

Divergent Pathway and Reactivity Control of Intramolecular Arene C–H Vinylation by Vinyl Cations

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1. Computational details

All DFT calculations were conducted with the Gaussian 09 software package.¹ Geometry optimizations of all the minima and transition states were performed using B3LYP^{2,3} functional with 6-31G(d) basis set, including solvation energy corrections and Grimme's D3 empirical dispersion corrections with BJ-damping.^{4,5} To confirm whether each optimized stationary point is an energy minimum or a transition state, as well as evaluate the zero-point vibrational energy and thermal corrections at 298 K, the vibrational frequencies were computed at the same level of theory as for the geometry optimizations. The solvation energies of dichloromethane were evaluated by a self-consistent reaction field (SCRF) using the SMD model.⁶ For critical transition states, IRC (intrinsic reaction coordinates) analysis was also performed at the same level of theory as geometry optimization to verify the proposed process. The single-point energies were computed with B3LYP functional and 6-311+G(d,p) basis set, with solvation energy corrections and Grimme's D3(BJ) dispersion corrections as well. Extensive conformational searches for the intermediates and transition states have been conducted to ensure that the lowest energy conformers were located. The 3D diagrams of molecules were generated using CYLView.⁷

It is worth pointing out that **TS25** is a second order saddle point, which involves a small imaginary frequency of phenyl ring rotation. All the attempts for the first order saddle point location led to this second order saddle point **TS25**.

2. IRC calculations of the transition states in Fig. 1.

The results of IRC calculations of **TS2**, **TS4** and **TS8** are included in **Fig. S1-S3**. The IRC calculation of the C-C bond formation transition state **TS6** was not successful despite extensive efforts, which could be related to the flat free energy surface around **TS6**. (Pre: preceding intermediate, TS: transition state, Post: post intermediate).

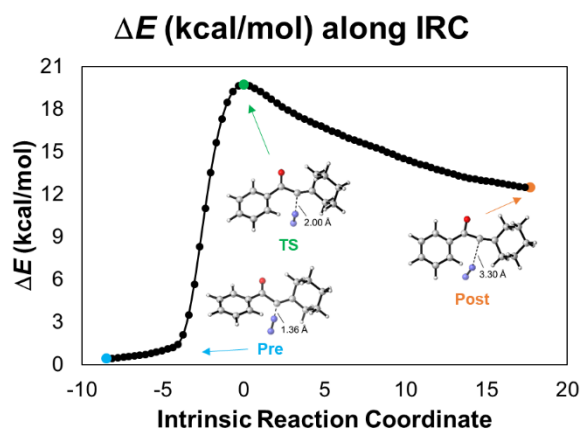


Fig. S1. IRC calculation of **TS2**.

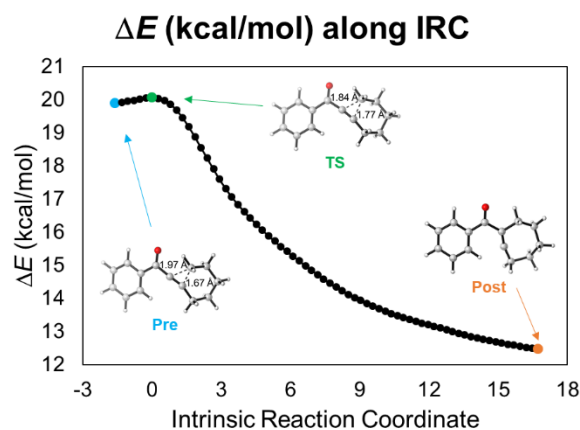


Fig. S2. IRC calculation of **TS4**.

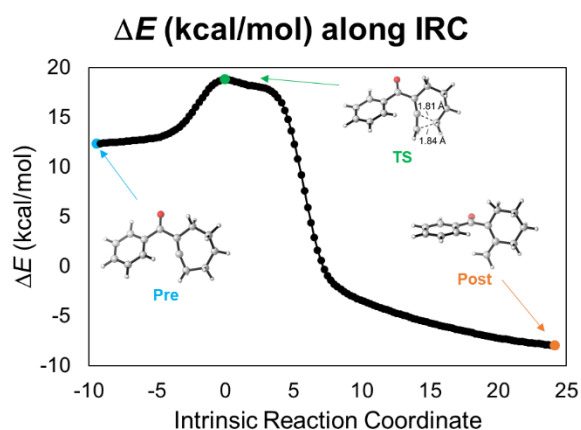


Fig. S3. IRC calculation of TS8.

3. DFT-computed free energy profile of intramolecular arene C-H vinylation by vinyl cation with *para*-nitro substitution.

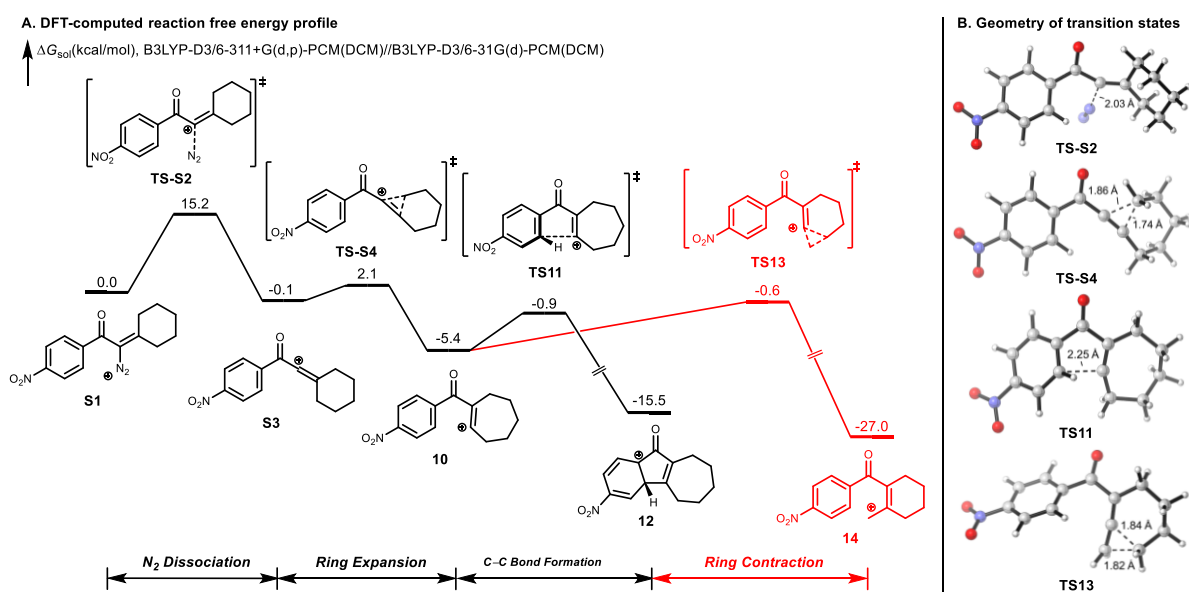


Fig. S4. DFT-calculated reaction energy profile of intramolecular arene C-H vinylation by vinyl cation with *para*-nitro substitution.

4. DFT-computed free energy profile of intramolecular arene C-H vinylation by vinyl cation with cyclopentane moiety.

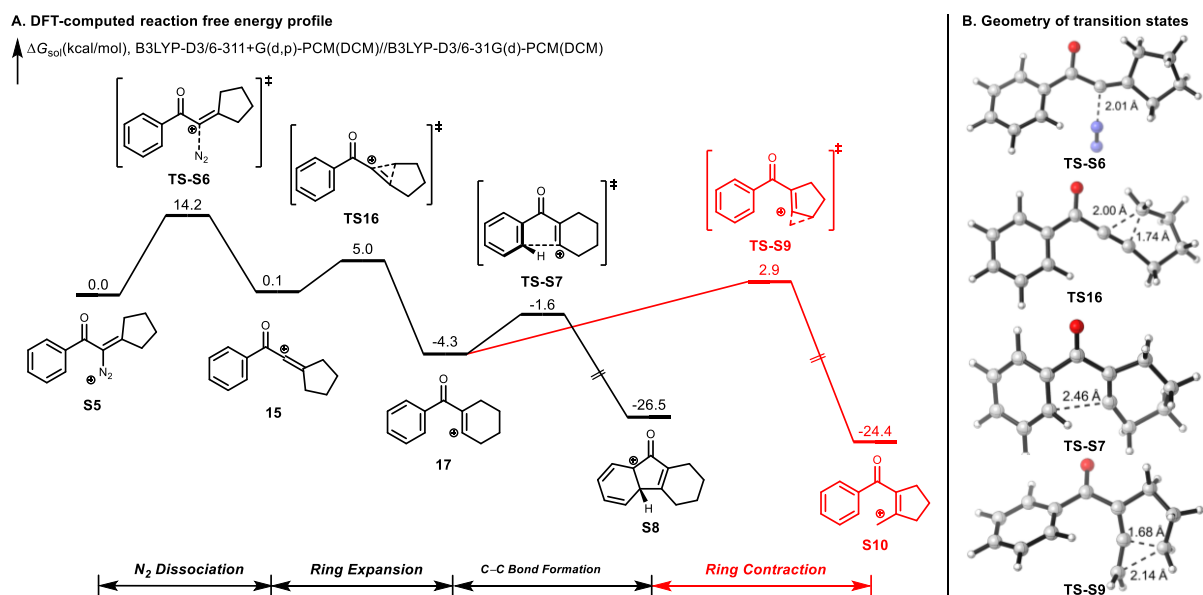


Fig. S5. DFT-calculated reaction energy profile of intramolecular arene C-H vinylation by vinyl cation with cyclopentane moiety.

5. IRC calculation of the transition states in Fig. 2.

The results of IRC calculations of TS19, TS23, TS25 and TS29 are included in Fig. S6-S8, and S10. The IRC calculation of the benzyl rotation transition state TS27 was not successful despite extensive efforts, which could be related to the flat free energy surface around TS27. We performed energy scan of the benzyl rotation of intermediate **26**, to confirm that the benzyl rotation leads to the C-C bond formation in spiro intermediate **28** (Fig. S9). (Pre: preceding intermediate, TS: transition state, Post: post intermediate)

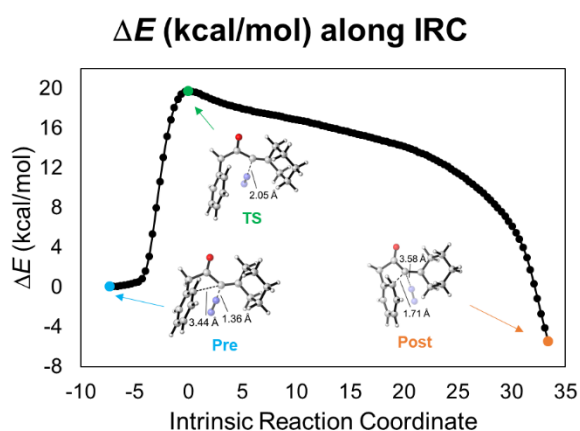


Fig. S6. IRC calculations of TS19

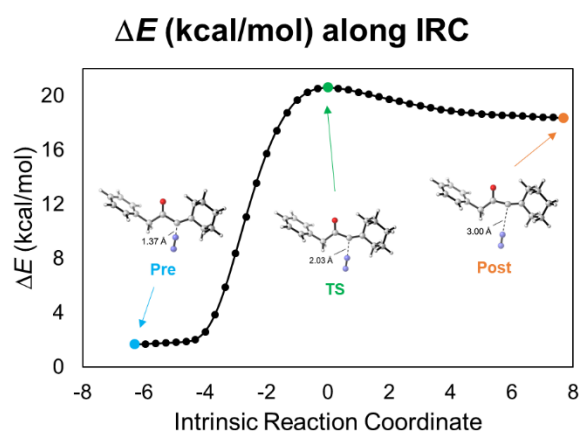


Fig. S7. IRC calculations of TS23.

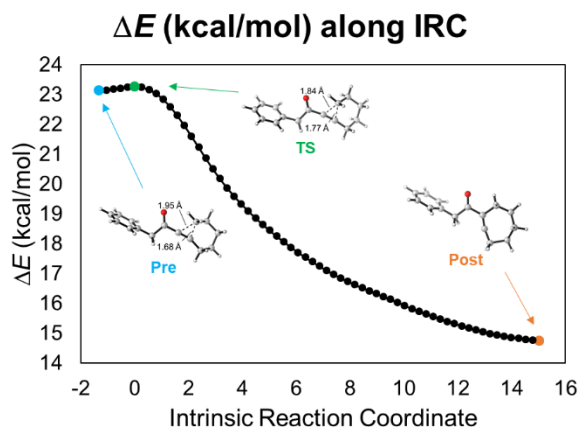


Fig. S8. IRC calculation of TS25.

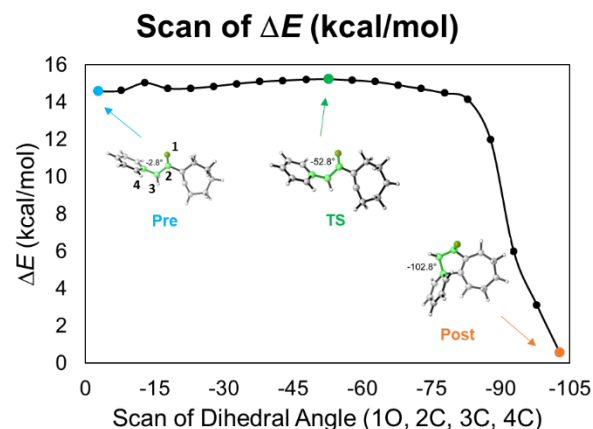


Fig S9. Energy scan of the benzyl rotation of intermediate **26**.

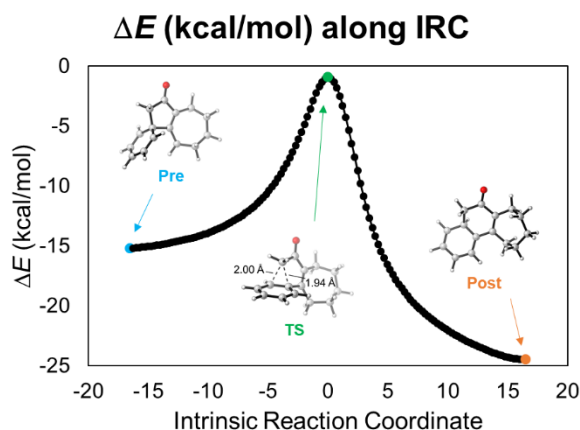


Fig. S10. IRC calculation of TS29.

6. References

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7. Energies, enthalpies, and free energy of the calculated structures

Zero-point correction (ZPE), thermal correction to enthalpy (ΔH), thermal correction to Gibbs free energy (ΔG), energies (E), enthalpies (H), Gibbs free energies (G) (in Hartree) and imaginary frequencies of the transition states calculated at the B3LYP-D3/6-311+G(d,p)-SMD(Dichloromethane)// B3LYP-D3/6-31G(d)-SMD(Dichloromethane)

Structures	ZPE	tcH	tcG	E	H	G	Imaginary Frequency
1	0.265505	0.281349	0.221694	-727.293683	-727.012334	-727.071989	
TS2	0.261661	0.278273	0.217445	-727.264944	-726.986671	-727.047499	-256.7i
3	0.253869	0.268375	0.211855	-617.718036	-617.449661	-617.506181	
TS4	0.252984	0.266893	0.212582	-617.71345	-617.446557	-617.500868	-138.7i
5	0.253948	0.268185	0.213333	-617.725172	-617.456987	-617.511839	
TS6	0.25359	0.267011	0.214618	-617.722704	-617.455693	-617.508086	-100.8i
7	0.256297	0.269476	0.217812	-617.756224	-617.486748	-617.538412	
TS8	0.252877	0.266792	0.212524	-617.716315	-617.449523	-617.503791	-217.3i
9	0.254128	0.268227	0.214027	-617.758785	-617.490558	-617.544758	
10	0.256172	0.272996	0.211359	-822.29011	-822.017114	-822.078751	
TS11	0.255759	0.271748	0.212772	-822.284449	-822.012701	-822.071677	-153.2i
12	0.257894	0.27382	0.21462	-822.309562	-822.035742	-822.094942	
TS13	0.255831	0.272123	0.212059	-822.283315	-822.011192	-822.071256	-222.3i
14	0.255963	0.272819	0.210108	-822.323334	-822.050515	-822.113226	
15	0.224046	0.237576	0.183631	-578.38031	-578.142734	-578.196679	
TS16	0.223635	0.236667	0.183531	-578.372439	-578.135772	-578.188908	-135i
17	0.224271	0.237382	0.184891	-578.388665	-578.151283	-578.203774	
18	0.294078	0.311122	0.24847	-766.62491	-766.313788	-766.37644	
TS19	0.290296	0.308052	0.244678	-766.598606	-766.290554	-766.353928	-197.7i
20	0.283951	0.298376	0.243394	-657.093319	-656.794943	-656.849925	
TS21	0.294374	0.310538	0.250148	-766.620404	-766.309866	-766.370256	-36.2i
22	0.294028	0.311169	0.246288	-766.622679	-766.31151	-766.376391	
TS23	0.290092	0.308026	0.24319	-766.597659	-766.289633	-766.354469	-220.2i
24	0.281813	0.297648	0.237867	-657.042468	-656.74482	-656.804601	
TS25	0.280785	0.295351	0.239107	-657.040688	-656.745337	-656.801581	-147.7i, -16.1i
26	0.281641	0.2975	0.237003	-657.053782	-656.756282	-656.816779	
TS27	0.281967	0.296755	0.2403	-657.052528	-656.755773	-656.812228	-22.3i
28	0.285652	0.300027	0.245461	-657.098231	-656.798204	-656.85277	
TS29	0.284216	0.298327	0.244611	-657.074944	-656.776617	-656.830333	-365.3i
30	0.286796	0.300801	0.247169	-657.110937	-656.810136	-656.863768	
N2	0.005607	0.008912	-0.012842	-109.55516	-109.546248	-109.568002	
S1	0.268092	0.286401	0.220692	-931.858918	-931.572517	-931.638226	
TS-S2	0.264027	0.283225	0.21562	-931.829624	-931.546399	-931.614004	-237.8i
S3	0.256286	0.273281	0.210217	-822.28068	-822.007399	-822.070463	
TS-S4	0.255557	0.27193	0.211532	-822.27841	-822.00648	-822.066878	-73.5i
S5	0.235054	0.250003	0.192879	-687.957755	-687.707752	-687.764876	
TS-S6	0.231324	0.247336	0.18606	-687.928242	-687.680906	-687.742182	-259.0i
TS-S7	0.224201	0.236473	0.186694	-578.386135	-578.149662	-578.199441	-95.0i
S8	0.226672	0.238779	0.18963	-578.428697	-578.189918	-578.239067	
TS-S9	0.223274	0.23606	0.184684	-578.376881	-578.140821	-578.192197	-150.0i
S10	0.224659	0.237799	0.185714	-578.421396	-578.183597	-578.235682	

8. Cartesian coordinates for the calculated structures

1

C	3.35887000	-1.56863900	0.11933600
C	4.45672800	-0.50744500	0.02727700
C	3.90467600	0.83373100	-0.45863600
C	2.71381900	1.31054200	0.42848900
C	1.69877200	0.22126400	0.44896900
C	2.17530500	-1.07313000	1.00477900
H	4.67058400	1.61486800	-0.42995100
H	4.92017700	-0.37543200	1.01367100
H	5.24325600	-0.84889900	-0.65559100
H	2.97072400	-1.81068300	-0.87648600
H	3.73728600	-2.49587700	0.56031400
H	3.07882000	1.45354600	1.45259500
H	2.32180500	2.26416400	0.06777900
H	2.56224400	-0.87500800	2.01219600
H	1.39327300	-1.82689200	1.06091600
H	3.55763300	0.74938500	-1.49525100
C	0.44393600	0.35233700	-0.10549100
C	-0.61412300	-0.74044400	-0.29107200
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N	0.11675600	1.56126000	-0.63192400
N	-0.21413000	2.51710700	-1.10780600
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C	-4.35524300	-0.92992200	-0.42055200
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TS2

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H	-2.86146000	1.35695300	1.62415600
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C	0.70042800	-0.96121800	-0.54489400
O	0.47797600	-2.10083900	-0.94183000
N	0.16873900	1.70823700	-1.00889200

N	0.61439300	2.55962900	-1.55275700
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C	3.15003500	-1.10836300	-0.45310300
C	2.03656400	0.56065000	0.93457800
C	4.37991500	-0.69493400	0.04370200
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H	1.12815000	1.02129100	1.31003100
C	4.44063800	0.33708000	0.98650100
H	5.29125200	-1.17382200	-0.29976600
H	3.32330900	1.74269600	2.18397500
H	5.40314000	0.65641600	1.37467800

3

C	3.28487500	1.60419100	0.45935300
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C	2.82722400	-1.19095300	-0.48952700
C	1.75071100	-0.12093700	-0.48837200
C	2.22088400	1.32726200	-0.61833000
H	4.68466600	-1.58805400	0.50305900
H	4.95908100	0.65338900	-0.52361100
H	5.13235100	0.78619500	1.22705400
H	2.80356500	1.60463900	1.44493400
H	3.67279400	2.61415800	0.28632900
H	3.28549000	-1.15672200	-1.48632000
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H	2.65742100	1.40781700	-1.62183700
H	1.38484400	2.02575500	-0.54787300
H	3.42388400	-0.97690100	1.57735400
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C	-0.79601100	-0.89295500	-0.12601400
O	-0.42927500	-2.08724800	-0.06293200
C	-2.09084300	-0.28957000	-0.02327500
C	-3.21403300	-1.10813900	0.20541900
C	-2.22083400	1.10627100	-0.15007600
C	-4.46599200	-0.52027600	0.30787400
H	-3.08770300	-2.18183700	0.29999000
C	-3.47999400	1.68146200	-0.04694500
H	-1.34336100	1.72159700	-0.32986500
C	-4.59678800	0.86924100	0.18202600
H	-5.34234900	-1.13465100	0.48560400
H	-3.59777600	2.75550600	-0.14381700
H	-5.58004000	1.32260900	0.26341700

TS4

C	-3.52317000	-1.44866500	0.55319700
C	-4.21279600	-0.08521000	0.45832900
C	-3.22933800	1.08548900	0.55787900
C	-2.19127500	1.10559800	-0.56013000
C	-1.50807000	-0.52398400	-0.51656600
C	-2.45612100	-1.63427200	-0.55062200
H	-3.76661000	2.03776300	0.47712500
H	-4.76201500	-0.01545500	-0.48976100
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H	-2.57843600	1.07729200	-1.58053400
H	-1.54182000	1.99216400	-0.48225000
H	-2.92512200	-1.65353400	-1.54214500
H	-1.88984000	-2.56156800	-0.41886500
H	-2.71358900	1.08646000	1.52464600
C	-0.56616400	0.26938000	-0.37563800
C	0.65895700	1.08051400	-0.18114800
O	0.55251100	2.29827700	-0.14020000
C	1.91040700	0.32478300	-0.04324100
C	3.09550600	1.04810400	0.18149200
C	1.94423800	-1.07714100	-0.13105300
C	4.29983800	0.37031800	0.31816800
H	3.05149700	2.12975900	0.24621800
C	3.15482300	-1.74840400	0.00640400
H	1.03495400	-1.64271000	-0.30980400
C	4.33011200	-1.02645100	0.23119500
H	5.21648500	0.92476600	0.49266200
H	3.18355200	-2.83110200	-0.06208100
H	5.27371300	-1.55295900	0.33896900

5

C	3.44178700	0.79414300	0.54962600
C	3.80970000	-0.33514400	-0.43292800
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C	1.59608800	-1.87951100	-0.53126300
C	1.06515800	-0.63615200	-0.15419500
C	2.11326700	1.50505300	0.29326200
H	3.62168500	-2.47625800	-0.72188000
H	3.61639700	-0.03158400	-1.47007000
H	4.88818000	-0.50931800	-0.35647900
H	3.44842800	0.39374900	1.57096300
H	4.21758000	1.56569900	0.51013000
H	1.50291100	-2.04974200	-1.60875100
H	1.20660600	-2.72564300	0.04123300
H	2.15401400	2.10388700	-0.62404800
H	1.86443600	2.17919700	1.11890600
H	3.23503300	-1.92409200	0.92716400
C	0.88616800	0.60247900	0.10667700
C	-0.48588600	1.29628400	0.03396400
O	-0.48866500	2.50019700	-0.11293300
C	-1.69553400	0.45314500	0.08537100
C	-2.88758300	0.98402500	-0.43596700
C	-1.68082800	-0.84406000	0.62026500
C	-4.03722200	0.20355400	-0.46192200
H	-2.88698800	1.99049500	-0.84003300
C	-2.83764300	-1.62087200	0.59278200
H	-0.79844200	-1.22929400	1.12283400
C	-4.01252400	-1.09962300	0.04817000
H	-4.95232000	0.60473200	-0.88605400
H	-2.82664200	-2.61998600	1.01628500
H	-4.91405300	-1.70460700	0.02907900

TS6

C	3.43525600	0.64820700	0.22197900
C	3.52041500	-0.62600000	-0.64058900
C	2.76508200	-1.83363200	-0.07383700
C	1.18817200	-1.85708200	-0.24187900

C	0.76082700	-0.53475400	0.07416300
C	2.17292100	1.49289400	0.04380200
H	3.07911200	-2.74795600	-0.58737800
H	3.19786900	-0.41913800	-1.66981600
H	4.57339600	-0.92175300	-0.69998000
H	3.54047800	0.37158700	1.27871500
H	4.28325600	1.29789100	-0.01835300
H	0.92104500	-2.09941400	-1.27716000
H	0.77405800	-2.61094900	0.43237900
H	2.15153300	1.95386600	-0.95227600
H	2.14101500	2.30807000	0.77500500
H	2.98602400	-1.94417100	0.99138400
C	0.85183600	0.75291600	0.17210200
C	-0.44362500	1.53711300	0.22462600
O	-0.46233800	2.74593800	0.14278800
C	-1.62815800	0.64243800	0.22832200
C	-1.51313100	-0.61874100	0.85308200
C	-2.75546100	0.96038300	-0.53000600
C	-2.50206200	-1.58978500	0.63572100
H	-0.79684300	-0.77677300	1.65589000
C	-3.73658900	-0.01094800	-0.72701600
H	-2.82450200	1.92992600	-1.01174000
C	-3.60288600	-1.28661700	-0.16054300
H	-2.43152900	-2.55041100	1.13526600
H	-4.59757100	0.21552300	-1.34808200
H	-4.37421600	-2.03216000	-0.32572000

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C	3.23847400	0.79572600	0.23850800
C	3.58752500	-0.66795600	-0.05822100
C	2.56620300	-1.70889200	0.41543600
C	1.22928000	-1.73015800	-0.35649000
C	0.37050500	-0.53249200	-0.11819600
C	2.05499600	1.35662500	-0.56562400
H	3.00764500	-2.70665300	0.30659600
H	3.75026600	-0.78907300	-1.13900300
H	4.54597900	-0.89572400	0.42494700
H	3.03779500	0.91746400	1.31136400
H	4.11479100	1.41454100	0.01097000
H	1.44296400	-1.79705300	-1.43342900
H	0.67853300	-2.63710900	-0.09106000
H	2.24188700	1.19651700	-1.63728000
H	1.99085000	2.44028900	-0.42006200
H	2.36116400	-1.56961200	1.48487800
C	0.71946500	0.77548600	-0.21123200
C	-0.43685500	1.63615200	0.10387700
O	-0.49210900	2.85424500	0.16681800
C	-1.60445300	0.70320800	0.26387500
C	-2.93052300	0.96477300	0.06912000
C	-1.07990800	-0.66183800	0.39169800
C	-3.79058000	-0.13744700	-0.14117400
H	-3.29882000	1.98073300	-0.02760500
C	-1.99877000	-1.74682000	0.01224400
C	-3.32936200	-1.46934900	-0.19674000
H	-4.84512400	0.05308800	-0.32111500
H	-1.63848300	-2.77062700	0.02725700
H	-4.03336500	-2.26711400	-0.40410800

H	-0.99519100	-0.86572400	1.49062000
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TS8

C	3.49780900	0.61459700	0.74790600
C	3.69740600	-0.41924300	-0.35886200
C	2.72824600	-1.61080200	-0.22915800
C	1.05794200	-1.88384700	-0.95195400
C	1.17111400	-0.69902300	-0.31095900
C	2.18814500	1.38697400	0.60123500
H	3.03466300	-2.37238600	-0.95320400
H	3.61890500	0.02595700	-1.35612000
H	4.69314100	-0.86854200	-0.27886900
H	3.52586500	0.10208400	1.71677000
H	4.33234100	1.32212600	0.73563400
H	1.13798300	-1.92896800	-2.03721400
H	0.72213900	-2.78070100	-0.43493700
H	2.28754200	2.19659200	-0.13136600
H	1.89677700	1.86286600	1.54366300
H	2.68427600	-2.04489000	0.76817100
C	1.04404300	0.53502600	0.11358500
C	-0.29619300	1.22549300	-0.09145100
O	-0.26920400	2.41187500	-0.38286200
C	-1.55719000	0.45931600	0.03824700
C	-2.69718500	0.95910900	-0.61487700
C	-1.65757900	-0.70636300	0.81560100
C	-3.90931700	0.28588200	-0.51739300
H	-2.61091300	1.86742600	-1.20163800
C	-2.87913400	-1.36866400	0.92276900
H	-0.79788200	-1.07446300	1.36403600
C	-4.00151900	-0.87950800	0.25138000
H	-4.78394100	0.66711300	-1.03568200
H	-2.95606700	-2.26171600	1.53540000
H	-4.95072600	-1.40117800	0.33184200

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C	-3.18884800	-0.48616700	0.96570600
C	-3.51265900	-1.05185800	-0.42052300
C	-3.12659400	-0.04658100	-1.50693800
C	-1.62887500	0.26289500	-1.45230400
C	-1.05616000	0.40171000	-0.09971600
C	-1.76045700	0.01136000	1.06830900
H	-3.36938300	-0.42884900	-2.50253100
H	-2.96674200	-1.99197200	-0.57501900
H	-4.58017900	-1.28441100	-0.47693900
H	-3.85556700	0.35932900	1.17957700
H	-3.35880100	-1.23131100	1.74873000
H	-1.03815100	-0.56470900	-1.89604600
H	-1.34151000	1.13499700	-2.05483400
H	-3.68942300	0.88396400	-1.36776000
C	0.29377800	1.06882600	-0.02941100
O	0.17789400	2.29004900	0.01538800
C	-1.09796100	0.07261000	2.26390400
H	-0.08145500	0.44119700	2.35480000
H	-1.58197500	-0.25308700	3.18127800
C	1.54371400	0.31604600	-0.06880200
C	2.75861300	1.02450400	-0.09324900
C	1.54052300	-1.08934600	-0.08301400

C	3.95901400	0.32763000	-0.13081600
H	2.74027700	2.10938400	-0.08340500
C	2.74777200	-1.78003600	-0.12143000
H	0.60346000	-1.63738600	-0.05782400
C	3.95320300	-1.07262900	-0.14479400
H	4.90006600	0.86809500	-0.14976900
H	2.75179200	-2.86528000	-0.13115900
H	4.89405100	-1.61412700	-0.17374600

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C	-4.52362800	0.27938600	-0.60701200
C	-4.70611600	-0.84209300	0.43330300
C	-3.79534800	-2.05672100	0.23245400
C	-2.23667600	-1.94059500	0.66523200
C	-1.94755200	-0.64530400	0.22497600
C	-3.35881900	1.23779700	-0.36286100
H	-4.12192300	-2.88508300	0.86765600
H	-4.60738800	-0.44984300	1.45359500
H	-5.72919100	-1.22242400	0.34391400
H	-4.42441100	-0.16815300	-1.60363800
H	-5.42856700	0.89500200	-0.62760300
H	-2.14240600	-2.03568800	1.75153900
H	-1.69136900	-2.72975800	0.14060800
H	-3.53725900	1.85984700	0.52188300
H	-3.21550700	1.90439800	-1.21890700
H	-3.80521200	-2.37455500	-0.81181300
C	-1.98889800	0.58982600	-0.10656000
C	-0.77416700	1.52217000	-0.06861300
O	-0.98234000	2.71221200	0.02050400
C	0.58251800	0.92173300	-0.09595200
C	1.64025600	1.68358400	0.42579200
C	0.82147400	-0.35623700	-0.62103000
C	2.92391400	1.15717700	0.46090900
H	1.44231100	2.67341100	0.82048300
C	2.10608900	-0.89066100	-0.59533000
H	0.03146100	-0.92336900	-1.10244600
C	3.13096100	-0.12428900	-0.04907000
H	3.75031300	1.71932700	0.87641300
H	2.31406700	-1.87108300	-1.00331800
N	4.49128200	-0.68662000	-0.01725900
O	5.38507700	0.00170000	0.47284300
O	4.65752000	-1.81395300	-0.48146800

TS11

C	4.34755400	-0.19444300	0.01057800
C	3.96580100	-1.47636200	-0.75212300
C	2.92159800	-2.34809100	-0.04691300
C	1.41604300	-1.88127400	-0.12110200
C	1.40098500	-0.47305700	0.14715100
C	3.39284100	0.98821300	-0.15370300
H	2.89643400	-3.34512100	-0.49892600
H	3.64020200	-1.23715100	-1.77347900
H	4.86758100	-2.09039000	-0.85086400
H	4.45376000	-0.43095000	1.07692700
H	5.32921100	0.14701100	-0.33421100
H	1.00986600	-2.06338500	-1.12379800
H	0.83472300	-2.44966500	0.60933700

H	3.41973000	1.36418200	-1.18513800
H	3.68783500	1.81974600	0.49609900
H	3.18449600	-2.45997400	1.00905700
C	1.93024500	0.71796400	0.14185300
C	0.96603000	1.86649900	0.26482200
O	1.28552100	3.02962200	0.16728500
C	-0.42895500	1.34422100	0.35502800
C	-0.59780200	0.10102900	1.01079400
C	-1.46051400	1.91725800	-0.38373000
C	-1.79476200	-0.61390900	0.83346600
H	0.03767000	-0.17642800	1.84843800
C	-2.65257000	1.21435500	-0.54295800
H	-1.30633900	2.86458400	-0.88839800
C	-2.78477100	-0.04774800	0.04682000
H	-1.96661300	-1.55353400	1.34254700
H	-3.45825200	1.61458400	-1.14586900
N	-4.03946400	-0.79478400	-0.15269100
O	-4.12796600	-1.90669700	0.36394900
O	-4.91810500	-0.26391800	-0.82783100

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C	-4.21864500	-0.06077500	-0.11834100
C	-4.06425300	-1.56375700	0.14486000
C	-2.79571600	-2.21290200	-0.41935400
C	-1.47703200	-1.81458500	0.28096700
C	-1.06773600	-0.40010500	0.04584900
C	-3.23572500	0.83755500	0.64972000
H	-2.88320300	-3.30106100	-0.31935100
H	-4.11311600	-1.74893300	1.22757800
H	-4.92706300	-2.07864200	-0.29572900
H	-4.12629400	0.13778500	-1.19435300
H	-5.23224900	0.24099500	0.17086900
H	-1.59382500	-1.96332300	1.36450900
H	-0.68228400	-2.49192200	-0.04371200
H	-3.29834100	0.60396600	1.72227500
H	-3.53166400	1.88639500	0.54163200
H	-2.71211500	-1.99925800	-1.49268000
C	-1.80646600	0.72649700	0.21383300
C	-0.99783300	1.92067800	-0.08835500
O	-1.32469300	3.09567400	-0.09391000
C	0.39893600	1.41070000	-0.32079600
C	1.58423800	2.07154500	-0.12591500
C	0.32125500	-0.03916400	-0.53692100
C	2.75123900	1.29861700	-0.00648000
H	1.61851600	3.14390100	0.03214700
C	1.54385300	-0.80270900	-0.26298300
H	0.23361400	-0.20482600	-1.64219800
C	2.70476100	-0.11068400	-0.05404400
H	3.70616400	1.78058300	0.17557100
H	1.54308000	-1.88452100	-0.33821200
N	3.96209100	-0.86395500	0.13927400
O	4.97350600	-0.21508600	0.38449100
O	3.90354800	-2.08545300	0.04748200

TS13

C	-4.60841000	0.12620500	-0.57033300
C	-4.51420300	-0.92082400	0.53950500

C	-3.37873400	-1.93092100	0.29864700
C	-1.64339000	-1.88883300	0.85302100
C	-1.97989400	-0.73181500	0.24448500
C	-3.45125500	1.12255000	-0.54419500
H	-3.48143500	-2.74119300	1.02743200
H	-4.41382800	-0.46342800	1.52942500
H	-5.42262700	-1.53246100	0.55411000
H	-4.63912000	-0.38886000	-1.53770600
H	-5.54947600	0.67486700	-0.46966800
H	-1.61396700	-1.93931700	1.94080100
H	-1.19151600	-2.71043600	0.30099700
H	-3.62439400	1.90572000	0.20352200
H	-3.34283700	1.63720600	-1.50433900
H	-3.34869400	-2.33644700	-0.71095900
C	-2.12667800	0.49963500	-0.17963300
C	-0.92780200	1.42715800	-0.10759600
O	-1.13918100	2.62372000	-0.01058500
C	0.45546200	0.87171300	-0.10997700
C	1.43342400	1.56189600	0.62359100
C	0.80390700	-0.27288100	-0.84268300
C	2.74070600	1.09602300	0.65936300
H	1.15674800	2.45384000	1.17427000
C	2.11496900	-0.73829700	-0.82920500
H	0.06750800	-0.78465800	-1.45148700
C	3.05650700	-0.05056900	-0.06847400
H	3.50412100	1.60450500	1.23393900
H	2.40585900	-1.61220300	-1.39774800
N	4.43901400	-0.54971400	-0.03589400
O	4.70459900	-1.55486400	-0.69535600
O	5.25619600	0.06297200	0.65088800

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C	-4.05621500	-0.88608200	0.91718900
C	-4.21175800	-1.53319200	-0.46233400
C	-4.00044600	-0.49181400	-1.56220800
C	-2.59680800	0.11094800	-1.47297000
C	-2.10852800	0.38513500	-0.10870500
C	-2.76628600	-0.10011800	1.04739100
H	-4.13005400	-0.93165800	-2.55500700
H	-3.48226600	-2.34578000	-0.57642700
H	-5.20771700	-1.97821100	-0.54327700
H	-4.89024300	-0.19451700	1.09339700
H	-4.09083300	-1.63601300	1.71311800
H	-1.83866400	-0.58712100	-1.88424800
H	-2.47050700	1.01461200	-2.08525300
H	-4.74061800	0.31063300	-1.46018000
C	-0.90372900	1.29208100	-0.02941200
O	-1.20113700	2.47775700	-0.04410200
C	-2.19542700	0.15122100	2.26732700
H	-1.27959600	0.72221200	2.38662400
H	-2.65611100	-0.22238300	3.17842600
C	0.46843100	0.75841300	-0.01531900
C	1.53660900	1.66438700	-0.11877300
C	0.70634800	-0.62075400	0.08707300
C	2.84194700	1.19446600	-0.12974800
H	1.33250000	2.72647100	-0.19598900
C	2.01094600	-1.10068900	0.07570300

H	-0.11856900	-1.31929000	0.17743400
C	3.05112600	-0.18151300	-0.03625300
H	3.68416100	1.86919400	-0.21216400
H	2.22331300	-2.15919200	0.14988400
N	4.43478000	-0.68675700	-0.06141900
O	4.60240800	-1.90361000	0.00643300
O	5.34428800	0.13627900	-0.15110200

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C	4.09931900	1.16036900	0.34940900
C	4.43969600	-0.21616200	-0.23002000
C	3.16880000	-1.05121600	0.01356200
C	2.04595500	-0.01426400	-0.04560400
C	2.64288900	1.39638900	-0.09515700
H	4.63274200	-0.13950800	-1.30556200
H	4.15421600	1.14024100	1.44336000
H	4.75090300	1.95988400	-0.01358500
H	2.99479100	-1.86461200	-0.69461600
H	3.14770900	-1.47378000	1.02578600
H	2.59906300	1.71427300	-1.14445000
H	2.07880800	2.11249400	0.50563500
H	5.30959100	-0.68008000	0.24261200
C	0.77842900	-0.25707900	-0.03271200
C	-0.50207800	-0.84584200	-0.00211900
O	-0.11565000	-2.03496300	0.02518100
C	-1.81533400	-0.27174800	-0.00103800
C	-2.93795700	-1.12057200	0.04936600
C	-1.96236000	1.12743000	-0.05012400
C	-4.20683100	-0.56038000	0.04989600
H	-2.79893600	-2.19618700	0.08859800
C	-3.23829500	1.67481200	-0.04945600
H	-1.08528700	1.76825600	-0.08789400
C	-4.35474900	0.83212500	0.00016000
H	-5.08295500	-1.19918000	0.08857900
H	-3.36926600	2.75098400	-0.08745800
H	-5.35108500	1.26374500	0.00057600

TS16

C	-4.22426900	-0.82473800	0.09336800
C	-3.82985900	0.60376200	0.48237500
C	-2.60645900	0.96930100	-0.36184100
C	-1.84660600	-0.58285700	-0.14991500
C	-2.88938900	-1.61118500	0.02703400
H	-4.60767500	1.34419600	0.26361200
H	-4.91502900	-1.27757500	0.80712800
H	-2.78671200	1.00680200	-1.43641200
H	-2.08126000	1.86399600	-0.02091900
H	-2.84699000	-2.33794500	-0.79021700
H	-2.66159900	-2.14086200	0.95938200
H	-3.57844200	0.67337000	1.54515300
C	-0.81628000	0.10773500	-0.14151000
C	0.36937700	0.98676300	-0.10672400
O	0.19019000	2.19735600	-0.11515900
C	1.66604700	0.30413600	-0.04005900
C	2.82062400	1.08798900	0.13144700
C	1.76510900	-1.09373400	-0.14096900
C	4.06287500	0.47161000	0.20460100

H	2.72339600	2.16546500	0.20819700
C	3.01371100	-1.70280400	-0.06834200
H	0.87694200	-1.70239500	-0.28533500
C	4.15956400	-0.92161800	0.10548200
H	4.95778300	1.07071300	0.33971000
H	3.09556900	-2.78186700	-0.14923100
H	5.13306700	-1.39917100	0.16334700
H	-4.69724600	-0.82974300	-0.89282600

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C	-3.64244900	0.42378200	0.32592900
C	-3.64838600	-0.99633100	-0.23142800
C	-2.31844600	-1.86535700	0.18899800
C	-1.41610500	-0.80123700	0.05823100
C	-2.45414800	1.24546400	-0.17513600
H	-4.47022500	-1.59905400	0.16414900
H	-3.63023700	0.39272900	1.42088800
H	-4.57158100	0.91948000	0.02291600
H	-2.40605700	-2.24467300	1.21049900
H	-2.21210500	-2.66974300	-0.54328400
H	-2.29660800	2.15796200	0.40728900
H	-2.54517400	1.51261900	-1.23314000
H	-3.67778900	-1.00082100	-1.32291500
C	-1.12145000	0.43732100	-0.04784500
C	0.20057200	1.18301700	-0.04978300
O	0.16647500	2.39881100	-0.04608200
C	1.44534800	0.38619700	-0.03881400
C	2.66426400	1.07666700	0.07890800
C	1.44880800	-1.00886600	-0.13063600
C	3.86010900	0.36943800	0.11697600
H	2.65160900	2.15873200	0.14954500
C	2.64391200	-1.71921200	-0.08867000
H	0.52044000	-1.56819500	-0.26740300
C	3.85173200	-1.02657600	0.03416800
H	4.80005500	0.90339900	0.21499700
H	2.63604700	-2.80162500	-0.16245000
H	4.78725800	-1.57714100	0.06217900

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C	-3.83450500	1.03667700	0.28170100
C	-4.57193700	-0.29442200	0.43649700
C	-3.72524800	-1.46882400	-0.05587700
C	-2.32659900	-1.48936800	0.64168500
C	-1.69413200	-0.16566700	0.39211300
C	-2.43471500	0.98399600	0.97170500
H	-4.20968200	-2.42728300	0.15448400
H	-4.82930200	-0.44827200	1.49235200
H	-5.51336800	-0.26207100	-0.12427700
H	-3.69183500	1.27865800	-0.77783600
H	-4.39421800	1.85970400	0.73608400
H	-2.48021900	-1.60102500	1.72091800
H	-1.73716400	-2.33648100	0.28670100
H	-2.58858700	0.76862400	2.03616100
H	-1.91419600	1.92982200	0.85696100
H	-3.57546300	-1.40488900	-1.14010800
C	-0.59001200	-0.00455400	-0.42660300
C	0.07855600	1.28185600	-0.89454300

O	-0.53826600	2.32132000	-0.80237900
N	-0.01348400	-1.15044400	-0.88683000
N	0.50888200	-2.04891400	-1.29549900
C	1.49036900	1.18946300	-1.43471300
H	1.47186000	0.62011300	-2.37329300
H	1.78861300	2.21256700	-1.68159400
C	2.44927700	0.54842600	-0.44692600
C	2.52287300	1.02158100	0.87035500
C	3.26407800	-0.52178900	-0.83384600
C	3.39897300	0.43488700	1.78338300
H	1.89838500	1.85597100	1.18028800
C	4.14343400	-1.10704000	0.07837900
H	3.21184500	-0.89280000	-1.85441900
C	4.21069400	-0.63138900	1.38948500
H	3.44867800	0.81183700	2.80084900
H	4.77326500	-1.93453900	-0.23520600
H	4.89309300	-1.08799000	2.10049300

TS19

C	-3.55237400	0.21363800	-1.35126800
C	-4.13612400	-1.10662100	-0.84293700
C	-3.10523700	-1.89210800	-0.02690200
C	-2.53400700	-1.03729900	1.13212000
C	-1.97921800	0.24727500	0.58448500
C	-2.98576200	1.07508400	-0.19717100
H	-3.54840600	-2.79412800	0.40624800
H	-5.01881700	-0.90475700	-0.22178500
H	-4.47742500	-1.71411500	-1.68735800
H	-2.75367400	0.02251500	-2.07860300
H	-4.31421700	0.80902500	-1.86442500
H	-3.34855700	-0.77293700	1.81865700
H	-1.79098500	-1.59812800	1.70316100
H	-3.79278900	1.31712600	0.50764100
H	-2.55073300	2.00196300	-0.56075200
H	-2.27818100	-2.21637100	-0.67079200
C	-0.71732700	0.66297000	0.65261500
C	0.16861100	1.79020100	0.24227400
O	-0.41497600	2.63580900	-0.40545900
N	0.25740900	-0.53403400	1.58421500
N	0.98775500	-1.17669700	2.10940900
C	1.63752300	1.82914000	0.57596100
H	1.76502900	1.82620700	1.66621400
H	1.99482900	2.79819500	0.21169000
C	2.39786800	0.67187200	-0.05048100
C	2.09159100	0.24169500	-1.34690200
C	3.40347300	0.01815300	0.67078400
C	2.77873900	-0.83449300	-1.91203000
H	1.33026400	0.75742200	-1.92742600
C	4.09114000	-1.05454800	0.10438300
H	3.65777000	0.35551600	1.67287500
C	3.77525200	-1.48669600	-1.18646900
H	2.53868200	-1.15648900	-2.92057500
H	4.87532900	-1.54966600	0.66858900
H	4.31065900	-2.32232400	-1.62583500

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C	2.83167800	-1.60571400	-0.83783200
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C	4.01495000	-0.77895300	-0.33103500
C	3.58910200	0.66617300	-0.06469400
C	2.38599600	0.72982400	0.89882200
C	1.23882700	-0.11744300	0.40721400
C	1.62697400	-1.54832500	0.13044300
H	4.41548400	1.24458500	0.36347500
H	4.39904100	-1.22297500	0.59816800
H	4.83250300	-0.80737100	-1.06134200
H	2.51238800	-1.22602700	-1.81785500
H	3.11651300	-2.65452600	-0.97785400
H	2.69590000	0.30939200	1.86739300
H	2.07512800	1.75808700	1.06926100
H	1.91274100	-2.02375200	1.07945800
H	0.80763300	-2.12821500	-0.29484200
H	3.31369000	1.15147200	-1.01074500
C	-0.00008900	0.37775800	0.17558700
C	-0.36338700	1.82353500	0.09473200
O	0.24548800	2.79365800	0.49942400
C	-1.68664000	1.93202900	-0.69706000
H	-2.31697900	2.77202300	-0.39560400
H	-1.39605900	2.08628000	-1.74881400
C	-2.30058900	0.60474600	-0.49940800
C	-1.24387800	-0.41261700	-0.27271200
C	-3.63624900	0.30363000	-0.34635200
C	-1.69592800	-1.65951500	0.38407300
C	-3.98953800	-0.95904000	0.14187700
H	-4.39917800	1.05106400	-0.53475400
C	-3.02866100	-1.92310800	0.53138800
H	-0.95858900	-2.40313900	0.66036200
H	-5.04260700	-1.19530500	0.26727000
H	-3.36121800	-2.86438400	0.95459700
H	-1.02572000	-0.79435000	-1.30382400

TS21

C	3.20097800	-1.99783200	-0.21383000
C	4.52341000	-1.32898300	0.16444100
C	4.42663700	0.19468800	0.08102600
C	3.23575300	0.73558100	0.93524300
C	2.00300300	0.04234600	0.47130000
C	2.02537100	-1.43298700	0.64434800
H	5.33734800	0.67546300	0.45094500
H	4.80127300	-1.62132000	1.18526800
H	5.31942000	-1.68204900	-0.50147200
H	2.97248300	-1.83256400	-1.27297400
H	3.23749200	-3.07875400	-0.04856000
H	3.40922800	0.46545300	1.98317900
H	3.18148000	1.82321800	0.86193500
H	2.25608000	-1.62813900	1.69933600
H	1.08739800	-1.91066900	0.37747200
H	4.28462600	0.51178400	-0.95891000
C	0.97096800	0.70320900	-0.17420800
C	-0.27444800	0.11577200	-0.82253500
O	-0.25061700	-1.05034700	-1.15081800
N	1.08144000	2.05826800	-0.25152000
N	1.12276000	3.16994400	-0.35429500
C	-1.49621300	1.00085300	-1.01094400
H	-1.33999200	2.00395800	-0.60862100

H	-1.64492200	1.09644000	-2.09324400
C	-2.70875200	0.36401600	-0.35999900
C	-3.42550700	-0.64123900	-1.01905200
C	-3.09533000	0.75080100	0.92791300
C	-4.51821900	-1.24737800	-0.39880200
H	-3.12790000	-0.94533900	-2.01829100
C	-4.18958400	0.14539800	1.54817600
H	-2.54170100	1.53179600	1.44321000
C	-4.90231900	-0.85606400	0.88613500
H	-5.07169900	-2.02307900	-0.92049400
H	-4.48445500	0.45687600	2.54631500
H	-5.75511300	-1.32686300	1.36689000

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C	-3.20599600	-2.02396400	0.35242600
C	-4.57051600	-1.35420100	0.51653400
C	-4.43718800	0.16193400	0.66158300
C	-3.61527200	0.77137800	-0.51798200
C	-2.30496300	0.06502300	-0.56879400
C	-2.40848600	-1.39243100	-0.83498500
H	-5.41545800	0.65210000	0.66657300
H	-5.19681400	-1.58479300	-0.35477800
H	-5.07873600	-1.76293000	1.39767500
H	-2.61342200	-1.92146700	1.26890000
H	-3.30692900	-3.09324300	0.14330900
H	-4.14789800	0.56385000	-1.45336400
H	-3.52967100	1.85321600	-0.40391500
H	-3.00496900	-1.52020400	-1.74646600
H	-1.44314800	-1.87375100	-0.95203800
H	-3.93644200	0.41319100	1.60412800
C	-1.10720800	0.68399700	-0.24780000
C	0.29656100	0.09820900	-0.15691100
O	0.43921600	-1.10039100	-0.25034400
N	-1.18379400	2.01645500	0.03600700
N	-1.18120000	3.10511800	0.28613500
C	1.43578900	1.07946200	0.05220000
H	1.38242800	1.83724300	-0.74173400
H	1.25088400	1.60898000	0.99655600
C	2.78569400	0.40917500	0.07414800
C	3.46462700	0.14804000	-1.12134300
C	3.36387300	0.01914600	1.28663100
C	4.70475700	-0.49052100	-1.10506100
H	3.01988900	0.44815700	-2.06691500
C	4.60485000	-0.61924400	1.30561400
H	2.84151500	0.21943400	2.21879100
C	5.27767200	-0.87563500	0.10932800
H	5.22420300	-0.68550100	-2.03911600
H	5.04606300	-0.91377500	2.25364900
H	6.24457700	-1.37060100	0.12296900

TS23

C	-3.42213900	-2.05677400	0.29460300
C	-4.74405000	-1.29378800	0.40919900
C	-4.50350100	0.19589200	0.67110900
C	-3.58332400	0.81623900	-0.40993700
C	-2.30463000	0.03175400	-0.49532700
C	-2.49688300	-1.44770400	-0.78642500

H	-5.44468400	0.75414700	0.67255500
H	-5.32121900	-1.41516400	-0.51690000
H	-5.35048000	-1.71629300	1.21674600
H	-2.89519200	-2.05620700	1.25656700
H	-3.59405600	-3.10419900	0.02708100
H	-4.07639100	0.74006500	-1.38758100
H	-3.40573700	1.87580300	-0.21162300
H	-2.99401700	-1.50044300	-1.76461800
H	-1.54711800	-1.97226100	-0.84806300
H	-4.04242800	0.33783800	1.65636500
C	-1.07382400	0.48557200	-0.27433000
C	0.35320700	0.05573900	-0.21358200
O	0.48977800	-1.13001800	-0.42524600
N	-1.13601100	2.25357500	0.07367800
N	-0.99946800	3.33057200	0.28290100
C	1.46888400	1.03614700	0.08052200
H	1.25421800	1.51932800	1.04427500
H	1.43121200	1.83039700	-0.67890500
C	2.82132000	0.36904400	0.10098000
C	3.32973200	-0.15051000	1.29496400
C	3.56095000	0.24252800	-1.07854900
C	4.56906100	-0.78811700	1.31060800
H	2.75984200	-0.05276000	2.21593800
C	4.80015900	-0.39513400	-1.06336300
H	3.17145900	0.64644700	-2.00995800
C	5.30497400	-0.91126300	0.13114200
H	4.96088900	-1.18397600	2.24230500
H	5.37219600	-0.48505500	-1.98149900
H	6.27201500	-1.40429900	0.14356300

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C	4.32589100	0.84774100	0.98371900
C	5.08777800	-0.33389900	0.37724100
C	4.13487700	-1.44463500	-0.07492800
C	3.08549700	-0.92930900	-1.07583800
C	2.38373900	0.27817600	-0.46871700
C	3.28046200	1.42209900	0.01126200
H	4.68535500	-2.25409800	-0.56682500
H	5.67806100	0.01334300	-0.48112900
H	5.79424200	-0.73224300	1.11334700
H	3.82286100	0.53979900	1.90825800
H	5.01075800	1.66315500	1.24185200
H	3.57447400	-0.56106400	-1.98655400
H	2.35874800	-1.69534000	-1.34709600
H	3.76210500	1.81220800	-0.89413500
H	2.69615300	2.22255900	0.46781800
H	3.62066000	-1.87908000	0.79066600
C	1.11199200	0.34995200	-0.27282400
C	-0.28575000	0.14371400	-0.16983000
O	-0.40864700	-0.96461900	-0.69870600
C	-1.31293100	1.02693100	0.44356300
H	-1.02400200	1.14419300	1.49893300
H	-1.20077400	2.02055500	-0.00976800
C	-2.71051300	0.47789000	0.28923300
C	-3.59692100	1.04933500	-0.62888100
C	-3.12191500	-0.62270200	1.05101900
C	-4.88517100	0.53318500	-0.77738100

H	-3.27971300	1.90230000	-1.22288100
C	-4.40738700	-1.14138900	0.89947300
H	-2.43486600	-1.06962000	1.76489800
C	-5.29163900	-0.56340900	-0.01466800
H	-5.56986000	0.98779900	-1.48752100
H	-4.71888000	-1.99441900	1.49539400
H	-6.29420100	-0.96517900	-0.13025300

TS25

C	4.59507200	0.68385600	0.85921500
C	4.88207500	-0.60162600	0.07983500
C	3.62501100	-1.44678200	-0.15140900
C	2.55834200	-0.73395800	-0.97750900
C	2.34244400	0.80305600	-0.13212500
C	3.55148200	1.57336500	0.14378400
H	3.87664700	-2.35284300	-0.71514800
H	5.33368200	-0.35279300	-0.88955000
H	5.61534500	-1.20097300	0.62885400
H	4.22555600	0.44383800	1.86234000
H	5.50615600	1.27761700	0.97416700
H	2.88058300	-0.33323500	-1.94058100
H	1.69944200	-1.39624000	-1.16979900
H	3.94768700	1.93541900	-0.81315900
H	3.26660500	2.43972800	0.74871300
H	3.18535000	-1.76970700	0.79888500
C	1.22769100	0.26262200	-0.19001700
C	-0.17482500	-0.20000600	-0.17879400
O	-0.46283800	-1.26055800	-0.69255600
C	-1.11803800	0.75457600	0.52348600
H	-0.89463300	1.76917600	0.17121100
H	-0.83884200	0.73270900	1.58693100
C	-2.57025000	0.40374100	0.32031900
C	-3.17644000	-0.59325000	1.09291000
C	-3.32123100	1.06266400	-0.65886800
C	-4.51676300	-0.92336500	0.89207800
H	-2.59743300	-1.10766800	1.85549300
C	-4.66262200	0.73426700	-0.86043600
H	-2.85436700	1.83792600	-1.26115600
C	-5.26268600	-0.25981600	-0.08524800
H	-4.97948900	-1.69590200	1.49967500
H	-5.23775800	1.25588500	-1.62026300
H	-6.30740700	-0.51453500	-0.23949800

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C	-3.84547800	-1.30357000	0.47034900
C	-4.58782300	-0.20798300	-0.32028700
C	-4.31212300	1.22416900	0.15019500
C	-2.90414300	1.91015800	-0.25342700
C	-2.02968800	0.82841900	-0.09345000
C	-2.39159200	-1.55459000	0.07097900
H	-5.02463100	1.91526700	-0.30926800
H	-4.39522600	-0.30359300	-1.39684200
H	-5.66303200	-0.36350800	-0.18183300
H	-3.89208500	-1.06591000	1.54038600
H	-4.37073000	-2.25459200	0.33518500
H	-2.93679800	2.26538700	-1.28792300
H	-2.72744500	2.73106200	0.44841100

H	-2.32960300	-2.00283900	-0.92787100
H	-1.89886900	-2.23285800	0.77502900
H	-4.39397800	1.29057300	1.23693100
C	-1.47949500	-0.31780200	0.00807000
C	0.04730400	-0.56578600	-0.00254400
O	0.43803200	-1.69445300	0.14126900
C	0.90074600	0.66842400	-0.21341800
H	0.62451900	1.05227600	-1.20616500
H	0.55523400	1.41350500	0.51627600
C	2.38083500	0.42760600	-0.10338600
C	3.03510700	0.59504300	1.12280500
C	3.11661900	0.01109900	-1.21914900
C	4.40459200	0.35224000	1.23193300
H	2.46930900	0.91880600	1.99281500
C	4.48552100	-0.23325200	-1.11193400
C	5.13236800	-0.06275300	0.11448700
H	4.90305500	0.48895000	2.18740100
H	5.04721200	-0.55389600	-1.98472700
H	6.19909600	-0.25030600	0.19820500
H	2.61321400	-0.12123600	-2.17350700

TS27

C	-3.59922800	-0.86822300	1.14863500
C	-4.42671100	0.03803300	0.21568700
C	-3.90498200	1.47239700	0.08334000
C	-2.60137500	1.74317300	-0.83958600
C	-1.81843800	0.62967000	-0.51567800
C	-2.34093600	-1.48528300	0.53908100
H	-4.64837300	2.09957700	-0.41708800
H	-4.54390200	-0.42227500	-0.77392300
H	-5.43315500	0.12814500	0.63807300
H	-3.32728500	-0.30276200	2.04850200
H	-4.22565900	-1.70340700	1.47816700
H	-2.88169000	1.75702200	-1.89729100
H	-2.17126000	2.69843000	-0.52353800
H	-2.59826200	-2.22400500	-0.22949300
H	-1.73806000	-1.98978000	1.30119900
H	-3.68236200	1.88923200	1.06752500
C	-1.37570500	-0.51303600	-0.15338100
C	0.05212300	-1.00560700	-0.43582200
O	0.37256000	-2.09385800	-0.02985200
C	0.96288200	-0.07787900	-1.22188900
H	1.12248100	-0.56033200	-2.19424900
H	0.43671500	0.86794400	-1.39977300
C	2.27865100	0.15386700	-0.51688800
C	2.42933100	1.24953700	0.34147700
C	3.34225700	-0.74147200	-0.67991400
C	3.63021900	1.45220700	1.02242600
H	1.60703900	1.94804300	0.47248200
C	4.54172900	-0.54089700	0.00319400
C	4.68829900	0.55622400	0.85556500
H	3.73897100	2.30854400	1.68188200
H	5.36245300	-1.23949500	-0.13220800
H	5.62415000	0.71415000	1.38399500
H	3.22901400	-1.59443000	-1.34293400

C	3.25124200	-0.63846100	0.39176400
C	2.76638800	-2.03389100	-0.02304900
C	1.28566500	-2.33982500	0.23897600
C	0.28491400	-1.56085300	-0.63625200
C	0.21885800	-0.09899200	-0.32319300
C	2.69145000	0.52047900	-0.44730100
H	1.11275200	-3.40638300	0.05185200
H	2.97840500	-2.18453900	-1.09156100
H	3.36433800	-2.77844000	0.51728300
H	3.01714000	-0.46418400	1.45056700
H	4.34418400	-0.61231100	0.30441500
H	0.57114300	-1.67249800	-1.69254700
H	-0.70870600	-2.00817700	-0.53555500
H	2.87797100	0.31844400	-1.51160500
H	3.22254700	1.44774600	-0.20533000
H	1.04874200	-2.16403600	1.29693900
C	1.22836100	0.78313000	-0.24462100
C	0.73070900	2.12953500	0.09855200
O	1.39782600	3.13312200	0.26724500
C	-0.79094400	2.08675600	0.20619400
H	-1.12461800	2.46890700	1.17365400
H	-1.23679200	2.71609300	-0.56914800
C	-1.17700000	0.58057500	0.00341200
C	-2.06147500	0.38896900	-1.16055400
C	-1.65428500	-0.03459100	1.25746400
C	-3.19295500	-0.37972600	-1.09660100
H	-1.76004000	0.86475900	-2.08951900
C	-2.78372400	-0.80793200	1.30384000
C	-3.54320200	-0.98230000	0.12904500
H	-3.82073000	-0.52484100	-1.96845200
H	-3.10609100	-1.27308700	2.22857600
H	-4.43821200	-1.59677800	0.17179400
H	-1.04865900	0.12710500	2.14462600

TS29

C	-2.96466700	-1.36781000	0.99548500
C	-3.87463100	-0.71059500	0.11901200
C	-3.41224400	0.10602000	-0.88471200
C	-2.01081800	0.30879700	-1.03704300
C	-1.08346100	-0.31987100	-0.14608700
C	-1.61075300	-1.19043400	0.86812000
H	-3.35344100	-2.02617400	1.76603800
H	-4.94030100	-0.87962100	0.23533800
H	-4.09388900	0.58162900	-1.58175200
H	-1.62501000	0.80916800	-1.91999400
H	-0.91447800	-1.70077300	1.52500400
C	-1.30819000	1.58349100	0.34087700
H	-1.70304100	1.37891100	1.33424100
H	-1.90357300	2.34774300	-0.15620700
C	0.17879800	1.93159300	0.24557200
O	0.49877400	3.05352800	0.57659400
C	1.04511300	0.85317300	-0.23877600
C	0.38752000	-0.31552900	-0.40659800
C	1.02666100	-1.62878100	-0.77867000
C	2.51425700	1.09756900	-0.41998800
C	2.16756500	-2.06794200	0.16490400
H	1.42486500	-1.53456100	-1.79986900

H	0.25975900	-2.40911900	-0.82162500
C	3.41144900	0.20094000	0.45502000
H	2.70535000	2.14967800	-0.18908200
H	2.77646800	0.95018700	-1.47694100
C	3.47059500	-1.26978700	0.02367100
H	2.37687300	-3.12097400	-0.05323400
H	1.81516700	-2.02878100	1.20453900
H	4.42527100	0.61371300	0.41713100
H	3.08651800	0.27458100	1.50100300
H	3.80926400	-1.32538000	-1.02076500
H	4.24083700	-1.77345000	0.61870300

30

C	3.06996000	-1.75760000	-0.34858900
C	3.90498000	-0.61532700	-0.27154400
C	3.35157200	0.57735100	0.08468600
C	1.91479600	0.70568100	0.39829400
C	1.08381600	-0.52398100	0.27384000
C	1.70248800	-1.72264700	-0.07258400
H	3.51084400	-2.70520700	-0.64531300
H	4.96219000	-0.70514800	-0.49449800
H	3.95314100	1.47844600	0.16244100
H	1.86710100	1.01686000	1.45843000
H	1.12825700	-2.63366000	-0.18431100
C	1.25453700	1.86129300	-0.41091700
H	1.33501300	1.62440000	-1.47874500
H	1.76755900	2.80733000	-0.22877500
C	-0.21009700	2.01181800	-0.06754100
O	-0.75747100	3.09979300	-0.17503000
C	-0.96982400	0.79839600	0.35621800
C	-0.34655900	-0.41642200	0.49271900
C	-1.15536300	-1.65620800	0.79901500
C	-2.45200800	0.96026200	0.50929300
C	-2.10609200	-2.07116600	-0.34533400
H	-1.74768200	-1.46246200	1.70274700
H	-0.49057700	-2.48445900	1.05001600
C	-3.26153300	0.24296300	-0.59865000
H	-2.67658200	2.02810600	0.49109400
H	-2.76341100	0.56743800	1.48633200
C	-3.41231900	-1.26827400	-0.39302300
H	-2.35589000	-3.12978600	-0.20893400
H	-1.57637900	-1.99294200	-1.30355800
H	-4.26116800	0.69210400	-0.62121800
H	-2.80146500	0.45291200	-1.57286900
H	-3.95675400	-1.43852500	0.54668000
H	-4.04456500	-1.67058300	-1.19457400

N2

N	0.00000000	0.00000000	0.55252600
N	0.00000000	0.00000000	-0.55252600

S1

C	4.43743400	-1.46517000	0.31235700
C	5.49914600	-0.37398600	0.17369100
C	4.91703700	0.89595100	-0.44677000
C	3.67211100	1.40002900	0.34887900
C	2.69821400	0.27722100	0.43535400

C	3.20697900	-0.94255600	1.11553100
H	5.64898800	1.70929400	-0.45699200
H	5.91600600	-0.14145700	1.16219900
H	6.32492800	-0.73888000	-0.44794600
H	4.09499800	-1.79955100	-0.67364700
H	4.82822000	-2.33964200	0.84115400
H	3.98920100	1.65222500	1.36779200
H	3.26180700	2.29868300	-0.11603300
H	3.55733000	-0.63686300	2.10971800
H	2.45564600	-1.72117300	1.22072300
H	4.61613600	0.70888000	-1.48432700
C	1.45197900	0.31323400	-0.15880300
C	0.44025300	-0.82321700	-0.26249600
O	0.86642400	-1.94772200	-0.43816900
N	1.09183200	1.46341600	-0.78923400
N	0.74079500	2.36845000	-1.34273400
C	-1.00388000	-0.50942900	-0.14343900
C	-1.91649000	-1.40364100	-0.72636000
C	-1.46358800	0.60515200	0.57439300
C	-3.28109000	-1.17887700	-0.61082000
H	-1.54762800	-2.26472500	-1.27182200
C	-2.82902200	0.83201500	0.70596800
H	-0.77141000	1.28075200	1.06553200
C	-3.71055100	-0.06265900	0.10562700
H	-4.00208400	-1.84933600	-1.06026100
H	-3.20535500	1.67816500	1.26579100
N	-5.15715000	0.17617800	0.24014300
O	-5.92309400	-0.63544300	-0.27726400
O	-5.51912000	1.17353100	0.86321100

TS-S2

C	-4.42471200	0.82348500	-1.37427200
C	-5.24278800	-0.44443600	-1.12641800
C	-4.35761600	-1.57716400	-0.59862700
C	-3.59988700	-1.15538000	0.67604000
C	-2.83134100	0.11259200	0.42070200
C	-3.66982800	1.28532700	-0.11532700
H	-4.95618800	-2.46014800	-0.35270300
H	-6.03752100	-0.23244300	-0.39911300
H	-5.73046300	-0.75893700	-2.05541800
H	-3.70271800	0.65828200	-2.18321700
H	-5.07067100	1.65397600	-1.68116700
H	-4.31995400	-0.92272400	1.47075100
H	-2.94079300	-1.95077900	1.02564700
H	-4.37102700	1.52242500	0.69478800
H	-3.05606800	2.16350000	-0.30706900
H	-3.63034300	-1.87661200	-1.36299500
C	-1.55157800	0.33871800	0.54107800
C	-0.40807500	1.24545300	0.37841700
O	-0.74045500	2.42298300	0.41032600
N	-0.73440300	-1.27365800	1.46063100
N	-0.29156100	-1.94217500	2.21934300
C	0.96518700	0.76186900	0.15056800
C	2.02231500	1.56593900	0.60443500
C	1.21815400	-0.42904600	-0.54824000
C	3.33472400	1.16612000	0.39005900
H	1.81119300	2.48720100	1.13586300

C	2.52913500	-0.82709600	-0.78005200
H	0.40189100	-1.02625100	-0.94070800
C	3.56040200	-0.02601100	-0.29561600
H	4.16789600	1.75876000	0.74483700
H	2.75241300	-1.73484100	-1.32535000
N	4.95081100	-0.45675700	-0.52324500
O	5.85161100	0.26950800	-0.10670700
O	5.13182800	-1.51942700	-1.11583500

S3

C	-4.12208200	-1.85848000	0.42723200
C	-5.38395700	-0.99200700	0.43080000
C	-5.04545000	0.48689400	0.64199400
C	-4.06131600	1.00745800	-0.41999200
C	-2.84718100	0.09216900	-0.46650000
C	-3.11488900	-1.40583900	-0.64401100
H	-5.94724600	1.10611800	0.58325900
H	-5.91505200	-1.11424200	-0.52239900
H	-6.06018200	-1.33128800	1.22269400
H	-3.63837300	-1.82692700	1.41085800
H	-4.36731400	-2.90585100	0.21854900
H	-4.51272700	0.94718100	-1.41868200
H	-3.75245400	2.03614500	-0.23301600
H	-3.54336400	-1.50352800	-1.64952800
H	-2.18984300	-1.98398000	-0.60442200
H	-4.61136400	0.63750000	1.63770300
C	-1.62868300	0.48135200	-0.31188600
C	-0.42594800	1.20474300	-0.12077600
O	-0.87258600	2.35847100	-0.01997100
C	0.93771300	0.72295200	-0.05964300
C	1.97801000	1.65106000	0.11252700
C	1.19599700	-0.65166300	-0.17595600
C	3.28880700	1.20001600	0.16576700
H	1.75359700	2.70866000	0.19874000
C	2.50607900	-1.10768600	-0.12328100
H	0.38312400	-1.35960100	-0.30705900
C	3.52274500	-0.16994000	0.04510600
H	4.11644700	1.88508000	0.29479700
H	2.74140700	-2.16006400	-0.21066300
N	4.91697100	-0.65156400	0.09650400
O	5.80468200	0.18452900	0.24999000
O	5.10858800	-1.86055200	-0.01810000

TS-S4

C	-4.34610900	-1.80210100	0.55129200
C	-5.23196700	-0.55478800	0.50791600
C	-4.42815300	0.74255100	0.63819200
C	-3.42286800	0.94833600	-0.49160500
C	-2.50982800	-0.53706700	-0.50173700
C	-3.27059600	-1.78464700	-0.56003800
H	-5.09704600	1.61023100	0.59538100
H	-5.79867600	-0.53616400	-0.43213900
H	-5.96302600	-0.60151300	1.32134400
H	-3.84708900	-1.87820000	1.52370800
H	-4.94397000	-2.70717300	0.41295000
H	-3.81693500	0.90095500	-1.50889100
H	-2.90500300	1.91364500	-0.38477600

H	-3.74115300	-1.84412700	-1.54958400
H	-2.56409400	-2.61444300	-0.46283600
H	-3.90141700	0.78692000	1.59792500
C	-1.65973900	0.35627100	-0.36293400
C	-0.56553400	1.33245400	-0.19779800
O	-0.83332800	2.52178300	-0.13704100
C	0.79905200	0.76986600	-0.11196600
C	1.85913000	1.66584100	0.10170500
C	1.04279500	-0.60552000	-0.24238200
C	3.16001400	1.19073400	0.18554700
H	1.65244400	2.72513100	0.20008700
C	2.34253300	-1.09003700	-0.16012100
H	0.23006100	-1.30320600	-0.41188200
C	3.37523100	-0.18048400	0.05181000
H	3.99428600	1.86027200	0.34974900
H	2.55636800	-2.14622100	-0.25812900
N	4.75441600	-0.69011000	0.13643300
O	5.65614700	0.12461200	0.32577400
O	4.92725200	-1.90186900	0.01186200

S5

C	4.17716900	-1.00705200	0.32469300
C	4.29178400	0.50004700	0.59795500
C	3.08383400	1.08788200	-0.15743900
C	2.03986100	0.02065000	-0.06844100
C	2.65886600	-1.27332400	0.34648100
H	4.18811800	0.70455200	1.66940700
H	4.57473800	-1.24304800	-0.66871100
H	4.70810900	-1.61972800	1.05658500
H	2.74170200	2.06815400	0.18860400
H	3.32504700	1.19194500	-1.22933300
H	2.30305600	-1.47844300	1.36980200
H	2.31346100	-2.10976200	-0.26378800
H	5.23426500	0.93317800	0.25632900
C	0.69667200	0.20828800	-0.30786800
C	-0.40547100	-0.83939700	-0.24239500
O	-0.07951700	-2.00140100	-0.40459900
N	0.34430800	1.45819300	-0.71186300
N	0.03770100	2.46524300	-1.08616600
C	-1.79534700	-0.40486000	0.00416500
C	-2.82949300	-1.19204800	-0.53083600
C	-2.10377700	0.71656400	0.79233800
C	-4.15541600	-0.84108800	-0.30519000
H	-2.57847100	-2.06163100	-1.12896300
C	-3.43462600	1.05093900	1.02919300
H	-1.31946900	1.30343500	1.26104400
C	-4.45865400	0.28013900	0.47404000
H	-4.95369700	-1.43978400	-0.73254000
H	-3.67194200	1.90826100	1.65110400
H	-5.49525800	0.54957800	0.65327400

TS-S6

C	-4.19970300	-0.86619700	0.69811600
C	-4.40109200	0.48920100	0.01170400
C	-2.99826600	1.12661300	0.03358500
C	-2.05347100	-0.05497600	-0.01421100
C	-2.84624800	-1.35598700	0.15236800

H	-4.72381000	0.34507700	-1.02519700
H	-4.13654300	-0.74022100	1.78461700
H	-4.99330500	-1.58636700	0.48154800
H	-2.80261900	1.82993900	-0.78042900
H	-2.81185200	1.65064400	0.98009400
H	-2.95041000	-1.77775400	-0.85573400
H	-2.32150700	-2.08827800	0.76795700
H	-5.13571900	1.12376900	0.51320000
C	-0.75316200	-0.09743800	-0.14767100
C	0.44152800	-0.93712900	-0.20890300
O	0.09724300	-2.09564200	-0.43664000
N	-0.18392200	1.78284900	-0.57087900
N	0.05584700	2.74807700	-1.04941800
C	1.80882100	-0.47114400	0.00921000
C	2.84803100	-1.19697400	-0.59963200
C	2.10025400	0.61702600	0.85009800
C	4.16729100	-0.81382500	-0.39187900
H	2.60637400	-2.03924700	-1.23962400
C	3.42531300	0.98114000	1.06618100
H	1.30415700	1.14370000	1.36597300
C	4.45535400	0.27435400	0.43891100
H	4.97201600	-1.36010100	-0.87333600
H	3.65617300	1.81076400	1.72654000
H	5.48771200	0.56875200	0.60233100

TS-S7

C	3.55960900	0.06441800	0.21076000
C	3.23283000	-1.19903400	-0.58935300
C	1.81642900	-1.87829600	-0.18997800
C	1.08162100	-0.68326100	-0.00880500
C	2.52862100	1.18120300	-0.00155000
H	3.18335700	-0.98393800	-1.65940600
H	3.61443500	-0.18016900	1.27770000
H	4.54895600	0.42331300	-0.09206400
H	1.48607900	-2.49282500	-1.03235300
H	1.89543100	-2.47587500	0.72280700
H	2.61705600	1.64327500	-0.99136700
H	2.61537600	1.97113100	0.75153000
H	3.96479300	-1.99246100	-0.41389100
C	1.10816100	0.60368400	0.09633900
C	-0.14667700	1.42349600	0.19039800
O	-0.12911800	2.63646900	0.14460700
C	-1.36638700	0.57286500	0.21083900
C	-1.27638200	-0.74826000	0.69198100
C	-2.54381800	1.02655200	-0.38405700
C	-2.33774300	-1.63769400	0.49271300
H	-0.48383500	-1.03909800	1.38323700
C	-3.60653000	0.13867700	-0.56064600
H	-2.59791600	2.04397200	-0.75677500
C	-3.49903800	-1.19132700	-0.13860800
H	-2.27400200	-2.65048900	0.87663000
H	-4.51140300	0.47742900	-1.05539800
H	-4.32956500	-1.87415500	-0.28769500

S8

C	3.40819500	-0.04180300	0.12014700
C	2.90551800	-1.37073100	-0.46229800

C	1.52935800	-1.75792200	0.10984600
C	0.62857300	-0.57419300	0.16745300
C	2.45623500	1.11670800	-0.22199500
H	3.61998100	-2.17448400	-0.25778300
H	3.48776200	-0.13273900	1.21158100
H	4.41127800	0.18082000	-0.25776600
H	1.06591200	-2.55712200	-0.48267700
H	1.62813500	-2.16344200	1.12932900
H	2.57864500	1.41642900	-1.27228600
H	2.68274000	2.00705400	0.37628800
C	1.03326800	0.70824700	0.00611500
C	-0.11113300	1.62811800	0.10647300
O	-0.13146500	2.84717500	0.05110100
C	-1.32349100	0.73611400	0.21946400
C	-2.61589900	1.00872100	-0.12674700
C	-0.86334300	-0.62878500	0.52001900
C	-3.48623100	-0.08849700	-0.32434700
H	-2.94372400	2.01978100	-0.34476100
C	-1.77166100	-1.72118100	0.13970000
H	-0.91816500	-0.73052200	1.63567900
C	-3.06595600	-1.43135900	-0.22298500
H	-4.51272300	0.10996800	-0.62022200
H	-1.44151700	-2.74687400	0.27388400
H	-3.77250400	-2.22639000	-0.43198000
H	2.82531000	-1.28048400	-1.55316000

TS-S9

C	-3.57403100	-0.04337900	-0.57560300
C	-3.15458100	-1.07895400	0.49177200
C	-1.24332800	-1.99927800	0.80334500
C	-1.51634800	-0.73137100	0.39677500
C	-2.62539000	1.15600300	-0.44577000
H	-3.43204900	-0.83180100	1.51843500
H	-3.48233200	-0.49467700	-1.56650400
H	-4.62742100	0.19759100	-0.39560800
H	-1.39614400	-2.30006100	1.84068000
H	-0.98579800	-2.77872700	0.08446900
H	-2.93169300	1.84828100	0.34778700
H	-2.53947500	1.73415500	-1.36975700
H	-3.48199000	-2.09086400	0.24115800
C	-1.32198900	0.49648400	-0.06984500
C	-0.01663200	1.23345100	-0.01432900
O	-0.06346600	2.45046000	0.11391900
C	1.25841700	0.47894100	-0.07689300
C	2.39071700	1.03605700	0.53836600
C	1.36573800	-0.74814600	-0.75103700
C	3.60567400	0.35887600	0.50695900
H	2.29871800	1.99078200	1.04569400
C	2.58843700	-1.41583100	-0.79209600
H	0.51207600	-1.15745500	-1.28130800
C	3.70511400	-0.86865200	-0.15562700
H	4.47623800	0.78603800	0.99543900
H	2.67183600	-2.35756400	-1.32609300
H	4.65497800	-1.39458300	-0.18184800

S10

C	-3.35735800	-0.93524500	0.06646300
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C	-3.54709600	0.21162700	-0.95051500
C	-2.10855200	0.65339500	-1.30043100
C	-1.30632900	0.28959900	-0.11608600
C	-2.01295700	-0.62757900	0.70207400
H	-4.15758400	-0.99390600	0.80779400
H	-3.29874500	-1.90620200	-0.44026800
C	-0.01296400	0.95788100	0.22493400
O	-0.23446900	2.07587700	0.68567800
C	-1.48461400	-1.11341800	1.86009000
H	-0.50892500	-0.79822900	2.21862500
H	-2.03106200	-1.82567500	2.47263400
C	1.28963400	0.33814100	0.02207600
C	2.44646800	1.08982000	0.29878700
C	1.39717100	-0.98257600	-0.44988200
C	3.69759300	0.52076000	0.10381500
H	2.34455100	2.10817600	0.65894100
C	2.65501500	-1.54455300	-0.64294600
H	0.50537700	-1.56550100	-0.65905300
C	3.80144900	-0.79444900	-0.36648300
H	4.59423900	1.09489700	0.31469500
H	2.74357500	-2.56324300	-1.00643100
H	4.78230600	-1.23511500	-0.51849900
H	-4.10838800	-0.09422200	-1.83479700
H	-4.07174500	1.04951200	-0.48147300
H	-1.68923500	0.04527800	-2.12676400
H	-1.97337500	1.69678400	-1.60220800