.51784400	-0.50789600
C	-2.55591700	-2.40049800	0.22667500	H	-4.64397500	3.51591200	1.13563900
H	-2.40130600	-1.61004000	-0.52131600	C	-5.12453900	2.95686200	-2.66376700
H	-2.03339500	-3.28815200	-0.15861900	H	-3.00250600	2.54980000	-2.71963900
C	-4.01570600	-2.69698200	0.41535400	C	-6.21756400	3.30567500	-1.87347800
C	-4.47753600	-4.01642900	0.43443100	H	-6.88545600	3.79980500	0.11764000
C	-4.93807400	-1.66283400	0.61191700	H	-5.25351500	2.80661200	-3.73362900
C	-5.82524900	-4.30033400	0.64201700	H	-7.20146400	3.42203000	-2.32206200
H	-3.76927100	-4.83107200	0.26655000	C	0.76174700	3.72094900	-1.15106700
C	-6.28466900	-1.94211600	0.81995100	F	-0.17839500	3.77339600	-2.11350300
H	-4.59547700	-0.62650000	0.59445100	F	1.93799100	4.06852500	-1.71847000
C	-6.73160000	-3.26221500	0.83699500	F	0.45123500	4.65616100	-0.23930700
H	-6.16754100	-5.33324900	0.64630300	C	4.66042600	-0.37965700	-1.22603300
H	-6.99053300	-1.12638800	0.96468200	C	3.46821900	0.36039500	-0.61413900
H	-7.78546300	-3.47985700	0.99679700	C	2.74779900	-1.45815900	-1.67143300
				H	5.31337300	-0.83731700	-0.47060300
				H	3.33168400	1.33174400	-1.11379000
				H	5.26492300	0.21430200	-1.91529700
				O	4.05363900	-1.45310400	-1.98166300
				N	2.31067200	-0.49130200	-0.94694000
				C	3.57457000	0.55640400	0.89502000
				H	2.60280200	0.92314300	1.26778500
				H	3.71872600	-0.43118400	1.35966800
				C	4.68243400	1.49696900	1.27908200
				C	5.74775700	1.06163800	2.07048900
				C	4.67659500	2.82524000	0.83364700
				C	6.77806900	1.93134700	2.42000400
				H	5.76226700	0.02841400	2.42102300
				C	5.70307000	3.69707200	1.18225800
				H	3.86442000	3.18727500	0.19708900
				C	6.75676600	3.25100400	1.97799900
				H	7.59925200	1.57631400	3.03928600
				H	5.68214600	4.72632200	0.82997300
				H	7.56054700	3.93157800	2.25010000
				C	2.03548100	-2.63883800	-2.27118500
				C	2.84795500	-3.90751300	-1.85661700
				H	3.79381700	-3.89588500	-2.40814300
				H	2.28787200	-4.79083600	-2.18054500
				C	2.01208900	-2.42717400	-3.82508300
				H	3.05391100	-2.41869300	-4.16753400
				H	1.52284300	-3.30078700	-4.27260500
				C	3.10968300	-3.91091600	-0.37037500
				C	4.38097500	-3.59891300	0.12336300
				C	2.07323500	-4.11160300	0.55007400
TS5							
Cu	0.35531900	-0.18521000	-0.33798900				
C	-2.71374800	-1.03570900	2.22437700				
C	-2.10759700	-0.32041900	1.19046300				
C	-0.73930700	-0.07087900	1.23327700				
C	0.00620700	-0.45993800	2.35158000				
C	-0.61151400	-1.18695900	3.36194900				
C	-1.98250600	-1.48989300	3.32611800				
H	-3.77911400	-1.24281000	2.13950300				
H	-2.71656700	-0.00505200	0.34661800				
H	1.06507600	-0.21234700	2.43654900				
H	-0.00891200	-1.51155600	4.21072200				
C	-2.61604400	-2.26597900	4.47600300				
C	-2.49418000	-1.43746700	5.76242900				
H	-3.01110400	-0.47464200	5.66402900				
H	-2.93992500	-1.97437700	6.60892300				
H	-1.44738100	-1.22939800	6.01551000				
C	-1.87491400	-3.59753700	4.65931400				
H	-2.32170300	-4.17330100	5.47903600				
H	-1.92842500	-4.21079800	3.75043100				
H	-0.81591100	-3.44931700	4.90317800				
C	-4.09232000	-2.56646100	4.22091500				
H	-4.50521800	-3.14176400	5.05739500				
H	-4.69018200	-1.65138900	4.12758300				
H	-4.23711000	-3.15875900	3.30803300				
C	0.89848700	2.32059900	-0.56971700				
H	0.93663100	1.67711700	-1.46028700				
H	1.87386300	2.27652600	-0.09132300				

C	4.60748700	-3.46756100	1.49158400	H	-7.54657800	-0.34259000	0.07804700
H	5.20116100	-3.45723700	-0.58032400	H	-6.37540600	0.87548600	-0.44509200
C	2.29171400	-3.96977200	1.91750900	H	-6.41402300	0.34647000	1.24928400
H	1.08310300	-4.39733700	0.19524200	C	0.31259900	1.13500500	1.83991400
C	3.55896500	-3.63831200	2.39302700	H	-0.26100400	2.06221800	1.93112700
H	5.60860900	-3.23779800	1.85375900	H	-0.09646600	0.43560900	2.57628400
H	1.46934600	-4.12853000	2.61363800	C	0.11482400	0.51570600	0.43408200
H	3.73278500	-3.53459700	3.46222300	C	0.28793900	1.50628100	-0.72213700
C	1.30476500	-1.14580800	-4.17548100	C	0.47513000	2.88143600	-0.56349000
C	-0.08144500	-1.12390700	-4.35746700	C	0.16521800	1.00736500	-2.02898300
C	1.99712800	0.07084100	-4.18005000	C	0.55255300	3.72550500	-1.67088500
C	-0.76397300	0.07961900	-4.50712700	H	0.57654300	3.31534200	0.42804400
H	-0.63072200	-2.06766500	-4.37090500	C	0.25002400	1.84375600	-3.13331800
C	1.31800900	1.27840100	-4.32412100	H	-0.00997400	-0.05953800	-2.17255000
H	3.08226500	0.06778600	-4.06087500	C	0.44502000	3.21296000	-2.95817800
C	-0.06722600	1.28482800	-4.47639600	H	0.70103500	4.79307000	-1.51804500
H	-1.84596900	0.07803000	-4.63108700	H	0.15393300	1.42614800	-4.13390100
H	1.87003800	2.21792400	-4.31721200	H	0.50688000	3.87421000	-3.82027300
H	-0.60012400	2.22858800	-4.57334400	C	1.10392000	-0.68303400	0.39061700
C	-1.24204400	-4.05083000	-1.60161400	O	0.89928700	-1.67775300	1.07137300
C	-1.46978700	-2.64772800	-1.01980800	N	2.22086200	-0.48551700	-0.37159500
C	0.61332300	-2.80947500	-1.81404000	H	2.28105900	0.40738700	-0.84626100
H	-1.94058400	-4.31744200	-2.40115100	C	3.35475100	-1.30362700	-0.50712200
H	-1.68979700	-2.69158100	0.05665800	C	4.38757200	-0.81077500	-1.31548500
H	-1.22768300	-4.85346700	-0.85533300	C	3.49120900	-2.55680000	0.10219700
O	0.08314600	-3.98809000	-2.18760000	C	5.54162900	-1.55392100	-1.51516000
N	-0.14758000	-2.00551900	-1.16870300	H	4.27792300	0.16620100	-1.78734300
C	-2.55770900	-1.83501400	-1.72593300	C	4.65560500	-3.28877000	-0.10975700
H	-2.24076700	-0.78631800	-1.75728500	H	2.69485400	-2.93770600	0.72993500
H	-2.60580400	-2.15336200	-2.78052900	C	5.68300900	-2.80220000	-0.91292500
C	-3.91868000	-1.92396600	-1.08764100	H	6.33341000	-1.15378100	-2.14604700
C	-4.76416200	-0.80886500	-1.12572300	H	4.75556100	-4.26221900	0.36750300
C	-4.36339700	-3.07301800	-0.42715600	H	6.58606800	-3.38883700	-1.06867900
C	-6.01620800	-0.83866200	-0.51960800	C	1.72983500	1.43153600	2.28243400
H	-4.42026900	0.09966100	-1.62477700	F	1.71671100	2.27256100	3.33683700
C	-5.61825300	-3.10892400	0.17795500	F	2.38848000	0.32334500	2.66581200
H	-3.72422800	-3.95671000	-0.37423700	F	2.48343100	2.01675400	1.32186800
C	-6.44714900	-1.99063600	0.13662100				
H	-6.65241700	0.04431500	-0.55639200	TS6	S**2 = 0.69		
H	-5.94786300	-4.01397900	0.68530200	C	-1.72328200	-2.01259600	3.19382400
H	-7.42522300	-2.01791700	0.61251900	C	-1.67414100	-1.02130800	2.02784600
				C	0.16710900	-2.26423500	2.01123900
4a				H	-2.57667500	-2.69925900	3.14930700
C	-3.70606000	0.59413500	0.45636300	H	-1.71163000	0.01510500	2.38987400
C	-2.36648500	0.94359300	0.59042900	H	-1.69105700	-1.54801900	4.18400000
C	-1.34166200	0.02710700	0.34331100	O	-0.51451600	-2.79472300	3.04266000
C	-1.71089800	-1.25609000	-0.07002100	N	-0.35548000	-1.25648500	1.41476400
C	-3.05097300	-1.59610300	-0.21080900	C	-2.73489700	-1.24171500	0.95443800
C	-4.08293900	-0.68827100	0.05114400	H	-2.50930800	-0.53552000	0.14641500
H	-4.46217800	1.34879900	0.66214300	H	-2.58127900	-2.24267900	0.52390000
H	-2.12099300	1.96951800	0.86706800	C	-4.14925300	-1.08348700	1.42578900
H	-0.95231700	-2.00910800	-0.26283700	C	-4.96867600	-2.20149800	1.60207100
H	-3.29661200	-2.60850100	-0.53295200	C	-4.68096900	0.18284100	1.69446300
C	-5.53724000	-1.11948900	-0.11865000	C	-6.28779300	-2.06165900	2.02657900
C	-5.76981400	-1.55544900	-1.57152000	H	-4.56972000	-3.19262300	1.37641800
H	-5.57380500	-0.73161100	-2.26894200	C	-5.99762000	0.32888400	2.11820100
H	-6.80910800	-1.87982300	-1.71442600	H	-4.05691900	1.06892800	1.55312900
H	-5.11969000	-2.39241600	-1.85383600	C	-6.80537500	-0.79529400	2.28414900
C	-5.82744400	-2.30358900	0.81287600	H	-6.91378200	-2.94321200	2.15114700
H	-6.86716400	-2.63758400	0.69790100	H	-6.39753000	1.32150000	2.31711300
H	-5.67429600	-2.02904200	1.86386100	H	-7.83612000	-0.68262300	2.61377700
H	-5.17756500	-3.15972900	0.59570400	C	1.46086400	-2.97779000	1.76201500
C	-6.51532400	0.00685600	0.21070800	C	1.14343500	-4.49625000	1.58500200

H	0.70631900	-4.85068400	2.52496100
H	2.10097900	-5.01187900	1.45215700
C	2.38683400	-2.78668700	3.01026900
H	1.78688600	-3.03870000	3.89364000
H	3.18413000	-3.53510800	2.93881700
C	0.22522400	-4.76470800	0.42493800
C	-1.16308900	-4.80160000	0.59538700
C	0.74462000	-4.93345700	-0.86307100
C	-2.00865200	-4.99552800	-0.49385000
H	-1.58102500	-4.69811500	1.59765800
C	-0.09716000	-5.12645600	-1.95422900
H	1.82623500	-4.93784500	-1.00319900
C	-1.47751300	-5.15479000	-1.77171200
H	-3.08672800	-5.03501900	-0.34109200
H	0.32527800	-5.27000600	-2.94667800
H	-2.13449300	-5.32158900	-2.62382000
C	2.98170700	-1.40849100	3.11551900
C	4.35269300	-1.21621200	2.91601400
C	2.18354400	-0.28625400	3.37228300
C	4.91162600	0.05973700	2.96664500
H	4.98696500	-2.08154600	2.71757300
C	2.73350800	0.99078200	3.39595300
H	1.11826900	-0.40654400	3.57014600
C	4.10004500	1.16900800	3.18979700
H	5.98328200	0.18761400	2.82348100
H	2.08943600	1.84874200	3.58234600
H	4.53272600	2.16759200	3.21848800
C	3.94809900	-2.69978400	-0.84327500
C	3.19849800	-1.39970200	-1.10735900
C	2.21871300	-2.49448100	0.55774500
H	5.02149000	-2.57194900	-0.67459900
H	2.91295900	-1.30582100	-2.15832000
H	3.78767200	-3.46836300	-1.60825700
O	3.35907300	-3.18392300	0.38818900
N	1.97870700	-1.53908000	-0.27186500
C	3.97903800	-0.16264600	-0.64589500
H	3.32079400	0.71020800	-0.73275300
H	4.19374900	-0.28050000	0.42495100
C	5.25202900	0.03729200	-1.41703700
C	6.48482800	-0.29831200	-0.84871500
C	5.22872000	0.51996400	-2.73021300
C	7.66775900	-0.15335900	-1.56957800
H	6.51320500	-0.66793100	0.17842200
C	6.40861700	0.66689800	-3.45255000
H	4.27655000	0.79281500	-3.18570000
C	7.63114900	0.32949400	-2.87456700
H	8.61895000	-0.41424100	-1.10960300
H	6.37489000	1.04965400	-4.47081200
H	8.55332800	0.44651000	-3.43985600
Cu	0.41580100	-0.17730300	-0.22998900
C	-0.94620400	3.10918600	1.96422300
C	-1.07878000	2.08104600	1.03300900
C	-0.02171900	1.71585800	0.19413900
C	1.14716200	2.49190400	0.24504100
C	1.28200700	3.51367200	1.18215300
C	0.23866400	3.85199500	2.05829500
H	-1.79692000	3.35523500	2.59765600
H	-2.04200700	1.57355000	0.94219800
H	1.97553500	2.29540200	-0.43922300
H	2.21965300	4.07041800	1.21912100
C	0.41213900	5.02276700	3.02275700
C	0.76913800	6.28516800	2.22544600
H	-0.01764600	6.53378000	1.50195200

H	0.88616600	7.14215000	2.89992100
H	1.70816200	6.17250700	1.67120300
C	1.55230100	4.70970200	4.00145000
H	1.72235100	5.55831900	4.67554200
H	1.31747000	3.83524300	4.62173700
H	2.49604900	4.51025000	3.47776600
C	-0.85769500	5.30217100	3.82437400
H	-0.69495400	6.15155600	4.49743700
H	-1.70373500	5.55700200	3.17296600
H	-1.15098400	4.44598900	4.44453200
C	0.13064500	2.35334200	-2.91866600
H	0.74785100	3.07135800	-2.35949600
H	-0.17817100	2.89864000	-3.82400600
C	-1.11155900	2.03949500	-2.12846000
C	-1.96244700	3.25769200	-2.02472900
C	-1.59270300	4.31163000	-1.17589800
C	-3.06321000	3.45434400	-2.88071300
C	-2.34042900	5.48279700	-1.12893300
H	-0.71132600	4.20705700	-0.54550800
C	-3.80518200	4.63177900	-2.83492000
H	-3.31230700	2.69997400	-3.62821900
C	-3.45628500	5.64421300	-1.94683000
H	-2.04447000	6.27982800	-0.44927100
H	-4.64781100	4.76013300	-3.51109100
H	-4.03723400	6.56288400	-1.90779700
C	-1.66157800	0.67355900	-2.02682100
O	-0.94456400	-0.34873700	-1.92565600
N	-3.02344000	0.59630300	-2.00501500
H	-3.51018100	1.48601100	-1.99971600
C	-3.87549200	-0.52389900	-2.01285200
C	-5.23473600	-0.26451400	-1.78596600
C	-3.44066800	-1.83484600	-2.24297900
C	-6.15448100	-1.30193700	-1.77900000
H	-5.56297200	0.75793300	-1.59612000
C	-4.38015300	-2.86113400	-2.23918500
H	-2.38943300	-2.04015300	-2.41281400
C	-5.73044500	-2.60922600	-2.00768300
H	-7.20325500	-1.08730200	-1.58637500
H	-4.04500300	-3.87870100	-2.43075500
H	-6.44893000	-3.42579800	-2.00836400
C	1.04782800	1.27191900	-3.41447700
F	1.66448200	0.60347800	-2.39839800
F	2.03990000	1.83316700	-4.13598100
F	0.44689300	0.37022800	-4.19436800

TS7

C	-1.26912200	-3.54064900	-1.87114900
C	-1.42118600	-2.56504000	-0.69560200
C	0.12316700	-1.79487400	-2.10054600
H	-2.16880800	-3.60788000	-2.49748700
H	-1.07021400	-3.01648800	0.24175500
H	-0.96009200	-4.54994800	-1.58556300
O	-0.21196000	-2.97108700	-2.67824100
N	-0.49379800	-1.47123200	-1.02558000
C	-2.84423700	-2.05656700	-0.48990000
H	-2.80627800	-1.28598600	0.29047800
H	-3.18470600	-1.56064800	-1.41068700
C	-3.76829700	-3.17776400	-0.10995800
C	-4.70124600	-3.68947900	-1.01600700
C	-3.66562000	-3.77268600	1.15361000
C	-5.51380300	-4.76811000	-0.67309400
H	-4.79650400	-3.22756600	-2.00043700
C	-4.47501500	-4.84961200	1.49802500

H	-2.94660500	-3.37390200	1.86999800
C	-5.40050900	-5.35258300	0.58476400
H	-6.23716300	-5.15138200	-1.39099400
H	-4.38513600	-5.29859900	2.48593000
H	-6.03307700	-6.19625600	0.85509100
C	1.13577000	-1.01913400	-2.89828500
C	0.40490800	-0.45750600	-4.16312500
H	0.00991600	-1.31432000	-4.72393200
H	1.17110400	0.02118200	-4.78545700
C	2.30584200	-1.95178200	-3.33960100
H	1.86738100	-2.88328500	-3.71608800
H	2.80431500	-1.46523000	-4.18609200
C	-0.67876200	0.51685800	-3.80167200
C	-1.98182100	0.08550500	-3.53942200
C	-0.37131100	1.86854300	-3.60755100
C	-2.94631400	0.97323700	-3.06862100
H	-2.23467600	-0.96637900	-3.69302500
C	-1.33324200	2.75792300	-3.14240600
H	0.63976900	2.21835800	-3.82155600
C	-2.62105800	2.30994100	-2.86237000
H	-3.95315900	0.61830500	-2.85134300
H	-1.07514300	3.80375400	-2.98058200
H	-3.36202500	2.99910400	-2.46104700
C	3.31868600	-2.21180100	-2.25356800
C	4.64949800	-1.82267100	-2.43874600
C	2.95987400	-2.78992400	-1.03051100
C	5.60144000	-2.02409200	-1.44286200
H	4.93631900	-1.34924900	-3.37858800
C	3.90518200	-2.97861600	-0.02638300
H	1.92847400	-3.08583000	-0.84081800
C	5.23030200	-2.60075200	-0.23032700
H	6.63440600	-1.72224100	-1.61238500
H	3.59410500	-3.41060900	0.92246900
H	5.96897700	-2.74548700	0.55594800
C	3.21037100	1.80687300	-1.98067600
C	2.58446300	1.49166100	-0.61825200
C	1.75624800	0.11986500	-2.14075700
H	4.30521300	1.77714900	-1.98599500
H	2.13091500	2.37162900	-0.14793000
H	2.87164400	2.75494000	-2.41612100
O	2.73537600	0.73802700	-2.83963000
N	1.52916600	0.51970000	-0.94723600
C	3.56010300	0.83135000	0.36381700
H	2.98011500	0.51329800	1.23824100
H	3.95623300	-0.07929000	-0.10978600
C	4.67977600	1.74967200	0.75416300
C	5.95592900	1.59894600	0.20326100
C	4.45577300	2.80441200	1.64725000
C	6.98578500	2.47744400	0.53180500
H	6.13915400	0.76835600	-0.48189600
C	5.48281700	3.68224000	1.97778800
H	3.46495600	2.91636600	2.08890600
C	6.75042900	3.52349500	1.41929400
H	7.97497400	2.34190100	0.09691500
H	5.29656100	4.49309800	2.68078200
H	7.55366600	4.21055900	1.68087200
Cu	-0.36162900	0.32616300	-0.03653500
S	0.18514300	-1.53350100	2.43133600
O	0.89377800	-2.52986900	1.65101700
O	-1.27577900	-1.48462200	2.42425600
O	0.81524900	-0.12991500	2.17113100
C	0.68837100	-1.84587500	4.18426100
F	2.01042700	-1.75517100	4.29844600

F	0.30042600	-3.08333400	4.49807900
F	0.10789000	-0.98192300	5.00810900
C	-3.88502800	2.36541200	0.91332900
C	-2.87740200	1.41562100	1.01026900
C	-1.53752700	1.68741400	0.66222000
C	-1.29229900	3.00872400	0.24948800
C	-2.29571000	3.97492800	0.15358100
C	-3.62111800	3.67235200	0.47423200
H	-4.90479200	2.08962800	1.19016200
H	-3.14431300	0.42090400	1.38052900
H	-0.27391000	3.29510100	-0.03218400
H	-2.03368400	4.97629900	-0.18941900
B	0.03515600	1.18636400	2.29279000
O	-0.88421900	1.27662400	3.31090300
H	-1.59978100	0.63529200	3.21026900
O	0.96538000	2.18963100	2.09822300
H	0.51391200	3.03157000	2.24512600
C	-4.75840100	4.68756800	0.38510500
C	-4.29448700	6.02378300	-0.19123400
H	-3.87529200	5.90696800	-1.19960200
H	-5.14155800	6.71743600	-0.26180000
H	-3.53106400	6.49837700	0.43779600
C	-5.32890700	4.93067900	1.78898200
H	-6.15609900	5.65270300	1.75351100
H	-5.71282900	4.00367600	2.23199300
H	-4.56103700	5.32727100	2.46456200
C	-5.87382600	4.13871600	-0.51476300
H	-6.70972100	4.84911500	-0.56927000
H	-5.51370700	3.96777300	-1.53773000
H	-6.27132900	3.18833600	-0.13972000

INT8

C	4.30778400	-0.90132800	-0.37152000
C	3.22597600	0.03915100	-0.91683800
C	2.27763200	-1.53621700	0.34420200
H	4.97907000	-0.41118100	0.34586600
H	3.12961500	-0.05559100	-2.00847100
H	4.90823900	-1.39897400	-1.13785300
O	3.57370800	-1.92241000	0.34546600
N	1.98495700	-0.47129900	-0.31103700
C	3.43521100	1.51031900	-0.55898500
H	2.56100400	2.06894000	-0.92848100
H	3.41848400	1.60143400	0.53657400
C	4.71995400	2.04640200	-1.12066700
C	5.82192500	2.28194100	-0.29297900
C	4.85698600	2.28241300	-2.49378000
C	7.02653000	2.74418100	-0.81744900
H	5.72389600	2.11012900	0.78051700
C	6.05806600	2.74382000	-3.02174900
H	4.00323200	2.11463100	-3.15189200
C	7.14804700	2.97529700	-2.18447700
H	7.87078700	2.92826800	-0.15491600
H	6.14273000	2.92988800	-4.09123800
H	8.08695400	3.34029700	-2.59663900
C	1.41151800	-2.35784500	1.26098400
C	1.83225700	-1.99156800	2.72146400
H	2.80315600	-2.46653400	2.91130200
H	1.10209500	-2.45999300	3.39219600
C	1.65683600	-3.88131000	1.04300500
H	2.73514200	-4.05997400	1.12828200
H	1.17141200	-4.40191400	1.87821900
C	1.93425600	-0.51059100	2.95471100
C	3.18416000	0.08719700	3.14248800

C	0.80301600	0.31170100	2.89631900	H	-4.61949300	6.97058100	-0.98769100
C	3.30329600	1.46916200	3.27429000	H	-2.94865500	6.61335500	-0.51207500
H	4.07323700	-0.54402600	3.18837700	H	-3.56104200	6.04108600	-2.07137100
C	0.91986300	1.69391200	3.00753400				
H	-0.18434900	-0.13029500	2.75872300	TfOB(OH)₂			
C	2.17076700	2.27694500	3.19616100	S	0.19075900	-0.66711900	-0.00004800
H	4.28390400	1.91625200	3.43372900	O	0.15913600	-1.35619000	-1.27052900
H	0.02880900	2.31389500	2.93186900	O	0.15945400	-1.35669800	1.27016200
H	2.26157800	3.35828600	3.28147700	O	-0.85652000	0.57109300	0.00034000
C	1.12112200	-4.38615000	-0.26594100	C	1.67770400	0.42794000	-0.00003200
C	-0.14971400	-4.96522600	-0.33251900	F	1.68610600	1.19063600	-1.08627600
C	1.84724200	-4.22941200	-1.45046500	F	2.75000800	-0.35986900	-0.00053900
C	-0.68271900	-5.37831300	-1.55004400	F	1.68661700	1.18996100	1.08668800
H	-0.72315000	-5.09175900	0.58749400	B	-2.24450600	0.36661900	0.00017200
C	1.31633100	-4.63944500	-2.66976500	O	-2.95466400	1.52225100	0.00021800
H	2.84470900	-3.78978000	-1.40993700	H	-3.90991500	1.40495300	0.00047400
C	0.04825800	-5.21268900	-2.72367600	O	-2.68823700	-0.91636500	-0.00004600
H	-1.67334800	-5.83087400	-1.58228000	H	-3.64385600	-1.03105200	-0.00037900
H	1.89696300	-4.51443100	-3.58227200				
H	-0.36632200	-5.53504300	-3.67690800	TS8 S**2 = 2.00			
C	-2.20261000	-2.38185900	1.61610900	Cu	0.06970200	-0.92074100	-0.86255300
C	-2.06078600	-1.50510700	0.36045700	C	-3.60005200	-0.70620800	-2.89040700
C	-0.05492500	-2.09678600	1.05907200	C	-2.23296800	-0.53383900	-2.65151500
H	-2.68064700	-3.34993700	1.40966900	C	-1.46005200	-1.45795700	-1.92813000
H	-2.36792000	-0.46486400	0.55489100	C	-2.15510400	-2.61636100	-1.52217200
H	-2.72106700	-1.90329700	2.45207100	C	-3.52071300	-2.78851400	-1.73455800
O	-0.84001400	-2.63976200	2.03157000	C	-4.28576800	-1.82093700	-2.40041800
N	-0.61839800	-1.47827200	0.09594800	H	-4.14417200	0.06923400	-3.43118000
C	-2.83943100	-2.02805800	-0.84281000	H	-1.77284200	0.40044400	-2.98915400
H	-2.55069800	-1.42455000	-1.71460800	H	-1.62572400	-3.39665100	-0.96389600
H	-2.51498700	-3.05734100	-1.05597500	H	-4.01298500	-3.68582600	-1.34927300
C	-4.32485600	-1.97204200	-0.61960800	C	-5.80080300	-1.98494400	-2.49453800
C	-5.09856600	-3.13404800	-0.56704700	C	-6.14675800	-3.30731600	-3.18967300
C	-4.95978700	-0.73760100	-0.43300400	H	-5.72897900	-4.16921700	-2.65531300
C	-6.47316500	-3.06934200	-0.34665700	H	-7.23547200	-3.44559400	-3.24273300
H	-4.61434500	-4.10199500	-0.71115600	H	-5.75240800	-3.33002900	-4.21334600
C	-6.33081100	-0.66976900	-0.21380100	C	-6.46091100	-0.84505900	-3.26831000
H	-4.36879800	0.17980400	-0.46358900	H	-7.54576400	-1.00387700	-3.31891200
C	-7.09349100	-1.83598900	-0.17134400	H	-6.29143100	0.12497500	-2.78298400
H	-7.06032100	-3.98588900	-0.31446500	H	-6.08575000	-0.78064400	-4.29777700
H	-6.80677400	0.30063500	-0.07834600	C	-6.37894500	-1.99632100	-1.07083300
H	-8.16763300	-1.78252800	-0.00192000	H	-7.46905200	-2.13535700	-1.09164300
Cu	0.33900100	0.61127200	-0.34437600	H	-5.94761300	-2.80895200	-0.47139500
C	-3.28549100	2.64785400	-1.07108300	H	-6.16694000	-1.05115400	-0.55148800
C	-2.22995800	1.73277400	-1.06634700	C	1.63987000	1.07688800	-2.65082700
C	-1.00619700	1.95704800	-0.40588900	C	2.74997500	2.98606400	-1.37028500
C	-0.92262100	3.21169800	0.23596600	C	3.78939100	3.83616700	-1.03114400
C	-1.96640200	4.13285300	0.24158700	C	4.99504400	3.70868200	-1.71823100
C	-3.18201300	3.87159700	-0.40526800	C	5.11758300	2.75595500	-2.72370100
H	-4.20084500	2.39278800	-1.60747900	C	4.04864400	1.92013300	-3.03209400
H	-2.37844600	0.79645700	-1.61493400	C	2.83094200	2.00122100	-2.34489000
H	0.00096000	3.48587900	0.75537200	H	3.68654300	4.57150900	-0.24007200
H	-1.83374400	5.08553900	0.76112200	H	5.83110000	4.35419600	-1.45736400
C	-4.30721000	4.90360000	-0.36472700	H	6.05426800	2.65485500	-3.26861700
C	-4.68791100	5.19098900	1.09379400	H	4.16180400	1.17581000	-3.81820200
H	-3.83428900	5.57326100	1.66648400	I	0.85900900	3.08177700	-0.33985500
H	-5.48808800	5.94228700	1.14686800	O	0.89311200	0.88752500	-1.47680400
H	-5.04284600	4.28174600	1.59558200	C	0.78481900	1.73620700	-3.74259900
C	-5.55781000	4.42333900	-1.09928200	H	1.36700400	1.93689700	-4.65161300
H	-6.34550200	5.18530700	-1.04032600	H	-0.04591900	1.07001500	-4.00167800
H	-5.35933200	4.23270200	-2.16144300	H	0.36376600	2.68780000	-3.39447700
H	-5.95699500	3.49847500	-0.66187800	C	2.12948200	-0.28373600	-3.14496500
C	-3.83102700	6.20588800	-1.02081000	H	1.26240500	-0.95083100	-3.22580700

H	2.61310300	-0.22445900	-4.12870200
H	2.83975800	-0.71919900	-2.43146900
C	1.42200000	5.35359600	0.52432600
F	0.26476400	5.73801000	1.09051100
F	1.75386300	6.25245800	-0.41303900
F	2.37098200	5.37739300	1.48089400
C	-1.82855500	1.94836300	2.02835100
C	-1.94502400	1.08944000	0.75784700
C	-0.37642000	0.24775900	2.06377000
H	-2.76760700	2.03057000	2.58800300
H	-1.83043000	1.67916700	-0.16416200
H	-1.42393400	2.95665800	1.86372500
O	-0.88314200	1.22577900	2.85822300
N	-0.82566500	0.15058400	0.87535500
C	-3.24530800	0.28173600	0.68633600
H	-3.14449100	-0.44306700	-0.13369100
H	-3.32914400	-0.29746500	1.61516600
C	-4.46370600	1.13545300	0.49580300
C	-5.41584500	1.26748200	1.51091300
C	-4.67666100	1.81496100	-0.71012800
C	-6.55864900	2.04307500	1.32556600
H	-5.26004400	0.73321500	2.45025000
C	-5.81562600	2.59078700	-0.89858400
H	-3.94901000	1.70428000	-1.51512100
C	-6.76265900	2.70530400	0.11850500
H	-7.29375500	2.12550900	2.12482700
H	-5.97061100	3.10219100	-1.84775700
H	-7.65700600	3.30750800	-0.03174000
C	0.53317600	-0.70270200	2.78748900
C	-0.32339200	-1.29149000	3.95893400
H	-0.38256200	-0.51320800	4.72920800
H	0.25126100	-2.12273800	4.38643500
C	1.77156000	0.02229200	3.41755900
H	1.46269300	1.05338900	3.63867600
H	1.97165300	-0.45373800	4.38592600
C	-1.71803900	-1.72123300	3.58409700
C	-2.81573800	-1.14900400	4.23565400
C	-1.96309200	-2.66579100	2.57915600
C	-4.11852200	-1.51883100	3.90935400
H	-2.63977200	-0.39884300	5.00762300
C	-3.26408600	-3.02111000	2.23433100
H	-1.13024600	-3.12388300	2.04507000
C	-4.34722400	-2.45172500	2.90048300
H	-4.95736900	-1.06700200	4.43726800
H	-3.43121300	-3.73552000	1.42999700
H	-5.36461400	-2.72408400	2.62493600
C	3.03865100	-0.00887100	2.60148300
C	4.22207900	-0.46487600	3.19092400
C	3.06832300	0.36326300	1.25176800
C	5.40808900	-0.53579400	2.46468700
H	4.20702800	-0.77777100	4.23567600
C	4.25272500	0.29326800	0.52213400
H	2.15306600	0.66515200	0.73964700
C	5.42647100	-0.15447600	1.12518900
H	6.31679000	-0.89345000	2.94628400
H	4.25106900	0.58525900	-0.52795800
H	6.35032300	-0.20790400	0.55124500
C	2.44039700	-3.55058800	1.69636200
C	1.77669500	-3.21191000	0.36319000
C	1.05571400	-1.81877300	1.92637700
H	3.48997700	-3.22046800	1.73660200
H	1.01935300	-3.96749700	0.09420500
H	2.37758900	-4.59902300	1.99589700

O	1.70065300	-2.76312500	2.65600900
N	1.06250700	-1.95517300	0.65027400
C	2.74858000	-3.04874300	-0.79846600
H	2.15792300	-2.79448000	-1.69058500
H	3.39483900	-2.18523100	-0.58124000
C	3.57440500	-4.28439400	-1.01446200
C	4.89785800	-4.34648000	-0.56682800
C	3.01911600	-5.41845900	-1.61802100
C	5.64916900	-5.50941400	-0.71852500
H	5.34180500	-3.46458500	-0.10092500
C	3.76694900	-6.58140700	-1.77150100
H	1.99072200	-5.38038500	-1.98009100
C	5.08472900	-6.63075400	-1.32032600
H	6.67980600	-5.53794700	-0.36849900
H	3.32125400	-7.45204400	-2.24965600
H	5.67087500	-7.53974200	-1.44260400

INT9 S**2 = 0.75

Cu	-0.15529500	0.25603200	0.26567300
C	-1.81680600	-3.76058100	0.36080500
C	-1.37688300	-2.51192600	0.81368900
C	-0.74001700	-1.60163500	-0.03215500
C	-0.54506800	-2.01168400	-1.36014000
C	-0.97231600	-3.25736800	-1.81260900
C	-1.62489600	-4.16166500	-0.96373200
H	-2.31092100	-4.42820200	1.06705500
H	-1.54135500	-2.26620900	1.86667500
H	-0.04848800	-1.34538200	-2.07286500
H	-0.79429100	-3.53062900	-2.85589900
C	-2.08233200	-5.51434100	-1.50596400
C	-3.04306100	-5.29559100	-2.68249600
H	-2.56600300	-4.73435300	-3.49577000
H	-3.37810900	-6.25693000	-3.09521800
H	-3.93227300	-4.73425900	-2.36780200
C	-2.80201300	-6.34896300	-0.44809000
H	-3.12189400	-7.30645100	-0.87813200
H	-2.15214500	-6.57162700	0.40724300
H	-3.69745500	-5.84089200	-0.06750800
C	-0.86258600	-6.30439700	-1.99809300
H	-1.16757200	-7.27907700	-2.40304500
H	-0.32645600	-5.76721400	-2.78991000
H	-0.15294600	-6.48310400	-1.18087700
C	1.58729800	0.18840000	2.60462100
C	3.72635800	-1.26102700	2.28360600
C	5.05380800	-1.56356800	2.58597700
C	5.75042100	-0.82623400	3.53737500
C	5.10475900	0.21671800	4.18740800
C	3.77977400	0.50438300	3.87824600
C	3.04322900	-0.21056500	2.92103400
H	5.54813700	-2.37942400	2.06380200
H	6.78775500	-1.07120100	3.75927600
H	5.62568000	0.81093400	4.93646200
H	3.29701900	1.32633200	4.40053500
I	2.88171100	-2.51165700	0.75734700
O	1.47469500	0.36673900	1.22994200
C	0.64112100	-0.89029700	3.15181000
H	0.76289700	-1.01673600	4.23596500
H	-0.39794200	-0.58565100	2.95684600
H	0.79710700	-1.85712300	2.66401400
C	1.19059700	1.51762000	3.26649300
H	0.16881200	1.75145000	2.93798500
H	1.19325100	1.49452300	4.36506100
H	1.84420700	2.33228300	2.92672000

C	2.14567300	3.32618200	-1.96469300
C	2.02244500	2.06381100	-1.09714600
C	-0.00482700	2.77140100	-1.65862000
H	2.63479200	3.14136900	-2.93010600
H	2.35976100	2.22645300	-0.06412900
H	2.63791300	4.17215800	-1.47573100
O	0.77292000	3.71963000	-2.23543400
N	0.57881200	1.82794100	-1.03206600
C	2.75020700	0.83932600	-1.64462200
H	2.39544400	-0.02811000	-1.06940400
H	2.45940400	0.68465700	-2.69523100
C	4.23817100	0.98026600	-1.50534500
C	5.07431600	1.15966600	-2.60904900
C	4.80561800	0.96645500	-0.22534400
C	6.44953900	1.31538200	-2.44261800
H	4.64248800	1.16495100	-3.61165200
C	6.17707300	1.11827600	-0.05624000
H	4.15250000	0.81759500	0.63674300
C	7.00363200	1.29498800	-1.16580200
H	7.08923700	1.44891300	-3.31387000
H	6.60052400	1.09074200	0.94693300
H	8.07825000	1.41212600	-1.03510500
C	-1.47492000	2.98502000	-1.87433500
C	-1.76968600	2.85877500	-3.39924500
H	-1.21218900	3.65789700	-3.90350200
H	-2.83800500	3.06224500	-3.54087500
C	-1.87405300	4.41299900	-1.38232600
H	-1.13962100	5.11827000	-1.78897900
H	-2.84522800	4.65444900	-1.83053200
C	-1.40335400	1.51285800	-3.96076000
C	-0.13457700	1.28784000	-4.50374200
C	-2.30530400	0.44453200	-3.90262300
C	0.22255200	0.03047500	-4.98365600
H	0.57535500	2.11524900	-4.55677800
C	-1.95102600	-0.81378700	-4.37933500
H	-3.29896500	0.60812000	-3.48296700
C	-0.68596300	-1.02335700	-4.92318300
H	1.21326200	-0.12586500	-5.40767400
H	-2.66186500	-1.63641000	-4.31746900
H	-0.40736300	-2.00783100	-5.29529300
C	-1.96818200	4.50270900	0.11652200
C	-3.22209400	4.52780100	0.73600900
C	-0.82545500	4.47836100	0.92458600
C	-3.33655200	4.52585500	2.12377300
H	-4.11767300	4.54534400	0.11408000
C	-0.93634900	4.47517800	2.31207900
H	0.16396600	4.46641500	0.46431600
C	-2.19174900	4.49368000	2.91647100
H	-4.32265000	4.55415600	2.58585200
H	-0.03704400	4.45481600	2.92444100
H	-2.27527000	4.48923000	4.00159900
C	-4.33556400	1.31318900	-0.40835100
C	-3.22023400	0.46337800	0.21032600
C	-2.32600800	2.00313700	-1.11919100
H	-4.84159400	1.95302500	0.32880100
H	-3.23211000	-0.57094100	-0.16637800
H	-5.08525600	0.74901200	-0.96931200
O	-3.64812300	2.18360600	-1.34149000
N	-1.99082800	1.09332600	-0.28501000
C	-3.22322200	0.44007300	1.73585000
H	-2.33666100	-0.13073700	2.05376400
H	-3.08751300	1.46947200	2.10186300
C	-4.48424500	-0.16218800	2.28550300

C	-5.41221900	0.61877300	2.97933900
C	-4.77360100	-1.51552200	2.07017300
C	-6.59825600	0.06466700	3.45608100
H	-5.19189700	1.67347600	3.15409200
C	-5.95699600	-2.07080500	2.54499400
H	-4.05438500	-2.13490500	1.53002900
C	-6.87346200	-1.28237300	3.23941600
H	-7.30734500	0.68697900	3.99966100
H	-6.16416600	-3.12619500	2.37534200
H	-7.79838000	-1.71874400	3.61224900

INT6-R S2 = 2.00**

C	-2.28077800	-3.45668800	2.06315100
C	-2.09123900	-2.02321400	1.55868500
C	-0.33301400	-3.26160100	0.97051400
H	-3.20132600	-3.93138900	1.70833200
H	-2.15430300	-1.28476300	2.36862100
H	-2.21056500	-3.56714800	3.15024800
O	-1.16026300	-4.18383100	1.48476200
N	-0.71594300	-2.03969700	1.03462400
C	-3.03693100	-1.63796100	0.42003600
H	-2.67963300	-0.69186100	-0.00616000
H	-2.92681700	-2.38263600	-0.38354700
C	-4.46969100	-1.52936400	0.85117200
C	-5.39676700	-2.51650400	0.50455800
C	-4.90566100	-0.43792200	1.61054500
C	-6.72970400	-2.41550000	0.89652300
H	-5.06716300	-3.36509400	-0.09903200
C	-6.23584900	-0.33240500	2.00299500
H	-4.19494900	0.34537000	1.88210500
C	-7.15193900	-1.32107600	1.64642700
H	-7.43933800	-3.19070800	0.61356300
H	-6.56174700	0.52662900	2.58674000
H	-8.19255800	-1.23767900	1.95314700
C	0.91244000	-3.85117000	0.37335900
C	0.46887100	-4.86633500	-0.72675700
H	0.06008800	-5.74449500	-0.21353800
H	1.37626900	-5.19267600	-1.25068100
C	1.70822700	-4.59134300	1.50041700
H	0.99341300	-5.23094800	2.03183800
H	2.43555300	-5.24934500	1.01201300
C	-0.55214900	-4.30022000	-1.67828900
C	-1.88298200	-4.72827700	-1.61639900
C	-0.21187000	-3.31101300	-2.60963900
C	-2.84798600	-4.19086300	-2.46548300
H	-2.15920700	-5.49960100	-0.89685200
C	-1.17718100	-2.76215800	-3.44816600
H	0.82316700	-2.97463900	-2.69505000
C	-2.49810000	-3.20059700	-3.38016400
H	-3.87395600	-4.55256800	-2.41751500
H	-0.89394900	-1.99985500	-4.17278200
H	-3.24726800	-2.78246300	-4.05050600
C	2.40650100	-3.63678800	2.43297600
C	3.78861900	-3.43885600	2.33838700
C	1.68685100	-2.87491000	3.36159100
C	4.43381300	-2.49604100	3.13495900
H	4.36203300	-4.03914800	1.63218900
C	2.32573500	-1.92482700	4.15367800
H	0.61469200	-3.03710200	3.47923600
C	3.70069000	-1.72803700	4.03736200
H	5.51059200	-2.35963300	3.04854500
H	1.74925900	-1.34503000	4.87207000
H	4.20187000	-0.99140500	4.66261600

C	3.88314200	-2.28960100	-1.00257700
C	3.04160300	-1.02748500	-0.77104800
C	1.85301800	-2.83922200	-0.22176900
H	4.78075400	-2.34306000	-0.37632900
H	2.91709700	-0.46057800	-1.70116100
H	4.15893900	-2.45433400	-2.04957300
O	3.01429400	-3.38195100	-0.60631600
N	1.72952100	-1.56756400	-0.36011100
C	3.53412800	-0.10486900	0.34136400
H	2.85952700	0.77110600	0.36034500
H	3.37809700	-0.61517200	1.30529700
C	4.96716700	0.34368800	0.24759100
C	5.58470000	0.87329200	1.38704100
C	5.71446700	0.25503300	-0.93027800
C	6.90149800	1.31668600	1.34705000
H	5.01653700	0.93447500	2.31681800
C	7.03682300	0.69380300	-0.97343000
H	5.26076800	-0.15174500	-1.83480900
C	7.63329100	1.22845700	0.16375500
H	7.36179200	1.72739600	2.24352900
H	7.60193700	0.61335200	-1.90037200
H	8.66557900	1.56999100	0.13153100
Cu	0.21603600	-0.39756700	0.27632100
C	-1.90832000	2.91559200	1.86406000
C	-1.63429800	1.69404300	1.24250700
C	-0.38209700	1.08966300	1.35435700
C	0.57042900	1.70661600	2.17671700
C	0.30072800	2.93483800	2.77850200
C	-0.93906700	3.57272400	2.62987300
H	-2.89725500	3.35524100	1.73712900
H	-2.41683600	1.24014000	0.63102900
H	1.54698800	1.24471200	2.34571000
H	1.07724800	3.40488900	3.38367800
C	-1.17203200	4.93437600	3.27991600
C	-0.16838800	5.93642000	2.69171400
H	-0.29278800	6.03537500	1.60572800
H	-0.31006200	6.92901900	3.13718800
H	0.86848100	5.63372500	2.88279800
C	-0.95361000	4.82824300	4.79457800
H	-1.10521700	5.80459400	5.27128700
H	-1.65570800	4.11885700	5.24934900
H	0.06219500	4.49673900	5.04042800
C	-2.58451300	5.45915200	3.02905200
H	-2.71039000	6.43581800	3.51013700
H	-2.78839400	5.59425900	1.95899600
H	-3.35048400	4.78973700	3.44026100
C	0.44239600	3.49074300	-1.01874800
H	1.38381000	3.56770300	-0.45860500
H	-0.35487300	3.52224400	-0.26405200
C	0.37939400	2.21216500	-1.80259000
C	1.49362400	1.69619900	-2.54005900
C	2.78590700	2.27385700	-2.44675600
C	1.32962600	0.61804500	-3.45486400
C	3.83738900	1.80801900	-3.21876200
H	2.96207200	3.10457400	-1.76744200
C	2.38619100	0.16172000	-4.22392500
H	0.35305100	0.15392000	-3.55950300
C	3.64962500	0.75050800	-4.11313900
H	4.81699200	2.27122300	-3.12074500
H	2.22323700	-0.65258100	-4.92845600
H	4.47682800	0.39815100	-4.72643100
C	-0.87071900	1.42610100	-1.76308300
O	-0.85327600	0.19632800	-1.51465800

N	-2.02195400	2.10017700	-1.98382300
H	-1.93213000	3.09326700	-2.17399300
C	-3.34107700	1.59040400	-1.90143800
C	-4.34512200	2.45365700	-1.45240800
C	-3.65589400	0.28236400	-2.28079500
C	-5.65832500	2.00503800	-1.36867400
H	-4.08922900	3.47330400	-1.16405200
C	-4.97303300	-0.15405100	-2.18436000
H	-2.87560700	-0.38661100	-2.63122400
C	-5.97650200	0.69773600	-1.72918400
H	-6.43381000	2.68058100	-1.01439400
H	-5.21423300	-1.17841200	-2.46557700
H	-7.00115800	0.34182300	-1.64916400
C	0.31791500	4.74846800	-1.85188200
F	0.40610300	5.84593000	-1.08850400
F	-0.89417600	4.79556000	-2.47999000
F	1.25027300	4.83146800	-2.80971600

TS4-R S**2 = 0.66

C	-2.23228500	-2.99270400	2.44184800
C	-2.08753200	-1.69437600	1.64410800
C	-0.27469400	-2.96178800	1.34964600
H	-3.13753500	-3.55863600	2.20023700
H	-2.18042500	-0.80366300	2.27981100
H	-2.16074100	-2.86944300	3.52777300
O	-1.08903200	-3.78870800	2.02451600
N	-0.70189000	-1.77037600	1.14245300
C	-3.05002200	-1.60330100	0.46074900
H	-2.74877300	-0.75245400	-0.16009100
H	-2.89591500	-2.48692200	-0.17581600
C	-4.48917900	-1.49363300	0.87098000
C	-5.38481300	-2.53478600	0.61073000
C	-4.96594400	-0.34791000	1.51808700
C	-6.72610400	-2.43346500	0.97235100
H	-5.02265700	-3.43103700	0.10186200
C	-6.30458300	-0.24192100	1.88084500
H	-4.28041000	0.47534200	1.72947300
C	-7.18915900	-1.28397400	1.60687600
H	-7.40980500	-3.25260400	0.75763100
H	-6.66149300	0.65844800	2.37780200
H	-8.23620400	-1.20045000	1.89080400
C	1.02078900	-3.61150700	0.95687900
C	0.68722500	-4.84572400	0.06301000
H	0.15409000	-5.57048400	0.68915700
H	1.64241900	-5.30228700	-0.22412200
C	1.76106600	-4.06380700	2.26181900
H	1.03022200	-4.59577300	2.88198500
H	2.52989300	-4.78727400	1.96930700
C	-0.13040400	-4.47725600	-1.14583500
C	-1.52007700	-4.63526500	-1.14023700
C	0.47376500	-3.91860700	-2.27869700
C	-2.28780100	-4.24133800	-2.23385600
H	-2.00257000	-5.07901100	-0.26764000
C	-0.29092800	-3.52906300	-3.37375300
H	1.55955900	-3.80417900	-2.31009900
C	-1.67505600	-3.68465800	-3.35296300
H	-3.36812400	-4.38079100	-2.21530600
H	0.19635700	-3.11712100	-4.25607300
H	-2.27224000	-3.38820400	-4.21348700
C	2.38713400	-2.90771100	2.99819100
C	3.77210900	-2.71046900	2.95496800
C	1.60339300	-1.96781400	3.67905000
C	4.35859100	-1.60150700	3.56022100

H	4.39472100	-3.44359500	2.44219200
C	2.18358700	-0.85260600	4.27757500
H	0.52619700	-2.11633900	3.76006900
C	3.56293400	-0.66281100	4.21409000
H	5.43860900	-1.46940100	3.51857000
H	1.55602200	-0.13548900	4.80357400
H	4.01793600	0.20426400	4.68943900
C	4.04338700	-2.27156700	-0.51797100
C	3.16423300	-1.01815000	-0.60881600
C	1.97137400	-2.71152300	0.21923000
H	4.88996700	-2.16613200	0.17045400
H	3.09783100	-0.66110400	-1.64169400
H	4.40480700	-2.63498600	-1.48551700
O	3.16548100	-3.28743900	0.02652100
N	1.83520300	-1.49830700	-0.18141700
C	3.56266100	0.12316000	0.32040000
H	2.84237100	0.94532900	0.15007100
H	3.38977400	-0.20461800	1.35859500
C	4.97300300	0.62874600	0.18729300
C	5.49289800	1.44818900	1.19673200
C	5.79374700	0.31582200	-0.90029400
C	6.78562600	1.95191600	1.11566200
H	4.86705400	1.68830200	2.05809200
C	7.09286000	0.81499800	-0.98307600
H	5.41700800	-0.31753600	-1.70458000
C	7.59157100	1.63606300	0.02271400
H	7.16938100	2.58873800	1.91024800
H	7.71671600	0.55640700	-1.83670900
H	8.60559700	2.02468800	-0.04029600
Cu	0.28118200	-0.25867400	0.18277100
C	-2.13899300	2.91595300	1.63381300
C	-1.73605400	1.71627800	1.03914500
C	-0.41693100	1.27490600	1.12862400
C	0.47857700	2.03019200	1.89487700
C	0.07411800	3.22872900	2.48018100
C	-1.23548400	3.71143400	2.34549700
H	-3.17601700	3.23052300	1.52002600
H	-2.47274100	1.15721000	0.45922500
H	1.51339700	1.70426500	2.03015400
H	0.80406300	3.80833900	3.04705300
C	-1.60484800	5.07251500	2.92984800
C	-0.74693000	6.14280400	2.23908600
H	-0.90546700	6.13988900	1.15245000
H	-1.00074100	7.14208100	2.61426700
H	0.32332500	5.98376500	2.41893900
C	-1.32027800	5.08808500	4.43687400
H	-1.56524200	6.06957100	4.86121500
H	-1.91963900	4.33527600	4.96329900
H	-0.26484400	4.88953100	4.65798500
C	-3.07749000	5.41397100	2.71063100
H	-3.30185900	6.39393600	3.14702700
H	-3.33312000	5.46586500	1.64464100
H	-3.74355200	4.68287700	3.18595100
C	0.31530300	3.04601200	-1.30675200
H	1.21149600	3.22220500	-0.69892300
H	-0.52723600	3.17957500	-0.61853400
C	0.31913500	1.65186500	-1.87512300
C	1.46096000	1.15254300	-2.59973600
C	2.71035800	1.82319000	-2.54776800
C	1.37090600	0.01180400	-3.44446700
C	3.78802700	1.39897000	-3.30653300
H	2.83491500	2.69497300	-1.91067500
C	2.45540800	-0.40322700	-4.19970800

H	0.43694700	-0.53851000	-3.50064100
C	3.67016900	0.28479800	-4.14124300
H	4.73030300	1.93862400	-3.24375400
H	2.35203100	-1.26734600	-4.85371900
H	4.51573300	-0.03952600	-4.74468700
C	-0.96029500	0.88855200	-1.95142800
O	-0.97589000	-0.34191800	-1.74497700
N	-2.08346600	1.59536100	-2.22184300
H	-1.97929800	2.59105500	-2.38185300
C	-3.41367700	1.10829000	-2.18402100
C	-4.41277100	1.99751100	-1.77514300
C	-3.74288400	-0.20259600	-2.54241100
C	-5.73422900	1.57195300	-1.70512200
H	-4.14558300	3.01870300	-1.50190100
C	-5.06788400	-0.61626000	-2.45583000
H	-2.96635300	-0.88977200	-2.86040300
C	-6.06600500	0.26092100	-2.03807300
H	-6.50496300	2.26712200	-1.37943100
H	-5.32085700	-1.64152700	-2.72234800
H	-7.09712200	-0.07747900	-1.96606800
C	0.23357100	4.18680400	-2.30292000
F	0.25609500	5.36204900	-1.65885800
F	-0.93551200	4.14127200	-3.00595700
F	1.22099600	4.18914700	-3.20666800

INT7-R

C	-2.58930200	1.03437500	3.06176900
C	-2.16562100	1.04345500	1.58907000
C	-0.64868700	-0.06800400	2.79855200
H	-3.52497800	0.49096900	3.24032900
H	-1.95206400	2.06320000	1.23605700
H	-2.65999700	2.02401900	3.52069600
O	-1.52729500	0.31556400	3.73838500
N	-0.89739300	0.29222300	1.59342600
C	-3.15850800	0.36657100	0.64639900
H	-2.73262200	0.41181000	-0.36705900
H	-3.21033400	-0.70091500	0.90482100
C	-4.52533300	0.98513500	0.65963100
C	-5.59206100	0.33611800	1.28636900
C	-4.75825900	2.22180500	0.04763900
C	-6.86527500	0.90079500	1.29410500
H	-5.42280200	-0.63808400	1.74972900
C	-6.02837600	2.78859800	0.05114700
H	-3.93312800	2.74037500	-0.44603600
C	-7.08607500	2.12724100	0.67391400
H	-7.68731300	0.37807500	1.77961100
H	-6.19635200	3.74750600	-0.43542400
H	-8.08039400	2.56882900	0.67474000
C	0.47884300	-0.87875800	3.35936000
C	-0.13111100	-2.13596600	4.05395000
H	-0.73593300	-1.77656600	4.89435300
H	0.70536500	-2.70532500	4.47471600
C	1.21472500	-0.02308900	4.44153800
H	0.46329900	0.26434900	5.18597400
H	1.93013900	-0.68660300	4.93979400
C	-0.95914500	-2.99182700	3.13743400
C	-2.34704000	-2.82755500	3.07243300
C	-0.36025800	-3.95698000	2.32113400
C	-3.11836000	-3.61809600	2.22560600
H	-2.82718800	-2.09186400	3.71970400
C	-1.12844600	-4.74869500	1.47292200
H	0.71869600	-4.10880900	2.37786200
C	-2.51066700	-4.58417400	1.42682200

H	-4.20003600	-3.49117300	2.20481600	C	-0.00968100	-0.72330200	-2.22719700
H	-0.64854900	-5.50984500	0.86009300	C	1.15504800	-1.63379000	-2.31192100
H	-3.11479800	-5.21876100	0.77966600	C	2.41082300	-1.13002900	-2.70366100
C	1.91223300	1.18769900	3.88812300	C	1.03782700	-3.02214600	-2.10285400
C	3.26976300	1.13735000	3.55628900	C	3.49353800	-1.97257300	-2.90152400
C	1.21560800	2.38304000	3.67481400	H	2.53728000	-0.05956200	-2.86161100
C	3.91794500	2.25288600	3.02943800	C	2.12292200	-3.86553900	-2.31234400
H	3.82791900	0.21722900	3.73585000	H	0.08807700	-3.44478700	-1.78774900
C	1.85907000	3.49914900	3.15000900	C	3.35291800	-3.34858000	-2.71366200
H	0.16200800	2.44507500	3.95155300	H	4.45540600	-1.55756400	-3.19627900
C	3.21345400	3.43701100	2.82771600	H	2.00052900	-4.93750300	-2.17052800
H	4.97999100	2.19963700	2.79342700	H	4.20256500	-4.00903200	-2.87595200
H	1.30437200	4.42388100	3.00057800	C	-1.27944600	-1.34104600	-1.73777600
H	3.72265400	4.31567000	2.43476800	O	-1.21838800	-1.87542200	-0.59496200
C	3.38505700	-2.42743600	1.86916400	N	-2.42699100	-1.19822900	-2.43133400
C	2.88669500	-1.65003500	0.64438100	H	-2.34378100	-0.83013000	-3.37143100
C	1.49898200	-1.31547400	2.34452500	C	-3.74579000	-1.51449900	-2.00921100
H	4.39913800	-2.15895300	2.18288300	C	-4.78395100	-0.73577900	-2.52726000
H	2.70854900	-2.31812400	-0.20672700	C	-4.01890200	-2.55910200	-1.12489200
H	3.31888000	-3.51702000	1.76650900	C	-6.09779000	-0.99810400	-2.15935800
O	2.48182000	-2.03285500	2.92503600	H	-4.55661000	0.08609600	-3.20651300
N	1.58807300	-1.08873800	1.08458400	C	-5.33994100	-2.80947000	-0.76528000
C	3.82090000	-0.52168200	0.23334700	H	-3.20908800	-3.15766900	-0.72132700
H	3.32572400	0.05465700	-0.56119100	C	-6.38043900	-2.03708000	-1.27607000
H	3.91375100	0.17526300	1.08277500	H	-6.89980400	-0.37965400	-2.55611200
C	5.18909700	-0.94301900	-0.23387300	H	-5.55637800	-3.63103700	-0.08383900
C	6.11725200	0.04921100	-0.57236300	H	-7.40838400	-2.24153100	-0.98502300
C	5.57211400	-2.27997700	-0.37417700	C	-0.12869700	-0.08188300	-4.72520300
C	7.38013700	-0.28168800	-1.04883300	F	-0.33629500	0.97891000	-5.51943500
H	5.83554500	1.09781100	-0.46277300	F	-1.15568000	-0.95343500	-4.94892900
C	6.83877900	-2.61726100	-0.84907800	F	0.98728600	-0.69127700	-5.13648700
H	4.86912500	-3.07995600	-0.13901300				
C	7.74569700	-1.61990400	-1.19053100				
H	8.08353500	0.50650100	-1.31010600	TS5-R			
H	7.11418800	-3.66535800	-0.95223400	Cu	0.25632100	0.13933900	-0.04143400
H	8.73394900	-1.88141600	-1.56242100	C	-2.27102600	-1.08558100	3.04407300
Cu	-0.01512700	-0.17092200	-0.19152300	C	-1.90500700	-0.27533900	1.96864300
C	-0.54668400	3.87734300	-1.21845900	C	-0.55878200	-0.04094300	1.70207300
C	-0.72902000	2.49671700	-1.10057700	C	0.41031500	-0.52206900	2.58708500
C	0.28822900	1.69429900	-0.59407200	C	0.03060300	-1.35707000	3.63581000
C	1.47835100	2.27906900	-0.17550800	C	-1.31444000	-1.66619900	3.88398300
C	1.65300100	3.65581500	-0.31746800	H	-3.33099400	-1.26536000	3.21194400
C	0.65455400	4.48486600	-0.84249800	H	-2.69039800	0.15131800	1.34445000
H	-1.36502100	4.47486800	-1.61664900	H	1.46674200	-0.28667200	2.44544000
H	-1.68465900	2.06753400	-1.41180200	H	0.80784600	-1.76890500	4.28008400
H	2.26354000	1.69086500	0.29805500	C	-1.67970200	-2.61398700	5.02254500
H	2.59736000	4.08966100	0.01356900	C	-1.11809300	-2.07988900	6.34634300
C	0.90539500	5.98626900	-0.97038600	H	-1.53793200	-1.09647500	6.58997400
C	2.10733900	6.21884700	-1.89543300	H	-1.36571000	-2.76316500	7.16769600
H	1.92032900	5.81912300	-2.89955900	H	-0.02642900	-1.98105500	6.32115000
H	2.31255400	7.29204600	-1.99368800	C	-1.06115500	-3.98758700	4.72460100
H	3.01705800	5.74256400	-1.51018300	H	-1.30466300	-4.69961400	5.52271800
C	1.21665300	6.56827500	0.41515700	H	-1.44324400	-4.39749100	3.78009800
H	1.40716700	7.64622700	0.34385000	H	0.03202500	-3.93511500	4.64931400
H	0.37738000	6.42097300	1.10682700	C	-3.19105900	-2.78444400	5.16780600
H	2.10658800	6.10675000	0.86158700	H	-3.41022200	-3.47141600	5.99289600
C	-0.30131300	6.72564700	-1.54542100	H	-3.69376400	-1.83499400	5.38986600
H	-0.08078700	7.79646000	-1.62159500	H	-3.64676500	-3.20748500	4.26263600
H	-0.55730800	6.37294400	-2.55229800	C	-0.65701100	2.58108600	2.28270400
H	-1.18971400	6.61971600	-0.90998800	H	0.14364000	2.28797700	2.96570700
C	-0.08615600	0.36737500	-3.27628000	H	-1.55272900	2.08992100	2.67157900
H	0.75950500	1.05704100	-3.19037100	C	-0.35819600	2.09919600	0.86673400
H	-0.97388600	0.98889800	-3.12379200	C	0.84982300	2.75610700	0.26703300
				C	1.88959100	3.21276400	1.10060300

C	0.94117000	3.05319400	-1.10905300	H	1.43395900	-3.76659600	-0.15786600
C	2.93929700	3.97252300	0.59536900	C	4.61447800	-3.79380100	1.02936900
H	1.87135200	3.00348500	2.16870700	H	6.38521100	-3.51240800	-0.16597500
C	1.99724300	3.80591300	-1.60719400	H	2.67862600	-4.06229100	1.94148600
H	0.17177200	2.70177000	-1.79057100	H	5.16452300	-3.94179000	1.95620600
C	2.99827400	4.28199300	-0.76148500	C	0.07509500	-0.52565600	-4.24581300
H	3.71555100	4.32723500	1.27039200	C	-1.28911600	-0.81097500	-4.35734100
H	2.02670000	4.03661800	-2.67155100	C	0.47919600	0.81399300	-4.23058300
H	3.81299500	4.88676400	-1.15294700	C	-2.22689500	0.21411900	-4.45210800
C	-1.53776100	2.01842900	-0.07729800	H	-1.61464400	-1.85262100	-4.38650400
O	-1.42494900	1.33342000	-1.10721800	C	-0.45582500	1.83995000	-4.33403900
N	-2.68311200	2.65605600	0.26598700	H	1.54279200	1.05299400	-4.16016600
H	-2.67056100	3.24113200	1.09250600	C	-1.81245000	1.54309800	-4.44108600
C	-3.91786500	2.68814900	-0.42519300	H	-3.28550900	-0.02756900	-4.54866400
C	-4.90065100	3.52810000	0.11186000	H	-0.12390000	2.87751000	-4.34414700
C	-4.19323400	1.92909900	-1.56879400	H	-2.54399500	2.34522200	-4.52043900
C	-6.14999500	3.61278800	-0.48643000	C	-1.42259600	-3.70066000	-1.38165800
H	-4.67776700	4.11895800	1.00108600	C	-1.55887600	-2.39471500	-0.59116800
C	-5.45189900	2.02866700	-2.15469900	C	0.25305000	-2.29838100	-1.87929100
H	-3.43310800	1.28711700	-1.99805800	H	-2.30279800	-3.94350500	-1.98480800
C	-6.43279200	2.86216500	-1.62556200	H	-1.55486500	-2.57007100	0.49325600
H	-6.90354700	4.27083900	-0.05993600	H	-1.14769500	-4.57193200	-0.77695300
H	-5.66270800	1.44019400	-3.04667400	O	-0.32049000	-3.44313300	-2.29021700
H	-7.41034700	2.92940300	-2.09694600	N	-0.32539700	-1.66025100	-0.92941600
C	-0.87422100	4.09283100	2.44123100	C	-2.78552200	-1.58694400	-0.99839900
F	-0.05128200	4.63219800	3.34528200	H	-2.69467800	-0.58247400	-0.56888800
F	-2.14996300	4.32598100	2.86355300	H	-2.74147400	-1.42230700	-2.08568600
F	-0.74116800	4.78505300	1.29393000	C	-4.09902000	-2.21812900	-0.62438400
C	4.08743900	0.49456800	-2.05188800	C	-5.18644100	-2.11794000	-1.49828600
C	3.30491000	0.64231000	-0.75670400	C	-4.28646400	-2.88586500	0.59204500
C	2.27195400	-0.80503400	-2.07880100	C	-6.42689500	-2.65395900	-1.16720400
H	5.14594200	0.25323500	-1.92176400	H	-5.05153800	-1.60566600	-2.45264300
H	3.12435100	1.69092700	-0.51671700	C	-5.52546800	-3.42700900	0.92553100
H	3.98508900	1.35618900	-2.72333800	H	-3.45795900	-2.98542200	1.29527800
O	3.45218900	-0.63919800	-2.69744800	C	-6.60032600	-3.31140000	0.04820100
N	2.02789300	-0.04032700	-1.07146000	H	-7.25891900	-2.56383400	-1.86282800
C	3.93783400	-0.07131400	0.44704800	H	-5.65041900	-3.94521900	1.87487900
H	3.21402800	-0.01843800	1.27389300	H	-7.56739100	-3.73647200	0.30815500
H	4.04854000	-1.13581600	0.19657000				
C	5.25544600	0.51718200	0.85927900	4a-R			
C	6.45626500	-0.00021900	0.36195800	C	3.71506100	0.52515600	0.55893200
C	5.31084500	1.61549200	1.72291800	C	2.37310700	0.86716000	0.69417700
C	7.67806800	0.57269100	0.70618300	C	1.35285100	-0.00188600	0.30167900
H	6.42717900	-0.87703400	-0.28757900	C	1.72983700	-1.22255200	-0.26600300
C	6.52867600	2.19077500	2.07119700	C	3.07173700	-1.55513700	-0.40598700
H	4.38224300	2.01214500	2.13537900	C	4.09899400	-0.69948400	0.00750000
C	7.71650000	1.67281000	1.55871300	H	4.46789700	1.23909200	0.88612000
H	8.60280500	0.15365100	0.31423500	H	2.12462700	1.85025100	1.09534000
H	6.55338600	3.04010700	2.75183700	H	0.97496700	-1.93639700	-0.58212700
H	8.67021700	2.11886600	1.83256700	H	3.32185000	-2.51993100	-0.84818300
C	1.49329700	-1.95490800	-2.65216200	C	5.55619100	-1.12192200	-0.15950200
C	2.45477100	-3.18892700	-2.66199800	C	5.84444300	-1.37711800	-1.64479600
H	3.17634100	-3.02928300	-3.47056800	H	5.68246800	-0.47096000	-2.24159600
H	1.85216900	-4.06184400	-2.93850800	H	6.88643500	-1.69339100	-1.78538400
C	1.07887800	-1.63676800	-4.12301700	H	5.20088600	-2.16471600	-2.05469200
H	2.00168600	-1.39589600	-4.66488600	C	5.80198700	-2.41489900	0.62931600
H	0.68351800	-2.56501200	-4.55330400	H	6.84301100	-2.74412200	0.51327300
C	3.19300200	-3.41715800	-1.36871000	H	5.61042700	-2.26907800	1.69952000
C	4.59029700	-3.35037700	-1.34345100	H	5.15519200	-3.23062400	0.28485100
C	2.52045900	-3.68120100	-0.16846400	C	6.52763800	-0.05616200	0.34469700
C	5.29726800	-3.55031800	-0.15982800	H	7.56086700	-0.39830700	0.20934400
H	5.12700800	-3.14229500	-2.26964200	H	6.41937400	0.88856500	-0.20289000
C	3.22260500	-3.85806000	1.02058000	H	6.38742900	0.15288300	1.41271400

C	-0.33176300	0.92967200	1.88399900
H	0.24494600	1.83531700	2.09416500
H	0.05499300	0.14657300	2.54436900
C	-0.10668400	0.46760700	0.42167200
C	-0.27364400	1.57489700	-0.62289100
C	-0.41701100	2.92884600	-0.30944200
C	-0.18173100	1.22167800	-1.97863900
C	-0.48148900	3.89396400	-1.31312700
H	-0.49412800	3.25069000	0.72590000
C	-0.25637600	2.17984400	-2.98135800
H	-0.04033000	0.17321200	-2.24431400
C	-0.40639600	3.52581300	-2.65142400
H	-0.59547600	4.94136800	-1.03962700
H	-0.18649000	1.87491200	-4.02390000
H	-0.45992000	4.28081100	-3.43330200
C	-1.08588500	-0.72652400	0.25295400
O	-0.87045200	-1.78218000	0.83089300
N	-2.21408300	-0.45899800	-0.47044800
H	-2.27134400	0.46510000	-0.88107200
C	-3.36982400	-1.24627900	-0.61379500
C	-4.38847400	-0.73125700	-1.42611700
C	-3.54543400	-2.48555400	0.01352900
C	-5.56797600	-1.43970100	-1.60964500
H	-4.24910500	0.23438300	-1.91310400
C	-4.73422100	-3.18196300	-0.18201000
H	-2.75915300	-2.88492600	0.64185000
C	-5.74858500	-2.67309100	-0.98810600
H	-6.34889300	-1.02250400	-2.24279400
H	-4.86430500	-4.14368500	0.31137300
H	-6.67168600	-3.23087200	-1.13111300
C	-1.75566100	1.18959200	2.32660600
F	-1.75668100	1.86757000	3.49300100
F	-2.44866600	0.05374500	2.52774700
F	-2.46759500	1.92563800	1.44124600

TS9 S**2 = 0.75

C	-1.61696400	-0.83914300	-0.86585800
H	-1.87124600	-1.90552800	-0.87045400
H	-1.40026900	-0.56290600	-1.90720100
C	-0.41314400	-0.61371600	0.01683200
C	0.02123100	0.76248200	0.30524400
C	0.52820700	1.12403500	1.56461100
C	0.03896400	1.73220400	-0.71331000
C	1.01963100	2.40299200	1.79883700
H	0.51161900	0.40145400	2.37966600
C	0.53355800	3.00666700	-0.47910200
H	-0.33687300	1.47759600	-1.70286000
C	1.02822800	3.34998800	0.77866000
H	1.39304600	2.66168600	2.78814700
H	0.53586700	3.73849200	-1.28503400
H	1.41368900	4.35117400	0.96163300
C	-0.28383600	-1.59774400	1.16758700
O	-1.17545200	-1.93399900	1.92265600
N	1.02011100	-2.07077100	1.25498700
H	1.32468300	-2.52611200	2.10563300
C	1.87781000	-1.62217600	0.25003400
C	3.14316700	-1.10484700	0.42388200
C	1.14127800	-1.45343800	-0.97408700
C	3.74673100	-0.41229400	-0.63798600
H	3.64299500	-1.18854900	1.38773300
C	1.78221100	-0.73055600	-2.02430600
H	0.48889100	-2.28287100	-1.26451200
C	3.04708800	-0.20216300	-1.83501600

H	4.74916300	-0.00854200	-0.51544200
H	1.27961800	-0.62427000	-2.98482500
H	3.52607400	0.34904900	-2.64233700
C	-2.88372700	-0.09663400	-0.48511500
F	-3.93785800	-0.62585100	-1.14679700
F	-2.82791200	1.20816800	-0.82827500
F	-3.15167600	-0.15423000	0.82376800

INT10 S**2 = 0.75

C	-1.19632700	-1.27744300	-0.86838200
H	-1.22606600	-2.36201900	-0.71263300
H	-0.99524200	-1.11952100	-1.93597900
C	-0.05880100	-0.68553400	-0.02516500
C	-0.18634900	0.81383400	0.22987800
C	-0.24710300	1.34470600	1.52108200
C	-0.22835100	1.70107600	-0.85205500
C	-0.32671300	2.72007300	1.72571000
H	-0.25481800	0.68112900	2.38383200
C	-0.30869600	3.07362000	-0.65082400
H	-0.22435900	1.31426200	-1.86891700
C	-0.35086700	3.59032200	0.64167300
H	-0.37657000	3.10846200	2.74133400
H	-0.34362300	3.74157400	-1.50952800
H	-0.41355600	4.66520200	0.80091800
C	0.08900400	-1.43591200	1.32046900
O	-0.78233000	-1.86437000	2.04800600
N	1.44909300	-1.51016000	1.58063300
H	1.79236400	-1.82422400	2.47913900
C	2.23524400	-1.07592300	0.53007400
C	3.54401200	-0.69026700	0.51658300
C	1.33447000	-1.04030900	-0.66453200
C	4.07308900	-0.13682200	-0.67178700
H	4.15656100	-0.76443300	1.41373500
C	1.91472500	-0.27182900	-1.79851300
H	1.20040200	-2.09835900	-0.99174600
C	3.23510700	0.09034000	-1.78830700
H	5.11620000	0.16758200	-0.70487000
H	1.30878700	-0.11672400	-2.69012500
H	3.65742700	0.57472300	-2.66755800
C	-2.59868100	-0.76094500	-0.62528300
F	-3.49668100	-1.64300400	-1.11921500
F	-2.82202100	0.40963000	-1.26311000
F	-2.88408600	-0.57057000	0.66790100

TS9' S**2 = 0.75

C	1.69036600	-0.61094000	1.07472600
C	0.45152300	-0.47990600	0.22255700
C	0.14785300	0.80611300	-0.42232900
C	-0.46156900	0.86733900	-1.68744200
C	0.35369700	2.01535500	0.26624200
C	-0.83895800	2.08426600	-2.24278200
H	-0.61614400	-0.04895300	-2.25693400
C	-0.02616300	3.22843100	-0.28844200
H	0.81549500	1.99904800	1.25186600
C	-0.62713800	3.27072300	-1.54599400
H	-1.29655500	2.10469600	-3.23034900
H	0.14506200	4.14945100	0.26611500
H	-0.92337600	4.22354100	-1.98053300
C	0.10866600	-1.71511200	-0.58460000
O	0.89499700	-2.36244300	-1.25313500
N	-1.24899800	-2.02014500	-0.49371300
C	-1.94929900	-1.19699200	0.38913700
C	-3.16957400	-0.60467300	0.14066100

C	-1.11009800	-0.79457300	1.48456200
C	-3.60499400	0.43250600	0.98079400
H	-3.75838700	-0.90048700	-0.72619600
C	-1.58208600	0.26909000	2.30818200
H	-0.52968200	-1.58434100	1.97118000
C	-2.79152900	0.88302900	2.02972400
H	-4.56611800	0.90678700	0.79542600
H	-0.99763900	0.57351900	3.17554800
H	-3.14030700	1.69612900	2.66394600
C	-1.87886200	-2.87857800	-1.46702400
H	-2.40873400	-2.29297400	-2.23266000
H	-1.09105000	-3.46131400	-1.94957700
H	-2.59290800	-3.54930000	-0.97897600
C	3.00086500	-0.19106700	0.43649700
F	3.13433800	1.15202700	0.38784000
F	3.14791000	-0.65197500	-0.80992000
F	4.03498400	-0.65586600	1.17413400
H	1.59726200	-0.02563500	2.00015300
H	1.81478600	-1.65736900	1.37678100

INT10' S**2 = 0.75

C	-1.28912700	1.00930500	1.21340900
H	-1.18539400	2.08709500	1.38355300
H	-1.24035700	0.53073400	2.20015900
C	-0.12273800	0.53187100	0.33738800
C	-0.37132900	-0.79939100	-0.36742300
C	-0.28466100	-0.93266800	-1.75599400
C	-0.66823400	-1.93952800	0.38848000
C	-0.47300500	-2.16911500	-2.36880100
H	-0.09019000	-0.06004900	-2.37764200
C	-0.85813500	-3.17403100	-0.22048800
H	-0.77796800	-1.85849600	1.46791100
C	-0.75455600	-3.29554500	-1.60385500
H	-0.40493500	-2.24579800	-3.45248200
H	-1.09266900	-4.04406300	0.39009400
H	-0.90302300	-4.26184100	-2.08227100
C	0.27276200	1.60153400	-0.70220700
O	-0.45449300	2.32553400	-1.35359200
N	1.65805700	1.56841700	-0.81914200
C	2.24223000	0.74482600	0.12369000
C	3.49732500	0.20664500	0.13333900
C	1.20766200	0.48796900	1.17162200
C	3.81778900	-0.73912100	1.13415200
H	4.21938600	0.46216300	-0.64073100
C	1.56090900	-0.65592500	2.05571500
H	1.14833300	1.40826000	1.79903800
C	2.82888000	-1.17329800	2.04770600
H	4.81296600	-1.17587300	1.16351300
H	0.83633300	-0.98736400	2.79830600
H	3.08743800	-1.94980800	2.76632400
C	-2.69632000	0.77814900	0.70434500
F	-3.55121800	1.60920700	1.34213800
F	-3.12311600	-0.47862700	0.96123500
F	-2.83317500	0.98334500	-0.61057500
C	2.35769900	2.23128400	-1.88962100
H	3.16353500	2.85901300	-1.49339700
H	2.78861400	1.49744800	-2.58330800
H	1.63215500	2.85229800	-2.42025100

INT11

C	-4.13933300	0.22810500	2.04393100
C	-2.99639400	0.81818600	1.21788500
C	-2.84601600	-1.41304400	1.21980600

H	-5.13371900	0.52424200	1.69454400
H	-2.39086700	1.52498500	1.79828000
H	-4.06291400	0.41110300	3.12042000
O	-4.01241800	-1.20782600	1.84402300
N	-2.17147400	-0.36460700	0.90271400
C	-3.44103000	1.44715600	-0.09878000
H	-2.53507400	1.66294700	-0.68379700
H	-3.98715700	0.68582100	-0.67559200
C	-4.28384000	2.67678800	0.07142500
C	-5.59199600	2.71017400	-0.41923000
C	-3.78369400	3.80931500	0.72502900
C	-6.38322700	3.84653100	-0.26925100
H	-5.98751100	1.83190700	-0.93404900
C	-4.57207500	4.94525500	0.87847300
H	-2.76429800	3.80015000	1.11628700
C	-5.87388700	4.96709900	0.38083600
H	-7.39878900	3.85609700	-0.66010600
H	-4.16952500	5.81888800	1.38773200
H	-6.48943300	5.85607500	0.50076900
C	-2.53073600	-2.86195400	1.01113500
C	-3.75880300	-3.55020000	0.34185900
H	-4.59622400	-3.45739900	1.04271100
H	-3.51713200	-4.61646200	0.26989100
C	-2.30973000	-3.53717300	2.40799900
H	-3.19477600	-3.29997400	3.01195600
H	-2.31846000	-4.61993700	2.23795600
C	-4.14571600	-3.01662900	-1.01105300
C	-5.06478500	-1.96820300	-1.13992600
C	-3.63105200	-3.59926400	-2.17503900
C	-5.46874000	-1.52503800	-2.39675800
H	-5.49888900	-1.52346600	-0.24358400
C	-4.03951300	-3.16359600	-3.43314300
H	-2.93832900	-4.43704100	-2.08846500
C	-4.96361200	-2.12682000	-3.54708600
H	-6.20150400	-0.72325500	-2.47757800
H	-3.64940000	-3.64721300	-4.32665400
H	-5.29346800	-1.79384400	-4.52943100
C	-1.04542000	-3.13724900	3.11485800
C	0.02838600	-4.03029900	3.19536400
C	-0.91214600	-1.87720900	3.71154600
C	1.20009300	-3.67835300	3.86177400
H	-0.06320300	-5.01824600	2.74083600
C	0.26345200	-1.51732200	4.36390300
H	-1.74863500	-1.17693000	3.69300700
C	1.32439900	-2.41770100	4.43993200
H	2.01506300	-4.39579900	3.94035200
H	0.34395200	-0.53552400	4.82750900
H	2.23745600	-2.14457900	4.96467300
C	0.12081600	-4.45278600	-0.88404900
C	0.70554400	-3.04027700	-0.79675900
C	-1.29792700	-3.09511600	0.18566500
H	0.76889300	-5.22817600	-0.46609500
H	0.96083600	-2.64212900	-1.78604100
H	-0.19693600	-4.74420100	-1.89102100
O	-1.07578600	-4.39063200	-0.05955200
N	-0.42192700	-2.25567700	-0.24366400
C	1.92362600	-2.93808200	0.13229300
H	2.31874400	-1.91836100	0.04923900
H	1.58086400	-3.06551600	1.16975100
C	2.97803900	-3.96345700	-0.18577900
C	3.39074000	-4.87323500	0.79153400
C	3.53294500	-4.06478100	-1.46720800
C	4.34671400	-5.84590600	0.50923900

H	2.95555400	-4.80830400	1.78992700
C	4.48462700	-5.03786300	-1.75421200
H	3.22899500	-3.36632900	-2.24569400
C	4.89648600	-5.93029100	-0.76640300
H	4.65977000	-6.54003100	1.28683500
H	4.91016900	-5.09781200	-2.75408200
H	5.64271500	-6.68923000	-0.99173000
Cu	-0.34875100	-0.24031100	0.10165400
C	0.39457800	3.77255600	1.38827100
C	-0.17939000	2.69252500	0.70795900
C	0.18025200	1.39274000	1.03840300
C	1.09488300	1.17205300	2.06784000
C	1.65953000	2.25762000	2.73770500
C	1.33211700	3.57921900	2.40669500
H	0.09443900	4.78016400	1.10380200
H	-0.89574700	2.89577200	-0.09155400
H	1.38832100	0.15954400	2.35426400
H	2.38049600	2.06204400	3.53326500
C	2.01493600	4.73336800	3.13847400
C	3.52131500	4.67559700	2.84889800
H	3.71910700	4.78839800	1.77517000
H	4.04655700	5.48304900	3.37428000
H	3.96297600	3.72560600	3.17551800
C	1.78290400	4.59778200	4.64876300
H	2.27425600	5.41871500	5.18541600
H	0.71374700	4.63037100	4.89167700
H	2.18731200	3.65892400	5.04528900
C	1.48804300	6.09506800	2.68911400
H	1.99638200	6.89254700	3.24307300
H	1.66761700	6.27433900	1.62165900
H	0.41204400	6.20055200	2.87655200
C	3.72208500	0.72600200	-0.13878300
H	3.01249600	0.16040800	0.47003600
H	4.28966100	1.37193400	0.54142700
C	2.99245200	1.50456400	-1.18696400
C	3.67080800	2.57184500	-1.89659800
C	4.70086200	3.30827200	-1.26624200
C	3.36806800	2.90645800	-3.23876600
C	5.34958000	4.34404000	-1.91828200
H	4.97899000	3.07942500	-0.24031800
C	4.03430300	3.93170500	-3.89257900
H	2.64220200	2.31014800	-3.78684100
C	5.01990400	4.66655100	-3.23470400
H	6.12426000	4.90293300	-1.39771800
H	3.79495500	4.14793900	-4.93161600
H	5.53858100	5.47275600	-3.74840400
C	1.67836900	1.08117200	-1.46116400
O	1.24907200	-0.05120600	-1.02005600
N	0.82292200	1.90382900	-2.16614900
H	1.11533000	2.87215700	-2.22849800
C	-0.49183400	1.65290400	-2.56095000
C	-1.32170100	2.76191600	-2.79909500
C	-1.00461800	0.36049500	-2.77346200
C	-2.62613800	2.58679400	-3.24421600
H	-0.92867800	3.76666000	-2.64004900
C	-2.31854700	0.20297000	-3.20442200
H	-0.36612100	-0.50792000	-2.64837500
C	-3.13619100	1.30491000	-3.44293000
H	-3.25021200	3.46054900	-3.42126700
H	-2.70103700	-0.80356400	-3.36541400
H	-4.16162000	1.16546300	-3.78083500
C	4.69953100	-0.26744400	-0.73145600
F	5.17740000	-1.09407800	0.21561200

F	5.74671300	0.33991000	-1.31553800
F	4.10292400	-1.03033100	-1.67349500

TS10

C	-4.39219900	-0.98159800	0.49801000
C	-3.20658500	-0.13816400	0.00377400
C	-2.49697400	-2.18340300	0.58096600
H	-5.15213300	-1.16668100	-0.27029800
H	-3.01161300	0.70646600	0.68419400
H	-4.87709600	-0.59127800	1.39897400
O	-3.81091500	-2.26593500	0.84615700
N	-2.06996400	-1.06688800	0.11579100
C	-3.31153300	0.38107600	-1.42677900
H	-2.28910800	0.55796100	-1.79589700
H	-3.70444700	-0.42630500	-2.06902100
C	-4.11860200	1.64170600	-1.57951200
C	-3.80162000	2.54494300	-2.59996900
C	-5.17462000	1.96093800	-0.72095300
C	-4.51726300	3.72712900	-2.76064600
H	-2.97139100	2.31172900	-3.26871900
C	-5.89507200	3.14350800	-0.87658700
H	-5.44812500	1.28580100	0.09097400
C	-5.56807700	4.03182000	-1.89706800
H	-4.25199300	4.41613500	-3.56032200
H	-6.71104000	3.37164100	-0.19263100
H	-6.12738400	4.95691700	-2.01840000
C	-1.74330800	-3.43614300	0.92422800
C	-2.38942500	-4.64279200	0.17832200
H	-3.44096700	-4.68285600	0.48488300
H	-1.90598500	-5.54959500	0.55837300
C	-1.88931900	-3.67812400	2.46195300
H	-2.95194200	-3.86788000	2.65327100
H	-1.34832100	-4.60455600	2.68899100
C	-2.27481500	-4.57158100	-1.31855400
C	-3.21933500	-3.86857800	-2.07455400
C	-1.22166500	-5.20710800	-1.98559700
C	-3.11990700	-3.80994500	-3.46135300
H	-4.06245800	-3.39559700	-1.56881900
C	-1.11770100	-5.14785200	-3.37338600
H	-0.49876900	-5.78385500	-1.40834100
C	-2.06764500	-4.44855700	-4.11481600
H	-3.87641200	-3.27715400	-4.03576400
H	-0.30429700	-5.66499400	-3.87874700
H	-1.99584900	-4.41380200	-5.20032100
C	-1.39412800	-2.54566800	3.31546900
C	-0.03953100	-2.44399300	3.65026500
C	-2.27690200	-1.57155400	3.79446500
C	0.42392100	-1.40124500	4.44821200
H	0.65217100	-3.21599900	3.30759800
C	-1.82016500	-0.53542600	4.60453200
H	-3.33902000	-1.65255400	3.55915500
C	-0.46882600	-0.44642000	4.93263200
H	1.47886000	-1.34648400	4.71130400
H	-2.52627100	0.19450600	4.99773700
H	-0.11267600	0.35663900	5.57555600
C	1.72261900	-4.37189400	0.36817900
C	1.82457400	-2.87707900	0.04143600
C	-0.27910600	-3.38161200	0.58120000
H	2.38180600	-4.69327800	1.18103100
H	2.17424800	-2.72644200	-0.99029000
H	1.86763700	-5.03124600	-0.49341900
O	0.35202500	-4.54425200	0.81604200
N	0.42927600	-2.40953400	0.13195000

C	2.72719300	-2.08465100	0.98994200	H	1.45247300	-0.96391000	-1.92765900
H	2.54467200	-1.01495900	0.82545800	C	-1.13778500	-0.94559500	-4.14026300
H	2.42262300	-2.30132100	2.02455800	H	-1.82594100	0.80472300	-5.19563400
C	4.17510100	-2.42061400	0.77518700	H	-0.20949400	-2.49760100	-2.96384900
C	4.83642200	-3.34298300	1.58980700	H	-1.82136600	-1.62467800	-4.64299000
C	4.87343600	-1.84586900	-0.29236000	C	4.16739500	2.08761200	1.68464700
C	6.16347100	-3.68819800	1.34340900	F	4.16969300	2.28689400	3.01806400
H	4.31133500	-3.78039800	2.44100900	F	5.33576200	2.54261300	1.20205100
C	6.19785700	-2.18687600	-0.54150600	F	4.14310600	0.75241900	1.48142600
H	4.37427700	-1.09935300	-0.91491700				
C	6.84498900	-3.11324800	0.27489900	6a			
H	6.66717100	-4.40178900	1.99239300	C	-2.96893700	-0.90022600	1.35255500
H	6.73162200	-1.72171600	-1.36786500	C	-1.63370600	-0.79229600	0.97017900
H	7.88281600	-3.37761300	0.08364700	C	-1.32205400	-0.63142700	-0.37326700
Cu	-0.18080200	-0.43747000	-0.15368100	C	-2.32951200	-0.58251300	-1.33087200
C	-1.89456700	3.27914100	0.41964900	C	-3.65253300	-0.69970100	-0.92882400
C	-0.99494200	2.43713900	-0.24125200	C	-4.00744000	-0.85761400	0.41835200
C	-0.36076900	1.46104800	0.51148900	H	-3.19132400	-1.02584600	2.40985700
C	-0.45086200	1.39986100	1.89678500	H	-0.83724000	-0.83642100	1.71089000
C	-1.36364900	2.24474200	2.51890100	H	-2.06301100	-0.45595900	-2.37783400
C	-2.10822600	3.19513600	1.80038000	H	-4.43201700	-0.66114400	-1.68974200
H	-2.45192700	3.99500300	-0.18178600	C	-5.48040800	-0.97563300	0.80378600
H	-0.88056200	2.49986700	-1.32203400	C	-6.09567600	-2.19157900	0.09848800
H	0.13019900	0.67863500	2.47291900	H	-5.59050700	-3.11937400	0.39415300
H	-1.48497000	2.15968100	3.59849900	H	-7.15889300	-2.28839400	0.35500300
C	-3.14766800	4.04415200	2.52650900	H	-6.02490600	-2.10833200	-0.99270100
C	-2.53183800	4.70152800	3.76765400	C	-6.22541800	0.29098800	0.36216400
H	-1.69214200	5.35335500	3.49858900	H	-7.28996800	0.22192400	0.62226400
H	-3.28185400	5.31585700	4.28002900	H	-5.81447000	1.18324200	0.85024800
H	-2.16574300	3.96675700	4.49424500	H	-6.15879200	0.44550500	-0.72148200
C	-4.29092100	3.11147400	2.95672100	C	-5.67090600	-1.14592900	2.30998000
H	-5.06092100	3.66807500	3.50564600	H	-6.73928200	-1.22693000	2.54428400
H	-4.76734300	2.65089700	2.08004600	H	-5.18236500	-2.05434700	2.68447900
H	-3.93071700	2.30438000	3.60902100	H	-5.27477600	-0.29083900	2.87209900
C	-3.72316900	5.14185000	1.63297400	C	2.12052100	-2.17636100	-0.06280900
H	-4.44448100	5.74159100	2.19994100	H	1.11593800	-2.58333500	-0.21384300
H	-2.94300600	5.82244100	1.26961300	H	2.59167300	-2.75869200	0.73891600
H	-4.25207100	4.73140700	0.76363600	C	2.06469300	-0.71411700	0.27058700
C	2.98033800	2.77281900	1.04821800	C	3.22741900	-0.07075300	0.90805800
H	2.08601400	2.39756400	1.55494800	C	3.96176500	-0.72774600	1.90849900
H	3.06874800	3.83605700	1.30138500	C	3.65856900	1.21133800	0.52105400
C	2.87900600	2.57420400	-0.43470500	C	5.06311700	-0.12685400	2.50732000
C	3.75863200	3.33106700	-1.33182000	H	3.65930000	-1.72250400	2.23392400
C	4.18455600	4.63141900	-1.00058700	C	4.75882600	1.81213800	1.12057900
C	4.23716700	2.78273100	-2.53927400	H	3.13563100	1.72543800	-0.28492500
C	5.01700200	5.35481200	-1.84423900	C	5.46673300	1.14841200	2.12057700
H	3.84857600	5.09405900	-0.07467400	H	5.60910800	-0.66019100	3.28378000
C	5.07635700	3.50490700	-3.37733600	H	5.07520200	2.80041500	0.79090600
H	3.97202100	1.75966900	-2.80088600	H	6.33150100	1.61685200	2.58635800
C	5.46680500	4.79903500	-3.03949300	C	0.94014900	-0.01636900	-0.03026900
H	5.31905600	6.36164600	-1.56292900	O	-0.01323600	-0.58536900	-0.83500400
H	5.44090000	3.04645700	-4.29468300	N	0.63054300	1.23665700	0.46551700
H	6.12511200	5.36417800	-3.69548500	H	1.16748900	1.50261700	1.28146600
C	1.93862800	1.68038200	-0.89620700	C	0.06509500	2.30129500	-0.25173800
O	1.37797600	0.82635300	-0.04672400	C	-0.29117300	3.45544400	0.45809400
N	1.49141900	1.70295600	-2.21248700	C	-0.14112700	2.25736100	-1.63653100
H	1.66002000	2.57737100	-2.69603200	C	-0.84583200	4.54279200	-0.20314800
C	0.63030300	0.80864600	-2.83767600	H	-0.13424000	3.48809400	1.53608800
C	-0.28319800	1.29091000	-3.78853500	C	-0.71137400	3.34920300	-2.28266900
C	0.66202800	-0.57086900	-2.56565000	H	0.15186200	1.37694100	-2.20162000
C	-1.13913300	0.41489700	-4.44602300	C	-1.06709200	4.49619200	-1.57826000
H	-0.30324300	2.35704300	-4.01734500	H	-1.11317800	5.43199400	0.36517200
C	-0.23523300	-1.43239100	-3.19837800	H	-0.86536000	3.30220300	-3.35950100

H	-1.50845200	5.34575100	-2.09449700
C	2.90756300	-2.46599700	-1.31905000
F	2.91723400	-3.79053800	-1.58423900
F	4.19248600	-2.07196000	-1.21002400
F	2.38868000	-1.84445700	-2.39455300

INT4'' S2 = 0.75**

C	1.77018400	-1.05034000	0.97517500
H	1.51800300	-2.06255000	1.30282900
H	2.19858100	-0.50988600	1.82818600
C	0.54041300	-0.38284900	0.43904100
C	0.54218400	1.02652200	0.13603400
C	-0.30770900	1.57433300	-0.85709800
C	1.42447100	1.91804700	0.79270300
C	-0.29049200	2.92748400	-1.15098600
H	-0.96360800	0.91457500	-1.41942800
C	1.42527200	3.27315900	0.50611900
H	2.10728900	1.53863800	1.54941200
C	0.56700400	3.78937500	-0.46556000
H	-0.94479300	3.31435000	-1.92975600
H	2.10381100	3.93447600	1.04149100
H	0.57528900	4.85304200	-0.69530400
C	-0.56021000	-1.30676400	0.12374700
O	-0.29781500	-2.49798400	-0.08391100
C	2.87621700	-1.19612400	-0.04865000
F	3.89673900	-1.91607000	0.46059700
F	3.38372900	-0.00113000	-0.42256200
F	2.45252700	-1.81419400	-1.16082100
C	-1.98369100	-0.86334100	0.12153700
C	-2.90312600	-1.60808600	-0.62689300
C	-2.44829100	0.19313800	0.91576300
C	-4.25285900	-1.28089400	-0.61257800
H	-2.53156500	-2.44672800	-1.21207300
C	-3.80276200	0.50542000	0.94752700
H	-1.74581500	0.76309000	1.52178300
C	-4.70556600	-0.22320600	0.17544800
H	-4.95762800	-1.85613500	-1.21025900
H	-4.15567300	1.31963200	1.57769700
H	-5.76455100	0.02865700	0.19379700

INT11''

C	3.31287300	-2.62543100	1.42445300
C	1.90052100	-2.28373200	0.94722600
C	3.20661400	-0.47012600	0.80142200
H	3.78145800	-3.44496800	0.86985000
H	1.14360300	-2.50028600	1.71150000
H	3.39041300	-2.82166100	2.49807700
O	4.08219400	-1.41675200	1.15426900
N	1.97146800	-0.82379600	0.74798900
C	1.50956200	-2.92689100	-0.38490700
H	0.55697300	-2.47481200	-0.70484300
H	2.25563800	-2.63244600	-1.13885400
C	1.39347900	-4.42014800	-0.31223800
C	2.34949700	-5.23980900	-0.91766100
C	0.33424100	-5.01787600	0.38014300
C	2.25452800	-6.62719200	-0.83490700
H	3.17025800	-4.77913700	-1.47228600
C	0.23706300	-6.40280600	0.46500800
H	-0.42252600	-4.38537700	0.84961500
C	1.19804100	-7.21067800	-0.14145000
H	3.00446300	-7.25244900	-1.31536900
H	-0.59350800	-6.85605100	1.00286800
H	1.12002500	-8.29383300	-0.07625800

C	3.82497800	0.87267800	0.55397000
C	5.06340800	0.70469200	-0.37679000
H	5.77788700	0.06939100	0.15850800
H	5.52162000	1.69631900	-0.46747600
C	4.32842300	1.43935200	1.92393300
H	5.09900700	0.74642800	2.28322900
H	4.82517300	2.39244400	1.70736000
C	4.78319300	0.13506000	-1.74141600
C	4.87262900	-1.24204600	-1.97893900
C	4.48594400	0.98008900	-2.81687700
C	4.69543300	-1.75713500	-3.26050800
H	5.12824200	-1.91063200	-1.15629800
C	4.31286200	0.46877600	-4.10033100
H	4.44386700	2.05740900	-2.65143800
C	4.42717300	-0.90152200	-4.32678100
H	4.79303600	-2.82814700	-3.43175700
H	4.11185900	1.14388400	-4.92987000
H	4.31267700	-1.30032800	-5.33299700
C	3.25386600	1.61637000	2.95794700
C	2.51819500	2.80411500	3.02924600
C	2.96183800	0.59223400	3.86553100
C	1.51610300	2.96591000	3.98287800
H	2.75646300	3.62132100	2.34534800
C	1.96705700	0.75302500	4.82606500
H	3.54497000	-0.32972600	3.83484300
C	1.24026300	1.94073900	4.88550400
H	0.96063000	3.90109000	4.03273200
H	1.76297100	-0.04823600	5.53413900
H	0.46738900	2.07210500	5.64030800
C	2.40200100	3.87009700	-0.93440200
C	1.11944200	3.04110300	-0.79852600
C	2.87110600	1.86124300	-0.05839600
H	2.36652100	4.82853200	-0.40714000
H	0.61237900	2.91426700	-1.76325500
H	2.72270800	4.03776000	-1.96737900
O	3.42653100	3.05436000	-0.29652000
N	1.62712400	1.72638100	-0.35620200
C	0.12287600	3.60412200	0.22460200
H	-0.75395000	2.94440900	0.24577300
H	0.58783900	3.55935300	1.22022600
C	-0.26889200	5.01705600	-0.10523800
C	0.17150900	6.08250800	0.68523100
C	-1.03916000	5.29699400	-1.23966800
C	-0.15604000	7.39694200	0.36064100
H	0.77004500	5.87521700	1.57504400
C	-1.36634200	6.60856000	-1.56754500
H	-1.40091300	4.47599700	-1.85872100
C	-0.92537900	7.66201800	-0.76847200
H	0.18840500	8.21349900	0.99215200
H	-1.97414600	6.80991300	-2.44747800
H	-1.18502100	8.68707400	-1.02419800
Cu	0.38564300	0.20640400	0.15690000
C	-2.51235600	-2.32582000	1.99829700
C	-1.70742300	-1.76260700	0.99981600
C	-0.82766200	-0.74929800	1.32877300
C	-0.72749900	-0.29066600	2.63889800
C	-1.55102500	-0.84856800	3.61647300
C	-2.45783900	-1.87569900	3.32010000
H	-3.19068300	-3.13069500	1.72003200
H	-1.79920200	-2.12940000	-0.02384500
H	-0.03244800	0.50447500	2.91448000
H	-1.48371100	-0.46012000	4.63407100
C	-3.34076400	-2.44676800	4.42848600

C	-4.22316400	-1.32485800	4.99227000	H	4.95891400	-2.10383400	-0.01327300
H	-4.87009000	-0.89869600	4.21541800	C	6.79715300	0.62841100	0.80423800
H	-4.86691200	-1.71015900	5.79264500	H	6.11852100	2.25053900	2.05129500
H	-3.62604200	-0.50722800	5.41356400	H	7.17955100	-1.12352900	-0.39228700
C	-2.45363400	-3.00437600	5.54938100	H	7.77884200	1.06333900	0.62951100
H	-3.07196500	-3.41002300	6.35959700	C	-0.82570700	-3.85072700	0.45743700
H	-1.80819800	-3.81220900	5.18268600	C	-0.97924700	-4.76736300	1.70709900
H	-1.80851300	-2.23124600	5.98402200	H	-0.20580500	-5.54071000	1.63089100
C	-4.24606700	-3.56918200	3.92429400	H	-1.94835800	-5.27083600	1.61473000
H	-4.85813900	-3.95215800	4.74876000	C	-0.96031800	-4.73977200	-0.82404000
H	-4.93308000	-3.22339400	3.14172000	H	-0.20510400	-5.53015900	-0.74217200
H	-3.67060200	-4.41370500	3.52451900	H	-1.94363200	-5.22146800	-0.77399600
C	-3.73867700	0.76823900	-0.08823200	C	-0.88189000	-4.05471600	3.02800200
H	-2.94705200	0.83289400	0.66501100	C	0.36232100	-3.82190500	3.62554100
H	-4.57677600	0.21746500	0.35511900	C	-2.03527400	-3.63349600	3.69855000
C	-3.22949400	0.08127500	-1.32027500	C	0.45167200	-3.20218600	4.86859400
C	-4.18031900	-0.44229600	-2.28986500	H	1.26734200	-4.17061500	3.12601500
C	-5.42916600	-0.95617800	-1.88494200	C	-1.95013200	-3.02009400	4.94630400
C	-3.89794600	-0.42169700	-3.67261600	H	-3.01156700	-3.82898500	3.25311900
C	-6.33030500	-1.46080800	-2.81105400	C	-0.70569900	-2.80686400	5.53622300
H	-5.68565500	-0.98851600	-0.82777800	H	1.42702300	-3.04741800	5.32728200
C	-4.80707200	-0.91136600	-4.59657200	H	-2.85860100	-2.72382900	5.46718600
H	-2.96273500	0.01590100	-4.01607200	H	-0.63927300	-2.34037700	6.51747100
C	-6.02552600	-1.44136700	-4.17115500	C	-0.79972600	-3.98172800	-2.11144000
H	-7.27971400	-1.86821600	-2.47039700	C	-1.89921900	-3.36858700	-2.72171500
H	-4.57188100	-0.86767600	-5.65784100	C	0.45539700	-3.85893900	-2.71788500
H	-6.73883800	-1.82552400	-4.89701900	C	-1.75109100	-2.64922500	-3.90508700
C	-1.84629400	0.06855700	-1.50716700	H	-2.88900000	-3.48175700	-2.27497800
O	-1.12383000	0.90251300	-0.80269100	C	0.60590700	-3.14941300	-3.90591900
C	-4.23522100	2.17529700	-0.33529200	H	1.31570000	-4.35628700	-2.26770100
F	-4.64649300	2.73890700	0.81475500	C	-0.49639900	-2.53914100	-4.50136700
F	-5.26788800	2.20348800	-1.19699000	H	-2.62098600	-2.18974600	-4.37232600
F	-3.26559000	2.96254600	-0.84699500	H	1.58519800	-3.08799900	-4.37803000
C	-1.09095900	-0.87747400	-2.36404100	H	-0.38231200	-1.99348400	-5.43635600
C	0.17302000	-0.49464600	-2.84074000	C	-4.12076600	-2.30931900	0.42820500
C	-1.51872500	-2.19592500	-2.59270300	C	-3.26390000	-1.04885500	0.25149900
C	0.97781300	-1.39406800	-3.53068800	C	-1.93988300	-2.83760500	0.44278000
H	0.51628600	0.52653100	-2.67434300	H	-4.81474500	-2.49127700	-0.39922500
C	-0.70354200	-3.10110300	-3.26212600	H	-3.45903300	-0.32393900	1.05486100
H	-2.49161700	-2.51607100	-2.22162900	H	-4.67116500	-2.34964200	1.37284800
C	0.54770700	-2.70308000	-3.73367800	O	-3.15767400	-3.39905700	0.44575300
H	1.94900900	-1.07173200	-3.89821300	N	-1.88670100	-1.55529700	0.39135800
H	-1.04012600	-4.12605100	-3.40430300	C	-3.42508700	-0.34571700	-1.10230600
H	1.18841500	-3.41486600	-4.25248500	H	-2.72364100	0.50003800	-1.13099000

TS10''

C	2.78929900	-3.41762700	0.42716300	C	-5.69527900	-0.61147900	-2.16467300
C	2.36988000	-1.94123800	0.34427600	C	-5.32807800	1.25207900	-0.68666400
C	0.54932900	-3.24636100	0.45093400	C	-7.01782900	-0.21363000	-2.34480500
H	3.35782500	-3.66334900	1.33146900	H	-5.31514800	-1.49136400	-2.68924000
H	2.65736700	-1.49629000	-0.62264100	C	-6.64838900	1.65195900	-0.86432400
H	3.33250300	-3.78349600	-0.45012800	H	-4.66007300	1.84145000	-0.05727100
O	1.53700400	-4.15391800	0.49234000	C	-7.49700900	0.91831300	-1.69157900
N	0.90185600	-2.01569300	0.37220700	H	-7.67199000	-0.78485500	-3.00048100
C	2.87521600	-1.04640100	1.47378800	H	-7.01515300	2.54508100	-0.36239400
H	2.16421200	-0.21292500	1.59297700	H	-8.52838700	1.23423000	-1.83297500
H	2.81385000	-1.60301800	2.42493800	Cu	-0.22070500	-0.40038700	0.07182000
C	4.25655300	-0.49216100	1.24872500	C	3.23714700	1.22380600	-1.54236800
C	4.60977300	0.73571300	1.81864000	C	2.12738700	1.31693900	-0.69973200
C	5.20100300	-1.14795400	0.45381400	C	0.96291500	0.68797800	-1.09708800
C	5.86601800	1.29219800	1.60149600	C	0.79246100	0.14360600	-2.36446300
H	3.87593500	1.26201500	2.43143300	C	1.92011600	0.06451900	-3.17887700
C	6.46122700	-0.59563800	0.23300900	C	3.16366500	0.58443100	-2.78549100

H	4.17541700	1.65226700	-1.19471200
H	2.20847200	1.81583900	0.26529300
H	-0.16358500	-0.26596900	-2.69389400
H	1.81382400	-0.41489100	-4.15196500
C	4.38151500	0.39655500	-3.68604200
C	4.07191200	0.86988300	-5.11141900
H	3.80460500	1.93312500	-5.12899400
H	4.95024000	0.73435900	-5.75390200
H	3.24727300	0.31039600	-5.56849300
C	4.72045200	-1.10198400	-3.70837900
H	5.58779700	-1.29421800	-4.35234100
H	4.96257200	-1.46406300	-2.69935300
H	3.88206100	-1.69978800	-4.08955200
C	5.60084300	1.16306200	-3.17543100
H	6.44411000	1.01665200	-3.86011600
H	5.40934500	2.24175800	-3.11579700
H	5.92024900	0.81737000	-2.18396400
C	-0.44245200	3.99949900	-1.29692200
H	-0.09361000	3.15637200	-1.90203400
H	0.12878900	4.88832600	-1.58742200
C	-0.29130000	3.71509700	0.16936800
C	-0.21871800	4.84857100	1.10117400
C	0.56149200	5.97744200	0.80079200
C	-0.94154200	4.84766600	2.30630600
C	0.64131300	7.04681200	1.68482600
H	1.13636800	6.00858800	-0.12402900
C	-0.86906600	5.92079500	3.18401700
H	-1.58635900	4.00132600	2.53776200
C	-0.07278700	7.02368900	2.88043700
H	1.26263000	7.90471000	1.43599000
H	-1.44903900	5.90327200	4.10459200
H	-0.01909200	7.86638200	3.56630900
C	-0.34491800	2.41164000	0.58344800
O	-0.68944300	1.47680900	-0.32958700
C	-1.87705200	4.27254200	-1.69510500
F	-1.96823800	4.50497900	-3.01680700
F	-2.37550100	5.34462300	-1.05403800
F	-2.68821500	3.22895500	-1.41357900
C	-0.00064400	1.89279300	1.92461700
C	-0.73491200	0.81608900	2.44603400
C	1.10759300	2.35426100	2.65129500
C	-0.35848700	0.18859000	3.63002800
H	-1.63830700	0.49511600	1.92802400
C	1.47655900	1.73783900	3.84265800
H	1.68362200	3.19690300	2.26843400
C	0.75576100	0.64522400	4.32823500
H	-0.94084200	-0.65073800	4.00684000
H	2.34072400	2.10689300	4.39263100
H	1.05661800	0.15977000	5.25507400

6c

C	2.82248000	-0.78044100	1.09704700
C	1.53588900	-0.83400500	0.56343800
C	1.32825900	-0.46412500	-0.76236900
C	2.40261100	-0.04217500	-1.54538300
C	3.67478200	-0.00373300	-0.99414200
C	3.92058000	-0.36858500	0.33778600
H	2.95790200	-1.07680700	2.13495600
H	0.69629600	-1.15842300	1.17638600
H	2.21773200	0.25244400	-2.57590300
H	4.50183300	0.32901500	-1.62169500
C	5.34217700	-0.30170400	0.89115400
C	5.86209900	1.13822500	0.78755100

H	5.23906000	1.82780000	1.37044500
H	6.88951900	1.20568000	1.16895300
H	5.87037500	1.49433000	-0.24967900
C	6.25224100	-1.22364600	0.06876500
H	7.28357300	-1.18148200	0.44319300
H	5.91457400	-2.26594600	0.12368700
H	6.27249500	-0.93669600	-0.98951900
C	5.41271200	-0.73552400	2.35417900
H	6.44735700	-0.67330500	2.71267600
H	4.80127100	-0.09438500	3.00162800
H	5.07934700	-1.77207100	2.49042300
C	-0.51252500	1.93623200	-0.12627700
H	0.56250000	1.72467200	-0.06676100
H	-0.73232300	2.64724900	0.67753300
C	-1.35169700	0.69268200	0.04767800
C	-2.44128400	0.76649800	1.04183000
C	-3.25678200	1.90469000	1.13784600
C	-2.64414800	-0.26845800	1.96997100
C	-4.25607200	1.98975200	2.10210100
H	-3.11813100	2.72234000	0.43377500
C	-3.63976300	-0.18163400	2.93369400
H	-2.00401000	-1.14898700	1.93000600
C	-4.45540500	0.94702000	3.00239600
H	-4.88323100	2.87851800	2.14772000
H	-3.77211900	-0.99563100	3.64442900
H	-5.23362900	1.01631300	3.76012900
C	-1.05449100	-0.44881600	-0.62817700
O	0.10448500	-0.53477600	-1.38565600
C	-0.73172500	2.67926200	-1.42390800
F	-0.04571100	3.84179400	-1.41532200
F	-2.03461700	2.99143300	-1.61911700
F	-0.33097700	1.98734200	-2.50320400
C	-1.87643700	-1.65995400	-0.75771600
C	-1.24737100	-2.90754400	-0.88218800
C	-3.27750300	-1.60455300	-0.81793100
C	-1.99800700	-4.06961200	-1.01991200
H	-0.16009300	-2.95805800	-0.86955700
C	-4.02369900	-2.76560000	-0.96381700
H	-3.77675000	-0.63936100	-0.76032200
C	-3.38835200	-4.00383200	-1.05747500
H	-1.49358600	-5.03042600	-1.10523800
H	-5.10907300	-2.70372100	-1.01698700
H	-3.97644000	-4.91248400	-1.17309100

TS2' S**2 = 0.75

C	1.53479600	-0.10021200	1.72081700
C	0.68803900	-0.16197900	0.67431500
C	-0.00184400	1.02565200	0.14068800
C	-0.04375200	1.25603600	-1.24204300
C	-0.61656000	1.95103300	0.99338300
C	-0.67928200	2.38069800	-1.75402600
H	0.43926400	0.54672400	-1.91406300
C	-1.26079500	3.07098700	0.48001500
H	-0.61517200	1.76127600	2.06682300
C	-1.29492600	3.28959400	-0.89546300
H	-0.69411800	2.54967300	-2.82954300
H	-1.74676400	3.77211100	1.15641400
H	-1.80187400	4.16490700	-1.29761100
C	0.60367000	-1.47292000	-0.05277900
O	1.59417100	-2.17896400	-0.21495600
N	-0.63136200	-1.81341800	-0.57538100
C	-1.84994400	-1.26498800	-0.08328100
C	-2.78577500	-0.73320600	-0.97349400

C	-2.11679800	-1.25708600	1.28746700
C	-3.96525400	-0.17831000	-0.49276800
H	-2.56250000	-0.72436900	-2.03943400
C	-3.29548800	-0.69121800	1.76443700
H	-1.38875200	-1.68729600	1.97332100
C	-4.22185600	-0.15026200	0.87743500
H	-4.68206400	0.24914100	-1.19140200
H	-3.49268300	-0.68195500	2.83494300
H	-5.14370700	0.29107700	1.25094000
C	-0.71664200	-3.00547600	-1.40226100
H	-1.03395500	-3.87766600	-0.81474600
H	-1.44131700	-2.84688600	-2.20754100
H	0.27108700	-3.20674700	-1.81940500
C	3.73617400	0.12025800	0.20891100
F	4.40516400	1.17363800	0.67551000
F	3.24726200	0.38463500	-0.99528000
F	4.51816300	-0.94608800	0.17818800
H	1.71219100	0.83091900	2.25609900
H	2.02865500	-0.99654400	2.08865700

1b

C	1.08288500	-2.14402800	-1.91893200
H	2.10460600	-2.22685100	-2.28113100
H	0.29864000	-2.62354900	-2.50132600
C	0.81317500	-1.49919400	-0.77550300
C	-0.55133600	-1.39068800	-0.22171100
C	-0.77114400	-1.54705800	1.15374200
C	-1.65133200	-1.13716200	-1.05000100
C	-2.05383800	-1.46123100	1.68233500
H	0.07675300	-1.74194700	1.81045500
C	-2.93325300	-1.04165400	-0.52044400
H	-1.48364300	-0.97859700	-2.11526200
C	-3.13948600	-1.20376000	0.84781100
H	-2.20694900	-1.59404900	2.75214000
H	-3.77456500	-0.82904000	-1.17797900
H	-4.14265100	-1.12514300	1.26303800
C	1.97668400	-0.93437800	-0.00411500
O	3.03059400	-1.54558600	0.12220100
N	1.77199600	0.29637200	0.59855400
C	0.77555900	1.21433300	0.15867600
C	-0.09844200	1.79057500	1.08350900
C	0.66825500	1.54648300	-1.19342000
C	-1.08331800	2.67184600	0.65493600
H	-0.02143700	1.51236300	2.13371600
C	-0.32703100	2.42137900	-1.61907000
H	1.36200800	1.10404300	-1.90633100
C	-1.20495500	2.98578700	-0.69811100
H	-1.77079500	3.10390300	1.37977300
H	-0.40908200	2.66887100	-2.67598500
H	-1.98192200	3.67070200	-1.03185800
C	2.82992400	0.81468100	1.44997900
H	3.38591900	-0.02697400	1.86577100
H	3.52761000	1.44736300	0.88413300
H	2.39271200	1.41341300	2.25526800

INT4' S2 = 0.75**

C	2.07133800	-0.47303000	1.01758500
C	0.84678700	-0.37229800	0.15998800
C	0.32364100	0.89896400	-0.26045500
C	-0.51526500	1.02052500	-1.39484900
C	0.61999000	2.08634500	0.45154900
C	-1.04575400	2.24288800	-1.76987800
H	-0.73206500	0.13488800	-1.98835200

C	0.07838000	3.30471700	0.07725900
H	1.27411500	2.04383300	1.31912600
C	-0.76271800	3.39365500	-1.03267600
H	-1.68387500	2.30234400	-2.64992200
H	0.31301900	4.19601300	0.65632000
H	-1.18563300	4.35251200	-1.32599500
C	0.33704600	-1.68506500	-0.29093900
O	1.12096500	-2.60914600	-0.51617600
N	-1.02727000	-1.87455600	-0.46948800
C	-2.02901900	-1.09100100	0.15839900
C	-3.18363300	-0.74288500	-0.54993400
C	-1.87878000	-0.65221100	1.47745600
C	-4.15707200	0.05177700	0.04338300
H	-3.29745800	-1.07392700	-1.58160000
C	-2.84450500	0.16285600	2.05722000
H	-0.99647100	-0.94933400	2.04212100
C	-3.98646600	0.51967500	1.34454700
H	-5.04640900	0.32247700	-0.52280000
H	-2.71008200	0.50595200	3.08136500
H	-4.74350700	1.15207500	1.80333600
C	-1.39917600	-3.15280800	-1.06458700
H	-0.89796600	-3.28380100	-2.02780800
H	-1.09434300	-3.98394900	-0.41708100
H	-2.48171500	-3.17973400	-1.20154200
C	3.36136600	-0.10867500	0.31104800
F	3.39959600	1.19492600	-0.04015600
F	3.55034200	-0.82717600	-0.80307600
F	4.41524500	-0.32664200	1.12693700
H	2.00778700	0.17014300	1.90556600
H	2.19416300	-1.50497300	1.35904700

INT6' S2 = 2.00**

C	-4.98806400	1.13902000	-0.07481900
C	-3.48443100	1.42526100	-0.14323600
C	-3.82025300	-0.75706000	0.18508100
H	-5.54559400	1.47541000	-0.95449200
H	-3.16739000	2.14713300	0.62148000
H	-5.47375800	1.51661100	0.83096900
O	-5.06941300	-0.31361000	-0.03014400
N	-2.88591000	0.12099700	0.18078600
C	-3.00786500	1.88881700	-1.52140000
H	-1.91312400	1.79326300	-1.54404100
H	-3.38029900	1.17916500	-2.27475100
C	-3.45507300	3.28477600	-1.85146700
C	-4.39810400	3.51570000	-2.85641700
C	-2.95494900	4.38121100	-1.13792100
C	-4.82910200	4.80762600	-3.14914200
H	-4.79085700	2.67050600	-3.42392700
C	-3.38331600	5.67248700	-1.42771200
H	-2.22360000	4.21952400	-0.34326600
C	-4.32212100	5.88906800	-2.43493900
H	-5.56120700	4.96837000	-3.93796900
H	-2.98331300	6.51439900	-0.86577100
H	-4.65645300	6.89916600	-2.66179000
C	-3.75112300	-2.23811100	0.44767600
C	-4.33229400	-3.00917000	-0.78692000
H	-5.32450500	-2.59286000	-0.99684100
H	-4.46869700	-4.05394300	-0.48278200
C	-4.59329800	-2.51549000	1.73104900
H	-5.63986900	-2.29569100	1.49139500
H	-4.52235400	-3.58626200	1.95219800
C	-3.40943200	-2.90348400	-1.96963500
C	-3.38971000	-1.74697100	-2.75501200

C	-2.45061100	-3.89289800	-2.21238100
C	-2.41349300	-1.56282700	-3.73019800
H	-4.15325100	-0.98336200	-2.59468100
C	-1.47346500	-3.71399800	-3.18826800
H	-2.47094000	-4.80985300	-1.62112200
C	-1.44324600	-2.54039100	-3.94012000
H	-2.40802100	-0.65223900	-4.32695000
H	-0.73342000	-4.49271800	-3.36650300
H	-0.67311700	-2.39446000	-4.69443600
C	-4.11600400	-1.67059600	2.88143000
C	-2.95853500	-2.01177700	3.59089700
C	-4.75495100	-0.46540500	3.18811400
C	-2.43946800	-1.15859400	4.56039800
H	-2.47249500	-2.96813400	3.39471700
C	-4.23827400	0.39074900	4.15721700
H	-5.67331500	-0.20402300	2.66110300
C	-3.07155800	0.05147400	4.83793500
H	-1.54407100	-1.44479000	5.11034100
H	-4.75361000	1.32119400	4.38839600
H	-2.66618800	0.71940200	5.59492700
C	-0.91561100	-4.38341500	1.21366400
C	-0.16275800	-3.18273500	0.63166200
C	-2.35210700	-2.75493700	0.64511400
H	-0.72691100	-4.53993700	2.28338800
H	0.26320200	-3.43827500	-0.34833600
H	-0.75782000	-5.32472400	0.68142600
O	-2.31518400	-4.02947300	1.06308200
N	-1.22543500	-2.19291400	0.38717600
C	0.90299800	-2.58009300	1.53070100
H	1.17753000	-1.59368400	1.11043900
H	0.43931300	-2.35171400	2.50473500
C	2.15110800	-3.39622300	1.72888800
C	3.04401900	-3.02407000	2.74001400
C	2.48033100	-4.48755100	0.91887800
C	4.23124800	-3.71772000	2.93476500
H	2.80596500	-2.16368700	3.36783200
C	3.67304400	-5.18464100	1.10991600
H	1.80504700	-4.81131600	0.12557200
C	4.55113900	-4.80214900	2.11810900
H	4.91327100	-3.40940600	3.72526100
H	3.90939900	-6.03344400	0.47136700
H	5.47898700	-5.34903800	2.27196900
Cu	-0.86654600	-0.18427300	0.25819900
C	0.66506600	3.61422800	1.24553600
C	-0.04558100	2.57174300	0.64647900
C	-0.13255500	1.31639900	1.24207000
C	0.46160800	1.14156400	2.49580900
C	1.18292800	2.17998600	3.08569000
C	1.30709300	3.43653300	2.47503200
H	0.70903600	4.57763700	0.73712500
H	-0.51547000	2.74822400	-0.32044700
H	0.39608900	0.18589200	3.01998500
H	1.66362100	2.00138700	4.04909700
C	2.12094600	4.53991500	3.14922700
C	3.58294000	4.08612900	3.25543500
H	4.00906900	3.88965800	2.26122000
H	4.19494700	4.86012100	3.73557600
H	3.68053900	3.17042100	3.85258700
C	1.56989700	4.80245700	4.55645500
H	2.15244500	5.58673100	5.05562000
H	0.52462800	5.13215800	4.51836000
H	1.61442900	3.90725700	5.18781800
C	2.08278700	5.84949000	2.36272100

H	2.66638600	6.61570600	2.88584800
H	2.51530700	5.74070900	1.35920300
H	1.06103400	6.23344200	2.25262500
C	1.79144600	-1.82957800	-1.80816100
H	0.69551200	-1.91104700	-1.82146500
H	2.19345600	-2.66372900	-1.21976500
C	2.18711200	-0.50515700	-1.22331700
C	3.26772600	-0.39805600	-0.28937000
C	4.27339200	-1.39465600	-0.22062700
C	3.34364400	0.68059800	0.62659900
C	5.30811500	-1.29985300	0.69427400
H	4.25995700	-2.22524000	-0.92278700
C	4.36776400	0.75005200	1.55562400
H	2.57127400	1.45028700	0.61345700
C	5.36037400	-0.23195300	1.59190800
H	6.07681300	-2.06971200	0.71444300
H	4.39278100	1.57964600	2.25983400
H	6.16849500	-0.16630700	2.31788800
C	1.27796400	0.59343900	-1.61115400
O	0.03327800	0.38014700	-1.60701000
N	1.77157300	1.78247900	-2.03903300
C	3.17141500	2.08548100	-2.12433600
C	4.01629400	1.34192000	-2.94422100
C	3.66540800	3.15339400	-1.37480700
C	5.37506300	1.64280400	-2.97350900
H	3.61174600	0.53311900	-3.54688500
C	5.02139500	3.45554200	-1.42056800
H	2.98917000	3.71285400	-0.72747600
C	5.87967300	2.69364000	-2.21151800
H	6.03945700	1.05616000	-3.60403300
H	5.41013900	4.27984100	-0.82578300
H	6.94194900	2.92539700	-2.24042300
C	2.23691600	-2.02149300	-3.23884700
F	1.81358300	-3.20184800	-3.72691400
F	3.57885000	-1.98909400	-3.36345700
F	1.74060000	-1.05012000	-4.03993400
C	0.87521800	2.81934900	-2.53923500
H	1.20186100	3.11568600	-3.54107600
H	-0.14043900	2.42530500	-2.58684000
H	0.89645600	3.70204600	-1.88917300

TS4' S**2 = 0.89

C	0.90566200	3.51723300	2.66520500
C	1.12762200	2.21216900	1.89041000
C	-0.98225700	2.88313000	1.62741600
H	1.48304300	4.36054500	2.26481900
H	1.39323400	1.38868500	2.56756100
H	1.07214600	3.44171000	3.74261500
O	-0.49843400	3.81966100	2.46061100
N	-0.18865400	1.92963600	1.30540400
C	2.12765000	2.29612000	0.73987400
H	1.99885700	1.37058100	0.15599400
H	1.81148700	3.11513500	0.07487900
C	3.56695100	2.45465400	1.13213500
C	4.31558400	3.54018200	0.66846800
C	4.20071300	1.49637200	1.93316300
C	5.66660100	3.66332500	0.98692400
H	3.82835200	4.29189700	0.04416700
C	5.54887500	1.61725400	2.25459400
H	3.63168300	0.63810700	2.29936700
C	6.28616900	2.70094600	1.77937000
H	6.23525200	4.51390900	0.61654300
H	6.02698100	0.86489700	2.87973000

H	7.34038100	2.79578500	2.03032900	C	0.16409400	-4.70404900	3.93233400
C	-2.38492000	3.17409000	1.17178600	C	0.09566200	-5.97132400	3.07012600
C	-2.37651300	4.64003300	0.62707400	H	0.89988400	-5.98572700	2.32338000
H	-2.29340700	5.30884100	1.49075200	H	0.19994300	-6.86706600	3.69506900
H	-3.35169600	4.82454900	0.16307100	H	-0.85735600	-6.05333600	2.53444700
C	-3.35944000	3.05543700	2.38760800	C	-0.99263700	-4.71536600	4.94133000
H	-2.94708700	3.67269600	3.19561200	H	-0.93168100	-5.59757300	5.59107800
H	-4.31202900	3.50681800	2.08527200	H	-0.96897000	-3.82428900	5.58172800
C	-1.24274000	4.89033200	-0.33304800	H	-1.96809300	-4.74050500	4.43938300
C	-0.13856800	5.65237200	0.06407300	C	1.48399800	-4.71539600	4.70136900
C	-1.22949800	4.31567100	-1.60978000	H	1.55119700	-5.62046700	5.31616100
C	0.95536600	5.82568700	-0.78075000	H	2.34941400	-4.71084100	4.02526200
H	-0.14439600	6.11742800	1.04971400	H	1.57558700	-3.85505400	5.37595100
C	-0.13669200	4.48220600	-2.45545700	C	0.00684300	-2.17238400	-1.84297500
H	-2.09089100	3.74346300	-1.95625500	H	-0.81638300	-1.44967800	-1.88923500
C	0.96364500	5.23115600	-2.04078200	H	-0.29186400	-2.95640200	-1.13953300
H	1.79683600	6.43672400	-0.45720500	C	1.26176700	-1.47137600	-1.39939300
H	-0.14925700	4.03125000	-3.44642900	C	2.23731900	-2.13707800	-0.59079300
H	1.81563000	5.36572600	-2.70582300	C	2.18232900	-3.53682500	-0.37613000
C	-3.55729100	1.62863900	2.81884300	C	3.25433900	-1.41771200	0.08657900
C	-4.68217100	0.91280500	2.39693800	C	3.10299800	-4.17147100	0.44103500
C	-2.58366300	0.96316000	3.57298100	H	1.42756900	-4.13438100	-0.88001000
C	-4.83008300	-0.43524200	2.71726500	C	4.17372700	-2.05805000	0.89624300
H	-5.45405200	1.42557900	1.82066500	H	3.30420200	-0.33521100	-0.01514700
C	-2.72366300	-0.38491800	3.88618200	C	4.10804500	-3.44123100	1.07811800
H	-1.70563300	1.50983800	3.92329100	H	3.04628700	-5.24973500	0.57491000
C	-3.84635800	-1.08834800	3.45556800	H	4.94721800	-1.47279400	1.39186700
H	-5.72019600	-0.97409900	2.39497500	H	4.83205700	-3.94628300	1.71437100
H	-1.94871000	-0.89315500	4.45793300	C	1.35259200	-0.06087700	-1.85309100
H	-3.95212600	-2.14398800	3.70040800	O	0.31470800	0.65203200	-1.77709600
C	-4.48542000	1.64200600	-1.36621100	N	2.51358900	0.46950700	-2.32651600
C	-3.30221200	0.66550900	-1.41569300	C	3.68204200	-0.28989100	-2.65682700
C	-2.89311300	2.25316700	0.09316500	C	3.58765700	-1.41063200	-3.47938400
H	-5.41090300	1.18174000	-0.99896100	C	4.92001500	0.11138500	-2.14913400
H	-2.77846700	0.71472500	-2.38321400	C	4.72748300	-2.16100000	-3.75140900
H	-4.69449900	2.15695300	-2.30725300	H	2.62830500	-1.68653200	-3.90670400
O	-4.08061500	2.64530500	-0.40012500	C	6.05598900	-0.63414000	-2.44191300
N	-2.38423800	1.17957500	-0.38897300	H	4.98868500	0.98139400	-1.49511400
C	-3.69286900	-0.78398400	-1.13061200	C	5.96142200	-1.77788500	-3.23288100
H	-2.77242900	-1.38730300	-1.11399000	H	4.64808300	-3.04111700	-4.38566000
H	-4.11644700	-0.83371400	-0.11620900	H	7.01775700	-0.32627100	-2.03737800
C	-4.66150400	-1.31787100	-2.14658100	H	6.85130300	-2.36302300	-3.45321200
C	-6.01773800	-1.45335900	-1.83769500	C	0.09344900	-2.76713100	-3.22972300
C	-4.22919600	-1.64223500	-3.43726200	F	-1.05301200	-3.38244300	-3.55998600
C	-6.92461400	-1.90263700	-2.79461200	F	1.09309300	-3.66141100	-3.34947600
H	-6.36151300	-1.21600100	-0.82889200	F	0.31340600	-1.79876100	-4.15246900
C	-5.13215200	-2.09243200	-4.39463000	C	2.56539500	1.89937900	-2.62125200
H	-3.17076900	-1.55507900	-3.68939600	H	2.80509200	2.04900900	-3.67922400
C	-6.48288500	-2.22136000	-4.07553400	H	1.59607500	2.34079400	-2.39171600
H	-7.97643800	-2.00875200	-2.53686100	H	3.33929000	2.38374700	-2.01244400
H	-4.78040000	-2.34922200	-5.39183600				
H	-7.18848400	-2.57618400	-4.82369000				
Cu	-0.58266700	0.27628700	0.15016600	INT7'			
C	0.97288800	-2.44405300	3.00876900	Cu	0.02262100	-0.19569100	0.04497100
C	0.80160500	-1.33228400	2.18115600	C	-0.70849600	3.39601500	2.10808400
C	-0.30565400	-1.21614500	1.34730500	C	-0.85548700	2.12400400	1.55069100
C	-1.27210300	-2.22462000	1.39285300	C	0.20104900	1.52777300	0.87999900
C	-1.09437900	-3.33817000	2.21205700	C	1.42196800	2.18658700	0.79678700
C	0.02876200	-3.47406100	3.03802200	C	1.55019200	3.46717500	1.33461300
H	1.86685700	-2.50076400	3.62749000	C	0.49054600	4.10433000	1.99033000
H	1.59254500	-0.57871200	2.16596900	H	-1.56332700	3.84024200	2.61449400
H	-2.18612900	-2.15716400	0.80041300	H	-1.83542100	1.64671200	1.60041300
H	-1.86467000	-4.11118600	2.21553900	H	2.28457700	1.71625100	0.32974700
				H	2.51277400	3.97265100	1.24105800

C	0.67032300	5.52546800	2.52006400	H	3.76287000	-0.05756500	-3.85227100
C	1.00047200	6.45288500	1.34277800	C	7.16110200	0.03457400	-3.81682600
H	0.19487200	6.44365900	0.59755000	H	8.37380500	0.29822900	-2.05494000
H	1.12912500	7.48602200	1.68922400	H	5.69903500	-0.20124800	-5.38278400
H	1.92658100	6.15533200	0.83627400	H	8.01171500	-0.02324400	-4.49256800
C	1.82650200	5.55830500	3.52780600	C	1.79493300	-2.66693000	2.10329600
H	1.97141900	6.57481800	3.91429300	C	2.75061400	-2.33081500	3.29202900
H	1.62965100	4.89975200	4.38371000	H	3.67790100	-2.89070000	3.12374100
H	2.77316500	5.24405500	3.07081900	H	2.28879600	-2.73083000	4.20277700
C	-0.58994800	6.04745300	3.20740100	C	1.65193000	-4.21796400	1.97808400
H	-0.42270300	7.06848800	3.56923400	H	2.65938100	-4.62569800	1.84776100
H	-1.44566100	6.07907400	2.52063300	H	1.27109000	-4.58649400	2.93714000
H	-0.87070700	5.43454000	4.07322400	C	3.03476100	-0.86113000	3.42403100
C	0.44779700	0.96993700	-2.36754300	C	4.17947300	-0.30465700	2.84464600
H	1.12439600	0.12672000	-2.19170600	C	2.14120400	-0.01352900	4.08829800
H	0.93504000	1.86124100	-1.95643700	C	4.43281300	1.06179100	2.93785200
C	-0.87077100	0.71264300	-1.65287500	H	4.88979300	-0.95781900	2.33329900
C	-1.78136900	1.83251900	-1.38860100	C	2.38747800	1.35260100	4.17777800
C	-1.43357000	3.16018200	-1.69316700	H	1.25241000	-0.43632400	4.56064400
C	-3.00274600	1.61990600	-0.72049900	C	3.53677000	1.89253700	3.60558000
C	-2.28273300	4.21305100	-1.37722200	H	5.33968100	1.47610400	2.49914800
H	-0.49663100	3.38139100	-2.19581900	H	1.68118500	1.99794000	4.69758800
C	-3.85754700	2.66792700	-0.41779800	H	3.73436300	2.96005100	3.68511000
H	-3.28916100	0.60889700	-0.43278900	C	0.75451300	-4.64403500	0.84764500
C	-3.50199500	3.97522800	-0.74665800	C	-0.62435600	-4.78360900	1.04226400
H	-1.98993600	5.22929000	-1.63327100	C	1.27563000	-4.89782600	-0.42565600
H	-4.80438700	2.45998000	0.07912700	C	-1.45827800	-5.16933700	-0.00317500
H	-4.16765300	4.80225700	-0.50919500	H	-1.04079600	-4.62255900	2.03830500
C	-1.35550300	-0.69720700	-1.83781900	C	0.44507700	-5.28538200	-1.47344000
O	-0.54788700	-1.55983800	-1.36270200	H	2.35091200	-4.82002300	-0.58406900
N	-2.53893100	-1.10278500	-2.34846100	C	-0.92474600	-5.42372700	-1.26462200
C	-3.54842200	-0.26832400	-2.92916600	H	-2.52646600	-5.29557600	0.17399000
C	-3.24656100	0.63185400	-3.94608600	H	0.87192200	-5.49931000	-2.45139300
C	-4.85706800	-0.38634700	-2.45408800	H	-1.57236400	-5.74838600	-2.07750600
C	-4.24913300	1.45375900	-4.45246700	C	-1.44131800	-2.07745600	3.64482300
H	-2.24161300	0.67922100	-4.34798700	C	-1.58892500	-1.17759800	2.41281900
C	-5.85517500	0.42523500	-2.97942800	C	0.43338400	-2.12101700	2.40380600
H	-5.08345200	-1.09019200	-1.65327600	H	-2.16207000	-2.90299000	3.67521100
C	-5.55167900	1.35606600	-3.97155600	H	-1.75494100	-0.13172700	2.70481600
H	-4.00759500	2.16271500	-5.24125100	H	-1.47016800	-1.54340400	4.59868900
H	-6.87227400	0.33562000	-2.60416400	O	-0.11765000	-2.65348700	3.50924400
H	-6.33264700	1.99532700	-4.37672200	N	-0.27713900	-1.27418200	1.75762500
C	0.40591900	1.10177400	-3.87309500	C	-2.66583500	-1.61557400	1.41968600
F	1.64850400	1.30665500	-4.34627600	H	-2.51213000	-1.02267900	0.50381100
F	-0.36495100	2.11346100	-4.31052500	H	-2.46728400	-2.65932600	1.13427300
F	-0.06221400	-0.03420800	-4.44282300	C	-4.07090800	-1.44562100	1.91632600
C	4.10892200	-2.24225200	-0.63748100	C	-4.89197800	-2.55293200	2.14190600
C	3.11305000	-1.13618500	-1.01588500	C	-4.58514700	-0.16632700	2.16042100
C	2.42613800	-2.14006100	0.83975200	C	-6.19786500	-2.38963600	2.59956700
H	5.10754400	-1.86027900	-0.39495300	H	-4.50162800	-3.55445400	1.95010500
H	2.60616800	-1.37976800	-1.96356900	C	-5.88848200	0.00080400	2.61583500
H	4.20854500	-3.03681400	-1.38277100	H	-3.95455100	0.70888000	1.98413900
O	3.55521900	-2.82274300	0.55939200	C	-6.69816400	-1.11257100	2.83682400
N	2.09340400	-1.18101800	0.05599400	H	-6.82531400	-3.26209100	2.76977500
C	3.79308700	0.23130700	-1.13769700	H	-6.27502800	1.00170600	2.79957900
H	3.05649200	0.97404600	-1.47250100	H	-7.71768000	-0.98329900	3.19347500
H	4.12023200	0.53924000	-0.13343400	C	-2.85475300	-2.53139400	-2.23828300
C	4.96611100	0.19247600	-2.07866500	H	-3.51667200	-2.80074300	-3.06315600
C	6.27206800	0.28994900	-1.59035300	H	-1.93281500	-3.11196600	-2.28178300
C	4.77501200	0.00992600	-3.45269500	H	-3.35514800	-2.75146200	-1.28547500
C	7.36396800	0.21431300	-2.45151300				
H	6.43087700	0.43675400	-0.52001300				
C	5.86366000	-0.06656700	-4.31554000				
				TS5'			
				Cu	-0.48420800	0.25000600	0.00719100

C	0.48541900	-2.27436500	3.06309000	N	-2.29160800	1.21351200	-0.39823200
C	0.70183600	-1.44338500	1.96898900	C	-3.75319300	-0.61357400	-1.22748000
C	-0.15448600	-1.46578300	0.86722400	H	-2.89531300	-1.29910300	-1.24014200
C	-1.21355400	-2.37828700	0.87182700	H	-4.17948500	-0.66382800	-0.21450500
C	-1.41431200	-3.21973000	1.96249100	C	-4.76214900	-1.01735900	-2.26442800
C	-0.56409600	-3.20305100	3.07466700	C	-6.13084900	-0.98835800	-1.98232600
H	1.17219200	-2.21368900	3.90501200	C	-4.34859500	-1.38547900	-3.54944800
H	1.58102500	-0.79929000	1.96787600	C	-7.06702400	-1.31640400	-2.95994400
H	-1.91015300	-2.44081400	0.03823600	H	-6.46333900	-0.71887800	-0.97790800
H	-2.25126200	-3.91779900	1.93010000	C	-5.28088900	-1.71539300	-4.52767800
C	-0.76209200	-4.21321400	4.20096000	H	-3.28231800	-1.43001500	-3.77973000
C	-0.49407900	-5.61682800	3.63799600	C	-6.64316700	-1.67853700	-4.23541700
H	0.52374300	-5.69279300	3.23449600	H	-8.12875400	-1.29488700	-2.72248300
H	-0.60619700	-6.37466900	4.42336800	H	-4.94372900	-2.00767000	-5.52017600
H	-1.19253100	-5.86782800	2.83033000	H	-7.37239200	-1.93893100	-4.99956300
C	-2.20284400	-4.14696100	4.72461500	C	-2.14641600	3.21753000	1.15174100
H	-2.35096900	-4.88785100	5.51965400	C	-3.15786200	3.15852300	2.34225100
H	-2.43442700	-3.15977500	5.14553200	H	-4.05380500	3.71222400	2.03695700
H	-2.93896600	-4.36119500	3.94061800	H	-2.70658300	3.70258300	3.18140400
C	0.18694800	-3.96388700	5.37195900	C	-2.02184300	4.68644900	0.63126400
H	-0.00765900	-4.68910100	6.17016700	H	-2.96586800	4.94400900	0.13895700
H	1.23877600	-4.07550200	5.08155200	H	-1.92293900	5.33575500	1.50814700
H	0.05465000	-2.96135600	5.79957100	C	-3.50637900	1.74329900	2.70763700
C	-0.11654800	-2.15208100	-1.92956800	C	-4.71041200	1.17921900	2.27537500
H	-0.94686100	-1.44112400	-2.00673400	C	-2.59084800	0.93079400	3.38619100
H	-0.50132000	-3.04986400	-1.44117000	C	-4.99087200	-0.16584200	2.50596100
C	0.99575400	-1.51004000	-1.11139900	H	-5.43566700	1.80776800	1.75633100
C	2.03537800	-2.36658000	-0.52077700	C	-2.86193200	-0.41528800	3.60583400
C	1.94883100	-3.76862400	-0.53971600	H	-1.65388400	1.35731300	3.74943700
C	3.09923500	-1.78951000	0.19685600	C	-4.05998000	-0.96954800	3.15953400
C	2.90265800	-4.55179500	0.09929200	H	-5.94027000	-0.58608100	2.17684700
H	1.14092500	-4.26300700	-1.07142200	H	-2.12949000	-1.03704500	4.11957200
C	4.05499700	-2.56739200	0.82752700	H	-4.27169400	-2.02315700	3.33449000
H	3.17280800	-0.70385800	0.25989200	C	-0.84268200	4.87449000	-0.28651200
C	3.96246200	-3.95849100	0.78096700	C	0.29059100	5.56586600	0.15531900
H	2.81872800	-5.63566300	0.05799200	C	-0.81960400	4.30624900	-1.56572400
H	4.87795900	-2.08470800	1.35300300	C	1.42020600	5.68141700	-0.65150300
H	4.71024000	-4.57519100	1.27493400	H	0.27928400	6.02062800	1.14585500
C	1.32985400	-0.16091200	-1.74729200	C	0.30917800	4.41298200	-2.37235200
O	0.37528200	0.63796800	-1.91806100	H	-1.69971300	3.78539500	-1.94495900
N	2.56255200	0.22392900	-2.17966500	C	1.43560800	5.09600800	-1.91605100
C	3.77320100	-0.54129600	-2.29635600	H	2.28573800	6.23763900	-0.29411400
C	3.82475500	-1.72055900	-3.03257700	H	0.30581000	3.96273500	-3.36347900
C	4.92222900	-0.04582600	-1.67313200	H	2.31579200	5.18508400	-2.55147700
C	5.01933900	-2.43370600	-3.09834600	C	1.11328100	3.32074900	2.73348800
H	2.94231300	-2.07922600	-3.55091200	C	1.27844500	2.03250500	1.91786500
C	6.11238600	-0.75649200	-1.75594900	C	-0.77852800	2.82464200	1.63299800
H	4.86803500	0.87659600	-1.09317900	H	1.74611900	4.14270900	2.37409300
C	6.16150900	-1.95917000	-2.46014400	H	1.48426000	1.17346200	2.57247100
H	5.05464500	-3.36158200	-3.66507900	H	1.25395500	3.19963400	3.81062700
H	7.00075000	-0.37324000	-1.25737100	O	-0.26566800	3.70591800	2.51233600
H	7.09197500	-2.51931400	-2.51969800	N	-0.03685200	1.83806300	1.29142400
C	0.20705300	-2.53346800	-3.35760600	C	2.30294200	2.10042000	0.79055600
F	-0.91169900	-2.95006200	-3.97648800	H	2.12562000	1.20902500	0.16760800
F	1.11118500	-3.52880700	-3.44773500	H	2.04553300	2.96264500	0.15564800
F	0.69506100	-1.49043900	-4.06683700	C	3.74971000	2.14858100	1.18351000
C	-4.32003400	1.87311100	-1.42095100	C	4.58701200	3.13714600	0.65809100
C	-3.22469100	0.80040100	-1.46005200	C	4.30994500	1.16510300	2.00804200
C	-2.69796300	2.34253800	0.05552200	C	5.95193400	3.13954300	0.93788400
H	-5.27667000	1.49552400	-1.03835600	H	4.15833800	3.90335100	0.00910800
H	-2.67000100	0.82549300	-2.41168000	C	5.67264700	1.16417900	2.28967600
H	-4.49506500	2.38660400	-2.36950400	H	3.67391400	0.38041000	2.42504600
O	-3.82605100	2.85119800	-0.47514400	C	6.49803400	2.15082300	1.75215400

H	6.58967900	3.91534200	0.51889400
H	6.09294900	0.39179300	2.93148900
H	7.56343800	2.15054800	1.97219400
C	2.60906900	1.57451500	-2.75495600
H	2.05532600	1.60005300	-3.70066000
H	2.14673400	2.29427900	-2.07377900
H	3.65289900	1.83462100	-2.93615800

F	-2.30868800	-2.85914200	0.46301400
F	-2.53440600	-2.34692500	-1.62445100
C	-1.95791400	-0.34264400	3.35932400
H	-2.33229500	-1.36467100	3.49017400
H	-1.01992400	-0.25997500	3.91499500
H	-2.68968200	0.36802500	3.74658100

4b

C	3.42889900	-0.18099600	-1.12209900
C	2.06902500	-0.47303600	-1.13458500
C	1.29822400	-0.42570000	0.02927700
C	1.94041500	-0.03691500	1.20770300
C	3.29667800	0.26806500	1.21198200
C	4.07970900	0.19656600	0.05506900
H	3.98031300	-0.24185000	-2.05793700
H	1.59605100	-0.71668800	-2.08639200
H	1.39149800	0.01275000	2.14424500
H	3.75656700	0.56492000	2.15511400
C	5.56810600	0.52896500	0.11896800
C	5.74711300	1.97027200	0.61369100
H	5.26719600	2.68544600	-0.06577500
H	6.81313200	2.22579600	0.67668600
H	5.31231000	2.11496800	1.60995300
C	6.25978600	-0.42770300	1.09916000
H	7.33177600	-0.19983600	1.16736600
H	6.15530600	-1.47067700	0.77584500
H	5.83884400	-0.34977500	2.10868400
C	6.24709200	0.39842200	-1.24333600
H	7.31280800	0.64214000	-1.15458200
H	5.81343400	1.08196500	-1.98412100
H	6.17450100	-0.62193000	-1.64031700
C	-0.32868500	-2.14620400	-0.67652500
H	0.07958300	-2.17582500	-1.69164700
H	0.31066000	-2.78090700	-0.05613400
C	-0.22267500	-0.71578000	-0.08191200
C	-0.74837900	0.40909300	-0.97203400
C	-1.21937900	0.20823800	-2.27044800
C	-0.62516600	1.72924700	-0.51698200
C	-1.60685300	1.28591700	-3.06705300
H	-1.30489000	-0.79393300	-2.67748500
C	-1.02356200	2.80226200	-1.29940600
H	-0.21818200	1.90921200	0.47894600
C	-1.52350100	2.58507600	-2.58328600
H	-1.97672200	1.09888000	-4.07391900
H	-0.93956500	3.81460000	-0.90719800
H	-1.83243300	3.42522500	-3.20257700
C	-0.76838800	-0.85994700	1.37071500
O	-0.22634800	-1.71208400	2.06821000
N	-1.73672900	-0.05900300	1.93748800
C	-2.72569100	0.75267600	1.30505600
C	-2.93728300	2.04695000	1.79050800
C	-3.51526900	0.27047500	0.26262400
C	-3.90746800	2.85935100	1.21782000
H	-2.31543400	2.41739500	2.60483600
C	-4.46756900	1.09829400	-0.32443400
H	-3.37807300	-0.74574700	-0.09298200
C	-4.66962300	2.39143400	0.14886300
H	-4.05864400	3.86769700	1.59913200
H	-5.06279000	0.71916900	-1.15316700
H	-5.42180300	3.03080400	-0.30886100
C	-1.66061300	-2.85756700	-0.72171200
F	-1.46555700	-4.14463900	-1.07070300

TS2'' S2 = 0.75**

C	1.39906600	-0.77380500	2.07461800
H	1.01950200	-1.61738600	2.64628000
H	2.47669000	-0.62130400	2.05618000
C	0.54837900	0.06065500	1.45073900
C	1.00734800	1.22167600	0.66890100
C	2.23242900	1.19694800	-0.01434900
C	0.23356200	2.39010600	0.60472200
C	2.67397200	2.30494300	-0.72707300
H	2.82994600	0.28536400	-0.00151700
C	0.67723100	3.49995600	-0.10464300
H	-0.72177200	2.42879400	1.12751400
C	1.89834400	3.46172400	-0.77400700
H	3.62361000	2.26204500	-1.25742900
H	0.06542600	4.39960200	-0.13522100
H	2.24188000	4.32820700	-1.33586500
C	-0.91960800	-0.24407900	1.60065300
O	-1.35235400	-0.64464500	2.67457000
C	1.67623900	-2.27130800	-0.52611000
F	0.52857000	-2.90465000	-0.34052000
F	2.70444600	-3.09287200	-0.36440200
F	1.71190900	-1.70904600	-1.73101400
C	-1.82762600	-0.10826500	0.42732700
C	-1.36635600	-0.06334400	-0.89517000
C	-3.20807600	-0.10577600	0.66867400
C	-2.26946200	-0.01051300	-1.95110000
H	-0.29876700	-0.08192400	-1.10408900
C	-4.10800000	-0.03309600	-0.38510700
H	-3.54645900	-0.16667500	1.70095300
C	-3.63924600	0.01421500	-1.69821800
H	-1.90241100	0.01286700	-2.97530600
H	-5.17827600	-0.01953800	-0.18728700
H	-4.34404800	0.06598300	-2.52649300

1c

C	1.17002300	2.74538100	-0.71888800
H	0.50622100	3.59703000	-0.84302400
H	2.21005200	2.86869000	-1.01460600
C	0.71050100	1.59811500	-0.19396300
C	1.57278600	0.42149200	0.02490500
C	1.36234700	-0.41785300	1.12888500
C	2.63517000	0.12548500	-0.84123100
C	2.19339800	-1.50657800	1.36579100
H	0.54246400	-0.20542400	1.81457600
C	3.46431500	-0.96513700	-0.60655500
H	2.79304000	0.74968700	-1.72034700
C	3.24731900	-1.78541000	0.49881200
H	2.01667000	-2.14054900	2.23272400
H	4.27883500	-1.18164500	-1.29569300
H	3.89388300	-2.64191400	0.68016200
C	-0.73951700	1.57667900	0.21603800
O	-1.25396800	2.57468200	0.70584900
C	-1.55684700	0.35295000	-0.02151500
C	-1.19228900	-0.64169900	-0.93826500
C	-2.77928500	0.24246400	0.65427500
C	-2.03234600	-1.72562200	-1.16839200

H	-0.25447600	-0.56223500	-1.48473200
C	-3.60718400	-0.85056300	0.43992300
H	-3.05597500	1.03741600	1.34376200
C	-3.23468900	-1.83698900	-0.47341700
H	-1.74666200	-2.48792400	-1.89067600
H	-4.54896000	-0.93441700	0.97923400
H	-3.88556300	-2.69245900	-0.64659000

INT6'' S2 = 2.00**

C	-4.69591400	-1.32276000	0.21963400
C	-3.53449700	-0.33246700	0.07726000
C	-2.73319600	-2.39605200	0.37748400
H	-5.38964600	-1.31895800	-0.62701400
H	-3.56411400	0.44794300	0.84971700
H	-5.25946400	-1.21889500	1.15246400
O	-4.04977500	-2.62691100	0.25395800
N	-2.35221100	-1.17295300	0.32351600
C	-3.44264700	0.31763100	-1.30492500
H	-2.45129900	0.78399100	-1.39102900
H	-3.46345800	-0.47558900	-2.06705000
C	-4.54350700	1.31074500	-1.54859000
C	-5.56884200	1.03949900	-2.45835700
C	-4.57597200	2.52004600	-0.84307600
C	-6.60007800	1.95296800	-2.66557500
H	-5.55038500	0.10452700	-3.02068300
C	-5.60403100	3.43436300	-1.04810000
H	-3.78538400	2.74493200	-0.12405500
C	-6.61950400	3.15274300	-1.96047700
H	-7.38768100	1.72691600	-3.38158300
H	-5.61357000	4.37125100	-0.49419200
H	-7.42306600	3.86831700	-2.12120400
C	-1.92963000	-3.64722900	0.61687900
C	-2.12154600	-4.62485500	-0.59312300
H	-3.20022400	-4.75347500	-0.74142200
H	-1.70993100	-5.59661500	-0.29464600
C	-2.45795200	-4.28066500	1.94042500
H	-3.48203600	-4.62367500	1.75458700
H	-1.84747300	-5.16454300	2.15580800
C	-1.43782700	-4.09964100	-1.82499400
C	-2.02634800	-3.08274100	-2.58324800
C	-0.13956000	-4.50877500	-2.14785300
C	-1.32630500	-2.46516100	-3.61574000
H	-3.04959100	-2.77606300	-2.35809300
C	0.56368700	-3.89606500	-3.18223800
H	0.32257200	-5.31512800	-1.57573600
C	-0.02393200	-2.86311400	-3.91109300
H	-1.79751700	-1.67085800	-4.19210000
H	1.57268900	-4.22613700	-3.42503300
H	0.52753900	-2.38012800	-4.71451300
C	-2.42409300	-3.28331800	3.06750000
C	-1.22270800	-2.96427700	3.71122100
C	-3.57614800	-2.57168300	3.41575300
C	-1.17048500	-1.94575400	4.65841200
H	-0.32400800	-3.53866800	3.48390300
C	-3.52704300	-1.55070300	4.36141200
H	-4.52261100	-2.83096000	2.94022700
C	-2.32064900	-1.22725200	4.97747800
H	-0.22973100	-1.71871300	5.15786600
H	-4.43575900	-1.01294100	4.62565500
H	-2.28034000	-0.43042000	5.71697900
C	1.63059800	-4.09510400	1.21924400
C	1.66517500	-2.71048100	0.56449600
C	-0.44889000	-3.40644700	0.72858900

H	1.92557600	-4.08572500	2.27625300
H	2.10645900	-2.77556300	-0.43971800
H	2.20322500	-4.86419800	0.69518100
O	0.23191400	-4.47912300	1.15893700
N	0.24148100	-2.37870600	0.38226000
C	2.34048000	-1.61772500	1.37484600
H	2.06286600	-0.64594000	0.92267400
H	1.87782600	-1.60193100	2.37556800
C	3.83707900	-1.69257400	1.49997600
C	4.46999700	-0.87470200	2.44310100
C	4.62948200	-2.50801100	0.68632200
C	5.85279000	-0.86935200	2.56976400
H	3.86177000	-0.22267600	3.07283000
C	6.01902600	-2.50181000	0.80805600
H	4.16968500	-3.16392700	-0.05443400
C	6.63392300	-1.68364500	1.74970100
H	6.32536800	-0.22537400	3.30932000
H	6.61873700	-3.14594100	0.16820100
H	7.71722300	-1.68386900	1.84984200
Cu	-0.44230700	-0.46191900	0.20917700
C	-0.88953500	3.60076600	1.33938000
C	-1.00679300	2.38262100	0.66426300
C	-0.45809800	1.21486800	1.18607600
C	0.18156400	1.28072400	2.42715700
C	0.30795500	2.50030300	3.09097500
C	-0.22992800	3.68537100	2.56923600
H	-1.32648300	4.48990600	0.88672700
H	-1.51601000	2.36977400	-0.29928200
H	0.60049300	0.38552500	2.89132900
H	0.83156300	2.52260500	4.04814600
C	-0.09287900	4.99133400	3.35114800
C	1.39276700	5.35372800	3.47563600
H	1.83381200	5.54630800	2.48860100
H	1.51934900	6.26209400	4.07805100
H	1.97005600	4.55321700	3.95558900
C	-0.68581200	4.81017900	4.75480300
H	-0.60024600	5.74141400	5.32846900
H	-1.74805400	4.54159800	4.70526700
H	-0.16948400	4.02640700	5.32155000
C	-0.81569800	6.15158200	2.66882600
H	-0.70139900	7.06424700	3.26508300
H	-0.40918500	6.36045800	1.67135900
H	-1.89094500	5.95964400	2.56514700
C	2.49559100	-0.65960900	-1.99196900
H	1.58801200	-1.27931400	-1.95755700
H	3.28419700	-1.16323800	-1.41915900
C	2.20230900	0.71147100	-1.46303300
C	3.13971000	1.42752400	-0.65346800
C	4.50211200	1.04028700	-0.57772500
C	2.71284000	2.51305300	0.15698900
C	5.38768600	1.71678800	0.24384800
H	4.87050500	0.22580400	-1.19698300
C	3.60288000	3.16347600	0.99312400
H	1.66432500	2.81230000	0.14640400
C	4.94519600	2.77603000	1.03861700
H	6.43141400	1.41113700	0.27130800
H	3.24780400	3.97717000	1.62257400
H	5.64183500	3.29629700	1.69295100
C	0.87972000	1.22665100	-1.84567700
O	-0.12310600	0.48225600	-1.68696700
C	2.92622100	-0.62158500	-3.44346700
F	3.17244000	-1.85951500	-3.90980600
F	4.04315200	0.11146400	-3.61350800

F	1.96773900	-0.07431600	-4.21940900	H	-2.19227800	-2.16271900	4.42935600
C	0.72873400	2.53368800	-2.49378300	H	-0.11917100	-1.61812000	5.68625200
C	-0.56116200	3.03747200	-2.73715200	C	3.57127200	-2.86469800	0.68715900
C	1.84185700	3.25985700	-2.95301200	C	2.94497100	-1.54048800	0.24321000
C	-0.73242400	4.25388900	-3.37826800	C	1.38760800	-3.13153500	0.25010800
H	-1.42358100	2.45192300	-2.42536600	H	3.87869400	-2.86525600	1.74083900
C	1.66654600	4.47494800	-3.60012800	H	3.33200700	-1.25676000	-0.74457100
H	2.84424400	2.85659900	-2.82200800	H	4.40467800	-3.20662400	0.06832300
C	0.38230500	4.97863500	-3.80437100	O	2.49735000	-3.82463000	0.54574300
H	-1.73487700	4.63758000	-3.55467200	N	1.51875900	-1.86693100	0.05878400
H	2.53255600	5.02795800	-3.95591400	C	3.10604700	-0.40148400	1.23780600
H	0.24806100	5.93232700	-4.31080200	H	2.36911400	0.38422700	0.98349900
TS4'' S**2 = 0.70				H	2.79321600	-0.76401900	2.22950200
C	-3.36626800	-3.26942800	-0.11031900	C	4.48353500	0.20347900	1.31882100
C	-2.81774600	-1.83643500	-0.17011600	C	4.88560400	0.81602700	2.51100400
C	-1.12197000	-3.28392500	-0.01489600	C	5.35525300	0.24914200	0.22362500
H	-3.92803300	-3.55677700	-1.00630400	C	6.11103400	1.46603900	2.60608600
H	-3.12013400	-1.24362700	0.70612600	H	4.21753700	0.78810900	3.37233700
H	-3.97062800	-3.49193700	0.77390300	C	6.58370000	0.90172200	0.31548300
O	-2.18198400	-4.10808100	-0.04831300	H	5.08606500	-0.22077000	-0.72394800
N	-1.35966000	-2.02663700	-0.08627300	C	6.96394400	1.51514000	1.50494600
C	-3.21872600	-1.09272100	-1.44124300	H	6.40310300	1.93383800	3.54429500
H	-2.63320300	-0.16772800	-1.49073500	H	7.24535700	0.92598800	-0.54789900
H	-2.90921600	-1.68839800	-2.31297400	H	7.92397200	2.02145900	1.57678000
C	-4.69519500	-0.81580900	-1.48792300	Cu	0.00588000	-0.48980900	-0.11531600
C	-5.51972000	-1.45031000	-2.42046100	C	-2.70591100	2.23559600	1.74066400
C	-5.27650200	0.06905200	-0.57121100	C	-2.04065600	1.50249500	0.75120000
C	-6.89108800	-1.20566800	-2.44392800	C	-0.93121600	0.72648700	1.06958500
H	-5.07787800	-2.13635300	-3.14476900	C	-0.50780800	0.67429100	2.39936200
C	-6.64539300	0.31461700	-0.59170900	C	-1.17416900	1.40799900	3.37878600
H	-4.64426800	0.57027000	0.16487700	C	-2.28686000	2.20378300	3.07371500
C	-7.45690900	-0.32279000	-1.52889700	H	-3.56613900	2.83770900	1.45054500
H	-7.51742500	-1.70562000	-3.18008900	H	-2.40085400	1.57249400	-0.27851100
H	-7.08184400	1.00773600	0.12522900	H	0.33594800	0.04619500	2.69544000
H	-8.52753900	-0.13009100	-1.54541100	H	-0.82169300	1.34446400	4.40969200
C	0.18217300	-4.01975900	0.11897400	C	-2.99285300	2.97175000	4.18966900
C	0.40510700	-4.87553700	-1.17778200	C	-1.99819300	3.93075500	4.85688900
H	-0.50071300	-5.47039400	-1.34434300	H	-1.61627300	4.66891900	4.14059100
H	1.22758500	-5.57131100	-0.97380800	H	-2.48285500	4.47770200	5.67531400
C	0.09394700	-4.90513600	1.40192100	H	-1.13682300	3.39920000	5.27880000
H	-0.78337300	-5.55322500	1.30061200	C	-3.50865000	1.97387800	5.23585400
H	0.97965200	-5.54872500	1.42521400	H	-4.01126000	2.50160200	6.05609500
C	0.72818900	-3.97975400	-2.34338100	H	-4.22904600	1.27354700	4.79492900
C	-0.28423500	-3.27862800	-3.00616000	H	-2.69373400	1.38363700	5.67318900
C	2.05932400	-3.69970500	-2.67302300	C	-4.17685600	3.78565000	3.67119200
C	0.02138200	-2.29255700	-3.94002800	H	-4.65299600	4.32253200	4.49976000
H	-1.32731600	-3.50696000	-2.77889900	H	-3.86713800	4.53396400	2.93060900
C	2.37049800	-2.71424400	-3.60656900	H	-4.94275200	3.14883800	3.21074100
H	2.85804900	-4.25549400	-2.17952500	C	2.23138900	0.91687600	-1.74215800
C	1.35153600	-1.99572600	-4.23057100	H	1.82847900	-0.07830200	-1.98166100
H	-0.78001000	-1.74685500	-4.43437500	H	3.07692500	0.79293400	-1.06253400
H	3.41115400	-2.50463300	-3.85020300	C	1.16287400	1.79567200	-1.15486800
H	1.59454200	-1.21684400	-4.95087200	C	1.47579800	2.82935500	-0.20878500
C	0.01767200	-4.05332100	2.64398200	C	2.80119700	3.04309400	0.24976100
C	1.17417500	-3.74932200	3.37115800	C	0.45408900	3.63806300	0.35498600
C	-1.19203100	-3.47614800	3.04919900	C	3.07906300	3.99453000	1.21739700
C	1.12729700	-2.88057900	4.45927500	H	3.62974100	2.47542600	-0.16744500
H	2.11679500	-4.21757100	3.08821800	C	0.74027600	4.58442600	1.32067000
C	-1.24195100	-2.60283400	4.13155300	H	-0.57593500	3.49082300	0.04439300
H	-2.10991100	-3.73125400	2.51907500	C	2.05319800	4.76835200	1.76287300
C	-0.07968100	-2.29653500	4.83587700	H	4.10717900	4.13599900	1.54427600
H	2.03534200	-2.67068300	5.02237500	H	-0.06755000	5.18155600	1.73883100
				H	2.27492100	5.51172600	2.52573400

C	-0.12003100	1.68626800	-1.90281300	H	-3.61364700	-3.65356000	-2.70090900
O	-0.59000300	0.54334500	-2.07418900	C	-0.76285100	-1.65161700	-4.38472500
C	2.80430800	1.45049000	-3.03885900	H	0.57732900	-2.87095600	-3.23161500
F	3.76689900	0.62427300	-3.49170800	C	-2.08900900	-1.36800700	-4.70555700
F	3.34788700	2.67196900	-2.88422700	H	-4.15193100	-1.89617200	-4.36264700
F	1.86074700	1.54806300	-3.99599500	H	0.04679200	-1.10641200	-4.86732700
C	-0.77913600	2.85336600	-2.50334100	H	-2.32233800	-0.59666100	-5.43726100
C	-2.12565900	2.74264100	-2.88819000	C	-3.94516500	-2.12917100	0.18577700
C	-0.08271200	4.04542700	-2.76311700	C	-3.05449100	-0.88527200	0.22962900
C	-2.76976800	3.81176900	-3.49195900	C	-1.79021200	-2.69347100	-0.05077600
H	-2.65321000	1.80831800	-2.69999500	H	-4.69626800	-2.10471800	-0.61025200
C	-0.72545300	5.10425000	-3.38987600	H	-3.22995200	-0.30843800	1.14457400
H	0.96975400	4.12912100	-2.49804500	H	-4.42957300	-2.37129100	1.13812200
C	-2.06928900	4.99254900	-3.74501500	O	-3.02417700	-3.20495500	-0.11796700
H	-3.81688900	3.72714800	-3.77343400	N	-1.68385300	-1.44614100	0.25172600
H	-0.17850300	6.01934800	-3.60418700	C	-3.19059300	0.02724500	-0.98059600
H	-2.57309600	5.82811500	-4.22675600	H	-2.43329400	0.82276000	-0.88976000

INT7''

C	2.77306300	-3.32590100	-1.24024800	C	-4.54662900	0.65055700	-1.17371300
C	2.49791000	-1.89923800	-0.74764100	C	-4.79506800	1.35742500	-2.35602800
C	0.63070500	-3.12476700	-0.59419900	C	-5.55803700	0.59248600	-0.21084000
H	3.53900100	-3.84698900	-0.65549500	C	-6.00814500	2.00276500	-0.52050000
H	2.62732600	-1.15951500	-1.55083700	H	-4.01295300	1.40893200	-3.11567900
H	3.02143200	-3.40527100	-2.30264100	C	-6.77989100	1.23189300	-0.41682900
O	1.51580400	-4.02553900	-1.03869600	H	-5.39783100	0.05901100	0.72766600
N	1.06068200	-1.92941700	-0.40247000	C	-7.00658600	1.94288100	-1.59019500
C	3.36424100	-1.50774200	0.44607900	H	-6.17877200	2.55274700	-3.48552800
H	3.02245300	-0.53950100	0.82855800	H	-7.55419400	1.17401600	0.34574300
H	3.19026000	-2.22836400	1.25856700	H	-7.95841700	2.44422700	-1.75132200
C	4.82154100	-1.47814200	0.07623100	Cu	0.05478900	-0.31213200	0.31838800
C	5.72374000	-2.38575700	0.63697900	C	2.74089200	2.29690600	-1.78179500
C	5.29609400	-0.55847200	-0.86712100	C	2.21725400	1.56755700	-0.70601700
C	7.06895800	-2.37246700	0.27504800	C	0.99404100	0.93342700	-0.83701100
H	5.36717000	-3.10369600	1.37738300	C	0.29469700	1.01476200	-2.04278000
C	6.63821300	-0.54372900	-1.23195800	C	0.83086900	1.74159300	-3.10323400
H	4.60337400	0.15762400	-1.31411600	C	2.06076200	2.40553800	-2.99637800
C	7.52896200	-1.45140100	-0.66133700	H	3.70210800	2.78950100	-1.64432500
H	7.75815600	-3.08299600	0.72696600	H	2.78930700	1.51621600	0.21837800
H	6.99253000	0.18099800	-1.96296100	H	-0.65830400	0.50262100	-2.18740100
H	8.57899000	-1.43877800	-0.94573300	H	0.26857800	1.78526800	-4.03739700
C	-0.73916200	-3.70736200	-0.40033000	C	2.59641400	3.20099800	-4.18443700
C	-0.66950500	-4.76860100	0.74440900	C	1.60378400	4.32045300	-4.52591900
H	0.09163900	-5.50599900	0.46224500	H	1.47454100	5.00814300	-3.68088300
H	-1.63614200	-5.28597700	0.76447700	H	1.96348300	4.90390500	-5.38247000
C	-1.17667900	-4.37652400	-1.74644300	H	0.61550200	3.92333500	-4.78827800
H	-0.37300100	-5.05691300	-2.04857700	C	2.74163800	2.26724900	-5.39373500
H	-2.06083300	-4.98728500	-1.53654100	H	3.11629800	2.82229900	-6.26255900
C	-0.37155700	-4.13693900	2.07530200	H	3.44713200	1.45313000	-5.18570200
C	0.93807900	-3.79635400	2.42972000	H	1.78384400	1.81573900	-5.68081700
C	-1.41103900	-3.79601500	2.94764500	C	3.95770600	3.82846500	-3.89051300
C	1.20402900	-3.11450100	3.61471000	H	4.30977700	4.38317300	-4.76768300
H	1.76031100	-4.08327500	1.77111500	H	3.91256400	4.53569600	-3.05307000
C	-1.14882800	-3.12822000	4.14050100	H	4.71642900	3.07069400	-3.65621000
H	-2.43483500	-4.07366000	2.69075200	C	-0.91527800	0.22007000	2.72641800
C	0.15873800	-2.77564900	4.47170700	H	-0.24653900	-0.65249100	2.77097100
H	2.22853400	-2.85300500	3.87304500	H	-1.91126600	-0.15752600	2.48953500
H	-1.96565900	-2.87707500	4.81360800	C	-0.40712200	1.22544700	1.68950300
H	0.36105900	-2.23984600	5.39706000	C	-1.35533900	2.21571100	1.14125200
C	-1.48496100	-3.36473700	-2.82062000	C	-2.71616100	2.24251900	1.50488200
C	-2.81109400	-3.08425600	-3.16929900	C	-0.92155500	3.16942400	0.19453600
C	-0.46542100	-2.64186000	-3.45266200	C	-3.59855000	3.15678000	0.93988100
C	-3.11328600	-2.09705400	-4.10472300	H	-3.09361800	1.56689100	2.26842600
				C	-1.80460500	4.07247700	-0.37538400

H	0.12501900	3.19122000	-0.09885300
C	-3.15296400	4.06638000	-0.01395600
H	-4.64370100	3.14946300	1.24164300
H	-1.43706400	4.78692000	-1.10950300
H	-3.84964600	4.76678200	-0.46973300
C	1.01396100	1.59808500	2.08644100
O	1.81696200	0.66811600	2.20320400
C	-0.98089500	0.74752900	4.15364300
F	-1.61878300	-0.13884900	4.94175400
F	-1.65685500	1.91228000	4.23700100
F	0.23636200	0.95612700	4.67811400
C	1.43155600	2.98019300	2.40823600
C	2.80911400	3.25505600	2.38920000
C	0.54320700	3.98407700	2.82595800
C	3.28355100	4.51193400	2.73094000
H	3.49552300	2.45706400	2.11253900
C	1.02519000	5.23461100	3.19347900
H	-0.52163300	3.78242600	2.89877600
C	2.39017900	5.50589900	3.13225900
H	4.35125900	4.71755200	2.69867600
H	0.33125600	6.00038400	3.53253100
H	2.76135800	6.49048700	3.40982300

TS5''

C	-2.74447000	-3.67950600	-0.19350000
C	-2.47818300	-2.16861200	-0.22308300
C	-0.56488200	-3.27180100	-0.53901000
H	-3.46856500	-4.01028400	-0.94533200
H	-2.73654100	-1.69006300	0.73318800
H	-3.04347300	-4.07109100	0.78444200
O	-1.46311600	-4.27249000	-0.52338700
N	-1.01382700	-2.08046100	-0.38088900
C	-3.22183100	-1.46556300	-1.35825100
H	-2.84705200	-0.43926700	-1.44200000
H	-2.95943600	-1.95471800	-2.30786300
C	-4.71152300	-1.49891200	-1.15554000
C	-5.54678400	-2.16610800	-2.05519100
C	-5.29080700	-0.87735800	-0.04271100
C	-6.92518600	-2.20506300	-1.85666600
H	-5.10999300	-2.65271500	-2.92838600
C	-6.66618400	-0.91532400	0.16034900
H	-4.65069400	-0.36028400	0.67472900
C	-7.48832000	-1.57973500	-0.74816000
H	-7.55973600	-2.72627600	-2.57067000
H	-7.09932400	-0.42409600	1.03006800
H	-8.56436400	-1.60967100	-0.59087600
C	0.83825200	-3.76604900	-0.76505300
C	0.94013000	-4.28551000	-2.24454500
H	0.10484600	-4.97459000	-2.41771500
H	1.86940200	-4.86139200	-2.32600900
C	1.13187500	-4.88655600	0.28527300
H	0.32517800	-5.62475200	0.23068300
H	2.06035700	-5.38668200	-0.00890300
C	0.93654800	-3.12157900	-3.19950100
C	-0.25908900	-2.47753700	-3.53189900
C	2.14096400	-2.55179900	-3.62898200
C	-0.25579400	-1.26788400	-4.22053200
H	-1.20628900	-2.92880200	-3.23237200
C	2.15099400	-1.34479100	-4.32361200
H	3.07990500	-3.05789900	-3.40152400
C	0.95280900	-0.68821900	-4.60260700
H	-1.19662100	-0.76985300	-4.44596900
H	3.09686900	-0.91482500	-4.64965000

H	0.95957400	0.26403700	-5.13004200
C	1.26520500	-4.28921900	1.66397100
C	2.52936600	-4.04668500	2.21294300
C	0.13995100	-3.85217000	2.37359100
C	2.66766100	-3.35771700	3.41582300
H	3.41315100	-4.40677400	1.68659200
C	0.27375400	-3.15493000	3.57039800
H	-0.85595300	-4.07189600	1.98911900
C	1.54004900	-2.89232800	4.08886600
H	3.66048000	-3.19031600	3.83164800
H	-0.61521100	-2.82010700	4.10260100
H	1.64526200	-2.34859800	5.02602800
C	4.08968000	-2.20717500	-0.46488700
C	3.22524600	-0.94621000	-0.36986800
C	1.91298100	-2.72585200	-0.60561900
H	4.62995000	-2.43003200	0.46450400
H	3.40217500	-0.30212900	-1.24429000
H	4.79408800	-2.21486400	-1.30061000
O	3.13684400	-3.27105400	-0.68241500
N	1.84051600	-1.45222900	-0.45186600
C	3.44751600	-0.15603900	0.91673800
H	2.66258400	0.61333700	0.99533500
H	3.28734400	-0.83280500	1.76949300
C	4.81177100	0.47218400	0.97624400
C	5.73310900	0.09469700	1.95567400
C	5.19263600	1.43637300	0.03386400
C	7.00085500	0.67004400	2.00195400
H	5.44661400	-0.65474600	2.69514600
C	6.45695500	2.01486300	0.07839900
H	4.49725900	1.73901100	-0.75411400
C	7.36457900	1.63224600	1.06430700
H	7.70516500	0.36574800	2.77347600
H	6.73509700	2.76479500	-0.65918400
H	8.35384300	2.08320900	1.09941600
Cu	0.09426800	-0.34638000	-0.28885200
C	-2.84655900	1.07383500	2.22385700
C	-2.16417400	0.99651400	1.00738000
C	-0.78551800	0.79082400	0.99773100
C	-0.09432100	0.72256800	2.21350100
C	-0.79443300	0.75997200	3.41159600
C	-2.18435300	0.95238400	3.44877100
H	-3.92246300	1.23835000	2.19968600
H	-2.72958000	1.08566300	0.08031600
H	0.99174900	0.63200900	2.23530800
H	-0.23664100	0.66058900	4.34327800
C	-2.89716500	1.04954300	4.79357800
C	-2.34296100	2.25599200	5.56425600
H	-2.51429900	3.18952100	5.01400400
H	-2.83413900	2.34533900	6.54106000
H	-1.26442000	2.16718400	5.74195300
C	-2.63505900	-0.23041400	5.59924400
H	-3.12892000	-0.17353800	6.57694900
H	-3.02354500	-1.11489800	5.07834400
H	-1.56490800	-0.38992100	5.78094000
C	-4.40690900	1.22210700	4.63592000
H	-4.88160800	1.27000700	5.62245400
H	-4.66197900	2.14864700	4.10674600
H	-4.86189600	0.38281200	4.09367500
C	1.44404700	1.55935900	-1.42535100
H	1.20687700	0.64377400	-1.98816700
H	2.32990900	1.35685600	-0.82780700
C	0.26445500	2.00903100	-0.54753100
C	0.57568400	3.07116800	0.44679400

C	1.89202700	3.32563600	0.86689000
C	-0.45626400	3.77653700	1.09747700
C	2.16555000	4.23638600	1.88297600
H	2.73684700	2.82663900	0.39881000
C	-0.18420200	4.69258900	2.10008000
H	-1.49156000	3.58168100	0.82747400
C	1.13090900	4.92470600	2.50576800
H	3.19839700	4.40610200	2.18014100
H	-1.00572500	5.22205800	2.57841600
H	1.34347800	5.63581200	3.30108500
C	-0.95555000	2.03863800	-1.45291300
O	-1.27174600	0.94916000	-1.94581000
C	1.88332000	2.53598300	-2.50257400
F	2.96479500	2.02573100	-3.12973200
F	2.22948700	3.74507100	-2.02622400
F	0.92561800	2.72569700	-3.42923400
C	-1.72252000	3.24983100	-1.78737500
C	-3.06425300	3.08206400	-2.16663500
C	-1.15468000	4.53311900	-1.81179600
C	-3.83210100	4.17859900	-2.52967900
H	-3.49041500	2.07951900	-2.16310800
C	-1.91892800	5.62291300	-2.20757100
H	-0.10924800	4.67457900	-1.54811100
C	-3.25838100	5.45002600	-2.55392300
H	-4.87623100	4.04470600	-2.80327500
H	-1.46910200	6.61231300	-2.24453400
H	-3.85699500	6.30950800	-2.84888000

4c

C	-3.31611600	1.05793700	-0.06172600
C	-1.94051400	1.26163200	0.00349200
C	-1.06153700	0.23023900	0.33868200
C	-1.61801900	-1.03226000	0.56971300
C	-2.98995100	-1.23329800	0.49327400
C	-3.87770600	-0.19619800	0.18513100
H	-3.95206300	1.90181800	-0.32063200
H	-1.55432800	2.25113700	-0.23954300
H	-0.98374400	-1.87649200	0.82784900
H	-3.37795400	-2.23389000	0.68583300
C	-5.37775700	-0.47046500	0.12298800
C	-5.65462300	-1.53520800	-0.94669500
H	-5.32975300	-1.19552900	-1.93791800
H	-6.72868300	-1.75694000	-0.99969300
H	-5.13248300	-2.47487800	-0.72979500
C	-5.85526600	-0.99117900	1.48508100
H	-6.93173000	-1.20591000	1.45865700
H	-5.67663400	-0.25326000	2.27680100
H	-5.33951100	-1.91572000	1.77086100
C	-6.17952500	0.78276200	-0.22342600
H	-7.24986400	0.54524800	-0.25332400
H	-5.90442400	1.18622800	-1.20606300
H	-6.03885000	1.57676400	0.52074000
C	0.71930400	1.78743200	1.11656600
H	0.25126100	2.65099500	0.63466700
H	0.22860900	1.66254100	2.08788500
C	0.46206200	0.49275000	0.30631900
C	0.80192800	0.57122800	-1.18150500
C	1.08592200	1.76392700	-1.84964300
C	0.71178600	-0.60215300	-1.94360500
C	1.31376300	1.77751800	-3.22530600
H	1.15117500	2.70094500	-1.30332000
C	0.94386500	-0.59418000	-3.31167600
H	0.45773100	-1.54015000	-1.44863600

C	1.25265900	0.60022100	-3.96116300
H	1.54104300	2.72062500	-3.71939700
H	0.87863900	-1.52354800	-3.87456400
H	1.43441900	0.61180400	-5.03416000
C	1.17910700	-0.64141500	1.10774700
O	0.72081800	-0.91739800	2.20517500
C	2.14334500	2.18252800	1.42163500
F	2.15404200	3.33498500	2.12133000
F	2.79047200	1.26050400	2.16105300
F	2.89786500	2.39033600	0.31749100
C	2.37164800	-1.37860300	0.60531600
C	2.55661000	-2.67768300	1.09939800
C	3.33651000	-0.83431400	-0.25316100
C	3.65847200	-3.43062800	0.71741700
H	1.81621200	-3.07664700	1.78987900
C	4.45467200	-1.57927300	-0.60941400
H	3.23037900	0.18031800	-0.62636900
C	4.61171100	-2.88100000	-0.13838700
H	3.78093000	-4.44441500	1.09407300
H	5.20621100	-1.14050600	-1.26272800
H	5.48136700	-3.46570000	-0.43366300

INT2'

C	2.61942000	-1.28118500	-2.98397700
C	2.35837500	-0.92719300	-1.51218700
C	0.42807900	-1.33339000	-2.52580700
H	3.13019900	-2.24664400	-3.10313200
H	2.60078100	0.12594900	-1.29921300
H	3.15505800	-0.51693700	-3.55417900
O	1.29725800	-1.41564800	-3.56360200
N	0.90862400	-1.07768000	-1.37068500
C	3.09752400	-1.80265300	-0.50609900
H	2.58746900	-1.67321500	0.45940900
H	2.97510100	-2.85768100	-0.78921600
C	4.54664300	-1.42579400	-0.39662500
C	5.56774800	-2.29823100	-0.77855400
C	4.89655300	-0.15489300	0.07936300
C	6.90487800	-1.91742700	-0.68047200
H	5.30734200	-3.29124700	-1.14891100
C	6.22908000	0.22820600	0.18151100
H	4.10252800	0.53081400	0.38410100
C	7.23919200	-0.65416400	-0.20007300
H	7.68846900	-2.61204600	-0.97894500
H	6.47772000	1.21769200	0.56371300
H	8.28378400	-0.35821400	-0.12092100
C	-0.98736700	-1.66610000	-2.89533000
C	-1.01751100	-3.19188200	-3.25034700
H	-0.63140000	-3.29050000	-4.27312400
H	-2.07068000	-3.49984000	-3.26910100
C	-1.41810100	-0.86215100	-4.15848200
H	-0.63630700	-1.00377800	-4.91409800
H	-2.33365200	-1.32578300	-4.54307900
C	-0.19922000	-4.03203700	-2.31118800
C	1.03453700	-4.54523700	-2.72376100
C	-0.60623500	-4.23306200	-0.98849900
C	1.84315900	-5.25195900	-1.83614300
H	1.36048300	-4.38405600	-3.75274500
C	0.20256600	-4.93296400	-0.09693000
H	-1.55847700	-3.83705600	-0.63495600
C	1.42913600	-5.44298900	-0.51935600
H	2.79787900	-5.65400600	-2.17491600
H	-0.12963700	-5.08005800	0.92978500
H	2.05947900	-5.99103800	0.17873900

C	-1.65319700	0.59763500	-3.88932000
C	-2.95332400	1.10963300	-3.83718700
C	-0.58347300	1.46831000	-3.64904900
C	-3.18224500	2.45481100	-3.55697200
H	-3.79233800	0.43890700	-4.02191900
C	-0.80966500	2.81111100	-3.36049900
H	0.43936800	1.09221900	-3.70953200
C	-2.11112000	3.30888600	-3.30983800
H	-4.20164100	2.83792000	-3.53911100
H	0.03441500	3.47926400	-3.19349500
H	-2.28487200	4.35928900	-3.08761700
C	-4.10325500	-1.17671800	-1.09814800
C	-3.13722300	-0.59275900	-0.06140200
C	-1.98213500	-1.34970000	-1.80675000
H	-4.83949300	-0.45788300	-1.47831500
H	-3.21710800	-1.13239000	0.88651100
H	-4.61846100	-2.07744100	-0.74933600
O	-3.25499500	-1.56349400	-2.20690600
N	-1.80711700	-0.86577100	-0.63014700
C	-3.27797800	0.91225500	0.18593100
H	-2.53592100	1.18397500	0.95374900
H	-3.00072300	1.45180600	-0.73388400
C	-4.66520000	1.29916100	0.61405500
C	-5.47602200	2.07183600	-0.22218000
C	-5.19278800	0.85678300	1.83328600
C	-6.77667900	2.40586900	0.14803700
H	-5.07024100	2.41882000	-1.17432000
C	-6.49193500	1.18749400	2.20491100
H	-4.57673000	0.25165000	2.49782700
C	-7.28829900	1.96342100	1.36435500
H	-7.39057000	3.01296000	-0.51548800
H	-6.88503100	0.83797600	3.15807100
H	-8.30417600	2.22172500	1.65777100
Cu	-0.10403400	-0.96949700	0.47356100
C	1.80554500	0.73854900	2.37658800
C	2.49611100	2.89253400	1.25239000
C	3.31023000	3.97859500	0.98808900
C	4.43307800	4.15620700	1.79670500
C	4.69228000	3.26132300	2.83021100
C	3.85226900	2.17343000	3.04987400
C	2.73168900	1.95364700	2.24206400
H	3.10638800	4.66824900	0.17515200
H	5.10216200	4.99269900	1.60583900
H	5.56686800	3.40066500	3.46255700
H	4.07661900	1.46824000	3.84824900
I	0.74443000	2.38023200	0.04004700
O	1.35099900	0.43889600	1.06824000
C	2.55555500	-0.47971100	2.90550600
H	2.83997400	-0.34611700	3.95640500
H	1.89715700	-1.35213100	2.84741200
H	3.46467900	-0.67305200	2.32371800
C	0.63630700	1.06760400	3.30701800
H	-0.02022400	0.19490400	3.36943800
H	0.98348500	1.31663800	4.31741100
H	0.04741600	1.91791200	2.93900300
C	0.56522900	4.61910200	-0.54271300
F	-0.67885700	4.82652500	-0.99720700
F	1.42489500	4.98350000	-1.51593700
F	0.76100600	5.42588700	0.50609600
S	-1.27054500	-3.01138100	2.52888400
O	-0.90588900	-4.20913000	3.27737100
O	-2.30319800	-3.13683700	1.48977300
O	-0.08594200	-2.17726900	2.11578600

C	-2.06024800	-1.89899800	3.76686400
F	-1.23287100	-1.63485300	4.78334300
F	-3.18360900	-2.42924600	4.25319400
F	-2.37994900	-0.71549700	3.18318900

TS1' S**2 = 1.48

C	1.78351800	2.06692000	2.88365200
C	1.45685200	1.74941100	1.41739600
C	-0.06538100	0.80876500	2.73898100
H	1.65885800	3.13028700	3.12928000
H	2.21558000	1.09918900	0.96008600
H	2.76991800	1.73140400	3.21615300
O	0.79118900	1.32903300	3.64570800
N	0.21604700	0.97565500	1.50394600
C	1.26171200	2.96627900	0.51825800
H	0.75367300	2.61596000	-0.39205600
H	0.57195400	3.67104800	1.00480300
C	2.57164400	3.61471600	0.17681100
C	2.90060500	4.89647000	0.62157600
C	3.51060200	2.90829700	-0.58635100
C	4.13340000	5.46508400	0.30590900
H	2.17474600	5.45637100	1.21389100
C	4.74059300	3.47238500	-0.90503100
H	3.25643900	1.90555200	-0.93746700
C	5.05591700	4.75516800	-0.45785700
H	4.37251800	6.46788400	0.65652500
H	5.45224100	2.90846300	-1.50703500
H	6.01765300	5.20063400	-0.70643200
C	-1.27729300	0.17449700	3.36010600
C	-2.03070100	1.30104000	4.14287200
H	-1.46479700	1.48698200	5.06391600
H	-3.00855200	0.89958100	4.43497500
C	-0.83493400	-0.93215400	4.36278400
H	-0.20210200	-0.45065100	5.11739800
H	-1.74013400	-1.28793000	4.87010900
C	-2.15356200	2.57440300	3.35261800
C	-1.34922500	3.67302600	3.67309800
C	-2.99156000	2.65953100	2.23535300
C	-1.37971300	4.82939700	2.89704500
H	-0.68906900	3.61124400	4.53949800
C	-3.01920100	3.81013600	1.45383800
H	-3.62848600	1.81868000	1.95621600
C	-2.21093700	4.89641800	1.78142400
H	-0.74933000	5.67737000	3.16409300
H	-3.65631100	3.83880300	0.57441200
H	-2.22654300	5.79114100	1.16200800
C	-0.10521300	-2.07178600	3.70994300
C	-0.81140000	-3.13852200	3.14222600
C	1.29034000	-2.07156200	3.61976200
C	-0.14398600	-4.17687200	2.50101100
H	-1.89949600	-3.15454800	3.22006200
C	1.96362000	-3.11702600	2.99023100
H	1.85211600	-1.24660100	4.06044600
C	1.24712700	-4.17089200	2.42388300
H	-0.71035400	-5.00032700	2.06889700
H	3.05236100	-3.11476400	2.94586500
H	1.77263200	-4.98492500	1.93065300
C	-4.08683500	-1.55543000	1.82455800
C	-3.27419400	-1.23624200	0.56368900
C	-2.20623200	-0.44549800	2.35175100
H	-4.15891900	-2.63070600	2.03831200
H	-3.78920200	-0.49773900	-0.06389400
H	-5.08989800	-1.12111600	1.83691700

O	-3.33466200	-0.94390900	2.90653300	C	4.46237400	1.19296900	0.55152200
N	-2.06897900	-0.57882300	1.08699900	C	5.44372900	1.80659300	1.33296300
C	-2.90881500	-2.44300900	-0.29618100	C	4.86368400	0.40297000	-0.53345700
H	-2.11939600	-2.11619500	-0.98978700	C	6.79603400	1.64409300	1.03637100
H	-2.47446100	-3.22965800	0.33983300	H	5.13958600	2.42889100	2.17697900
C	-4.09825700	-2.95410400	-1.05810700	C	6.21139500	0.23807900	-0.83109200
C	-4.70787700	-4.17108400	-0.74777100	H	4.09962800	-0.07762500	-1.14775700
C	-4.64184000	-2.16823800	-2.08132600	C	7.18286800	0.85856800	-0.04569800
C	-5.83480700	-4.60050500	-1.44671600	H	7.54869500	2.13409800	1.65229200
H	-4.28898500	-4.79284600	0.04559400	H	6.50347800	-0.37672600	-1.68156100
C	-5.76564900	-2.59413600	-2.77926900	H	8.23875800	0.73106500	-0.27855700
H	-4.16857000	-1.21723400	-2.32572200	C	-0.73718100	0.13412300	3.25648600
C	-6.36625600	-3.81255800	-2.46360300	C	-0.64489000	1.40374100	4.16818300
H	-6.29691400	-5.55411600	-1.19600200	H	-0.11476800	1.09914800	5.07929300
H	-6.17281600	-1.97062100	-3.57383800	H	-1.67215100	1.65581900	4.46258200
H	-7.24611100	-4.14714600	-3.01045600	C	-1.11463700	-1.07770200	4.16140700
Cu	-0.68450800	0.25493200	-0.20514800	H	-0.25396200	-1.26519900	4.81445200
C	1.30568900	0.12032900	-2.46601800	H	-1.94280200	-0.75088800	4.80139500
C	3.58366100	-0.85742200	-1.84950600	C	0.05747700	2.57095500	3.53429600
C	4.95622300	-1.00907500	-1.98036200	C	1.31694100	2.96422100	3.99773600
C	5.59556100	-0.38011700	-3.04626200	C	-0.50243800	3.25149100	2.44702600
C	4.85208200	0.37288600	-3.94853100	C	1.99761300	4.02074600	3.39646900
C	3.48039500	0.51920100	-3.77336300	H	1.76333100	2.43381800	4.84030600
C	2.80696100	-0.08129100	-2.70274800	C	0.18350200	4.29432400	1.83228800
H	5.53214800	-1.58791200	-1.26601100	H	-1.48468000	2.97365400	2.06282900
H	6.67300500	-0.48086900	-3.15881300	C	1.43469000	4.68209500	2.30768000
H	5.34347600	0.86504500	-4.78549300	H	2.97317300	4.32203200	3.77629200
H	2.91284700	1.13146300	-4.47137300	H	-0.26134800	4.78893700	0.97304000
I	2.55195900	-1.79080300	-0.20857900	H	1.97086600	5.49734100	1.82586000
O	1.08552800	0.05409200	-1.07364300	C	-1.50557500	-2.32184200	3.41296800
C	0.86692500	1.50341300	-2.94991100	C	-2.85343500	-2.67324100	3.27714100
H	0.84202200	1.56699900	-4.04502700	C	-0.53877100	-3.14716300	2.82914800
H	-0.14396300	1.70675600	-2.58714600	C	-3.22819400	-3.81423000	2.57238000
H	1.53403200	2.28747400	-2.57079200	H	-3.61289900	-2.04330300	3.74008400
C	0.51672300	-0.96734900	-3.20259100	C	-0.91068900	-4.29460500	2.13233600
H	-0.55626100	-0.79178000	-3.05956400	H	0.51891200	-2.90073100	2.93869800
H	0.72922000	-0.96413700	-4.27937700	C	-2.25655200	-4.62684700	1.99362200
H	0.76354600	-1.96364800	-2.81235400	H	-4.28172800	-4.07617400	2.48650300
C	4.46383000	-3.48549500	0.02383900	H	-0.14349200	-4.94002300	1.70648500
F	3.97973700	-4.48242900	0.78443200	H	-2.54400700	-5.52297700	1.44759400
F	5.54309000	-2.98180100	0.65129300	C	-3.99382900	0.49749300	1.67859700
F	4.85676000	-4.00341900	-1.14538900	C	-3.12955600	0.35180200	0.42282700
S	-2.84528100	1.73716500	-1.63139100	C	-1.83057100	0.30126600	2.24123000
O	-1.93761700	2.86422800	-1.39736300	H	-4.73945300	-0.29746100	1.79931500
O	-4.08916400	1.68486100	-0.85443700	H	-3.22873800	1.22417500	-0.22979600
O	-2.12530600	0.41070700	-1.70707400	H	-4.48063800	1.47320500	1.76752400
C	-3.39154500	1.91176400	-3.38210800	O	-3.05396600	0.38627000	2.78443200
F	-2.34026800	1.86020400	-4.20949600	N	-1.76072900	0.33048200	0.96100800
F	-4.01784300	3.07788800	-3.55758500	C	-3.36106200	-0.92509700	-0.38740900
F	-4.23587200	0.92256700	-3.71142300	H	-2.57243800	-0.97066300	-1.15390800
				H	-3.21992900	-1.79813200	0.26851300
				C	-4.71925100	-0.93631100	-1.02470200
				C	-5.74510600	-1.74708500	-0.53313100
				C	-4.99115800	-0.08326200	-2.10076500
				C	-7.01540300	-1.71409300	-1.10466000
				H	-5.53715500	-2.42110300	0.30014900
				C	-6.25807400	-0.04846600	-2.67278700
				H	-4.19449300	0.55339600	-2.48880900
				C	-7.27410700	-0.86381500	-2.17575600
				H	-7.80289500	-2.35656400	-0.71407100
				H	-6.45354100	0.61625700	-3.51235800
				H	-8.26493100	-0.83745000	-2.62556800
				Cu	-0.17106300	0.37398300	-0.28055700
INT3'	S**2 = 0.75						
C	2.81549400	-0.45114000	2.72771700				
C	2.41564200	-0.01734100	1.31243300				
C	0.61180400	-0.06315900	2.62745500				
H	3.56404800	0.19904100	3.19366900				
H	2.65518800	-0.77701800	0.55934600				
H	3.14162600	-1.49442100	2.80091700				
O	1.58972500	-0.33278600	3.50852000				
N	0.95458400	0.07853200	1.40239400				
C	3.00128000	1.32510200	0.87015800				
H	2.43805600	1.65155200	-0.01496200				
H	2.83142600	2.07095600	1.65948300				

C	1.40209500	-0.32841400	-2.66920000
C	2.49510800	-2.60822800	-2.04639700
C	3.51489000	-3.54986200	-2.17379000
C	4.55618700	-3.34364000	-3.07249500
C	4.55924600	-2.19465800	-3.85220800
C	3.53638900	-1.26385400	-3.71175900
C	2.47721200	-1.42728400	-2.80581400
H	3.49526900	-4.45121800	-1.56570000
H	5.35046500	-4.08281100	-3.15802800
H	5.35880100	-2.01315400	-4.56846600
H	3.56297800	-0.36304000	-4.31945700
I	0.99548700	-3.16628000	-0.59521600
O	1.31762400	-0.09630800	-1.29335100
C	1.80752700	0.97841000	-3.35390900
H	1.85033700	0.90266200	-4.44840200
H	1.06204900	1.73621000	-3.09689700
H	2.77773300	1.33259200	-2.98363600
C	0.09788800	-0.83160600	-3.30685300
H	-0.66358200	-0.04536500	-3.26947400
H	0.26213900	-1.09856900	-4.35870000
H	-0.28969400	-1.71897400	-2.79345900
S	-1.23161700	2.91028200	-1.39774100
O	0.12808900	3.43912100	-1.32608700
O	-2.20732900	3.37239700	-0.40417400
O	-1.27778900	1.40516600	-1.61691900
C	-1.90581200	3.45237100	-3.02400600
F	-1.16028800	2.97371800	-4.02391400
F	-1.91414700	4.78473500	-3.08925900
F	-3.16088000	3.00741100	-3.17660900

INT2''

C	-0.96509400	3.19803900	-2.44107900
C	-1.23901700	2.34652000	-1.19052600
C	0.92884000	2.26268800	-1.68134500
H	-1.12450300	4.27159000	-2.27741100
H	-1.82304100	1.44640300	-1.44204500
H	-1.51131700	2.89132700	-3.33662100
O	0.45212900	3.00282100	-2.70875600
N	0.09394000	1.88679900	-0.79256100
C	-1.94765200	3.05626000	-0.03505600
H	-1.64918900	2.52951600	0.88327900
H	-1.57109800	4.08699700	0.04964600
C	-3.44382800	3.02769300	-0.17548000
C	-4.18618700	4.16143300	-0.50733400
C	-4.11514200	1.81181300	0.00702100
C	-5.57109700	4.08524800	-0.64769100
H	-3.67739000	5.11621400	-0.64798100
C	-5.49630000	1.73295900	-0.12809400
H	-3.53128600	0.92766100	0.27217900
C	-6.22879900	2.87299700	-0.45775100
H	-6.13829900	4.97827400	-0.90286200
H	-6.00130700	0.78053200	0.03072300
H	-7.31034200	2.81736500	-0.56306200
C	2.40811000	1.99933300	-1.74794900
C	3.15496300	3.36340100	-1.63161600
H	2.81777300	3.98965800	-2.46645500
H	4.22283700	3.16585000	-1.78072400
C	2.74102200	1.35156300	-3.12915700
H	2.30003400	1.99079600	-3.90285400
H	3.82854800	1.38913100	-3.25559300
C	2.92197200	4.04855000	-0.31512600
C	1.79887100	4.86049300	-0.11743800
C	3.80051900	3.85071100	0.75578600

C	1.56010900	5.46185200	1.11687600
H	1.11770400	5.03905200	-0.95072400
C	3.57183200	4.45747400	1.98841200
H	4.68593400	3.23024400	0.60959000
C	2.44810800	5.26118000	2.17443400
H	0.68888900	6.10064900	1.25001000
H	4.27515600	4.30709300	2.80558500
H	2.27047100	5.74086800	3.13492100
C	2.25682900	-0.06794100	-3.24882800
C	3.15833500	-1.13237600	-3.13809900
C	0.90142300	-0.35944500	-3.44378700
C	2.72124200	-2.45230300	-3.21865000
H	4.21848600	-0.91641700	-3.00294600
C	0.46074100	-1.67873200	-3.51920700
H	0.18839300	0.45654500	-3.57162800
C	1.36926300	-2.73032300	-3.40118000
H	3.44029300	-3.26711700	-3.15362900
H	-0.59237500	-1.88782900	-3.70850200
H	1.02851900	-3.75975500	-3.47751500
C	4.59617400	-0.13269100	0.22565600
C	3.26907400	-0.45418300	0.92039100
C	2.92222700	1.06582600	-0.67642200
H	5.07947000	-1.00226600	-0.23306100
H	3.32209900	-0.25460300	1.99981100
H	5.32070600	0.38247400	0.86465200
O	4.22853300	0.78097300	-0.83872100
N	2.32167700	0.49354200	0.30760600
C	2.75831600	-1.88278100	0.70502100
H	1.75025800	-1.93259100	1.14749700
H	2.63512100	-2.04526900	-0.37703300
C	3.66981300	-2.91171300	1.30633800
C	4.57058800	-3.62470800	0.50990800
C	3.67021400	-3.13911100	2.68692900
C	5.45136300	-4.54319900	1.07615300
H	4.56835100	-3.46488600	-0.57009800
C	4.54747400	-4.05609800	3.25636300
H	2.96353000	-2.59676000	3.31876200
C	5.44213600	-4.75914300	2.45128900
H	6.14202000	-5.09470800	0.44133400
H	4.53049200	-4.22778700	4.33083100
H	6.12652800	-5.47858800	2.89559900
Cu	0.42989000	0.59905100	0.84007000
C	-1.93763100	-0.47914200	2.34118300
C	-3.37278100	-1.92951100	0.83190400
C	-4.52421100	-2.58504100	0.43309600
C	-5.61430800	-2.56042500	1.30279600
C	-5.51686700	-1.89576600	2.52066900
C	-4.34329000	-1.23646600	2.87106000
C	-3.23367400	-1.22803800	2.01909000
H	-4.60340100	-3.09099300	-0.52280400
H	-6.53663400	-3.05830700	1.01295300
H	-6.36624900	-1.87785200	3.19948500
H	-4.28624400	-0.70564300	3.81934300
I	-1.59017500	-1.84889000	-0.42494800
O	-1.37906000	-0.09158400	1.09770900
C	-2.21485400	0.79409700	3.13376900
H	-2.54871900	0.57811500	4.15526400
H	-1.29405500	1.38393100	3.19445400
H	-2.98035700	1.40310800	2.63803000
C	-0.97731700	-1.39247200	3.10656900
H	-0.02792500	-0.85964000	3.26541100
H	-1.38090400	-1.68802000	4.08236900
H	-0.75674400	-2.30930300	2.54407300

C	-2.29487800	-3.69394300	-1.61660600
F	-1.24358600	-4.13062700	-2.31611800
F	-3.27310000	-3.38200400	-2.47334900
F	-2.71387300	-4.67009400	-0.81511500
O	0.71075400	2.31981900	2.37847000
C	1.67379600	2.03644300	3.38138700
H	1.79436900	2.87808300	4.07613600
H	1.29890000	1.17210100	3.93907100
H	2.65574100	1.78775800	2.95095100
H	1.01753300	3.09548800	1.87605700

MeOH

C	0.65525800	-0.01935500	0.00000100
H	1.03695200	-0.54227400	-0.89272200
H	1.07267400	0.99144500	-0.00065600
H	1.03706400	-0.54116800	0.89333200
O	-0.74424800	0.12174900	0.00000300
H	-1.12425100	-0.76586900	0.00001200

TS1'' S**2 = 1.04

C	-4.14829900	0.71946200	2.17810500
C	-3.20335400	1.21022700	1.07340000
C	-2.86705000	-0.96510900	1.43412800
H	-5.20903600	0.87291800	1.95303400
H	-2.55214600	2.02091900	1.42812300
H	-3.93021300	1.12528600	3.17072400
O	-3.91264400	-0.71372300	2.23763100
N	-2.37046100	0.02972400	0.79199200
C	-3.91507600	1.65421900	-0.20878300
H	-3.14159000	1.89271300	-0.95181000
H	-4.47350900	0.79264800	-0.60564400
C	-4.83463100	2.81822200	0.02410900
C	-6.21929300	2.63396200	0.07778200
C	-4.32126700	4.10156700	0.24133100
C	-7.07339000	3.70353100	0.33578900
H	-6.63172100	1.63807200	-0.09717400
C	-5.17058600	5.17239600	0.49947900
H	-3.24308400	4.26318200	0.19852800
C	-6.54952400	4.97547500	0.54791400
H	-8.14917700	3.54311400	0.36723700
H	-4.75610000	6.16573000	0.65958100
H	-7.21386800	5.81352100	0.74704400
C	-2.47222400	-2.41778700	1.41758800
C	-3.73198200	-3.23929300	1.00536000
H	-4.48030800	-3.11546200	1.79597400
H	-3.44175000	-4.29606900	0.98890600
C	-1.98947700	-2.84129200	2.84372000
H	-2.72486200	-2.46815600	3.56688400
H	-2.01730900	-3.93647700	2.88578200
C	-4.28466600	-2.80817400	-0.32709900
C	-5.36043300	-1.91663900	-0.40443700
C	-3.69671200	-3.24840100	-1.52102400
C	-5.83341900	-1.47237900	-1.63793300
H	-5.83847200	-1.57821500	0.51568600
C	-4.16553300	-2.80338600	-2.75547000
H	-2.87913800	-3.96894400	-1.48147100
C	-5.23294000	-1.90819700	-2.81678500
H	-6.68107800	-0.79055500	-1.67945500
H	-3.70357000	-3.16666200	-3.67201900
H	-5.60499400	-1.56539500	-3.78017400
C	-0.60038900	-2.34343000	3.13720700
C	0.48796300	-3.21956300	3.07187000
C	-0.35389900	-0.98757700	3.38437400

C	1.79000800	-2.75567600	3.24587800
H	0.30588100	-4.27940600	2.89113700
C	0.94638600	-0.51694900	3.54284700
H	-1.18991900	-0.29156000	3.46882800
C	2.02254500	-1.40065600	3.47133200
H	2.62324400	-3.45608100	3.21609400
H	1.11921000	0.54038100	3.73507600
H	3.03844200	-1.03643900	3.61724400
C	0.11603500	-4.14965700	-0.45949900
C	0.36912500	-2.72021700	-0.95598100
C	-1.35333000	-2.72796200	0.46346800
H	0.92655500	-4.53386600	0.17282100
H	0.15234200	-2.61599700	-2.03042400
H	-0.10297400	-4.87824400	-1.24363300
O	-1.06989900	-4.03727900	0.37599000
N	-0.62868300	-1.92528000	-0.22415200
C	1.76999400	-2.18868500	-0.66670700
H	1.78065600	-1.12575300	-0.95272900
H	1.92830200	-2.22191400	0.42290000
C	2.84082300	-2.95370900	-1.38810800
C	3.63099700	-3.88865600	-0.71365900
C	3.03747400	-2.77351600	-2.76191300
C	4.59582300	-4.62853600	-1.39321300
H	3.49477000	-4.02589000	0.36078200
C	4.00088200	-3.50981100	-3.44334500
H	2.43265700	-2.03979400	-3.29819900
C	4.78115400	-4.44104100	-2.75999900
H	5.20702900	-5.34871400	-0.85291700
H	4.14791900	-3.35389500	-4.51025300
H	5.53655200	-5.01513700	-3.29219500
Cu	-0.58116000	0.07823200	-0.17754700
C	0.83300700	2.21917200	-1.39079600
C	3.02179600	3.01371500	-0.30200500
C	4.02521800	3.94594300	-0.06924700
C	3.96496100	5.18017500	-0.70959000
C	2.90694800	5.45531300	-1.56617600
C	1.91093600	4.50659300	-1.76821400
C	1.92920800	3.25708700	-1.13532600
H	4.84335000	3.72721300	0.61038400
H	4.74488000	5.91627300	-0.52941900
H	2.84805700	6.41458000	-2.07524300
H	1.08621900	4.74621900	-2.43540200
I	3.20388500	1.12612500	0.70693300
O	0.58306400	1.52691100	-0.18709000
C	-0.48623200	2.87469200	-1.80765300
H	-0.43060900	3.36048400	-2.78875500
H	-1.24501200	2.08583700	-1.87221600
H	-0.80845500	3.61300500	-1.06459200
C	1.29099400	1.25746400	-2.49554100
H	0.52968100	0.47479200	-2.63641600
H	1.44055700	1.77560300	-3.45130400
H	2.23882400	0.77239500	-2.22818800
C	6.00338400	1.37533500	0.85877900
F	6.40929300	0.15816200	1.17453000
F	6.37378900	2.24720800	1.78733600
F	6.45627500	1.73656200	-0.32864600
C	-2.46142000	0.30099600	-3.49255800
H	-1.67103300	0.90743000	-3.94431800
H	-2.78657700	-0.44825900	-4.22747300
H	-3.31384400	0.95568700	-3.25315500
O	-1.90611700	-0.30337100	-2.33565000
H	-2.57571900	-0.89878300	-1.95812700

INT3'' S**2 = 0.75

C	1.30265200	-3.84048900	-0.43187600
C	1.30658700	-2.37773500	-0.89283800
C	-0.45181000	-2.75096400	0.44238400
H	2.12982200	-4.07596200	0.24952200
H	1.10905200	-2.28839700	-1.97233100
H	1.27507600	-4.57895400	-1.23597600
O	0.06618200	-3.97840500	0.32870600
N	0.14898100	-1.80629300	-0.18437400
C	2.57374400	-1.60739500	-0.53821900
H	2.41286800	-0.55250200	-0.80720800
H	2.69351000	-1.63153900	0.55611400
C	3.78991600	-2.15815800	-1.22487000
C	4.71750200	-2.93389300	-0.52446000
C	3.99504900	-1.93439900	-2.59086400
C	5.82564000	-3.47600600	-1.17133000
H	4.57510100	-3.09933500	0.54506700
C	5.10061100	-2.47391800	-3.23974100
H	3.28515200	-1.31869400	-3.14657400
C	6.01767000	-3.24820700	-2.53094200
H	6.54300800	-4.07179900	-0.61056300
H	5.25234900	-2.28428500	-4.30048300
H	6.88464000	-3.66673400	-3.03751400
C	-1.64870800	-2.67468700	1.34730500
C	-1.15508200	-3.02744400	2.79077600
H	-1.00704800	-4.11324800	2.82672700
H	-1.96866900	-2.78671600	3.48616900
C	-2.71808800	-3.70129800	0.86308700
H	-2.23436200	-4.68428800	0.83037000
H	-3.50282800	-3.74646100	1.62623900
C	0.12518800	-2.31463900	3.13297700
C	1.33676100	-3.01276200	3.12691000
C	0.15107700	-0.93130700	3.35252300
C	2.54452200	-2.34847500	3.33118700
H	1.32752400	-4.09157400	2.96743800
C	1.35750000	-0.26033400	3.53174500
H	-0.78432600	-0.37067600	3.39624200
C	2.55834900	-0.96853000	3.51919900
H	3.47594600	-2.91220600	3.34840000
H	1.36198900	0.81669600	3.68718000
H	3.49980200	-0.44438500	3.67213000
C	-3.29578500	-3.33230400	-0.47816300
C	-4.53252800	-2.68497600	-0.57383900
C	-2.57973600	-3.57899600	-1.65803300
C	-5.03686700	-2.28581800	-1.81050900
H	-5.10997700	-2.50347800	0.33332300
C	-3.07991900	-3.17725800	-2.89524700
H	-1.63316400	-4.11825500	-1.60884400
C	-4.30769300	-2.52056600	-2.97375100
H	-6.00841100	-1.79806800	-1.86749200
H	-2.51559600	-3.39137700	-3.80147600
H	-4.70272700	-2.21257500	-3.93967700
C	-3.89849600	0.09652300	2.05257300
C	-3.01322400	0.76989000	0.99690900
C	-2.30315000	-1.32028700	1.36088800
H	-4.96001300	0.06793800	1.78694500
H	-2.54766200	1.68566000	1.38539300
H	-3.78925000	0.50773600	3.06065800
O	-3.41860900	-1.27712100	2.09648500
N	-1.95935900	-0.23385300	0.76434600
C	-3.73269700	1.07806800	-0.32116400
H	-2.98891300	1.48194900	-1.02129500
H	-4.08149100	0.12637700	-0.75069200

C	-4.88293800	2.02494100	-0.13191500
C	-6.19901300	1.55314600	-0.13062000
C	-4.65905900	3.38682200	0.09685900
C	-7.26817000	2.41823900	0.08892000
H	-6.38546400	0.49341800	-0.31665900
C	-5.72415500	4.25418100	0.31670500
H	-3.63828300	3.77221400	0.09263000
C	-7.03156500	3.77122200	0.31419700
H	-8.28661700	2.03539100	0.07981900
H	-5.53454900	5.31208100	0.48655600
H	-7.86424100	4.45033800	0.48346200
Cu	-0.17943600	0.13834700	-0.07109500
C	0.86993300	2.59468700	-1.10515500
C	2.89371900	3.69134900	0.07985400
C	3.64781800	4.81049200	0.42617100
C	3.24519200	6.07865800	0.02228000
C	2.08786400	6.21704700	-0.73134500
C	1.34563600	5.09108900	-1.06656000
C	1.71428900	3.79664300	-0.67227800
H	4.55513400	4.69083200	1.01225500
H	3.84076000	6.94608100	0.29798300
H	1.75615100	7.19907500	-1.06086400
H	0.44176000	5.22758700	-1.65445900
I	3.70773600	1.83141100	0.77437500
O	0.70143700	1.72662700	-0.00360000
C	-0.54047500	2.99652700	-1.55278600
H	-0.53398300	3.58862900	-2.47450200
H	-1.10332200	2.07723700	-1.75222700
H	-1.05633900	3.56482600	-0.77024000
C	1.55470900	1.85105800	-2.26053500
H	0.97367400	0.95068100	-2.51259200
H	1.62383600	2.48604200	-3.15208400
H	2.57032800	1.54312500	-1.98618300
C	-1.81986200	0.17005100	-3.50088900
H	-1.11778900	0.92967000	-3.85613600
H	-1.92876600	-0.59435100	-4.28204900
H	-2.79778600	0.64554200	-3.32986600
O	-1.27236100	-0.37321100	-2.30849400
H	-1.85026700	-1.10087700	-2.02043800