



Supporting Information

Understanding Regioselectivities of Corey–Chaykovsky Reactions of Dimethylsulfoxonium Methylide (DMSOM) and Dimethylsulfonium Methylide (DMSM) toward Enones: A DFT Study

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1. Diastereoselectivities and regioselectivities of DMSM derivatives toward enones

For **Ar-DMSM**, two competing pathways of cyclopropanation are shown in **Figure S1**, the rate determining transition states **TS9-1** and **TS9-2** are close in energy, and subsequent nucleophilic substitutions via **TS10-1** and **TS10-2** give the cyclopropanation products **Ar-PR1-1** and **Ar-PR1-2**. These calculations suggest that, the reaction would give a mixture of both cyclopropane products. These calculation results agree with experimental observations.^[1]

The potential energy surfaces of two competing pathways of epoxidation for **Ar-DMSM** are shown in **Figure S2**. The epoxidations having activation free energies of 27.7 and 30.0 kcal/mol are not favored compared to cyclopropanations, agreeing with experiments.

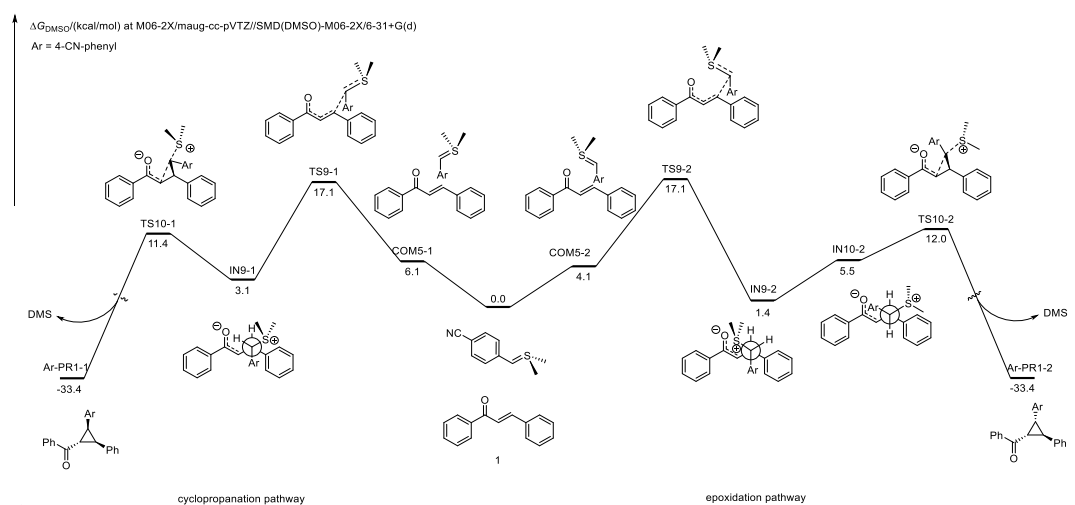


Figure S1. DFT computed energy surfaces of cyclopropanation reactions of **Ar-DMSM** with enone

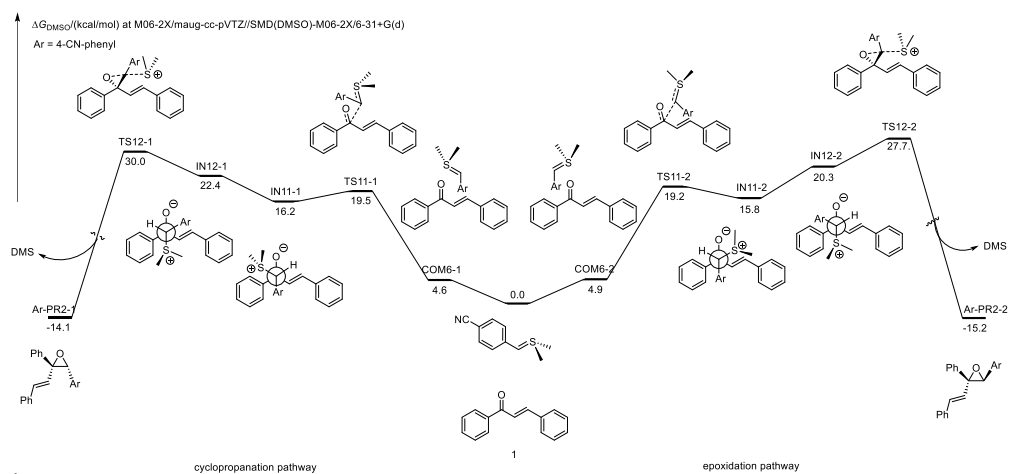


Figure S2. DFT computed energy surfaces of epoxidation reactions of **Ar-DMSM** with enone

For **E-DMSM**, two competing pathways of cyclopropanation are shown in **Figure S3**. In the rate determining step, **TS13-1** is 0.4 kcal/mol higher than **TS13-2** in energy, and subsequent nucleophilic substitutions via **TS14-1** and **TS14-2** give the cyclopropanation products **E-PR1-1** and **E-PR1-2**. Therefore, the reaction would give a mixture of both cyclopropane products. These calculation results are in agreement with experimental observations.^[2]

Two competing pathways of epoxidation are shown in **Figure S4**. The epoxidations having activation free energies of 34.0 and 35.5 kcal/mol are not favored compared to cyclopropanations, agreeing with experiments.

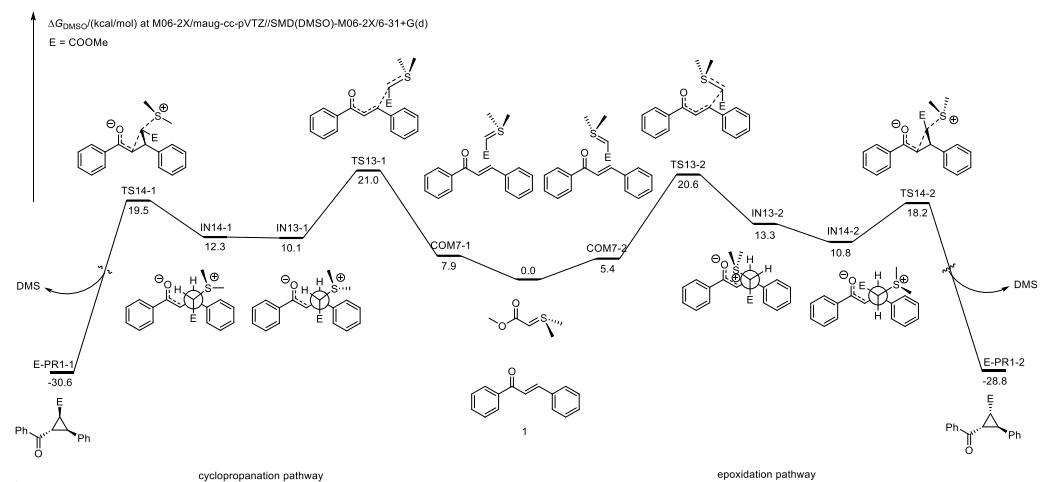


Figure S3. DFT computed energy surfaces of cyclopropanation reactions of **E-DMSM** with enone

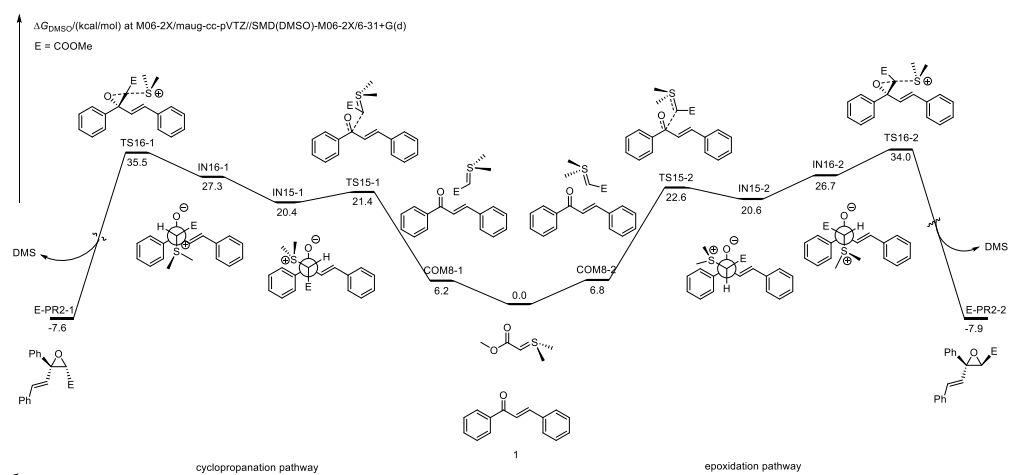


Figure S4. DFT computed energy surfaces of epoxidation reactions of **E-DMSM** with enone

2. Discussion on solvation effects

It is shown here (Figure S5) that the computed potential energy surfaces at the SMD(DMSO)-M06-2X/maug-cc-pVTZ//SMD(DMSO)-M06-2X/6-31+G(d) level are similar to those from M06-2X/maug-cc-pVTZ//SMD(DMSO)-M06-2X/6-31+G(d) (which used in the main text of this paper, Figure 1). Therefore calculations at M06-2X/maug-cc-pVTZ//SMD(DMSO)-M06-2X/6-31+G(d) level were used in order to reduce the computing times at SMD(DMSO)-M06-2X/maug-cc-pVTZ//SMD(DMSO)-M06-2X/6-31+G(d) level. The computed activation free energies are close to 16.6 kcal/mol measured experimentally (this value is computed based on the relative reaction rate of DMSOM toward *trans*-PhCH=CHCOPh and *trans*-PhCH=CHCOCH₃, the latter reaction had a measured activation free energy of 18.4 kcal/mol).^[3]

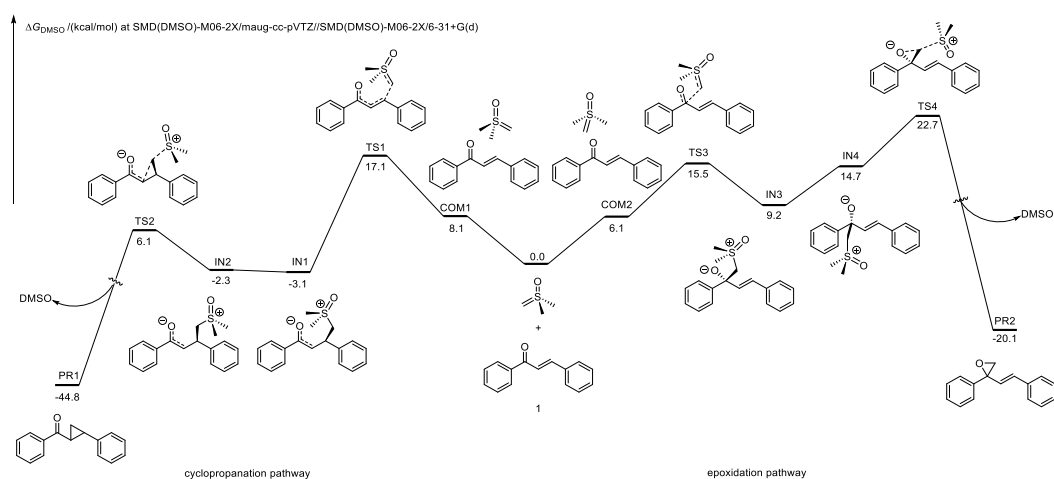


Figure S5. DFT computed energy surfaces at SMD(DMSO)-M062X/maug-cc-pVTZ// SMD(DMSO)-M062X/6-31+G(d)

We point out here that our calculation methods (low level geometry optimization in solvent, and high level gas phase calculations to obtain free energies in solutions) at M06-2X/maug-cc-pVTZ//SMD(DMSO)-M06-2X/6-31+G(d) level can help us roughly appreciate how solvent affects each step. For example, we present the free energy surfaces in both DMSO and gas phase together, for both ylides' reactions with enone (Figures S6 and S7) and we can see that, high-dielectric constant solvent DMSO influences the shapes of energy surfaces significantly. Especially DMSO is found to stabilize the zwitterionic species dramatically and this can promote the epoxidation reaction pathways significantly. Here we use an assumption that the thermal corrections to Gibbs free energy computed in solution phase are close to those from gas phase calculations.

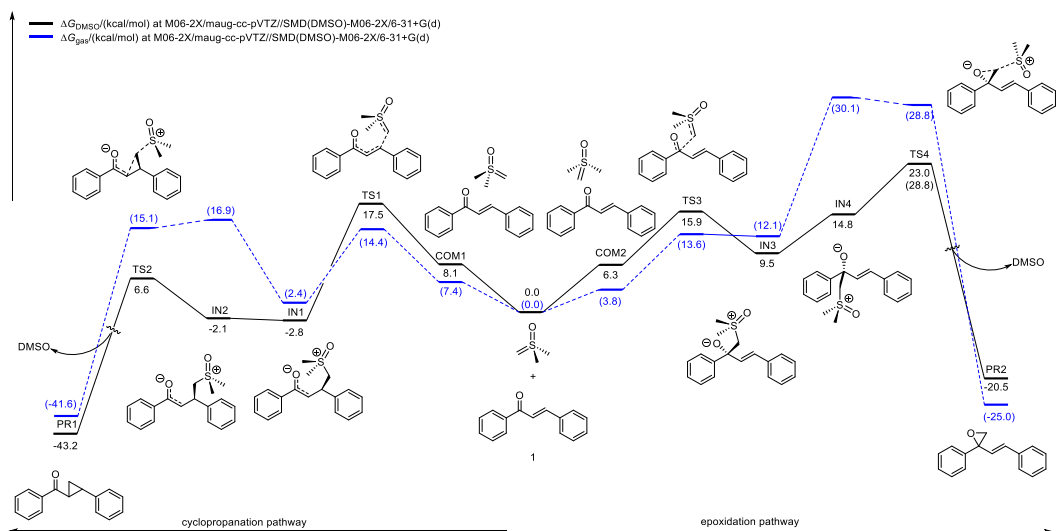


Figure S6. Comparison of gas-phase and sol-phase energy surfaces for DMSOM with enone

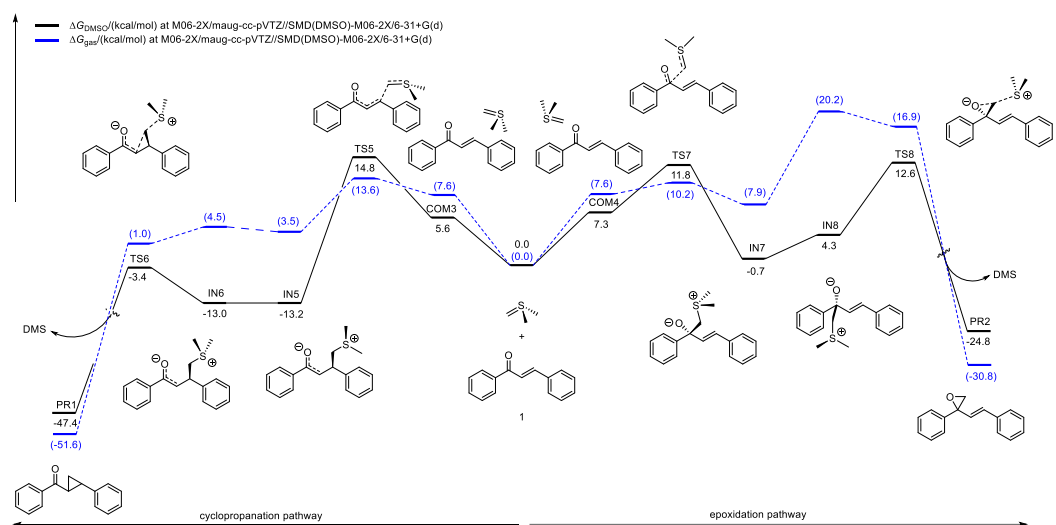


Figure S6. Comparison of gas-phase and sol-phase energy surfaces for DMSM with enone

3. HOMOs of sulfur ylides

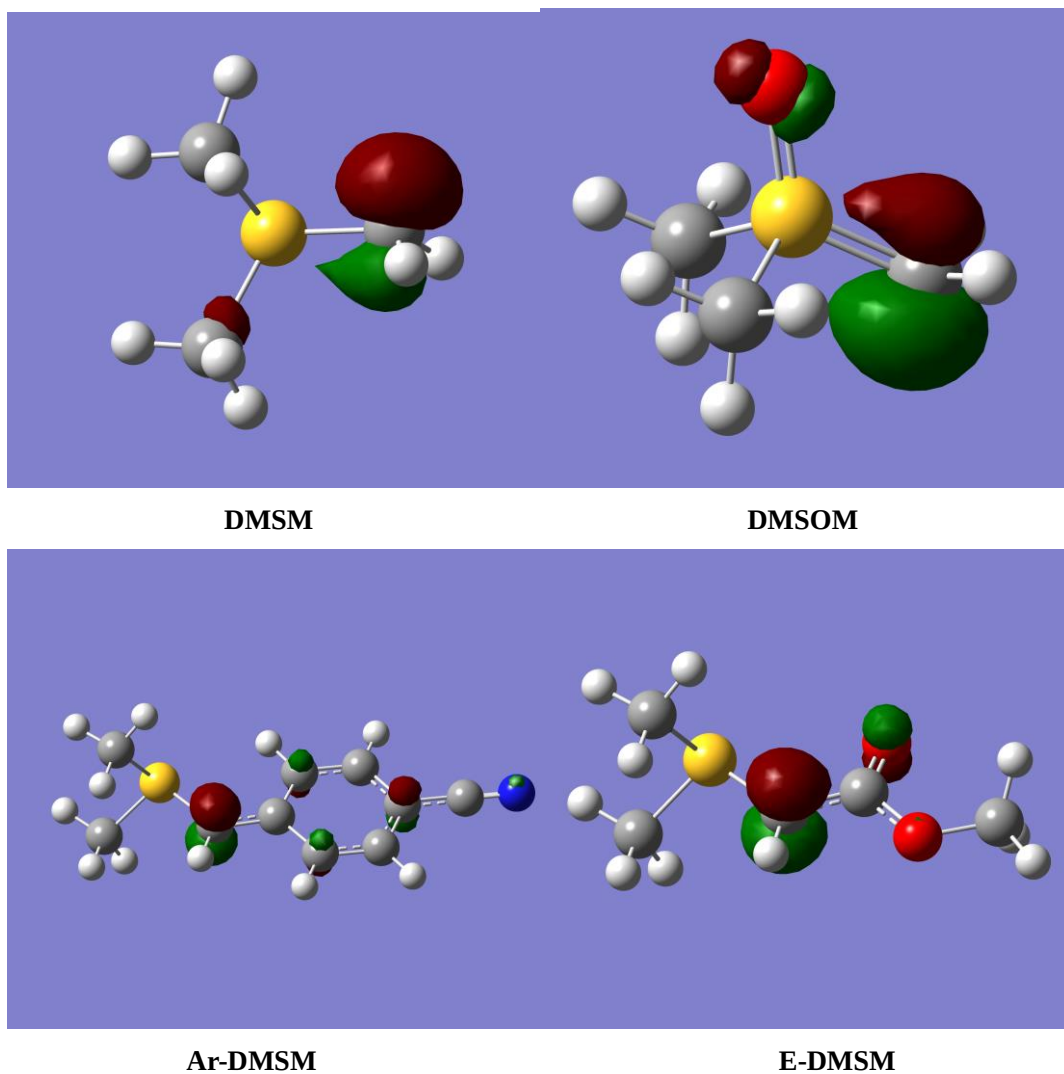


Figure S7. HOMOs of sulfur ylides

4. References

- [1] R. Appel, N. Hartmann, H. Mayr, *J. Am. Chem. Soc.* **2010**, *132*, 17894–17900.
- [2] a) G. A. Tolstikov, F. Z. Galin, V. N. Iskandarova, L. M. Khalilov, A. A. Panasenkov, *Russ. Chem. Bull.* **1985**, *34*, 2117–2122; b) M. F. Oswald, S. A. Raw, R. J. K. Taylor, *Org. Lett.* **2004**, *6*, 3997–4000.
- [3] F. Rocquet, A. Sevin, *Bulletin de la Societe Chimique de France* **1974**, *174*, 881.

5. Computed Energies of All of the Stationary Points

Table S1 Computed Energies of All Stationary Points

	TCG ^a (a.u.)	ΔG_{solv}^a (a.u.)	SPE ^b (a.u.)
enone	0.184504	-0.01921	-653.98727
DMSOM	0.078058	-0.01753	-592.417277
DMSO	0.051544	-0.01503	-553.189262
DMS	0.049855	-0.00435	-477.996036
DMSM	0.073962	-0.01174	-517.212464
PR1	0.21418	-0.01986	-693.291568
PR2	0.212251	-0.01706	-693.256349
COM1	0.283799	-0.03259	-1246.414055
COM2	0.283304	-0.02973	-1246.419226
TS1	0.284602	-0.02886	-1246.403604
IN1	0.290252	-0.04212	-1246.428343
IN2	0.288579	-0.06406	-1246.40359
TS2	0.284958	-0.04726	-1246.402828
TS3	0.28613	-0.03002	-1246.406431
IN3	0.287676	-0.0381	-1246.410219
IN4	0.287835	-0.05823	-1246.38179
TS4	0.284209	-0.04292	-1246.380288
COM3	0.276003	-0.031061	-1171.205152
TS5	0.278717	-0.02796	-1171.195986
IN5	0.284988	-0.05456	-1171.22072
IN6	0.285188	-0.05573	-1171.219325
TS6	0.283203	-0.03486	-1171.222911
COM4	0.279724	-0.02849	-1171.208884
TS7	0.278477	-0.02532	-1171.203565
IN7	0.284911	-0.04153	-1171.21366
IN8	0.283835	-0.05326	-1171.192928
TS8	0.281694	-0.03486	-1171.196011
Ar-DMSM	0.143737	-0.02612	-840.512292
COM5-1	0.352911	-0.042636	-1494.514199
COM5-2	0.351275	-0.036772	-1494.521622
COM6-1	0.350172	-0.037224	-1494.519301
COM6-2	0.351671	-0.036525	-1494.520897
TS9-1	0.354532	-0.043766	-1494.497093
TS9-2	0.356021	-0.037937	-1494.504452
IN9-1	0.356489	-0.052079	-1494.513104
IN9-2	0.357676	-0.049488	-1494.519589
IN10-2	0.357211	-0.061422	-1494.500602
TS10-1	0.354584	-0.039427	-1494.510573
TS10-2	0.355737	-0.04343	-1494.506873
TS11-1	0.355079	-0.041246	-1494.496395

TS11-2	0.353859	-0.039022	-1494.497948
IN11-1	0.356481	-0.04481	-1494.499449
IN11-2	0.357094	-0.044242	-1494.501231
IN12-1	0.355651	-0.05974	-1494.473858
IN12-2	0.355264	-0.055369	-1494.481178
TS12-1	0.355102	-0.043258	-1494.47772
TS12-2	0.354166	-0.040391	-1494.483307
Ar-PR-1-1	0.284685	-0.028543	-1016.575504
Ar-PR-1-2	0.284562	-0.030099	-1016.573843
Ar-PR-2-1	0.284007	-0.026967	-1016.545578
Ar-PR-2-2	0.282851	-0.026168	-1016.547016
E-DMSM	0.111315	-0.020334	-745.118765
COM-7-1	0.31753	-0.040042	-1399.111712
COM-7-2	0.318303	-0.031325	-1399.125039
COM-8-1	0.317592	-0.033136	-1399.121316
COM-8-2	0.319019	-0.033913	-1399.12109
TS13-1	0.319897	-0.042169	-1399.090995
TS13-2	0.32079	-0.034656	-1399.100127
IN13-1	0.324018	-0.052234	-1399.102371
IN13-2	0.324541	-0.041288	-1399.108852
IN14-1	0.324253	-0.052861	-1399.098583
IN14-2	0.323553	-0.064617	-1399.088544
TS14-1	0.321805	-0.036857	-1399.100597
TS14-2	0.321307	-0.040418	-1399.098574
TS-15-1	0.320515	-0.03498	-1399.098165
TS-15-2	0.322651	-0.036239	-1399.097156
IN15-1	0.322006	-0.04034	-1399.095857
IN15-2	0.323748	-0.042446	-1399.095259
IN16-1	0.322236	-0.05163	-1399.073854
IN16-2	0.322582	-0.049498	-1399.077355
TS-16-1	0.319642	-0.03729	-1399.074886
TS-16-2	0.321939	-0.037231	-1399.074816
E-PR-1-1	0.250344	-0.024449	-921.173856
E-PR-1-2	0.251109	-0.025551	-921.170605
E-PR-2-1	0.249353	-0.024224	-921.136909
E-PR-2-2	0.249372	-0.023518	-921.137168
CH ₃ ⁺	0.013307	-0.131107	-39.466889
SMe ₃ ⁺	0.087471	-0.09363	-517.643048
SOMe ₃ ⁺	0.090828	-0.107501	-592.821031

^aComputed at SMD(DMSO)-M06-2X/6-31+G(d) level, $\Delta G_{\text{solv}} = SPE_{\text{DMSO}}(\text{DZ}) - SPE_{\text{gas}}(\text{DZ})$

^bComputed at M06-2X/maug-cc-pVTZ//SMD(DMSO)-M06-2X/6-31+G(d) Level

$G_{\text{total}} = TCG(\text{DZ}) + \Delta G_{\text{solv}}(\text{DZ}) + SPE(\text{TZ}) + 1.89 \text{ kcal/mol}$

6. Cartesian Coordinates of All Stationary Points

enone

C	-1.18817600	-0.99872200	-0.00098000
C	0.07720000	-0.22963500	-0.08928000
H	0.01787000	0.83274200	-0.30243900
C	1.25771400	-0.84962400	0.08083300
H	1.24050000	-1.91735600	0.30015200
C	2.59102100	-0.24110000	0.01254200
C	3.70585200	-1.05026100	0.27945400
C	2.79942400	1.11180600	-0.30664200
C	4.99644500	-0.52647000	0.23332700
H	3.55257400	-2.09860700	0.52502200
C	4.08727900	1.63397300	-0.35277300
H	1.95437400	1.75936700	-0.52297900
C	5.18997100	0.81765000	-0.08246200
H	5.84833900	-1.16679800	0.44375200
H	4.23499200	2.68119700	-0.60113800
H	6.19424000	1.23030500	-0.11983500
C	-2.48120700	-0.24029700	0.00981500
C	-2.55422100	1.10534600	0.39045900
C	-3.65384200	-0.91909200	-0.34743800
C	-3.78529400	1.75998400	0.41536000
H	-1.66208800	1.64586000	0.69221300
C	-4.87881600	-0.25979900	-0.33898300
H	-3.59166400	-1.96383000	-0.63767800
C	-4.94614400	1.08204900	0.04434600
H	-3.83584800	2.80022100	0.72368500
H	-5.78162700	-0.78958300	-0.62942500
H	-5.90277100	1.59696300	0.05514500
O	-1.19651600	-2.22316600	0.04850600

DMSOM

C	0.00001400	1.65060300	-0.47377200
S	0.00000000	0.09911600	0.12971700
O	-0.00000200	-0.24047700	1.58935600
H	-0.91779400	2.17430700	-0.20127800
H	0.91782700	2.17429400	-0.20127200
C	-1.40944000	-0.72130200	-0.59940300
H	-1.33020700	-0.69383500	-1.68629700
H	-1.42420700	-1.74746400	-0.22659700
H	-2.30264700	-0.18792200	-0.26325900
C	1.40942900	-0.72132300	-0.59940300

H	1.33019000	-0.69386100	-1.68629700
H	2.30264300	-0.18794900	-0.26326800
H	1.42418800	-1.74748300	-0.22659100

DMSM

S	0.14241700	-0.03640100	-0.46789200
C	-1.10529500	-1.17803100	0.21933400
H	-1.13044000	-1.07217800	1.30780100
H	-2.08687800	-0.95881500	-0.21052100
H	-0.80070800	-2.19139800	-0.05178100
C	-0.55984900	1.48680400	0.19924700
H	0.05305800	2.31542300	-0.15906000
H	-1.58697000	1.59712400	-0.15667000
H	-0.53665300	1.44610300	1.29201400
C	1.65850700	-0.18424200	0.30290500
H	1.57750800	-0.39530700	1.37279500
H	2.27223700	-0.90572500	-0.23721800

DMSO

S	0.00000100	0.21740200	-0.44750000
C	1.35123700	-0.79630100	0.18903400
H	1.24382200	-0.89555500	1.27304900
H	1.32728500	-1.77684600	-0.29483900
H	2.28824900	-0.28975100	-0.05365100
C	-1.35124100	-0.79629500	0.18903400
H	-2.28825100	-0.28974100	-0.05365200
H	-1.32729400	-1.77684000	-0.29483800
H	-1.24382600	-0.89554800	1.27305000
O	0.00000400	1.50017800	0.38030800

DMS

S	0.00000000	0.00000000	0.66570700
C	0.00000000	1.37509300	-0.51538200
H	0.89403500	1.34790100	-1.14471300
H	-0.89403500	1.34790100	-1.14471300
H	0.00000000	2.30682300	0.05606100
C	0.00000000	-1.37509300	-0.51538200
H	0.89403500	-1.34790100	-1.14471300
H	0.00000000	-2.30682300	0.05606100
H	-0.89403500	-1.34790100	-1.14471300

PR1

C	-1.31939800	1.21601800	0.00376000
C	1.23567100	1.26494100	0.14718900

H	1.02624700	1.70592600	1.11870700	H	3.43194100	1.83732600	-1.13585000
C	2.40049900	0.33764800	0.12450900	C	4.20280600	-1.63564900	0.38393800
C	3.10690500	0.09993500	1.30984100	H	2.14991200	-1.67028000	1.00001400
C	2.81727000	-0.31141900	-1.04607300	C	5.21591500	-0.92264100	-0.26315100
C	4.20435000	-0.76110000	1.32842600	H	5.71418700	0.89438700	-1.31113900
H	2.79302200	0.59760000	2.22467100	H	4.41587900	-2.60846000	0.81877600
C	3.91194000	-1.17368200	-1.02797500	H	6.21651100	-1.33940200	-0.33623300
H	2.28692500	-0.14710800	-1.98167200	C	-2.37246900	0.06052100	0.08907800
C	4.61115600	-1.40245900	0.15892400	C	-2.56222600	-1.22686400	0.60494900
H	4.73971700	-0.93018300	2.25888600	C	-3.33580700	0.60274400	-0.76555800
H	4.21979400	-1.66890900	-1.94501900	C	-3.69953900	-1.95910500	0.26812300
H	5.46439200	-2.07489800	0.17034900	H	-1.83000800	-1.65946900	1.28198700
C	-2.37887800	0.15653400	0.00856800	C	-4.47191100	-0.13342500	-1.10442900
C	-2.08058400	-1.19446400	-0.20521500	H	-3.19141200	1.60209800	-1.16517200
C	-3.70217800	0.53927900	0.26368900	C	-4.65726200	-1.41611600	-0.58997900
C	-3.09499100	-2.15018900	-0.16030200	H	-3.83750900	-2.95569700	0.67849600
H	-1.05852500	-1.51405300	-0.38602800	H	-5.21152600	0.29770600	-1.77371100
C	-4.71554900	-0.41355300	0.29154800	H	-5.54179600	-1.98917800	-0.85370200
H	-3.92545800	1.58879900	0.43212500				
C	-4.41218100	-1.76108000	0.08142400	COM1			
H	-2.85513500	-3.19819000	-0.31486400	C	0.80763600	-1.04691500	0.76327500
H	-5.74144700	-0.10893900	0.47794400	C	2.47379400	1.88698300	-0.62917900
H	-5.20250300	-2.50628000	0.10736900	O	-1.35873900	0.54619000	1.57060400
O	-1.52054200	2.29300600	0.54874800	S	1.33659000	3.07814400	-0.40056400
C	-0.02153600	0.92716800	-0.66093000	O	1.54546100	4.52549300	-0.73124800
H	0.04147300	0.04334600	-1.28543200	H	2.68924400	1.73738600	-1.68811300
C	0.85254700	2.09311500	-1.03276300	H	3.34830100	2.04538600	0.00340100
H	1.44083700	1.98902500	-1.93966200	C	-0.12355200	2.55050500	-1.28463200
H	0.44473200	3.07965700	-0.83507300	H	-0.40089300	1.54207300	-0.97603600
				H	-0.91918100	3.26764700	-1.07167600
PR2				H	0.12203200	2.57116700	-2.34989500
C	-1.33617400	2.01540400	1.38736400	C	0.86248300	2.99290900	1.31820100
O	-1.14838000	2.20310700	-0.01158100	H	0.41297000	2.02012100	1.52712700
C	-1.15812800	0.86516300	0.46641800	H	1.76880900	3.14360500	1.91103600
H	-2.33441700	2.25115100	1.75280000	H	0.15416300	3.80336500	1.50336400
H	-0.49738000	2.32144400	2.01002500	C	-0.42807900	-1.18684400	0.25016000
C	0.15917400	0.16491100	0.42038800	H	-0.62937400	-1.87583600	-0.56378800
H	0.15903000	-0.87130900	0.75090600	C	-1.54664300	-0.36801200	0.77278300
C	1.27985100	0.76078700	-0.00436400	H	0.94351400	-0.32794700	1.57198800
H	1.21619400	1.79227200	-0.34998800	C	2.01907100	-1.76387800	0.35084600
C	2.62089300	0.15175600	-0.06963200	C	3.23977800	-1.39495100	0.93646900
C	3.64861000	0.86022600	-0.70945500	C	2.01147200	-2.79225400	-0.60607900
C	2.92013000	-1.10478700	0.48245400	C	4.42660400	-2.02625000	0.57094700
C	4.93404100	0.32916800	-0.80857300	H	3.25098700	-0.59921000	1.67829800

C	3.19664200	-3.42282000	-0.97061000	H	-2.50475800	-1.11743900	-1.71212700
H	1.07830100	-3.10527500	-1.06609100	C	-5.69317600	-0.72721200	-0.60015700
C	4.40758700	-3.04101600	-0.38584100	H	-6.25401800	-0.25003200	1.42632200
H	5.36370700	-1.72599000	1.03108800	H	-4.82829000	-1.18492100	-2.52251700
H	3.17795900	-4.21665500	-1.71208300	H	-6.71621600	-0.75506500	-0.96457700
H	5.33052100	-3.53638700	-0.67430100	C	1.94569000	-1.53120800	0.37051000
C	-2.93353800	-0.65673600	0.28697800	C	1.81111500	-2.60842500	-0.51267100
C	-3.29733800	-1.90311600	-0.23768300	C	3.22560300	-1.12468900	0.77044700
C	-3.89846300	0.35365000	0.39610100	C	2.94321300	-3.26867000	-0.99053300
C	-4.61124100	-2.13483500	-0.64252300	H	0.82819900	-2.95115700	-0.82215000
H	-2.57037800	-2.70615800	-0.31245500	C	4.35427500	-1.77518900	0.28265600
C	-5.20471400	0.12634900	-0.02477600	H	3.32688200	-0.29190700	1.46074200
H	-3.60967500	1.31666200	0.80728000	C	4.21432900	-2.84972900	-0.60003200
C	-5.56329400	-1.12053800	-0.54334200	H	2.83010300	-4.10922300	-1.66914500
H	-4.89018800	-3.10818200	-1.03550800	H	5.34376600	-1.44736700	0.58866500
H	-5.94473500	0.91792400	0.05138700	H	5.09542300	-3.35947500	-0.97992000
H	-6.58452000	-1.30085100	-0.86741800				
COM2				TS1			
C	0.75869300	-0.80218200	0.92248300	C	0.93373300	-0.50095900	0.56421700
C	1.24170400	1.38846100	-1.40554700	C	1.97135300	1.26517300	-0.48530600
O	0.87590800	-0.11340900	1.93230600	O	-1.40283500	0.79290200	1.50491800
S	1.16794600	2.77413000	-0.49560900	S	1.22969900	2.78143900	-0.40740300
O	1.28944600	4.16222100	-1.05088600	O	1.86584900	4.02152400	-0.94597300
H	0.40527800	1.31631300	-2.10168300	H	2.02816600	0.92104400	-1.51958300
H	2.23059000	1.24133900	-1.84192100	H	2.93066200	1.28858200	0.03469300
C	-0.37357800	2.69613600	0.40300400	C	-0.34379000	2.56365800	-1.20882100
H	-0.35829500	1.82942800	1.06742300	H	-0.80493300	1.63803600	-0.85927500
H	-0.47352400	3.62665000	0.96597900	H	-0.96275300	3.43344600	-0.97637800
H	-1.17840700	2.61274800	-0.33274400	H	-0.14588800	2.51620500	-2.28277000
C	2.41259600	2.59947700	0.77327800	C	0.86480700	3.05131500	1.31482400
H	2.16757500	1.74065700	1.40087300	H	0.17466300	2.27535800	1.65595000
H	3.37414300	2.45966600	0.27182600	H	1.81679900	3.00478200	1.85146900
H	2.42358500	3.52533900	1.35238600	H	0.42925200	4.04929700	1.40339300
C	-0.55044900	-0.95461900	0.24257200	C	-0.34029700	-0.79314100	0.11189700
H	-0.55779900	-1.33958400	-0.77217600	H	-0.48998500	-1.50783300	-0.69023700
C	-1.68249900	-0.60809700	0.87750400	C	-1.48606100	-0.14892100	0.69478100
H	-1.60019700	-0.25307300	1.90528600	H	1.01011500	0.05885800	1.49380100
C	-3.04543800	-0.65766300	0.33451400	C	2.10018400	-1.36055000	0.25294400
C	-4.11968100	-0.40702400	1.20170700	C	3.12923400	-1.47598800	1.19660400
C	-3.31875300	-0.93534600	-1.01570000	C	2.20388000	-2.07554700	-0.94879800
C	-5.43424400	-0.44389500	0.74036400	C	4.22816200	-2.29993000	0.95719100
H	-3.91558300	-0.18481700	2.24669900	H	3.06320300	-0.91399000	2.12609800
C	-4.63080300	-0.97090200	-1.47587300	C	3.30451900	-2.89387000	-1.19190800
				H	1.42744500	-1.98279400	-1.70433300

C	4.31903700	-3.01237400	-0.23874000	H	4.52453900	-2.72209200	2.06366200
H	5.01383400	-2.38241800	1.70330500	H	3.69200500	-3.14329400	-2.13402900
H	3.37350500	-3.43862000	-2.12959600	H	4.98305200	-3.82317000	-0.11958900
H	5.17627500	-3.65160500	-0.43073800	C	-2.63125500	-0.74729100	0.24852600
C	-2.85704800	-0.61881600	0.28326000	C	-2.75880100	-2.00826600	-0.35274800
C	-3.10073100	-1.91754200	-0.18114700	C	-3.79908000	-0.03027200	0.53881100
C	-3.92661100	0.27901000	0.38801500	C	-4.01427200	-2.52584200	-0.66906300
C	-4.39227400	-2.30891000	-0.53276400	H	-1.87265400	-2.60249900	-0.55975000
H	-2.28918000	-2.63671300	-0.24874900	C	-5.05674000	-0.54179100	0.21794100
C	-5.21407400	-0.10641000	0.02215800	H	-3.70225300	0.93647500	1.02474300
H	-3.73369600	1.28342200	0.75415900	C	-5.16979500	-1.79290900	-0.38937000
C	-5.44995700	-1.40369400	-0.43744900	H	-4.09154800	-3.50859600	-1.12715900
H	-4.57265900	-3.32290300	-0.87883400	H	-5.94971600	0.03523100	0.44513600
H	-6.03394200	0.60286200	0.09645200	H	-6.14791100	-2.19765500	-0.63515200
H	-6.45457300	-1.70846300	-0.71768800				
IN1				IN2			
C	1.18167000	0.02180800	0.25638700	C	-0.87152300	-1.08698700	-0.53084900
C	1.67659700	1.21008400	-0.60077600	C	0.93092300	0.44112600	0.11373800
O	-1.31190600	0.77681400	1.52603500	S	-2.47311900	-1.83262000	-0.16629100
S	0.85066700	2.79049800	-0.36950600	O	1.74344800	-1.60798400	0.93429000
O	1.60495200	3.84612800	-1.07823200	O	-2.68309400	-2.08015800	1.27337100
H	1.58896200	1.02088500	-1.67716000	H	-0.15388700	-1.90717600	-0.40093100
H	2.71568900	1.48078500	-0.37260000	H	-0.92131000	-0.78068600	-1.58133400
C	-0.82751500	2.71069500	-0.93684400	C	-3.76313600	-0.82815100	-0.86927400
H	-1.39304500	2.08137400	-0.24374300	H	-3.50847900	-0.60597900	-1.90875200
H	-1.18721800	3.74410800	-0.91782300	H	-4.68210100	-1.41784100	-0.80709600
H	-0.81985400	2.31978500	-1.95667100	H	-3.84643300	0.08321900	-0.27340700
C	0.74406300	3.07695400	1.37365100	C	-2.52276700	-3.32724300	-1.12299900
H	0.08337100	2.30171000	1.78609600	H	-2.34642600	-3.07606900	-2.17245300
H	1.75842800	3.03020300	1.77835000	H	-1.73874300	-3.98549700	-0.74028500
H	0.32207300	4.07851600	1.49790600	H	-3.51073400	-3.77486000	-0.98539300
C	-0.18297700	-0.50028900	-0.10750000	C	-0.49591400	0.06251700	0.42594500
H	-0.24823600	-1.22077400	-0.91735400	H	1.12112700	1.41419900	-0.32562200
C	-1.29847200	-0.12569000	0.60627600	C	1.93846800	-0.45987400	0.40234200
H	1.15876600	0.35441500	1.30132000	H	-0.55091300	-0.35227300	1.44174100
C	2.25353300	-1.05357800	0.14426800	C	-1.46818000	1.21756600	0.31990500
C	2.98897800	-1.43909300	1.26884800	C	-2.24373900	1.59670500	1.41924300
C	2.52098400	-1.67770800	-1.08132800	C	-1.64228800	1.89645200	-0.89349800
C	3.96556300	-2.43285300	1.17763500	C	-3.18486400	2.62302600	1.30968800
H	2.79303800	-0.95904400	2.22532800	H	-2.11765600	1.07600200	2.36621200
C	3.49764800	-2.66790400	-1.17625400	C	-2.58063200	2.92021900	-1.00738300
H	1.95887200	-1.39242900	-1.96863000	H	-1.04646700	1.61319400	-1.75961100
C	4.22296800	-3.05029500	-0.04566300	C	-3.35946600	3.28356600	0.09425100
				H	-3.78307300	2.90122100	2.17322600

H	-2.70832200	3.43337400	-1.95682700	H	4.21469300	3.96831000	0.16895700
H	-4.09505900	4.07815900	0.00431100	C	-3.42331800	-0.05637100	-0.16564800
C	3.37498000	-0.07558300	0.10148200	C	-3.71817800	0.49703200	1.08798700
C	3.73764300	0.92321100	-0.81466100	C	-4.48497700	-0.39602200	-1.01296300
C	4.39718000	-0.76534000	0.76545100	C	-5.03978600	0.71299600	1.47723100
C	5.07811200	1.23031900	-1.04573800	H	-2.91664300	0.74631200	1.77780900
H	2.97154800	1.45911600	-1.36878500	C	-5.80689300	-0.17177900	-0.63097400
C	5.73946400	-0.45706000	0.54246500	H	-4.25497700	-0.83821500	-1.97802400
H	4.11530700	-1.55128400	1.46022000	C	-6.08953700	0.38444600	0.61751300
C	6.08662400	0.54443500	-0.36505100	H	-5.25007400	1.13463500	2.45666500
H	5.33660600	2.00328100	-1.76511600	H	-6.61761300	-0.43299200	-1.30627700
H	6.51582600	-1.00052600	1.07552700	H	-7.11886000	0.55558500	0.92085200
H	7.13094800	0.78405700	-0.54661100				
TS2				TS3			
C	0.57805100	-0.96354300	0.40364800	C	0.81396000	-0.31670600	0.57022100
C	-0.96101500	0.40053600	-0.06170100	C	1.40901800	0.99511000	-0.99658600
S	2.53074300	-1.86755100	0.17623500	O	0.90950100	0.23063900	1.70157000
O	-1.85332700	-1.17099100	-1.56602700	S	1.38853100	2.61952700	-0.46260000
O	2.92916000	-2.15854900	-1.23825400	O	1.66369300	3.73637500	-1.40784100
H	0.00445300	-1.86073100	0.17252300	H	0.71953900	0.88581600	-1.83724300
H	0.67977200	-0.71992700	1.46107600	H	2.43845900	0.75124300	-1.27078200
C	3.78745400	-0.87626500	0.98054300	C	-0.18953700	2.86964800	0.31250800
H	3.46086500	-0.65811100	2.00114900	H	-0.29271800	2.12553400	1.10791500
H	4.71888900	-1.44977600	0.98231500	H	-0.19424700	3.88857800	0.70728300
H	3.90258000	0.04573000	0.40505200	H	-0.96025900	2.75337300	-0.45363500
C	2.57396900	-3.36365000	1.15679600	C	2.54512700	2.65053200	0.88133600
H	2.32178500	-3.10962200	2.19015200	H	2.27061200	1.84095300	1.56707000
H	1.83301900	-4.05132900	0.74186100	H	3.53923000	2.49401700	0.45397900
H	3.57781000	-3.79262300	1.09124700	H	2.48002000	3.63309700	1.35477100
C	0.44565700	0.16707100	-0.54976600	C	-0.56211800	-0.54644800	0.00060400
H	-1.11762500	1.12185400	0.73142800	H	-0.63984000	-0.93694500	-1.01039200
C	-2.01203000	-0.32080400	-0.64681300	C	-1.65662000	-0.29160000	0.72969200
H	0.44367800	-0.18633200	-1.58407800	H	-1.51103900	0.07569300	1.74575900
C	1.45199900	1.27155300	-0.35142900	C	-3.05590000	-0.46653400	0.30332400
C	2.30220200	1.63165200	-1.40117700	C	-4.07343900	-0.34010200	1.26138400
C	1.60545000	1.90450300	0.88875700	C	-3.42258900	-0.75107100	-1.02314700
C	3.29226300	2.59888400	-1.21787100	C	-5.41351700	-0.50734600	0.91448900
H	2.19421500	1.14171000	-2.36642900	H	-3.80519500	-0.11203600	2.29073700
C	2.59271600	2.87035800	1.07483700	C	-4.75992300	-0.91752500	-1.37057600
H	0.95725700	1.63584000	1.72064500	H	-2.65965300	-0.83665400	-1.79240900
C	3.44256100	3.21815300	0.02231400	C	-5.76223700	-0.79942800	-0.40365300
H	3.94685400	2.86388000	-2.04377100	H	-6.18407300	-0.40883300	1.67436600
H	2.70184500	3.35042300	2.04362500	H	-5.02317900	-1.13661400	-2.40191300
				H	-6.80513800	-0.92926900	-0.67900400

C	1.85941700	-1.36676300	0.20375100	C	-1.77461400	-2.10066600	1.15960900
C	1.82718800	-2.10205800	-0.98883600	C	-2.20646500	-2.09647200	-1.20863500
C	2.89154100	-1.60751600	1.11440600	C	-2.37502400	-3.35488000	1.26982600
C	2.80774100	-3.05427000	-1.26077200	H	-1.37615300	-1.62398700	2.05362200
H	1.04760100	-1.92714200	-1.72523500	C	-2.80335000	-3.35505300	-1.10297900
C	3.87585800	-2.55917300	0.84267700	H	-2.13285200	-1.57839500	-2.16039200
H	2.90945700	-1.03937600	2.03952500	C	-2.89023600	-3.98883500	0.13658600
C	3.83716800	-3.28739900	-0.34587000	H	-2.43995900	-3.83903900	2.24098100
H	2.76895400	-3.61454300	-2.19117000	H	-3.20436300	-3.84002800	-1.98978600
H	4.67167800	-2.73351500	1.56219500	H	-3.35643800	-4.96676400	0.22187700
H	4.60089700	-4.03004100	-0.55974400				
IN3				IN4			
C	-1.02162900	-0.06206500	-0.27049500	C	1.21261400	1.08547300	1.25686100
C	-1.78412800	0.86342600	0.76417500	O	0.38458100	-0.78733700	2.37046500
O	-1.12250500	0.42437000	-1.51363900	S	1.82922400	1.95581400	-0.19675700
S	-1.64206700	2.60470200	0.36101400	C	0.53793900	-0.36264300	1.11920300
O	-2.07545600	3.45123200	1.49627600	O	0.90475800	1.96538600	-1.34955600
H	-1.44366600	0.80037200	1.80412300	H	2.08920000	0.99509100	1.90756500
H	-2.86730000	0.69561300	0.73131000	H	0.48999900	1.77919800	1.70104800
C	0.02259600	2.98378600	-0.12067000	C	2.18836900	3.60541900	0.36149500
H	0.26168200	2.36618600	-0.98872200	H	2.88908500	3.54762500	1.19842000
H	0.03115700	4.05320000	-0.35051400	H	2.62404300	4.15108400	-0.47960300
H	0.67206800	2.76532600	0.73007400	H	1.24300400	4.05643700	0.67210900
C	-2.63280200	2.90247900	-1.07823900	C	3.42927800	1.30595500	-0.63193400
H	-2.29556200	2.18695300	-1.83338000	H	4.04697800	1.26103600	0.26820100
H	-3.67168700	2.72573300	-0.78708300	H	3.28947400	0.31771700	-1.07498900
H	-2.47872300	3.94750700	-1.36018900	H	3.85268500	2.00085100	-1.36260100
C	0.42295900	-0.23137100	0.23324600	C	-0.76655200	-0.15551800	0.34217600
H	0.55281300	-0.51183400	1.27982900	H	-0.70181400	0.27668500	-0.65557500
C	1.47082200	-0.08602700	-0.58388800	C	-1.94946000	-0.45491800	0.88921100
H	1.24912000	0.19950200	-1.61315300	H	-1.93066300	-0.85521800	1.90302800
C	2.89642300	-0.24969500	-0.24391200	C	-3.27986900	-0.29090600	0.27209200
C	3.85823400	-0.00561200	-1.23631900	C	-4.41911200	-0.57474100	1.04060400
C	3.34500600	-0.63743000	1.03059100	C	-3.46735300	0.13436000	-1.05460300
C	5.22088500	-0.13953900	-0.97072300	C	-5.70206600	-0.43347600	0.51187900
H	3.52817400	0.29371400	-2.22891300	H	-4.29211900	-0.90914700	2.06815800
C	4.70436600	-0.77190200	1.29740200	C	-4.74672700	0.27564700	-1.58443100
H	2.62712300	-0.83800800	1.82156400	H	-2.60729100	0.35394600	-1.68199500
C	5.65053200	-0.52318800	0.29890700	C	-5.87183000	-0.00608800	-0.80430600
H	5.94529800	0.05547900	-1.75697400	H	-6.56784600	-0.65857500	1.12904000
H	5.02904800	-1.07386600	2.28968600	H	-4.86808300	0.60511200	-2.61303000
H	6.71073100	-0.62957200	0.51115300	H	-6.86884800	0.10429200	-1.22160500
C	-1.68420200	-1.45831500	-0.08322100	C	1.52903500	-1.22783200	0.29574800
				C	1.36288500	-1.56614900	-1.05160600

C	2.68678700	-1.66665100	0.95249900
C	2.33765400	-2.30739600	-1.72909000
H	0.47521600	-1.25515800	-1.59470200
C	3.66467300	-2.39510900	0.28059400
H	2.80221600	-1.42599600	2.00636900
C	3.49539500	-2.71520200	-1.07019200
H	2.18743500	-2.56174900	-2.77525900
H	4.55965500	-2.71715200	0.80731500
H	4.25541300	-3.28485200	-1.59825200

TS4

C	1.18345100	0.79678600	1.48958600
O	0.43438600	-0.83187800	2.31998400
S	1.81171100	2.15433900	-0.08178300
C	0.57181700	-0.48599900	1.01178100
O	1.02827600	2.13553100	-1.36117000
H	2.16756400	0.70399400	1.94599400
H	0.49066400	1.49067800	1.96184700
C	1.80663100	3.80451100	0.60944000
H	2.39849800	3.80141600	1.52891800
H	2.22925400	4.49367700	-0.12693300
H	0.76734400	4.06244100	0.82732100
C	3.55251700	1.91042900	-0.41614300
H	4.10293700	2.01022900	0.52347900
H	3.67456800	0.90497300	-0.82642400
H	3.87249900	2.66602500	-1.13875300
C	-0.72516200	-0.28018300	0.24900900
H	-0.64952000	0.05046000	-0.78571900
C	-1.91060700	-0.48354100	0.83427000
H	-1.89942800	-0.80634200	1.87511100
C	-3.24106500	-0.31414500	0.22030300
C	-4.37822600	-0.60724800	0.98772200
C	-3.42780400	0.13298300	-1.09871600
C	-5.66134600	-0.46151500	0.46095000
H	-4.24974500	-0.95363100	2.01104000
C	-4.70753000	0.27925700	-1.62594000
H	-2.56787700	0.37085400	-1.71943800
C	-5.83147100	-0.01677100	-0.84938400
H	-6.52673400	-0.69514000	1.07535500
H	-4.83032900	0.62746700	-2.64807400
H	-6.82885600	0.09924000	-1.26422300
C	1.55477900	-1.35063500	0.21014200
C	1.78249400	-1.15994100	-1.15939000
C	2.27132900	-2.34470800	0.88067500

C	2.71340000	-1.94611400	-1.83932800
H	1.24479300	-0.38831900	-1.70571800
C	3.19869900	-3.13623600	0.20049100
H	2.08498500	-2.48303900	1.94163800
C	3.42415000	-2.93850400	-1.16199100
H	2.88212700	-1.78311500	-2.90071000
H	3.74571800	-3.90854300	0.73539700
H	4.14653400	-3.55254400	-1.69297800

COM3

C	0.16341000	-1.04706600	0.95530900
C	1.79926500	2.18525600	1.04611900
O	-2.00537400	0.33118100	2.08691500
S	3.16201400	2.49777800	0.06040900
H	1.77271400	2.90742100	1.86361100
H	0.86489800	2.14217800	0.47783600
C	3.33106100	1.01547200	-0.95674300
H	2.37888500	0.81453000	-1.45564800
H	4.12189800	1.17408300	-1.69436800
H	3.59565600	0.19102200	-0.29186200
C	2.79292900	3.66100600	-1.29811800
H	1.90446200	3.31597000	-1.83471100
H	2.60344500	4.63710100	-0.84575100
H	3.65020200	3.72565400	-1.97450300
C	-0.97173800	-0.79784100	0.27896800
H	-1.07468700	-1.04302800	-0.77297600
C	-2.11406700	-0.14551200	0.96291200
H	0.19176600	-0.77427100	2.01033000
C	1.39387300	-1.64810300	0.42800300
C	2.46750500	-1.84103900	1.31088600
C	1.55501400	-2.01128500	-0.91932400
C	3.67112900	-2.38411500	0.86545900
H	2.35302000	-1.55486900	2.35403400
C	2.75855100	-2.54669900	-1.36576700
H	0.74448500	-1.86569100	-1.62808400
C	3.82035400	-2.73592100	-0.47599500
H	4.49176400	-2.52628900	1.56287600
H	2.87161100	-2.81724600	-2.41192600
H	4.75858800	-3.15403600	-0.82999200
C	-3.42405500	-0.05836700	0.23801900
C	-3.74965300	-0.90965400	-0.82526700
C	-4.35811000	0.89382100	0.66735600
C	-4.99439700	-0.80978300	-1.44615200
H	-3.05101300	-1.66906100	-1.16297700

C	-5.59322600	1.00310200	0.03665200
H	-4.10099600	1.54833700	1.49497500
C	-5.91372400	0.14894500	-1.02156500
H	-5.24414400	-1.48135200	-2.26245300
H	-6.30730600	1.75150600	0.36831200
H	-6.87920500	0.23084600	-1.51309000

COM4

C	0.09656200	-0.66613300	1.06737700
C	1.41646400	2.00654400	-1.12506600
O	0.20553900	-0.12885300	2.16526000
S	2.94764400	1.50659600	-0.54273800
H	1.28911800	3.09323800	-1.10123400
H	1.25194000	1.57707400	-2.11496200
C	4.26380000	2.69677100	-0.97018300
H	3.95681800	3.70221800	-0.66781300
H	5.19510500	2.41422500	-0.47054400
H	4.39833800	2.65639500	-2.05348200
C	2.89342100	1.85681700	1.22724600
H	2.66320600	2.91589200	1.37783200
H	2.10757600	1.23535700	1.66202400
H	3.86139100	1.61071700	1.67140600
C	-1.20039500	-0.69889400	0.34915400
H	-1.28200000	-1.30137300	-0.54906300
C	-2.24818000	-0.00437100	0.82510200
H	-2.09188500	0.59031000	1.72511900
C	-3.59950600	0.05396800	0.25711300
C	-4.53076100	0.92366000	0.84495200
C	-4.00120300	-0.72097800	-0.84449500
C	-5.82742000	1.02628600	0.34481300
H	-4.22854200	1.52361500	1.70031200
C	-5.29559500	-0.61933000	-1.34218100
H	-3.30323800	-1.40982000	-1.31215900
C	-6.21278100	0.25503900	-0.75087600
H	-6.53484800	1.70636700	0.81076900
H	-5.59374700	-1.22483600	-2.19344800
H	-7.22310600	0.33044400	-1.14310000
C	1.28654700	-1.32895900	0.44151700
C	1.33427300	-1.66387400	-0.91778800
C	2.40553300	-1.57552800	1.24799800
C	2.48450900	-2.23526900	-1.45894500
H	0.49143700	-1.46077800	-1.57108800
C	3.55132800	-2.15171100	0.70839000
H	2.36544000	-1.31153100	2.30095200

C	3.59259000	-2.48147200	-0.64820300
H	2.51625600	-2.48311800	-2.51608800
H	4.41170100	-2.34526700	1.34292500
H	4.48729800	-2.92923100	-1.07218300

TS5

C	0.36546300	-0.54179800	0.84414600
C	1.13941600	1.59355300	0.04349400
O	-1.86057200	0.84719400	1.84782800
S	2.70321300	2.30774200	0.13907800
H	0.43652100	2.14981300	0.66320800
H	0.80732400	1.43382900	-0.98554900
C	3.76134500	1.11882900	-0.71455900
H	3.32516900	0.88568900	-1.68982000
H	4.75177100	1.56407800	-0.83671100
H	3.82893400	0.22015100	-0.09886400
C	2.90890600	3.69064700	-1.04158800
H	2.61735300	3.35462700	-2.04057400
H	2.25413500	4.49841900	-0.70783800
H	3.95006800	4.02626900	-1.03368300
C	-0.87951900	-0.62074700	0.27591700
H	-1.02981600	-1.14715700	-0.66115700
C	-1.98726600	0.10479300	0.86508700
H	0.43375700	-0.11887200	1.84203400
C	1.52704800	-1.34123900	0.41088300
C	2.51192100	-1.67430900	1.35102300
C	1.68514900	-1.77537800	-0.91304600
C	3.62933600	-2.42124200	0.98058100
H	2.40160800	-1.33495200	2.37897300
C	2.80575400	-2.51235100	-1.28681900
H	0.94260900	-1.50965900	-1.66167500
C	3.78320900	-2.83809800	-0.34229200
H	4.38283700	-2.67104000	1.72266700
H	2.92164600	-2.82985200	-2.31970900
H	4.65757500	-3.41187400	-0.63675700
C	-3.35054400	-0.03573600	0.23660300
C	-3.71456600	-1.14857500	-0.53178800
C	-4.29147500	0.97875800	0.45307300
C	-4.99685900	-1.24334100	-1.07240200
H	-3.00891000	-1.95810500	-0.69464900
C	-5.56685500	0.89238800	-0.09923000
H	-4.00759100	1.83682100	1.05562100
C	-5.92307600	-0.22128300	-0.86289700
H	-5.27220400	-2.11732400	-1.65614800

H	-6.28433400	1.69155100	0.06565100				
H	-6.91960400	-0.29306200	-1.29000200				
				IN6			
				C	-0.70868800	-0.38097800	-0.00137500
IN5				C	1.07778700	1.14976000	-0.70324000
C	0.61916200	0.01725800	0.53579900	S	2.78694600	1.77725300	-0.46857600
C	0.96592400	1.27123600	-0.28527300	O	-1.55451400	1.58149000	0.98473700
O	-1.70773400	1.52375400	1.20096700	H	0.40256400	2.00009400	-0.56476200
S	2.57736400	2.01229300	0.19396600	H	1.05298500	0.80670700	-1.74196700
H	0.22796000	2.04975700	-0.06448700	C	2.71253600	3.32718800	-1.38733400
H	1.01251800	1.07753500	-1.36194900	H	1.88694300	3.93439600	-1.01014600
C	3.78562500	1.17375700	-0.85465800	H	3.66727400	3.84128300	-1.25853900
H	3.39824400	1.10352700	-1.87361900	H	2.56347600	3.08058200	-2.44079400
H	4.69850800	1.77379800	-0.82693000	C	2.74340000	2.38694600	1.22775500
H	3.98265800	0.18534300	-0.43583500	H	1.82574800	2.95760700	1.38880000
C	2.47700200	3.60414300	-0.64865300	H	2.79732800	1.52786300	1.89934300
H	2.23829200	3.44372000	-1.70244500	H	3.62436700	3.01761600	1.36687200
H	1.69840900	4.19089700	-0.15747100	C	0.71598600	0.02658200	0.28237700
H	3.44238500	4.10282500	-0.53969800	H	-0.88447500	-1.32525600	-0.50529900
C	-0.78750300	-0.38675700	0.17394200	C	-1.73166900	0.46529700	0.38488100
H	-0.93448800	-1.27841200	-0.42642600	H	0.75264100	0.46221700	1.29002700
C	-1.83944400	0.42335000	0.56024500	C	1.70271700	-1.12064500	0.21846800
H	0.64945200	0.32072400	1.59270300	C	2.42810000	-1.49647300	1.35364900
C	1.65022000	-1.06953400	0.31833500	C	1.91763800	-1.82102900	-0.97647000
C	2.52211700	-1.44021700	1.34629900	C	3.34705000	-2.54710000	1.30203800
C	1.80081700	-1.67044800	-0.93906300	H	2.26960400	-0.96168300	2.28830800
C	3.53072600	-2.38163100	1.12538200	C	2.83304100	-2.87062300	-1.03211000
H	2.41676700	-0.98016300	2.32699000	H	1.36177600	-1.54494600	-1.87075400
C	2.80411100	-2.61059400	-1.16363500	C	3.55229600	-3.23694900	0.10818600
H	1.13507700	-1.38845900	-1.75277100	H	3.90106100	-2.82400300	2.19511400
C	3.67698500	-2.96612500	-0.13164300	H	2.98629200	-3.40428900	-1.96639800
H	4.20172400	-2.65410900	1.93567000	H	4.26730300	-4.05390700	0.06408300
H	2.91058100	-3.06352100	-2.14583400	C	-3.16925100	0.05436300	0.11410100
H	4.46294500	-3.69533900	-0.30781400	C	-3.53832200	-0.95522000	-0.78812800
C	-3.25052000	0.01143400	0.18246600	C	-4.18770200	0.73134200	0.79677200
C	-3.61966000	-1.30971300	-0.11178700	C	-4.87860400	-1.28301300	-0.98823100
C	-4.24239800	0.99938300	0.13658200	H	-2.77855100	-1.48667200	-1.35469200
C	-4.93335200	-1.62750000	-0.45545800	C	-5.53023300	0.40321200	0.60420100
H	-2.88123000	-2.10510300	-0.05521200	H	-3.90119300	1.52372900	1.48202800
C	-5.55681100	0.68739300	-0.21182500	C	-5.88271900	-0.60760600	-0.29030800
H	-3.96159300	2.01931400	0.38308700	H	-5.14077700	-2.06522000	-1.69621700
C	-5.90876900	-0.62943400	-0.51093900	H	-6.30248300	0.93911500	1.15083000
H	-5.19829000	-2.65940200	-0.67193900	H	-6.92708100	-0.86353300	-0.44788300
H	-6.30844900	1.47231400	-0.24728200				
H	-6.93282600	-0.87798000	-0.77662800	TS6			

C	-0.64024700	-0.42424100	0.00711600	O	-0.47825500	-0.06823800	2.03224200
C	0.76154500	0.97185400	-0.61744100	S	-2.66724900	-1.70817700	-0.53803900
S	2.67655100	2.09038800	-0.57868100	H	-0.38776800	-2.34229200	-0.34846600
O	-1.54170100	1.16191400	1.48927700	H	-0.72029200	-1.11113800	-1.66732800
H	0.13910700	1.83873600	-0.40374000	C	-3.19338600	-3.32799000	-1.19529200
H	0.82562700	0.66642900	-1.65860000	H	-2.57645800	-4.11399600	-0.75193100
C	2.08565100	3.62364700	-1.32957000	H	-4.25033300	-3.48578900	-0.96022200
H	1.14362800	3.92605200	-0.86344000	H	-3.05269600	-3.30060800	-2.27817000
H	2.83486600	4.40879600	-1.20494800	C	-2.88180700	-2.07163700	1.21446400
H	1.92900100	3.43595500	-2.39421400	H	-2.30433700	-2.96549300	1.46726500
C	2.62086600	2.55091700	1.16522500	H	-2.50582500	-1.21667200	1.77860600
H	1.59795800	2.81412800	1.45093100	H	-3.94355700	-2.23295700	1.41279600
H	2.96425200	1.69462700	1.75028000	C	0.93140100	0.36573500	0.17183200
H	3.28979900	3.39726400	1.33836100	H	0.95605600	0.66806600	-0.87002100
C	0.77504100	-0.09524400	0.40964000	C	2.05686900	0.04888900	0.82996000
H	-0.79488400	-1.19179600	-0.74201200	H	1.96610800	-0.23203600	1.87893300
C	-1.70053900	0.27089800	0.61067300	C	3.42291900	0.03879400	0.28327300
H	0.79828400	0.31785800	1.42144400	C	4.49157800	-0.23444700	1.15129600
C	1.81462600	-1.17055300	0.23454700	C	3.71234800	0.28888800	-1.06944700
C	2.63734300	-1.52063900	1.30976100	C	5.80724200	-0.25355200	0.69046700
C	1.98974900	-1.82986400	-0.98921800	H	4.28249100	-0.43321000	2.20017200
C	3.61356900	-2.50931100	1.17141300	C	5.02522900	0.27067600	-1.53005900
H	2.50966800	-1.01499600	2.26473600	H	2.90815900	0.49507000	-1.77053800
C	2.96322000	-2.81741700	-1.13024100	C	6.07984600	0.00047600	-0.65317300
H	1.36049500	-1.57552800	-1.83992200	H	6.61824000	-0.46699200	1.38145500
C	3.77946200	-3.16046400	-0.04999500	H	5.22845700	0.46608600	-2.57953400
H	4.24287700	-2.76829200	2.01867700	H	7.10330800	-0.01372100	-1.01723300
H	3.08546400	-3.32081300	-2.08557400	C	-1.50109000	1.21984200	0.32010400
H	4.53814500	-3.93017800	-0.16142000	C	-1.49893800	1.75651400	-0.97517200
C	-3.11682500	-0.06717800	0.19610700	C	-2.58351700	1.50166500	1.16060400
C	-3.43533000	-0.69245500	-1.01736600	C	-2.56139300	2.54035200	-1.41902000
C	-4.15962100	0.27923800	1.06388100	H	-0.68052500	1.55176400	-1.65844900
C	-4.76131100	-0.97149000	-1.34713300	C	-3.65010600	2.28412200	0.71670300
H	-2.65065200	-0.94899600	-1.72357100	H	-2.57828100	1.10319500	2.17097300
C	-5.48536100	-0.00738800	0.74146400	C	-3.64450800	2.80427800	-0.57679900
H	-3.91169800	0.77707900	1.99685100	H	-2.54598800	2.94358400	-2.42803000
C	-5.79146500	-0.63458900	-0.46723800	H	-4.48322100	2.48972000	1.38372600
H	-4.99045600	-1.44863900	-2.29638300	H	-4.47327400	3.41350800	-0.92701200
H	-6.28083800	0.26102600	1.43187500				
H	-6.82408300	-0.85455900	-0.72439500	IN7			
				C	0.68362900	0.23693800	0.25272700
TS7				C	1.35283300	1.16534000	-0.80996600
C	-0.38879400	0.34840600	0.87023700	O	0.79585500	0.81475200	1.45909200
C	-0.96693300	-1.47090400	-0.66769600	S	2.96355500	1.62782400	-0.09735800

H	0.78453800	2.09373200	-0.92968200	C	-0.03743700	3.14360100	-0.37494000
H	1.55865300	0.72593600	-1.79175000	H	-0.16584000	3.61582700	0.60177200
C	3.79725200	2.29962000	-1.55204300	H	-0.00353200	3.89257700	-1.16920700
H	3.14475100	3.01610900	-2.05620800	H	-0.84258000	2.43270800	-0.57045300
H	4.71549700	2.78741700	-1.21716000	C	2.66030200	3.55737900	0.10561700
H	4.04402700	1.46848200	-2.21561900	H	2.34215300	3.95301100	1.07274600
C	2.60645100	3.15454700	0.79080700	H	3.66013200	3.12419400	0.17291000
H	2.14462800	3.87196900	0.10839500	H	2.64219000	4.33496800	-0.66101500
H	1.92705800	2.87135800	1.59458000	C	-0.44538000	-0.20280700	0.26062000
H	3.55253500	3.54015000	1.17742800	H	-0.43636100	0.06996600	-0.79672900
C	-0.75425800	0.03053200	-0.24290700	C	-1.60114900	-0.49294800	0.86792400
H	-0.88313800	-0.41948600	-1.22866800	H	-1.53709100	-0.77605800	1.91880100
C	-1.80572800	0.38191900	0.50545500	C	-2.94904000	-0.47683500	0.26855300
H	-1.58122800	0.82659000	1.47558800	C	-4.03875200	-0.89187400	1.04921900
C	-3.23300300	0.23336600	0.16268600	C	-3.20143500	-0.05979200	-1.05001000
C	-4.19712300	0.69877700	1.07009500	C	-5.33521300	-0.89913400	0.53524100
C	-3.68122700	-0.35411200	-1.03316000	H	-3.86126700	-1.21488600	2.07282100
C	-5.56047300	0.58730400	0.79757700	C	-4.49488500	-0.06529700	-1.56456700
H	-3.86786800	1.15471400	2.00150000	H	-2.38210400	0.27372400	-1.68178900
C	-5.04124200	-0.46705800	-1.30674600	C	-5.56927800	-0.48611200	-0.77576900
H	-2.96235800	-0.72935000	-1.75683800	H	-6.16156000	-1.22747300	1.16003900
C	-5.98931800	0.00291900	-0.39341000	H	-4.66721700	0.26113600	-2.58679600
H	-6.28636000	0.95679500	1.51707600	H	-6.57742900	-0.48919300	-1.18067400
H	-5.36515100	-0.92605900	-2.23717800	C	1.91009000	-1.06794700	0.17402500
H	-7.05005100	-0.08743900	-0.61041300	C	2.02595300	-1.00507400	-1.22237400
C	1.37432200	-1.15823100	0.17437000	C	2.78256900	-1.91303700	0.86753300
C	1.47590800	-1.89961400	-1.01147200	C	2.98984300	-1.75728300	-1.89845300
C	1.91157200	-1.69907300	1.34407500	H	1.36403200	-0.37598100	-1.81183100
C	2.09886600	-3.14816600	-1.02406200	C	3.74799200	-2.66569900	0.19788800
H	1.06671800	-1.50670900	-1.94087200	H	2.67068200	-1.96621600	1.94637200
C	2.53342600	-2.94982800	1.33820700	C	3.85699900	-2.59022100	-1.19146900
H	1.83079600	-1.10760600	2.25146000	H	3.05717500	-1.69395100	-2.98167700
C	2.63007300	-3.67973000	0.15332800	H	4.41368700	-3.31599700	0.76054800
H	2.16970400	-3.70674800	-1.95408500	H	4.60518100	-3.17675500	-1.71805600
H	2.94638200	-3.35369700	2.25962100				
H	3.11537100	-4.65206500	0.14445200	TS8			
IN8				C	1.39267400	1.09995700	1.22926000
C	1.44010000	1.22727600	1.12377100	O	0.83496900	-0.45623300	2.25927300
O	0.79483700	-0.66268900	2.28475500	S	1.76843800	2.44311500	-0.50668200
S	1.52860000	2.24693900	-0.40585700	C	0.88545700	-0.26541000	0.90902700
C	0.88884500	-0.24608200	1.01930000	H	2.41223600	1.14273600	1.60345000
H	2.47026900	1.19190300	1.49264900	H	0.66972400	1.77583100	1.67911800
H	0.81244100	1.78829300	1.82259500	C	0.07149200	2.95597500	-0.85669300
				H	-0.49394400	3.05647800	0.07455900

H	0.08790600	3.90810000	-1.39255600	H	1.72446200	1.77184800	0.04289500
H	-0.38934800	2.19593600	-1.49129700	C	0.00651200	0.42440700	-0.00404300
C	2.32198700	3.85491400	0.47712000	C	-0.94675500	1.49211000	0.03486200
H	1.66889600	3.98631900	1.34476600	C	-0.53539300	-0.89894400	-0.04300200
H	3.34208200	3.65037700	0.80966600	C	-2.30420400	1.26211100	0.03486700
H	2.31609700	4.75751500	-0.13811000	H	-0.58035700	2.51522500	0.06535200
C	-0.45319500	-0.27404200	0.19506800	C	-1.89494300	-1.12659500	-0.04288000
H	-0.44456200	-0.14580600	-0.88689100	H	0.13242600	-1.75533200	-0.07326000
C	-1.60173300	-0.43867800	0.86045500	C	-2.81011800	-0.05483000	-0.00341300
H	-1.53506500	-0.58109700	1.93896000	H	-2.99467800	2.10107400	0.06527300
C	-2.95873300	-0.45601000	0.28229900	H	-2.26771800	-2.14714600	-0.07276400
C	-4.04162200	-0.78226200	1.11237700	C	-4.21238900	-0.29654300	-0.00151000
C	-3.22249200	-0.15455300	-1.06468100	N	-5.35897900	-0.49387800	0.00024100
C	-5.34485400	-0.81765800	0.61714900				
H	-3.85394800	-1.01313300	2.15881300	COM5-1			
C	-4.52266100	-0.18911400	-1.56055200	C	0.46805700	-0.40054100	1.61646800
H	-2.40740700	0.11289900	-1.73216800	C	-0.96661200	-1.72246200	-1.14240300
C	-5.59097100	-0.52183700	-0.72298300	O	2.75437100	-1.85076200	0.85927400
H	-6.16707100	-1.07542400	1.27925700	S	-1.91854300	-3.04958400	-0.64475500
H	-4.70534100	0.04755600	-2.60538000	H	0.06069000	-1.94504700	-1.41835500
H	-6.60459200	-0.54689700	-1.11313900	C	-0.88168400	-3.97817500	0.51078100
C	1.90704900	-1.13432200	0.16879000	H	-0.81686400	-3.40635900	1.43733800
C	2.12667200	-1.02631600	-1.21097400	H	-1.35456000	-4.94533900	0.69905300
C	2.66321600	-2.05226300	0.90064400	H	0.10940600	-4.11393400	0.07048500
C	3.08773400	-1.81706600	-1.84063100	C	-1.92022400	-4.24898800	-2.00935000
H	1.55103200	-0.32391300	-1.81019100	H	-2.47218200	-3.79646900	-2.83526900
C	3.61997100	-2.85124400	0.27127800	H	-0.88861200	-4.45666000	-2.30407100
H	2.48617200	-2.12378200	1.96975100	H	-2.42103100	-5.16155600	-1.67571300
C	3.83708000	-2.73473600	-1.10136500	C	1.54297700	0.17669700	1.05003000
H	3.24969700	-1.71833600	-2.91083700	H	1.54591900	1.22895400	0.78365100
H	4.19726700	-3.56414900	0.85464600	C	2.74534000	-0.63050800	0.73830700
H	4.58298900	-3.35318900	-1.59322600	H	0.52508000	-1.46429400	1.84846200
				C	-0.80001300	0.25636600	1.94881500
Ar-DMSM				C	-1.84932300	-0.52780600	2.45247900
S	2.58920900	-0.46222300	-0.02387700	C	-1.01650400	1.63153300	1.75924600
C	3.74065300	-0.00259800	-1.34433200	C	-3.08651200	0.04048200	2.75089300
H	4.04764800	1.03712800	-1.20702600	H	-1.68828100	-1.59203400	2.60994500
H	4.60535300	-0.66966900	-1.30285000	C	-2.24923800	2.20005500	2.06306600
H	3.21484900	-0.12583500	-2.29268100	H	-0.22040700	2.26217200	1.37255500
C	3.67237600	-0.14322900	1.39553400	C	-3.28953100	1.40661100	2.55569100
H	3.09383200	-0.34906300	2.29784500	H	-3.88954600	-0.58211300	3.13549100
H	4.53313100	-0.81422600	1.33735900	H	-2.40371500	3.26478900	1.90905700
H	3.99243000	0.90136500	1.37288600	H	-4.25254900	1.85388800	2.78611500
C	1.38161700	0.74200200	-0.00153100	C	3.97114000	0.07922200	0.24508400

C	4.19827700	1.43859400	0.49352600	H	3.92421600	0.07211800	-1.89296500
C	4.93065100	-0.66083400	-0.45866600	C	3.12707800	3.47289100	-0.22152400
C	5.37153300	2.04592900	0.04699100	H	1.06097100	2.96078900	-0.47984100
H	3.47913500	2.02694100	1.05531200	C	4.45684000	3.08473300	-0.40892400
C	6.09271200	-0.04966300	-0.91842200	H	5.77430500	1.55375800	-1.16423300
H	4.75116700	-1.71555200	-0.64536600	H	2.90046300	4.43010300	0.23980800
C	6.31572600	1.30595100	-0.66409100	H	5.26429200	3.73850600	-0.09123000
H	5.54654300	3.09748600	0.25521200	C	-2.40000400	-0.28989000	-1.51882600
H	6.82631600	-0.62737500	-1.47353700	C	-2.94700600	0.98688200	-1.34412500
H	7.22502500	1.78314400	-1.01889300	C	-3.23033000	-1.41370800	-1.42666600
C	-1.49910400	-0.42604100	-1.28839200	C	-4.30659400	1.13497900	-1.07163200
C	-2.85074100	-0.04981300	-1.00460400	H	-2.32459200	1.87311600	-1.42651100
C	-0.63588900	0.62369700	-1.74010600	C	-4.58403100	-1.26620500	-1.14050100
C	-3.28966500	1.24718800	-1.15821100	H	-2.79726400	-2.40123500	-1.55943700
H	-3.55858800	-0.79710600	-0.65543700	C	-5.12360100	0.01005400	-0.95816900
C	-1.07763700	1.92004800	-1.89224700	H	-4.72470500	2.12899000	-0.94002900
H	0.39997600	0.38282400	-1.96863800	H	-5.21891400	-2.14335700	-1.05293200
C	-2.41658400	2.26079700	-1.60652900	H	-6.17962700	0.12616400	-0.73032700
H	-4.32264200	1.49529200	-0.92670300	C	0.51486300	-0.64508700	1.61967300
H	-0.38990600	2.68904600	-2.23514500	C	0.77905600	0.70167100	2.02999300
C	-2.87326800	3.60109200	-1.74482400	C	-0.86316700	-1.00150500	1.48034300
N	-3.24742500	4.69744800	-1.85497800	C	-0.23096100	1.61537000	2.22992700
COM5-2				H	1.81342500	1.01320800	2.15825300
C	1.31203600	0.46687600	-1.64495500	C	-1.87277000	-0.08725100	1.69000800
C	1.60249400	-1.50019200	1.35426400	H	-1.13367200	-2.00876900	1.17358300
O	-0.53961700	-1.56971200	-2.22612600	C	-1.58245900	1.24266300	2.05565700
S	1.37727300	-3.09162100	0.77298000	H	0.01149400	2.63631200	2.51516600
C	2.54881100	-4.10677300	1.70644700	H	-2.90884700	-0.38812000	1.54690400
H	2.21609600	-4.11577100	2.74572600	C	-2.63287100	2.19007300	2.20799300
H	2.53697800	-5.11980600	1.29729400	N	-3.49908900	2.95919900	2.31988400
H	3.54703300	-3.66939500	1.62602700	H	2.62962700	-1.15069000	1.41863600
C	2.16726900	-3.18353700	-0.85708700	COM-6-1			
H	1.52359800	-2.63439800	-1.54810100	C	-0.39286600	0.45941300	1.93988300
H	3.16216400	-2.73437400	-0.79805300	C	-0.08880600	1.21423600	-1.40755100
H	2.23212500	-4.23387500	-1.15458100	O	-0.76884000	1.48246200	2.50641300
C	0.00243000	0.56646200	-1.35837100	S	-0.08936400	2.84935100	-0.90324200
H	-0.38756900	1.39423700	-0.77346600	H	-1.03380600	0.83575900	-1.78797600
C	-0.93656700	-0.50768200	-1.75425400	C	-0.28964000	3.89191600	-2.38335300
H	1.64852900	-0.40044600	-2.21339800	H	-1.17062300	3.55823900	-2.93714800
C	2.36423400	1.39978400	-1.22784600	H	-0.39358200	4.93400200	-2.06902400
C	3.70369800	1.02717100	-1.42081500	H	0.61296900	3.76824900	-2.98568500
C	2.08899600	2.63957600	-0.62512900	C	-1.73516400	3.07774100	-0.19558600
C	4.74323200	1.85967200	-1.01117400	H	-2.47477600	2.64984400	-0.87746200

H	-1.75522400	2.57902300	0.77513200	O	1.39607300	-0.41053500	-2.53051500
H	-1.90184600	4.15055100	-0.07281200	S	2.05655800	-2.81925600	0.51735000
C	-1.33093700	-0.37213200	1.14812700	C	3.22549900	-2.72311200	-0.85971400
H	-0.91221000	-1.11127000	0.47106000	H	4.15973900	-2.28225400	-0.50285700
C	-2.65745400	-0.18695700	1.25699400	H	3.39824100	-3.73396900	-1.23754000
H	-3.01272400	0.55352600	1.97426800	H	2.76745100	-2.10008900	-1.63089700
C	-3.69971800	-0.88713700	0.49766500	C	3.03725700	-3.86518100	1.63250400
C	-5.04060200	-0.70108300	0.86718100	H	4.00585400	-3.39137100	1.81044500
C	-3.41016700	-1.72652900	-0.59188200	H	2.47667500	-3.95388000	2.56509900
C	-6.06683100	-1.34669100	0.18009700	H	3.16381700	-4.84932800	1.17349400
H	-5.27319300	-0.04626300	1.70395700	C	-0.44374200	0.58706100	-1.41743400
C	-4.43485500	-2.36909600	-1.27856900	H	-0.72652300	1.33577700	-0.68308300
H	-2.38076000	-1.87328200	-0.90824700	C	-1.34463500	-0.28346500	-1.90379700
C	-5.76615800	-2.18376300	-0.89405400	H	-0.99603800	-1.04561100	-2.60109100
H	-7.09924200	-1.19476800	0.48208600	C	-2.76489500	-0.34579900	-1.54224700
H	-4.19715500	-3.01380300	-2.12010200	C	-3.49246600	-1.49595900	-1.88311100
H	-6.56341000	-2.68732000	-1.43356300	C	-3.41722600	0.68492800	-0.84369300
C	1.03911100	0.03667100	2.03890400	C	-4.83050300	-1.62857000	-1.51581600
C	1.45444200	-1.27031400	1.75283200	H	-2.99609800	-2.29352000	-2.43130000
C	1.98351200	0.98304300	2.45850200	C	-4.75428700	0.55541700	-0.48388600
C	2.79576000	-1.62458700	1.89375300	H	-2.88070500	1.59513400	-0.58762100
H	0.73757000	-2.02445100	1.44134700	C	-5.46362600	-0.60380900	-0.81316000
C	3.32394700	0.63187700	2.58356700	H	-5.37768800	-2.52911800	-1.78007400
H	1.65482100	1.99530000	2.67597100	H	-5.24782200	1.36037600	0.05384300
C	3.73152700	-0.67480200	2.30344900	H	-6.50757500	-0.70149300	-0.52846900
H	3.10986200	-2.64204800	1.67725600	C	1.93117800	1.52250600	-1.27684100
H	4.05219200	1.37416800	2.89815600	C	1.50069200	2.78339000	-0.84527900
H	4.77821200	-0.95094100	2.40055200	C	3.29283900	1.20032400	-1.20985600
C	1.08237500	0.43460500	-1.44631000	C	2.42179200	3.70820900	-0.35526200
C	0.98812000	-0.93306200	-1.86149800	H	0.45195100	3.06034600	-0.90172600
C	2.38996200	0.89529800	-1.09001100	C	4.20875300	2.11625400	-0.70136100
C	2.08811000	-1.76165400	-1.90518000	H	3.62155900	0.22104800	-1.54734000
H	0.01416700	-1.32318900	-2.14845700	C	3.77329200	3.37288900	-0.27302800
C	3.48648200	0.06261600	-1.12925200	H	2.08190400	4.68800000	-0.03210700
H	2.53317400	1.92584900	-0.77444000	H	5.26095500	1.85346100	-0.63839400
C	3.36313200	-1.28177500	-1.53961800	H	4.48770800	4.08985300	0.12213800
H	1.97415900	-2.79590900	-2.22019200	C	0.81934700	-0.61534200	1.54739800
H	4.46251200	0.44525700	-0.84082600	C	0.85781600	0.75235300	1.96794000
C	4.49629500	-2.14118900	-1.54715200	C	-0.47183400	-1.23272200	1.52822100
N	5.42314000	-2.84510100	-1.54699000	C	-0.28696100	1.45357700	2.27547400
COM-6-2				H	1.82106600	1.25712000	2.01001500
C	0.98244500	0.49236400	-1.80936600	C	-1.61561500	-0.52951700	1.83602800
C	2.02476400	-1.24670800	1.17919200	H	-0.56681300	-2.27800200	1.24599300
				C	-1.55189700	0.83068000	2.20577900

H	-0.21918100	2.49947700	2.56517100
H	-2.58218300	-1.02651800	1.79114000
H	2.98325500	-0.74513900	1.28036200
C	-2.74157200	1.55865600	2.48560400
N	-3.71879300	2.15307600	2.70079900

TS9-1

C	-0.32517700	-1.42337700	0.78654000
C	-1.01580700	-0.76181600	-1.21147300
O	1.82441300	-2.47959000	-0.66791900
S	-2.60680100	-1.41811200	-1.55263800
H	-0.23258100	-1.30376000	-1.74143500
C	-2.29279100	-3.19308100	-1.53796800
H	-2.20279200	-3.52913600	-0.50514700
H	-3.15189600	-3.67870800	-2.00587800
H	-1.37864500	-3.40120700	-2.09911500
C	-2.86912500	-1.18902500	-3.33558200
H	-2.95418900	-0.11530700	-3.51647800
H	-2.01863500	-1.60884600	-3.87761400
H	-3.80046800	-1.68984600	-3.61300000
C	0.97627500	-0.94161900	0.90330500
H	1.17994400	-0.03709800	1.46540200
C	2.02284500	-1.54991900	0.13955000
H	-0.42721900	-2.45306100	0.44955400
C	-1.43032100	-0.91328100	1.62586700
C	-2.50254500	-1.75506500	1.96132900
C	-1.44798400	0.40974400	2.09534800
C	-3.56051600	-1.29188200	2.74121000
H	-2.49596600	-2.78954300	1.62437600
C	-2.50588300	0.87390200	2.87529100
H	-0.63357800	1.08474900	1.84350000
C	-3.56690700	0.02702500	3.19916100
H	-4.37754700	-1.96178200	2.99509700
H	-2.50353500	1.90247800	3.22642100
H	-4.39106000	0.39093900	3.80651900
C	3.42674000	-1.01202000	0.28013700
C	3.85533100	-0.29448000	1.40462900
C	4.33786400	-1.25324200	-0.75557600
C	5.16684300	0.17253800	1.48809700
H	3.17388500	-0.11323500	2.23106600
C	5.64511800	-0.77738900	-0.67915000
H	4.00452500	-1.81693800	-1.62222200
C	6.06377400	-0.06320100	0.44505300
H	5.48903200	0.71861900	2.37056200

H	6.33851400	-0.96425600	-1.49477900
H	7.08409700	0.30494000	0.50937300
C	-0.90096800	0.66631600	-1.14123900
C	-1.97350000	1.54128200	-0.83186500
C	0.39393200	1.23289700	-1.26389900
C	-1.76585800	2.89577300	-0.65006200
H	-2.98424700	1.15497300	-0.72125900
C	0.60916200	2.58721200	-1.06787800
H	1.22792500	0.59245000	-1.53687200
C	-0.46935900	3.43079300	-0.75864700
H	-2.60137600	3.54858000	-0.41454000
H	1.60891600	3.00109000	-1.16481500
C	-0.25328900	4.83267800	-0.56844900
N	-0.07810700	5.96940400	-0.41221900

TS9-2

C	1.14449100	-0.82810100	-1.11906600
C	1.52481600	-0.63183400	1.08154000
O	-0.90227300	-2.48152500	-0.25558600
S	1.09851700	-2.11519900	1.92815600
C	2.26443100	-2.15458600	3.31829200
H	2.03033700	-1.30605800	3.96484500
H	2.11915900	-3.09018700	3.86507800
H	3.28747200	-2.08125300	2.94125200
C	1.80590300	-3.45729200	0.95335100
H	1.12227900	-3.65709100	0.12878500
H	2.80117800	-3.17312300	0.60258800
H	1.86944200	-4.32807200	1.61040300
C	-0.19511100	-0.53202200	-1.35785800
H	-0.49799200	0.44362800	-1.72241600
C	-1.18894300	-1.44526300	-0.89605500
H	1.40674200	-1.87841800	-1.03263300
C	2.25119400	0.04301000	-1.56835900
C	3.54351700	-0.49521000	-1.67721000
C	2.06492600	1.39900900	-1.87502900
C	4.61595000	0.29045000	-2.08894800
H	3.70045500	-1.54423300	-1.43242000
C	3.13918900	2.18858800	-2.28570000
H	1.07833100	1.84639000	-1.79374400
C	4.41675300	1.63946200	-2.39427000
H	5.60719600	-0.14690700	-2.17181900
H	2.97563200	3.23719400	-2.51951700
H	5.25178700	2.25646200	-2.71440200
C	-2.64174800	-1.11918500	-1.12221200

C	-3.07193800	-0.29394700	-2.16906600	H	-1.49698900	-3.49657900	0.88592800
C	-3.59390100	-1.66500600	-0.25273400	C	-2.31575500	-0.52339600	3.22219800
C	-4.42848300	-0.01939800	-2.34001300	H	-0.74419000	0.52680000	2.20415900
H	-2.35081400	0.12255400	-2.86732800	C	-3.05248000	-1.70517300	3.32063300
C	-4.94845400	-1.38139900	-0.41500900	H	-3.31593700	-3.70053400	2.54616000
H	-3.25651700	-2.31070300	0.55348700	H	-2.53781700	0.31294500	3.87980600
C	-5.36946800	-0.55733000	-1.46069200	H	-3.84685700	-1.79483400	4.05653100
H	-4.75103500	0.61336100	-3.16241000	C	3.68467500	0.03798700	0.25116100
H	-5.67675600	-1.80274200	0.27282100	C	3.94424500	0.59615800	1.51229500
H	-6.42570700	-0.33854300	-1.59196500	C	4.64844800	0.19685500	-0.75248800
C	0.70021400	0.50931800	1.37181800	C	5.12130200	1.30294000	1.75368300
C	1.26547000	1.80702300	1.30119000	H	3.23166300	0.46760500	2.32266200
C	-0.70123100	0.41197300	1.55504200	C	5.82578800	0.90760400	-0.51663500
C	0.48346500	2.94124600	1.42063000	H	4.45486100	-0.25060400	-1.72309500
H	2.33836500	1.90803100	1.15736600	C	6.06737600	1.46589300	0.73884600
C	-1.48853800	1.54525600	1.68798900	H	5.30432000	1.72211200	2.73990900
H	-1.17533400	-0.56477800	1.60273100	H	6.55682700	1.02340400	-1.31311400
C	-0.90401000	2.81834100	1.61927900	H	6.98508700	2.01620000	0.92858600
H	0.93608100	3.92738700	1.36984600	C	-1.21174100	0.59917900	-0.80813500
H	-2.56106300	1.44935200	1.83394700	C	-2.55426900	0.65270900	-0.40951600
C	-1.71692000	3.98942900	1.74995500	C	-0.51084500	1.79150100	-1.02217100
N	-2.37442800	4.93969600	1.85730800	C	-3.18860300	1.87474600	-0.22594800
H	2.60420600	-0.47993500	1.07735800	H	-3.11668400	-0.26039500	-0.22624200
IN9-1				C	-1.12794100	3.02244600	-0.82793800
C	-0.46894800	-0.69935500	-0.97415400	H	0.52651700	1.75364400	-1.34364600
O	2.44735100	-1.47343200	-1.12714200	C	-2.46909600	3.05858600	-0.43103900
S	-1.52429100	-1.89180600	-1.92100700	H	-4.22879300	1.91526600	0.08134600
H	0.40187100	-0.56859800	-1.62593100	H	-0.58138100	3.94619000	-0.98952500
C	-0.30705500	-3.17481600	-2.30116700	C	-3.11876000	4.32749800	-0.23629000
H	-0.35088700	-3.93435100	-1.51933800	N	-3.64186500	5.34890200	-0.08032200
H	-0.59586800	-3.61381000	-3.25884700	C	0.07274900	-1.35098000	0.34630200
H	0.68698600	-2.71745500	-2.34660400	H	0.38317300	-2.36568600	0.06103400
C	-1.62170100	-1.05177900	-3.51555700	IN9-2			
H	-2.24509800	-0.16440000	-3.39064100	C	-0.00196000	-1.46027600	0.03934500
H	-0.61546600	-0.78251000	-3.84619700	C	0.79577400	-0.76416900	1.19534100
H	-2.09308100	-1.73972200	-4.22073300	O	-2.61326600	-1.25403200	1.12462900
C	1.31211600	-0.59143600	0.73116500	S	-0.33215500	-0.34213500	2.59734400
H	1.28583700	0.10126500	1.56382300	C	0.90217200	0.20626200	3.80058800
C	2.42356200	-0.73505300	-0.07826500	H	1.25642100	1.19573700	3.50538800
C	-0.99200100	-1.46874400	1.41570500	H	0.40019300	0.27328000	4.76878200
C	-1.73203000	-2.65148400	1.53189800	H	1.72867600	-0.50724900	3.84446200
C	-1.29681900	-0.40698000	2.27769400	C	-0.69135800	-1.97164600	3.27834000
C	-2.75641800	-2.77188900	2.47263400	H	-1.39627000	-2.44233900	2.59384100

H	0.23868400	-2.53502100	3.38654700	C	1.00437200	1.05732600	-0.53523500
H	-1.16048700	-1.81229100	4.25259400	S	2.24481100	2.38672000	-0.05322800
C	-1.09902900	-0.63031200	-0.56212100	O	-1.01844200	-1.25641300	1.95280700
H	-0.89432500	-0.03498900	-1.44436600	H	1.24237400	0.91391100	-1.59660200
C	-2.34185500	-0.62963700	0.03490300	C	2.33829600	2.28220300	1.74241600
H	-0.45997300	-2.34127200	0.50855600	H	2.72097100	1.30849900	2.05188200
C	1.03189100	-1.97003600	-0.95380000	H	3.00870800	3.08098000	2.06805700
C	1.54574200	-3.26366300	-0.80780400	H	1.33719700	2.46053800	2.14215700
C	1.52629700	-1.17035900	-1.99226300	C	3.89618600	1.84570400	-0.54805700
C	2.51944000	-3.75467900	-1.67822100	H	4.22185900	0.97990300	0.02814500
H	1.17389400	-3.89438600	-0.00223200	H	3.86881800	1.62682800	-1.61768700
C	2.50087600	-1.65621900	-2.86413600	H	4.55099300	2.70167400	-0.36524900
H	1.15612500	-0.15595300	-2.12232500	C	1.11081100	-0.27686700	0.23253500
C	3.00074300	-2.95036200	-2.71132700	H	-0.04186400	-1.49944700	-1.22880600
H	2.89840600	-4.76516000	-1.55019700	C	-0.95949200	-1.61286700	0.72517400
H	2.87141100	-1.02055900	-3.66409700	H	0.97568700	-0.08266600	1.30279200
H	3.75775100	-3.32860700	-3.39286300	C	2.46363800	-0.94288800	0.04424900
C	-3.46531900	0.17147200	-0.59088300	C	3.24030000	-1.28559600	1.15596200
C	-3.46320200	0.60222100	-1.92641800	C	2.94862200	-1.25676200	-1.23274100
C	-4.57473200	0.48776300	0.20356400	C	4.48315200	-1.90312000	1.00036000
C	-4.52932900	1.33740800	-2.44292100	H	2.87026600	-1.06073600	2.15472700
H	-2.63200400	0.34929600	-2.57916900	C	4.18968600	-1.86893700	-1.39286400
C	-5.64213300	1.22634600	-0.30820100	H	2.35592000	-1.01686800	-2.11378400
H	-4.58226600	0.13894800	1.23209400	C	4.96632100	-2.18858500	-0.27595400
C	-5.62361900	1.65618800	-1.63529400	H	5.07329900	-2.15635600	1.87718200
H	-4.51022500	1.65512100	-3.48232300	H	4.55321300	-2.09758700	-2.39126100
H	-6.49055500	1.46443200	0.32873900	H	5.93533200	-2.66358500	-0.40176200
H	-6.45503700	2.22717300	-2.03987400	C	-2.04878000	-2.55160600	0.23775000
C	1.54056500	0.47866100	0.77746800	C	-1.92426000	-3.36686900	-0.89730100
C	2.93298400	0.40873800	0.65562800	C	-3.24000600	-2.62025700	0.97179200
C	0.88118000	1.67425400	0.46248500	C	-2.96465200	-4.20621500	-1.29429200
C	3.66310500	1.50208200	0.20557000	H	-1.00127700	-3.36434900	-1.47096900
H	3.44895200	-0.51545700	0.90422200	C	-4.28638500	-3.45305300	0.57430800
C	1.59942700	2.77780400	0.01641700	H	-3.32690400	-2.00604100	1.86341500
H	-0.19778100	1.74879800	0.55850000	C	-4.15376700	-4.25030600	-0.56321500
C	2.99001300	2.68657800	-0.11581200	H	-2.84306600	-4.83439300	-2.17315100
H	4.74216700	1.44272600	0.10457400	H	-5.20527600	-3.48277900	1.15477900
H	1.08923600	3.70416000	-0.22841100	H	-4.96371600	-4.90521400	-0.87315200
C	3.73562800	3.82669300	-0.57896500	C	-0.32833700	1.77442600	-0.41768900
N	4.33356600	4.74503500	-0.95370700	C	-1.13394700	1.63608500	0.71884300
H	1.50285000	-1.48188400	1.63007500	C	-0.73202500	2.62651200	-1.45301500
IN10-2				C	-2.32627600	2.34453400	0.81950500
C	-0.01535100	-1.18328600	-0.18973000	H	-0.86673300	0.93591400	1.50815300
				C	-1.92139100	3.33900800	-1.36431000

H	-0.11331500	2.72958500	-2.34143600
C	-2.71578600	3.19712100	-0.22052100
H	-2.95776900	2.23323200	1.69560100
H	-2.23539800	3.99544700	-2.16965300
C	-3.94875300	3.93119700	-0.11556900
N	-4.94025900	4.52369700	-0.02979700

TS10-1

C	-1.13294100	-0.88202000	-0.58180000
C	0.39364800	-0.51762200	0.85092200
S	2.00212500	-1.17588500	2.23601400
O	-2.34583500	-1.92981100	1.13790100
H	-0.34809700	-0.53825200	1.64997600
C	1.68082500	0.04961500	3.52312000
H	0.60232100	0.18603500	3.65079900
H	2.13082600	-0.28802700	4.45964800
H	2.14495400	0.98944700	3.21542300
C	1.09762500	-2.58304000	2.91484300
H	0.02779800	-2.35227700	2.96122700
H	1.26528800	-3.44355800	2.26357000
H	1.48061200	-2.80590300	3.91352900
C	0.13750300	-1.57630200	-0.17938200
H	-1.11441700	-0.15104100	-1.37926200
C	-2.29406600	-1.12149400	0.16847000
H	-0.10256200	-2.51448400	0.33198900
C	1.20872000	-1.81028200	-1.21636900
C	2.23820700	-2.71307300	-0.92016400
C	1.23866900	-1.14390500	-2.44523300
C	3.28640900	-2.92692600	-1.81372500
H	2.21316800	-3.26654700	0.01724000
C	2.28440300	-1.35850100	-3.34514800
H	0.45240100	-0.44248200	-2.70811500
C	3.31496900	-2.24358600	-3.03063300
H	4.07519400	-3.63093000	-1.56298900
H	2.29249500	-0.82912800	-4.29414400
H	4.12883400	-2.40770800	-3.73138900
C	-3.55592200	-0.37530500	-0.19967900
C	-3.54735000	0.86682600	-0.84910700
C	-4.78832200	-0.94266900	0.14657600
C	-4.74320300	1.51709700	-1.15373800
H	-2.60478200	1.34402200	-1.10575600
C	-5.98500300	-0.30010800	-0.16629400
H	-4.79180400	-1.89738900	0.66482100
C	-5.96631000	0.93424500	-0.81818900

H	-4.71891200	2.48410600	-1.64911900
H	-6.93276700	-0.76043500	0.10075900
H	-6.89701900	1.44121100	-1.05823300
C	0.88337400	0.85146100	0.50431100
C	2.09979200	1.06451200	-0.15933800
C	0.12581700	1.95509300	0.92031700
C	2.53551800	2.35580000	-0.43329000
H	2.72215000	0.22404800	-0.45246600
C	0.54862400	3.25041900	0.65266100
H	-0.81038900	1.79061100	1.44836000
C	1.75525100	3.44604600	-0.03095900
H	3.47663500	2.52107900	-0.94831400
H	-0.04382800	4.10328700	0.96857200
C	2.20429300	4.78337800	-0.31319500
N	2.56591400	5.85985800	-0.54077500

TS10-2

C	0.02346700	-1.36551100	-0.01335400
C	0.82772600	0.59883200	-0.54492400
S	2.33735500	2.25382200	-0.54322200
O	-1.29030600	-0.92674800	1.89718300
H	1.00661000	0.34198400	-1.58935200
C	2.56447900	2.50644800	1.22963900
H	2.72878700	1.55176600	1.73574500
H	3.42680600	3.16162400	1.37746900
H	1.67034700	2.99573200	1.62102100
C	3.96681500	1.60368100	-0.99011500
H	4.29610600	0.84993800	-0.27263000
H	3.89516600	1.17376900	-1.99142000
H	4.66838100	2.44228800	-1.00480400
C	1.17487400	-0.49707700	0.41655500
H	0.12618900	-1.91097200	-0.94546000
C	-1.13575300	-1.46816200	0.76795900
H	1.03088100	-0.18670400	1.45528100
C	2.54875000	-1.09900700	0.23844400
C	3.42375000	-1.17573400	1.32604900
C	2.97570700	-1.58193200	-1.00477900
C	4.70758200	-1.70334500	1.17517900
H	3.09889400	-0.81012100	2.29819000
C	4.25738600	-2.10605300	-1.16017500
H	2.30904300	-1.54166200	-1.86438000
C	5.13074900	-2.16291300	-0.07146700
H	5.37616900	-1.75020000	2.03062700
H	4.57725400	-2.46863200	-2.13345500

H	6.13125100	-2.56831000	-0.19454400	C	5.34351100	0.07937600	0.48522600
C	-2.27561600	-2.30478600	0.22944800	C	3.89048600	1.72865700	-0.50307700
C	-2.51213300	-2.47619300	-1.14103900	C	6.45770600	0.82911000	0.11024900
C	-3.15011800	-2.90810100	1.14172600	H	5.47731600	-0.85993900	1.01764300
C	-3.58894900	-3.24366700	-1.58617300	C	5.00177000	2.47779500	-0.87818400
H	-1.86532700	-1.99284700	-1.86888800	H	2.89701600	2.08850400	-0.75830700
C	-4.22071400	-3.68355300	0.70027700	C	6.29136400	2.03337900	-0.57270500
H	-2.97571100	-2.76003800	2.20376100	H	7.45502800	0.47135500	0.35158900
C	-4.44404700	-3.85417200	-0.66753000	H	4.86272700	3.41226900	-1.41528000
H	-3.76455800	-3.35863200	-2.65258800	H	7.15652800	2.62035900	-0.86810400
H	-4.88370500	-4.15314300	1.42240600	C	-0.63070200	-0.35356100	1.74456100
H	-5.28169700	-4.45305900	-1.01471600	C	-0.88096400	1.02293000	1.82532800
C	-0.37975900	1.44348900	-0.33929900	C	-1.52205000	-1.23176700	2.37152600
C	-0.83795100	1.78676000	0.94038700	C	-2.00596700	1.50286600	2.49796000
C	-1.03190800	1.96753000	-1.46786400	H	-0.20715900	1.73803800	1.36331200
C	-1.93935900	2.62255700	1.08945800	C	-2.64753700	-0.75522000	3.04286200
H	-0.34883300	1.39350100	1.82342100	H	-1.31723800	-2.29754900	2.32036400
C	-2.13248300	2.79874000	-1.33161100	C	-2.89768900	0.61662600	3.10381500
H	-0.67125200	1.71019100	-2.46080100	H	-2.18501000	2.57409300	2.54691700
C	-2.58611400	3.12450800	-0.04486700	H	-3.33089300	-1.45479200	3.51771400
H	-2.29792800	2.88579600	2.07973000	H	-3.77486000	0.99253900	3.62365900
H	-2.63983900	3.19490700	-2.20555400	C	-1.43952100	-0.14192700	-1.06210600
C	-3.72678700	3.98618100	0.11014200	C	-1.15937900	1.13742700	-1.58921000
N	-4.64654600	4.67922000	0.23609000	C	-2.75510500	-0.39986400	-0.61958100
TS11-1				C	-2.13095800	2.12320900	-1.64339900
C	0.54053300	-0.96026500	0.98619800	H	-0.15529700	1.35529800	-1.94542300
C	-0.33165100	-1.07051900	-0.88017800	C	-3.73530700	0.57766100	-0.67311300
O	0.88515300	-2.13936500	1.31761600	H	-3.01693600	-1.37007100	-0.20345400
S	-0.75864000	-2.80388900	-0.87069000	C	-3.42736600	1.84941600	-1.17990000
H	0.49147000	-0.92096700	-1.58131200	H	-1.89568500	3.10439900	-2.04523700
C	-1.62521000	-3.07651900	-2.43875300	H	-4.73980600	0.36443700	-0.31909100
H	-1.06275200	-2.61606900	-3.25346900	C	-4.43759100	2.86482200	-1.22847700
H	-1.70703600	-4.15677400	-2.58499300	N	-5.25512700	3.68686400	-1.26401700
H	-2.62359200	-2.64157100	-2.36301700	TS11-2			
C	0.83403500	-3.53796800	-1.29219900	C	0.91617500	-1.58678500	-0.52336400
H	1.16637700	-3.13654500	-2.25257900	C	1.28754900	-0.39878000	1.15665800
H	1.51385100	-3.27485900	-0.48125000	O	1.00029500	-2.78957600	-0.13151400
H	0.69475700	-4.61969600	-1.34832100	S	0.48225100	-1.40758300	2.38582200
C	1.60519200	0.00528600	0.54283300	C	1.77270900	-2.61973800	2.73314300
H	1.28483400	0.96285600	0.13711800	H	2.66419600	-2.09549900	3.08523900
C	2.90385300	-0.31616100	0.61647000	H	1.39029400	-3.29896300	3.49812700
H	3.15486600	-1.29000500	1.03705500	H	1.95489900	-3.14917400	1.79775800
C	4.04261700	0.51584200	0.19097000	C	0.57489200	-0.45441900	3.92492300

H	1.58989300	-0.07371800	4.05596100	C	-0.35484700	1.26517400	0.14990900
H	-0.14408300	0.36467500	3.87040700	C	0.58876600	0.78280300	-1.07201500
H	0.30242900	-1.12658300	4.74284600	O	-0.73590300	2.51538800	-0.13160400
C	-0.44432500	-1.02625800	-0.81789400	S	1.53982900	2.31373000	-1.47907700
H	-0.51595200	0.00464800	-1.15209800	H	-0.07210100	0.64180600	-1.93432900
C	-1.55078900	-1.75732300	-0.62452100	C	2.80557400	1.69881700	-2.62105200
H	-1.42101700	-2.78794200	-0.29409100	H	2.36715200	0.99627700	-3.33380000
C	-2.94048700	-1.30783900	-0.81674400	H	3.20129900	2.57228300	-3.14528000
C	-3.97404600	-2.25306700	-0.73052300	H	3.60742800	1.22561700	-2.05410200
C	-3.28384400	0.03082400	-1.07503500	C	0.49138700	3.12824900	-2.70426900
C	-5.30622800	-1.88240300	-0.91019200	H	0.30235000	2.43774500	-3.52983800
H	-3.72428900	-3.29148100	-0.52336900	H	-0.42399900	3.39911500	-2.18169400
C	-4.61316500	0.40206600	-1.25376100	H	1.03432800	4.00937700	-3.05531200
H	-2.50863700	0.79122000	-1.13122100	C	-1.48854100	0.23693400	0.17570900
C	-5.63133800	-0.55251500	-1.17461400	H	-1.22796100	-0.80935200	0.33442300
H	-6.08909400	-2.63305100	-0.84261800	C	-2.76025000	0.60845200	-0.00684800
H	-4.85785800	1.44216500	-1.45228000	H	-2.93881900	1.67204600	-0.16618700
H	-6.66796800	-0.25858100	-1.31365700	C	-3.94968400	-0.26417800	-0.01135700
C	2.07422700	-1.02089600	-1.33023800	C	-5.21270500	0.32075300	-0.18830100
C	1.96266500	0.06997500	-2.20055300	C	-3.88380600	-1.65865600	0.15224300
C	3.32658100	-1.63432200	-1.18513600	C	-6.37277800	-0.45342200	-0.19929800
C	3.07884500	0.53912500	-2.89984100	H	-5.28122600	1.39888200	-0.31719000
H	1.01061100	0.56839100	-2.35342300	C	-5.04024400	-2.43307000	0.14129000
C	4.44008200	-1.16485100	-1.87509700	H	-2.92129800	-2.14471700	0.29000900
H	3.40936100	-2.48706800	-0.51649400	C	-6.29170700	-1.83538400	-0.03394000
C	4.32042500	-0.07092400	-2.73781700	H	-7.33900100	0.02476700	-0.33663500
H	2.97075800	1.38510500	-3.57360600	H	-4.96649400	-3.50964900	0.27074800
H	5.40288800	-1.65240200	-1.74494700	H	-7.19226400	-2.44311300	-0.04122500
H	5.18691600	0.29654500	-3.28082500	C	0.44882900	1.16572700	1.47500900
C	0.81150700	0.96747900	1.03130700	C	0.67027700	-0.02923900	2.17471400
C	1.70079900	1.94697300	0.53366500	C	1.00120300	2.34290600	1.98949700
C	-0.52728900	1.35502000	1.27289000	C	1.42795200	-0.04507200	3.34649800
C	1.27737100	3.23966600	0.27289800	H	0.26844600	-0.96939100	1.80505200
H	2.73762000	1.67578000	0.35035700	C	1.76885200	2.33161000	3.15564600
C	-0.95759800	2.64639900	1.02083700	H	0.80504200	3.26786600	1.45551100
H	-1.25211900	0.63221400	1.64305700	C	1.98659100	1.13514200	3.83949900
C	-0.05795700	3.59866300	0.51514200	H	1.58578200	-0.98373100	3.87187100
H	1.97537400	3.97770700	-0.11147500	H	2.19219700	3.25898100	3.53390500
H	-1.99095800	2.92353100	1.20859500	H	2.57947600	1.12208400	4.75027500
H	2.36836800	-0.49873800	1.26932200	C	1.46388600	-0.42293400	-0.89690300
C	-0.50206900	4.93532500	0.25391300	C	1.03049300	-1.64114900	-1.43482700
N	-0.86259400	6.01725600	0.04101700	C	2.65251400	-0.39194300	-0.15245800
				C	1.75340700	-2.81055600	-1.22836700
				H	0.11328300	-1.67366100	-2.01739300

IN11-1

C	3.39618000	-1.54649200	0.04685300
H	3.00403300	0.53865300	0.28948200
C	2.93916600	-2.75867900	-0.48712800
H	1.40970800	-3.75327100	-1.64238700
H	4.31748900	-1.51677000	0.62005500
C	3.70004500	-3.96057700	-0.27578400
N	4.31453500	-4.92798900	-0.10768700

IN12-1

C	0.88089600	-1.33323800	-0.15643500
O	0.83903900	-0.10379400	-2.14775300
S	1.64195700	-1.63324200	1.51916300
C	1.17425400	0.09483400	-0.87891800
H	1.51125600	-2.01357900	-0.74163800
C	0.60190000	-0.88706200	2.78971700
H	-0.40360800	-1.30937400	2.76154700
H	1.08296000	-1.11791100	3.74378800
H	0.58400900	0.19425100	2.64709900
C	1.26935000	-3.37671500	1.80564700
H	0.18929200	-3.53818900	1.79658700
H	1.76020800	-3.95566100	1.02041100
H	1.69187400	-3.64080800	2.77810000
C	0.38320900	1.20528100	-0.18501400
H	0.58284700	1.42186900	0.86362800
C	-0.53677200	1.91669700	-0.84491600
H	-0.68649300	1.66851800	-1.89543800
C	-1.37559600	2.99508200	-0.28970300
C	-2.14653600	3.77479900	-1.16572400
C	-1.45288400	3.27403000	1.08593400
C	-2.95375200	4.80857100	-0.69194700
H	-2.10534300	3.56598900	-2.23266600
C	-2.25892100	4.30495600	1.56100000
H	-0.88352500	2.67668000	1.79411400
C	-3.01207500	5.07987200	0.67474300
H	-3.53807500	5.40069500	-1.39124200
H	-2.30409900	4.50282400	2.62872300
H	-3.64108900	5.88297600	1.04859400
C	2.69790900	0.36034200	-0.67767600
C	3.26035800	0.98904400	0.44216900
C	3.55913800	-0.07975200	-1.68803300
C	4.64176900	1.16883600	0.54576300
H	2.63502800	1.35273600	1.25457900
C	4.94005800	0.09119100	-1.58705800
H	3.11167100	-0.54627200	-2.56108900

C	5.48832600	0.71861100	-0.46707100
H	5.05456000	1.66403200	1.42106700
H	5.58923800	-0.25977400	-2.38566300
H	6.56278700	0.86032000	-0.38666500
C	-0.54425300	-1.80678400	-0.22608400
C	-1.59915500	-1.13556200	0.40993200
C	-0.82680500	-2.96595900	-0.96161200
C	-2.90350800	-1.60633700	0.30961300
H	-1.41603900	-0.23118100	0.97980900
C	-2.12529900	-3.44644800	-1.07642900
H	-0.01708500	-3.49547500	-1.45641100
C	-3.16452700	-2.76145100	-0.43627600
H	-3.71633200	-1.08194200	0.80225800
H	-2.33588500	-4.34144900	-1.65348100
C	-4.51340500	-3.24901600	-0.54580200
N	-5.59912200	-3.64285500	-0.63364700

IN12-2

C	0.43290800	-0.85607300	0.11784500
O	-0.06049500	0.14185700	-1.93622500
S	0.16751300	-1.05959000	1.95040200
C	-0.27811400	0.39470100	-0.65344700
H	-0.04333500	-1.74303600	-0.31280600
C	-1.51068300	-1.72469100	2.07461500
H	-1.69912400	-2.40171100	1.23812100
H	-1.55738700	-2.26196700	3.02509600
H	-2.22483100	-0.90220800	2.08652600
C	1.08655100	-2.58451000	2.28047800
H	0.81083500	-3.33931300	1.54011200
H	2.15319400	-2.36109100	2.23644500
H	0.81895900	-2.91055600	3.28803000
C	-1.75590200	0.38897300	-0.24595900
H	-2.02907400	0.78618900	0.73121700
C	-2.70153400	-0.07302500	-1.07137300
H	-2.36760500	-0.42746900	-2.04663000
C	-4.14778400	-0.16090500	-0.79740100
C	-4.99292500	-0.67935600	-1.79071000
C	-4.72629000	0.24021400	0.41955500
C	-6.36686100	-0.79511700	-1.58228400
H	-4.56139100	-0.99509100	-2.73820900
C	-6.09763600	0.12548700	0.62936500
H	-4.10234300	0.64934800	1.21016500
C	-6.92597200	-0.39334000	-0.36971800
H	-6.99956500	-1.19961300	-2.36786500

H	-6.52370800	0.44268700	1.57752500	C	0.68841900	3.30290800	-0.25682700
H	-7.99578500	-0.48152300	-0.20223700	C	0.57944700	4.38918000	-1.13791300
C	0.36787100	1.71204000	-0.14711500	C	0.71782100	3.56706400	1.12317700
C	0.15751000	2.25325800	1.12872200	C	0.52031500	5.69881600	-0.66246900
C	1.24673800	2.37350100	-1.00841500	H	0.54513600	4.19942000	-2.20859900
C	0.82420100	3.41059000	1.53602300	C	0.65692100	4.87371500	1.59937900
H	-0.52500700	1.78194600	1.83279600	H	0.77886900	2.74498200	1.83236300
C	1.91290100	3.53298800	-0.60962700	C	0.56080100	5.94683100	0.70923000
H	1.39642300	1.94256900	-1.99428400	H	0.44036100	6.52439500	-1.36456600
C	1.70856300	4.05399600	0.66884100	H	0.67857800	5.05681000	2.67039800
H	0.64943500	3.80996600	2.53184700	H	0.51190900	6.96538000	1.08403200
H	2.59624200	4.02849000	-1.29520900	C	2.47651300	-1.16085700	-0.62519100
H	2.22743200	4.95495000	0.98529200	C	3.15027900	-1.17070300	0.60340800
C	1.91815000	-0.89064400	-0.12507900	C	3.08743600	-1.75900800	-1.72942700
C	2.81316900	-0.07244100	0.57931800	C	4.40339600	-1.77166300	0.72265500
C	2.41341800	-1.75363500	-1.10871400	H	2.70943400	-0.70924000	1.48460600
C	4.17507200	-0.11227200	0.30680000	C	4.34443600	-2.35611500	-1.61500800
H	2.45482300	0.60926400	1.34766100	H	2.55746000	-1.74097000	-2.67712400
C	3.77148300	-1.79780400	-1.40025100	C	5.00637200	-2.36592600	-0.38754400
H	1.72432800	-2.39098300	-1.65418500	H	4.91073800	-1.77184600	1.68381300
C	4.65172600	-0.97475100	-0.68782500	H	4.80682400	-2.81365600	-2.48606100
H	4.86519400	0.52106500	0.85540900	H	5.98440000	-2.83031300	-0.29485700
H	4.15104700	-2.46502800	-2.16785900	C	-1.45468800	-1.17917500	-0.47680200
C	6.06022600	-1.02083200	-0.97488600	C	-1.98886300	-0.02230200	0.10950600
N	7.19489800	-1.05805900	-1.20516100	C	-2.32492000	-2.10248600	-1.07499800
TS12-1				C	-3.35821800	0.21355900	0.08542300
C	-0.00688400	-1.51901400	-0.44624900	H	-1.34049200	0.70536600	0.58353900
O	0.63210800	-0.54981100	-2.09755800	C	-3.69473500	-1.87849600	-1.10955400
S	0.21214400	-2.35598900	1.65507500	H	-1.91895600	-3.00536900	-1.52341300
C	1.08160800	-0.53245500	-0.81617400	C	-4.20950000	-0.71475300	-0.52585900
H	0.21968400	-2.49803600	-0.86405300	H	-3.76838300	1.10997300	0.53971700
C	-0.12391100	-1.00604100	2.80490700	H	-4.36166500	-2.59413700	-1.57990500
H	-1.02855000	-0.46622600	2.51382400	C	-5.62732000	-0.47259600	-0.54905900
H	-0.25328100	-1.43130500	3.80392800	N	-6.76897800	-0.27823100	-0.56679200
H	0.73517800	-0.33207600	2.81371500	TS12-2			
C	-1.31979400	-3.29362700	1.85476000	C	0.46185700	-0.69481900	-0.18596600
H	-2.18644600	-2.63904600	1.72907100	O	-0.07741800	0.21993400	-1.87752400
H	-1.33435200	-4.08577100	1.10241100	S	0.35083400	-1.19183400	2.00573500
H	-1.32869900	-3.74015100	2.85222500	C	-0.34236900	0.52256200	-0.57755200
C	1.04640700	0.82380600	-0.13496000	H	-0.05158700	-1.61353600	-0.46589400
H	1.30466700	0.87026700	0.92195900	C	-1.24956800	-2.03400800	2.05297800
C	0.74815500	1.93777400	-0.81115700	H	-1.39232400	-2.62349700	1.14273000
H	0.51231100	1.83287200	-1.86974600	H	-1.27585400	-2.68449500	2.93097100

H	-2.03647400	-1.28281300	2.14090900
C	1.43436100	-2.63976600	2.02929200
H	1.21345900	-3.28764400	1.17576500
H	2.46868100	-2.29279200	1.98055400
H	1.27678500	-3.18225600	2.96474800
C	-1.80153800	0.40009500	-0.16736100
H	-2.06927600	0.71018200	0.84224400
C	-2.72722900	-0.06131200	-1.01498200
H	-2.38968500	-0.33837000	-2.01355700
C	-4.16425400	-0.24302500	-0.73736500
C	-4.98937000	-0.73854600	-1.75814600
C	-4.74962000	0.04871200	0.50660600
C	-6.35376200	-0.93793300	-1.54995200
H	-4.55043000	-0.96923800	-2.72646600
C	-6.11133500	-0.14950100	0.71584100
H	-4.14009200	0.43581100	1.31914300
C	-6.92093200	-0.64413300	-0.31063100
H	-6.97216300	-1.32269800	-2.35645200
H	-6.54479900	0.08265700	1.68497300
H	-7.98323800	-0.79805400	-0.14292300
C	0.22014500	1.86545900	-0.09800800
C	0.08540700	2.30987200	1.22373800
C	0.92300500	2.65788100	-1.00670700
C	0.66407400	3.51206900	1.63015400
H	-0.45592700	1.71624900	1.95719500
C	1.49366700	3.86748300	-0.60600100
H	1.02725000	2.29695000	-2.02554800
C	1.37187600	4.29551400	0.71589400
H	0.56135100	3.83778200	2.66196800
H	2.04013400	4.47228700	-1.32528800
H	1.82161100	5.23251100	1.03304200
C	1.94492900	-0.73657800	-0.36446200
C	2.81016000	0.16472700	0.27156100
C	2.48335800	-1.76721000	-1.14468100
C	4.18588600	0.05495100	0.10850700
H	2.41860500	0.94833000	0.91290700
C	3.85596700	-1.88716800	-1.32024100
H	1.81502500	-2.47668100	-1.62469200
C	4.70614500	-0.96934500	-0.69195800
H	4.85531800	0.75208300	0.60264400
H	4.26891500	-2.68313300	-1.93190300
C	6.13006800	-1.08714300	-0.86033600
N	7.27645100	-1.18182600	-0.99570900

Ar-PR-1-1			
C	0.99263300	0.27582500	-0.52843600
C	-0.20871900	0.51097100	-1.39447400
O	2.49718900	0.85665100	-2.25688400
H	0.01375500	0.91972800	-2.37869400
C	0.28491200	-0.90104000	-1.19470200
H	0.85332600	0.37082200	0.54322300
C	2.33905000	0.61641400	-1.06884600
H	0.81429600	-1.30698800	-2.05355900
C	-0.46193400	-1.92320700	-0.40796500
C	-0.71087900	-3.16444900	-1.00865500
C	-0.94711800	-1.70002500	0.88837300
C	-1.42812800	-4.15537000	-0.33933000
H	-0.33729100	-3.35203300	-2.01288000
C	-1.66441700	-2.69047300	1.55844700
H	-0.76887200	-0.75164200	1.38915100
C	-1.90977500	-3.92138100	0.94854900
H	-1.60785000	-5.11044600	-0.82549700
H	-2.03051000	-2.49755600	2.56323100
H	-2.46784900	-4.69123200	1.47402100
C	3.50214000	0.62748200	-0.12704200
C	3.46124000	-0.03597000	1.10517000
C	4.67047700	1.29569000	-0.51531200
C	4.58114100	-0.03453700	1.93582300
H	2.57016400	-0.57514600	1.41502500
C	5.78082800	1.31044500	0.32272000
H	4.69437600	1.80560900	-1.47404600
C	5.73777600	0.64208800	1.54892500
H	4.54906700	-0.56194600	2.88469200
H	6.68034500	1.84004300	0.02216200
H	6.60636500	0.64877200	2.20160400
C	-1.49995400	0.96752600	-0.79697400
C	-2.70383900	0.46185400	-1.30506600
C	-1.53489200	1.88831600	0.25440500
C	-3.92316700	0.86088300	-0.77361100
H	-2.68124500	-0.25991000	-2.11795600
C	-2.74696100	2.29942500	0.79901300
H	-0.60613100	2.28438100	0.65593900
C	-3.94036900	1.78004900	0.28425200
H	-4.85520800	0.46395600	-1.16383300
H	-2.77265200	3.01353400	1.61648200
C	-5.19746100	2.19375700	0.84750000
N	-6.20958900	2.52588700	1.30277600

Ar-PR-1-2

C	0.90533200	0.81354600	-0.02324900
C	0.74772800	-0.57088500	0.61251700
O	-0.34564200	0.80081900	-2.04171600
H	1.13039300	-0.60915700	1.63053300
C	1.77145500	-0.33449300	-0.46006400
H	1.34185200	1.56639100	0.62712900
C	-0.18644600	1.27925500	-0.92954000
H	1.52248600	-0.71669500	-1.44676300
C	3.23002800	-0.35823900	-0.14428700
C	4.11906900	-0.91045200	-1.07376600
C	3.74466800	0.15416000	1.05424000
C	5.48915100	-0.95390700	-0.81450000
H	3.73182600	-1.30961300	-2.00846500
C	5.11334100	0.11096700	1.31426700
H	3.07969900	0.59309300	1.79517900
C	5.99200000	-0.44354800	0.38171900
H	6.16228800	-1.38715000	-1.54938700
H	5.49438900	0.51306800	2.24911200
H	7.05837900	-0.47578900	0.58668700
C	-1.11465200	2.32877500	-0.40641300
C	-1.22522600	2.58611700	0.96529500
C	-1.91135500	3.03969900	-1.31267200
C	-2.12805000	3.54417600	1.42461400
H	-0.62321900	2.03092100	1.67969000
C	-2.80071200	4.00573200	-0.85329900
H	-1.82066800	2.83101600	-2.37484500
C	-2.91106500	4.25721000	0.51684600
H	-2.21850200	3.73398800	2.49019400
H	-3.40913300	4.56291900	-1.55986200
H	-3.60861500	5.00885800	0.87584900
C	-0.49819800	-1.36633500	0.41801000
C	-0.79710200	-2.04853200	-0.76734000
C	-1.41197400	-1.42169900	1.48185400
C	-1.98153100	-2.76636700	-0.89365600
H	-0.10316300	-2.03258500	-1.60110400
C	-2.59807800	-2.13394700	1.37166600
H	-1.18525700	-0.89920400	2.40794100
C	-2.88222600	-2.80758800	0.17631400
H	-2.20675600	-3.29697000	-1.81363400
H	-3.30034200	-2.17256300	2.19874000
C	-4.10596800	-3.55144300	0.04890500
N	-5.09166600	-4.15147100	-0.05400400

Ar-PR-2-1

C	0.98253800	-1.70095400	-0.57653700
O	1.27469000	-0.81651600	-1.64543300
C	1.55928100	-0.33626300	-0.33525300
H	1.68222300	-2.53187700	-0.47265700
C	0.68205700	0.75909400	0.16241000
H	0.67584100	0.90750500	1.24006600
C	-0.06618800	1.51035900	-0.65291800
H	-0.01915900	1.31275300	-1.72366700
C	-0.97763800	2.59867900	-0.25530500
C	-1.66800500	3.29101400	-1.26073800
C	-1.18928400	2.97429800	1.08158200
C	-2.54395300	4.32958900	-0.94625800
H	-1.51260400	3.00914800	-2.29998200
C	-2.06304400	4.01050000	1.39599600
H	-0.67144500	2.45581000	1.88398200
C	-2.74445500	4.69344600	0.38437400
H	-3.06843000	4.85267200	-1.74115500
H	-2.21503600	4.28725700	2.43571100
H	-3.42578300	5.50171000	0.63479900
C	3.02532200	-0.26090700	-0.00096900
C	3.48931000	0.48499000	1.08804600
C	3.94823500	-0.96208400	-0.78658600
C	4.85093200	0.51836900	1.39123700
H	2.79700400	1.04471000	1.70932000
C	5.30793500	-0.92266400	-0.48545600
H	3.59962500	-1.53269200	-1.64294900
C	5.76480500	-0.18379200	0.60692800
H	5.19493200	1.10038300	2.24172400
H	6.01182700	-1.46849600	-1.10771100
H	6.82501100	-0.15321200	0.84190100
C	-0.44154100	-2.04323000	-0.32275200
C	-1.47696300	-1.48721400	-1.08044200
C	-0.73757400	-2.94874200	0.70333800
C	-2.79948600	-1.81953000	-0.80972000
H	-1.24525700	-0.80142800	-1.88871100
C	-2.05435800	-3.28396200	0.98854100
H	0.06964200	-3.39175800	1.28106000
C	-3.08490900	-2.71413300	0.22868400
H	-3.60735200	-1.39368500	-1.39667300
H	-2.28843500	-3.98142200	1.78659300
C	-4.45168000	-3.06000100	0.51288300
N	-5.55259200	-3.33806000	0.74218500

Ar-PR-2-2

C	-0.38254100	-1.14861800	0.38092900
O	0.12270500	-0.52837300	1.55531600
C	0.35935100	0.15207000	0.33116500
H	0.17653400	-2.02684600	0.05819400
C	1.77035900	0.15678600	-0.14883000
H	1.94249600	0.70190500	-1.07519300
C	2.76222200	-0.45580800	0.50942100
H	2.52201100	-0.96711200	1.44165900
C	4.17881700	-0.50748500	0.10585700
C	5.09785400	-1.12565500	0.96639200
C	4.65293800	0.03240500	-1.10132600
C	6.45131800	-1.19989300	0.63912600
H	4.74301800	-1.55018300	1.90295300
C	6.00325300	-0.04162400	-1.42878300
H	3.96491900	0.51084300	-1.79306600
C	6.90948700	-0.65683300	-0.56030900
H	7.14593300	-1.68173800	1.32172800
H	6.35192400	0.38069300	-2.36730800
H	7.96289900	-0.71237200	-0.82014900
C	-0.40418100	1.42900200	0.13188100
C	-0.74560100	1.83638200	-1.16128800
C	-0.77112700	2.21453500	1.22531800
C	-1.45469400	3.02045000	-1.35719200
H	-0.46686300	1.21900200	-2.01328200
C	-1.47814200	3.40142900	1.02791200
H	-0.51111100	1.89106100	2.23000400
C	-1.82208600	3.80537100	-0.26220900
H	-1.72536400	3.32737900	-2.36365000
H	-1.76210800	4.00830700	1.88328500
H	-2.37627300	4.72726400	-0.41492700
C	-1.85705200	-1.22904600	0.21527100
C	-2.36778100	-1.92760100	-0.88503800
C	-2.73174000	-0.60824400	1.11303600
C	-3.73769200	-1.99598000	-1.10143400
H	-1.68690900	-2.41818300	-1.57599600
C	-4.10537800	-0.67397400	0.91121800
H	-2.33495800	-0.08055900	1.97447300
C	-4.60488500	-1.36483200	-0.19981800
H	-4.13770500	-2.53344100	-1.95544000
H	-4.78930800	-0.19725500	1.60653700
C	-6.02527600	-1.43512000	-0.41385100
N	-7.16933100	-1.49115700	-0.58671900

E-DMSM

S	1.45793300	-0.02608800	-0.37493900
C	2.52083600	1.35366300	0.11759900
H	2.62041900	1.36459300	1.20581400
H	3.49751300	1.23346600	-0.35769400
H	2.04407800	2.27144000	-0.23103400
C	2.43242600	-1.37317900	0.34889100
H	1.88293800	-2.30031300	0.17568500
H	3.40316600	-1.41413000	-0.15159400
H	2.55694900	-1.19705100	1.42017800
C	0.04159100	0.11849500	0.55101500
H	0.12494400	0.22225400	1.62657300
C	-1.20177800	0.00740400	-0.11579400
O	-1.41344000	-0.15234400	-1.32165200
O	-2.24728600	0.10553700	0.76578300
C	-3.54581900	0.00485600	0.19244200
H	-3.68438300	-0.95873500	-0.30594900
H	-4.24575600	0.09252700	1.02472100
H	-3.72453100	0.81037900	-0.52564100

COM7-1

C	0.28213900	-0.57632500	-1.30853600
C	-1.61465900	1.62244100	0.88289000
O	2.29090500	1.36669200	-1.62493200
S	-2.91853700	1.87439800	-0.18332500
H	-0.81941100	2.35931600	0.90173000
C	-2.14801000	2.44855800	-1.71373500
H	-1.59337600	1.61354800	-2.14285000
H	-2.93468400	2.76991600	-2.40067500
H	-1.47360000	3.27851900	-1.48759400
C	-3.72191000	3.43683700	0.28413800
H	-4.19815800	3.27656500	1.25354600
H	-2.96793900	4.22501100	0.35413400
H	-4.47594300	3.68639200	-0.46706500
C	1.42169100	-0.58216400	-0.59525300
H	1.58352600	-1.28264100	0.21806800
C	2.49139200	0.39713900	-0.90184800
H	0.20327300	0.14504400	-2.12215800
C	-0.88133300	-1.45140200	-1.12754000
C	-1.95033500	-1.33399500	-2.02981000
C	-0.97486300	-2.39199400	-0.08870600
C	-3.08184900	-2.13764300	-1.90483600
H	-1.88661900	-0.60773500	-2.83731700
C	-2.10070700	-3.19923700	0.03081500

H	-0.16670300	-2.49349600	0.63092500	C	-2.70820700	-0.68767400	0.88385800
C	-3.15776600	-3.07526600	-0.87493900	C	-4.68199700	-2.11914300	-0.47996800
H	-3.90018500	-2.03464500	-2.61202800	H	-3.05025500	-3.13237200	-1.45727400
H	-2.16033000	-3.92416600	0.83822100	C	-4.05218200	-0.43020000	1.13024400
H	-4.03675700	-3.70616400	-0.77501800	H	-1.94567700	-0.12778300	1.41996300
C	3.84379200	0.18597300	-0.29151200	C	-5.04328900	-1.14427700	0.44976900
C	4.26730100	-1.06980100	0.16043500	H	-5.44739400	-2.67770200	-1.01134600
C	4.71507200	1.27963800	-0.20514000	H	-4.33137400	0.33183700	1.85298800
C	5.54903400	-1.22797200	0.68664600	H	-6.09216300	-0.93948800	0.64561700
H	3.61409400	-1.93406000	0.08363500	C	2.69039700	-1.19648800	0.43324100
C	5.98706600	1.12404100	0.33616400	C	2.59557700	-0.79376800	1.77060800
H	4.38036500	2.25014000	-0.55959700	C	3.92970200	-1.14153400	-0.21782600
C	6.40654400	-0.13223900	0.78126300	C	3.73020500	-0.34876200	2.44846600
H	5.87635000	-2.20745200	1.02319500	H	1.64678000	-0.84079600	2.29642700
H	6.65315200	1.97888100	0.41114800	C	5.05746800	-0.68201500	0.45467900
H	7.40150500	-0.25596100	1.19991400	H	3.99428200	-1.45585300	-1.25564400
C	-1.62090100	0.56428200	1.82236800	C	4.95872100	-0.28618800	1.79112900
O	-0.72861000	0.33851800	2.64605400	H	3.65294700	-0.04877800	3.48959300
O	-2.73940800	-0.22583900	1.77745100	H	6.01290700	-0.63071300	-0.05964700
C	-2.79537400	-1.27061300	2.73923900	H	5.83933000	0.06980800	2.31873100
H	-2.89509600	-0.86237500	3.75049700	C	-0.96442300	2.07925200	0.42518100
H	-3.68204500	-1.85795300	2.49455300	O	-0.22299500	1.71928700	1.34927100
H	-1.90587600	-1.90356300	2.69674500	O	-2.19560400	2.61491400	0.69608900
COM7-2				C	-2.52360000	2.74946700	2.07402500
C	-0.92986300	-1.95368500	-0.37251100	H	-1.86891500	3.47866500	2.56158600
C	-0.72667400	2.00754300	-0.96515000	H	-3.55415500	3.10657400	2.10046500
O	1.67448500	-2.37143900	-1.34793500	H	-2.44605200	1.79506100	2.60210600
S	0.79191100	1.43688900	-1.48477000	COM8-1			
H	-1.40497200	2.42857700	-1.69820800	C	-0.83652000	-0.78931300	-1.22964000
C	1.64074200	2.81571800	-2.30587000	C	0.00980000	1.98334000	0.82331600
H	1.88496200	3.54719900	-1.53323700	O	-0.72529800	-0.15833400	-2.27581900
H	2.55646500	2.44049400	-2.77034100	S	0.42250400	3.09722600	-0.39175200
H	0.97741600	3.25547100	-3.05461500	H	0.80103600	1.40803800	1.29084300
C	0.44315000	0.43578900	-2.94874000	C	1.61711200	4.23415400	0.35684600
H	-0.10733200	-0.44758700	-2.61997500	H	2.41562600	3.65830300	0.83116500
H	-0.15781200	1.02118200	-3.64920100	H	2.02170000	4.88473300	-0.42266000
H	1.39148400	0.14363600	-3.40578200	H	1.08206500	4.82761400	1.10048500
C	0.15044900	-1.34828000	0.15186500	C	1.54976200	2.24722100	-1.52764400
H	0.06320000	-0.55711800	0.89308300	H	2.36931500	1.79991900	-0.95842100
C	1.50665200	-1.70381500	-0.33277500	H	0.96548200	1.47877100	-2.03978400
H	-0.76722900	-2.72784600	-1.12309100	H	1.93547300	2.97616700	-2.24545000
C	-2.33168300	-1.66391400	-0.05458700	C	0.34854800	-1.13791400	-0.40830200
C	-3.33516300	-2.37549200	-0.72985100	H	0.18893800	-1.37446500	0.63931300

C	1.57367100	-1.13248300	-0.95824000	H	-2.12534800	4.53675800	0.61055900
H	1.65285900	-0.90444200	-2.02156900	H	-3.50602000	4.19937400	-0.47945200
C	2.84642800	-1.38697000	-0.27283300	C	0.44911400	-1.56857900	-0.41169800
C	4.02615800	-1.38983100	-1.03267500	H	0.53754800	-1.97748400	0.58968000
C	2.93575200	-1.60362100	1.11283900	C	1.51657500	-1.09349200	-1.07576900
C	5.26349300	-1.61117200	-0.43050800	H	1.35104900	-0.67360400	-2.06822000
H	3.96618100	-1.21576900	-2.10481000	C	2.89904800	-1.04698400	-0.59009300
C	4.17049700	-1.82586100	1.71299100	C	3.85829500	-0.38691300	-1.37282900
H	2.03884900	-1.59688400	1.72630000	C	3.29521100	-1.60317300	0.63778100
C	5.33836600	-1.83131000	0.94435900	C	5.17603000	-0.26554300	-0.93569500
H	6.16682200	-1.61066200	-1.03397900	H	3.55824800	0.04551100	-2.32475200
H	4.22510400	-1.99309800	2.78506700	C	4.61060900	-1.48493700	1.07241300
H	6.30059600	-2.00381100	1.41838700	H	2.57300500	-2.12394900	1.26062400
C	-2.18484700	-1.24505900	-0.76554600	C	5.55426100	-0.81128400	0.29072300
C	-2.33347400	-2.28366800	0.16127600	H	5.90465500	0.25583500	-1.55007500
C	-3.32374500	-0.64403000	-1.31608400	H	4.90358200	-1.91513000	2.02611700
C	-3.60653400	-2.72174800	0.52447000	H	6.57977100	-0.71706800	0.63696900
H	-1.46192100	-2.76947500	0.59043900	C	-2.08936800	-1.79434100	-0.17123200
C	-4.59387500	-1.07155600	-0.94206500	C	-2.05668900	-1.63371100	1.21916300
H	-3.20036600	0.16312000	-2.03150000	C	-3.29282800	-2.14661600	-0.79600800
C	-4.73658900	-2.11420900	-0.02240400	C	-3.21627400	-1.81587700	1.97255200
H	-3.71455000	-3.53506300	1.23644400	H	-1.13951600	-1.33851000	1.72077400
H	-5.47343800	-0.59472700	-1.36548600	C	-4.44507200	-2.34411400	-0.04211900
H	-5.72827800	-2.45093300	0.26738100	H	-3.31379200	-2.26080900	-1.87614600
C	-1.36087100	1.69021800	1.01928000	C	-4.40912000	-2.17356600	1.34458500
O	-2.34331500	2.23047900	0.50281700	H	-3.18727200	-1.67440700	3.04913100
O	-1.52154700	0.67819200	1.93236800	H	-5.37247700	-2.62639300	-0.53241100
C	-2.86657000	0.37351200	2.28058300	H	-5.31055100	-2.31975500	1.93330200
H	-3.46336100	0.13647800	1.39608500	C	0.59872700	1.96819600	0.46926300
H	-2.81562800	-0.49205800	2.94332600	O	1.24826700	2.56115800	-0.39779300
H	-3.33065900	1.21173900	2.81140600	O	1.23006400	1.39399300	1.54173500
COM8-2				C	2.62468800	1.65673600	1.65048200
C	-0.89395800	-1.51725800	-1.03163200	H	2.80552700	2.72435000	1.81547400
C	-0.80412800	1.78320900	0.53923800	H	2.96654500	1.09252700	2.51968200
O	-1.04885700	-1.24944600	-2.21936500	H	3.16772400	1.33531400	0.75819300
S	-1.76846600	2.54327800	-0.63748200	TS13-1			
H	-1.29180400	1.33786200	1.39882000	C	0.20985200	0.29711800	-0.98088400
C	-3.07281500	1.36035000	-1.05111900	C	0.96783300	-1.24011500	0.31904400
H	-3.50751800	0.96157000	-0.13007000	O	-1.94257500	-1.43323900	-1.39413500
H	-3.83352000	1.88020500	-1.63948400	S	2.48807500	-1.89379100	-0.26829400
H	-2.61925700	0.56584100	-1.64625000	H	0.12874000	-1.92156800	0.19772900
C	-2.79566800	3.76447500	0.22837800	C	1.97784700	-2.67272600	-1.81226200
H	-3.32073300	3.27439700	1.05232500	H	1.79315100	-1.89232500	-2.55171100

H	2.80466400	-3.30305000	-2.14714900	S	0.19111000	2.41304300	-0.08760800
H	1.08054200	-3.27179900	-1.64128300	H	-2.03131600	1.85625800	-0.84472700
C	2.80851300	-3.38489900	0.71487400	C	-0.25587800	3.93278000	0.79538500
H	3.02892500	-3.05978900	1.73364600	H	-0.47664600	3.65490400	1.82793200
H	1.92507400	-4.02685000	0.69582400	H	0.60397300	4.60763300	0.77049900
H	3.67676200	-3.89512300	0.28947500	H	-1.12645700	4.39079300	0.32102000
C	-1.08276600	0.58887500	-0.54321200	C	0.27154900	3.05834300	-1.76667200
H	-1.26704300	1.43051400	0.11377000	H	0.48074800	2.21398300	-2.42355500
C	-2.13014700	-0.34236200	-0.81582700	H	-0.67071500	3.55091000	-2.01650300
H	0.27243400	-0.39182500	-1.82038800	H	1.10064000	3.76841400	-1.80422100
C	1.31421500	1.28439300	-0.90618900	C	0.62864900	-0.83773200	-0.41391500
C	2.35298900	1.22815300	-1.84528800	H	0.62758900	-1.46992200	0.46610800
C	1.36604000	2.26446200	0.09543000	C	1.87054200	-0.32486400	-0.90367200
C	3.41344600	2.13244100	-1.79366300	H	-0.47504300	0.04092000	-1.98364600
H	2.32238000	0.47401100	-2.63022600	C	-1.83762300	-1.19733100	-0.84022800
C	2.42732500	3.16451700	0.15244500	C	-2.86457800	-1.02049700	-1.77749100
H	0.57870600	2.31622900	0.84384500	C	-2.05299500	-2.07121900	0.23356200
C	3.45460900	3.10299500	-0.79218700	C	-4.07614600	-1.69522300	-1.64843400
H	4.20620600	2.07899700	-2.53499200	H	-2.70749700	-0.34123900	-2.61326800
H	2.45471500	3.91540600	0.93792400	C	-3.26639900	-2.74334500	0.36800800
H	4.28030700	3.80786700	-0.74756100	H	-1.27565800	-2.22652800	0.97697900
C	-3.53196800	-0.01067100	-0.35919400	C	-4.28300500	-2.55767400	-0.56989300
C	-3.95041300	1.29787800	-0.08427300	H	-4.85918200	-1.54832600	-2.38752700
C	-4.45434700	-1.05569100	-0.22506000	H	-3.41889100	-3.41338400	1.21017500
C	-5.26085800	1.55264500	0.31937900	H	-5.22766200	-3.08399400	-0.46337300
H	-3.26115600	2.12918100	-0.20227100	C	3.14769400	-0.78494200	-0.24354500
C	-5.76107300	-0.80485600	0.18830200	C	3.25393100	-2.00455400	0.43764400
H	-4.12988600	-2.06794000	-0.44807400	C	4.27579600	0.03973200	-0.33493500
C	-6.16860500	0.50223500	0.46152500	C	4.46358700	-2.38755600	1.01668200
H	-5.57369900	2.57378900	0.51983100	H	2.39990300	-2.67304500	0.50168400
H	-6.46301900	-1.62753700	0.29616700	C	5.48117500	-0.33541800	0.25437000
H	-7.18844600	0.70160300	0.77929200	H	4.19227000	0.98008700	-0.87244400
C	1.04558700	-0.53609900	1.57837500	C	5.57836400	-1.55247200	0.93178300
O	0.07666300	-0.24075000	2.26274200	H	4.53612600	-3.34130900	1.53224500
O	2.30657000	-0.14775000	1.90200600	H	6.34551700	0.31962500	0.18493600
C	2.42915100	0.67510300	3.06160900	H	6.51860400	-1.85011300	1.38791400
H	2.11293000	0.13079500	3.95551500	C	-1.71022200	1.04470600	1.15253900
H	3.48703400	0.92846300	3.13328300	O	-0.97502500	0.91840800	2.12945500
H	1.83282000	1.58514800	2.95749200	O	-3.02429100	0.73780000	1.19267200
TS13-2				C	-3.49993100	0.19315100	2.42329400
C	-0.56692000	-0.45448100	-1.01825500	H	-3.42841200	0.93480800	3.22416200
C	-1.28396100	1.46335900	-0.15896300	H	-4.54456100	-0.06465700	2.24731300
O	1.95836500	0.49336600	-1.84292800	H	-2.93526200	-0.69968300	2.70284400

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C	-0.37646400	-0.16973200	-0.74541800
C	-0.77845500	1.00395900	0.22341300
O	1.88191600	1.42127300	-1.09729200
S	-2.03961700	2.09599900	-0.55260900
H	0.10486600	1.63485200	0.36257500
C	-1.06454500	2.77340400	-1.91980300
H	-1.24258900	2.15747700	-2.80255300
H	-1.43160900	3.78668100	-2.09863100
H	-0.00463600	2.76248100	-1.64513800
C	-2.00906000	3.49314800	0.59093700
H	-2.46268500	3.17241800	1.53066200
H	-0.97652400	3.81768400	0.73951100
H	-2.60790500	4.29140100	0.14723700
C	1.00292700	-0.63282500	-0.37852100
H	1.13521800	-1.58173900	0.12720600
C	2.04365300	0.24729000	-0.60314400
H	-0.31954200	0.29586000	-1.73872900
C	-1.44941500	-1.23857200	-0.78755600
C	-2.40990800	-1.21821200	-1.80452300
C	-1.54185700	-2.22788200	0.20033100
C	-3.44253300	-2.15682400	-1.83620000
H	-2.34535400	-0.46202400	-2.58585600
C	-2.57370000	-3.16516700	0.17450100
H	-0.80576500	-2.26716700	1.00043000
C	-3.52894900	-3.13198500	-0.84314500
H	-4.17651800	-2.12622300	-2.63698700
H	-2.63036500	-3.92403300	0.95056700
H	-4.33105200	-3.86465600	-0.86348500
C	3.45340800	-0.15705200	-0.22494400
C	3.84359400	-1.48716200	-0.00691200
C	4.42319100	0.84517100	-0.09679600
C	5.15646100	-1.80044300	0.34162100
H	3.12340900	-2.29228400	-0.12539800
C	5.73746000	0.53658200	0.25618800
H	4.12515100	1.87307400	-0.28147700
C	6.11047700	-0.78918400	0.47828600
H	5.43786800	-2.83850000	0.49978000
H	6.47213900	1.33197200	0.35531800
H	7.13418500	-1.03461500	0.74811600
C	-1.28641400	0.50191100	1.55928000
O	-0.55509100	0.16234100	2.45864200
O	-2.61867300	0.43712000	1.60698100
C	-3.18199100	-0.15213300	2.78991500

H	-2.93987500	0.45522200	3.66473700
H	-4.25774400	-0.16843300	2.62306000
H	-2.79928400	-1.16704900	2.91907700

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C	-0.66378600	-0.16361400	-0.81125700
C	-1.22136300	1.16314500	-0.17477300
O	1.88373900	0.76179200	-1.64538900
S	0.04822900	2.48381700	-0.23631300
H	-2.08286200	1.52900500	-0.74422800
C	-0.88410000	3.83309800	0.52766300
H	-0.89711000	3.67222300	1.60672900
H	-0.34764400	4.75916700	0.30666200
H	-1.89747900	3.87207700	0.12060300
C	-0.08121100	2.98928300	-1.96240200
H	0.35085600	2.18117300	-2.55196100
H	-1.12506500	3.19039600	-2.21235300
H	0.52306000	3.89356000	-2.06926500
C	0.63346500	-0.63519900	-0.22443300
H	0.62457200	-1.33153700	0.60542100
C	1.81581300	-0.14128400	-0.73459300
H	-0.48441200	0.10471800	-1.86050200
C	-1.79392800	-1.18299600	-0.78609700
C	-2.69569400	-1.23670900	-1.85403600
C	-1.99226600	-2.04471500	0.29934300
C	-3.76867800	-2.12874400	-1.84434900
H	-2.55404600	-0.57089000	-2.70342300
C	-3.06673600	-2.93346900	0.31683500
H	-1.31130000	-2.02324100	1.14738700
C	-3.95923900	-2.97934400	-0.75535000
H	-4.45436000	-2.15854200	-2.68702800
H	-3.20588200	-3.59175000	1.17042500
H	-4.79389600	-3.67497000	-0.74277100
C	3.12753300	-0.65497800	-0.17878800
C	3.25981500	-1.88745700	0.47865500
C	4.27316700	0.13397900	-0.34157500
C	4.49532300	-2.30727000	0.96997700
H	2.39660400	-2.53760000	0.59443100
C	5.51050100	-0.28016100	0.15231800
H	4.17320700	1.07964900	-0.86654800
C	5.62702100	-1.50396600	0.81236000
H	4.57718300	-3.26906300	1.47001100
H	6.38543400	0.35141600	0.01933400
H	6.58998200	-1.83361800	1.19320000

C	-1.60667700	0.97479000	1.28086000
O	-0.83442900	1.04668300	2.21133300
O	-2.89935700	0.69117500	1.39370100
C	-3.34700000	0.31305800	2.70559300
H	-3.20888200	1.14063700	3.40455200
H	-4.40477300	0.07937000	2.59662000
H	-2.79623600	-0.56513500	3.05084000

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C	0.81311900	-0.83510800	-0.33199800
C	-0.86395700	0.96088100	-0.48461900
S	-2.54815200	1.47639800	-1.00857700
O	1.72898400	0.58450600	-1.96919300
H	-0.20240900	1.53086200	-1.14823200
C	-3.66855800	1.16273500	0.37396700
H	-3.39353600	1.78038200	1.22938300
H	-4.66528300	1.42521700	0.01074100
H	-3.62864600	0.10108000	0.62359000
C	-2.43275100	3.27736500	-0.93836100
H	-2.17815300	3.60001100	0.07358900
H	-1.67134500	3.59010800	-1.65564100
H	-3.40663800	3.67608000	-1.23131400
C	-0.58439800	-0.54014800	-0.80352200
H	0.95601500	-1.45270700	0.54723900
C	1.86709700	-0.21979300	-0.98446200
H	-0.59963500	-0.56642400	-1.90250500
C	-1.66402700	-1.48372800	-0.31081800
C	-2.69023000	-1.85902100	-1.18791200
C	-1.69950700	-1.97014100	1.00206900
C	-3.74086500	-2.67398500	-0.76263200
H	-2.66528200	-1.51228100	-2.21941300
C	-2.74537000	-2.78682400	1.42991600
H	-0.91538300	-1.69729400	1.70109200
C	-3.77472400	-3.13483700	0.55249000
H	-4.52670500	-2.95023600	-1.46045700
H	-2.75836500	-3.15120600	2.45370500
H	-4.58984500	-3.76906900	0.89011700
C	3.28134100	-0.47661700	-0.49835800
C	3.64371800	-1.57695300	0.29308700
C	4.28321800	0.42908200	-0.86863900
C	4.96207700	-1.75538700	0.71038300
H	2.89752200	-2.31499200	0.57481600
C	5.60265100	0.25810300	-0.44831600
H	4.00481600	1.27113200	-1.49559200

C	5.94834900	-0.83601600	0.34530300
H	5.22193400	-2.61935900	1.31682800
H	6.36219800	0.97808300	-0.74296700
H	6.97569500	-0.97654800	0.67063600
C	-0.58456000	1.35925000	0.95414700
O	-1.11641900	0.86604700	1.92330200
O	0.31008600	2.34312300	1.01209700
C	0.68381900	2.77218400	2.33132400
H	1.13567600	1.94301700	2.88023300
H	1.40862200	3.57119400	2.18455200
H	-0.19070300	3.14493000	2.86888800

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C	-0.78307100	-0.30067300	-0.18832300
C	1.35908800	0.86732000	-0.41101900
S	3.17330900	0.86443200	-0.07043900
O	-1.62027700	-0.68555800	1.99437600
H	1.31425100	0.81610900	-1.50411600
C	3.66371000	2.54770400	-0.50012300
H	3.13894800	3.27266900	0.12636600
H	4.74109500	2.61768300	-0.33400200
H	3.44469300	2.69921400	-1.55957600
C	3.30979200	0.89636300	1.72694600
H	2.70157300	1.70344500	2.13641300
H	2.99037100	-0.07646100	2.10571000
H	4.36981800	1.04627700	1.94677700
C	0.66267700	-0.35055000	0.22544200
H	-1.00409100	-0.19853900	-1.24765800
C	-1.78920600	-0.45766900	0.75152800
H	0.68880600	-0.22785200	1.31496600
C	1.37525200	-1.64750500	-0.12970000
C	1.84548700	-2.49330500	0.87957700
C	1.54958600	-2.03469000	-1.46601300
C	2.47191400	-3.70234200	0.56599600
H	1.71465200	-2.20514300	1.92105700
C	2.18056900	-3.23526800	-1.78237200
H	1.18217300	-1.39489200	-2.26669700
C	2.64348400	-4.07543000	-0.76560300
H	2.82640900	-4.34903400	1.36430300
H	2.30913600	-3.51931600	-2.82349300
H	3.13307000	-5.01337400	-1.01270500
C	-3.22589700	-0.37975700	0.26256300
C	-3.61792900	0.33850800	-0.87634000
C	-4.21572200	-1.04082500	1.00070700

C	-4.95471900	0.37778900	-1.27345300	H	-4.47107600	-3.98447200	0.79695100
H	-2.87766100	0.88937900	-1.45140000	C	3.35318300	-0.42349400	-0.47681600
C	-5.55244100	-1.01093400	0.60359200	C	3.68886300	-1.27348500	0.58587500
H	-3.91479900	-1.57917600	1.89505500	C	4.35746400	0.37153200	-1.04243100
C	-5.92836000	-0.30097100	-0.53790500	C	4.99399700	-1.31786600	1.07541400
H	-5.23800700	0.94774500	-2.15480200	H	2.93642500	-1.92264900	1.02536200
H	-6.30287900	-1.53940600	1.18648700	C	5.66097700	0.33557400	-0.54955300
H	-6.96972500	-0.26946200	-0.84702200	H	4.09842300	1.01926400	-1.87495300
C	0.72101300	2.16010700	0.07483600	C	5.98383900	-0.51032300	0.51281900
O	0.64713300	2.47790100	1.24062500	H	5.23927900	-1.98907000	1.89419800
O	0.28882800	2.90215200	-0.93861100	H	6.42609000	0.96606500	-0.99509200
C	-0.37229600	4.12799100	-0.57967200	H	7.00023000	-0.54499700	0.89563600
H	0.31738700	4.78335200	-0.04352000	C	-0.62018400	1.18270500	1.00181300
H	-0.67629500	4.58249000	-1.52083200	O	-1.02018000	0.51054100	1.92579500
H	-1.24492500	3.91224500	0.04059500	O	-0.18698400	2.44186100	1.12976000
TS14-1				C	-0.25700100	2.99744300	2.45170700
C	0.87456000	-0.74162500	-0.25633500	H	0.38245400	2.43146100	3.13240700
C	-0.61120800	0.77799700	-0.44542400	H	0.10147700	4.02145500	2.35905500
S	-2.52885000	1.59559800	-1.08811300	H	-1.28787500	2.98659500	2.81347600
O	1.83313900	0.11670000	-2.22656800	TS14-2			
H	-0.00494400	1.42089600	-1.08327900	C	-0.63510100	-0.74078600	-0.06239500
C	-3.62238000	1.39729800	0.33773200	C	0.86356600	0.73285800	-0.41188500
H	-3.22541500	1.93158500	1.20431100	S	2.91056400	1.49927800	-0.35889200
H	-4.60550600	1.79374200	0.07245000	O	-1.60681700	-0.33600000	2.05530800
H	-3.70308200	0.32940100	0.55519600	H	0.81428900	0.62637300	-1.49320100
C	-2.27304800	3.38463100	-1.06724400	C	2.72425500	3.27998200	-0.61456500
H	-1.97750200	3.71733800	-0.07016900	H	2.02131300	3.70075800	0.10952300
H	-1.48775300	3.61681100	-1.79022400	H	3.70259300	3.75121700	-0.49145600
H	-3.20331400	3.87117100	-1.37099700	H	2.36959000	3.44273600	-1.63431300
C	-0.51416900	-0.66633200	-0.82171200	C	3.21436400	1.46332200	1.41999600
H	1.01113100	-1.02595900	0.77900100	H	2.37134900	1.91006700	1.95230600
C	1.95861300	-0.33904600	-1.05819200	H	3.34622400	0.42085000	1.71794700
H	-0.46408600	-0.71369000	-1.91383800	H	4.13454400	2.01638500	1.62441700
C	-1.58877500	-1.61186600	-0.33181100	C	0.78877100	-0.52925900	0.37694300
C	-2.70478100	-1.82635300	-1.15127900	H	-0.79965400	-1.07709000	-1.08075300
C	-1.52003700	-2.28576000	0.89137800	C	-1.71536400	-0.56791400	0.82681500
C	-3.74178800	-2.66887500	-0.74942500	H	0.80343300	-0.31319100	1.44939100
H	-2.75729300	-1.33731500	-2.12239000	C	1.79510800	-1.59823800	0.02264400
C	-2.55096600	-3.13470400	1.29370400	C	2.46289800	-2.28815200	1.03967300
H	-0.66474300	-2.14253100	1.54365000	C	2.06362200	-1.93709100	-1.30985600
C	-3.66894700	-3.32371700	0.47976900	C	3.37717300	-3.29844300	0.73632200
H	-4.59825700	-2.82022200	-1.40088900	H	2.26268600	-2.03110100	2.07794800
H	-2.48014400	-3.64967200	2.24810800	C	2.97846600	-2.94330000	-1.61578700

H	1.55363800	-1.41707800	-2.11857700	C	3.82734600	-0.60534200	0.91074400
C	3.63861000	-3.62789900	-0.59316800	C	5.97319200	0.19839200	-0.67831500
H	3.88599500	-3.82456700	1.53955600	H	4.48123200	0.81175800	-2.10488200
H	3.17660500	-3.19330500	-2.65460100	C	5.13299800	-0.77242200	1.36269800
H	4.35112900	-4.41232700	-0.83265100	H	3.00272200	-0.91831000	1.54573300
C	-3.11101900	-0.70180400	0.25305300	C	6.21319400	-0.37232000	0.57095600
C	-3.41595700	-0.40432100	-1.08173100	H	6.80419200	0.51504200	-1.30286800
C	-4.14460100	-1.11635800	1.10170400	H	5.31013300	-1.21495100	2.33937000
C	-4.72170500	-0.52897600	-1.55727600	H	7.23088600	-0.50315900	0.92805100
H	-2.63551900	-0.05356100	-1.75227700	C	-1.24549600	-1.11174200	-1.01309000
C	-5.44800300	-1.25196800	0.62697300	C	-1.10281000	-2.26970900	-0.23826300
H	-3.90942200	-1.33248000	2.14003600	C	-2.34502600	-1.01307300	-1.87328600
C	-5.74114600	-0.95790600	-0.70619400	C	-2.04444800	-3.29789200	-0.31753400
H	-4.94371700	-0.28463900	-2.59276600	H	-0.25940700	-2.38826900	0.43557700
H	-6.23674800	-1.58523100	1.29648700	C	-3.28863400	-2.03589300	-1.95052900
H	-6.75759100	-1.05691000	-1.07753700	H	-2.44151900	-0.12180100	-2.48648700
C	0.09767200	1.90548200	0.12693500	C	-3.14269400	-3.18402700	-1.16941600
O	0.02684300	2.19741000	1.30016700	H	-1.91452100	-4.19105600	0.28844400
O	-0.41684400	2.64325100	-0.86248000	H	-4.13701200	-1.93989300	-2.62342600
C	-1.11271500	3.83015600	-0.45600200	H	-3.87461900	-3.98511600	-1.22886600
H	-0.44618000	4.49024000	0.10467500	C	-1.81439700	0.25655200	1.45278600
H	-1.43521900	4.31207900	-1.37776600	O	-3.02726900	0.11380900	1.40263600
H	-1.97717200	3.56872900	0.15872100	O	-1.03447400	-0.41869500	2.31636800
TS15-1				C	-1.70322700	-1.37586400	3.14365700
C	-0.26296200	0.05932000	-0.98339600	H	-2.22255300	-2.11675800	2.53038700
C	-1.01571900	1.09687500	0.56457800	H	-0.91973000	-1.85416500	3.73082300
O	-0.27876000	0.83131800	-1.99511100	H	-2.41804400	-0.87819600	3.80375500
S	-2.02807600	2.28021800	-0.29528100	TS15-2			
H	-0.16192000	1.58505800	1.03393800	C	0.78707600	0.50103400	-0.72220700
C	-2.87028000	3.21575300	1.00614500	C	1.27017000	-1.14470600	0.37709600
H	-2.14710500	3.52529200	1.76332600	O	0.97294900	0.19375700	-1.93871700
H	-3.33336500	4.08586800	0.53342900	S	2.16361500	-2.08205300	-0.83827700
H	-3.63833700	2.57166800	1.43491000	H	1.90889800	-0.86305000	1.21321500
C	-0.77533100	3.49258400	-0.75961700	C	3.67231300	-1.11375700	-1.01226700
H	-0.29040700	3.87020700	0.14356400	H	4.03636900	-0.80803900	-0.02834600
H	-0.07258700	2.96993300	-1.40943700	H	4.40655300	-1.75060000	-1.51142500
H	-1.27746200	4.29930400	-1.29783100	H	3.43074200	-0.25410700	-1.63618300
C	1.06199000	-0.23680200	-0.32368200	C	2.81348200	-3.48055400	0.10919100
H	1.04792200	-0.77066000	0.62396500	H	3.34546200	-3.11699600	0.99075200
C	2.21082300	0.16675600	-0.88038700	H	1.96627800	-4.10608800	0.39721900
H	2.14558000	0.69996800	-1.82875500	H	3.48288300	-4.04723100	-0.54331700
C	3.57025900	-0.03438800	-0.34751800	C	-0.62591600	0.68208500	-0.22213700
C	4.66441400	0.36545600	-1.12975800	H	-0.75353000	1.01854800	0.80411900

C	-1.68067000	0.44449700	-1.01107300	H	-0.70486300	3.16067900	-1.62007600
H	-1.48001400	0.12030000	-2.03239500	H	-2.16107200	4.19331900	-1.34241600
C	-3.09991800	0.58446500	-0.63970300	C	1.04368500	-0.07246100	-0.14152000
C	-4.07904700	0.41100200	-1.62944600	H	1.10320400	-0.61952500	0.79812500
C	-3.52279000	0.87897500	0.66833800	C	2.14900600	0.35377000	-0.76168600
C	-5.43580100	0.53370900	-1.33046700	H	2.00661400	0.90430800	-1.69150800
H	-3.76779000	0.17751400	-2.64540600	C	3.54383000	0.15935600	-0.32196800
C	-4.87603900	1.00272200	0.96787900	C	4.57937100	0.65163600	-1.13069100
H	-2.79012700	1.00663600	1.46152700	C	3.89131600	-0.49530000	0.87231100
C	-5.84018500	0.83147500	-0.02982400	C	5.91668300	0.49823900	-0.76540600
H	-6.17558800	0.39628000	-2.11453300	H	4.32771100	1.16137500	-2.05840300
H	-5.18186000	1.22997000	1.98569000	C	5.22517800	-0.64889100	1.23888300
H	-6.89595400	0.92682900	0.20818100	H	3.11408400	-0.88740700	1.52311200
C	1.75693000	1.50796300	-0.09000300	C	6.24589600	-0.15314200	0.42248800
C	1.78460200	1.79166500	1.28189200	H	6.70003000	0.88863300	-1.40961200
C	2.61484100	2.21290800	-0.93696700	H	5.47148600	-1.15812100	2.16693700
C	2.65786100	2.74927700	1.79322300	H	7.28596500	-0.27470700	0.71203500
H	1.13381100	1.24974400	1.96558000	C	-1.11635000	-1.11872800	-0.91887500
C	3.49183000	3.17365200	-0.42896800	C	-0.95329300	-2.24926500	-0.10588300
H	2.58548000	1.99593200	-2.00116900	C	-2.05187700	-1.17873500	-1.95629600
C	3.51729800	3.44447800	0.93832200	C	-1.71500300	-3.39983000	-0.31911200
H	2.67065100	2.95158300	2.86097200	H	-0.23016900	-2.25125400	0.70567600
H	4.15350400	3.71144400	-1.10319400	C	-2.81924400	-2.32447900	-2.16959000
H	4.19941900	4.19014100	1.33762500	H	-2.15465600	-0.30826600	-2.59746200
C	0.05282500	-1.86730400	0.74166500	C	-2.65557600	-3.44095100	-1.34855600
O	-0.49595100	-2.72070600	0.05940100	H	-1.56906800	-4.26629900	0.32118700
O	-0.45285200	-1.43402400	1.91057200	H	-3.54338100	-2.34755200	-2.98040300
C	-1.74218800	-1.94835600	2.25654700	H	-3.24878800	-4.33643400	-1.51348800
H	-1.68920400	-3.02367400	2.44592300	C	-1.78017500	0.19268800	1.51082900
H	-2.03698400	-1.42329000	3.16502700	O	-2.95661300	-0.10391600	1.52289100
H	-2.46004500	-1.75258400	1.45595700	O	-0.88799000	-0.26319800	2.38928800
IN15-1				C	-1.37998100	-1.22473700	3.33670100
C	-0.34230800	0.21560800	-0.72411800	H	-1.83697900	-2.06881800	2.81465200
C	-1.11446100	1.04770600	0.46830000	H	-0.50790700	-1.55159100	3.90089200
O	-0.34725100	0.98135100	-1.80993700	H	-2.11039900	-0.75793200	4.00108000
S	-2.37926000	2.03050800	-0.40831000	IN15-2			
H	-0.41170700	1.75657700	0.91735200	C	0.77418100	0.28798700	-0.51085400
C	-3.30244100	2.78785500	0.95599300	C	1.33509300	-1.05131300	0.25417600
H	-2.61322400	3.11699800	1.73758200	O	0.92635500	0.11597700	-1.81894800
H	-3.82979000	3.64699900	0.53398100	S	2.51088300	-1.77842800	-0.92628700
H	-4.01808400	2.06487700	1.34282000	H	1.86252200	-0.84723100	1.19019200
C	-1.44504000	3.49810100	-0.89748200	C	3.84460400	-0.56541900	-0.93673200
H	-0.98130400	3.94148200	-0.01296800	H	4.03447500	-0.20306600	0.07625300

H	4.72680000	-1.07748200	-1.32952900	C	0.75263400	0.36674500	-0.80752500
H	3.53989100	0.24170700	-1.60085900	H	2.52640600	-0.85770700	-0.50479300
C	3.28667100	-3.02268200	0.13763200	C	0.20388200	-1.01135800	2.53646500
H	3.64785900	-2.56797100	1.06232700	H	-0.48693200	-1.61128300	1.94217200
H	2.54893900	-3.79961300	0.34795600	H	0.39952400	-1.47855000	3.50537600
H	4.11692700	-3.45758100	-0.42408900	H	-0.16581800	0.00232400	2.69305800
C	-0.67691200	0.46392700	-0.03937900	C	2.41570300	-2.59425700	1.97898200
H	-0.83663200	0.68877100	1.01486800	H	1.64842300	-3.32198200	1.70511300
C	-1.70455200	0.34824000	-0.88611200	H	3.32093100	-2.72384300	1.38255200
H	-1.46288400	0.14814900	-1.93017100	H	2.65845400	-2.67952500	3.04048900
C	-3.13378900	0.47771200	-0.54328400	C	-0.62631600	0.56729300	-0.17347000
C	-4.07251700	0.63055400	-1.57468200	H	-0.68750400	0.94186400	0.84624300
C	-3.60380800	0.43878900	0.78074500	C	-1.74736900	0.33597100	-0.86264400
C	-5.43312500	0.76092700	-1.29746400	H	-1.63267100	0.00145800	-1.89326200
H	-3.72580600	0.65082900	-2.60568800	C	-3.12495400	0.49429000	-0.36060800
C	-4.96164200	0.56893900	1.05934000	C	-4.18810100	0.50798300	-1.27644700
H	-2.90397600	0.29304600	1.60034600	C	-3.42717500	0.61771900	1.00660600
C	-5.88371700	0.73311400	0.02200700	C	-5.50661900	0.66081700	-0.84882600
H	-6.14084100	0.88204300	-2.11327100	H	-3.97229000	0.40186800	-2.33752600
H	-5.30424000	0.53393900	2.09017300	C	-4.74304300	0.76944500	1.43562200
H	-6.94312000	0.83091300	0.24226800	H	-2.62777300	0.58147300	1.74323400
C	1.55664000	1.50412200	0.06572500	C	-5.78991500	0.79492000	0.51014000
C	1.67526500	1.76033800	1.43742400	H	-6.31238200	0.67304900	-1.57803300
C	2.12279200	2.40942600	-0.83327100	H	-4.95489600	0.86000300	2.49780500
C	2.35835000	2.88632400	1.89820600	H	-6.81599900	0.91062900	0.84805600
H	1.23316300	1.07865600	2.16315100	C	1.63429300	1.60718200	-0.48516400
C	2.80489400	3.53967000	-0.37861100	C	1.66356600	2.24927200	0.76051800
H	2.02405900	2.19762700	-1.89439800	C	2.46006800	2.09468300	-1.50166200
C	2.92802400	3.78130700	0.99003300	C	2.50275700	3.34257700	0.98378200
H	2.44442600	3.06584200	2.96688600	H	1.02685200	1.91704000	1.57843600
H	3.24276900	4.23172100	-1.09393500	C	3.29910000	3.18870100	-1.28478000
H	3.46092500	4.65841200	1.34733700	H	2.41665000	1.59445900	-2.46485400
C	0.25553800	-2.08030900	0.47586600	C	3.32517700	3.81666600	-0.03875000
O	-0.03839100	-2.95611100	-0.31020800	H	2.50825200	3.82628400	1.95717200
O	-0.36184400	-1.88294900	1.63967100	H	3.93218900	3.55369200	-2.08993700
C	-1.54540200	-2.66548300	1.85627100	H	3.97596600	4.66963900	0.13401400
H	-1.29486100	-3.72769200	1.89985100	C	0.83371800	-2.17692900	-0.54313800
H	-1.94840900	-2.33256200	2.81147300	O	-0.25583900	-2.54421800	-0.15852400
H	-2.26459500	-2.48594800	1.05311400	O	1.61002400	-2.88915100	-1.35660600
IN16-1				C	1.04315700	-4.11456400	-1.84201300
C	1.50641600	-0.89060300	-0.11112600	H	0.13108500	-3.91016300	-2.40716200
O	0.72549800	0.03641500	-2.09228900	H	1.80077400	-4.55180200	-2.49063600
S	1.80810700	-0.91231200	1.70655300	H	0.82169000	-4.78561800	-1.00878900

IN16-2

C	1.01426600	-1.01901300	0.31317300
O	0.26712700	-0.58098300	-1.89131200
S	1.48171300	-0.30623600	1.93230700
C	0.23301400	-0.00624300	-0.69701300
H	0.30458600	-1.80510600	0.58999300
C	1.91238000	-1.76554300	2.90576400
H	2.69364700	-2.33751900	2.40014900
H	2.26469200	-1.41523000	3.87891300
H	1.00611700	-2.36095700	3.03042500
C	3.10651000	0.47515100	1.77921400
H	3.87616100	-0.28815100	1.66901400
H	3.09772800	1.14590000	0.91956800
H	3.24342600	1.04217400	2.70322400
C	-1.16739100	0.13270400	-0.08258400
H	-1.25476700	0.48549300	0.94609000
C	-2.25816200	-0.19882400	-0.78049800
H	-2.09247500	-0.56366600	-1.79441300
C	-3.66014500	-0.13359300	-0.32550500
C	-4.66969700	-0.58293900	-1.19009300
C	-4.03955100	0.35758400	0.93555900
C	-6.01204800	-0.55012200	-0.81276900
H	-4.39299900	-0.96318200	-2.17120800
C	-5.37847200	0.39091200	1.31420500
H	-3.28386500	0.72025600	1.62758500
C	-6.37267300	-0.06330800	0.44290000
H	-6.77465800	-0.90510500	-1.50084000
H	-5.64983900	0.77476700	2.29411700
H	-7.41678600	-0.03502400	0.74179700
C	0.95282300	1.37136600	-0.64475500
C	1.94510200	1.61619200	-1.60025200
C	0.69440500	2.36350200	0.31217400
C	2.68315000	2.79856100	-1.58474700
H	2.12281200	0.84973800	-2.34777700
C	1.42949800	3.55242000	0.32952600
H	-0.08247300	2.22983100	1.06002900
C	2.43264200	3.77098900	-0.61298600
H	3.45603500	2.96461400	-2.33135100
H	1.21142400	4.30753600	1.08042100
H	3.00635600	4.69386500	-0.59861700
C	2.18826800	-1.63570100	-0.41649200
O	3.22591100	-1.06344600	-0.66667900
O	1.94335900	-2.90561700	-0.73371100
C	2.95052500	-3.55246000	-1.52301900

H	3.89987500	-3.57874300	-0.98342900
H	2.58445000	-4.56368200	-1.69484400
H	3.07531700	-3.02748400	-2.47295700

TS16-1

C	0.99497900	-0.92259600	-0.39311300
O	0.28835500	0.00682300	-1.97720700
S	1.37947300	-1.36354000	1.73451100
C	0.19275600	0.31572500	-0.65059300
H	0.42468400	-1.83539700	-0.54762400
C	1.67895300	-3.14576400	1.67671400
H	2.47900400	-3.37054000	0.96734700
H	1.94999700	-3.49055400	2.67735600
H	0.75181100	-3.63062200	1.36270900
C	3.04590100	-0.77393600	2.11289500
H	3.77562800	-1.22261600	1.43466300
H	3.05268600	0.31269700	2.00496200
H	3.27884600	-1.04347800	3.14621000
C	-1.20458500	0.21924000	-0.05836600
H	-1.30792600	0.42032500	1.00765400
C	-2.26320900	-0.08116700	-0.81803500
H	-2.07557600	-0.27831700	-1.87357100
C	-3.66660200	-0.18470000	-0.37527600
C	-4.62711800	-0.64634300	-1.28746000
C	-4.09107000	0.16038600	0.91895600
C	-5.96739500	-0.76967200	-0.92224200
H	-4.31455500	-0.91178900	-2.29517300
C	-5.42829200	0.03777400	1.28495100
H	-3.37457500	0.53584500	1.64490800
C	-6.37358500	-0.42899100	0.36724800
H	-6.69288100	-1.13094700	-1.64613600
H	-5.73668100	0.31202900	2.29031400
H	-7.41687000	-0.52105800	0.65615000
C	0.82326200	1.64756000	-0.23237600
C	1.27878000	2.51880500	-1.22228400
C	0.92561300	2.03335400	1.10886500
C	1.83721300	3.75096600	-0.88225500
H	1.20168500	2.20321100	-2.25844500
C	1.49947600	3.25794900	1.45407400
H	0.55517900	1.38583800	1.90214200
C	1.95583800	4.12250100	0.45827300
H	2.18793000	4.42018400	-1.66392800
H	1.58158400	3.53840000	2.50097700
H	2.39729500	5.07888600	0.72522600

C	2.40772100	-0.96532300	-0.90891800	C	2.71650000	4.24974400	0.02821300
O	3.19344300	-0.04760600	-0.90733600	H	2.21595600	3.94624400	2.10449100
O	2.71152700	-2.20603500	-1.30828000	H	3.05646000	4.27146700	-2.09964900
C	4.06379500	-2.40707000	-1.74491100	H	3.24165000	5.18423900	0.20618100
H	4.76030800	-2.18437300	-0.93309300	C	1.02633700	-2.03836900	-0.73755100
H	4.12858600	-3.45777000	-2.02349000	O	-0.02725900	-2.48134600	-0.33859500
H	4.28108400	-1.77096300	-2.60562600	O	1.91913000	-2.75336500	-1.42595100
TS16-2				C	1.54922900	-4.11092800	-1.70375400
C	1.56104500	-0.65911200	-0.45811500	H	0.64589900	-4.13923900	-2.31702200
O	0.68231200	0.11466200	-2.03253900	H	2.38970600	-4.53861500	-2.24832800
S	2.20247000	-0.94663200	1.64261700	H	1.38207500	-4.65866800	-0.77289900
C	0.64805100	0.50582500	-0.72485600	E-PR-1-1			
H	2.57209300	-0.48473300	-0.81494500	C	0.37365900	-0.38330700	0.23259900
C	0.65757000	-1.17131900	2.55431700	C	-0.72097500	-1.37576000	0.55915100
H	-0.05448700	-1.74128500	1.95197400	O	1.75834200	-1.19022500	1.96084800
H	0.88680000	-1.70147700	3.48235300	H	-0.48262400	-2.16412900	1.26485600
H	0.25548400	-0.18543100	2.79511500	C	-0.77495500	0.02405300	1.11598000
C	2.81118800	-2.65145100	1.64648600	H	0.34999100	-0.00485400	-0.78289400
H	2.02951400	-3.34103600	1.31647000	C	1.69591000	-0.60811700	0.88800900
H	3.67804400	-2.70754000	0.98471200	H	-0.53019200	0.06308300	2.17628700
H	3.11523400	-2.90555400	2.66488300	C	-1.78809500	1.02346100	0.65283800
C	-0.72246600	0.50272700	-0.07739100	C	-3.14394700	0.81764700	0.93201500
H	-0.78040400	0.77173600	0.97556800	C	-1.40161300	2.18131500	-0.02637400
C	-1.82751900	0.25171400	-0.78475000	C	-4.09786400	1.75446700	0.53711000
H	-1.70306500	0.01048300	-1.83974100	H	-3.45204600	-0.08349800	1.45914500
C	-3.21145100	0.26243900	-0.27634300	C	-2.35468800	3.12122000	-0.42140200
C	-4.26959700	0.19490500	-1.19514000	H	-0.34977700	2.34634300	-0.24950800
C	-3.52381900	0.32570300	1.09237000	C	-3.70469900	2.90978400	-0.14119100
C	-5.59699600	0.20814600	-0.76815000	H	-5.14792900	1.58131000	0.75658400
H	-4.04328900	0.13591000	-2.25765600	H	-2.04140700	4.01731900	-0.95022700
C	-4.84834800	0.33737100	1.52038100	H	-4.44730700	3.63967800	-0.45134900
H	-2.72614700	0.35606500	1.83070600	C	2.93776000	-0.10688300	0.22036600
C	-5.89227600	0.28161100	0.59266100	C	2.90601500	0.81377500	-0.83413200
H	-6.39957000	0.15920900	-1.49925200	C	4.17280500	-0.57231000	0.69265000
H	-5.06878200	0.38422600	2.58357800	C	4.09601700	1.26481900	-1.40423300
H	-6.92483500	0.28954900	0.93035600	H	1.96337200	1.20003200	-1.20881700
C	1.35788600	1.83504300	-0.43044000	C	5.35767500	-0.13235600	0.11296000
C	1.46079400	2.35850800	0.86493300	H	4.19026000	-1.28489800	1.51195900
C	1.94026000	2.53329100	-1.48951700	C	5.32051300	0.79008200	-0.93597700
C	2.14044100	3.55481500	1.09346600	H	4.06440400	1.98676000	-2.21506900
H	1.00877500	1.84365700	1.71089900	H	6.31065500	-0.50495700	0.47743100
C	2.61203800	3.73642100	-1.26429200	H	6.24591100	1.13758600	-1.38680500
H	1.85669500	2.11479600	-2.48815100	C	-1.65681600	-1.73817400	-0.54013200

O	-1.76815700	-1.14546400	-1.59221400
O	-2.38816200	-2.80932400	-0.21498600
C	-3.34181600	-3.23593300	-1.19783800
H	-2.83233600	-3.51863000	-2.12182100
H	-3.84531500	-4.09884600	-0.76426600
H	-4.06115700	-2.43888500	-1.39909200

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C	0.02320300	0.44363500	0.98863400
C	-0.61515400	1.67750300	0.40626500
O	2.25791400	1.14602500	1.33471200
H	-1.41310400	2.14368400	0.97431900
C	-0.85991100	0.31051900	-0.20966900
H	-0.39862000	0.10898600	1.93651900
C	1.52214300	0.26585300	0.92673000
H	-0.33506800	0.16355600	-1.15183200
C	-2.18829800	-0.35977300	-0.12390700
C	-2.60062100	-1.18666000	-1.17533800
C	-3.03287200	-0.20590600	0.98348200
C	-3.82981000	-1.84494700	-1.12537600
H	-1.95098200	-1.31440500	-2.03843000
C	-4.26184100	-0.86112100	1.03265800
H	-2.73636500	0.42867500	1.81624800
C	-4.66562200	-1.68352000	-0.02107700
H	-4.13236100	-2.48307300	-1.95124900
H	-4.90603000	-0.72844000	1.89757700
H	-5.62372000	-2.19386900	0.02014900
C	2.06543900	-1.02761000	0.41333100
C	1.23621000	-2.13053900	0.17372500
C	3.44417700	-1.13395800	0.18812400
C	1.78468000	-3.32902800	-0.28036500
H	0.16598500	-2.06355700	0.34971500
C	3.98737400	-2.32688500	-0.27676600
H	4.07858600	-0.27286400	0.37737700
C	3.15711400	-3.42660300	-0.50996500
H	1.13969800	-4.18458800	-0.45827800
H	5.05566200	-2.40276500	-0.45791300
H	3.58123800	-4.35930600	-0.87138300
C	0.25312400	2.59928400	-0.37470700
O	1.04669800	2.24667900	-1.22266400
O	0.04874300	3.87531700	-0.03703700
C	0.84134100	4.84299000	-0.73879200
H	0.64993400	4.78504600	-1.81258300
H	0.53158800	5.81263000	-0.35128300

H	1.90266700	4.67671300	-0.54094200
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C	-1.04972700	-1.54476500	0.35813500
O	-0.65655400	-0.89337800	1.54637400
C	-0.52588100	-0.14566700	0.34963100
H	-0.39229600	-2.33713100	0.00593400
C	0.86694200	0.09502600	-0.12715100
H	0.94686900	0.67880300	-1.04208900
C	1.94354100	-0.35622500	0.52710400
H	1.78893300	-0.91889300	1.44764900
C	3.35053100	-0.16341700	0.13329800
C	4.35494500	-0.64801000	0.98372800
C	3.73337200	0.48320800	-1.05357200
C	5.70326300	-0.49147100	0.66475000
H	4.07116900	-1.15213400	1.90502900
C	5.07874800	0.64001200	-1.37218600
H	2.97873900	0.86553300	-1.73558300
C	6.07033800	0.15401200	-0.51514200
H	6.46497600	-0.87441600	1.33831700
H	5.35667500	1.14289600	-2.29448800
H	7.11951000	0.27799800	-0.76838300
C	-1.48253100	1.00026900	0.17972600
C	-1.97051600	1.68532600	1.29261800
C	-1.86800600	1.39292400	-1.10504200
C	-2.83900200	2.76341400	1.12111100
H	-1.67805300	1.36722100	2.28943900
C	-2.73974400	2.46792500	-1.27454600
H	-1.49189300	0.85229500	-1.97165300
C	-3.22507400	3.15598500	-0.16106300
H	-3.21727800	3.29434900	1.99034400
H	-3.04202900	2.76549900	-2.27477300
H	-3.90451300	3.99346200	-0.29266900
C	-2.52091200	-1.77763600	0.18002700
O	-3.38667300	-1.41094200	0.93874100
O	-2.73906400	-2.43238700	-0.96164700
C	-4.11487900	-2.68058800	-1.28847100
H	-4.64757800	-1.73508900	-1.41296800
H	-4.09939500	-3.23411700	-2.22593200
H	-4.58794900	-3.27456200	-0.50366000

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C	1.37884300	1.63283100	0.51809700
O	1.17607600	0.80645800	1.64025600

C	1.18552100	0.15489600	0.37855700	C	-1.09240900	1.18267200	0.27078500
H	2.38527300	2.02912100	0.38691900	H	-1.00351400	1.07758600	1.35422400
C	-0.12068200	-0.39562900	-0.08303400	H	-0.79474400	2.18237600	-0.05210300
H	-0.11070600	-0.87305700	-1.05949100	H	-2.11104300	0.97328800	-0.06155600
C	-1.23630600	-0.32725300	0.65299100	C	1.57052200	0.35444600	0.27094900
H	-1.17974900	0.14938300	1.63009700	H	2.29050900	-0.39592900	-0.06201700
C	-2.56487700	-0.83872700	0.27125100	H	1.89326100	1.34657400	-0.05164200
C	-3.59597400	-0.79018300	1.22084300	H	1.43742000	0.31713900	1.35426700
C	-2.84998000	-1.36662500	-0.99897600	C	-0.47824600	-1.53726000	0.27080400
C	-4.87257900	-1.26336000	0.91987900	H	-0.43507800	-1.40527800	1.35410700
H	-3.38924600	-0.37777600	2.20598100	H	-1.49163600	-1.78096200	-0.05502100
C	-4.12386300	-1.83870600	-1.30005500	H	0.21394500	-2.31484600	-0.05843400
H	-2.07700500	-1.40491300	-1.76197100				
C	-5.14084900	-1.79126200	-0.34219800	SOMe ₃ ⁺			
H	-5.65600400	-1.21812700	1.67146200	C	-1.49472200	0.65286200	-0.53839200
H	-4.32675300	-2.24291300	-2.28810500	S	-0.00042700	0.00104200	0.15478500
H	-6.13431200	-2.15967200	-0.58218500	O	-0.00448700	0.00857300	1.62587400
C	2.41160500	-0.66991900	0.09260100	H	-2.31725000	0.02983200	-0.17770800
C	2.60756100	-1.24337800	-1.16883900	H	-1.59572600	1.68114700	-0.18107300
C	3.37455800	-0.85477100	1.08804800	C	0.18111800	-1.62534800	-0.52536800
C	3.75343400	-1.99388100	-1.42689800	H	0.17553600	-1.55011800	-1.61588100
H	1.87639600	-1.09796500	-1.95963300	H	1.13054700	-2.02619200	-0.16034100
C	4.51749100	-1.61149200	0.82835300	H	-0.66010200	-2.22344500	-0.16552400
H	3.22581700	-0.40799100	2.06652100	C	1.31792500	0.96386800	-0.53369100
C	4.71022600	-2.18339000	-0.42860700	H	1.25819000	0.91028400	-1.62383100
H	3.89839900	-2.43047100	-2.41114700	H	1.18888100	1.98982100	-0.17910500
H	5.25690100	-1.75322700	1.61178800	H	2.25555400	0.53742000	-0.16719900
H	5.60079400	-2.77170100	-0.63102100	H	-1.41883100	0.61770000	-1.62819300
C	0.26097100	2.57550800	0.18143800				
O	-0.71304400	2.77841300	0.86691900				
O	0.49802500	3.15972800	-0.99354700				
C	-0.50264300	4.08369000	-1.44861200				
H	-0.61352000	4.90249900	-0.73437700				
H	-0.14177300	4.45994500	-2.40456700				
H	-1.45770500	3.56997500	-1.57832500				
CH ₃ ⁺							
C	0.00000000	0.00000700	0.00000000				
H	0.00000100	1.08788400	0.00000000				
H	0.94159000	-0.54396400	0.00000000				
H	-0.94159100	-0.54396200	0.00000000				
SMe ₃ ⁺							
S	0.00010500	0.00005600	-0.53731600				