

Supporting Information

Computational Insights into Different Regioselectivities in Ir-Porphyrin-Catalyzed C–H Insertion Reaction of Quinoid Carbene

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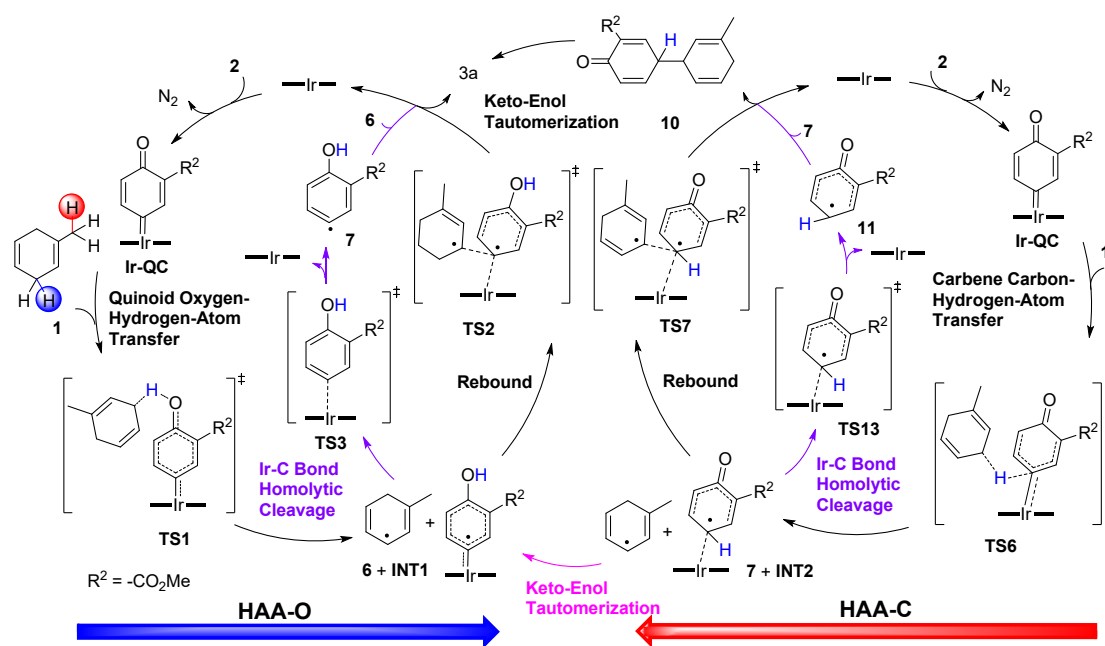
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Table of Contents

Proposed catalytic cycle for Ir-porphyrin-catalyzed C–H insertion reaction	2
Gibbs free energy profiles for HAA-O and HAA-C catalytic cycles of insertion reaction of Ir-QC to 1-methyl-1,3-cyclohexadiene 1 (M06)	2
Gibbs free energy profiles for HAA-O and HAA-C catalytic cycles of insertion reaction of Ir-QC to 1-methylcyclohexene 4 (M06).....	4
Gibbs free energy profiles for HAA-O and HAA-C catalytic cycles of insertion reaction of Ir-QC to 1-methyl-1,3-cyclohexadiene 1 (MN15)	6
Gibbs free energy profiles for HAA-O and HAA-C catalytic cycle of insertion reaction of Ir-QC to 1-methylcyclohexene 4 (MN15).....	8
Rebound transition states	10
Gibbs free energy profiles for HAA-O and HAA-C catalytic cycle of insertion reaction of Ir-QC to 1-methyl-1,3-cyclohexadiene 1 (B3LYP-D3).....	10
Different conformers for the hydrogen-atom abstraction by quinoid oxygen of the ^{OSS} Ir-QC (with substrate 1).....	11
Different conformers for the hydrogen-atom abstraction by carbene carbon of the ^{OSS} Ir-QC (with substrate 1).....	11
Localized molecular orbitals (LMOs) analysis	12
Energies and free energies of calculated structures	12
Cartesian coordinates of the structures	14



Scheme S1. Proposed catalytic cycle for Ir-porphyrin-catalyzed C–H insertion reaction of QC.

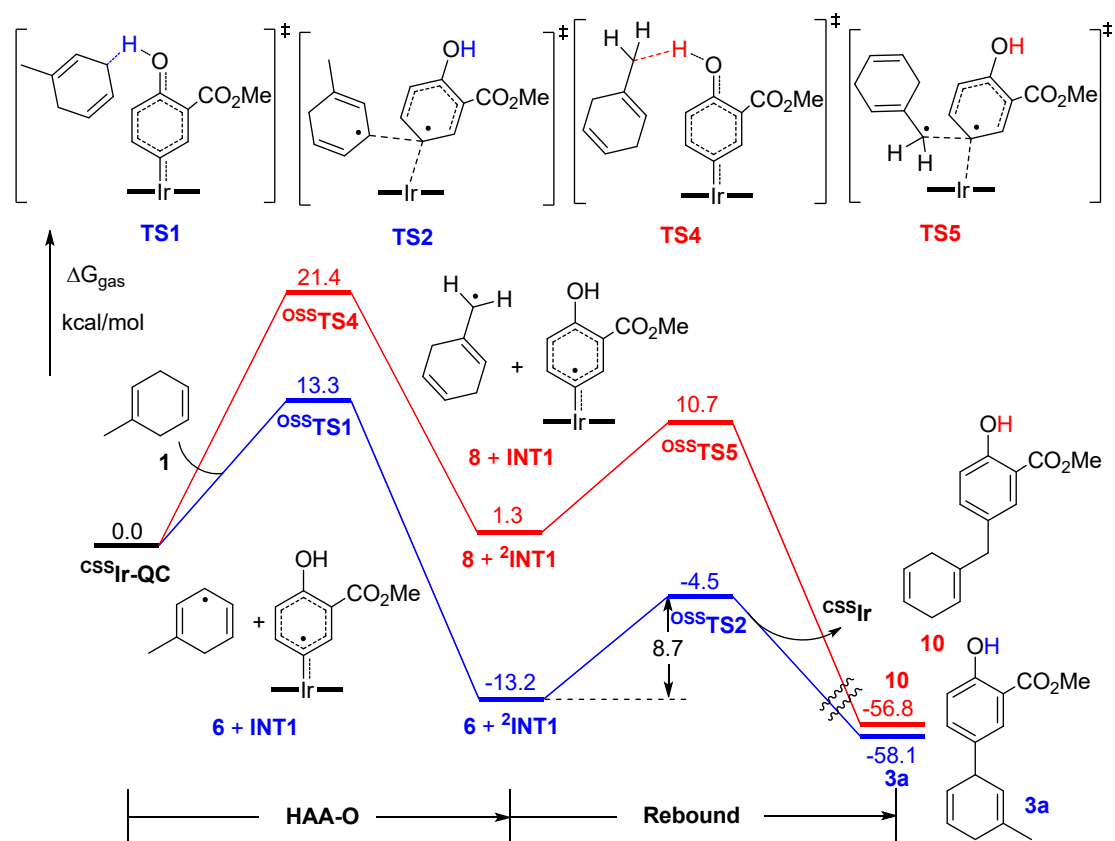


Figure S1. Gibbs free energy profiles for HAA-O catalytic cycle of insertion reaction of CSSIr-QC to **1**. CSS is closed-shell singlet and OSS is open-shell singlet. Gibbs free energy obtained at the (U)M06/6-311+G(d,p)-SDD/(U)M06/6-31G(d)-LANL2DZ level.

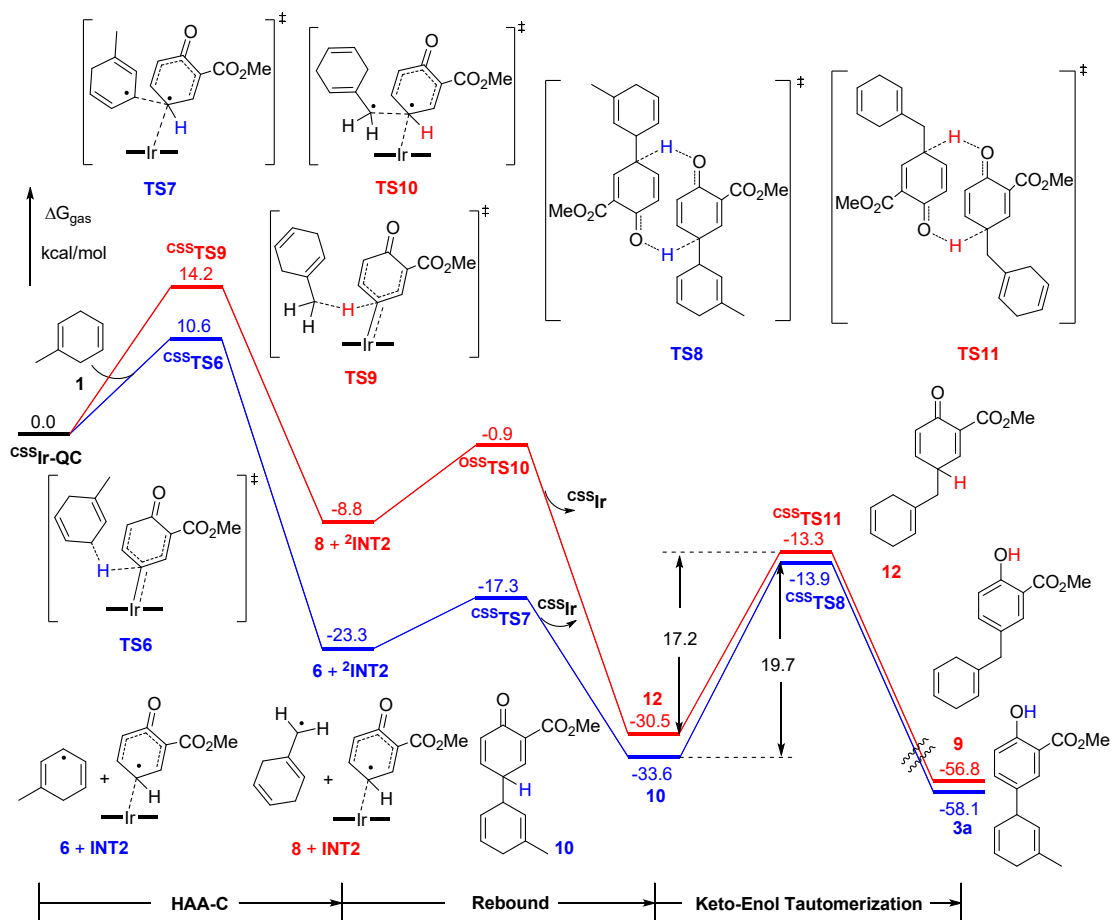


Figure S2. Gibbs free energy profiles for HAA-C catalytic cycle of insertion reaction of CSSIr-QC to **1**. The free energy of CSSTS8 is given with respect to **10**, and CSSTS11 is given with respect to **12**. Gibbs free energy obtained at the (U)M06/6-311+G(d,p)-SDD/(U)M06/6-31G(d)-LANL2DZ level.

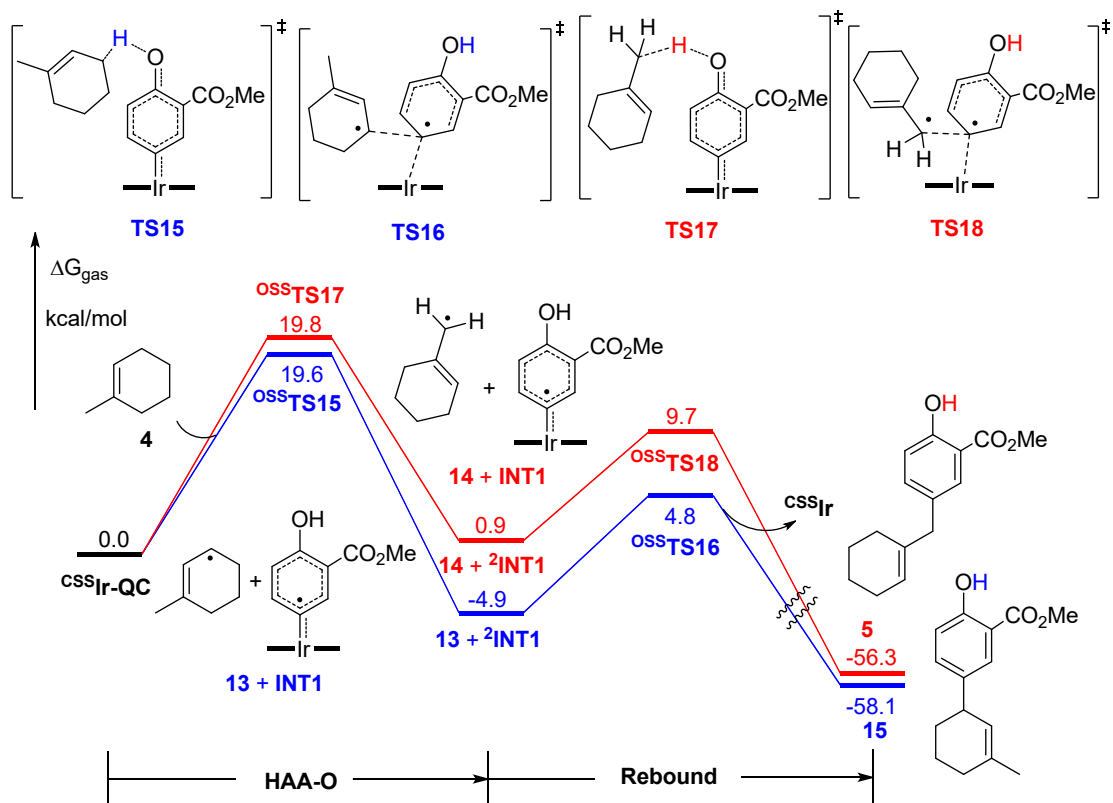


Figure S3. Gibbs free energy profiles for HAA-O catalytic cycle of insertion reaction of $^{CSS}Ir-QC$ to **4**. Gibbs free energy obtained at the (U)M06/6-311+G(d,p)-SDD// (U)M06/6-31G(d)-LANL2DZ level.

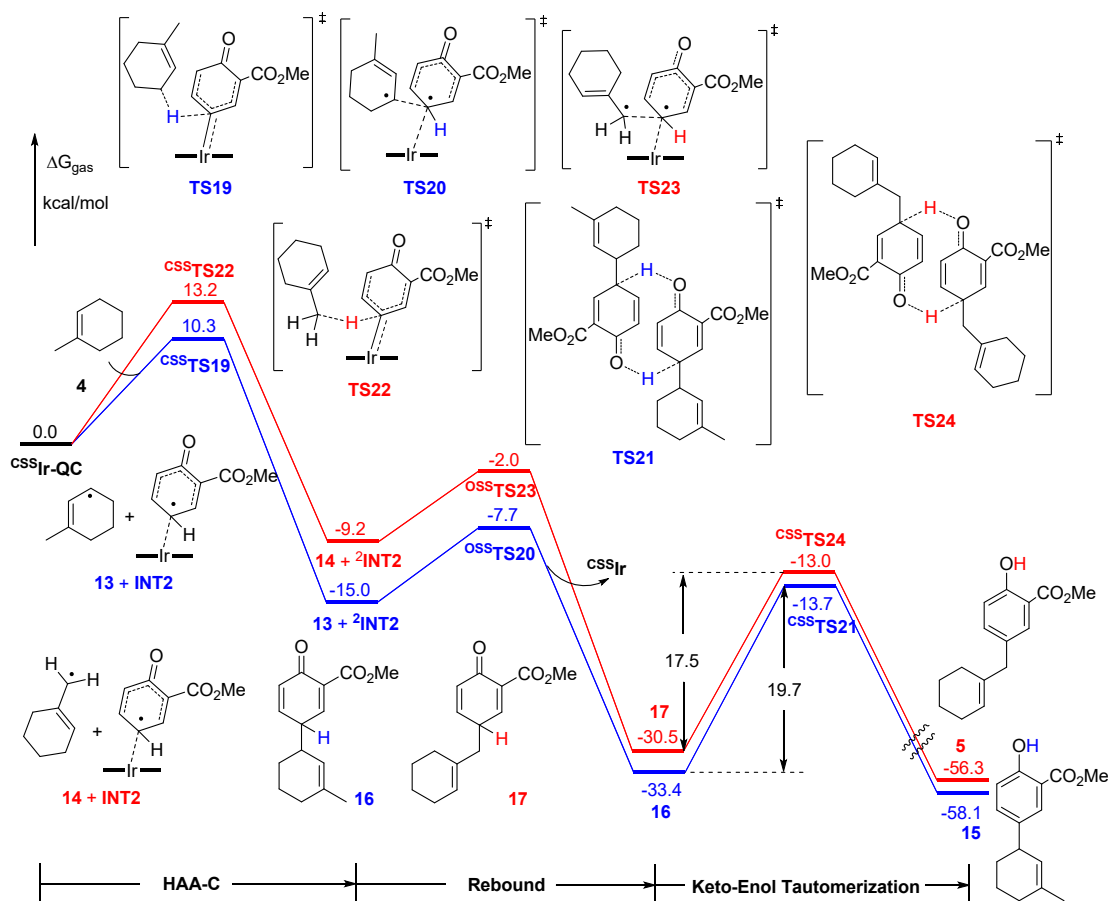


Figure S4. Gibbs free energy profiles for HAA-C catalytic cycle of insertion reaction of CSSIr-QC to **4**. The free energy of $\text{CSS}^{\ddagger}\text{TS21}$ is given with respect to **16** and $\text{CSS}^{\ddagger}\text{TS24}$ is given with respect to **17**. Gibbs free energy obtained at the (U)M06/6-311+G(d,p)-SDD/(U)M06/6-31G(d)-LANL2DZ level. $\text{OSS}^{\ddagger}\text{TS23}$ were subjected to a loose convergence threshold.

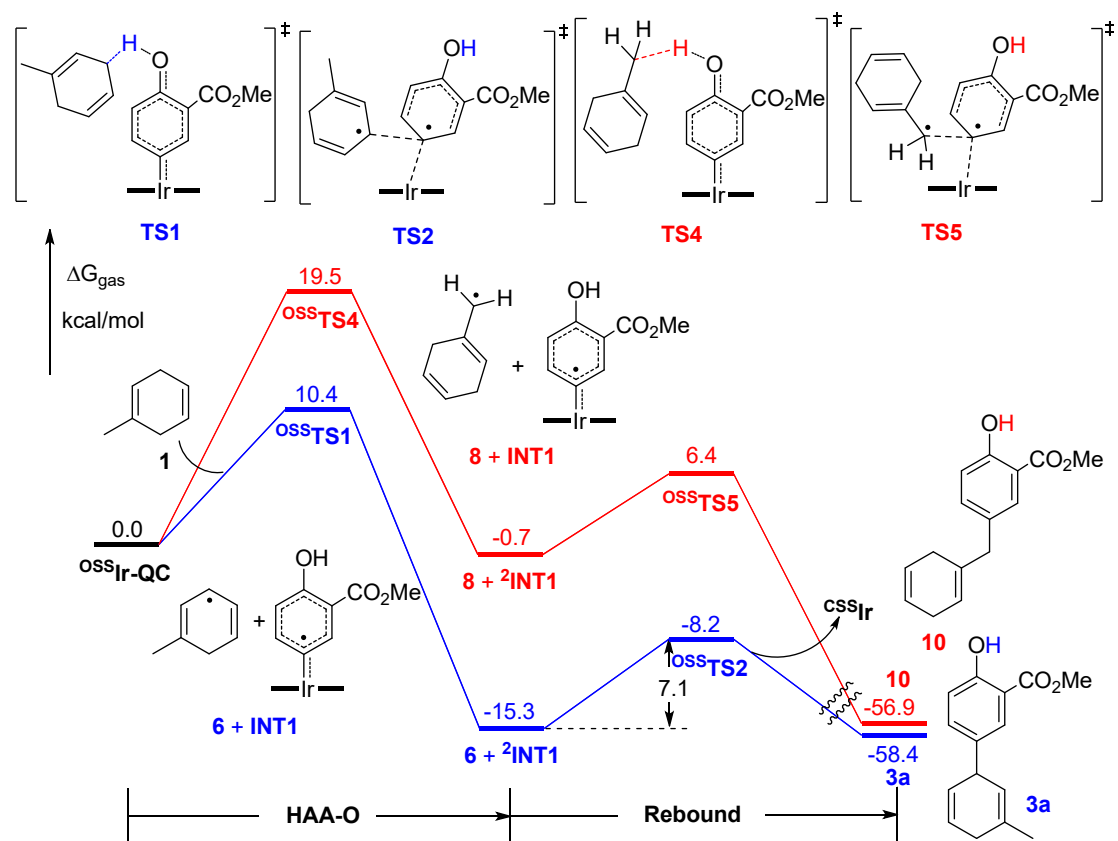


Figure S5. Gibbs free energy profiles for HAA-O catalytic cycle of insertion reaction of $^{OSS}Ir\text{-}QC$ to **1**. CSS is closed-shell singlet and OSS is open-shell singlet. Gibbs free energy obtained at the (U)MN15/6-311+G(d,p)-SDD//((U)MN15/6-31G(d)-LANL2DZ level.

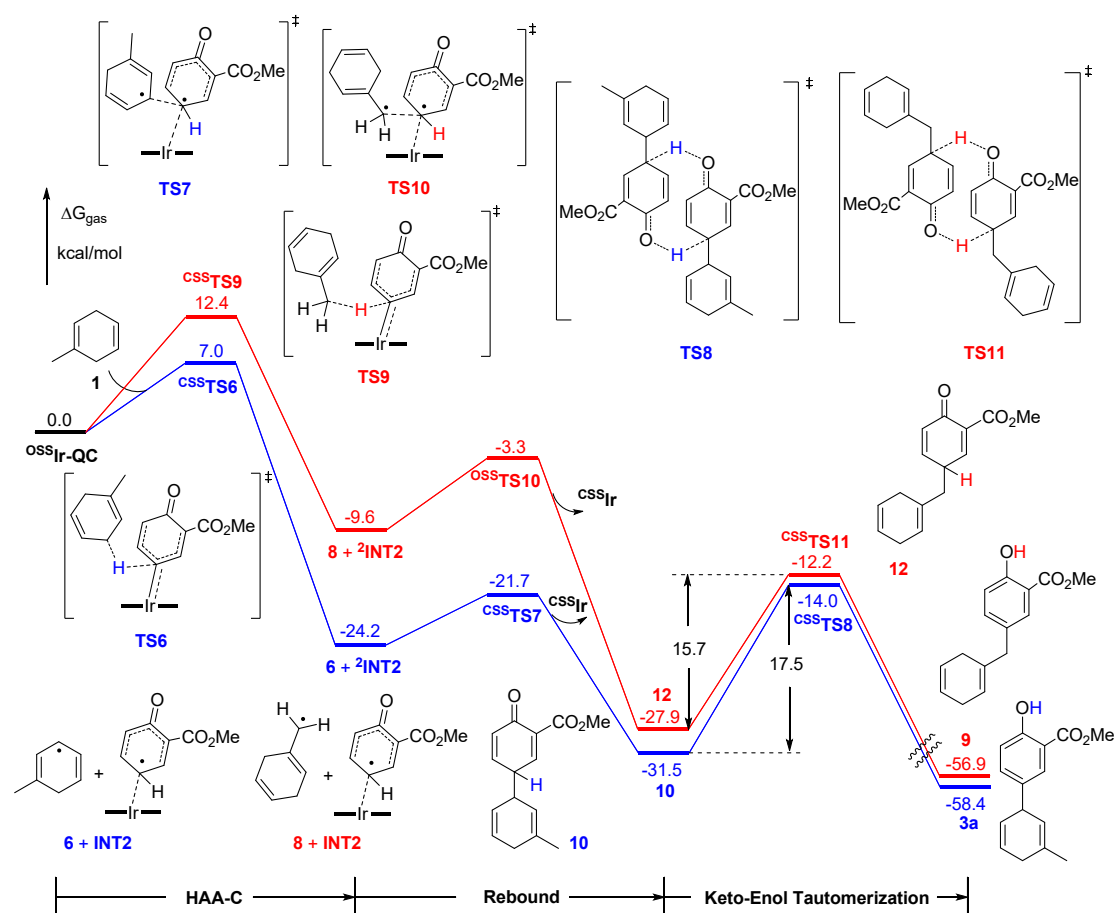


Figure S6. Gibbs free energy profiles for HAA-C catalytic cycle of insertion reaction of ${}^{\text{OSS}}\text{Ir-QC}$ to **1**. The free energy of ${}^{\text{CSS}}\text{TS8}$ is given with respect to **10**, and ${}^{\text{CSS}}\text{TS11}$ is given with respect to **12**. Gibbs free energy obtained at the (U)MN15/6-311+G(d,p)-SDD//((U)MN15/6-31G(d)-LANL2DZ level.

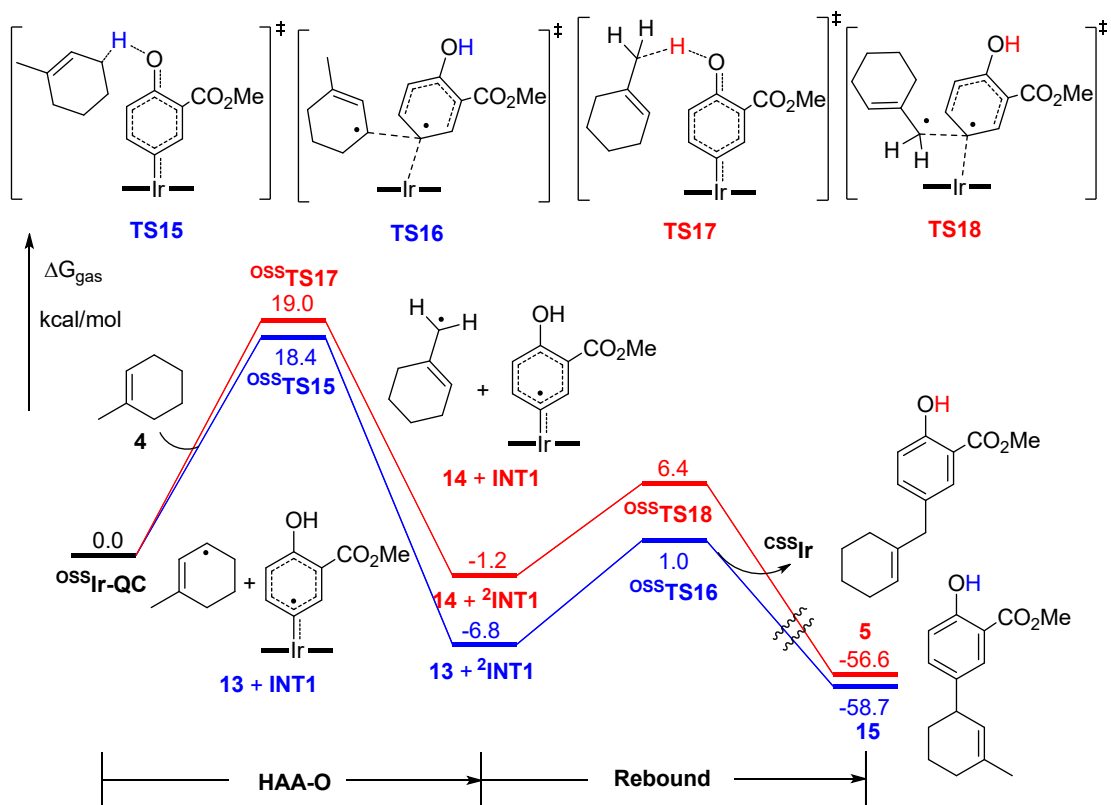


Figure S7. Gibbs free energy profiles for HAA-O catalytic cycle of insertion reaction of OSSIr-QC to **4**. Gibbs free energy obtained at the (U)MN15/6-311+G(d,p)-SDD/(U)MN15/6-31G(d)-LANL2DZ level.

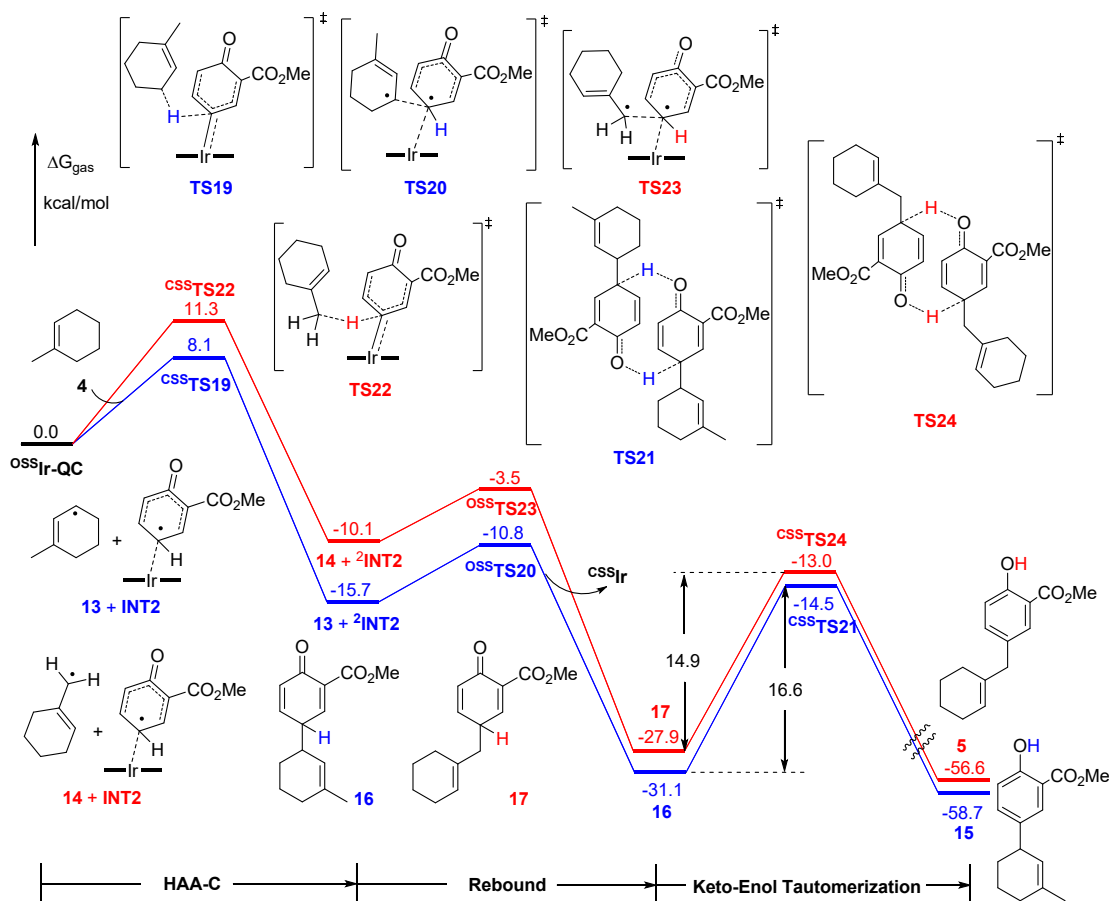


Figure S8. Gibbs free energy profiles for HAA-C catalytic cycle of insertion reaction of OSSIr-QC to **4**. The free energy of $\text{CSS}^{\dagger}\text{TS21}$ is given with respect to **16** and $\text{CSS}^{\dagger}\text{TS24}$ is given with respect to **17**. Gibbs free energy obtained at the (U)MN15/6-311+G(d,p)-SDD//((U)MN15/6-31G(d)-LANL2DZ level.

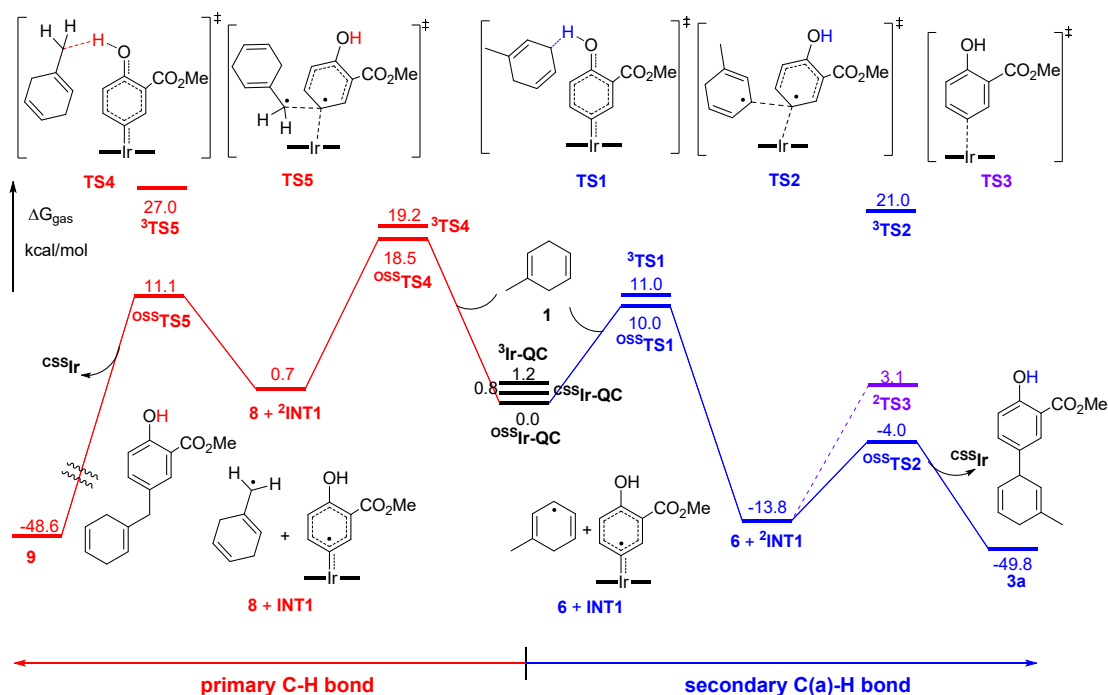


Figure S9. Gibbs free energy profiles for HAA-O catalytic cycle of insertion reaction of ^{OSS}Ir -QC to **1**. Gibbs free energy obtained at the (U)B3LYP-D3/6-311+G(d,p)-SDD// (U)B3LYP-D3/6-31G(d)-LANL2DZ level.

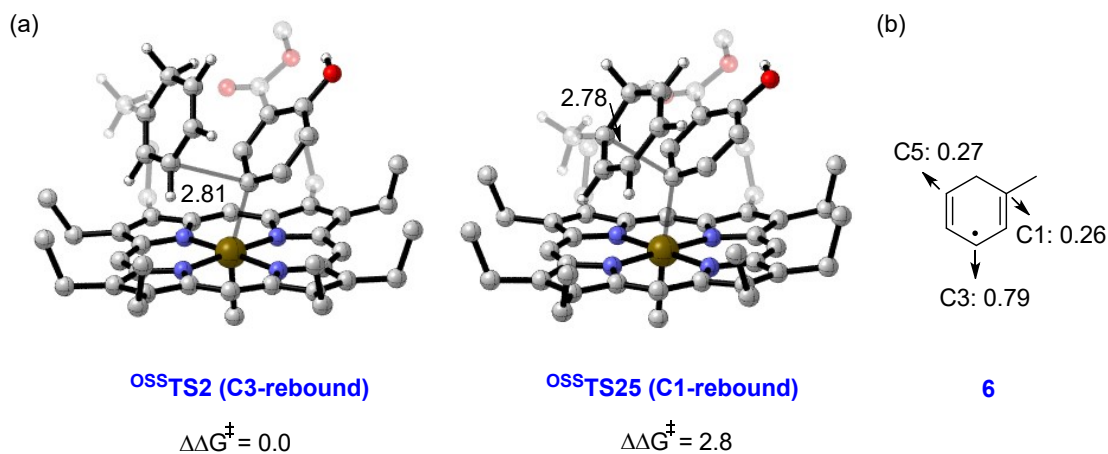


Figure S10. (a) Optimized geometries of transition states $^{OSS}TS2$ and $^{OSS}TS25$. (b) Populations of spin densities for radical intermediate **6**. Hydrogen atoms on the catalyst are omitted for clarity. The distances are in Å, and energies are shown in kcal mol⁻¹.

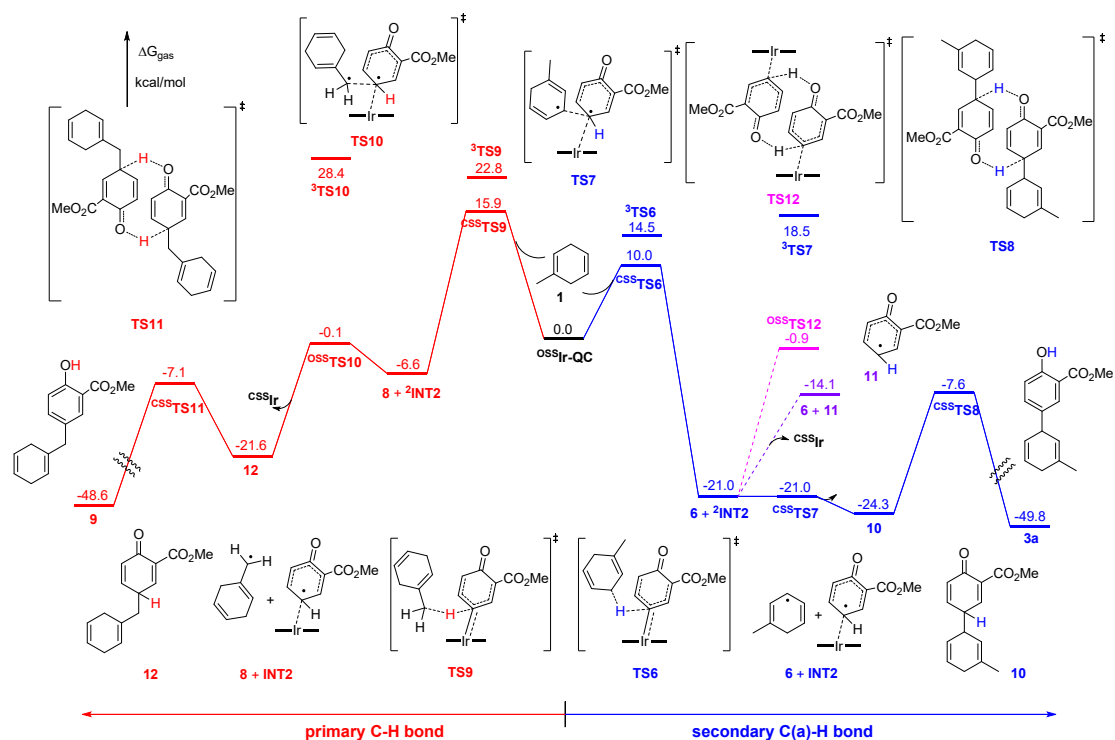


Figure S11. Gibbs free energy profiles for HAA-C catalytic cycle of insertion reaction of $^{OSS}Ir\text{-}QC$ to **1**. The free energy of $^{CSS}TS8$ is given with respect to **10**, and $^{CSS}TS11$ is given with respect to **12**. Gibbs free energy obtained at the (U)B3LYP-D3/6-311+G(d,p)-SDD//((U)B3LYP-D3/6-31G(d)-LANL2DZ level.

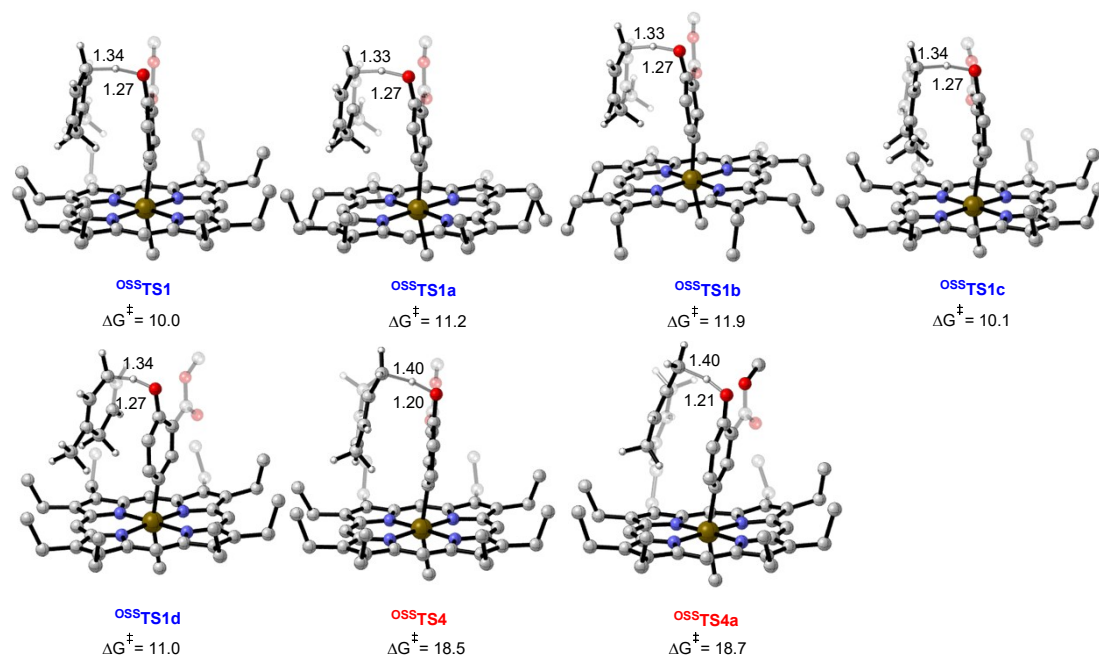


Figure S12. Different conformers for the hydrogen-atom abstraction by quinoid oxygen of the $^{OSS}Ir\text{-}QC$ (with substrate **1**). The distances are shown in Å. The energies are shown in kcal mol⁻¹. Gibbs free energy obtained at the (U)B3LYP-D3/6-311+G(d,p)-SDD//((U)B3LYP-D3/6-31G(d)-LANL2DZ level.

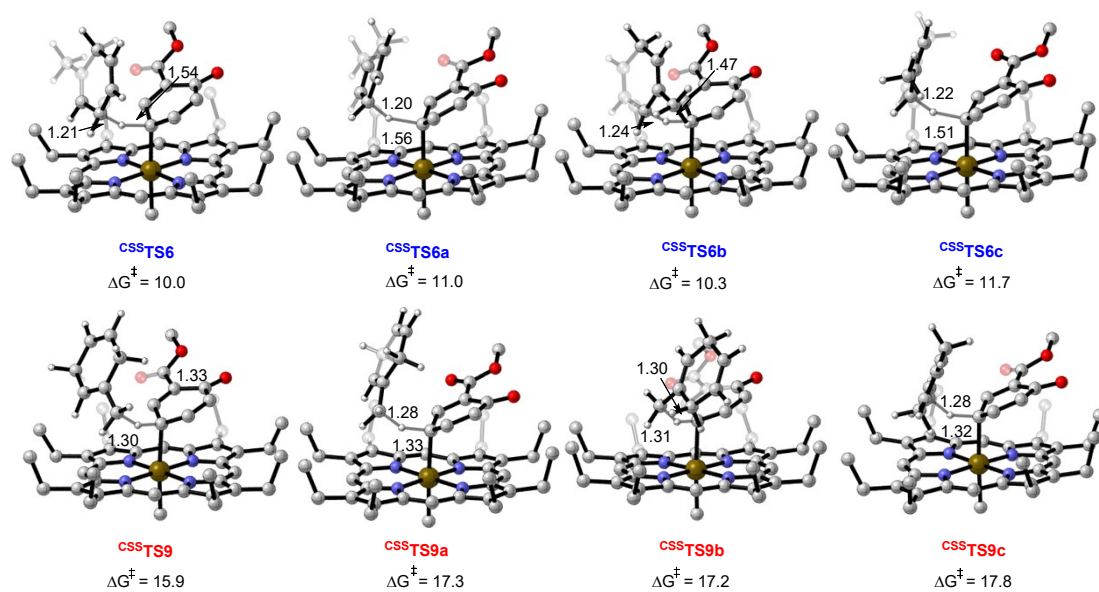


Figure S13. Different conformers for the hydrogen-atom abstraction by carbene carbon of the ^oSSIr-QC (with substrate **1**). The distances are shown in Å. The energies are shown in kcal mol⁻¹. Gibbs free energy obtained at the (U)B3LYP-D3/6-311+G(d,p)-SDD//((U)B3LYP-D3/6-31G(d)-LANL2DZ level.

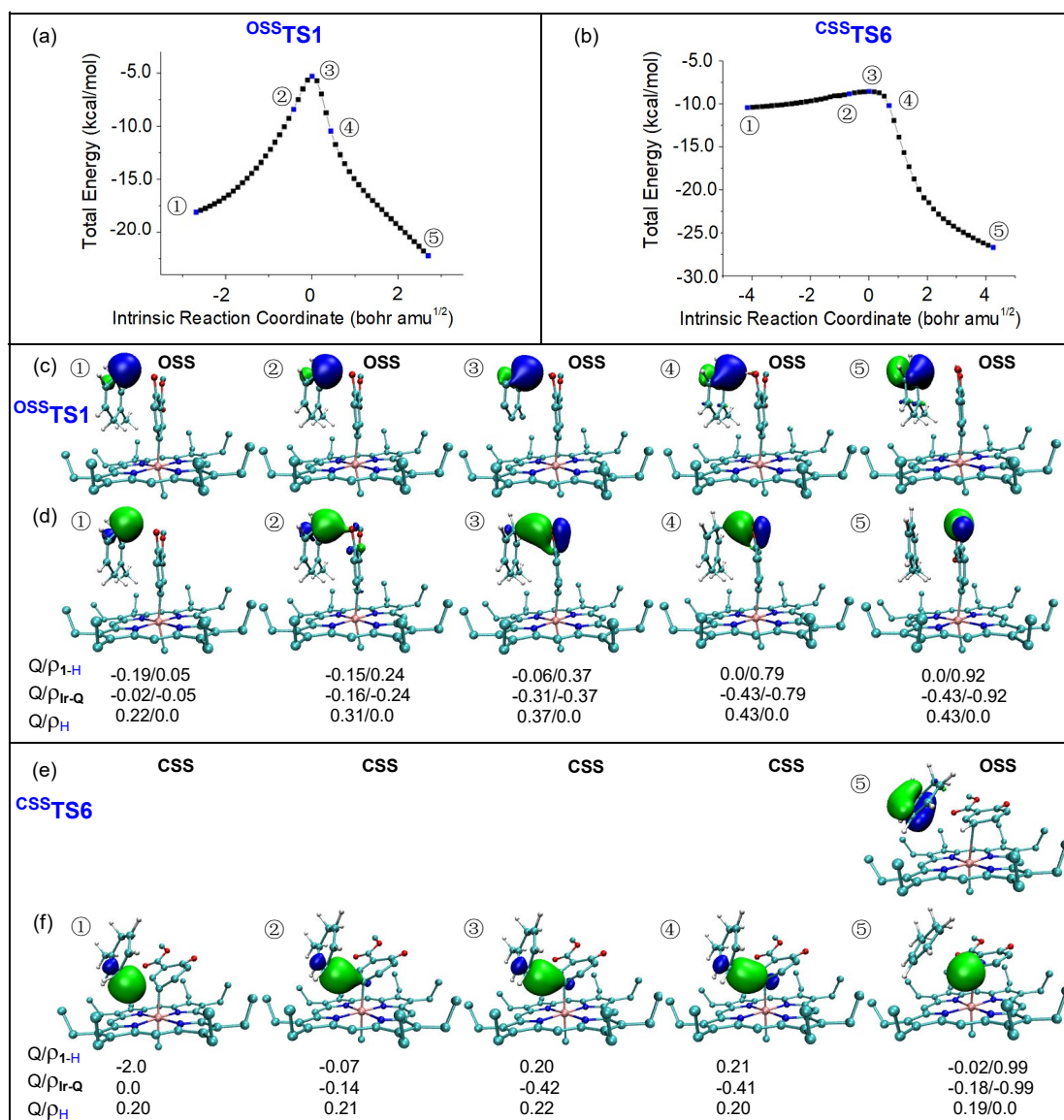


Figure S14. Plots of the change in electronic energies along the intrinsic reaction coordinate (IRC) for ^{oss}TSS1 (a) and ^{css}TSS6 (b). (c) α-LMOs and (d) β-LMO analysis along the IRC between quinoid oxygen of the Ir-QC and **1**, and the Mulliken charges (Q) and spin densities (ρ) on the hydrogen-atom abstracted moieties (1-H) and on the Ir-QC. (e) α-LMOs and (f) LMO analysis along the IRC between carbene carbon of the Ir-QC and **1**, and the Mulliken charges (Q) and spin densities (ρ) on the hydrogen-atom abstracted moieties (1-H) and on the Ir-QC.

Table S1. Electronic Energies and Free Energies (in Hartree) of the Structures Calculated at the (U)B3LYP-D3/6-311+G(d,p)-SDD//(U)B3LYP-D3/6-31G(d)-LANL2DZ Level of Theory

Structures	ZPVE	TCE	TCH	TCG	E _{gas}	G _{gas} (E _{gas} +TCG)	Imaginary Frequenc y	ΔG _{gas} (kcal/mol)
^{oss} Ir-QC	0.89475	0.948951	0.949896	0.818098	-2296.593992	-2295.775894	—	—
^{css} Ir-QC	0.895536	0.949566	0.950510	0.819079	-2296.593686	-2295.774607	—	—

³ Ir-QC	0.893948	0.948393	0.949337	0.81601	-2296.590055	-2295.774045	—	—
1	0.150651	0.157387	0.158331	0.120221	-272.823116	-272.702895	—	—
osSTS1	1.041722	1.103034	1.103978	0.959249	-2569.422176	-2568.462927	1713.04i	10.0
³ TS1	1.041242	1.102879	1.103824	0.95745	-2569.4187	-2568.46125	1651.76i	11.0
6	0.137144	0.143721	0.144666	0.10635	-272.196611	-272.090261	—	—
² INT1	0.90738	0.961729	0.962673	0.829899	-2297.24035	-2296.410451	—	—
osSTS2	1.047302	1.108757	1.109701	0.964309	-2569.449403	-2568.485094	158.11i	-4.0
³ TS2	1.046964	1.107977	1.108921	0.963571	-2569.408883	-2568.445312	482.38i	21.0
3a	0.280012	0.2967	0.297644	0.237568	-807.149171	-806.911603	—	—
cssIr	0.769757	0.812275	0.813219	0.703127	-1762.349742	-1761.646615	—	—
² TS3	0.907473	0.96106	0.962004	0.830493	-2297.214069	-2296.383576	29.05i	3.1
osSTS4	1.041845	1.103001	1.103945	0.959576	-2569.408918	-2568.449342	1825.03i	18.5
³ TS4	1.041681	1.102909	1.103854	0.958244	-2569.406451	-2568.448207	1868.79i	19.2
8	0.136912	0.14344	0.144385	0.10617	-272.173432	-272.067262	—	—
osSTS5	1.047258	1.108507	1.109451	0.964602	-2569.425627	-2568.461025	218.85i	11.1
³ TS5	1.047125	1.107931	1.108875	0.963937	-2569.399768	-2568.435831	452.51i	27.0
9	0.280628	0.297079	0.298023	0.238337	-807.147976	-806.909639	—	—
cssTS6	1.044781	1.106056	1.107000	0.962122	-2569.424986	-2568.462864	265.08i	10.0
³ TS6	1.042446	1.103865	1.104809	0.958396	-2569.414041	-2568.455645	1186.91i	14.5
² INT2	0.907099	0.961535	0.962479	0.829209	-2297.251192	-2296.421983	—	—
cssTS7	1.048843	1.11005	1.110995	0.965949	-2569.478221	-2568.512272	26.81i	-21.0
³ TS7	1.04638	1.107227	1.108171	0.962749	-2569.412132	-2568.449383	707.08i	18.5
10	0.279018	0.295851	0.296795	0.236599	-807.107428	-806.870829	—	—
11	0.135003	0.144756	0.145700	0.099430	-534.863879	-534.764449	—	—
cssTS8	0.553821	0.588167	0.589112	0.495167	-1614.210201	-1613.715034	1167.81i	-7.6
cssTS9	1.044015	1.10501	1.105954	0.961606	-2569.415028	-2568.453422	781.7i	15.9
³ TS9	1.042675	1.103875	1.10482	0.958727	-2569.401113	-2568.442386	1547.82i	22.8
osSTS10	1.046782	1.108486	1.10943	0.96353	-2569.44246	-2568.47893	132.26i	-0.1
³ TS10	1.04582	1.107043	1.107987	0.961398	-2569.39497	-2568.433572	884.94i	28.4
12	0.279545	0.296364	0.297308	0.236849	-807.103384	-806.866535	—	—
cssTS11	0.555525	0.589419	0.590363	0.496824	-1614.206863	-1613.710039	1316.41i	-7.1
osSTS12	1.812411	1.921867	1.922811	1.689328	-4594.501271	-4592.811943	1458.61i	-0.9
osSTS14	1.041421	1.10288	1.103824	0.958824	-2569.419301	-2568.460477	-1770.65i	11.5
4	0.175197	0.182162	0.183106	0.144637	-274.055283	-273.910646	—	—
osSTS15	1.065891	1.127684	1.128628	0.982986	-2570.642842	-2569.659856	1900.33i	16.7
13	0.161184	0.168234	0.169179	0.129842	-273.414207	-273.284365	—	—
osSTS16	1.07071	1.132822	1.133766	0.987086	-2570.66628	-2569.679194	112.98	4.6
15	0.304613	0.321449	0.322393	0.262104	-808.381588	-808.119484	—	—

^{oss} TS17	1.066604	1.128011	1.128955	0.983978	-2570.642371	-2569.658393	1830.52i	17.7
14	0.161559	0.168254	0.169198	0.130676	-273.406300	-273.275624	—	—
^{oss} TS18	1.071484	1.133095	1.134039	0.988482	-2570.657453	-2569.668971	171.23i	11.0
5	0.305114	0.321801	0.322745	0.262777	-808.379861	-808.117084	—	—
^{css} TS19	1.068491	1.129916	1.13086	0.985775	-2570.655697	-2569.669922	585.54i	10.4
^{oss} TS20	1.067029	1.128644	1.129588	0.982663	-2570.640904	-2569.658241	13.28i	-8.6
16	0.161184	0.168234	0.169179	0.129842	-273.414207	-273.284365	—	—
^{css} TS21	0.907099	0.961535	0.962479	0.829209	-2297.251192	-2296.421983	1222.13i	-8.2
^{css} TS22	1.068562	1.129811	1.130755	0.985991	-2570.649675	-2569.663684	712.49i	14.3
^{oss} TS23	0.161559	0.168254	0.169198	0.130676	-273.406300	-273.275624	38.31i	-1.9
17	0.907099	0.961535	0.962479	0.829209	-2297.251192	-2296.421983	—	—
^{css} TS24	1.071228	1.133125	1.134069	0.987891	-2570.67748	-2569.689589	1283.35i	-6.6
^{oss} TS25	1.047096	1.108387	1.109331	0.964119	-2569.444793	-2568.480674	91.74i	-1.2

ZPVE = zero-point vibrational energy; TCE = thermal correction to energy; TCH = thermal correction to enthalpy; TCG = thermal correction to Gibbs free energy.

Cartesian coordinates of the structures

(U)B3LYP-D3/6-311+G(d,p)-SDD/(U)B3LYP-D3/6-31G(d)-LANL2DZ

^{oss}Ir-QC

N	1.03832900	-1.27039100	-1.34038900
N	0.80342400	1.62500800	-1.22442200
N	-1.99297000	1.39159500	-0.55234100
N	-1.80045600	-1.50363800	-0.63772700
C	0.94137900	-2.63670500	-1.28347600
C	2.24439400	-3.22278000	-1.55527700
C	3.10873800	-2.18146400	-1.77802400
C	2.33075800	-0.96068000	-1.65139700
C	2.83223900	0.33711400	-1.75578000
C	2.14330300	1.52279900	-1.53648800
C	2.73811000	2.84720600	-1.55492500
C	1.73529100	3.73840000	-1.27504100
C	0.52526600	2.96144400	-1.07089200
C	-0.72470100	3.48152700	-0.75539000
C	-1.89233600	2.76268800	-0.52289300
C	-3.18676900	3.33839200	-0.21016200
C	-4.06343400	2.29399000	-0.05979300
C	-3.30947400	1.07430200	-0.27671300

C	-3.82824400	-0.21156500	-0.19946900
C	-3.13342900	-1.41127800	-0.35707200
C	-3.69741100	-2.74350200	-0.22187700
C	-2.67099000	-3.62812600	-0.43642100
C	-1.48245400	-2.83516700	-0.70656900
C	-0.22170500	-3.34843800	-1.00319700
H	-0.79759300	4.56082300	-0.68669500
H	3.88854900	0.42841000	-1.97876200
H	-0.13605300	-4.42917800	-1.01692600
H	-4.88651400	-0.29212900	0.02167600
C	-0.95227300	-0.25099000	-2.99742900
H	-0.18801000	0.27183100	-3.57941000
H	-0.95054600	-1.31707500	-3.22738600
H	-1.94643200	0.17711900	-3.15904300
Ir	-0.48138600	0.08139700	-0.89130300
C	4.20646100	3.11264200	-1.71355800
C	4.96963200	2.91168000	-0.38686500
H	4.36265900	4.13598900	-2.07493700
H	4.62772300	2.45311300	-2.48324600
H	6.04862700	3.03762000	-0.53422900
H	4.63920700	3.64514600	0.35718900
H	4.78585900	1.91873500	0.03676300
C	1.83085400	5.22693500	-1.10669800
C	1.87615300	5.65574600	0.37343000
H	0.97905500	5.71416600	-1.60013100
H	2.72788800	5.59579800	-1.61722600
H	1.93793400	6.74624000	0.46430100
H	0.98236300	5.31600800	0.90822100
H	2.74566900	5.21802900	0.87533200
C	-3.44407400	4.80565500	-0.02501900
C	-2.98160100	5.31741500	1.35367800
H	-4.51428000	5.00963500	-0.14551900
H	-2.93639600	5.37633100	-0.81377000
H	-3.17129200	6.39180300	1.45759400
H	-3.51214100	4.79483100	2.15723500
H	-1.90990300	5.14172600	1.49806400
C	-5.51174300	2.34317100	0.33280000
C	-5.72830600	2.05130800	1.83085000
H	-6.08685600	1.62383700	-0.26506800
H	-5.92350100	3.33065800	0.09458300
H	-6.79305500	2.08457600	2.08837600
H	-5.34098100	1.06159100	2.09729200
H	-5.20158300	2.78800000	2.44733200
C	-5.11891800	-3.03319800	0.16394300

C	-5.36572000	-2.86503800	1.67622000
H	-5.37987300	-4.05565400	-0.13278000
H	-5.79995900	-2.37423700	-0.39094300
H	-6.41062700	-3.07537300	1.93146800
H	-4.72714500	-3.54656800	2.24902000
H	-5.13244600	-1.84431100	1.99989000
C	-2.69629700	-5.12632000	-0.34526500
C	-2.13962700	-5.64581000	0.99508800
H	-2.11932700	-5.56194100	-1.17171400
H	-3.72423300	-5.48502900	-0.47295500
H	-2.16116000	-6.74096200	1.03202600
H	-1.10523600	-5.31674700	1.14389700
H	-2.73090800	-5.26131800	1.83351800
C	2.55075700	-4.69111900	-1.49446700
C	2.67397600	-5.21238400	-0.04882900
H	3.48487000	-4.89185100	-2.03175700
H	1.77076900	-5.25877800	-2.01967400
H	2.89189600	-6.28645700	-0.03577600
H	3.47749200	-4.69098500	0.48232300
H	1.74701100	-5.04254600	0.50995300
C	4.59637000	-2.22319500	-1.97073700
C	5.35209300	-2.04400400	-0.63698700
H	4.90639300	-1.44137000	-2.67606900
H	4.88570600	-3.17582600	-2.43043800
H	6.43519500	-2.00862400	-0.80302300
H	5.04593700	-1.12812200	-0.12047200
H	5.13769700	-2.88067000	0.03744700
C	0.08290200	-0.26182600	1.04694500
C	-0.84604300	-0.59280900	2.08158400
C	1.45885600	-0.22046500	1.40110300
C	-0.44606900	-0.59214000	3.38927700
H	-1.89297700	-0.74113900	1.83864500
C	1.91027500	-0.20536200	2.70169600
H	2.21103400	-0.11408000	0.63326700
C	0.94520300	-0.37408800	3.80717000
O	1.23683400	-0.34914000	5.01309100
H	-1.15725300	-0.71788900	4.20141600
C	3.38146800	-0.02714400	2.86438100
O	4.14335300	0.20666000	1.93364100
O	3.81583700	-0.16777200	4.12720200
C	5.23036000	-0.01710400	4.30420400
H	5.77623200	-0.76957000	3.72642400
H	5.55792400	0.97586500	3.98126400
H	5.40348300	-0.15133500	5.37251900

cssIr-QC

N	0.99836500	-1.34226200	-1.31342200
N	0.86521800	1.56378100	-1.24401400
N	-1.93845400	1.43971900	-0.57457400
N	-1.84645400	-1.46527100	-0.60938900
C	0.85175800	-2.70391600	-1.24205600
C	2.13300000	-3.33843900	-1.50884900
C	3.03373100	-2.33109100	-1.74340100
C	2.30011900	-1.08183700	-1.63030700
C	2.84739900	0.19596900	-1.74971700
C	2.20024700	1.40866800	-1.55098700
C	2.84196600	2.71074100	-1.58884500
C	1.87080900	3.64142700	-1.32614400
C	0.63363600	2.91120000	-1.11252800
C	-0.59776200	3.48013200	-0.80869200
C	-1.79065100	2.80615000	-0.56941800
C	-3.06636500	3.43145100	-0.27479800
C	-3.97906600	2.42044800	-0.11164400
C	-3.26582600	1.17196700	-0.30257800
C	-3.82893600	-0.09390900	-0.20460300
C	-3.17659100	-1.32004700	-0.33825900
C	-3.78891700	-2.62908100	-0.18844700
C	-2.79457400	-3.55324400	-0.38802000
C	-1.57680200	-2.80796100	-0.66321700
C	-0.33575800	-3.37047000	-0.95443400
H	-0.63298600	4.56229600	-0.75814700
H	3.90667300	0.24666400	-1.97135500
H	-0.28955400	-4.45365500	-0.95720500
H	-4.89064300	-0.13360200	0.01091300
C	-0.95933500	-0.26702300	-2.96233600
H	-0.19406700	0.23570000	-3.56202600
H	-0.97729000	-1.33361600	-3.19208200
H	-1.94761300	0.17207100	-3.13412700
Ir	-0.47028100	0.07056700	-0.87890900
C	4.31900800	2.92167800	-1.74837900
C	5.07192800	2.71908800	-0.41608800
H	4.51156200	3.93199700	-2.12839800
H	4.71856700	2.23359000	-2.50447900
H	6.15489500	2.80554500	-0.56279500
H	4.76508600	3.47708600	0.31337300
H	4.85338900	1.74090600	0.02497800
C	2.01853100	5.12826200	-1.18211300
C	2.07525600	5.57988300	0.29082600

H	1.18570800	5.63693000	-1.68616600
H	2.92929800	5.45662300	-1.69596600
H	2.17475500	6.66893100	0.36365100
H	1.16891700	5.28044200	0.82854300
H	2.92780300	5.12076400	0.80261500
C	-3.27405500	4.90964100	-0.11656000
C	-2.80349800	5.42831100	1.25679200
H	-4.33574400	5.14824800	-0.24832000
H	-2.74166100	5.44890400	-0.91106100
H	-2.95708100	6.51009900	1.34173700
H	-3.35687700	4.93740000	2.06489800
H	-1.73941700	5.21861200	1.41173000
C	-5.42712900	2.52612300	0.27063500
C	-5.66258100	2.26974800	1.77235700
H	-6.02293300	1.81585100	-0.31771100
H	-5.80343700	3.52246700	0.01156300
H	-6.72717200	2.34375000	2.02192000
H	-5.31070700	1.27264500	2.05963100
H	-5.11509900	2.99955200	2.37888100
C	-5.22176000	-2.86200300	0.19391400
C	-5.46990400	-2.66270100	1.70219700
H	-5.51782200	-3.87867900	-0.08933600
H	-5.87588900	-2.18732300	-0.37426700
H	-6.52305500	-2.83124400	1.95451100
H	-4.85960000	-3.35838800	2.28869000
H	-5.20151200	-1.64637000	2.01221500
C	-2.87518700	-5.04826300	-0.27913800
C	-2.33997900	-5.57126000	1.06852400
H	-2.31339200	-5.51469700	-1.09917900
H	-3.91544600	-5.37032600	-0.40442100
H	-2.40289500	-6.66423700	1.11944700
H	-1.29403700	-5.27958500	1.21458300
H	-2.91728400	-5.15385500	1.90093900
C	2.38680400	-4.81609300	-1.43368100
C	2.49322100	-5.32724500	0.01687300
H	3.31241800	-5.05529500	-1.96988500
H	1.58631400	-5.36046400	-1.95259600
H	2.67235900	-6.40827700	0.04016600
H	3.31577800	-4.83002600	0.54203600
H	1.57367700	-5.11878600	0.57485400
C	4.51865200	-2.42754800	-1.93710300
C	5.28169500	-2.25763400	-0.60627900
H	4.85473800	-1.66618000	-2.65278600
H	4.77378300	-3.39555400	-2.38471500

H	6.36514300	-2.26209800	-0.77361700
H	5.00816100	-1.32512800	-0.10125400
H	5.03915700	-3.07765200	0.07896400
C	0.07130900	-0.27929400	1.04885300
C	-0.87204000	-0.57156400	2.09016700
C	1.44986700	-0.29887100	1.40512200
C	-0.48271100	-0.48660800	3.39335500
H	-1.91791800	-0.72157300	1.84512800
C	1.89164900	-0.19072700	2.70181300
H	2.20932100	-0.28664800	0.63697700
C	0.91209000	-0.25134900	3.81214900
O	1.19133500	-0.13723000	5.01009400
H	-1.20239100	-0.54255600	4.20581700
C	3.36442300	-0.03610100	2.86212200
O	4.14090200	0.08760900	1.92177200
O	3.78352500	-0.06352300	4.13774200
C	5.19968200	0.06810000	4.31565500
H	5.73106400	-0.75132600	3.82153000
H	5.55629900	1.01566700	3.90017200
H	5.35937600	0.03584900	5.39397700

³Ir-QC

N	0.89828700	-1.46161600	-1.28422000
N	0.89882400	1.46137200	-1.28420500
N	-1.92400200	1.44170100	-0.60573500
N	-1.92455300	-1.44091900	-0.60581000
C	0.71755200	-2.81132700	-1.17488900
C	1.97679700	-3.49630100	-1.41676200
C	2.90838400	-2.52522500	-1.67877300
C	2.21451100	-1.24957000	-1.60366000
C	2.80714900	-0.00047300	-1.77524600
C	2.21496100	1.24883200	-1.60367700
C	2.90927900	2.52424700	-1.67892100
C	1.97802700	3.49567000	-1.41704600
C	0.71854800	2.81114900	-1.17504300
C	-0.49521800	3.42659300	-0.87362200
C	-1.70994100	2.80647200	-0.61303800
C	-2.94944800	3.49223500	-0.29936200
C	-3.90357400	2.52611200	-0.10695600
C	-3.25107400	1.24469100	-0.30012900
C	-3.85998500	0.00074600	-0.17167500
C	-3.25158100	-1.24342200	-0.30033500
C	-3.90459700	-2.52461500	-0.10735400
C	-2.95083600	-3.49108600	-0.29979700

C	-1.71100700	-2.80576000	-0.61318800
C	-0.49647000	-3.42632300	-0.87358000
H	-0.48986700	4.51019200	-0.83716000
H	3.86518000	-0.00066400	-2.00952100
H	-0.49151500	-4.50992200	-0.83709200
H	-4.91631800	0.00094300	0.07190000
C	-0.69137100	0.00035900	-3.13528700
H	0.31004000	-0.00011300	-3.56336500
H	-1.24466800	-0.90920400	-3.37809700
H	-1.24370100	0.91058400	-3.37780500
Ir	-0.52615000	0.00014100	-0.91695800
C	4.39027600	2.67576200	-1.86794700
C	5.15964700	2.49174800	-0.54274600
H	4.61205200	3.66513600	-2.28573200
H	4.75234100	1.94870700	-2.60633800
H	6.24209500	2.54156300	-0.70946200
H	4.88749400	3.28030200	0.16787100
H	4.92127300	1.53432400	-0.06785600
C	2.18208900	4.97814300	-1.29772100
C	2.26648900	5.45046500	0.16730100
H	1.36553000	5.51076100	-1.80398400
H	3.10081900	5.26408500	-1.82287000
H	2.40859200	6.53587600	0.22287800
H	1.35288100	5.19480500	0.71547100
H	3.10370500	4.96614700	0.68123000
C	-3.08697700	4.97956800	-0.14802700
C	-2.56663700	5.48568200	1.21190300
H	-4.13943300	5.26460300	-0.26059000
H	-2.54746800	5.48978300	-0.95685400
H	-2.67050000	6.57373400	1.29235400
H	-3.12499600	5.02468100	2.03409300
H	-1.51004200	5.22993000	1.34765700
C	-5.33604300	2.69811500	0.30768200
C	-5.54723600	2.46024900	1.81617800
H	-5.97586600	2.01091500	-0.26174700
H	-5.67460900	3.70856700	0.05116500
H	-6.60159000	2.58093300	2.08985800
H	-5.23180800	1.45049900	2.10180200
H	-4.95519600	3.16929000	2.40521800
C	-5.33718800	-2.69611800	0.30707400
C	-5.54846100	-2.45863500	1.81562000
H	-5.67617100	-3.70633600	0.05018400
H	-5.97663500	-2.00844700	-0.26220500
H	-6.60290500	-2.57892000	2.08913200

H	-4.95682300	-3.16812800	2.40451900
H	-5.23260600	-1.44911700	2.10159700
C	-3.08896800	-4.97838500	-0.14867700
C	-2.56908400	-5.48485200	1.21129500
H	-2.54948500	-5.48870800	-0.95745200
H	-4.14151000	-5.26300700	-0.26148800
H	-2.67336500	-6.57287600	1.29159600
H	-1.51242000	-5.22950700	1.34727900
H	-3.12743000	-5.02374200	2.03343000
C	2.18035700	-4.97882700	-1.29725100
C	2.26421900	-5.45105800	0.16783500
H	3.09914400	-5.26509700	-1.82212000
H	1.36376800	-5.51123800	-1.80368800
H	2.40598900	-6.53650600	0.22352700
H	3.10143600	-4.96694700	0.68195600
H	1.35054200	-5.19509200	0.71574300
C	4.38931900	-2.67733500	-1.86782400
C	5.15875200	-2.49411100	-0.54255500
H	4.75171600	-1.95018000	-2.60595000
H	4.61065600	-3.66665400	-2.28597400
H	6.24118100	-2.54432600	-0.70928000
H	4.92076600	-1.53674500	-0.06735400
H	4.88627000	-3.28279600	0.16779100
C	0.14949100	-0.00015700	1.05233500
C	-0.80419600	-0.00022500	2.10696000
C	1.51715400	-0.00030900	1.39812200
C	-0.39159600	-0.00054600	3.41782300
H	-1.86568400	-0.00005200	1.87649200
C	1.97944000	-0.00058200	2.70144400
H	2.26914600	-0.00019500	0.62338100
C	1.01516700	-0.00081200	3.81089900
O	1.32235900	-0.00131300	5.02228100
H	-1.10478300	-0.00067300	4.23794800
C	3.46350000	-0.00060300	2.85134500
O	4.23920400	-0.00114700	1.90271900
O	3.89211500	0.00015400	4.12372400
C	5.31639700	0.00017300	4.28559800
H	5.75930500	-0.88871200	3.82567500
H	5.75937200	0.88860000	3.82484800
H	5.48426200	0.00067100	5.36316000
1			
C	0.22601300	-1.21007600	-0.00003800
C	0.95292500	-0.08696500	0.00001200

C	0.30596400	1.28074800	-0.00021000
C	-1.19944300	1.24628700	0.00013900
C	-1.90882900	0.11633700	0.00011500
C	-1.27965100	-1.25132600	-0.00009700
H	0.66698900	1.85580000	0.87017300
H	0.73535500	-2.17367500	0.00017300
H	-1.70938200	2.20859600	0.00036800
H	-2.99701900	0.15744900	0.00025500
H	-1.63775900	-1.82599800	0.87108700
H	-1.63774700	-1.82569000	-0.87151300
H	0.66658100	1.85512100	-0.87124300
C	2.45907000	-0.09487100	0.00010700
H	2.85650400	0.42944500	0.88098800
H	2.86344900	-1.11249700	-0.00052300
H	2.85673700	0.43065400	-0.87993800

osTS1

N	2.67980200	0.61504200	-0.53958700
N	0.27959200	2.08476100	-1.34228700
N	-1.05701300	-0.43237000	-1.88776700
N	1.29334900	-1.88585900	-1.05337700
C	3.70077900	-0.23918700	-0.23211200
C	4.86273800	0.52289700	0.19559000
C	4.50891600	1.84624700	0.13336100
C	3.13223100	1.89064400	-0.33491500
C	2.38521000	3.04960900	-0.53489700
C	1.06834800	3.14392500	-0.97589900
C	0.31212300	4.38021200	-1.11143600
C	-0.93296000	4.03431100	-1.56759100
C	-0.93214900	2.58824900	-1.72245100
C	-2.00754300	1.81950200	-2.16523900
C	-2.06508500	0.43457700	-2.25942800
C	-3.19413200	-0.32375500	-2.76739900
C	-2.84588000	-1.64908600	-2.70502700
C	-1.51146700	-1.70726600	-2.13400900
C	-0.80271400	-2.87126700	-1.85714500
C	0.48449700	-2.95959000	-1.33783400
C	1.19345300	-4.19433800	-1.04974700
C	2.44468300	-3.84197900	-0.61381500
C	2.50468600	-2.39101100	-0.63227500
C	3.61454000	-1.63043900	-0.28095600
H	-2.90091900	2.36081400	-2.45399100
H	2.88450600	3.98634500	-0.31355000
H	4.50474900	-2.17950600	0.00473400

H	-1.30378100	-3.80808800	-2.07386100
C	1.67165200	0.35763600	-3.15966500
H	2.18001200	1.32279300	-3.20544600
H	2.38019100	-0.46134900	-3.31570400
H	0.85176700	0.31903800	-3.88408100
C	0.24169600	0.27415300	0.82732500
C	0.98666200	-0.33415100	1.86658700
C	-0.90751900	0.99347400	1.20104100
C	0.48511500	-0.39525800	3.15159600
H	1.92279400	-0.83377700	1.64240900
C	-1.44185300	0.95361100	2.48878800
H	-1.46485700	1.55616400	0.46426600
C	-0.75607100	0.20932700	3.50993700
O	-1.22522300	0.01989400	4.71677800
Ir	0.77984500	0.08438800	-1.17847200
H	0.99834300	-0.94438800	3.93537600
C	-2.73944500	1.66243800	2.66604600
O	-3.37844600	2.14748700	1.74258100
O	-3.16891700	1.73249100	3.94244700
C	-4.42374500	2.40023500	4.12090800
H	-4.37321900	3.43128000	3.75832400
H	-5.22005200	1.87998300	3.57846400
H	-4.61349900	2.37824300	5.19487100
C	0.81572200	5.73785600	-0.71597900
C	0.79713700	5.95482200	0.81020200
H	0.20452500	6.50972400	-1.19809800
H	1.83808100	5.88270900	-1.09061800
H	1.17518700	6.95016000	1.07096300
H	-0.22184700	5.85928000	1.20053900
H	1.41510500	5.20719900	1.31959000
C	-2.14041900	4.90598400	-1.75136000
C	-3.05512600	4.88772400	-0.50869400
H	-2.71071600	4.57914300	-2.63087100
H	-1.82780300	5.93604100	-1.96084800
H	-3.96374200	5.47647700	-0.68221000
H	-3.34306200	3.86731300	-0.23588500
H	-2.53262400	5.31181600	0.35602800
C	-4.49261800	0.28408500	-3.21278100
C	-5.40468600	0.66756300	-2.02961900
H	-5.02423700	-0.41827800	-3.86563500
H	-4.29599600	1.17532900	-3.82300000
H	-6.31902100	1.15742900	-2.38378800
H	-5.69082900	-0.22246800	-1.45955600
H	-4.89339300	1.34620900	-1.33832600

C	-3.63912900	-2.84776700	-3.14444500
C	-4.36796800	-3.57703100	-2.00016600
H	-2.97126200	-3.55590500	-3.65235900
H	-4.37587000	-2.53958900	-3.89556900
H	-4.86846200	-4.47995400	-2.36854300
H	-3.66860700	-3.87233900	-1.20996000
H	-5.12679800	-2.93021500	-1.54746500
C	0.59482800	-5.56674100	-1.15609200
C	-0.32135100	-5.90653600	0.03579100
H	1.39445500	-6.31371300	-1.22061300
H	0.02254500	-5.65536200	-2.08913100
H	-0.75011700	-6.90994600	-0.06740800
H	0.23977700	-5.86835300	0.97640800
H	-1.14451400	-5.18812400	0.11372000
C	3.54510800	-4.73401900	-0.11722500
C	3.61270200	-4.78170500	1.42213500
H	4.51182100	-4.39487800	-0.51256900
H	3.40038800	-5.74940900	-0.50402200
H	4.42799100	-5.43048000	1.76234000
H	3.77382700	-3.78044800	1.83702200
H	2.67300000	-5.16329100	1.83720600
C	6.14661200	-0.08080900	0.68635700
C	6.04767900	-0.57569200	2.14296700
H	6.95339700	0.65758000	0.61074900
H	6.44030200	-0.91695400	0.03785200
H	6.99337000	-1.01984300	2.47459400
H	5.80143300	0.25324000	2.81571900
H	5.25911800	-1.32952800	2.24734000
C	5.31433800	3.04741700	0.53593200
C	4.94157100	3.56586900	1.93901500
H	5.17739500	3.85335200	-0.19718200
H	6.38179000	2.79830200	0.51504100
H	5.53736300	4.44673100	2.20475800
H	3.88185800	3.83993200	1.98662900
H	5.11499400	2.79171700	2.69469300
C	-1.75405200	-2.96383000	3.99157800
C	-2.79548200	-2.00003100	4.34742900
C	-3.58713200	-1.46747400	3.24632000
C	-3.22001200	-1.60597300	1.94670500
C	-2.01347000	-2.42198100	1.56746400
C	-1.36458800	-3.13877300	2.71124100
H	-4.44917800	-0.85142300	3.49279100
H	-2.27872500	-3.13190100	0.76469700
H	-1.27524600	-1.75930800	1.07859900

C	-3.93982900	-0.93099200	0.82174900
H	-4.27313100	-1.65766000	0.07259400
H	-4.80010000	-0.35070800	1.16645600
H	-3.26178500	-0.24058800	0.30246800
H	-2.06472700	-0.92883700	4.66783200
H	-3.31950500	-2.16904900	5.29135500
H	-1.24324800	-3.48740100	4.79627800
H	-0.54629600	-3.81325300	2.46942100

³TS1

N	2.71025600	0.54121500	-0.52863700
N	0.36598000	2.08913600	-1.34911700
N	-1.04022700	-0.37692700	-1.91923000
N	1.25234400	-1.90998300	-1.07347400
C	3.69866700	-0.34589000	-0.20779500
C	4.87629500	0.37635700	0.24479400
C	4.56482600	1.71052900	0.18588500
C	3.19867100	1.80004700	-0.30543100
C	2.48931100	2.98236600	-0.50566500
C	1.18193000	3.12093800	-0.96183100
C	0.46283200	4.38049900	-1.08207000
C	-0.79065800	4.07726200	-1.54491000
C	-0.83100800	2.63444700	-1.72040900
C	-1.92965500	1.90305500	-2.16813600
C	-2.02757400	0.52168100	-2.27450300
C	-3.18190300	-0.19904700	-2.77837900
C	-2.87064400	-1.53437700	-2.73409000
C	-1.53653600	-1.63757800	-2.17113900
C	-0.86663700	-2.82406100	-1.89753300
C	0.41275800	-2.95682800	-1.36846100
C	1.07688800	-4.21478200	-1.07468200
C	2.33296000	-3.90460600	-0.62146900
C	2.44057300	-2.45643800	-0.63516700
C	3.56871800	-1.73354200	-0.26501800
H	-2.80948100	2.47256900	-2.44375900
H	3.01263300	3.90146200	-0.26648500
H	4.43590200	-2.31217500	0.03293000
H	-1.39848400	-3.74305100	-2.11736800
C	1.78208500	0.33622100	-3.16336200
H	2.27118400	1.31026000	-3.19006700
H	2.49944100	-0.48093100	-3.26618100
H	0.97062600	0.27168500	-3.89349200
C	0.24496800	0.26238500	0.82575400
C	0.95178300	-0.37886200	1.86029500

C	-0.92631900	0.94912000	1.15811200
C	0.44809700	-0.39435100	3.15055500
H	1.87577300	-0.90550300	1.64755900
C	-1.45608000	0.95752500	2.45361400
H	-1.49261200	1.47518200	0.40193000
C	-0.77351100	0.24687000	3.49462200
O	-1.24074000	0.10629200	4.71589800
Ir	0.80449200	0.07558200	-1.20289900
H	0.95800200	-0.92580900	3.94869600
C	-2.74395600	1.68798600	2.60660300
O	-3.37569500	2.15484400	1.66749600
O	-3.17761700	1.80126000	3.87850200
C	-4.42450700	2.48855700	4.03190300
H	-4.36197400	3.50668300	3.63593100
H	-5.22624300	1.96023500	3.50529000
H	-4.61675200	2.50388600	5.10561300
C	1.00403000	5.71711400	-0.66487600
C	0.98409900	5.91364500	0.86411100
H	0.41801700	6.51309900	-1.13901500
H	2.03202300	5.83735800	-1.03286000
H	1.38975300	6.89389500	1.14002700
H	-0.03907500	5.84267900	1.24844700
H	1.57708300	5.14151300	1.36652500
C	-1.97318300	4.98515600	-1.71513900
C	-2.88448800	4.97938500	-0.46962200
H	-2.55519200	4.68459200	-2.59632700
H	-1.63176400	6.00810300	-1.91433900
H	-3.77773600	5.59332800	-0.63536200
H	-3.19872100	3.96461300	-0.20459900
H	-2.34852300	5.38296700	0.39668900
C	-4.46875300	0.44967300	-3.19850400
C	-5.35452600	0.83474300	-1.99568400
H	-5.02635800	-0.22738500	-3.85643500
H	-4.25657300	1.34619800	-3.79562600
H	-6.25752600	1.35980800	-2.32780000
H	-5.66092700	-0.05897100	-1.44227700
H	-4.81475500	1.48087400	-1.29494000
C	-3.70028100	-2.70428300	-3.18364300
C	-4.46186700	-3.41207100	-2.04779100
H	-3.05251000	-3.43220800	-3.68955100
H	-4.42034300	-2.36860300	-3.93923900
H	-4.98668400	-4.29846400	-2.42232200
H	-3.77973900	-3.72925000	-1.25107700
H	-5.20381100	-2.74163100	-1.60218900

C	0.43421200	-5.56625100	-1.19136400
C	-0.50525900	-5.87842000	-0.01012100
H	1.20926300	-6.33916000	-1.24994100
H	-0.13080800	-5.63315800	-2.13066200
H	-0.96705900	-6.86612800	-0.12164700
H	0.04697900	-5.86268600	0.93627700
H	-1.30397800	-5.13243400	0.06237500
C	3.39634300	-4.83319600	-0.11128200
C	3.44022300	-4.88617200	1.42880400
H	4.37929000	-4.52533600	-0.49203400
H	3.22379700	-5.84248200	-0.50261900
H	4.22876000	-5.56225900	1.77868600
H	3.62824400	-3.89178400	1.84882100
H	2.48268500	-5.23735100	1.82954600
C	6.13149700	-0.27031800	0.75466400
C	5.99135700	-0.76818500	2.20690100
H	6.96254400	0.44232300	0.69669700
H	6.40978800	-1.11251600	0.10716700
H	6.91669600	-1.24331100	2.55263800
H	5.75948300	0.06511600	2.87927900
H	5.17776400	-1.49717000	2.29407500
C	5.39918100	2.88348100	0.61212200
C	5.01812300	3.40191500	2.01303200
H	5.29956900	3.69903400	-0.11641400
H	6.45877600	2.60206200	0.60730400
H	5.63591400	4.26193000	2.29616800
H	3.96661900	3.70790000	2.04527200
H	5.15470100	2.61688900	2.76496700
C	-1.80520000	-2.91195900	4.00261000
C	-2.81678400	-1.92284900	4.38239700
C	-3.64504700	-1.40162000	3.29822300
C	-3.33558700	-1.57549800	1.99012400
C	-2.15893200	-2.42193300	1.57820800
C	-1.47399700	-3.12401200	2.71223400
H	-4.48627500	-0.76604100	3.56616500
H	-2.47641700	-3.14996100	0.81152800
H	-1.43048100	-1.78645100	1.04188100
C	-4.09959100	-0.92003400	0.88025500
H	-4.52067000	-1.66755000	0.19793300
H	-4.90720600	-0.28395100	1.25292900
H	-3.43177500	-0.28735800	0.28173600
H	-2.08412000	-0.86982300	4.67910400
H	-3.31927700	-2.08639400	5.33976800
H	-1.26946200	-3.42684500	4.79680900

H	-0.67758800	-3.81794400	2.45263300
6			
C	0.20760300	1.24111800	0.00059400
C	0.92760200	0.07539600	0.00055000
C	0.22348200	-1.25996600	0.00097000
C	-1.27646100	-1.16966300	-0.00053500
C	-1.92798200	0.03118100	-0.00052000
C	-1.21072200	1.25553700	0.00031700
H	0.56964000	-1.85878100	-0.86537600
H	0.74220800	2.18971600	0.00011200
H	-1.83588000	-2.10199400	-0.00177400
H	-3.01564200	0.05378600	-0.00152400
H	-1.74332700	2.20127100	-0.00034200
H	0.56775400	-1.85648200	0.86977500
C	2.42762600	0.04398400	-0.00087300
H	2.81402500	-0.49035300	-0.88204400
H	2.85881300	1.05055500	0.00033200
H	2.81551800	-0.49323700	0.87782800
INT1			
N	1.00942700	-1.26945500	-1.39279000
N	0.78792600	1.62464800	-1.26695300
N	-2.00010900	1.39339300	-0.55861600
N	-1.81956100	-1.49200500	-0.67124600
C	0.91171500	-2.63345400	-1.33770500
C	2.21332100	-3.22463300	-1.60590700
C	3.08125200	-2.18546600	-1.82242600
C	2.30523700	-0.96312100	-1.69503600
C	2.81091100	0.33238000	-1.80327700
C	2.12596400	1.52063300	-1.58313900
C	2.72527900	2.84387700	-1.60362300
C	1.72662800	3.73671500	-1.31739600
C	0.51579400	2.96046000	-1.10832000
C	-0.72967300	3.48249900	-0.77715600
C	-1.89316700	2.76607700	-0.52198400
C	-3.17487300	3.34531100	-0.16737200
C	-4.05099000	2.30391700	0.00431400
C	-3.30966900	1.08262200	-0.24322900
C	-3.83202100	-0.20158400	-0.16244800
C	-3.14464100	-1.40022500	-0.34988700
C	-3.70884400	-2.73206800	-0.20455400
C	-2.69144400	-3.61768000	-0.44892000
C	-1.50790300	-2.82570400	-0.74566500

C	-0.25285000	-3.34256700	-1.05412300
H	-0.79920500	4.56192100	-0.70392800
H	3.86677200	0.41995500	-2.03142000
H	-0.17052400	-4.42374500	-1.06895800
H	-4.88363100	-0.28075800	0.08939700
C	-0.93182200	-0.21175000	-3.09341700
H	-0.09308400	0.21322400	-3.64933300
H	-1.05034500	-1.27550200	-3.30254800
H	-1.86252700	0.33528900	-3.27228100
C	0.11902000	-0.20686600	1.04201100
C	-0.79517700	-0.46508400	2.08135400
C	1.46038200	-0.10307800	1.38704700
C	-0.37726000	-0.56475200	3.40483400
H	-1.85326800	-0.57130600	1.86192800
C	1.91835400	-0.20063300	2.71569200
H	2.21878500	0.07289900	0.63774200
C	0.97637100	-0.43736700	3.74777800
O	1.28672700	-0.55609900	5.06254800
Ir	-0.50937700	0.08138700	-0.95602000
H	-1.08732600	-0.74497600	4.20672600
C	3.37344800	-0.05031500	2.90558200
O	4.19715500	0.14916200	2.03146400
O	3.76264800	-0.15910600	4.22128400
C	5.17263600	-0.02396900	4.46429900
H	5.72707200	-0.79840000	3.92776000
H	5.52327700	0.95734300	4.13410100
H	5.29692600	-0.13617600	5.54198900
C	4.19370600	3.10494800	-1.77026100
C	4.96855700	2.88239700	-0.45417700
H	4.35225800	4.13286600	-2.11763300
H	4.60639900	2.45460300	-2.55252000
H	6.04639700	3.01397400	-0.60614600
H	4.64056000	3.59945700	0.30684100
H	4.79185900	1.87987800	-0.04996000
C	1.82624700	5.22457900	-1.14494900
C	1.88509200	5.64882700	0.33592600
H	0.97084700	5.71530800	-1.62869800
H	2.71929500	5.59456500	-1.66203600
H	1.94730400	6.73914400	0.43102100
H	0.99635000	5.30610200	0.87720800
H	2.75950600	5.20923400	0.82802700
C	-3.42021100	4.81227300	0.03607500
C	-2.91601700	5.31175700	1.40452900
H	-4.49257800	5.02220000	-0.05185100

H	-2.93274500	5.38723400	-0.76237100
H	-3.09685800	6.38641700	1.52248100
H	-3.42592100	4.78515400	2.21885000
H	-1.84160200	5.12897200	1.51623700
C	-5.48578700	2.35651500	0.44323300
C	-5.65641200	2.05043300	1.94436800
H	-6.08345400	1.64554800	-0.14257900
H	-5.90036200	3.34828800	0.22825500
H	-6.71238900	2.08462000	2.23631500
H	-5.26420700	1.05678700	2.18799800
H	-5.10734000	2.77901200	2.55107400
C	-5.11954600	-3.01956800	0.22057400
C	-5.32305100	-2.85704600	1.73988900
H	-5.39208900	-4.04025300	-0.07243100
H	-5.81465600	-2.35636400	-0.31154000
H	-6.36133100	-3.06373200	2.02430800
H	-4.67119700	-3.54382000	2.29115400
H	-5.07535100	-1.83890800	2.06079500
C	-2.71770200	-5.11610400	-0.36045800
C	-2.13546700	-5.64052500	0.96704300
H	-2.15811600	-5.55130700	-1.19911100
H	-3.74872600	-5.47302900	-0.46814600
H	-2.15636700	-6.73598900	1.00131800
H	-1.09851400	-5.31149000	1.09676100
H	-2.71036200	-5.25818900	1.81783600
C	2.51462900	-4.69415000	-1.54734200
C	2.63666700	-5.21824200	-0.10269000
H	3.44779400	-4.89835300	-2.08537000
H	1.73230700	-5.25885100	-2.07236700
H	2.84902500	-6.29366500	-0.09028500
H	3.44346200	-4.70102700	0.42792400
H	1.71106400	-5.04328300	0.45674400
C	4.56933800	-2.23138500	-2.01126500
C	5.32364900	-2.04318600	-0.67828000
H	4.88326200	-1.45569000	-2.72184400
H	4.85844800	-3.18830200	-2.46239900
H	6.40766500	-2.01448700	-0.84094700
H	5.02021000	-1.12006600	-0.17322500
H	5.10236600	-2.87111700	0.00475500
H	2.25283800	-0.44988400	5.15555100

ossTS2

N	1.44947700	2.06938800	-0.90735600
N	-1.11864400	0.92135700	-1.70426500

N	0.00356100	-1.73703600	-1.40576200
N	2.53660900	-0.59414500	-0.60508600
C	2.69625800	2.41639100	-0.45766000
C	2.79164600	3.86409500	-0.35178900
C	1.58017200	4.36807400	-0.74873200
C	0.74433300	3.22910600	-1.09423500
C	-0.59949900	3.30210200	-1.45268800
C	-1.47048600	2.24306100	-1.69077000
C	-2.90270800	2.36851000	-1.91708000
C	-3.38731800	1.09881800	-2.09016200
C	-2.25323200	0.19840200	-1.94775200
C	-2.31708100	-1.19230100	-1.99810800
C	-1.27649600	-2.08647200	-1.77127100
C	-1.36559300	-3.52991500	-1.91980200
C	-0.10839100	-4.03027800	-1.70043800
C	0.74171200	-2.89618000	-1.37360400
C	2.08581400	-2.97169100	-1.02267800
C	2.90602900	-1.91908400	-0.62622900
C	4.27524200	-2.05138800	-0.15950800
C	4.72568500	-0.78567000	0.11518800
C	3.63688200	0.12531400	-0.19481100
C	3.70077400	1.51295000	-0.12060800
H	-3.28302500	-1.62369100	-2.23537600
H	-1.02725400	4.29667500	-1.51087800
H	4.63988800	1.93675000	0.21810300
H	2.53285100	-3.95977000	-1.02296100
C	1.26260700	0.27954500	-3.17148000
H	1.05240600	1.28819800	-3.53793500
H	2.33304600	0.06241100	-3.25783000
H	0.67728200	-0.45363300	-3.73574500
C	-0.34108200	0.57438900	0.88894700
C	-0.16801900	1.79696500	1.56284700
C	-1.53043900	-0.10134900	1.11825500
C	-1.17821900	2.35801900	2.34099500
H	0.76523800	2.34367100	1.46901800
C	-2.58723700	0.44447000	1.87950900
H	-1.70078400	-1.07836900	0.68122800
C	-2.41487900	1.71901600	2.47829700
O	-3.36716300	2.36612000	3.20292900
Ir	0.71200200	0.16113900	-1.11417700
H	-1.04223800	3.31664600	2.83408700
C	-3.80046600	-0.37519200	1.99235200
O	-3.90346000	-1.55529300	1.69657800
O	-4.88687900	0.31550700	2.47935100

C	-6.10055400	-0.44408200	2.60985800
H	-6.43162900	-0.79386800	1.62913700
H	-5.94530200	-1.30554400	3.26462000
H	-6.83053200	0.24288200	3.03948700
C	-3.67140200	3.65089400	-1.79186800
C	-3.88616200	4.03916000	-0.31354700
H	-4.64416300	3.55364600	-2.28844800
H	-3.14603600	4.46500800	-2.30903000
H	-4.43876000	4.98219500	-0.22739500
H	-4.44573900	3.25968700	0.21543200
H	-2.92766200	4.14826100	0.20494600
C	-4.81125400	0.66322500	-2.28268600
C	-5.46422900	0.16061500	-0.98002100
H	-4.86133600	-0.13069300	-3.04015200
H	-5.39835900	1.49866700	-2.68195600
H	-6.50830500	-0.12926400	-1.15116900
H	-4.92776200	-0.70481100	-0.57907000
H	-5.44420600	0.94189100	-0.21204900
C	-2.64006700	-4.27561900	-2.18744700
C	-3.51116900	-4.40885100	-0.92101500
H	-2.41229300	-5.27452700	-2.57829400
H	-3.21528800	-3.76659800	-2.97210300
H	-4.46255100	-4.90439200	-1.14794200
H	-2.99081500	-4.99996900	-0.15929400
H	-3.72512300	-3.42921400	-0.47961500
C	0.35411400	-5.45901200	-1.75202000
C	0.43514600	-6.13574400	-0.37061600
H	1.33990300	-5.50634200	-2.23331300
H	-0.32076200	-6.03817400	-2.39342400
H	0.83656600	-7.15262000	-0.45278900
H	1.08077400	-5.56811500	0.30937300
H	-0.55759500	-6.19949100	0.08789500
C	4.97289600	-3.36144800	0.06391400
C	4.51356000	-4.05357100	1.36278100
H	6.05691500	-3.20282300	0.10310400
H	4.79581600	-4.03289500	-0.78692100
H	5.02160600	-5.01506900	1.50134100
H	4.72868100	-3.42177400	2.23199600
H	3.43277900	-4.23403500	1.34806400
C	6.04475600	-0.36995200	0.69870400
C	5.94663600	-0.05000700	2.20340500
H	6.43115700	0.50934300	0.16617000
H	6.78399300	-1.16493400	0.54608700
H	6.91757400	0.25939200	2.60749200

H	5.22685300	0.75641000	2.38379400
H	5.60547100	-0.92891900	2.76231100
C	3.98336000	4.60535200	0.18141400
C	4.06924900	4.56119000	1.71994300
H	3.94442900	5.65071200	-0.14697500
H	4.90592500	4.18822900	-0.24422800
H	4.95312900	5.09848200	2.08333400
H	3.18016100	5.01841700	2.16857600
H	4.12451600	3.52698800	2.07803800
C	1.11138300	5.79398600	-0.72902400
C	0.30046600	6.12237800	0.54115300
H	0.49802800	6.00124600	-1.61562700
H	1.97296800	6.46934100	-0.79205700
H	-0.05688700	7.15870000	0.52690400
H	-0.56648200	5.45892700	0.63415600
H	0.91707100	5.98367500	1.43644200
C	0.88871900	-0.44629900	3.57483300
C	1.24322900	-1.18088500	2.40490000
C	0.53901400	-2.35906500	2.05982800
C	-0.57327000	-2.75663600	2.74855200
C	-1.02923300	-1.99181200	3.95594300
C	-0.18674300	-0.81118900	4.31843000
H	0.84607700	-2.90579900	1.17749700
H	-2.07053900	-1.66650900	3.78842300
H	-1.10786600	-2.68010400	4.81871400
C	-1.42438800	-3.90896400	2.31407400
H	-2.43029300	-3.54535000	2.06565000
H	-1.01139400	-4.39881300	1.42956000
H	-1.53504200	-4.65589800	3.11348800
H	-4.18901900	1.84317400	3.15500100
H	2.10568400	-0.88451100	1.82401000
H	-0.47721600	-0.23564300	5.19335000
H	1.46391300	0.43695600	3.83496500

³TS2

N	1.14461900	2.17372300	-0.93270100
N	-1.28691400	0.65427200	-1.53475000
N	0.23749100	-1.81460400	-1.31102100
N	2.60103300	-0.30408000	-0.65535500
C	2.35052800	2.70853000	-0.57812500
C	2.24080700	4.15527200	-0.49467700
C	0.94235700	4.46878000	-0.80581500
C	0.26021300	3.21491200	-1.07959800
C	-1.09458800	3.08934900	-1.37216500

C	-1.81713900	1.91335900	-1.56019600
C	-3.24089700	1.83380100	-1.84591300
C	-3.53088300	0.50759800	-2.04043400
C	-2.29146400	-0.22346600	-1.83534000
C	-2.14637100	-1.60685400	-1.89149500
C	-0.99119000	-2.34186800	-1.64575900
C	-0.88528900	-3.78655500	-1.75972300
C	0.43118500	-4.10772800	-1.55279300
C	1.12403100	-2.86200500	-1.27077600
C	2.47326100	-2.74080600	-0.95381300
C	3.14879700	-1.57087700	-0.62948200
C	4.53472900	-1.49134000	-0.21289100
C	4.82058900	-0.16383600	-0.01524400
C	3.61348100	0.57923400	-0.31611100
C	3.49164300	1.96070700	-0.28688800
H	-3.03473800	-2.17520700	-2.14210500
H	-1.65863900	4.01294100	-1.43740900
H	4.37942300	2.51859800	-0.01073400
H	3.05112900	-3.65767400	-0.92759000
C	0.89097800	0.37639800	-3.20079700
H	0.61568600	1.39025000	-3.49874900
H	1.94770600	0.18354100	-3.41673000
H	0.24983300	-0.36046600	-3.69092900
C	-0.12869600	0.36675500	1.03093900
C	-0.12364400	1.73025000	1.55932600
C	-1.42209600	-0.27855800	1.15548400
C	-1.21655700	2.31638900	2.13918600
H	0.80490000	2.29068600	1.52773200
C	-2.53410300	0.29358200	1.76381100
H	-1.53178700	-1.28709800	0.78206100
C	-2.45474800	1.63444100	2.23886600
O	-3.48118200	2.32208700	2.79579700
Ir	0.68628500	0.16753100	-1.05543900
H	-1.17090500	3.32789500	2.53352200
C	-3.72767900	-0.56683800	1.87869300
O	-3.77517100	-1.76250900	1.65853800
O	-4.85130400	0.11581500	2.29102200
C	-6.01787500	-0.69187700	2.53012600
H	-6.34025100	-1.17581100	1.60599900
H	-5.80116100	-1.45731000	3.27978700
H	-6.78182400	-0.00193200	2.89025600
C	-4.18916300	2.99456600	-1.78506200
C	-4.52688100	3.37355000	-0.32811300
H	-5.11298200	2.74792800	-2.32153900

H	-3.76245400	3.86658600	-2.29853200
H	-5.22781300	4.21564800	-0.29059800
H	-4.97589000	2.52399200	0.19809600
H	-3.62461600	3.64776900	0.22747500
C	-4.86151800	-0.11833800	-2.34447500
C	-5.57738100	-0.64926100	-1.08878100
H	-4.73054600	-0.93939300	-3.06153100
H	-5.50401700	0.61696600	-2.84335200
H	-6.54731300	-1.09130600	-1.34670200
H	-4.97365100	-1.40763900	-0.58114500
H	-5.74755600	0.16496000	-0.37570100
C	-2.05373400	-4.70406200	-1.96966900
C	-2.88167400	-4.88446900	-0.67993400
H	-1.70040500	-5.68256100	-2.31565300
H	-2.70091200	-4.31543200	-2.76737700
H	-3.75657700	-5.51993500	-0.86072700
H	-2.27354500	-5.35041800	0.10284600
H	-3.22565500	-3.92033300	-0.28937600
C	1.08281700	-5.46118800	-1.57550700
C	1.28050300	-6.07636500	-0.17715400
H	2.05641200	-5.38847200	-2.07831000
H	0.48115600	-6.14512100	-2.18569300
H	1.81392700	-7.03198000	-0.24089700
H	1.85448800	-5.40570800	0.47207700
H	0.31470800	-6.25704300	0.30608100
C	5.41073000	-2.68287600	0.04139700
C	5.09133500	-3.36092500	1.38909700
H	6.46378000	-2.37900600	0.02826300
H	5.29596200	-3.41379700	-0.77010000
H	5.72377200	-4.24214200	1.54679800
H	5.25658400	-2.66472600	2.21874100
H	4.04266700	-3.67521300	1.43024600
C	6.09255200	0.44948900	0.49368500
C	6.00991500	0.81651700	1.98864500
H	6.33484100	1.34854300	-0.08857900
H	6.92559200	-0.24544800	0.33733500
H	6.94523300	1.27046000	2.33577100
H	5.19450600	1.52493700	2.17240500
H	5.81378800	-0.07536900	2.59401300
C	3.34572900	5.07164300	-0.05530700
C	3.53105500	5.08237000	1.47510000
H	3.13823600	6.09131100	-0.40049300
H	4.28973500	4.77666400	-0.53273100
H	4.34923400	5.74961500	1.77002100

H	2.61487200	5.42099900	1.97160900
H	3.75612800	4.07717100	1.84901000
C	0.27376800	5.81226500	-0.77033200
C	-0.50665400	6.04094400	0.53998300
H	-0.40988400	5.91534600	-1.62323800
H	1.02454200	6.60269000	-0.88692700
H	-1.00535900	7.01704800	0.53835900
H	-1.26592700	5.26453800	0.68379800
H	0.16958500	6.00191000	1.40145600
C	0.75078700	-0.13311300	3.58307300
C	1.06585200	-0.68273300	2.25821600
C	0.68468100	-2.08459000	2.07727100
C	-0.22400300	-2.70403600	2.85829400
C	-0.80422100	-2.02383000	4.07529300
C	-0.13144900	-0.72052300	4.40950800
H	1.07382000	-2.60174800	1.20878100
H	-1.88648600	-1.86677300	3.91669800
H	-0.75427300	-2.70928000	4.94056900
C	-0.75799000	-4.07427600	2.55161600
H	-1.84173000	-4.02319600	2.37191400
H	-0.29136000	-4.49554800	1.65697300
H	-0.60477600	-4.77252300	3.38784700
H	-4.27250200	1.74934400	2.77740500
H	2.02868700	-0.39267300	1.84594600
H	-0.38145400	-0.25909200	5.36309200
H	1.20311700	0.81576800	3.86178100

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C	-0.52397200	0.14465400	-0.20595100
C	-0.56438800	-1.26152900	-0.27003600
C	0.71510700	0.75267800	-0.08149300
C	0.59285600	-2.01904000	-0.21147700
H	-1.52814500	-1.75445900	-0.36731700
C	1.91385300	0.01117500	-0.01860300
H	0.79701600	1.83434200	-0.02774300
C	1.84934800	-1.40146900	-0.08515800
O	2.92001700	-2.22583700	-0.03605700
H	0.56497500	-3.10287600	-0.26084200
C	3.16092500	0.79469100	0.11483100
O	3.23633000	2.00456400	0.17393800
O	4.28841000	0.00914500	0.16977600
C	5.53341400	0.71861500	0.30010500
H	5.68003900	1.38628400	-0.55262500
H	5.53897100	1.30818100	1.22033400

H	6.30664400	-0.04971900	0.32778000
C	-2.51495300	0.73958400	-1.59722000
C	-1.81951700	0.95447400	-0.27224100
C	-2.71552700	0.62433700	0.90047800
C	-3.96308200	0.15048900	0.80387000
C	-4.62726700	-0.07728500	-0.53455500
C	-3.75799200	0.26892000	-1.71249100
H	-2.27179500	0.77214500	1.88437300
H	-4.95634100	-1.12800400	-0.60712000
H	-4.19300000	0.12546000	-2.70044400
H	-1.52975200	2.01582200	-0.20129000
H	-1.93065700	0.97086500	-2.48592200
H	-5.56477700	0.50310800	-0.57985000
C	-4.79741200	-0.18148500	2.01323000
H	-5.10102500	-1.23798400	2.00455600
H	-4.25837500	0.00948900	2.94677700
H	-5.72453100	0.40897000	2.02687200
H	3.72433500	-1.67745400	0.05144200

²TS3

N	1.45168500	-0.18174100	-1.18525800
N	-0.38424500	2.00385500	-0.74515600
N	-2.56980100	0.12032200	-0.47137000
N	-0.71894700	-2.07093600	-0.84583000
C	2.17241000	-1.34496200	-1.31512900
C	3.56406000	-1.02978500	-1.58262400
C	3.65895900	0.33679100	-1.64016400
C	2.33368000	0.85948600	-1.35810200
C	2.01604200	2.20412800	-1.20564700
C	0.77448000	2.73204500	-0.87253400
C	0.50631900	4.13410400	-0.59882700
C	-0.83312600	4.23443400	-0.32929600
C	-1.38480600	2.89357300	-0.43579800
C	-2.72103700	2.55786300	-0.24542800
C	-3.27490100	1.28222600	-0.26334200
C	-4.67123500	0.96874400	-0.01145300
C	-4.78838500	-0.39577000	-0.07078900
C	-3.46311400	-0.91925000	-0.35605500
C	-3.13017000	-2.26757500	-0.43584200
C	-1.86052400	-2.80476800	-0.62450400
C	-1.53000900	-4.21919100	-0.56883900
C	-0.17675400	-4.31711800	-0.76389500
C	0.32000200	-2.96544600	-0.95435100

C	1.64580100	-2.62535000	-1.19457800
H	-3.40078600	3.37764200	-0.04117300
H	2.83105000	2.91119300	-1.31278500
H	2.34787300	-3.44700800	-1.27941000
H	-3.94053900	-2.97567000	-0.30214600
C	-0.88770100	0.09160400	-2.90574700
H	-0.11483100	0.72958000	-3.34614100
H	-0.83524600	-0.91433800	-3.33440200
H	-1.87705300	0.52559800	-3.08205900
C	-0.29556400	1.17494000	2.35030300
C	-0.72714100	-0.13457000	2.20299500
C	1.01245700	1.56526200	2.34945000
C	0.25276800	-1.12414300	2.08044100
H	-1.77915200	-0.39982700	2.17078000
C	2.01201100	0.56454300	2.23560100
H	1.32325400	2.60134900	2.43282800
C	1.61914800	-0.79182700	2.10568200
O	2.48023000	-1.83052700	1.99273200
Ir	-0.56636800	-0.03054700	-0.87615500
H	-0.01717000	-2.16550400	1.94242700
C	3.41047300	1.03679300	2.31001000
O	3.76071200	2.19925300	2.36566400
O	4.32304000	0.01218200	2.36145500
C	5.67315000	0.37793500	2.70339600
H	6.02464300	1.19435900	2.07371900
H	5.71540000	0.68388200	3.75283100
H	6.26875000	-0.52126000	2.54331700
C	1.55744800	5.20316000	-0.52626500
C	2.32372600	5.18284700	0.81212400
H	1.09350800	6.18717100	-0.66396300
H	2.26978900	5.08694300	-1.35399500
H	3.09908600	5.95787700	0.83330900
H	1.63756300	5.36691700	1.64729500
H	2.80159100	4.21332400	0.98762900
C	-1.61128600	5.44410900	0.09977400
C	-1.84852300	5.48066100	1.62252200
H	-2.57941900	5.47216700	-0.41830500
H	-1.07878800	6.35268100	-0.20496400
H	-2.43409500	6.36131600	1.91140900
H	-2.38491900	4.58487200	1.95476200
H	-0.89390500	5.51051500	2.15961400
C	-5.72616700	1.98141800	0.32930400
C	-5.66369800	2.43097600	1.80249200
H	-6.71851100	1.56335600	0.12256000

H	-5.62612900	2.85988900	-0.32185800
H	-6.43487600	3.17897100	2.02061200
H	-5.81381500	1.57709700	2.47271300
H	-4.68619500	2.86670600	2.03735800
C	-6.00252600	-1.23996800	0.18962900
C	-6.03254200	-1.81248600	1.62054900
H	-6.04597200	-2.06648100	-0.53200900
H	-6.90779200	-0.64448900	0.02202500
H	-6.92198700	-2.43317100	1.77995900
H	-5.14632100	-2.42728900	1.81431700
H	-6.04115000	-1.00325300	2.35936800
C	-2.50848200	-5.31315400	-0.25256000
C	-2.83072000	-5.40435100	1.25200400
H	-2.10813400	-6.27492400	-0.59422600
H	-3.43990100	-5.15684000	-0.81313800
H	-3.55462200	-6.20230300	1.45456300
H	-1.92188900	-5.60992600	1.82875900
H	-3.24873400	-4.46022900	1.61905700
C	0.69776600	-5.53378600	-0.67909700
C	1.39935300	-5.64304200	0.69037200
H	1.45474500	-5.51012900	-1.47434900
H	0.10112400	-6.43649600	-0.85583700
H	2.07920900	-6.50269700	0.72056400
H	1.97264400	-4.73531300	0.90940100
H	0.65988200	-5.76300000	1.49043800
C	4.66975800	-2.04043900	-1.66958400
C	5.10350600	-2.54099600	-0.27638900
H	5.53422100	-1.60001800	-2.18061900
H	4.35775200	-2.89813700	-2.28002300
H	5.91717100	-3.27176600	-0.35070400
H	5.44716000	-1.70082300	0.33827300
H	4.26290300	-3.00970100	0.24625800
C	4.87292600	1.17459500	-1.92600500
C	5.65623100	1.57441300	-0.66394500
H	4.57352000	2.07932300	-2.46963000
H	5.54010300	0.62650500	-2.60290300
H	6.50454900	2.22250400	-0.91426400
H	5.01539400	2.10330000	0.04927000
H	6.04721300	0.68050300	-0.16632500
H	3.39231100	-1.48378800	2.03238200

ossTS4

N	-2.67830400	-0.75727300	-0.45926700
N	-0.20483100	-1.90160600	-1.53376600

N	0.83874300	0.77797500	-1.92396100
N	-1.58739500	1.90368300	-0.84152400
C	-3.75228900	-0.04431500	-0.00721700
C	-4.79676200	-0.95653600	0.42905900
C	-4.32016000	-2.22562200	0.22328600
C	-2.98628800	-2.08640000	-0.34035900
C	-2.14917500	-3.14067500	-0.69767700
C	-0.86484200	-3.06265400	-1.22902600
C	-0.00994900	-4.20008700	-1.53356700
C	1.16463500	-3.69202700	-2.02407400
C	1.02213000	-2.24486000	-2.02635400
C	1.99830600	-1.33359900	-2.42640400
C	1.91888800	0.05288100	-2.38341800
C	2.96269900	0.96279600	-2.81968000
C	2.48123800	2.23608300	-2.64910500
C	1.15344900	2.10875000	-2.07352400
C	0.33804100	3.16615300	-1.68720700
C	-0.91899000	3.07751200	-1.09951700
C	-1.73346000	4.20449800	-0.68294400
C	-2.90600400	3.68960500	-0.19268900
C	-2.81321000	2.24560100	-0.30687900
C	-3.80924200	1.34775800	0.05799600
H	2.92925300	-1.75273000	-2.78983600
H	-2.53961000	-4.13894500	-0.53417600
H	-4.72626000	1.77611500	0.44679500
H	0.72588800	4.16427200	-1.85559200
C	-1.86353600	-0.22600000	-3.11259900
H	-2.32309200	-1.21366600	-3.17335300
H	-2.61789600	0.56282600	-3.18580500
H	-1.08167600	-0.11090000	-3.86886300
C	-0.17962000	-0.32017700	0.77939400
C	-0.93373600	0.00970800	1.92813500
C	1.07819600	-0.90579400	0.98695800
C	-0.39388100	-0.13050700	3.19469300
H	-1.92890400	0.42929900	1.82424700
C	1.64776900	-1.07151700	2.25175600
H	1.68393600	-1.21668200	0.14776900
C	0.90385200	-0.67298600	3.41095500
O	1.33579500	-0.79188600	4.65051800
Ir	-0.88921100	0.01990300	-1.16132000
H	-0.94437000	0.17573400	4.08016800
C	3.00773800	-1.67599100	2.25908300
O	3.62411100	-1.98884100	1.25138400
O	3.52670600	-1.86690300	3.49382600

C	4.81583900	-2.49333200	3.51423000
H	4.77776700	-3.47438400	3.03174100
H	5.55648000	-1.87820100	2.99307300
H	5.07267000	-2.59263000	4.56972600
C	-0.35975400	-5.63227200	-1.25119200
C	-0.21933000	-5.99282400	0.24122300
H	0.28617600	-6.29037600	-1.84404500
H	-1.38728500	-5.83971500	-1.57940500
H	-0.48572300	-7.04108800	0.41948500
H	0.81009700	-5.83540700	0.58051100
H	-0.86799800	-5.36259800	0.85954900
C	2.42564500	-4.42448100	-2.37819300
C	3.41112000	-4.48303100	-1.19262800
H	2.91221600	-3.94140400	-3.23560500
H	2.18404100	-5.44332900	-2.70450300
H	4.35194600	-4.96187200	-1.48928000
H	3.63010500	-3.48423600	-0.80262000
H	2.98016400	-5.05936300	-0.36630800
C	4.33686000	0.53124000	-3.24052400
C	5.22790400	0.20309800	-2.02330500
H	4.81013200	1.32022400	-3.83660700
H	4.27392100	-0.34770300	-3.89491600
H	6.20673500	-0.17312400	-2.34240100
H	5.38797300	1.10046500	-1.41509500
H	4.75802900	-0.54839900	-1.37904000
C	3.17000700	3.54155600	-2.93138900
C	3.75386200	4.22091000	-1.67681000
H	2.46453100	4.22921300	-3.41692900
H	3.97579400	3.37624900	-3.65599600
H	4.22391500	5.17631200	-1.93667900
H	2.97386900	4.41423700	-0.93245300
H	4.50568900	3.58516300	-1.19880300
C	-1.28948800	5.63758800	-0.72904500
C	-0.31917600	5.99116100	0.41550300
H	-2.16376500	6.29669300	-0.67749700
H	-0.80661100	5.85005200	-1.69219300
H	-0.00405300	7.03926300	0.35658500
H	-0.79528100	5.82859400	1.38891300
H	0.57607000	5.36058400	0.37749100
C	-4.05948200	4.42296200	0.42812700
C	-4.02919200	4.37256100	1.96844300
H	-5.00846600	4.00248500	0.06963900
H	-4.05043900	5.46906000	0.10084500
H	-4.88543500	4.90520400	2.39795300

H	-4.05373100	3.33710400	2.32602600
H	-3.11072900	4.83190100	2.35069200
C	-6.09150000	-0.53320500	1.05992000
C	-5.92713400	-0.14914600	2.54379700
H	-6.82436700	-1.34423000	0.97656300
H	-6.51713000	0.31664800	0.50981900
H	-6.88306300	0.16411900	2.97923500
H	-5.54682300	-0.99863500	3.12181400
H	-5.21196800	0.67336200	2.65805300
C	-4.96867000	-3.53384500	0.57181300
C	-4.43659400	-4.12262900	1.89342600
H	-4.81084700	-4.25828300	-0.23815400
H	-6.05384700	-3.39776500	0.64799300
H	-4.91837500	-5.08072200	2.12015900
H	-3.35429300	-4.28487800	1.84235700
H	-4.62672500	-3.43576600	2.72558200
C	3.22148800	1.79945500	0.87536800
C	1.99746800	2.40580100	1.50381500
C	1.94746900	2.22823600	2.98706300
C	2.96440600	1.69410200	3.73464600
C	4.29155600	1.34779100	3.08776700
C	4.25009600	1.33104500	1.58250600
H	1.01407200	2.48555700	3.48312400
H	5.05137800	2.06542800	3.44087500
H	4.62603400	0.37320200	3.46453300
C	2.75869400	1.30645200	5.10128400
H	3.63883200	1.06057400	5.69706600
H	1.97462800	1.82409100	5.65615400
H	2.11566500	0.08057200	4.90963500
H	1.09562600	1.95176400	1.06471500
H	1.91803700	3.47513400	1.23606200
H	3.22952400	1.72961900	-0.20610600
H	5.09910100	0.88021500	1.07322100

³TS4

N	-2.70295600	-0.72030400	-0.46386700
N	-0.24573900	-1.90691500	-1.52275900
N	0.83947900	0.75976400	-1.92056500
N	-1.57368700	1.91531000	-0.84339500
C	-3.76356900	0.00619900	0.00135700
C	-4.81841500	-0.89140700	0.44327900
C	-4.36250700	-2.16652500	0.23207400
C	-3.03005300	-2.04667800	-0.33961100
C	-2.20802100	-3.11385500	-0.68939400

C	-0.91999100	-3.05714200	-1.21635100
C	-0.07944000	-4.20691200	-1.51182000
C	1.10378600	-3.71564800	-1.99985700
C	0.97924800	-2.26707100	-2.00852600
C	1.96774500	-1.37015700	-2.41201700
C	1.90890900	0.01774800	-2.37492700
C	2.96626200	0.91062600	-2.81794300
C	2.50108200	2.19062000	-2.65856700
C	1.17142000	2.08288100	-2.08040000
C	0.36814200	3.15191200	-1.69903300
C	-0.88677800	3.08170600	-1.10625700
C	-1.68001700	4.21949700	-0.68333300
C	-2.85632200	3.72324800	-0.18107600
C	-2.78958500	2.27943600	-0.29587700
C	-3.79729100	1.39784500	0.07502900
H	2.89355700	-1.80394700	-2.77143800
H	-2.61276700	-4.10558400	-0.52089800
H	-4.70311600	1.83983200	0.47459400
H	0.76812100	4.14467000	-1.87101300
C	-1.77564200	-0.25300800	-3.17180300
H	-2.40409800	-1.14404000	-3.16693900
H	-2.36146800	0.65408600	-3.34697500
H	-0.94322400	-0.34904400	-3.87170400
C	-0.14892200	-0.32807400	0.78055200
C	-0.89121200	0.02061400	1.92606400
C	1.11857300	-0.88011700	0.97051400
C	-0.35542000	-0.15459500	3.19354600
H	-1.88249900	0.45117500	1.82696500
C	1.67982700	-1.08568000	2.23720800
H	1.73180600	-1.15842900	0.12578800
C	0.93334600	-0.71437600	3.40021600
O	1.37052700	-0.85198800	4.64028700
Ir	-0.91125700	0.02826400	-1.16455400
H	-0.91155900	0.12745500	4.08356400
C	3.03599800	-1.69665900	2.23265700
O	3.65207300	-1.99016900	1.21789200
O	3.55753500	-1.91336400	3.46195200
C	4.84793100	-2.53661700	3.46659900
H	4.81298600	-3.50569200	2.96013600
H	5.58705200	-1.90681900	2.96080600
H	5.10539700	-2.66099600	4.51932800
C	-0.44912700	-5.63318900	-1.22484300
C	-0.32128000	-5.98884800	0.26989500
H	0.19138100	-6.30221100	-1.81133500

H	-1.47753500	-5.82898800	-1.55757300
H	-0.60186300	-7.03287900	0.45117500
H	0.70812200	-5.84289400	0.61419700
H	-0.96513800	-5.34782000	0.88213200
C	2.35593500	-4.46663400	-2.34673800
C	3.33328900	-4.54146000	-1.15536900
H	2.85511400	-3.99036000	-3.20066300
H	2.10072200	-5.48135200	-2.67567200
H	4.26807400	-5.03491400	-1.44713400
H	3.56612600	-3.54658600	-0.76334400
H	2.88846200	-5.11231700	-0.33254500
C	4.33522200	0.45683200	-3.23206900
C	5.21861300	0.12704900	-2.00953700
H	4.82054700	1.23429000	-3.83365000
H	4.26202600	-0.42672200	-3.87921900
H	6.19191900	-0.26776600	-2.32308000
H	5.39210900	1.02829700	-1.41079900
H	4.73636200	-0.60971400	-1.35743700
C	3.20188500	3.48590000	-2.95859800
C	3.79800700	4.17744800	-1.71667500
H	2.50086600	4.17373800	-3.45049900
H	4.00282900	3.30347200	-3.68451700
H	4.27040100	5.12740400	-1.99183700
H	3.02497100	4.38376000	-0.96851100
H	4.55088200	3.54441700	-1.23680400
C	-1.21630200	5.64624600	-0.73490100
C	-0.23503000	5.98916900	0.40338500
H	-2.08119900	6.31732200	-0.68019300
H	-0.73603700	5.84981200	-1.70125200
H	0.09290700	7.03307300	0.34067700
H	-0.70739700	5.83431000	1.37983400
H	0.65191400	5.34741200	0.36136800
C	-3.99137700	4.47561500	0.45079600
C	-3.94679400	4.42406600	1.99077900
H	-4.95052200	4.07071300	0.10155400
H	-3.96835600	5.52147600	0.12355500
H	-4.79034700	4.97003400	2.42850300
H	-3.98422400	3.38903000	2.34837500
H	-3.01762700	4.86872500	2.36433200
C	-6.10155100	-0.44969900	1.08511300
C	-5.92012000	-0.07272900	2.56886800
H	-6.84762700	-1.24892800	1.00496800
H	-6.51789100	0.40838100	0.54064500
H	-6.86767600	0.25480700	3.01200100

H	-5.54968200	-0.93001400	3.14169000
H	-5.19073300	0.73751600	2.68053400
C	-5.02785300	-3.46536500	0.58418700
C	-4.50005400	-4.06030300	1.90480800
H	-4.88298300	-4.19274900	-0.22557100
H	-6.11076900	-3.31397700	0.66373900
H	-4.99427900	-5.01154700	2.13352100
H	-3.42022000	-4.23733400	1.85127200
H	-4.67860300	-3.37034800	2.73692500
C	3.25499000	1.80830200	0.87237400
C	2.03755500	2.43664600	1.49243600
C	1.96471100	2.24244200	2.97364700
C	2.96230000	1.68288300	3.72679100
C	4.29193600	1.32287800	3.09270600
C	4.26697900	1.31592700	1.58699500
H	1.02776200	2.50573500	3.45983700
H	5.05789300	2.02740600	3.45897400
H	4.60804300	0.34110100	3.46660900
C	2.73742400	1.28500800	5.09012500
H	3.61363700	1.04892700	5.69632600
H	1.94891600	1.80626100	5.63589400
H	2.12120400	0.06456200	4.90629400
H	1.13113100	2.00969100	1.03570400
H	1.98948100	3.51108200	1.23881000
H	3.27090300	1.74142100	-0.20922300
H	5.11123200	0.84945100	1.08403100

8

C	-0.27744600	-1.22482600	0.00020300
C	-1.04607600	-0.06805700	0.00005400
C	-0.36711600	1.29662500	-0.00037600
C	1.13705800	1.24591400	0.00022200
C	1.84704500	0.11651500	0.00029500
C	1.22110300	-1.25241200	-0.00032700
H	-0.71322000	1.87217500	-0.87296300
H	-0.78895600	-2.18605900	0.00048900
H	1.65015100	2.20655400	0.00051700
H	2.93492700	0.15790900	0.00067700
H	1.58475300	-1.82661500	-0.87110800
H	1.58541000	-1.82783600	0.86932000
H	-0.71387000	1.87303900	0.87138100
C	-2.43711600	-0.11395600	0.00014800
H	-2.96929600	-1.06093400	0.00013600
H	-3.03461400	0.79294500	0.00023800

OSST5

N	1.87666300	1.87120900	-0.69151300
N	-0.75889300	1.16536500	-1.75593300
N	-0.08240800	-1.64481800	-1.49040400
N	2.55419900	-0.93326200	-0.52936200
C	3.13472300	2.00682400	-0.16826500
C	3.42175400	3.41482100	0.05672800
C	2.31343100	4.11158900	-0.34977800
C	1.35137400	3.13032400	-0.82524400
C	0.06985900	3.42209600	-1.28375900
C	-0.91141500	2.52254300	-1.69113300
C	-2.26886300	2.87801100	-2.07313200
C	-2.91143500	1.70772200	-2.38333100
C	-1.95047400	0.63724900	-2.16692500
C	-2.22132200	-0.72542700	-2.27982500
C	-1.36990900	-1.77769000	-1.96277100
C	-1.69738900	-3.18801300	-2.09184900
C	-0.57314100	-3.89094100	-1.74423000
C	0.43976600	-2.91105500	-1.38460600
C	1.74443000	-3.20418200	-0.99885200
C	2.72396500	-2.29811300	-0.60273200
C	4.05487700	-2.65006000	-0.14226600
C	4.68126200	-1.47856800	0.19709900
C	3.73917100	-0.40509800	-0.06373300
C	3.99508400	0.94924900	0.11533000
H	-3.21520400	-0.99341200	-2.61949100
H	-0.20467400	4.47075000	-1.30340300
H	4.97255800	1.21050600	0.50542200
H	2.02152800	-4.25240800	-0.98769900
C	1.54691500	0.28578000	-3.08756100
H	1.54910700	1.34139900	-3.36936700
H	2.55958200	-0.12732000	-3.14392800
H	0.86133400	-0.27796600	-3.72676900
C	-0.28843000	0.58926400	0.84545900
C	0.06449200	1.66033700	1.68078800
C	-1.60014200	0.14696200	0.90333700
C	-0.88572700	2.30677200	2.47454900
H	1.08967500	2.01665200	1.71279500
C	-2.58583600	0.77130000	1.69015100
H	-1.91478700	-0.72245400	0.34086600
C	-2.22317900	1.89460300	2.47834400
O	-3.08278200	2.59823200	3.26102700
Ir	0.88671400	0.10576800	-1.06721400

H	-0.60958900	3.14614900	3.10641100
C	-3.92550000	0.16465100	1.64376200
O	-4.24277100	-0.83527600	1.02260200
O	-4.86034800	0.84610200	2.38567800
C	-6.17822500	0.27397700	2.39620700
H	-6.58793900	0.24503500	1.38326500
H	-6.14585500	-0.74201200	2.79850900
H	-6.77551200	0.92465500	3.03599200
C	-2.84475300	4.25981200	-1.97203500
C	-3.18199200	4.63037800	-0.51246800
H	-3.75151000	4.33107000	-2.58425800
H	-2.14201100	4.99763400	-2.38182500
H	-3.58909100	5.64605900	-0.44542800
H	-3.91887800	3.93361700	-0.09796100
H	-2.29165200	4.56972600	0.12267900
C	-4.34884400	1.51167100	-2.77097100
C	-5.24515000	1.13564100	-1.57449900
H	-4.42577000	0.73058500	-3.53903100
H	-4.72967200	2.42908300	-3.23561100
H	-6.28784400	1.01034300	-1.89089700
H	-4.90984900	0.20669900	-1.10524700
H	-5.21113900	1.91865800	-0.80770700
C	-3.05736100	-3.71353700	-2.44695000
C	-4.01842500	-3.69388400	-1.24047400
H	-2.97248700	-4.73776200	-2.82908700
H	-3.48743000	-3.12042200	-3.26453700
H	-5.01974900	-4.03442700	-1.52962300
H	-3.64909500	-4.35695400	-0.44955800
H	-4.10161500	-2.68914600	-0.81297400
C	-0.38960200	-5.37938900	-1.66619200
C	-0.48749300	-5.92375500	-0.22746400
H	0.58395400	-5.65828200	-2.09129800
H	-1.14372200	-5.87419700	-2.28918800
H	-0.34125200	-7.00990000	-0.20566700
H	0.26830900	-5.46377000	0.41891900
H	-1.47027800	-5.70141500	0.20349400
C	4.55901000	-4.05590800	0.00868100
C	4.03087500	-4.73489900	1.28822200
H	5.65514700	-4.05577000	0.02688500
H	4.27084300	-4.65427700	-0.86571800
H	4.39836900	-5.76437400	1.37019300
H	4.35279700	-4.18245600	2.17802900
H	2.93539100	-4.75915800	1.29525800
C	6.04446700	-1.29050000	0.79717900

C	5.99241900	-1.06083500	2.32054100
H	6.55064300	-0.44104300	0.31964700
H	6.66468700	-2.16945900	0.58610400
H	6.99764800	-0.91600400	2.73300900
H	5.39132900	-0.17705800	2.56199500
H	5.53410700	-1.91935400	2.82422800
C	4.67398600	3.93939100	0.69728100
C	4.67190200	3.76632500	2.22897800
H	4.79497000	5.00163700	0.45447800
H	5.55201200	3.43084300	0.27683500
H	5.59988000	4.14639300	2.67190500
H	3.83034800	4.30708100	2.67636600
H	4.56799300	2.71019400	2.50208200
C	2.04228700	5.58352200	-0.23679800
C	1.19503300	5.92303700	1.00639800
H	1.52682100	5.94232700	-1.13731800
H	2.98956600	6.13364400	-0.19064800
H	0.98020800	6.99671300	1.05857200
H	0.24372000	5.37975300	0.99153500
H	1.72348900	5.63325600	1.92167800
C	-3.04794200	-2.50628800	3.69210400
C	-2.59067300	-3.25569000	2.46960500
C	-1.21053200	-2.88610100	2.02823700
C	-0.40549300	-1.97693800	2.67544900
C	-0.87845100	-1.27323900	3.93464000
C	-2.28676200	-1.61920700	4.33627500
H	-0.85523900	-3.32550500	1.09943500
H	-0.19106600	-1.50236900	4.76451400
H	-0.79472700	-0.18853600	3.78058100
C	0.81694500	-1.59604900	2.10740900
H	1.46072300	-0.86102800	2.57632600
H	1.20435300	-2.11312300	1.24487500
H	-3.96557300	2.19068500	3.17891100
H	-3.28933800	-3.05840800	1.64179700
H	-2.65348000	-4.34544900	2.64074900
H	-4.06155600	-2.70629100	4.03577600
H	-2.68159600	-1.09661900	5.20620500

³TS5

N	1.72398500	1.93951900	-0.75663600
N	-0.89990400	1.01567000	-1.67447000
N	0.02657700	-1.73128200	-1.46405200
N	2.61568100	-0.80445000	-0.59394000
C	2.99621400	2.18389100	-0.32427000

C	3.17389500	3.60966600	-0.10060000
C	1.97720000	4.20605400	-0.40378500
C	1.07350500	3.14726100	-0.82325300
C	-0.25629800	3.32814400	-1.18934500
C	-1.17272400	2.35109800	-1.57251500
C	-2.55424200	2.59263400	-1.95214300
C	-3.07585600	1.38402700	-2.33934600
C	-2.02772200	0.39728400	-2.13799600
C	-2.17422900	-0.98193400	-2.27588100
C	-1.25231500	-1.96217200	-1.92555800
C	-1.49786500	-3.39420000	-1.97449600
C	-0.33853300	-4.01121000	-1.58354100
C	0.61744400	-2.95662600	-1.28701300
C	1.93869900	-3.14786700	-0.89455200
C	2.86620900	-2.16081200	-0.57945400
C	4.22822200	-2.39846300	-0.14384500
C	4.79503900	-1.17107500	0.09052600
C	3.78325800	-0.17472000	-0.19907100
C	3.95261800	1.19777900	-0.08358400
H	-3.13682200	-1.33115800	-2.63163600
H	-0.62482700	4.34762000	-1.16984500
H	4.92773400	1.53873000	0.24582500
H	2.27778300	-4.17460500	-0.81711200
C	1.33252600	0.38852600	-3.17634400
H	1.25357900	1.44902100	-3.42483900
H	2.36159100	0.03734900	-3.31139900
H	0.63452400	-0.20240700	-3.77513600
C	-0.08309300	0.30919100	0.89890700
C	0.23096400	1.49848000	1.66694400
C	-1.48998700	-0.00096000	0.87730800
C	-0.72089700	2.22929500	2.34150500
H	1.26700000	1.81599200	1.73140300
C	-2.46586000	0.70968400	1.56651800
H	-1.82301200	-0.87163800	0.33219300
C	-2.08933400	1.87745500	2.29123900
O	-2.95259600	2.69400800	2.94160700
Ir	0.87407200	0.08888100	-1.08112100
H	-0.45110900	3.10883000	2.91958600
C	-3.83565100	0.16616200	1.49394400
O	-4.16278700	-0.89671700	1.00144700
O	-4.77757100	0.99728700	2.05519000
C	-6.11909200	0.47885900	2.09230300
H	-6.49232400	0.32214000	1.07769300
H	-6.14118200	-0.46952100	2.63510000

H	-6.71091300	1.23558000	2.60845300
C	-3.26803500	3.90106600	-1.78156100
C	-3.61808900	4.16264600	-0.30081600
H	-4.18675500	3.90373800	-2.37986800
H	-2.65368700	4.72869000	-2.16096700
H	-4.15002500	5.11384500	-0.18248000
H	-4.24949000	3.35993200	0.09626100
H	-2.71544800	4.19130200	0.31814100
C	-4.47007600	1.08778000	-2.81428800
C	-5.42912700	0.68328200	-1.67907300
H	-4.44282900	0.28894800	-3.56656200
H	-4.87077900	1.96969800	-3.32887800
H	-6.43410500	0.48243500	-2.06948800
H	-5.07141000	-0.20854100	-1.15760600
H	-5.50415100	1.48723900	-0.93747900
C	-2.83277000	-4.01282600	-2.26887600
C	-3.77342700	-3.95245600	-1.04688900
H	-2.69931200	-5.05669600	-2.57638200
H	-3.30571800	-3.50466700	-3.11959300
H	-4.75888400	-4.36764400	-1.28902000
H	-3.35453500	-4.52939700	-0.21471300
H	-3.90448300	-2.92410600	-0.69387900
C	-0.07673400	-5.47709600	-1.39281100
C	-0.15910600	-5.90868600	0.08491800
H	0.91432300	-5.73438200	-1.79043600
H	-0.79745800	-6.05820700	-1.97977000
H	0.06092700	-6.97680800	0.19571100
H	0.55051200	-5.34429100	0.69967700
H	-1.16035900	-5.72003600	0.48734900
C	4.82244500	-3.75809900	0.08182800
C	4.37118700	-4.37996100	1.41875900
H	5.91646600	-3.69111600	0.06505000
H	4.54715100	-4.42880900	-0.74274500
H	4.80184100	-5.37880400	1.55371500
H	4.68492500	-3.75287700	2.26056500
H	3.27992000	-4.46577000	1.46273400
C	6.16393200	-0.86550100	0.62590400
C	6.15166200	-0.55475300	2.13575500
H	6.59735900	-0.01493400	0.08331600
H	6.83061000	-1.71508500	0.43806900
H	7.16006800	-0.32596700	2.49931500
H	5.50485800	0.30241300	2.35356000
H	5.76694900	-1.41006000	2.70215700
C	4.41979400	4.23888800	0.45191500

C	4.54096000	4.06894400	1.97928200
H	4.43298800	5.30715500	0.20585200
H	5.30521500	3.80582700	-0.03246400
H	5.46189900	4.52834400	2.35666300
H	3.68998100	4.53620500	2.48731000
H	4.54806200	3.00850900	2.25555600
C	1.58368500	5.64525100	-0.24078500
C	0.80162800	5.88788000	1.06618600
H	0.97405800	5.96850100	-1.09477800
H	2.47867900	6.27838100	-0.25069300
H	0.49558500	6.93659700	1.15556800
H	-0.09515200	5.26001600	1.10779200
H	1.41906800	5.63472300	1.93546900
C	-2.93035800	-2.51184700	3.97307400
C	-2.50547200	-3.27554500	2.74757500
C	-1.18991900	-2.81029200	2.19167400
C	-0.41429900	-1.84492300	2.74599300
C	-0.81650700	-1.16970400	4.04272400
C	-2.17679500	-1.57090700	4.54663600
H	-0.88819200	-3.23794800	1.23705100
H	-0.05703700	-1.37553100	4.81631700
H	-0.78176000	-0.07988900	3.90170700
C	0.71853800	-1.29504000	2.03399400
H	1.45973700	-0.73208700	2.59840800
H	1.13962200	-1.91023100	1.25106400
H	-3.85395000	2.33651300	2.81998300
H	-3.27868600	-3.16762000	1.97017700
H	-2.47632200	-4.35700400	2.97316900
H	-3.90714600	-2.75504300	4.39005700
H	-2.54067300	-1.04937600	5.43148200

9

C	0.38574100	0.23524400	0.91831600
C	0.40782100	1.55866300	0.43661200
C	-0.79675100	-0.47777800	0.79093100
C	-0.71282500	2.13870100	-0.13389000
H	1.33089700	2.12915700	0.50614700
C	-1.95589100	0.08129000	0.21336800
H	-0.86187200	-1.50399100	1.13993600
C	-1.91212100	1.41616400	-0.25564100
O	-2.94969200	2.06828500	-0.82701000
H	-0.69725700	3.15887100	-0.50383100
C	-3.14174100	-0.80018800	0.14376600
O	-3.19653000	-1.94815800	0.53352100

O	-4.23442200	-0.18992800	-0.42551300
C	-5.41939400	-1.00095300	-0.51996800
H	-5.22479800	-1.88621900	-1.13058100
H	-5.74207600	-1.31724400	0.47512800
H	-6.17225000	-0.36575800	-0.98759200
C	4.98311300	-0.40629000	-1.27236000
C	5.13046200	0.42113400	-0.02298000
C	3.92139800	0.35766300	0.87289000
C	2.82327400	-0.36033100	0.60982900
C	2.68982500	-1.19028100	-0.64703200
C	3.89370600	-1.12555400	-1.54806300
H	3.97009800	0.93931700	1.79358200
H	2.48349100	-2.23866100	-0.36999900
H	1.78972700	-0.87373800	-1.19829900
C	1.63074500	-0.37488500	1.54272400
H	1.40553300	-1.40966200	1.83735200
H	1.88399500	0.16549700	2.46455200
H	3.84437800	-1.70546600	-2.46843600
H	5.82107500	-0.39960400	-1.96759600
H	5.33986900	1.47038100	-0.29184900
H	6.02544900	0.09864600	0.53580200
H	-3.71527100	1.46127700	-0.85331500

Ir

N	1.59372700	1.28187300	-0.23452400
N	-1.28237000	1.59468200	-0.23812600
N	-1.59627600	-1.28043000	-0.23810600
N	1.27951800	-1.59568200	-0.23439000
C	2.92482300	0.93279700	-0.24023400
C	3.74629900	2.13109000	-0.22812800
C	2.88842600	3.19976800	-0.22779500
C	1.54081900	2.65703300	-0.23990700
C	0.37099800	3.40830300	-0.25469200
C	-0.93343900	2.92647700	-0.24300600
C	-2.13183600	3.74732100	-0.23093900
C	-3.20053400	2.88923200	-0.23141900
C	-2.65811900	1.54181100	-0.24361400
C	-3.40990300	0.37225000	-0.25613800
C	-2.92822400	-0.93199000	-0.24360800
C	-3.74859200	-2.13061000	-0.23139400
C	-2.89019400	-3.19908000	-0.23150100
C	-1.54292100	-2.65618600	-0.24314400
C	-0.37319500	-3.40817900	-0.25440400
C	0.93117700	-2.92706000	-0.23963200

C	2.12992100	-3.74774400	-0.22732700
C	3.19816900	-2.88930700	-0.22826000
C	2.65460400	-1.54199100	-0.24020700
C	3.40590900	-0.37186700	-0.25479200
H	-4.48787600	0.48991500	-0.26885500
H	0.48830200	4.48631500	-0.26814600
H	4.48387300	-0.48954400	-0.26960100
H	-0.49123500	-4.48611000	-0.26769200
C	0.05004200	-0.00420600	-2.35907700
H	-0.34716900	0.94822100	-2.72244200
H	1.08903900	-0.12812000	-2.67857200
H	-0.56048600	-0.83533300	-2.72438400
Ir	-0.00178600	0.00009400	-0.29830600
C	-2.13908200	5.24696200	-0.15671400
C	-1.86766700	5.77298300	1.26637500
H	-3.10712200	5.62791400	-0.50284400
H	-1.38872800	5.65970600	-0.84430300
H	-1.86807700	6.86902300	1.28915000
H	-2.63390200	5.41389000	1.96256200
H	-0.89709400	5.42180100	1.63410100
C	-4.66318800	3.22016300	-0.15750700
C	-5.23489000	3.06847700	1.26571400
H	-5.22814200	2.57652200	-0.84502700
H	-4.82623600	4.24760600	-0.50363600
H	-6.30494300	3.30563300	1.28916500
H	-5.10132500	2.04483400	1.63296400
H	-4.71822500	3.73878600	1.96173900
C	-5.24823700	-2.13821200	-0.15747700
C	-5.77442300	-1.86678000	1.26554500
H	-5.62899600	-3.10630900	-0.50364100
H	-5.66093300	-1.38790900	-0.84513800
H	-6.87046300	-1.86711200	1.28818400
H	-5.41547200	-2.63300500	1.96181600
H	-5.42320100	-0.89622200	1.63327700
C	-3.22082400	-4.66181200	-0.15752200
C	-3.06924100	-5.23358500	1.26568000
H	-2.57713700	-5.22672500	-0.84505500
H	-4.24824400	-4.82497100	-0.50366900
H	-3.30658400	-6.30359900	1.28904200
H	-2.04562300	-5.10023300	1.63306200
H	-3.73952600	-4.71684100	1.96167000
C	2.13728000	-5.24734400	-0.15316900
C	1.86439100	-5.77339800	1.26962200
H	3.10565400	-5.62827100	-0.49838000

H	1.38757300	-5.66004000	-0.84150900
H	1.86462800	-6.86944200	1.29236800
H	2.62995600	-5.41440700	1.96660300
H	0.89349200	-5.42207900	1.63637800
C	4.66105100	-3.21932000	-0.15514500
C	5.23419900	-3.06536200	1.26724300
H	5.22511500	-2.57648700	-0.84420800
H	4.82422200	-4.24719700	-0.49992900
H	6.30430000	-3.30240100	1.28995300
H	5.10094800	-2.04119600	1.63315200
H	4.71826100	-3.73466900	1.96476700
C	5.24597800	2.13774000	-0.15512400
C	5.77317600	1.86458000	1.26719300
H	5.62699400	3.10595900	-0.50067200
H	5.65784600	1.38791600	-0.84384600
H	6.86924000	1.86459500	1.28903900
H	5.41490500	2.63012200	1.96456400
H	5.42197500	0.89369700	1.63411300
C	3.21908500	4.66243600	-0.15368200
C	3.06544200	5.23447800	1.26919400
H	2.57632900	5.22723100	-0.84218800
H	4.24699100	4.82551600	-0.49843800
H	3.30261400	6.30453300	1.29274100
H	2.04129900	5.10104900	1.63510300
H	3.73479200	4.71790500	1.96620900

CSS^{TS6}

N	-0.94090600	1.60648300	-1.33406500
N	-0.78709200	-1.29403600	-1.52368300
N	2.06118800	-1.16720000	-0.95020600
N	1.91555300	1.73270700	-0.78719900
C	-0.81196900	2.96630000	-1.19907600
C	-2.12208700	3.58852500	-1.28752800
C	-3.02816300	2.57704500	-1.48336600
C	-2.27191500	1.33678500	-1.53245800
C	-2.80942500	0.07080400	-1.75478500
C	-2.12691300	-1.14126000	-1.77589400
C	-2.71722500	-2.44030000	-2.06804900
C	-1.70269400	-3.35849000	-1.99902900
C	-0.49277900	-2.62502700	-1.65807000
C	0.76667100	-3.18845900	-1.47364800
C	1.93819700	-2.52466600	-1.11572200
C	3.20789400	-3.16320300	-0.82224400
C	4.08818300	-2.16189300	-0.48753200

C	3.36168400	-0.90996600	-0.59256300
C	3.89941700	0.35528400	-0.36995300
C	3.23966300	1.57735400	-0.47159400
C	3.83557900	2.88155800	-0.22615100
C	2.84439700	3.81039600	-0.41407800
C	1.64074000	3.07450300	-0.76672900
C	0.38526500	3.63911000	-0.97434400
H	0.83994500	-4.26303900	-1.59907400
H	-3.87762100	0.02600000	-1.93169200
H	0.32518000	4.71964300	-0.91534700
H	4.94971400	0.39335500	-0.10306700
C	0.97931100	0.30108400	-3.19264800
H	0.19304100	0.86610000	-3.70744800
H	1.94555400	0.78995800	-3.36298800
H	1.01128700	-0.71601600	-3.60077500
C	0.10318200	0.20644200	0.99366000
C	0.56068200	1.33726500	1.77727900
C	-1.21194700	-0.27790900	1.29976000
C	-0.36950000	2.21164600	2.23326400
H	1.61960300	1.57348900	1.80907600
C	-2.18289300	0.54921300	1.78641800
H	-1.47668700	-1.29594300	1.03887400
C	-1.82167100	1.94560000	2.14232300
O	-2.64061500	2.84033100	2.36262000
Ir	0.55669500	0.21853200	-1.11747300
H	-0.09916300	3.19273900	2.61373200
C	-3.53309700	-0.04281600	1.95999000
O	-3.84027700	-1.15639600	1.55447100
O	-4.38147100	0.73102200	2.65701400
C	-5.69111500	0.18024200	2.85270500
H	-6.18631800	0.01981500	1.89050400
H	-5.63664400	-0.77395800	3.38523200
H	-6.23091900	0.92251000	3.44125900
C	-4.17212800	-2.68798700	-2.34468700
C	-4.99100200	-2.93605800	-1.06294700
H	-4.27425700	-3.55163500	-3.01371600
H	-4.59725900	-1.83598300	-2.88999700
H	-6.05203300	-3.07881300	-1.30102400
H	-4.63323000	-3.83457300	-0.54722100
H	-4.89143700	-2.10393400	-0.36103700
C	-1.77769400	-4.84609200	-2.18787900
C	-1.78970600	-5.62427300	-0.85784900
H	-0.93094900	-5.18806400	-2.79810500
H	-2.68132600	-5.09657300	-2.75571800

H	-1.84677400	-6.70501900	-1.03233400
H	-0.88317700	-5.42109800	-0.27625400
H	-2.64905900	-5.32783300	-0.24678800
C	3.44311200	-4.64638700	-0.82095100
C	2.94264300	-5.32998100	0.46658700
H	4.51384900	-4.84853700	-0.94191900
H	2.95009700	-5.10356300	-1.68878600
H	3.12799500	-6.40994700	0.43780000
H	3.45048600	-4.91777200	1.34585600
H	1.86778000	-5.17060600	0.60422800
C	5.50857000	-2.28792100	-0.01833900
C	5.63441700	-2.15273400	1.51229100
H	6.13312700	-1.52516700	-0.50167200
H	5.91712500	-3.25626500	-0.32967700
H	6.67909400	-2.23503200	1.83369300
H	5.24648500	-1.18501500	1.85032000
H	5.05695000	-2.93569400	2.01712700
C	5.24989600	3.10255900	0.22628800
C	5.44118400	2.81647800	1.72895200
H	5.54735000	4.13654500	0.01609000
H	5.93277600	2.46704000	-0.35304900
H	6.48247600	2.97372000	2.03331900
H	4.80425400	3.47482400	2.33057800
H	5.16681200	1.78241600	1.96711700
C	2.90372600	5.29527300	-0.20165300
C	2.34389000	5.71301100	1.17295100
H	2.34435100	5.81103100	-0.99301100
H	3.94057500	5.64073800	-0.28905500
H	2.38333900	6.80060900	1.30312300
H	1.30203700	5.39208000	1.28421600
H	2.92134600	5.24896800	1.98067700
C	-2.38098800	5.05523800	-1.09576000
C	-2.28520200	5.49580500	0.37882200
H	-3.37668200	5.30249400	-1.48139400
H	-1.67151300	5.63902500	-1.69858100
H	-2.51162200	6.56393200	0.47923400
H	-2.97331500	4.92253700	1.00539200
H	-1.27950500	5.32009200	0.77593500
C	-4.52628100	2.66372600	-1.52098700
C	-5.17326600	2.13524300	-0.22373300
H	-4.91876300	2.10357500	-2.38110900
H	-4.82556600	3.70639700	-1.67539300
H	-6.25424400	2.31963800	-0.22387500
H	-5.01469300	1.05618100	-0.12420700

H	-4.72978500	2.60990400	0.65700500
C	1.48576900	-1.27551100	3.53065500
C	1.32116100	-1.87119000	2.18097200
C	0.26851200	-2.90820800	2.07487700
C	-0.68570000	-3.07643900	3.00789000
C	-0.66543100	-2.28499100	4.29347800
C	0.56683400	-1.44601800	4.48901000
H	0.98024800	-0.98210300	1.44032000
H	0.22029500	-3.46218200	1.14208300
H	-1.56071300	-1.64097900	4.32810500
H	0.69467500	-0.97496700	5.46139800
H	2.26331500	-2.14196400	1.69256300
H	2.36171200	-0.65525100	3.70496300
H	-0.79101500	-2.97077700	5.14762300
C	-1.86542600	-3.98460000	2.80422700
H	-2.77107900	-3.37820400	2.65629900
H	-1.74223800	-4.61650500	1.92039800
H	-2.03925900	-4.62931900	3.67589900

³TS6

N	-1.13997000	1.11404400	-1.55399900
N	-0.21432500	-1.64171300	-1.49075000
N	2.43789300	-0.74580800	-0.79359400
N	1.56310300	2.00904900	-0.87769700
C	-1.37976200	2.45776900	-1.46614000
C	-2.79953800	2.71252000	-1.65555600
C	-3.38968900	1.49686200	-1.88767400
C	-2.33281100	0.50057300	-1.81384800
C	-2.50721000	-0.87652500	-1.94228300
C	-1.54012900	-1.86354900	-1.79957900
C	-1.77038400	-3.28974300	-1.95707700
C	-0.55973200	-3.90938500	-1.78697800
C	0.40761800	-2.86602600	-1.49182000
C	1.75167500	-3.07060100	-1.19965600
C	2.68258000	-2.10217100	-0.84122500
C	4.04491300	-2.36471500	-0.42106100
C	4.61758800	-1.14976200	-0.13612300
C	3.61207600	-0.13739600	-0.39161000
C	3.79808300	1.23271500	-0.25804100
C	2.85507600	2.23299800	-0.48599400
C	3.06900700	3.65820800	-0.29612800
C	1.87871400	4.27612900	-0.58274000
C	0.93817200	3.22900500	-0.94524200
C	-0.41189800	3.42772900	-1.21982000

H	2.10210900	-4.09641000	-1.21744500
H	-3.51352100	-1.21618800	-2.15770700
H	-0.75894500	4.45447700	-1.20286500
H	4.78277500	1.55828200	0.05827500
C	0.96318400	0.45705500	-3.23920000
H	0.19597700	-0.10469600	-3.77811500
H	0.89718100	1.52180100	-3.47267400
H	1.96330000	0.07319100	-3.46632000
C	-0.16387700	0.44229900	0.96686300
C	0.10169800	1.67345200	1.65273300
C	-1.44806400	-0.13834600	1.15804600
C	-0.89416800	2.34258600	2.30173000
H	1.10491700	2.08846000	1.62623100
C	-2.48041200	0.49640400	1.81856900
H	-1.64270600	-1.12237100	0.75071800
C	-2.27231400	1.84957500	2.37074200
O	-3.16439800	2.55654100	2.87312000
Ir	0.66938600	0.17322300	-1.15482000
H	-0.71712400	3.29978700	2.78541900
C	-3.74811500	-0.26836700	1.92342400
O	-3.87370700	-1.43278600	1.55471200
O	-4.77098400	0.41594300	2.46510500
C	-5.99263400	-0.32020300	2.60604100
H	-6.37928500	-0.62147100	1.62811700
H	-5.83807300	-1.21681200	3.21394400
H	-6.68523400	0.36428300	3.09716100
C	-3.11873600	-3.91572600	-2.16068100
C	-3.89890400	-4.04476100	-0.83565400
H	-3.00221100	-4.90688900	-2.61518500
H	-3.70544900	-3.32283200	-2.87439700
H	-4.89906800	-4.45842600	-1.01052600
H	-3.37012100	-4.71098700	-0.14461200
H	-4.00123400	-3.07783900	-0.33301100
C	-0.24616700	-5.37747800	-1.83380500
C	-0.18752100	-6.03475200	-0.44154400
H	0.71148900	-5.53386800	-2.34784600
H	-1.00066500	-5.89184900	-2.44036800
H	0.08139000	-7.09464900	-0.51776000
H	0.55161600	-5.54024900	0.19886000
H	-1.15906200	-5.96454200	0.05871300
C	4.62745700	-3.73625000	-0.23980300
C	4.16359400	-4.39943000	1.07287200
H	5.72196800	-3.67781700	-0.24863400
H	4.35172000	-4.37661500	-1.08799900

H	4.58403200	-5.40625800	1.17633800
H	4.47858600	-3.80482000	1.93760700
H	3.07125900	-4.47664800	1.10922800
C	5.98184200	-0.87199000	0.42514900
C	5.94528600	-0.59742700	1.94178400
H	6.43237400	-0.01266900	-0.08892000
H	6.64300700	-1.72351700	0.22765900
H	6.94841200	-0.38694400	2.32980800
H	5.30238300	0.26083800	2.16746100
H	5.54237200	-1.46246000	2.48041000
C	4.34307900	4.27092700	0.20899400
C	4.50423200	4.12664200	1.73534500
H	4.37088800	5.33395200	-0.05728100
H	5.20516000	3.81063600	-0.29198400
H	5.44487500	4.57323800	2.07763000
H	3.67822900	4.62127400	2.25833000
H	4.49758300	3.07156700	2.03173300
C	1.52422400	5.72823000	-0.44405500
C	0.80730300	6.02822100	0.88819600
H	0.88490500	6.04110000	-1.27981200
H	2.43208000	6.33908600	-0.51220700
H	0.53602000	7.08755900	0.96086200
H	-0.10596000	5.43105500	0.98586400
H	1.45413700	5.78024500	1.73726400
C	-3.45437100	4.05058700	-1.47488800
C	-3.57973900	4.43268100	0.01493500
H	-4.45028300	4.03749200	-1.93264100
H	-2.88666600	4.82673800	-2.00637900
H	-4.08132400	5.40070800	0.12850800
H	-4.14307900	3.67939500	0.57399300
H	-2.59492500	4.49825900	0.48927100
C	-4.84488200	1.19198000	-2.09694800
C	-5.53388900	0.65394800	-0.82822600
H	-4.95929800	0.46213200	-2.91002700
H	-5.36031400	2.09943600	-2.43191500
H	-6.60166000	0.48188300	-1.00906500
H	-5.08393800	-0.29033400	-0.50638400
H	-5.43167700	1.36179900	0.00078000
C	1.30981200	-0.79527700	3.55844400
C	1.31843000	-1.45621400	2.24344700
C	0.40086600	-2.59327700	2.09570700
C	-0.63728600	-2.80012700	2.93381600
C	-0.83017500	-1.93448800	4.15534200
C	0.30528800	-0.98815400	4.42961700

H	0.80544500	-0.57692500	1.45441600
H	0.50738700	-3.20922200	1.20797300
H	-1.76701600	-1.36166600	4.03955300
H	0.28609400	-0.45142600	5.37566300
H	2.30010700	-1.57481200	1.78051300
H	2.10509200	-0.08740700	3.78028700
H	-1.00966200	-2.57421700	5.03612900
C	-1.68366400	-3.84889700	2.68753800
H	-2.65005000	-3.36562700	2.49163400
H	-1.43571500	-4.46751200	1.82017800
H	-1.81189300	-4.50479100	3.55990000

²INT2

N	0.90534900	-1.34002900	-1.05077000
N	1.05051800	1.54464900	-0.90222900
N	-1.80692300	1.66617200	-0.45419200
N	-1.96420200	-1.22473700	-0.67085400
C	0.63822800	-2.68988000	-1.09202900
C	1.88067900	-3.43315600	-1.21883500
C	2.89067200	-2.50793600	-1.27174100
C	2.26530700	-1.19861400	-1.18154500
C	2.93772000	0.01917100	-1.23266000
C	2.38632700	1.28892900	-1.11386300
C	3.12459300	2.54060300	-1.15627500
C	2.21419300	3.54250500	-0.95128300
C	0.91628600	2.91039900	-0.80049200
C	-0.28113300	3.58031100	-0.57653500
C	-1.53912200	3.01319300	-0.39826200
C	-2.76057800	3.74522400	-0.11302000
C	-3.76371100	2.81647600	-0.00731500
C	-3.15722100	1.51576700	-0.23162600
C	-3.83166800	0.29870700	-0.21357500
C	-3.28767400	-0.96811800	-0.40307100
C	-4.02017900	-2.21972200	-0.31844200
C	-3.11470200	-3.22384200	-0.55204400
C	-1.82971000	-2.58530300	-0.77539600
C	-0.62698900	-3.25387400	-0.99536600
H	-0.22640700	4.66182700	-0.52314300
H	4.01148000	-0.03133500	-1.36938100
H	-0.67961300	-4.33447600	-1.06171900
H	-4.89841700	0.34175200	-0.02293600
C	-0.80621400	0.27124600	-2.84917800
H	-0.14881400	1.03189400	-3.28208500
H	-0.59664600	-0.70673500	-3.29315300

H	-1.85439200	0.54103600	-3.01155400
C	-0.72554300	-0.25088300	2.07706700
C	-0.94125700	-1.64614700	2.18972000
C	0.58453800	0.26785400	2.08136300
C	0.13120500	-2.49879700	2.22691300
H	-1.95674300	-2.03097600	2.19227800
C	1.69473900	-0.56246600	2.16275200
H	0.74348100	1.33970200	2.03086500
C	1.50786200	-2.01898400	2.16939600
O	2.44832000	-2.84324700	2.10026900
Ir	-0.45596800	0.16627600	-0.81877700
H	0.00808300	-3.57598300	2.26354800
C	3.01982300	0.11160400	2.25350900
O	3.18898400	1.29422400	2.00118000
O	4.00247400	-0.69000900	2.69974200
C	5.28413200	-0.06749000	2.85782100
H	5.68765600	0.23723800	1.88786800
H	5.21245400	0.81260700	3.50345700
H	5.92119700	-0.82970500	3.30738500
C	4.61045900	2.67864400	-1.33782300
C	5.35820600	2.94305500	-0.01706300
H	4.81628300	3.49746500	-2.04009500
H	5.01460300	1.77613400	-1.81103900
H	6.44379200	2.93048100	-0.17241000
H	5.08566600	3.92213500	0.39100400
H	5.08874500	2.19673100	0.73422400
C	2.47267900	5.01489600	-0.81479900
C	2.42255500	5.49181400	0.65102800
H	1.74222200	5.58455900	-1.40580800
H	3.45650200	5.25114700	-1.23724200
H	2.64159900	6.56354100	0.72329300
H	1.43382600	5.31426500	1.08818300
H	3.14935700	4.94449600	1.25994600
C	-2.83655600	5.23005400	0.09622800
C	-2.34944300	5.65763600	1.49463200
H	-3.86936800	5.56952800	-0.04514000
H	-2.24121500	5.74698200	-0.66816400
H	-2.40607100	6.74541700	1.61727100
H	-2.96122600	5.19120500	2.27509400
H	-1.31140500	5.34739400	1.65878600
C	-5.20614800	3.03627400	0.34690400
C	-5.50587400	2.73247600	1.82802300
H	-5.84793500	2.41110000	-0.28814700
H	-5.48506400	4.07379200	0.12890200

H	-6.56605300	2.89014800	2.05765200
H	-5.25267700	1.69473900	2.07309900
H	-4.91216800	3.38090700	2.48215700
C	-5.47170600	-2.33774800	0.04666000
C	-5.71553200	-2.18329900	1.56085600
H	-5.85718800	-3.30963400	-0.28297600
H	-6.05721200	-1.58142100	-0.49286600
H	-6.78231500	-2.26033200	1.80081100
H	-5.18164300	-2.96130300	2.11852700
H	-5.35315600	-1.21234800	1.91725200
C	-3.33067300	-4.70836400	-0.49263100
C	-2.88115300	-5.31472600	0.85167300
H	-2.78881600	-5.20076100	-1.31081900
H	-4.39132600	-4.93459600	-0.65307500
H	-3.03650100	-6.39954300	0.86978000
H	-1.81818400	-5.11846900	1.03193100
H	-3.44516600	-4.87315000	1.68124400
C	1.98344500	-4.93134100	-1.20473100
C	1.75166400	-5.54021100	0.19329600
H	2.97515900	-5.22868400	-1.56373800
H	1.26409000	-5.36265000	-1.91504700
H	1.91929700	-6.62352600	0.17751100
H	2.41471500	-5.08055000	0.93079200
H	0.72520100	-5.36157400	0.53276600
C	4.37220600	-2.74274200	-1.33634400
C	5.08403700	-2.45555000	0.00043300
H	4.81438000	-2.11996800	-2.12694700
H	4.56171500	-3.78130100	-1.63027500
H	6.14963000	-2.70560900	-0.06633700
H	4.99518800	-1.39861100	0.26782900
H	4.62656000	-3.02123800	0.81577600
H	-1.57167100	0.42697200	2.04355100

CSS^{TS7}

N	-2.39679200	-0.89938000	-0.94488500
N	0.30448300	-1.79896300	-1.46064700
N	1.18730300	0.94438800	-1.71184300
N	-1.49863100	1.85465800	-1.09450100
C	-3.58413100	-0.27886200	-0.63290100
C	-4.59541000	-1.27891100	-0.33770200
C	-3.99440800	-2.50345700	-0.48113100
C	-2.61546600	-2.25259800	-0.86070100
C	-1.63843600	-3.22956600	-1.02178400
C	-0.28458200	-3.02420900	-1.24902900

C	0.72781000	-4.06670300	-1.27581900
C	1.92181100	-3.45196700	-1.54135400
C	1.64305200	-2.02919300	-1.66765100
C	2.59015800	-1.04708400	-1.94032000
C	2.39024700	0.32914200	-1.96275100
C	3.42057600	1.33532000	-2.17313300
C	2.81711500	2.55413400	-2.01614100
C	1.41790400	2.29883700	-1.72946300
C	0.46552600	3.27596400	-1.46424800
C	-0.87133500	3.07657800	-1.13512600
C	-1.80553000	4.12030800	-0.75307300
C	-3.00599400	3.50614900	-0.50304900
C	-2.80468300	2.08534300	-0.72705700
C	-3.76740600	1.09741900	-0.54365200
H	3.60042900	-1.39520900	-2.12123200
H	-1.95786600	-4.25903100	-0.90781700
H	-4.76114200	1.43591500	-0.27137800
H	0.80747700	4.30436200	-1.49377600
C	-0.99964100	0.03685800	-3.39651000
H	-0.92602800	1.06708000	-3.75991000
H	-0.26043100	-0.59249400	-3.90257400
H	-2.00778100	-0.35230100	-3.57225100
C	-0.77894900	0.12878400	1.59516200
C	-1.27231300	-1.16701300	1.97243900
C	0.59422400	0.28451600	1.33071800
C	-0.41311900	-2.19888900	2.17496300
H	-2.34560300	-1.30882600	2.07503700
C	1.51371700	-0.72015300	1.60813200
H	0.97173100	1.25323000	1.02532900
C	1.04106900	-2.06858200	2.01072800
O	1.78195400	-3.04266800	2.21671500
Ir	-0.61388200	0.02180900	-1.37214400
H	-0.76188600	-3.19032200	2.44696000
C	2.93752200	-0.35142000	1.50271600
O	3.33859800	0.77191200	1.20182200
O	3.79292700	-1.33107700	1.86769400
C	5.18374000	-0.99291000	1.85626100
H	5.53884900	-0.85261200	0.83189200
H	5.37341700	-0.07694400	2.42368500
H	5.68935600	-1.84457800	2.31294400
C	0.47488200	-5.50579600	-0.93077300
C	0.22713400	-5.71249400	0.57847400
H	1.33516300	-6.11004700	-1.24010100
H	-0.38402400	-5.88906100	-1.49963700

H	0.15702300	-6.77982900	0.81989900
H	1.02621900	-5.25827400	1.17232000
H	-0.70829300	-5.23282500	0.88736900
C	3.29110000	-4.06526700	-1.59251600
C	4.12787200	-3.75403900	-0.33598400
H	3.82743000	-3.71578200	-2.48632100
H	3.19556400	-5.15120300	-1.70516300
H	5.07429200	-4.30828200	-0.35136900
H	4.35507600	-2.68627000	-0.27940000
H	3.57571100	-3.99912100	0.57577500
C	4.87619300	1.06508300	-2.43870600
C	5.78294200	1.40645600	-1.23999400
H	5.20279000	1.64172400	-3.31506300
H	5.01637800	0.01296700	-2.71057900
H	6.80065000	1.02804900	-1.39498200
H	5.84734500	2.48951600	-1.09456800
H	5.37286000	0.98343800	-0.31968500
C	3.45561900	3.91281500	-2.01702600
C	3.65266900	4.46853900	-0.59105300
H	2.84848800	4.61913900	-2.59975700
H	4.42685300	3.85856000	-2.52294800
H	4.15842300	5.44124500	-0.61260000
H	2.68911600	4.59418900	-0.08499400
H	4.24596100	3.77529100	0.01348500
C	-1.43570600	5.56224900	-0.55952400
C	-0.69449100	5.79978300	0.77202900
H	-2.33734200	6.18538100	-0.58698800
H	-0.80404800	5.90575100	-1.38939800
H	-0.40660400	6.85133900	0.88668200
H	-1.33227300	5.52491000	1.62068100
H	0.21187500	5.18575100	0.82531600
C	-4.27528900	4.11641600	0.01691100
C	-4.44205500	3.92184000	1.53723500
H	-5.14167200	3.68222800	-0.49946100
H	-4.29242200	5.18829900	-0.21287400
H	-5.38016900	4.36199400	1.89496400
H	-4.44271700	2.85646000	1.79470700
H	-3.61368600	4.39392600	2.07849200
C	-5.98916600	-0.97334900	0.12991100
C	-6.04410000	-0.60147900	1.62503100
H	-6.63663700	-1.83997100	-0.04850000
H	-6.41306400	-0.15168500	-0.46256400
H	-7.06815400	-0.36853000	1.93961300
H	-5.67573800	-1.42943200	2.24150600

H	-5.41472700	0.27154200	1.83262100
C	-4.56646200	-3.86195800	-0.19625200
C	-4.18136000	-4.37879600	1.20447700
H	-4.22517500	-4.58015100	-0.95314800
H	-5.65925000	-3.82929800	-0.28070300
H	-4.59064200	-5.37956100	1.38505000
H	-3.09249300	-4.42773600	1.31586600
H	-4.56329900	-3.70647200	1.98132500
C	0.24981500	0.23972400	4.42766700
C	-0.61293300	1.17901200	3.81145000
C	-0.12477700	2.48669800	3.45280800
C	1.18939500	2.77445100	3.57198400
C	2.18196300	1.75792500	4.03597800
C	1.60324200	0.44223400	4.47763700
H	-0.82525700	3.22097700	3.06418700
H	2.90277400	1.58626200	3.21334200
H	2.80366100	2.17201900	4.84884500
H	-1.68413600	1.02111400	3.86821000
H	-0.16324300	-0.70559200	4.76428600
H	-1.47867100	0.90814900	1.32401000
H	1.57042600	3.75458100	3.29726700
C	2.54309100	-0.59794400	5.01205600
H	3.10790500	-1.06254300	4.19296700
H	3.26978000	-0.16073400	5.70877100
H	2.00209000	-1.39984500	5.52263700

³TS7

N	-1.84331800	0.61792100	-1.20435200
N	-0.19697500	-1.77236500	-1.45228100
N	2.18396100	-0.15040400	-1.26817100
N	0.56207700	2.21897600	-0.92815900
C	-2.44103900	1.82819600	-1.01023200
C	-3.87889700	1.70003900	-1.16373400
C	-4.12217300	0.39407100	-1.51011200
C	-2.83651500	-0.28311400	-1.49348300
C	-2.63990500	-1.65063200	-1.64480900
C	-1.43442100	-2.34690300	-1.55912500
C	-1.30491600	-3.79280800	-1.57570400
C	0.03655800	-4.07008100	-1.50805700
C	0.72002800	-2.79012000	-1.44215700
C	2.09927300	-2.60364700	-1.38430500
C	2.78056000	-1.39364600	-1.31104100
C	4.22060900	-1.24504200	-1.21742000
C	4.47853100	0.09894400	-1.12186200

C	3.19623900	0.77765500	-1.15060100
C	3.00442700	2.14477500	-0.98008100
C	1.79090100	2.81826800	-0.85367300
C	1.63417400	4.23402400	-0.56631900
C	0.28810700	4.47136300	-0.47478300
C	-0.37962700	3.20409600	-0.72144100
C	-1.75465800	3.01884100	-0.75614800
H	2.70871000	-3.50055100	-1.39972300
H	-3.52961600	-2.24903400	-1.80541800
H	-2.36396400	3.89536800	-0.57427300
H	3.90079700	2.74929700	-0.89552700
C	0.02684900	0.50477700	-3.29483900
H	-0.69297000	-0.21636500	-3.69369900
H	-0.31332700	1.52544800	-3.49618900
H	1.01005400	0.33963100	-3.74814300
C	1.52090300	0.26747300	1.76158800
C	1.49891800	1.65810400	2.20236300
C	0.28478100	-0.27632300	1.25129200
C	0.33797300	2.33097600	2.35538800
H	2.44667400	2.14061600	2.43230600
C	-0.96102800	0.33623100	1.65554600
H	0.25894400	-1.34903700	1.09581300
C	-0.97490100	1.73111600	2.06798200
O	-2.00599300	2.44044700	2.16072700
Ir	0.19880200	0.23233500	-1.21406700
H	0.31593900	3.36504800	2.68295500
C	-2.14070300	-0.53833800	1.69163100
O	-2.08705200	-1.75310800	1.50061900
O	-3.29143900	0.07910500	2.03745600
C	-4.38455200	-0.78655100	2.34718700
H	-4.54920500	-1.52015800	1.55736000
H	-4.19642500	-1.31669400	3.28788600
H	-5.25195900	-0.13363700	2.45405200
C	-2.46318100	-4.74349100	-1.50773700
C	-3.00883400	-4.85902700	-0.06852000
H	-2.15965000	-5.73371900	-1.86758300
H	-3.26704000	-4.41185200	-2.17824200
H	-3.90960100	-5.48340800	-0.03627100
H	-2.25555600	-5.30823200	0.58863800
H	-3.24011600	-3.87062900	0.34220200
C	0.70940800	-5.40985600	-1.43401800
C	1.15657000	-5.77361200	-0.00531900
H	1.58207600	-5.42876400	-2.10118000
H	0.02729800	-6.18238400	-1.80740400

H	1.63593500	-6.75904800	0.02146000
H	1.86740700	-5.03376700	0.37642900
H	0.29894000	-5.78661800	0.67650200
C	5.19100600	-2.38887200	-1.15194200
C	5.24429100	-3.04168900	0.24368400
H	6.19333200	-2.03904400	-1.42496300
H	4.92274400	-3.14956100	-1.89702800
H	5.93724200	-3.89071500	0.25781300
H	5.57667100	-2.31633600	0.99507500
H	4.25395500	-3.39917800	0.54622200
C	5.79748800	0.78156900	-0.90324500
C	6.03907900	1.12613200	0.58031500
H	5.85082900	1.69980300	-1.50288200
H	6.61054200	0.13912600	-1.26088800
H	7.00008700	1.63482400	0.71787900
H	5.24713600	1.77946900	0.96392900
H	6.04087500	0.21633600	1.19115600
C	2.76831600	5.18453800	-0.31495200
C	3.36079000	5.03463400	1.10039600
H	2.42083500	6.21511000	-0.45161000
H	3.56194000	5.03131200	-1.05869200
H	4.18599700	5.73801700	1.26094700
H	2.59391300	5.22278600	1.85977600
H	3.74041800	4.01899800	1.26007400
C	-0.41998400	5.74160700	-0.10316100
C	-0.83894200	5.76721500	1.38144500
H	-1.31041600	5.86820800	-0.73309400
H	0.22517400	6.60183700	-0.31785800
H	-1.42008000	6.66909600	1.60685600
H	-1.43541200	4.88632300	1.64267700
H	0.04814300	5.76697800	2.02599900
C	-4.86837900	2.78516100	-0.86219900
C	-5.18344700	2.84030100	0.64826500
H	-5.79276000	2.62048800	-1.42947000
H	-4.47977200	3.75722100	-1.19160400
H	-5.82672600	3.69658300	0.88345400
H	-5.70285100	1.92598800	0.95759900
H	-4.26320500	2.90256000	1.23725800
C	-5.43334500	-0.23993500	-1.88339200
C	-6.10572800	-1.05601500	-0.76567900
H	-5.28210400	-0.88872200	-2.75667400
H	-6.12425000	0.54619800	-2.21015400
H	-7.06024600	-1.47087300	-1.10985900
H	-5.47045600	-1.88888000	-0.44612200

H	-6.29969800	-0.42882500	0.10986000
C	0.69151000	-0.93165800	4.17110900
C	1.93748900	-0.78590800	3.41866100
C	2.50650100	-2.02039400	2.87996000
C	1.78491500	-3.15335200	2.79679400
C	0.37720000	-3.25136500	3.31384000
C	-0.06361500	-2.04801600	4.11478200
H	2.43185100	-0.04140800	1.25967700
H	3.52081700	-1.98794800	2.48841800
H	-0.32694300	-3.38302700	2.47405800
H	2.65938100	-0.08142700	3.83200800
H	0.33709800	-0.06765700	4.72945300
H	0.26336100	-4.16687700	3.92036400
H	2.22226100	-4.04981300	2.36397500
C	-1.39503500	-2.16795900	4.79952000
H	-2.17251000	-2.39756800	4.05925800
H	-1.39670700	-2.98795200	5.53212000
H	-1.67334300	-1.24368200	5.31657600

10

C	1.06932400	1.48533100	-1.09491200
C	0.67627900	2.69455200	-0.30573000
C	0.00178700	0.44742800	-1.14960500
C	-0.43793600	2.74155800	0.43963700
H	1.36936000	3.53476300	-0.31689000
C	-1.11210600	0.46591300	-0.39372500
H	0.19447400	-0.42036100	-1.77362000
C	-1.38838200	1.60767500	0.52780500
O	-2.31238800	1.61823000	1.33236800
H	-0.69311200	3.60499500	1.04763600
C	-1.99741900	-0.73845500	-0.45856300
O	-1.58159800	-1.86568500	-0.66971600
O	-3.29515500	-0.44667000	-0.29610600
C	-4.18738900	-1.57189200	-0.32940800
H	-4.14090300	-2.07216400	-1.30135300
H	-3.92474600	-2.29149500	0.45124700
H	-5.18097500	-1.15904400	-0.15394000
C	2.13300700	0.32787500	0.92040500
C	2.39762400	0.82262400	-0.47857900
C	2.89071300	-0.27626200	-1.38619400
C	2.69426300	-1.56727800	-1.10779900
C	1.99787200	-2.02808200	0.14531300
C	1.91614300	-0.95942300	1.21338700
H	1.34108300	1.78609700	-2.11896500

H	3.38201100	0.02530900	-2.30993100
H	0.97282800	-2.35614200	-0.10172500
H	3.13478700	1.63836200	-0.45531400
H	2.04174000	1.08383600	1.69723000
H	2.49903100	-2.92134000	0.54771800
H	3.03374200	-2.33473200	-1.80093400
C	1.54144500	-1.42966400	2.59227300
H	0.56733300	-1.93767300	2.57128600
H	2.26898100	-2.15845400	2.97560300
H	1.47614300	-0.60034800	3.30375500

11

C	2.40198100	-1.30561600	0.12894500
C	3.03041500	-0.04376400	0.10991200
C	1.00191100	-1.40970200	0.05358300
C	2.26583800	1.09643000	0.00748700
H	4.11334200	0.02176400	0.17079300
C	0.19448100	-0.28699000	-0.03270000
H	0.52515100	-2.38476800	0.06498900
C	0.81202300	1.04523400	-0.08638800
O	0.16493900	2.10655200	-0.23696000
H	2.70678000	2.08768700	-0.02790700
C	-1.28128600	-0.53237100	-0.08308200
O	-1.75864100	-1.61885700	-0.36091100
O	-2.01783500	0.53930000	0.24061700
C	-3.43949600	0.33388800	0.20822300
H	-3.76086200	0.03263100	-0.79292000
H	-3.73266200	-0.44250700	0.92121100
H	-3.87559200	1.29500900	0.48095600
H	3.00092900	-2.20843000	0.20502800

CSS^{TS8}

C	2.80540500	1.33977400	-0.17757700
C	2.38473400	2.72335200	-0.24627300
C	2.16168200	0.54181300	0.80972200
C	1.26531700	3.15058800	0.39492300
H	2.94434800	3.40169700	-0.88888400
C	0.97755500	0.91169200	1.41866800
H	2.54717200	-0.45415100	0.99876900
C	0.41079700	2.25526700	1.18523900
O	-0.71223200	2.63723300	1.55425900
H	0.89824300	4.16716300	0.28752900
C	0.31199800	-0.16461600	2.19623700
O	0.85491400	-1.21685600	2.50495500

O	-0.99072700	0.06922800	2.46171000
C	-1.69059400	-1.03707300	3.05455200
H	-1.63302700	-1.91376800	2.40230100
H	-1.26683900	-1.28742600	4.03105200
H	-2.72321200	-0.69931900	3.15828100
C	5.24226500	1.18469600	0.37152400
C	4.19892000	0.94632500	-0.69637400
C	4.23835500	-0.46682700	-1.23024500
C	5.09940700	-1.41078000	-0.83064100
C	6.12571100	-1.15103000	0.24784200
C	6.08689000	0.24660400	0.80196700
H	1.83776100	0.85212500	-1.20389700
H	3.50312900	-0.70156800	-1.99903900
H	5.98934600	-1.88149700	1.06330500
H	6.79867800	0.47933600	1.59234700
H	4.40446900	1.62779300	-1.54035900
H	5.25563900	2.18040600	0.81161100
H	7.13314300	-1.36881400	-0.14640000
C	5.12598300	-2.79090000	-1.43535200
H	4.97236300	-3.56488200	-0.66976300
H	4.35974000	-2.91534400	-2.20756800
H	6.10431600	-2.99727900	-1.89173900
C	-2.83340600	1.30700500	-0.29969500
C	-2.11653700	2.31632100	-1.13050800
C	-2.15073700	-0.00999000	-0.27556000
C	-0.92207100	2.06541700	-1.70632400
H	-2.58554400	3.29069300	-1.24534300
C	-0.92858500	-0.26002000	-0.80691200
H	-2.66647900	-0.82219200	0.22483800
C	-0.21932400	0.81718700	-1.49429300
O	0.97096600	0.69869800	-1.97295900
H	-0.38643400	2.81620700	-2.27723400
C	-0.38450400	-1.63523700	-0.55054500
O	-1.07808500	-2.55127400	-0.14597600
O	0.93648500	-1.73527800	-0.73968200
C	1.53108100	-2.95465200	-0.25014200
H	1.31606900	-3.05545100	0.81613500
H	1.14164300	-3.81730200	-0.79690200
H	2.59860400	-2.82882600	-0.41932400
C	-4.49422100	0.48951000	-2.03175600
C	-4.35847200	1.14508700	-0.68095700
C	-5.07615600	0.38655400	0.40535500
C	-5.59676400	-0.83778100	0.25793300
C	-5.54956700	-1.56211500	-1.06833800

C	-5.00944200	-0.72943000	-2.19909200
H	-2.80171200	1.68135900	0.73799100
H	-5.12234100	0.87769700	1.37738800
H	-4.94362900	-2.47791000	-0.96055900
H	-5.04949500	-1.16997800	-3.19367200
H	-4.75771200	2.17072400	-0.72594300
H	-4.10063500	1.04153400	-2.88337400
H	-6.55829800	-1.92757300	-1.32145000
C	-6.26042100	-1.57773600	1.38869400
H	-5.75904200	-2.53791100	1.57340300
H	-6.24647400	-1.00113300	2.31922100
H	-7.30615900	-1.81244200	1.14639600

CSST9

N	0.22563900	-1.85505300	-1.25528200
N	1.05417200	0.92127700	-1.52945300
N	-1.64683800	1.77280900	-0.88241100
N	-2.48381100	-0.99867500	-0.64197900
C	-0.35198200	-3.09049700	-1.10030600
C	0.66107600	-4.12340500	-1.24191400
C	1.84546600	-3.48214400	-1.50058500
C	1.55479500	-2.05735100	-1.53117800
C	2.47628000	-1.05290000	-1.81741100
C	2.24981500	0.31901500	-1.83416100
C	3.23558500	1.33661000	-2.17146100
C	2.60328000	2.54773200	-2.06380200
C	1.23102800	2.27294200	-1.66713200
C	0.24465000	3.23294800	-1.45870400
C	-1.07677600	3.00893600	-1.08027000
C	-2.05081300	4.04299200	-0.78417700
C	-3.20981400	3.40349600	-0.41286100
C	-2.95080800	1.97866500	-0.49583900
C	-3.87597200	0.97396600	-0.22338200
C	-3.66840400	-0.40052900	-0.29906000
C	-4.66136900	-1.42243600	-0.00568200
C	-4.04864800	-2.63430600	-0.19570100
C	-2.67907000	-2.35455500	-0.59646000
C	-1.69804400	-3.31426900	-0.82910600
H	0.53828800	4.26752800	-1.59871400
H	3.48369600	-1.37769100	-2.04809300
H	-2.00826300	-4.35014200	-0.75702300
H	-4.86969600	1.29798800	0.06543300
C	-1.14030000	-0.10424100	-3.11624100
H	-0.24072700	-0.40359800	-3.66578600

H	-1.94272300	-0.82493600	-3.31027300
H	-1.45422600	0.88979300	-3.45553300
C	-0.22587500	-0.13107500	1.14450400
C	-0.94606700	-1.14201900	1.89444600
C	1.19720100	-0.11522000	1.30287000
C	-0.29542700	-2.28385400	2.22966800
H	-2.02220600	-1.05148900	2.00998300
C	1.89790100	-1.22905100	1.66429200
H	1.74928200	0.77809400	1.03769600
C	1.15816300	-2.46078600	2.03260700
O	1.68644200	-3.56619900	2.18223500
Ir	-0.71121300	-0.04055300	-1.05749300
H	-0.82371200	-3.15700400	2.60151900
C	3.37466600	-1.08804700	1.70338900
O	3.98013200	-0.16542000	1.17637700
O	3.98843900	-2.03892100	2.42800300
C	5.41363300	-1.91239300	2.51620100
H	5.86797100	-1.99015100	1.52392300
H	5.69093400	-0.95052500	2.95784700
H	5.73845800	-2.73833400	3.14969900
C	4.66779300	1.08088400	-2.54758200
C	5.64089100	1.19686100	-1.35871700
H	4.96685700	1.79031700	-3.33030200
H	4.76211300	0.08561300	-2.99826500
H	6.66773800	0.97872900	-1.67657600
H	5.62321000	2.21235900	-0.94625200
H	5.36120900	0.51250900	-0.55425900
C	3.17650400	3.91800600	-2.28580500
C	3.49325600	4.66834300	-0.97754700
H	2.48068900	4.52059600	-2.88537800
H	4.09468500	3.83507800	-2.87901200
H	3.91492600	5.65896500	-1.18379800
H	2.59054400	4.80391700	-0.37154200
H	4.21438100	4.10675600	-0.37447300
C	-1.77596300	5.51926100	-0.82132500
C	-1.05465600	6.02717800	0.44227400
H	-2.71934600	6.06529300	-0.93880400
H	-1.17329700	5.76485500	-1.70538000
H	-0.87214000	7.10654300	0.38676500
H	-1.65433900	5.82625600	1.33736000
H	-0.08987200	5.52504400	0.57292700
C	-4.49528200	4.01172500	0.06807900
C	-4.62815900	3.96694900	1.60327000
H	-5.34935700	3.49096700	-0.38437400

H	-4.56158300	5.05262200	-0.26921500
H	-5.57704800	4.40594200	1.93228200
H	-4.58295000	2.93435200	1.96753500
H	-3.81018600	4.52170800	2.07711400
C	-6.05233000	-1.14549400	0.48653500
C	-6.08847200	-0.78618900	1.98510900
H	-6.68709600	-2.02191200	0.31122300
H	-6.49944100	-0.32676300	-0.09288300
H	-7.11168600	-0.57778300	2.31869200
H	-5.69160600	-1.61055700	2.58846100
H	-5.47454100	0.09863800	2.18874000
C	-4.59942800	-4.00855900	0.05235500
C	-4.16688700	-4.57539400	1.41941000
H	-4.27495600	-4.69267500	-0.74259900
H	-5.69437200	-3.98347200	0.00205700
H	-4.56633700	-5.58420700	1.57465800
H	-3.07467200	-4.62403900	1.49353400
H	-4.52583700	-3.93456400	2.23288800
C	0.41042200	-5.59150700	-1.04822300
C	0.20107500	-5.98143600	0.42903700
H	1.25556600	-6.15980400	-1.45290300
H	-0.46679700	-5.89830900	-1.63513300
H	0.07519600	-7.06614200	0.52819000
H	1.04559400	-5.65760200	1.04237800
H	-0.69108600	-5.49625100	0.84031400
C	3.21897400	-4.07429300	-1.63170900
C	4.10755700	-3.78242300	-0.40453300
H	3.70986800	-3.69406500	-2.53870000
H	3.13358700	-5.15839800	-1.76541900
H	5.05567700	-4.32920400	-0.47303400
H	4.33839800	-2.71403400	-0.33811500
H	3.59741100	-4.06058100	0.52239300
C	3.25358800	2.48856700	3.69419000
C	2.88849500	3.22124900	2.43135200
C	1.43548800	3.10836200	2.07916500
C	0.54058100	2.38641300	2.78823300
C	0.91964900	1.66407500	4.06307900
C	2.37587100	1.79396800	4.41996300
H	1.11964800	3.55442900	1.13861600
H	0.28912800	2.02850300	4.89098300
H	0.65757900	0.59899000	3.95782300
C	-0.78339000	2.10576800	2.23891600
H	-1.53981400	1.74696600	2.93862900
H	-1.17679900	2.81488800	1.51188900

H	-0.68033200	1.08578300	1.44097400
H	2.70316800	1.27253300	5.31736900
H	4.29771200	2.53087100	3.99725000
H	3.47474000	2.81193800	1.59107400
H	3.18947800	4.28006400	2.49308100

³TS9

N	0.41891400	-1.71222400	-1.40492700
N	0.88607900	1.13469700	-1.58124000
N	-1.84770800	1.65427800	-0.81645000
N	-2.35865400	-1.20582800	-0.68427100
C	-0.00931900	-3.01196300	-1.27652900
C	1.12179600	-3.91640700	-1.42164500
C	2.22491700	-3.13496400	-1.64230500
C	1.76392700	-1.75393600	-1.65342200
C	2.56012200	-0.63618800	-1.89167200
C	2.16113200	0.69342900	-1.88486600
C	3.01363200	1.83239600	-2.16944000
C	2.23723400	2.95622800	-2.03397800
C	0.90799500	2.51246500	-1.66466200
C	-0.17389300	3.34338100	-1.40274400
C	-1.44283700	2.95463300	-0.98263700
C	-2.51980300	3.85537700	-0.61043800
C	-3.57822400	3.07017500	-0.22936400
C	-3.15375100	1.68919100	-0.37965300
C	-3.94462400	0.57428000	-0.12637200
C	-3.58652500	-0.76495800	-0.26970500
C	-4.44482200	-1.90436000	0.00500300
C	-3.70628900	-3.02877000	-0.26991200
C	-2.39666500	-2.57290400	-0.70161200
C	-1.31348600	-3.39999300	-0.99976300
H	-0.00245100	4.40891100	-1.50612200
H	3.60719700	-0.82443500	-2.09566400
H	-1.49773500	-4.46717400	-0.95789800
H	-4.95732300	0.76866400	0.20931900
C	-1.43227100	-0.17905200	-3.08846000
H	-0.76186900	0.41088600	-3.72190900
H	-1.41828800	-1.22969400	-3.38898900
H	-2.44987100	0.21845200	-3.12847600
C	-0.25089000	-0.38002200	1.23433700
C	-0.80356900	-1.56101500	1.82465600
C	1.15888700	-0.22241900	1.24805000
C	0.01434600	-2.58038400	2.22111600
H	-1.88251600	-1.65573800	1.91212000

C	2.01520000	-1.21268000	1.67666100
H	1.59250500	0.71444700	0.92497300
C	1.47420600	-2.51594100	2.09452400
O	2.17597000	-3.52313600	2.30918900
Ir	-0.71630600	-0.02309600	-1.12136300
H	-0.38293400	-3.51054400	2.61821900
C	3.45429400	-0.85303300	1.71575300
O	3.93731300	0.08561500	1.09663400
O	4.18316500	-1.62662700	2.53729400
C	5.57174800	-1.28331200	2.62127200
H	6.05312900	-1.38340600	1.64367900
H	5.69424400	-0.25378300	2.97160100
H	6.00217300	-1.98875900	3.33279300
C	4.47479200	1.76540100	-2.51217100
C	5.39200900	1.91211200	-1.28228400
H	4.71156600	2.55384100	-3.23809100
H	4.69486200	0.81822800	-3.01926100
H	6.44571300	1.83196600	-1.57546200
H	5.24610200	2.89056000	-0.81027300
H	5.17002600	1.14909300	-0.53249200
C	2.64993500	4.39242400	-2.18456600
C	2.86720600	5.10860700	-0.83676500
H	1.89341700	4.93846800	-2.76437500
H	3.57578900	4.44418800	-2.76904100
H	3.17631900	6.14866000	-0.99177900
H	1.95037700	5.11227000	-0.23738100
H	3.64028300	4.60313300	-0.24925300
C	-2.40510300	5.35189500	-0.57189600
C	-1.67259000	5.85621900	0.68745600
H	-3.40523200	5.79912800	-0.61034400
H	-1.87915500	5.71114400	-1.46631400
H	-1.59445800	6.94948700	0.68748700
H	-2.20652800	5.54918700	1.59361100
H	-0.66103600	5.43996300	0.74810000
C	-4.90442700	3.49925900	0.32794500
C	-4.96597600	3.36816700	1.86273300
H	-5.71134400	2.90415100	-0.11997800
H	-5.10382100	4.53959500	0.04609000
H	-5.94407300	3.67931000	2.24720100
H	-4.78763500	2.33265300	2.17356200
H	-4.19651300	3.99006500	2.33359700
C	-5.83622900	-1.81321100	0.56130800
C	-5.84957000	-1.52837400	2.07622800
H	-6.37307800	-2.74867900	0.36545700

H	-6.39819200	-1.02677600	0.04000200
H	-6.87515800	-1.45668700	2.45632300
H	-5.33543000	-2.32674600	2.62313400
H	-5.33337300	-0.58828100	2.30155900
C	-4.08505600	-4.46711400	-0.06647900
C	-3.55261200	-5.02826900	1.26739400
H	-3.70388800	-5.07769400	-0.89532000
H	-5.17629000	-4.56982000	-0.09201900
H	-3.82308800	-6.08331500	1.38931100
H	-2.46122200	-4.94550800	1.31802500
H	-3.96590000	-4.46738500	2.11330300
C	1.04623900	-5.40669000	-1.25063500
C	0.88449600	-5.83836000	0.22115000
H	1.95330100	-5.86424600	-1.66147300
H	0.21221000	-5.80746300	-1.84389200
H	0.88894500	-6.93144900	0.30544600
H	1.68326600	-5.42749800	0.84443800
H	-0.05956200	-5.46930000	0.63685100
C	3.66162700	-3.55749900	-1.74984800
C	4.47449200	-3.21911100	-0.48230200
H	4.13125600	-3.08349500	-2.62330400
H	3.70680100	-4.63717800	-1.93077900
H	5.48124400	-3.64943600	-0.54275600
H	4.57696200	-2.13568000	-0.36461300
H	3.97969600	-3.60003000	0.41711600
C	3.11483200	2.37194600	3.54483100
C	2.64594900	3.14042700	2.33929500
C	1.17264500	2.99876900	2.08419900
C	0.33295400	2.25786300	2.84312100
C	0.81851000	1.53184500	4.08047300
C	2.29953500	1.65441600	4.31990100
H	0.78905200	3.44835000	1.17062700
H	0.25869000	1.89229800	4.95972700
H	0.54809800	0.46712900	3.99343000
C	-1.01836800	1.93752200	2.38748000
H	-1.72558900	1.61047600	3.15378800
H	-1.46301700	2.61260200	1.65883600
H	-0.83608400	0.82445800	1.69017100
H	2.70044300	1.10709900	5.17131600
H	4.18075600	2.40776600	3.76227600
H	3.19054200	2.77967900	1.45049500
H	2.92467000	4.20401600	2.42897300

osSTs10

N	-1.86477700	-0.43755900	-1.30822600
N	0.91331000	-1.23439000	-1.51445500
N	1.73021100	1.48609100	-0.99358700
N	-1.05493400	2.29609100	-0.84918000
C	-3.11442500	0.12879000	-1.20411200
C	-4.13007800	-0.91185900	-1.23845600
C	-3.46868700	-2.10413400	-1.36877900
C	-2.04875900	-1.79306400	-1.43779800
C	-1.03026600	-2.72029000	-1.62929600
C	0.33591500	-2.46936400	-1.68305800
C	1.36678100	-3.46282600	-1.93378100
C	2.56597800	-2.80009200	-1.92451100
C	2.27248200	-1.40211300	-1.65598200
C	3.21647900	-0.38693200	-1.53974800
C	2.97717900	0.94320300	-1.20217800
C	3.99511000	1.95367800	-0.97087900
C	3.33727600	3.09717100	-0.59008700
C	1.91701300	2.80147700	-0.63421400
C	0.89491800	3.71534500	-0.39130400
C	-0.47460100	3.49311100	-0.49805300
C	-1.50976800	4.47832800	-0.23745800
C	-2.71284200	3.85658100	-0.45712500
C	-2.41479000	2.48572300	-0.83333600
C	-3.36102400	1.48556400	-1.03755300
H	4.25331900	-0.66974800	-1.68876700
H	-1.33556000	-3.75306900	-1.74864800
H	-4.40154300	1.78556000	-0.99314900
H	1.20036100	4.71730700	-0.11006100
C	-0.04899800	0.87064500	-3.26011800
H	0.98513300	0.80042500	-3.61279600
H	-0.66597600	0.11011400	-3.74865000
H	-0.44967900	1.86906800	-3.46088100
C	-0.34507500	0.74785600	1.75502300
C	-1.61335500	1.30579000	2.07636100
C	-0.20056500	-0.65987300	1.68835400
C	-2.68667700	0.48783100	2.29275900
H	-1.72571000	2.38630600	2.09592900
C	-1.25281100	-1.51534900	1.94499300
H	0.76959500	-1.08889000	1.46316800
C	-2.59642100	-0.97064100	2.20244400
O	-3.62095500	-1.67227300	2.31608800
Ir	-0.07341400	0.53554200	-1.22647200

H	-3.67580600	0.88441600	2.49910000
C	-0.93012600	-2.96733100	1.96563600
O	0.06634700	-3.44745500	1.44819900
O	-1.80526000	-3.70347500	2.67618800
C	-1.49630700	-5.09973200	2.76548800
H	-1.51344900	-5.56480700	1.77549200
H	-0.50669300	-5.25182500	3.20745200
H	-2.27396100	-5.52800000	3.39873700
C	1.12379800	-4.93396600	-2.11235200
C	1.12837800	-5.70741400	-0.77909900
H	1.88860000	-5.35359400	-2.77802800
H	0.16522300	-5.09333700	-2.62205400
H	0.88691800	-6.76490900	-0.94153000
H	2.11518700	-5.65046200	-0.30617600
H	0.41314000	-5.27651700	-0.07371200
C	3.94130400	-3.37532900	-2.10695400
C	4.69289100	-3.59947700	-0.78054500
H	4.53983600	-2.71887800	-2.75318900
H	3.86421200	-4.33184800	-2.63722400
H	5.67144400	-4.06165300	-0.95580600
H	4.85421900	-2.65257400	-0.25507000
H	4.11566900	-4.25092700	-0.11571200
C	5.47620000	1.75199300	-1.12983600
C	6.15662000	1.09222900	0.08342000
H	5.95058000	2.72231300	-1.31885100
H	5.67081200	1.14489400	-2.02380400
H	7.24115700	1.02774200	-0.06227900
H	5.96752100	1.66760900	0.99704800
H	5.77639600	0.07943200	0.24344300
C	3.92178500	4.40493600	-0.14156300
C	3.90018200	4.55685900	1.39258300
H	3.37298000	5.24073000	-0.59541800
H	4.95516600	4.49179200	-0.49679900
H	4.32056400	5.52017500	1.70371600
H	2.87501300	4.49120200	1.77532800
H	4.48295800	3.75859200	1.86679200
C	-1.25626700	5.87159100	0.26127600
C	-0.92913400	5.90914700	1.76724200
H	-2.13443000	6.49867000	0.06798500
H	-0.42917000	6.32707700	-0.29958500
H	-0.73131600	6.93282200	2.10577400
H	-1.76504100	5.50986000	2.35297600
H	-0.04714000	5.29773100	1.98970500
C	-4.09567000	4.40183200	-0.24569500

C	-4.67956400	4.00926600	1.12616900
H	-4.76527300	4.04550400	-1.03922100
H	-4.07979200	5.49482700	-0.33139800
H	-5.69597500	4.39981300	1.25152800
H	-4.71470100	2.91991400	1.23677500
H	-4.05770600	4.40484600	1.93745600
C	-5.60346200	-0.67051700	-1.07213600
C	-6.00675200	-0.32583600	0.37583200
H	-6.15301600	-1.56260200	-1.39338000
H	-5.92515100	0.13839300	-1.74332600
H	-7.09575700	-0.23133700	0.46175200
H	-5.65379000	-1.08938900	1.07393800
H	-5.55889500	0.62280600	0.69173400
C	-4.03354500	-3.49500100	-1.35026000
C	-3.71454400	-4.24248300	-0.03936600
H	-3.64797100	-4.07057400	-2.20391700
H	-5.12005000	-3.44682600	-1.48356100
H	-4.22209400	-5.21420900	-0.01205900
H	-2.63798800	-4.41960600	0.05069600
H	-4.01389500	-3.65257300	0.83159700
C	3.45951500	-2.33105400	2.66866600
C	3.96046400	-1.02385300	2.11799200
C	3.17460800	0.16226200	2.58190300
C	2.16297400	0.09464300	3.51373000
C	1.82931800	-1.21763100	4.20626100
C	2.50464300	-2.41561000	3.59502800
H	3.37189600	1.11013100	2.08244400
H	2.09243900	-1.14218000	5.27367300
H	0.73999300	-1.36225100	4.18779700
C	1.33357600	1.19988800	3.75854100
H	0.52715700	1.15286200	4.48255100
H	1.56877400	2.17581000	3.34431400
H	0.46439000	1.39025300	1.43957800
H	2.16560500	-3.39064500	3.93766500
H	3.90128800	-3.23468000	2.25541700
H	3.91860100	-1.04680700	1.01858300
H	5.03127800	-0.89083400	2.35315700

³TS10

N	-0.19129800	-2.02905500	-1.20342700
N	1.40063900	0.34532400	-1.70797700
N	-0.91514900	2.01281400	-1.21192200
N	-2.51605700	-0.36941900	-0.83518500
C	-1.07925300	-3.02193500	-0.90433400

C	-0.38522500	-4.30232500	-0.82841800
C	0.92703400	-4.05503100	-1.12484800
C	1.03537900	-2.62998300	-1.39193500
C	2.18750800	-1.97631000	-1.80414100
C	2.36546100	-0.60253100	-1.95047000
C	3.62011100	0.04605200	-2.26732200
C	3.40198500	1.39655000	-2.15852200
C	2.00126500	1.57154700	-1.82214100
C	1.36924500	2.79490500	-1.63136400
C	0.02568300	3.00368100	-1.33435200
C	-0.59567400	4.29716100	-1.10834000
C	-1.92570400	4.06182600	-0.87111500
C	-2.11520800	2.62328500	-0.94399100
C	-3.31328800	1.95236000	-0.71735700
C	-3.50034800	0.57433500	-0.65406200
C	-4.74859000	-0.08510100	-0.31919300
C	-4.50122900	-1.43635200	-0.31287100
C	-3.10342100	-1.61008400	-0.63995900
C	-2.43983900	-2.82707700	-0.68812200
H	1.98739300	3.68017400	-1.72809000
H	3.05554900	-2.59879800	-1.98576400
H	-3.03352800	-3.71330100	-0.49864400
H	-4.18666500	2.56828200	-0.53502400
C	-0.88373300	-0.09383800	-3.32899300
H	-0.30273700	-0.92088800	-3.74784800
H	-1.95176700	-0.25723300	-3.50591900
H	-0.56935300	0.85571200	-3.77168500
C	-1.00633000	0.63615600	1.74009400
C	-1.78662600	-0.48481500	2.25583500
C	0.25783200	0.32053100	1.13115500
C	-1.24842700	-1.71829900	2.38040100
H	-2.82131300	-0.30249400	2.53864200
C	0.92964800	-0.89260600	1.51994500
H	0.90203600	1.14958100	0.86012100
C	0.15250700	-2.01478000	2.02799200
O	0.58815800	-3.18047500	2.16417100
Ir	-0.56378300	-0.01209600	-1.25723900
H	-1.82468200	-2.56272000	2.74756600
C	2.40044700	-0.87853800	1.46066300
O	3.05741000	-0.01657100	0.88524600
O	2.97940200	-1.85748000	2.19195400
C	4.40053800	-1.77082600	2.32349200
H	4.89505900	-1.90837500	1.35925100
H	4.68731000	-0.79960900	2.73679400

H	4.67577000	-2.57660700	3.00597400
C	4.91125300	-0.66217700	-2.55820200
C	5.60839800	-1.19501100	-1.29231300
H	5.58869900	0.02353200	-3.08042600
H	4.73232900	-1.49500000	-3.25133700
H	6.58078900	-1.63747800	-1.53793300
H	5.75696100	-0.39129900	-0.56457500
H	4.99549200	-1.96006400	-0.80694500
C	4.40690400	2.50754000	-2.21806000
C	4.82810300	2.96800000	-0.80653700
H	4.00142600	3.36231100	-2.77557900
H	5.29386400	2.17649000	-2.77036200
H	5.58244200	3.76169500	-0.85892800
H	3.96501900	3.34629300	-0.24809900
H	5.23776600	2.12807500	-0.23604200
C	0.14741200	5.60039900	-1.05485100
C	0.93064900	5.77740000	0.26148400
H	-0.55705500	6.43222500	-1.17053600
H	0.84305800	5.67217800	-1.90162800
H	1.46618000	6.73358900	0.27877700
H	0.25147000	5.74859900	1.12127600
H	1.66223400	4.97215900	0.39167100
C	-2.99369300	5.04277200	-0.48351000
C	-3.23927300	5.06796300	1.03852800
H	-3.93293600	4.80171300	-0.99878000
H	-2.71350000	6.04758400	-0.82047300
H	-4.02666500	5.78340300	1.30240500
H	-3.53940300	4.07815400	1.40122700
H	-2.32438000	5.35154000	1.57125300
C	-6.01556900	0.62903100	0.04980800
C	-5.99008100	1.15561400	1.49918300
H	-6.87020100	-0.04602200	-0.07354700
H	-6.18806500	1.46746900	-0.63768400
H	-6.91750300	1.68626500	1.74291300
H	-5.87171300	0.32812600	2.20769100
H	-5.15073300	1.84365900	1.65031400
C	-5.43026000	-2.55075400	0.07272600
C	-5.22371400	-3.00518700	1.53170700
H	-5.28771400	-3.40785100	-0.59805200
H	-6.46971900	-2.23002300	-0.06282900
H	-5.89539000	-3.83279000	1.78657000
H	-4.19220500	-3.33567100	1.69530000
H	-5.41897100	-2.17876800	2.22441500
C	-1.02776800	-5.58962500	-0.40243500

C	-1.36640000	-5.62592400	1.10228200
H	-0.35768100	-6.42322000	-0.64076000
H	-1.94272400	-5.76118200	-0.98766300
H	-1.75572600	-6.61086000	1.38572500
H	-0.48510300	-5.39172400	1.70411000
H	-2.12353800	-4.87473700	1.35220800
C	2.09914800	-4.98852500	-1.04717200
C	2.96436700	-4.71861400	0.20198300
H	2.71756500	-4.90205500	-1.95195300
H	1.73971200	-6.02347700	-1.02470800
H	3.75681800	-5.47061800	0.29542200
H	3.43066900	-3.72987200	0.14717100
H	2.34954400	-4.71555500	1.10578600
C	3.62857200	1.53986400	3.97982000
C	3.11952900	2.59378200	3.03478100
C	1.62149000	2.66487000	2.98311700
C	0.78761800	1.81732300	3.63634200
C	1.32939400	0.70822400	4.51494400
C	2.82822800	0.69649100	4.63550100
H	1.19143000	3.42532500	2.33159000
H	0.87101600	0.77395800	5.51513200
H	0.98868200	-0.26011300	4.11451800
C	-0.63762200	1.83099800	3.39131300
H	-1.27484900	1.34895600	4.13097100
H	-1.05142100	2.75912500	2.99929600
H	-1.57831000	1.43817300	1.28862000
H	3.25513600	-0.06002700	5.29166800
H	4.70832700	1.47322200	4.10430500
H	3.49766500	2.37830300	2.02158600
H	3.54212700	3.57806400	3.29857700

12

C	0.34582700	-0.28820300	-0.46077700
C	0.40634600	1.19827600	-0.63792500
C	-1.03400200	-0.79526600	-0.19930500
C	-0.66791600	1.98807700	-0.50079600
H	1.38460800	1.62217900	-0.85210300
C	-2.12960700	-0.01891800	-0.07475400
H	-1.15244900	-1.87169500	-0.08917500
C	-2.01500000	1.47062700	-0.16215000
O	-2.94222500	2.23908900	0.05929000
H	-0.60709500	3.06806400	-0.60293400
C	-3.42844600	-0.72824600	0.17522400
O	-3.49818500	-1.85884600	0.62261500

O	-4.49949400	-0.01034400	-0.19209500
C	-5.76634700	-0.65499600	0.01276500
H	-5.83097600	-1.57475700	-0.57642200
H	-5.90422600	-0.90303000	1.06907300
H	-6.51426400	0.06758700	-0.31441200
C	5.52765000	0.02840200	-0.21475400
C	4.87358400	0.84235800	0.86917800
C	3.42754500	0.48444100	1.08485700
C	2.76987700	-0.46053800	0.40167500
C	3.44268300	-1.27635800	-0.68146700
C	4.88808400	-0.91716200	-0.90491200
H	2.90169200	1.04219800	1.85942600
H	3.35632700	-2.34846200	-0.43465800
H	2.89146400	-1.17270900	-1.63162100
C	1.31698200	-0.76817100	0.67572300
H	1.18235800	-1.85314300	0.79111300
H	0.99509400	-0.30091400	1.61269300
H	0.69703600	-0.76528700	-1.39183800
H	5.41291900	-1.47619200	-1.67770900
H	6.57446600	0.24034600	-0.42516400
H	4.95910900	1.91689300	0.63549200
H	5.42961300	0.72378700	1.81427400

CSS TS11

C	2.35704400	1.28822300	-0.75931200
C	1.98390800	0.18184400	-1.61679900
C	1.34454500	2.26748800	-0.54367000
C	0.69398500	-0.02346200	-1.99450300
H	2.76346300	-0.51585300	-1.91263600
C	0.00626100	2.04873600	-0.82328500
H	1.60236300	3.17623600	-0.00479800
C	-0.40561600	0.81883800	-1.52413800
O	-1.58097900	0.42366700	-1.65146000
H	0.39951800	-0.89403700	-2.57259300
C	-0.92900800	3.08594900	-0.31829200
O	-0.58362300	4.07347600	0.31106500
O	-2.23501300	2.84164800	-0.59276600
C	-3.15004800	3.82802600	-0.10010400
H	-3.07858700	3.91680400	0.98893000
H	-2.94396300	4.80742600	-0.54137600
H	-4.14000100	3.47504700	-0.39376300
H	2.02762000	0.70664500	0.57590600
C	-2.47115800	0.12365300	1.34280200
C	-1.56041500	-0.93569700	0.83577300

C	-1.83695500	1.01139100	2.36121300
C	-0.21167400	-0.91301500	1.01769600
H	-1.99364200	-1.74091600	0.25172600
C	-0.50051000	1.06261300	2.51850200
H	-2.48277200	1.69808100	2.90429200
C	0.37257800	0.21745200	1.71911500
O	1.61641000	0.52804800	1.67546600
H	-2.60986400	0.78153800	0.46240400
H	-0.01225600	1.78807400	3.16073200
C	0.57821300	-2.02792700	0.40012500
O	0.07057700	-2.91400000	-0.25712300
O	1.89614000	-1.96686800	0.66788500
C	2.69607600	-2.98280800	0.03514400
H	2.56396400	-2.94048900	-1.04959100
H	3.72637000	-2.75391400	0.30730500
H	2.40360500	-3.97470100	0.39005400
C	6.50741500	-1.68037400	0.22079800
C	6.47791500	-1.15246000	-1.18893800
C	5.53309000	0.00762200	-1.36401600
C	4.77340400	0.52490200	-0.39007100
C	4.80139400	-0.02699300	1.01942700
C	5.76493000	-1.16867300	1.20563100
H	5.48546200	0.44306500	-2.36218300
H	5.04521400	0.78737200	1.72246700
H	3.79597600	-0.35307400	1.31884300
C	3.83652500	1.68518200	-0.65350500
H	3.93517100	2.43018900	0.14868500
H	4.13677900	2.18704100	-1.58335300
H	5.83274100	-1.58643900	2.20915600
H	7.18069700	-2.51227100	0.42162900
H	6.20864300	-1.96248400	-1.88793500
H	7.49449000	-0.85454900	-1.49625900
C	-6.03835500	-2.15680700	-1.64693100
C	-5.69618500	-3.05732800	-0.48973400
C	-4.96337400	-2.34307400	0.61417500
C	-4.59562200	-1.05672000	0.56850500
C	-4.86146500	-0.18661500	-0.64244500
C	-5.67056400	-0.87621200	-1.70840700
H	-4.73651800	-2.93142600	1.50349600
H	-5.37226400	0.73857000	-0.32144300
H	-3.91051300	0.15461300	-1.08142500
C	-3.88265800	-0.40117400	1.72759100
H	-4.46424200	0.46478100	2.07772600
H	-3.79886300	-1.09462400	2.57250600

H	-5.93591900	-0.27538600	-2.57643000
H	-6.60747000	-2.59992300	-2.46232600
H	-5.09238800	-3.91029900	-0.84300500
H	-6.61295300	-3.51834400	-0.08535300

OSS*TS12

N	-3.72525700	0.97230000	1.89220300
N	-2.98843400	-1.80330200	1.54047100
N	-5.00696700	-2.08290700	-0.51940200
N	-5.72446500	0.70267100	-0.19184600
C	-4.19997300	2.26186600	1.89583200
C	-3.42487400	3.06596600	2.82656800
C	-2.47389500	2.23836800	3.36351200
C	-2.67023900	0.92767800	2.76964500
C	-1.87221100	-0.18585000	3.00714400
C	-2.00440100	-1.44220400	2.43083700
C	-1.10454800	-2.56226300	2.64661600
C	-1.59739700	-3.61191800	1.91863600
C	-2.76821000	-3.11959700	1.21292900
C	-3.47499000	-3.83418000	0.25445600
C	-4.48480800	-3.35231200	-0.56908100
C	-5.10428900	-4.09744700	-1.65198500
C	-6.01712000	-3.25925900	-2.23642100
C	-5.94919000	-1.99737900	-1.51648200
C	-6.68959200	-0.85930900	-1.81915800
C	-6.58627900	0.39054500	-1.21645500
C	-7.34718500	1.56986700	-1.59228000
C	-6.93388800	2.58659400	-0.77099100
C	-5.91755300	2.03095100	0.10650700
C	-5.22230700	2.73951600	1.08165000
H	-3.15743300	-4.85549900	0.08244500
H	-1.03149800	-0.04739900	3.67693400
H	-5.48447700	3.78547200	1.19835500
H	-7.40970200	-0.95069600	-2.62485200
C	-5.79702500	-1.05335300	2.15880700
H	-6.44873200	-1.84487600	1.77431700
H	-5.27767600	-1.40027200	3.05815600
H	-6.38852800	-0.16136800	2.39112900
C	-2.66444900	-0.17819500	-1.68518500
C	-2.27699900	0.93364700	-0.91653700
C	-1.89717900	-1.34114200	-1.63574300
C	-1.13577500	0.86976500	-0.12988000
H	-2.87329400	1.84147600	-0.93392400
C	-0.75639000	-1.43897600	-0.82663300

H	-2.18964800	-2.21192400	-2.21102300
C	-0.35007700	-0.30693600	-0.04530800
O	0.72555000	-0.28804300	0.71763500
Ir	-4.40173000	-0.57088500	0.72322600
H	-0.82071400	1.71483100	0.47307500
C	-0.07230200	-2.75810700	-0.83604200
O	-0.47181600	-3.73048500	-1.46061700
O	1.06364200	-2.81327200	-0.09982800
C	1.79422500	-4.04020000	-0.20507300
H	1.19032700	-4.88974400	0.11925400
H	2.10827700	-4.21308700	-1.24035200
H	2.66153100	-3.91322100	0.44235000
C	0.16369700	-2.49095800	3.44229000
C	-0.04040800	-2.60670000	4.96287100
H	0.67092400	-1.55258200	3.19187400
H	0.84027200	-3.28566800	3.10559400
H	0.91755000	-2.55306500	5.49734300
H	-0.68395100	-1.80330000	5.33905800
H	-0.51833700	-3.55851500	5.22108000
C	-1.06851700	-5.01123700	1.81188400
C	-1.90818300	-6.02824100	2.60804400
H	-0.03472000	-5.03876300	2.17626200
H	-1.03153800	-5.30776000	0.75569100
H	-1.50560100	-7.04262300	2.50132600
H	-1.91697400	-5.77095800	3.67335900
H	-2.94754100	-6.03404600	2.26217100
C	-4.68590000	-5.47416700	-2.07945300
C	-3.38604700	-5.45575100	-2.91104500
H	-5.48740000	-5.93973600	-2.66562300
H	-4.54428700	-6.11405600	-1.19812400
H	-3.08602800	-6.47288000	-3.19077300
H	-3.53188100	-4.87927200	-3.83209100
H	-2.56231500	-4.99094100	-2.35872700
C	-6.86820500	-3.50633900	-3.44830700
C	-6.26868000	-2.89245400	-4.72888800
H	-7.87596100	-3.09930600	-3.28914400
H	-6.99717700	-4.58549500	-3.59287300
H	-6.91337400	-3.07699600	-5.59633000
H	-6.14152400	-1.80951800	-4.61947100
H	-5.28180100	-3.32112900	-4.93559100
C	-8.32533300	1.62836700	-2.72989900
C	-7.63194300	1.74108600	-4.10199900
H	-8.99761500	2.48407300	-2.59523000
H	-8.96538600	0.73609200	-2.72083600

H	-8.36567600	1.76933500	-4.91612700
H	-7.02609400	2.65295800	-4.15326100
H	-6.96317100	0.88983100	-4.27187400
C	-7.34983600	4.02908300	-0.79069400
C	-6.34473900	4.92461600	-1.54157300
H	-7.46740600	4.39988200	0.23631800
H	-8.33623500	4.12270400	-1.26035300
H	-6.66142700	5.97423400	-1.52881600
H	-5.35016900	4.85957300	-1.08641300
H	-6.25191000	4.60644800	-2.58622300
C	-3.68727200	4.51114100	3.13630400
C	-4.87138000	4.70438400	4.10334200
H	-3.88416800	5.06417400	2.20788300
H	-2.78848100	4.96394600	3.57224600
H	-5.05050000	5.76741300	4.30389600
H	-5.78816100	4.27295900	3.68675400
H	-4.67438200	4.20188900	5.05705700
C	-1.42279700	2.55440800	4.38434400
C	-1.77859100	2.04737700	5.79453800
H	-1.25980300	3.63785500	4.42231300
H	-0.46874900	2.11465600	4.06853800
H	-0.98958600	2.29359900	6.51620800
H	-2.71340100	2.50002200	6.14355100
H	-1.91651800	0.96071000	5.79507400
H	-3.54652300	-0.13240500	-2.31509300
N	5.18729500	0.01914800	-1.57607700
N	4.45779600	-1.21827000	0.95592400
N	3.27764900	1.25516900	1.83899500
N	3.96169100	2.52389600	-0.67002600
C	5.29434000	0.73830900	-2.73474000
C	5.90837000	-0.08761400	-3.75965400
C	6.19299300	-1.29650400	-3.17474000
C	5.72980800	-1.21440600	-1.80068400
C	5.75244100	-2.25145000	-0.86694800
C	5.16169300	-2.26443300	0.39188100
C	5.13940700	-3.40123800	1.29642200
C	4.41147800	-3.02213300	2.39650900
C	4.00287500	-1.64695100	2.17686100
C	3.30423000	-0.85816400	3.08408500
C	2.99046400	0.48652600	2.94571500
C	2.35827500	1.30896600	3.95819300
C	2.28689800	2.58358000	3.45265500
C	2.84086400	2.53981400	2.11421300
C	2.88610200	3.60992700	1.23178500

C	3.37177600	3.60154500	-0.07556100
C	3.28063000	4.69892300	-1.02465100
C	3.83467500	4.25133300	-2.19619300
C	4.27092100	2.88449000	-1.95989200
C	4.87440400	2.05814400	-2.90160000
H	3.00277100	-1.33403500	4.00917800
H	6.24535400	-3.16650500	-1.17612500
H	5.03945400	2.49108800	-3.88135300
H	2.46872000	4.54532900	1.58598400
C	6.14067000	1.28211900	0.64440400
H	6.77718600	0.40066500	0.76020700
H	6.53264200	1.93720400	-0.13532800
H	6.05088600	1.82910200	1.58920100
C	2.47986200	0.11018400	-1.06544100
C	1.69792300	1.19534500	-1.64683500
C	2.61249100	-1.07823900	-1.90657400
C	1.12051700	1.13125100	-2.87284100
H	1.46344100	2.04348500	-1.01471400
C	2.13733000	-1.13749200	-3.17026400
H	3.12610500	-1.93075000	-1.48183700
C	1.43794700	0.00340200	-3.78816000
O	1.18372600	0.02672900	-4.99166600
Ir	4.17373800	0.63116200	0.14535700
C	5.83485500	-4.70774300	1.04475800
C	7.34908100	-4.63725800	1.32186500
H	5.66905400	-5.02542800	0.00655400
H	5.38840700	-5.48697400	1.67311200
H	7.83087200	-5.60071200	1.12053200
H	7.82685900	-3.87597300	0.69544500
H	7.53687500	-4.37037200	2.36776600
C	4.11440300	-3.80930600	3.63990100
C	5.06213000	-3.46371100	4.80515700
H	4.18705200	-4.88113500	3.42203700
H	3.07630700	-3.63348100	3.95048200
H	4.81254500	-4.04604100	5.69923700
H	6.10194400	-3.67743700	4.53387700
H	4.99930700	-2.39992000	5.06013700
C	1.94734900	0.81855600	5.31614400
C	3.13491000	0.68030600	6.28854400
H	1.43800800	-0.14858700	5.22154500
H	1.20933100	1.50405400	5.74569400
H	2.79971800	0.31037200	7.26400500
H	3.88638700	-0.01478000	5.89787000
H	3.62644900	1.64815100	6.43778600

C	1.82458300	3.83596100	4.13955700
C	2.99858000	4.72405300	4.59611200
H	1.21510800	3.57385400	5.00992300
H	1.16641900	4.40896000	3.47303200
H	2.63279900	5.63255100	5.08778500
H	3.63675200	4.18345300	5.30406700
H	3.62393700	5.02084300	3.74731400
C	2.59656900	6.00578800	-0.74695700
C	1.05888300	5.87997600	-0.74298000
H	2.89731600	6.74093300	-1.50210100
H	2.93525000	6.40786100	0.21820000
H	0.59177200	6.85766600	-0.57642800
H	0.69882200	5.46560400	-1.68787400
H	0.72260500	5.20135600	0.04880900
C	3.91323500	4.94890100	-3.52312600
C	2.83631100	4.46050000	-4.51352700
H	4.90966700	4.80461500	-3.96264600
H	3.80296900	6.02904800	-3.37416800
H	2.91455700	4.99692000	-5.46611700
H	2.94212800	3.38857900	-4.71546800
H	1.83525900	4.60954600	-4.10059500
C	6.05392400	0.31304600	-5.19862800
C	4.71682700	0.22268600	-5.96320200
H	6.79661400	-0.32855000	-5.68687100
H	6.44573200	1.33663000	-5.26791000
H	4.84370200	0.52090500	-7.00993200
H	4.32404900	-0.79932700	-5.94224700
H	3.95295400	0.86515600	-5.51361200
C	6.73927200	-2.53833900	-3.81660400
C	5.62462700	-3.52907200	-4.20859300
H	7.44641200	-3.03431400	-3.13839800
H	7.31498900	-2.26918900	-4.70953700
H	6.04160900	-4.43232300	-4.66822300
H	5.04171400	-3.82795200	-3.32995200
H	4.93288200	-3.06743500	-4.92160600
H	1.82404900	-0.16668700	0.02175100
H	2.27260900	-2.00969200	-3.80323400
C	0.12280100	2.18328000	-3.21939500
O	0.15571500	3.32588800	-2.79490700
O	-0.87044200	1.70325700	-3.98159100
C	-1.94333200	2.61961300	-4.24240100
H	-1.57393200	3.50797500	-4.76265500
H	-2.64796700	2.07021500	-4.86680900
H	-2.41663900	2.92424500	-3.30437700

OSST^STS14

N	2.78631200	0.48439900	-0.33004000
N	0.56239100	2.10558600	-1.32861500
N	-0.87212400	-0.32428900	-2.01716000
N	1.32432000	-1.92186400	-1.04558700
C	3.71449500	-0.43223100	0.07503000
C	4.86755500	0.25401800	0.63486100
C	4.60596900	1.59709900	0.54618300
C	3.29309300	1.72907700	-0.06657200
C	2.64626700	2.93329400	-0.33467000
C	1.38332100	3.11230800	-0.89263300
C	0.71545400	4.39305700	-1.07013400
C	-0.51514700	4.12520200	-1.61134600
C	-0.59035100	2.68332000	-1.78000300
C	-1.69528700	1.98116200	-2.26033600
C	-1.83614400	0.60269100	-2.35519800
C	-3.02615100	-0.08377500	-2.82315200
C	-2.74579200	-1.42622800	-2.80666200
C	-1.39607000	-1.56695000	-2.28814200
C	-0.74685600	-2.77246900	-2.04801600
C	0.49928900	-2.94297000	-1.45433300
C	1.12030100	-4.22114100	-1.15497100
C	2.33058300	-3.94877400	-0.57038100
C	2.45824100	-2.50378900	-0.51748100
C	3.55671800	-1.81520100	-0.01642300
H	-2.55265200	2.57467200	-2.55496500
H	3.18072100	3.83589400	-0.05987600
H	4.37852800	-2.41985100	0.35053700
H	-1.28219200	-3.67453000	-2.32261800
C	2.01574600	0.35393000	-3.04889000
H	2.60315200	1.27280200	-3.00444000
H	2.66441200	-0.51745900	-3.17844100
H	1.25931600	0.41360300	-3.83728900
C	0.17861100	0.27006700	0.77695800
C	0.76705300	-0.36073300	1.89688100
C	-1.00227700	0.99693100	0.99870900
C	0.08920100	-0.43035000	3.10206600
H	1.71806800	-0.87341100	1.79392300
C	-1.70123400	0.95943200	2.20287000
H	-1.45730300	1.56451000	0.20078700
C	-1.18004800	0.18783600	3.29356700
O	-1.84226200	-0.02143700	4.40840300
Ir	0.93419400	0.07438100	-1.16337400

H	0.48211700	-1.00142100	3.93803700
C	-2.97782600	1.72401700	2.22172800
O	-3.58482900	2.06280800	1.21472100
O	-3.39649600	2.06721700	3.45644600
C	-4.57991800	2.87676800	3.49061500
H	-4.42186500	3.81499400	2.95008400
H	-5.42470400	2.34992300	3.03743000
H	-4.76893600	3.06803100	4.54767100
C	1.27195900	5.71604600	-0.62988400
C	1.14948100	5.93604400	0.89106400
H	0.75067900	6.52518600	-1.15473100
H	2.32732800	5.79503300	-0.92372300
H	1.57211800	6.90409900	1.18408500
H	0.09923300	5.91038500	1.20120100
H	1.67425100	5.14941000	1.44433600
C	-1.65584700	5.06783800	-1.86109400
C	-2.65173800	5.08944500	-0.68188400
H	-2.18425500	4.78509500	-2.78091500
H	-1.27173500	6.08053000	-2.03261900
H	-3.50699100	5.73893800	-0.90304900
H	-3.02573300	4.08582800	-0.45222600
H	-2.16175100	5.46635500	0.22306200
C	-4.33263700	0.59206200	-3.11857800
C	-5.13303700	0.86180100	-1.82612300
H	-4.93037800	-0.02776400	-3.79745500
H	-4.15972100	1.53878700	-3.64613300
H	-6.05312800	1.41738300	-2.04247100
H	-5.41257800	-0.08476500	-1.34838600
H	-4.54215400	1.42950600	-1.09963300
C	-3.64713000	-2.56321300	-3.19745600
C	-4.32257100	-3.26300200	-2.00261900
H	-3.07793900	-3.30487500	-3.77392400
H	-4.42318900	-2.18761200	-3.87451100
H	-5.00946200	-4.04527800	-2.34552400
H	-3.58089600	-3.72901200	-1.34614700
H	-4.89075500	-2.54658000	-1.39980500
C	0.48159500	-5.55917400	-1.39156200
C	-0.53378800	-5.93687000	-0.29534300
H	1.25711800	-6.33217500	-1.44486300
H	-0.01995700	-5.56710500	-2.36815000
H	-0.98713900	-6.91432400	-0.49627500
H	-0.04590400	-5.98044500	0.68495500
H	-1.33616200	-5.19426700	-0.23045600
C	3.32765900	-4.91453600	0.00094600

C	3.22223300	-5.02807200	1.53477100
H	4.34666000	-4.60880800	-0.27098800
H	3.18014100	-5.90483900	-0.44532900
H	3.96495400	-5.72970900	1.93150900
H	3.38084500	-4.05371800	2.01023500
H	2.22627400	-5.37949700	1.82725700
C	6.05043000	-0.43079100	1.25563200
C	5.75867800	-0.93506000	2.68283800
H	6.90222600	0.25872600	1.28409200
H	6.36635700	-1.27595300	0.62954700
H	6.63343000	-1.43824600	3.11084200
H	5.48600600	-0.10044800	3.33819800
H	4.92118400	-1.64189000	2.68432100
C	5.43655200	2.74429000	1.04388900
C	4.94998600	3.27954600	2.40513200
H	5.42798000	3.56001800	0.30886400
H	6.48290000	2.42940000	1.13304300
H	5.56673400	4.12117300	2.74100100
H	3.90975900	3.61796900	2.34365000
H	4.99537100	2.49342100	3.16697900
C	-2.14859400	-3.05119800	3.54471800
C	-3.23720600	-2.11875700	3.82175300
C	-3.93813800	-1.54061400	2.67025400
C	-3.40038300	-1.64502400	1.43049500
C	-2.14486600	-2.40476900	1.13839300
C	-1.60885300	-3.16210000	2.31134800
H	-2.29619800	-3.08063800	0.28226400
H	-1.37373700	-1.70605400	0.76453700
H	-2.56224900	-1.03885800	4.24967600
H	-3.84805700	-2.32760700	4.70430200
H	-1.72500600	-3.60424600	4.38008400
H	-0.75316200	-3.81005600	2.13606100
H	-3.86871100	-1.13296800	0.59257400
C	-5.18366400	-0.73954300	2.94484700
H	-5.99772400	-1.38276900	3.30470300
H	-4.98272400	0.00185800	3.72692500
H	-5.52683300	-0.20889100	2.05121400

4

C	-0.30636100	1.22361900	0.09018500
C	-1.00959100	0.08677300	-0.00361800
C	-0.33003300	-1.26625800	-0.08091100
C	1.15363300	-1.21496300	0.31311400
C	1.84752900	-0.02082800	-0.35299000

C	1.20168600	1.29582600	0.10488800
H	-0.86663800	-1.98141100	0.55958200
H	-0.84103000	2.17142400	0.15961100
H	1.23489800	-1.11317900	1.40449900
H	1.64886600	-2.15593500	0.04375000
H	2.92105200	-0.01714100	-0.12784700
H	1.74946000	-0.11240200	-1.44388600
H	1.54729200	1.54657900	1.12105100
H	1.53863700	2.12527600	-0.53253400
H	-0.43352900	-1.65851200	-1.10579300
C	-2.51566000	0.06937900	-0.05101600
H	-2.93197400	-0.49642400	0.79463900
H	-2.93976400	1.07882200	-0.02743700
H	-2.87448600	-0.42838500	-0.96354200

OSS^{TS15}

N	2.77749800	0.28926400	-0.49131100
N	0.59738400	2.05279200	-1.33327600
N	-1.01064600	-0.27207700	-1.97364400
N	1.11389200	-2.01366400	-1.08515900
C	3.68170700	-0.68704800	-0.18169000
C	4.91309200	-0.07821800	0.29449500
C	4.71845700	1.27880100	0.26176100
C	3.37023900	1.49712200	-0.23931900
C	2.77027600	2.74059500	-0.42648400
C	1.49038600	3.00132200	-0.90788400
C	0.89149100	4.32168400	-1.03575200
C	-0.36525600	4.13787700	-1.55033400
C	-0.52895300	2.70617400	-1.74654900
C	-1.66522200	2.08178500	-2.25863000
C	-1.88460800	0.71583400	-2.38431100
C	-3.07293400	0.10552900	-2.95159400
C	-2.90027400	-1.25340100	-2.87537300
C	-1.61320200	-1.47967500	-2.24345300
C	-1.07329500	-2.72329600	-1.93385700
C	0.17653000	-2.97446600	-1.37797000
C	0.70975200	-4.28857000	-1.06462700
C	1.99118300	-4.10075100	-0.61542500
C	2.24136500	-2.67010100	-0.64049900
C	3.42997700	-2.05685100	-0.26025100
H	-2.47108300	2.73236300	-2.57807000
H	3.36804500	3.60594800	-0.16257500
H	4.23912900	-2.71462400	0.03672100
H	-1.68569500	-3.58862000	-2.16118500

C	1.84436100	0.21763800	-3.13736900
H	2.47179800	1.11036000	-3.13229300
H	2.44500200	-0.68340200	-3.29022000
H	1.04878200	0.30477000	-3.88365800
C	0.28790100	0.22940900	0.80841700
C	0.91686700	-0.50660800	1.83847800
C	-0.75641200	1.08422900	1.17787100
C	0.38447400	-0.53357400	3.11431500
H	1.78549800	-1.11779400	1.62002600
C	-1.30857400	1.09077200	2.46521800
H	-1.22060600	1.73710200	0.45036700
C	-0.77060200	0.21559700	3.46369200
O	-1.30693700	0.02478500	4.65361900
Ir	0.84753500	0.00467200	-1.19603800
H	0.80428900	-1.17152300	3.88752700
C	-2.45873500	2.01226100	2.66177800
O	-3.03488800	2.59129100	1.75146400
O	-2.81932800	2.17972300	3.95256100
C	-3.92136600	3.07032800	4.16134100
H	-3.69647700	4.06832900	3.77336400
H	-4.82183800	2.69876800	3.66075500
H	-4.06926800	3.10069300	5.24164500
C	1.53383200	5.59920800	-0.57924400
C	1.47944500	5.77397100	0.95150600
H	1.03650600	6.45067900	-1.05821100
H	2.58030800	5.63314000	-0.91141900
H	1.95867000	6.71097600	1.25808000
H	0.44141100	5.78622900	1.30103400
H	1.98648500	4.94557500	1.45839000
C	-1.45310400	5.15102400	-1.75407300
C	-2.41598900	5.20733900	-0.54957800
H	-2.01956600	4.91786000	-2.66538400
H	-1.01332200	6.14211600	-1.91820000
H	-3.24078700	5.90453000	-0.73919900
H	-2.83284500	4.22114000	-0.32157800
H	-1.88519300	5.54063400	0.34905100
C	-4.26115700	0.87022100	-3.45867500
C	-5.18014800	1.36115800	-2.32183200
H	-4.84006500	0.23957900	-4.14374200
H	-3.92449800	1.73130900	-4.05068700
H	-6.01411200	1.95083800	-2.71951900
H	-5.59275800	0.51265600	-1.76615100
H	-4.62775300	1.98080900	-1.60722900
C	-3.82249000	-2.34370700	-3.34396900

C	-4.68421900	-2.96127600	-2.22603300
H	-3.23138200	-3.13693100	-3.82015300
H	-4.48258500	-1.95090200	-4.12625000
H	-5.27618800	-3.80086700	-2.60827800
H	-4.06139700	-3.32719200	-1.40211800
H	-5.37631400	-2.21905500	-1.81443900
C	-0.07522600	-5.56508300	-1.14730800
C	-1.07135200	-5.71655600	0.02018900
H	0.60966200	-6.42078800	-1.15202000
H	-0.62290300	-5.60997000	-2.09837100
H	-1.63319800	-6.65437600	-0.05917300
H	-0.54310700	-5.71105800	0.98032700
H	-1.78592800	-4.88660000	0.03485500
C	2.95597500	-5.12485400	-0.09220000
C	2.98734100	-5.16902400	1.44840700
H	3.96593000	-4.91799900	-0.47052400
H	2.68694500	-6.11548100	-0.47670200
H	3.70301000	-5.91733400	1.80789200
H	3.27198300	-4.19471700	1.86115900
H	1.99760400	-5.41907200	1.84658800
C	6.10301800	-0.84122200	0.80007800
C	5.90797000	-1.35249900	2.24129700
H	6.99328500	-0.20259500	0.76180300
H	6.31243400	-1.69195900	0.13803500
H	6.78531100	-1.91336800	2.58372600
H	5.74432500	-0.51503400	2.92843600
H	5.03308500	-2.00901000	2.30875600
C	5.64736100	2.36596300	0.71876000
C	5.29905300	2.88768900	2.12689700
H	5.62577500	3.20131500	0.00639300
H	6.67858300	1.99372200	0.71655000
H	5.98549800	3.68583700	2.43228100
H	4.27734300	3.28204500	2.15693500
H	5.36087100	2.07928700	2.86382200
C	-2.98128600	-2.79846600	4.16474800
C	-3.46460200	-1.35887900	4.26250200
C	-3.89287800	-0.74434800	3.03401600
C	-3.53517200	-1.19975900	1.79483500
C	-2.78333900	-2.49756300	1.62636200
C	-2.11467800	-3.01422800	2.91263700
H	-4.44441500	0.19110600	3.09989200
H	-3.49602200	-3.24559400	1.23690200
H	-2.02871600	-2.37735100	0.83695400
C	-3.85676700	-0.43914500	0.54978200

H	-4.39423000	-1.06308800	-0.17326300
H	-4.43593200	0.46577800	0.74947600
H	-2.92435300	-0.13296100	0.05544700
H	-2.37196500	-0.58523200	4.53033100
H	-4.06181200	-1.12002800	5.14691400
H	-2.41593200	-3.07281500	5.06327900
H	-3.85907600	-3.46395100	4.13016500
H	-1.86724800	-4.07675400	2.79962800
H	-1.16811400	-2.48396800	3.04397900

13

C	-1.92486400	0.08438200	0.19102500
C	-1.09771300	1.32646000	0.00232300
C	0.28711500	1.25698900	-0.08387700
C	1.00064400	0.06436100	0.01591400
C	0.24910500	-1.23085100	0.20915600
C	-1.18604700	-1.15642200	-0.33980300
H	-2.15174300	-0.05567600	1.26260900
H	0.84816500	2.18164100	-0.21937800
H	0.79310900	-2.05806600	-0.26866900
H	-1.73830600	-2.06993100	-0.08895700
H	-1.59721300	2.29052300	-0.04414300
H	-2.89822500	0.18916200	-0.30666800
H	-1.14011000	-1.09588700	-1.43503100
H	0.22050500	-1.47881500	1.28481200
C	2.49797700	0.01214200	-0.01508600
H	2.86102800	-0.61941200	-0.84063800
H	2.94282200	1.00670300	-0.12957600
H	2.90266700	-0.43260700	0.90772700

osST16

N	1.13175200	1.85502200	-1.28767900
N	-1.47203600	0.59663300	-1.72808300
N	-0.25758600	-2.00581300	-1.28365300
N	2.32741200	-0.75296300	-0.94089600
C	2.41918500	2.26173300	-1.06036600
C	2.47323900	3.71388800	-1.01365000
C	1.19601200	4.16194100	-1.23089100
C	0.36302500	2.98419700	-1.41287200
C	-1.01387100	3.00046900	-1.61515400
C	-1.86554800	1.90622600	-1.73856700
C	-3.31238600	1.97782400	-1.86345400
C	-3.76477200	0.68746100	-1.96129300
C	-2.59487300	-0.17073600	-1.85750400

C	-2.62144900	-1.56310700	-1.79072200
C	-1.55528400	-2.40879300	-1.50676100
C	-1.64601900	-3.85449100	-1.37259000
C	-0.38103200	-4.30834900	-1.10960800
C	0.48635300	-3.14133200	-1.07974400
C	1.86509600	-3.16553200	-0.89424800
C	2.72075400	-2.06961700	-0.83601100
C	4.15373700	-2.13460100	-0.62262500
C	4.61780700	-0.84354800	-0.62879700
C	3.46875100	0.01696200	-0.83780200
C	3.50219800	1.40535700	-0.88041000
H	-3.58963600	-2.03369600	-1.91807000
H	-1.48059300	3.97801500	-1.66018800
H	4.47300600	1.87111000	-0.75219600
H	2.32051200	-4.14216100	-0.77458600
C	0.66763100	-0.11071900	-3.39287200
H	1.69935300	-0.41165700	-3.60443300
H	-0.04107400	-0.83284200	-3.80755700
H	0.47098500	0.88926700	-3.78643700
C	-0.45588100	0.42588000	0.75812000
C	-0.16686000	1.64975700	1.38814000
C	-1.63223400	-0.20671700	1.13063300
C	-1.07719200	2.26599400	2.24365100
H	0.77705700	2.15065300	1.19745200
C	-2.57996400	0.38640100	1.99427700
H	-1.89312100	-1.17664000	0.72740000
C	-2.31400800	1.67190700	2.52678500
O	-3.16819700	2.37474800	3.31695600
Ir	0.43619700	-0.08141400	-1.26218200
H	-0.85941000	3.23009600	2.69477000
C	-3.80017900	-0.39614900	2.24542300
O	-3.98827300	-1.55685300	1.92913300
O	-4.78701900	0.32429800	2.88233600
C	-6.00749200	-0.38996300	3.14032800
H	-6.47151800	-0.69499700	2.19898800
H	-5.81076600	-1.27783400	3.74662800
H	-6.64916000	0.31071200	3.67599400
C	-4.11437700	3.23800700	-1.72259000
C	-4.22079200	3.67677600	-0.24628300
H	-5.12039900	3.08772000	-2.13177400
H	-3.66384600	4.04835800	-2.31132400
H	-4.80206500	4.60116800	-0.14874100
H	-4.70271400	2.89880200	0.35614500
H	-3.22817200	3.84264700	0.18572200

C	-5.18463600	0.20528600	-2.04258400
C	-5.76172400	-0.19346600	-0.67003200
H	-5.24975400	-0.65299700	-2.72445800
H	-5.81073600	0.98935100	-2.48498700
H	-6.80345900	-0.52366700	-0.76445800
H	-5.18180300	-1.00195200	-0.21619700
H	-5.73157900	0.65641500	0.02171600
C	-2.93020400	-4.63059900	-1.40110700
C	-3.66574100	-4.57825500	-0.04596000
H	-2.72741000	-5.67508700	-1.66674700
H	-3.58734700	-4.24127300	-2.18961200
H	-4.62772200	-5.10168000	-0.10142800
H	-3.06211800	-5.05641300	0.73398200
H	-3.84620400	-3.54676200	0.27365400
C	0.06620600	-5.70737300	-0.80144000
C	0.28711000	-5.93387300	0.70756500
H	0.99573200	-5.93359400	-1.34152800
H	-0.67945100	-6.42199700	-1.16866500
H	0.62261900	-6.95784700	0.90918400
H	1.04058500	-5.24170000	1.10026100
H	-0.64133100	-5.75914000	1.26234500
C	4.91389900	-3.39728600	-0.33965700
C	4.73809400	-3.86459200	1.11926200
H	5.97979700	-3.24300800	-0.54402400
H	4.58713000	-4.19525500	-1.01934800
H	5.28794000	-4.79424100	1.30622600
H	5.10343200	-3.10070600	1.81462300
H	3.68079900	-4.03669700	1.34950400
C	6.01722800	-0.35797200	-0.38247300
C	6.22635000	0.15049100	1.05757200
H	6.26585200	0.44471100	-1.08931200
H	6.72728900	-1.16848500	-0.58359700
H	7.26061200	0.47745600	1.21532000
H	5.56493700	0.99685000	1.27251000
H	5.99819800	-0.63780700	1.78351800
C	3.70075200	4.50885500	-0.67567800
C	4.01464100	4.48948700	0.83388900
H	3.57162200	5.54677400	-1.00412700
H	4.56592800	4.12086300	-1.23010900
H	4.92201600	5.06222600	1.05844800
H	3.18472400	4.92067900	1.40497300
H	4.15866700	3.46281300	1.18900800
C	0.67822700	5.56961500	-1.17496500
C	0.04065800	5.89826200	0.19042600

H	-0.06140300	5.73138700	-1.97001400
H	1.49445200	6.27443300	-1.37287600
H	-0.35920700	6.91881400	0.20611100
H	-0.77477100	5.20305900	0.41869800
H	0.78261500	5.80748900	0.99194000
C	0.33720000	-1.81148000	3.26645700
C	1.30060900	-1.38830300	2.20242800
C	2.24896800	-0.39292000	2.43321400
C	2.34028500	0.28520700	3.63513800
C	1.42848400	-0.08180500	4.77898500
C	0.10456100	-0.69877500	4.29898100
H	2.92113500	-0.12269400	1.62531400
H	1.95991600	-0.79094700	5.43808400
H	1.22952500	0.80367100	5.39806600
C	3.34806200	1.36905800	3.86121800
H	3.99536700	1.14320000	4.72241600
H	3.98663600	1.52581900	2.98613300
H	2.84913900	2.32154300	4.09540800
H	-3.99340200	1.86017500	3.39834300
H	1.31000600	-1.93601300	1.27209600
H	-0.61244300	-2.11685100	2.81101100
H	0.73984500	-2.71342300	3.76244200
H	-0.46751000	-1.08106100	5.15244600
H	-0.49501000	0.08588500	3.83004300

15

C	0.58970300	1.25631400	-0.39569700
C	-0.08079900	2.49472300	-0.41639500
C	-0.18391500	0.11294800	-0.24563400
C	-1.45798900	2.58011400	-0.28932800
H	0.49691700	3.40940900	-0.53565700
C	-1.58642800	0.16311200	-0.11165200
H	0.28543800	-0.86464500	-0.23694700
C	-2.23576600	1.42100500	-0.13380700
O	-3.57100500	1.60423900	-0.01910100
H	-1.97158400	3.53598200	-0.31020400
C	-2.27285300	-1.13835800	0.04254700
O	-1.73604500	-2.22627000	0.06971500
O	-3.63808100	-1.01728100	0.16074000
C	-4.35939000	-2.25245900	0.31513800
H	-4.19492600	-2.89814800	-0.55118800
H	-4.02906900	-2.77418600	1.21690900
H	-5.40976400	-1.97038000	0.39384300
C	2.76648000	1.44139100	0.90581800

C	2.11396800	1.21078200	-0.48116600
C	2.62037400	-0.07038600	-1.10382400
C	3.25207400	-1.04664300	-0.43745300
C	3.52956500	-0.95417200	1.04917900
C	2.73299100	0.15970100	1.74285400
H	3.81049700	1.74997600	0.75657800
H	2.42425300	-0.19405400	-2.16881300
H	3.31542800	-1.92410600	1.52019100
H	3.13319600	0.34237700	2.74722800
H	2.41791300	2.04435000	-1.13183600
H	2.25569900	2.26176900	1.42380900
H	1.69022800	-0.15913200	1.86898800
H	4.60997900	-0.79064400	1.19390800
C	3.74908700	-2.29402400	-1.12144800
H	3.26922700	-3.18919100	-0.70216500
H	3.55608100	-2.27690000	-2.19910700
H	4.83076000	-2.41990600	-0.97028300
H	-3.99183400	0.72762800	0.07910400

OSS^{TS17}

N	-2.76811000	-0.34094500	-0.50468100
N	-0.54375700	-2.00929300	-1.42566700
N	1.01060600	0.39538000	-1.94421200
N	-1.16946500	2.02590000	-0.99367500
C	-3.68130500	0.59069700	-0.09718900
C	-4.88908400	-0.07574900	0.36167800
C	-4.67309400	-1.42216400	0.21845600
C	-3.33322900	-1.57723200	-0.32641300
C	-2.71112700	-2.79394600	-0.59498200
C	-1.42068200	-2.99999200	-1.07628500
C	-0.78685300	-4.29619400	-1.26444700
C	0.47888300	-4.05217600	-1.73141800
C	0.61034900	-2.60861800	-1.84199300
C	1.74924100	-1.92894100	-2.27128500
C	1.93795900	-0.55280000	-2.31856600
C	3.14938800	0.10559200	-2.77318700
C	2.91617200	1.45514200	-2.71764000
C	1.57666800	1.62530000	-2.17710600
C	0.96482400	2.84195600	-1.89609200
C	-0.28970900	3.03298600	-1.32688400
C	-0.87671900	4.31820400	-0.99913000
C	-2.11920400	4.06809700	-0.47219900
C	-2.30472700	2.63087000	-0.48805000
C	-3.45676800	1.96676900	-0.08601600

H	2.59168800	-2.54112400	-2.57073100
H	-3.29256700	-3.68531300	-0.38728700
H	-4.27012100	2.58659500	0.27436900
H	1.53566500	3.73585400	-2.12231200
C	-1.72820800	-0.18285900	-3.18227600
H	-2.49755800	-0.95649200	-3.16487700
H	-2.16085000	0.79446900	-3.41991900
H	-0.92238500	-0.44532500	-3.87227000
C	-0.21515100	-0.38399200	0.76882800
C	-0.99185000	-0.12255900	1.92054500
C	1.02779400	-1.00024600	0.97134300
C	-0.48326900	-0.35365700	3.18830500
H	-1.97876800	0.31776300	1.82542300
C	1.57011500	-1.24855100	2.23399100
H	1.64259300	-1.28184800	0.12945100
C	0.80568000	-0.91575900	3.39898600
O	1.22221800	-1.10205200	4.63364300
Ir	-0.85420200	0.03378500	-1.18559500
H	-1.05198600	-0.09882200	4.07844000
C	2.92724900	-1.85622300	2.23069200
O	3.52512900	-2.19011500	1.21661400
O	3.47694500	-2.00300300	3.45620300
C	4.78297700	-2.59461700	3.46802600
H	4.76163900	-3.59005000	3.01524400
H	5.49452900	-1.97381600	2.91437000
H	5.06301600	-2.65558100	4.52041100
C	-1.40927300	-5.61293700	-0.90092200
C	-1.38153300	-5.88233800	0.61674800
H	-0.88392600	-6.42229100	-1.42127900
H	-2.44789000	-5.64793100	-1.25671700
H	-1.84762200	-6.84565500	0.85421700
H	-0.35073400	-5.89704700	0.98690100
H	-1.91502900	-5.09725400	1.16387400
C	1.59865000	-5.02436900	-1.96053500
C	2.53628800	-5.11622800	-0.73805000
H	2.17859300	-4.72979000	-2.84501000
H	1.19041800	-6.01727000	-2.18415600
H	3.38176100	-5.78390300	-0.94207200
H	2.92670900	-4.13231200	-0.45685500
H	1.99321600	-5.50810600	0.12946400
C	4.42500300	-0.60828100	-3.10994100
C	5.19882700	-1.01587600	-1.83740500
H	5.05846100	0.03421700	-3.73319200
H	4.21317300	-1.50221700	-3.71104200

H	6.09966300	-1.58614100	-2.09280600
H	5.50437700	-0.12620800	-1.27538300
H	4.57919700	-1.61986600	-1.16638200
C	3.84511800	2.56524000	-3.12411200
C	4.74095100	3.09232400	-1.98770800
H	3.26421900	3.39768600	-3.54171800
H	4.48441700	2.20921600	-3.94128100
H	5.41902300	3.87058900	-2.35700300
H	4.14406400	3.51806700	-1.17599800
H	5.34617300	2.28391300	-1.56423000
C	-0.19186700	5.64365900	-1.16884000
C	0.78111000	5.96897000	-0.01885400
H	-0.94454900	6.43769100	-1.23831800
H	0.35404000	5.66234500	-2.12115300
H	1.25870500	6.94362400	-0.17216800
H	0.25066400	5.99400000	0.93969300
H	1.56596400	5.21006300	0.05853700
C	-3.10456100	5.04863600	0.09420400
C	-3.07076400	5.09072300	1.63483500
H	-4.11999900	4.79723300	-0.23975200
H	-2.89633600	6.05039800	-0.29897300
H	-3.80268600	5.80639600	2.02651500
H	-3.29333200	4.10455400	2.05729200
H	-2.07687200	5.38493400	1.99027200
C	-6.07862500	0.62426700	0.95204800
C	-5.85340100	1.03505100	2.42073500
H	-6.95765300	-0.02798300	0.89112600
H	-6.32172200	1.51598500	0.35898400
H	-6.73128200	1.55145600	2.82593400
H	-5.65528900	0.15395000	3.04111100
H	-4.98969800	1.70340800	2.51206300
C	-5.57113100	-2.55782400	0.61532300
C	-5.18500800	-3.16688200	1.97789400
H	-5.54649200	-3.34164700	-0.15318100
H	-6.60952100	-2.20856200	0.65725800
H	-5.84707800	-4.00055300	2.23884500
H	-4.15400500	-3.53718100	1.96352400
H	-5.25208300	-2.41291100	2.77004500
C	2.76205800	2.85529700	1.25437200
C	1.44083500	2.67125000	2.01210000
C	1.63911900	2.10518900	3.38329300
C	2.78351800	1.47500300	3.80492700
C	3.98076200	1.35237300	2.87749900
C	3.64958700	1.61449300	1.40077200

H	0.79888500	2.16185500	4.07275100
H	4.74140700	2.07177500	3.21881200
H	4.43174500	0.36129000	3.00190200
C	2.83877100	0.83729100	5.09326500
H	3.81405100	0.49361900	5.44030600
H	2.20989500	1.25623300	5.88089200
H	2.11280700	-0.32465100	4.87298300
H	0.78721400	1.98533000	1.44767800
H	0.88587500	3.61826500	2.06597300
H	2.54706700	3.04314000	0.19960300
H	3.29315900	3.73549800	1.64497800
H	4.57652100	1.73328900	0.82740900
H	3.12724400	0.74957700	0.97817200

14

C	1.80126300	-0.03151500	0.31393000
C	1.14175600	1.29844000	-0.08533100
C	-0.35876000	1.23835500	-0.05325600
C	-1.10389600	0.06371800	0.02395100
C	-0.38076000	-1.27535000	0.13644600
C	1.07447600	-1.20869900	-0.34770300
H	-0.89533300	2.18239600	-0.14112700
H	-0.39251700	-1.59461600	1.18911400
H	-0.93561400	-2.04066600	-0.42015700
C	-2.49417900	0.08065100	0.01402500
H	-3.07314300	-0.83687100	0.06270600
H	-3.04670100	1.01478700	-0.03818200
H	1.58521800	-2.15418800	-0.12804100
H	1.09457700	-1.08067700	-1.43943400
H	2.86335500	-0.02161700	0.04098900
H	1.75322700	-0.15088000	1.40542400
H	1.46789600	1.57473200	-1.10378400
H	1.49963600	2.11400000	0.56012500

OSST18

N	-1.85318600	-1.92772200	-0.68246500
N	0.77857700	-1.20832600	-1.74943200
N	0.05792100	1.59740700	-1.55416700
N	-2.56721900	0.87087600	-0.58146400
C	-3.11366200	-2.06999500	-0.16818900
C	-3.37907900	-3.47530800	0.09582900
C	-2.25248200	-4.16368400	-0.27307500
C	-1.30223100	-3.18028000	-0.76716100
C	-0.00878400	-3.46206700	-1.19745800

C	0.95854700	-2.55852600	-1.62876300
C	2.32529200	-2.90029500	-1.98792700
C	2.94275200	-1.73165500	-2.35181900
C	1.96046800	-0.67309100	-2.17787800
C	2.21022100	0.69085900	-2.32424000
C	1.34628100	1.73741700	-2.02349500
C	1.66004000	3.14940500	-2.16806500
C	0.52553300	3.84494700	-1.84010900
C	-0.47839800	2.85926800	-1.47090800
C	-1.78575300	3.14373100	-1.08898100
C	-2.75302200	2.23278100	-0.67561700
C	-4.08816400	2.57593700	-0.22193800
C	-4.70269000	1.40233500	0.13163300
C	-3.74857500	0.33587400	-0.11171700
C	-3.99019300	-1.01799100	0.08655000
H	3.20001900	0.96587700	-2.67033100
H	0.28735000	-4.50475500	-1.17391700
H	-4.96687900	-1.28404800	0.47530600
H	-2.07485700	4.18868800	-1.09382500
C	-1.53082700	-0.40417700	-3.12091500
H	-1.51186700	-1.46671800	-3.37355700
H	-2.55041200	-0.01072300	-3.19069600
H	-0.85082300	0.15603600	-3.76881700
C	0.25531700	-0.56904900	0.82533500
C	-0.12656000	-1.58630500	1.71449300
C	1.57399700	-0.14614300	0.87994000
C	0.80063400	-2.21151300	2.54994000
H	-1.15899500	-1.92038100	1.75288700
C	2.54467300	-0.77336300	1.68550200
H	1.91401500	0.68663100	0.27839600
C	2.15212400	-1.85049500	2.52161200
O	2.99652000	-2.55426800	3.32117100
Ir	-0.88779000	-0.15583100	-1.09416800
H	0.50020000	-3.01037400	3.22190900
C	3.91088400	-0.23947300	1.58324500
O	4.24280400	0.79194500	1.02326300
O	4.85424800	-1.03424700	2.19205100
C	6.20637200	-0.54825900	2.13504500
H	6.54313600	-0.49286500	1.09690900
H	6.27495700	0.44437700	2.58758800
H	6.80077500	-1.27135800	2.69466100
C	2.93542500	-4.25902500	-1.80754200
C	3.25990200	-4.53958900	-0.32459700
H	3.85297400	-4.33785700	-2.40252000

H	2.25907000	-5.03740900	-2.18542200
H	3.69856100	-5.53609800	-0.19669200
H	3.96572600	-3.79718300	0.06431400
H	2.35727300	-4.47504900	0.29251900
C	4.37353600	-1.52656000	-2.75978200
C	5.28008300	-1.10315100	-1.58765200
H	4.43035700	-0.76813800	-3.55176900
H	4.76155200	-2.45216500	-3.20173200
H	6.31752200	-0.97770400	-1.92098600
H	4.94129200	-0.16279400	-1.14452800
H	5.26316100	-1.86104300	-0.79551400
C	3.02207900	3.68348300	-2.50123800
C	3.96108800	3.66368200	-1.27694500
H	2.93774000	4.70883800	-2.88034400
H	3.46961400	3.09603000	-3.31368600
H	4.96357500	4.01783700	-1.54483900
H	3.56989900	4.31275000	-0.48530900
H	4.04806800	2.65649000	-0.85597700
C	0.32516300	5.33227500	-1.78325400
C	0.41725900	5.89955200	-0.35298900
H	-0.65171600	5.59300100	-2.21222400
H	1.07297800	5.82632300	-2.41441300
H	0.25113800	6.98303400	-0.34767300
H	-0.32665500	5.43477800	0.30338500
H	1.40508600	5.70182300	0.07803400
C	-4.60608500	3.97838400	-0.08784800
C	-4.08340300	4.67654000	1.18368800
H	-5.70214800	3.96804500	-0.06925800
H	-4.32375800	4.56917800	-0.96926900
H	-4.45803200	5.70438900	1.25266400
H	-4.40230000	4.13277000	2.07986900
H	-2.98815700	4.70773000	1.19153800
C	-6.06479600	1.20791900	0.73215200
C	-6.01269300	1.00046600	2.25871500
H	-6.56093900	0.34637500	0.26586500
H	-6.69406000	2.07702300	0.50757200
H	-7.01703900	0.85085200	2.67160100
H	-5.40261600	0.12670700	2.51364700
H	-5.56425900	1.87080500	2.75079600
C	-4.62958400	-4.00246500	0.73768400
C	-4.64704900	-3.78737600	2.26399200
H	-4.73058100	-5.07287800	0.52323700
H	-5.51108600	-3.52036900	0.29403600
H	-5.57350500	-4.17055600	2.70740300

H	-3.80176800	-4.30159200	2.73492400
H	-4.56339200	-2.72262600	2.50916200
C	-1.95538300	-5.62560500	-0.10764900
C	-1.12121100	-5.90738000	1.15866700
H	-1.41934400	-6.00359700	-0.98807700
H	-2.89271600	-6.19218300	-0.05747500
H	-0.88565900	-6.97416800	1.24880800
H	-0.18113200	-5.34500800	1.14112700
H	-1.66982300	-5.59939300	2.05592700
C	2.72891700	3.26756300	3.87976500
C	2.51146000	3.48435200	2.37430300
C	1.17589800	2.99057700	1.91351700
C	0.37110700	2.13461300	2.64024200
C	0.82173000	1.60520000	3.99455900
C	2.31310000	1.84496300	4.27520100
H	0.85033400	3.28405300	0.91869000
H	0.21979500	2.08573500	4.77998200
H	0.59755500	0.53251500	4.04402200
C	-0.83838500	1.68927500	2.09999000
H	-1.46982500	0.97988800	2.62314800
H	-1.21689800	2.10104000	1.17897100
H	3.90198200	-2.22676700	3.16492600
H	3.28839200	2.94701800	1.80690000
H	2.62922500	4.54582400	2.10922700
H	3.77896900	3.45153400	4.13759300
H	2.12790300	3.99271800	4.44663100
H	2.52633200	1.65659000	5.33444900
H	2.90803000	1.12692800	3.69887900

5

C	0.26800100	1.52759000	0.53036000
C	-0.45920000	2.65305800	0.10603300
C	-0.39085800	0.30391800	0.54514000
C	-1.78987800	2.55677100	-0.27585200
H	0.03082600	3.62394000	0.07507300
C	-1.73866100	0.16998100	0.16241800
H	0.13772600	-0.59405400	0.84937300
C	-2.45342800	1.32094000	-0.25471500
O	-3.74800500	1.32524300	-0.64741400
H	-2.34899700	3.42692600	-0.60448700
C	-2.30194600	-1.19748200	0.22449900
O	-1.70521300	-2.19631600	0.56835800
O	-3.62193800	-1.25440900	-0.15674500
C	-4.22364600	-2.56083000	-0.11665600

H	-3.69335700	-3.24289600	-0.78600800
H	-4.19182800	-2.96137400	0.89969500
H	-5.25372900	-2.41891800	-0.44493400
C	4.52668500	-1.25934500	-0.74133600
C	4.03809800	-1.50756100	0.69424600
C	3.14885000	-0.39511000	1.19383900
C	2.60469100	0.54719100	0.41155100
C	2.82127200	0.56662100	-1.08814400
C	3.37326100	-0.76279700	-1.62165200
H	2.94446100	-0.37665600	2.26483500
H	1.87484100	0.81226800	-1.58781000
H	3.51199300	1.38866100	-1.33721500
C	1.72068900	1.63908200	0.97399400
H	1.77118500	1.62236700	2.07125200
H	2.10651900	2.62115200	0.66315700
H	2.56956100	-1.51242300	-1.61884800
H	3.69810800	-0.64657200	-2.66280600
H	5.31958300	-0.49820900	-0.72811100
H	4.96917100	-2.17379200	-1.15473000
H	4.89438400	-1.63031300	1.37206400
H	3.48552400	-2.45952500	0.74175700
H	-4.08830000	0.41111200	-0.58819300

CSSTS19

N	-1.11537200	1.52038500	-1.29080100
N	-0.69787600	-1.34836300	-1.52376400
N	2.13660800	-0.96292700	-1.00541200
N	1.72512000	1.90700100	-0.80293300
C	-1.10896100	2.88764700	-1.16379500
C	-2.46966400	3.39065400	-1.25111800
C	-3.28185200	2.30241700	-1.44354200
C	-2.41757800	1.13394200	-1.48944100
C	-2.83977000	-0.17385700	-1.71661100
C	-2.05034800	-1.31871300	-1.75272500
C	-2.52422900	-2.66497900	-2.04312400
C	-1.42928200	-3.48691300	-1.99319000
C	-0.28552100	-2.64669200	-1.67230500
C	1.02471100	-3.09186800	-1.52271600
C	2.13802000	-2.32468700	-1.18562100
C	3.46689900	-2.84514000	-0.92357700
C	4.25708600	-1.76966700	-0.59345900
C	3.41565100	-0.58974000	-0.66979100
C	3.83583500	0.71685200	-0.43405100
C	3.06265500	1.87249900	-0.50584300

C	3.53790400	3.22329800	-0.24982600
C	2.46296700	4.05830900	-0.41642100
C	1.32860200	3.21792200	-0.76469600
C	0.02444400	3.66647700	-0.95404600
H	1.19425700	-4.15394200	-1.66122400
H	-3.90073500	-0.31388100	-1.88698900
H	-0.13257200	4.73709600	-0.89285600
H	4.88237100	0.84982000	-0.18307300
C	0.85598600	0.42723400	-3.20647500
H	-0.03774900	0.82447200	-3.70172700
H	1.70478600	1.09285700	-3.40095900
H	1.07497500	-0.56823300	-3.61002200
C	0.11578000	0.19001900	1.05785700
C	0.42923600	1.40493800	1.78265900
C	-1.15493100	-0.40575600	1.33573200
C	-0.60033200	2.18923500	2.19128800
H	1.45446200	1.76018200	1.81513300
C	-2.21855200	0.33270500	1.77377200
H	-1.31048600	-1.45440100	1.10953600
C	-2.01365800	1.76607000	2.09774300
O	-2.92637500	2.57268300	2.29550900
Ir	0.50838700	0.27812800	-1.13179700
H	-0.44188700	3.20684900	2.53683500
C	-3.49885100	-0.39832500	1.94286700
O	-3.67794700	-1.54734900	1.55949100
O	-4.43614700	0.29262700	2.61356600
C	-5.67835200	-0.39520100	2.81106000
H	-6.14439900	-0.62914100	1.84927800
H	-5.52459000	-1.32657200	3.36427500
H	-6.30268500	0.29468000	3.37954400
C	-3.95313200	-3.04529800	-2.30628100
C	-4.72578700	-3.40863900	-1.02361400
H	-3.98115300	-3.89531200	-2.99979500
H	-4.46724900	-2.22401600	-2.82102100
H	-5.77107200	-3.64749800	-1.25449100
H	-4.27563400	-4.28281600	-0.53928800
H	-4.69730500	-2.59096200	-0.29883700
C	-1.37356100	-4.97582400	-2.17747900
C	-1.27289000	-5.74367000	-0.84487500
H	-0.51860000	-5.24343200	-2.81305800
H	-2.26824700	-5.31062600	-2.71518300
H	-1.24622300	-6.82664400	-1.01288600
H	-0.36549200	-5.46220300	-0.29818100
H	-2.13073900	-5.51452000	-0.20341300

C	3.83733800	-4.30035500	-0.93957200
C	3.42573100	-5.03480900	0.35151400
H	4.91959200	-4.40303000	-1.08162100
H	3.37156200	-4.79541200	-1.80161900
H	3.70543900	-6.09387500	0.31038000
H	3.91284300	-4.58463300	1.22400800
H	2.34392700	-4.97181800	0.51126100
C	5.69088800	-1.76871500	-0.14854100
C	5.82904100	-1.64432000	1.38203100
H	6.23325600	-0.94377500	-0.62883400
H	6.18314800	-2.68988400	-0.48131700
H	6.88194600	-1.63146100	1.68650200
H	5.35627000	-0.72322400	1.74155000
H	5.33728700	-2.48654400	1.88258900
C	4.93004700	3.56888200	0.19322900
C	5.16115900	3.28126000	1.68996300
H	5.12816400	4.62884800	-0.00429100
H	5.66349800	3.00761100	-0.40085400
H	6.18631900	3.52954600	1.98849000
H	4.47181600	3.87003900	2.30580500
H	4.98506000	2.22313400	1.91522400
C	2.38627400	5.53966100	-0.18570900
C	1.79899700	5.88737900	1.19693000
H	1.77617900	6.01091800	-0.96734200
H	3.38607600	5.98078200	-0.27457200
H	1.73785100	6.97230500	1.34042300
H	0.79224600	5.46953400	1.30929000
H	2.42203600	5.46954800	1.99601700
C	-2.85691100	4.83024000	-1.06998500
C	-2.78679800	5.29466200	0.39866900
H	-3.87474700	4.98268000	-1.44679900
H	-2.20922100	5.46876000	-1.68688800
H	-3.11472700	6.33692800	0.49073900
H	-3.40731900	4.66299100	1.03913700
H	-1.76397400	5.22266800	0.78441000
C	-4.78148600	2.25616300	-1.49242900
C	-5.39152000	1.66651100	-0.20407400
H	-5.11514800	1.66826900	-2.35900800
H	-5.17011900	3.26916300	-1.64529500
H	-6.48452300	1.75515600	-0.21458100
H	-5.13971300	0.60514100	-0.10745700
H	-4.99798900	2.17234200	0.68267800
C	1.81096700	-1.14627700	3.50666100
C	1.56342400	-1.71539000	2.11919100

C	0.62896100	-2.84425100	2.04444700
C	-0.22713000	-3.15974700	3.04109800
C	-0.19958700	-2.43643600	4.36848800
C	0.51325000	-1.07607900	4.32182800
H	2.53831700	-1.80130400	4.01014600
H	1.05027100	-0.81459000	1.41641500
H	0.57221000	-3.37332100	1.09738000
H	-1.22789600	-2.30979500	4.73267900
H	0.72257700	-0.72675700	5.33934000
H	2.47039200	-1.84485300	1.52401200
H	2.27927500	-0.15805900	3.43256500
H	-0.15293800	-0.33671100	3.86571500
H	0.29034300	-3.09993600	5.10007700
C	-1.27701000	-4.22083800	2.87956700
H	-2.25932500	-3.73703800	2.76953100
H	-1.10841900	-4.83728800	1.99221200
H	-1.33220600	-4.87369100	3.76057600

osSTS20

N	-0.26248100	-2.02149600	-1.25548800
N	1.50167200	0.24432300	-1.63687200
N	-0.73653600	2.04161400	-1.25790400
N	-2.52123000	-0.23408400	-0.98259300
C	-1.24154000	-2.96155100	-1.03102700
C	-0.64071200	-4.28218300	-0.93090600
C	0.70562200	-4.11922800	-1.12065700
C	0.92958600	-2.69824400	-1.33962100
C	2.16432900	-2.11135200	-1.59756800
C	2.43653200	-0.75621500	-1.74771000
C	3.74461500	-0.17782300	-2.01082700
C	3.57568600	1.18060700	-2.04721000
C	2.16699800	1.43612200	-1.80499100
C	1.58378300	2.69468600	-1.71244200
C	0.25395300	2.98161700	-1.41797900
C	-0.29087000	4.30976900	-1.19756700
C	-1.62129700	4.14796700	-0.90332400
C	-1.89552100	2.72345100	-0.96483800
C	-3.13677600	2.13062500	-0.74977000
C	-3.43250000	0.77082200	-0.75693500
C	-4.73211400	0.19311100	-0.46042400
C	-4.58139900	-1.16910900	-0.51591600
C	-3.18818100	-1.42451100	-0.83820200
C	-2.59423000	-2.68287400	-0.88795000
H	2.24168400	3.54451900	-1.85592500

H	3.00812800	-2.78679400	-1.67473500
H	-3.24926800	-3.53417100	-0.74292600
H	-3.96246300	2.80258700	-0.54253000
C	-0.79090600	-0.02297200	-3.38896700
H	-0.36899600	0.89485300	-3.81157200
H	-0.27854100	-0.89674900	-3.80429400
H	-1.86274600	-0.07784000	-3.60464000
C	-0.80980000	0.25223900	1.51508500
C	-1.71372900	-0.72324700	2.01579500
C	0.56129900	-0.05377300	1.43229400
C	-1.25995700	-1.96833000	2.35302300
H	-2.77261700	-0.48476600	2.07269400
C	1.07049500	-1.28792200	1.81709700
H	1.26183500	0.70598100	1.11115900
C	0.14619900	-2.35795700	2.22997300
O	0.48603200	-3.53652500	2.46172500
Ir	-0.51463500	0.00193400	-1.34497200
H	-1.93267900	-2.75104500	2.68940300
C	2.54779300	-1.40482600	1.83760400
O	3.30854600	-0.54487400	1.40479000
O	2.99750900	-2.52236200	2.43714000
C	4.41987800	-2.65189300	2.52953600
H	4.86135000	-2.78870200	1.53794200
H	4.86563000	-1.76746200	2.99469100
H	4.58946300	-3.53941600	3.14027600
C	5.03193200	-0.94186900	-2.14320000
C	5.89588300	-0.87197900	-0.86903500
H	5.60667200	-0.55100500	-2.99354200
H	4.82294700	-1.99024100	-2.38491000
H	6.76136600	-1.54167200	-0.94194800
H	6.26829900	0.14591500	-0.71119500
H	5.30313600	-1.13658300	0.01049000
C	4.62589400	2.23651700	-2.24169400
C	5.01726000	2.95757400	-0.93670300
H	4.27926500	2.98082200	-2.97202900
H	5.52055100	1.77694800	-2.67831600
H	5.81895400	3.68395400	-1.11446700
H	4.16185500	3.49295700	-0.51236700
H	5.35781100	2.23990800	-0.18328800
C	0.50995000	5.58026700	-1.22536700
C	1.34036200	5.79850400	0.05404500
H	-0.16235000	6.43466300	-1.36638300
H	1.18188500	5.57872800	-2.09398400
H	1.90830800	6.73472400	0.00410000

H	0.69124200	5.83762000	0.93631700
H	2.05036000	4.97724600	0.20135400
C	-2.61771800	5.18926700	-0.48405000
C	-2.83262900	5.20680600	1.04294200
H	-3.58061400	5.01589700	-0.98263900
H	-2.28078500	6.17966600	-0.81154300
H	-3.56417000	5.96934300	1.33448200
H	-3.19444200	4.23346800	1.39463800
H	-1.89026900	5.41782200	1.56184900
C	-5.95008600	0.98205100	-0.07493300
C	-5.91279100	1.44731900	1.39436700
H	-6.84918700	0.37603100	-0.23722400
H	-6.05315800	1.85807200	-0.72905000
H	-6.80337200	2.03395400	1.64835900
H	-5.86534600	0.58572200	2.07002400
H	-5.02852000	2.06620600	1.58497800
C	-5.59119500	-2.23260500	-0.19453500
C	-5.45187100	-2.75848000	1.24823100
H	-5.49079700	-3.07076600	-0.89635800
H	-6.60383000	-1.83722500	-0.33793300
H	-6.18321800	-3.54828200	1.45518400
H	-4.44925300	-3.16561400	1.41962400
H	-5.60790300	-1.94874000	1.97022400
C	-1.38968700	-5.53222400	-0.56872300
C	-1.79680300	-5.57223200	0.91892200
H	-0.76687600	-6.40535400	-0.79376800
H	-2.28609800	-5.63083500	-1.19716900
H	-2.25436900	-6.53617700	1.17130300
H	-0.93095500	-5.40101300	1.56487200
H	-2.52233600	-4.78297700	1.14557200
C	1.79347600	-5.15083500	-1.03738900
C	2.63607200	-5.02920800	0.24819400
H	2.45081800	-5.07369500	-1.91539400
H	1.34687600	-6.15054500	-1.08315800
H	3.35525300	-5.85420700	0.31930100
H	3.19283900	-4.08756300	0.26070700
H	1.99871400	-5.02200600	1.13617900
C	0.87261400	0.88281100	4.82667900
C	2.14653600	1.68159200	4.50100600
C	2.05583700	2.44646200	3.20557900
C	0.81777000	2.83652000	2.71739500
C	-0.37561100	2.47660500	3.33836600
C	-0.40029200	1.72327200	4.63443600
H	0.82136700	0.01730100	4.15971600

H	2.35596900	2.40232900	5.31032500
H	-1.31374100	2.85492600	2.94069200
H	-1.28882400	1.08192600	4.68132300
H	3.01445900	1.01032100	4.46865000
H	0.92205300	0.49707500	5.85094600
H	-0.50649200	2.44981900	5.45982800
H	-1.17827100	1.21262000	1.18703600
H	0.77130300	3.38816000	1.78012600
C	3.32102700	2.69789600	2.45494500
H	4.12448100	3.04824900	3.11741700
H	3.66199500	1.75037500	2.00722900
H	3.18685000	3.42322100	1.64756800

16

C	0.60202300	1.44153100	-0.96567700
C	-0.12456500	2.69041700	-0.57150100
C	-0.22628300	0.21157400	-0.82045900
C	-1.36277500	2.68400700	-0.05661300
H	0.41442900	3.62849500	-0.69876900
C	-1.47123000	0.18330000	-0.30368800
H	0.23933300	-0.72589800	-1.11379600
C	-2.13167900	1.43667400	0.16749800
O	-3.21734900	1.45932500	0.73465500
H	-1.86890000	3.59632300	0.24653000
C	-2.10755100	-1.16348800	-0.15569600
O	-1.46820900	-2.18546000	0.02466500
O	-3.44177800	-1.13337200	-0.27988000
C	-4.09994300	-2.40159500	-0.13242100
H	-3.76925400	-3.10007700	-0.90699600
H	-3.88273800	-2.83371900	0.84855100
H	-5.16445600	-2.18871900	-0.23245300
C	1.80768100	1.06455900	1.32650200
C	1.97712000	1.30122500	-0.18968700
C	2.84776200	0.25315000	-0.83788200
C	3.28143500	-0.86687900	-0.24253800
C	2.91771300	-1.20365000	1.18801800
C	1.69821000	-0.42243900	1.69291100
H	2.68538700	1.48620800	1.83446600
H	0.88786400	1.53174800	-2.02832100
H	3.13848000	0.45085700	-1.87095700
H	2.73491000	-2.28347400	1.27395400
H	1.60786600	-0.52836000	2.78063000
H	2.46677200	2.27670700	-0.33121700
H	0.93564100	1.61688100	1.69549100

H	0.78935400	-0.85725700	1.26319000
H	3.79303300	-1.00039000	1.82615800
C	4.18304400	-1.84881000	-0.94404600
H	3.70419800	-2.83492500	-1.01683900
H	4.44685700	-1.51995900	-1.95464600
H	5.11414500	-1.99583700	-0.37881900

CSSTS21

C	2.81326900	1.29741800	-0.23265400
C	2.39389000	2.68190100	-0.13151000
C	2.21658300	0.40209400	0.69900800
C	1.32037700	3.04186900	0.61797900
H	2.92025500	3.42307000	-0.73141500
C	1.07717900	0.71094800	1.42008200
H	2.58461200	-0.61628600	0.74358000
C	0.50693000	2.07014100	1.36199300
O	-0.59112000	2.41234500	1.83113800
H	0.95522300	4.06468700	0.63910600
C	0.45214000	-0.44065400	2.11747200
O	1.00554400	-1.52042200	2.28022800
O	-0.82917600	-0.23448600	2.48786600
C	-1.49795900	-1.39484600	3.00864500
H	-1.50254100	-2.19490800	2.26211500
H	-1.00525200	-1.75368000	3.91651500
H	-2.51468800	-1.06440300	3.22779700
C	5.36051300	1.37354200	0.01270300
C	4.16377800	0.98783600	-0.89133200
C	4.26734100	-0.45109200	-1.34503200
C	5.09215800	-1.36213800	-0.80895200
C	5.99897800	-1.03636800	0.36014200
C	5.63954400	0.28527600	1.05306100
H	1.79184500	0.90217100	-1.23633900
H	3.61185200	-0.73946100	-2.16682800
H	5.97063900	-1.86447800	1.08267700
H	4.74981600	0.14322200	1.67938000
H	4.21092600	1.62033700	-1.79100000
H	6.25036100	1.50394800	-0.61894700
H	7.03892300	-1.00041100	-0.00328100
C	5.20422100	-2.76506500	-1.34927100
H	4.92810000	-3.50775700	-0.58744800
H	4.57028300	-2.92087500	-2.22874700
H	6.24114500	-2.98863300	-1.63739900
C	-2.83833600	1.33882500	-0.06255500
C	-2.12989200	2.41640700	-0.81077200

C	-2.16280700	0.02379200	-0.17095400
C	-0.96917000	2.20744800	-1.46627800
H	-2.58490300	3.40409600	-0.80756600
C	-0.97769200	-0.19294400	-0.79630700
H	-2.65160000	-0.81961400	0.30386300
C	-0.28425200	0.93208300	-1.41967100
O	0.87483800	0.84023300	-1.97189300
H	-0.44527700	3.00431900	-1.98301800
C	-0.45229500	-1.59538300	-0.71004100
O	-1.15071700	-2.53622100	-0.37496500
O	0.85401000	-1.70087800	-0.97740200
C	1.43908200	-2.98216000	-0.66850100
H	1.30875700	-3.18694200	0.39669900
H	0.97268800	-3.77063900	-1.26453900
H	2.49356600	-2.87261700	-0.91422900
C	-4.66725900	0.87031900	-1.86659900
C	-4.37696000	1.26766900	-0.40447900
C	-5.08787400	0.37032300	0.57785000
C	-5.68911200	-0.78649100	0.26532100
C	-5.72222600	-1.31452300	-1.15406100
C	-4.68418400	-0.65055200	-2.06871600
H	-2.77681900	1.60792100	1.00613600
H	-5.08702900	0.70681500	1.61536200
H	-5.57202300	-2.40278700	-1.14210100
H	-3.69349500	-1.06895600	-1.85567400
H	-4.73854300	2.29487900	-0.24939800
H	-5.65166000	1.27258500	-2.14082300
H	-6.73616700	-1.16160200	-1.55763600
C	-6.39856900	-1.62459500	1.29655500
H	-5.94065400	-2.62043000	1.37198100
H	-6.37927100	-1.16199200	2.28874900
H	-7.44875500	-1.78506600	1.01487100
H	5.16305600	2.33717000	0.49691000
H	6.45014600	0.59222700	1.72448800
H	-3.93522600	1.33996300	-2.53483700
H	-4.89970500	-0.88693300	-3.11752600

CSS TS22

N	-0.02025300	-1.92470800	-1.21331600
N	1.14482300	0.72180800	-1.54300100
N	-1.42671700	1.91468200	-0.90901200
N	-2.59748600	-0.72596600	-0.60250500
C	-0.75046900	-3.07528700	-1.04724300
C	0.11957800	-4.23005400	-1.19479600

C	1.37388400	-3.74749300	-1.46792800
C	1.26976800	-2.29720400	-1.49795300
C	2.31034100	-1.41949900	-1.79384800
C	2.25571900	-0.03021800	-1.83365600
C	3.35444000	0.84944000	-2.20841900
C	2.87143000	2.13030200	-2.14816700
C	1.47993900	2.03662700	-1.73368400
C	0.61658700	3.11469600	-1.55960000
C	-0.71730600	3.06546400	-1.16160900
C	-1.56095100	4.21881100	-0.90739100
C	-2.78210100	3.73599600	-0.50009500
C	-2.69343600	2.28824400	-0.52556600
C	-3.73039300	1.41207800	-0.21535700
C	-3.69449500	0.02115800	-0.26019700
C	-4.80339600	-0.86347700	0.06188600
C	-4.34922100	-2.14552500	-0.11276300
C	-2.96062500	-2.04567000	-0.53231900
C	-2.11098500	-3.12412300	-0.76151100
H	1.02953900	4.10051700	-1.74387700
H	3.26753000	-1.87103000	-2.02628600
H	-2.54883600	-4.11168000	-0.67467500
H	-4.67384000	1.86281200	0.07215600
C	-1.16790800	-0.04180200	-3.09875900
H	-0.34159600	-0.51576000	-3.64043600
H	-2.09045700	-0.60654600	-3.27437700
H	-1.29400700	0.98420800	-3.46358200
C	-0.23826900	-0.11893400	1.15781600
C	-1.08150200	-1.02118400	1.91592700
C	1.17437200	-0.26927700	1.33202700
C	-0.57906200	-2.23487000	2.25282900
H	-2.13756900	-0.79523700	2.03020600
C	1.73013700	-1.46576300	1.68821500
H	1.82905800	0.55920500	1.08432500
C	0.83863900	-2.59710800	2.04541700
O	1.21702000	-3.76330900	2.18564000
Ir	-0.72110000	-0.00417200	-1.04302000
H	-1.21264500	-3.03382800	2.62692800
C	3.21205100	-1.50982000	1.74203400
O	3.92905900	-0.60426500	1.33443300
O	3.70580100	-2.60644000	2.34018400
C	5.13516700	-2.65761500	2.43984600
H	5.58999900	-2.66012800	1.44485000
H	5.51669700	-1.79887000	3.00023400
H	5.35428000	-3.58963700	2.96150000

C	4.74519000	0.40547000	-2.56161300
C	5.69192700	0.36413100	-1.34656800
H	5.15989600	1.08047600	-3.32119000
H	4.71177800	-0.58545000	-3.03101700
H	6.68520900	0.00348500	-1.64035400
H	5.80744600	1.36563400	-0.91632100
H	5.29516200	-0.28073900	-0.55824400
C	3.59966200	3.41350900	-2.42791800
C	4.02572700	4.16400200	-1.15175400
H	2.96935200	4.07329800	-3.03956200
H	4.49051700	3.20166400	-3.03070000
H	4.55535400	5.09170300	-1.39805300
H	3.15600300	4.42121500	-0.53746600
H	4.68748800	3.54175400	-0.54015000
C	-1.12799200	5.65195400	-1.03406800
C	-0.34967200	6.16461600	0.19276200
H	-2.00933300	6.28590700	-1.18714800
H	-0.50902100	5.77569800	-1.93219400
H	-0.07602800	7.21926300	0.07306700
H	-0.95238400	6.06747200	1.10290700
H	0.57066200	5.59086900	0.34429800
C	-3.98398200	4.51051500	-0.04262600
C	-4.10960100	4.54673300	1.49339900
H	-4.89648300	4.07479700	-0.47022500
H	-3.93054000	5.53691400	-0.42379800
H	-4.99858600	5.10676100	1.80559500
H	-4.18164600	3.53242900	1.90204500
H	-3.22915300	5.02226800	1.94065900
C	-6.14313100	-0.40637400	0.56177800
C	-6.11609700	-0.01684200	2.05294000
H	-6.88404000	-1.20005100	0.41045800
H	-6.49197100	0.45051200	-0.02987000
H	-7.10140500	0.32337100	2.39221800
H	-5.81721900	-0.87256700	2.66899100
H	-5.39469800	0.78853800	2.23242500
C	-5.06409400	-3.43583200	0.16573900
C	-4.68569100	-4.03160100	1.53657200
H	-4.83995600	-4.16744600	-0.62153500
H	-6.14786400	-3.27412400	0.12933400
H	-5.20709900	-4.97913600	1.71456400
H	-3.60741100	-4.21724000	1.59706400
H	-4.94817400	-3.33794900	2.34355900
C	-0.31611300	-5.65319500	-0.99433500
C	-0.54986500	-6.01173300	0.48721100

H	0.44153400	-6.32653200	-1.41099200
H	-1.23509900	-5.84393300	-1.56621500
H	-0.81503600	-7.07057100	0.59130800
H	0.34004200	-5.80057600	1.08523300
H	-1.36329600	-5.41326600	0.91215100
C	2.65507900	-4.51474900	-1.62176900
C	3.59037500	-4.35297700	-0.40624400
H	3.17932100	-4.19568800	-2.53365500
H	2.42505000	-5.57693200	-1.76089900
H	4.45722100	-5.01930300	-0.49103800
H	3.96055400	-3.32487700	-0.33593300
H	3.05985200	-4.56561700	0.52625200
C	3.45153000	2.94813000	3.75581600
C	3.14304700	3.34553600	2.30504800
C	1.69660200	3.15099000	1.95129600
C	0.82973100	2.42230600	2.69069500
C	1.26141900	1.70847100	3.95808200
C	2.78829400	1.60488700	4.08559700
H	1.34956400	3.57365000	1.01131900
H	0.84194400	2.24073300	4.82595100
H	0.81174600	0.70668000	3.97312400
C	-0.53383800	2.18673000	2.21436600
H	-1.26254300	1.88721200	2.96975400
H	-0.93516000	2.90944300	1.50418500
H	-0.53539200	1.16552800	1.44593200
H	3.05698700	1.27297500	5.09528000
H	3.16153900	0.84736900	3.38510800
H	4.53587500	2.89285100	3.90568400
H	3.07167700	3.72259700	4.43696600
H	3.74201900	2.72824800	1.61610700
H	3.44204100	4.38387200	2.10607100

OSS^{TS23}

N	-1.71786000	-1.14845100	-1.19847300
N	1.13791000	-0.86507800	-1.59191900
N	0.91571100	1.98019100	-1.12885900
N	-1.95684500	1.70582500	-0.80413600
C	-3.07764800	-1.08381900	-0.99817000
C	-3.63472500	-2.42681700	-0.97184400
C	-2.59130500	-3.29127500	-1.17192100
C	-1.39585300	-2.47733400	-1.33237700
C	-0.12044400	-2.96543500	-1.59701200
C	1.05110000	-2.22918200	-1.73229400
C	2.36236500	-2.77411600	-2.04385200

C	3.22932500	-1.71470800	-2.09537300
C	2.45302600	-0.52111900	-1.80761400
C	2.95991200	0.77217900	-1.74075500
C	2.26329700	1.92762300	-1.39731800
C	2.84887400	3.24610700	-1.22540200
C	1.83490800	4.07955100	-0.82434500
C	0.62177400	3.28207700	-0.79255000
C	-0.65145200	3.76176700	-0.49784300
C	-1.84384500	3.04403000	-0.50765800
C	-3.15179200	3.58171000	-0.17524400
C	-4.04624800	2.54810400	-0.29255300
C	-3.28342600	1.37496300	-0.68185300
C	-3.79879600	0.08777800	-0.80733700
H	4.01780900	0.88828800	-1.94875000
H	-0.03202500	-4.03955800	-1.70869400
H	-4.87001400	-0.01991800	-0.68215600
H	-0.72424800	4.81433400	-0.24667600
C	-0.64671000	0.69582700	-3.26786200
H	0.32725500	0.95096100	-3.69810000
H	-1.02092500	-0.23348400	-3.70874400
H	-1.35930500	1.50863500	-3.43914300
C	-0.49146000	0.66575400	1.69846900
C	-1.84675600	0.66630700	2.12163100
C	0.21542500	-0.55412200	1.61756600
C	-2.47982900	-0.51694600	2.38496100
H	-2.38512900	1.60845500	2.17445300
C	-0.38137300	-1.76809100	1.91291900
H	1.26058600	-0.54580400	1.33194600
C	-1.81278400	-1.81251300	2.25432900
O	-2.46339600	-2.86630800	2.41084700
Ir	-0.41514600	0.42184800	-1.23716200
H	-3.52863700	-0.55639100	2.66138600
C	0.50087400	-2.96224700	1.86866100
O	1.61591300	-2.96064600	1.36263100
O	-0.00563600	-4.03908800	2.49340800
C	0.84706600	-5.19035100	2.52612100
H	1.02317900	-5.57139200	1.51602200
H	1.81060000	-4.94782200	2.98434600
H	0.30931700	-5.93014700	3.11987900
C	2.68612700	-4.23175000	-2.21033100
C	3.26316300	-4.86056500	-0.92712300
H	3.40421600	-4.35758200	-3.03125000
H	1.78868800	-4.78296100	-2.51499100
H	3.39919200	-5.94228600	-1.04676700

H	4.23749300	-4.41989600	-0.68848300
H	2.60656000	-4.66808600	-0.07459000
C	4.70845500	-1.74640600	-2.35556700
C	5.56314000	-1.55435200	-1.08739500
H	4.97705900	-0.97296100	-3.08855900
H	4.96933900	-2.70550500	-2.81820200
H	6.63056300	-1.65922500	-1.31435400
H	5.40703800	-0.56176500	-0.65287500
H	5.29665300	-2.29305500	-0.32383000
C	4.29677700	3.58249900	-1.44546300
C	5.21663500	3.15463700	-0.28767300
H	4.39792600	4.66263000	-1.60316700
H	4.64607200	3.10928900	-2.37299800
H	6.25798600	3.43192300	-0.48829900
H	4.91009500	3.63101300	0.65062000
H	5.17526900	2.07151200	-0.13886500
C	1.91790800	5.52028500	-0.41167400
C	1.91198300	5.68722900	1.12111900
H	1.08068500	6.08650700	-0.84082600
H	2.82982600	5.97189000	-0.81911400
H	1.96641200	6.74392700	1.40736400
H	0.99931500	5.26217700	1.55502200
H	2.76587800	5.16541800	1.56853900
C	-3.40429500	4.98640800	0.29087900
C	-3.01807400	5.19656800	1.76843400
H	-4.46346400	5.23537000	0.15674500
H	-2.84489100	5.69592600	-0.33339200
H	-3.19475500	6.23199400	2.08200400
H	-3.60508300	4.53685300	2.41763000
H	-1.95942400	4.96454700	1.93145400
C	-5.51354200	2.54463700	0.02557900
C	-5.80747400	2.00498300	1.43965000
H	-6.05672600	1.94024200	-0.71251600
H	-5.91380400	3.56161000	-0.06244000
H	-6.88425600	1.99252600	1.64396800
H	-5.42496800	0.98474500	1.55448800
H	-5.32152300	2.62840600	2.19893900
C	-5.07222800	-2.74725400	-0.67774500
C	-5.44016100	-2.55696200	0.80801300
H	-5.27770000	-3.78399600	-0.96730100
H	-5.73000600	-2.12469100	-1.30052000
H	-6.46941100	-2.88361900	0.99796900
H	-4.75723700	-3.11574100	1.45370100
H	-5.36043600	-1.50340400	1.09813400

C	-2.60442500	-4.79261400	-1.15511200
C	-1.95696900	-5.38133600	0.11432400
H	-2.08765400	-5.18194000	-2.04402000
H	-3.63914600	-5.14559200	-1.22946300
H	-2.07058500	-6.47183500	0.13764500
H	-0.88821200	-5.14936200	0.14704100
H	-2.39767600	-4.94916700	1.01654200
C	4.70024100	-0.54159400	3.25800900
C	4.42174900	0.44641600	2.11608000
C	3.25151800	1.34135000	2.38775400
C	2.31201800	1.10444400	3.37707000
C	2.43393200	-0.11537500	4.28255700
C	3.39195500	-1.18281800	3.73305000
H	3.10539000	2.19135200	1.72198100
H	2.78133900	0.21797300	5.27150900
H	1.43624700	-0.54540900	4.43530200
C	1.20912000	1.94801600	3.53111200
H	0.46298700	1.77220900	4.29901100
H	1.11748700	2.86142000	2.95002900
H	-0.02024600	1.58676000	1.38923600
H	3.58708400	-1.93439400	4.50770200
H	2.92411500	-1.70721400	2.89166500
H	5.40901200	-1.30704700	2.92081800
H	5.17526900	-0.00955300	4.09444500
H	4.21301800	-0.11317600	1.18938400
H	5.31293700	1.05087400	1.89805600

17

C	0.25602500	1.54260900	-0.39161000
C	-0.62008200	2.74344600	-0.20629500
C	-0.49384700	0.25267600	-0.33190100
C	-1.93062600	2.65419800	0.06051400
H	-0.13505400	3.71645300	-0.27345700
C	-1.81548900	0.14285800	-0.08775600
H	0.08509300	-0.65649500	-0.47122300
C	-2.64104700	1.35906500	0.18788200
O	-3.81568000	1.32239500	0.53225300
H	-2.54969800	3.53266200	0.21975700
C	-2.37964500	-1.24749600	-0.07038500
O	-1.70556500	-2.24215700	0.12784700
O	-3.69158500	-1.28544000	-0.34668300
C	-4.27590300	-2.59703300	-0.35617200
H	-3.81077800	-3.22130500	-1.12513400
H	-4.14710600	-3.08155400	0.61595600

H	-5.33314700	-2.44097800	-0.57183100
C	4.72073100	-1.27991100	0.00856200
C	3.54911800	-1.73610700	0.89157000
C	2.53063400	-0.64281200	1.09841000
C	2.47827400	0.49018500	0.38343000
C	3.45924800	0.77185200	-0.73824500
C	4.20581500	-0.48813400	-1.19963300
H	1.78960500	-0.80802700	1.88077000
H	2.93647400	1.22978600	-1.59040200
H	4.17964500	1.53257700	-0.39688100
C	1.43162000	1.54677500	0.65002500
H	0.99707600	1.42395500	1.64809900
H	1.89346800	2.54396200	0.61870100
H	0.72569700	1.60849300	-1.38822600
H	3.52032000	-1.12164000	-1.77991500
H	5.03050100	-0.21398700	-1.86837200
H	5.39094500	-0.63794900	0.59724100
H	5.31125400	-2.14516200	-0.31515500
H	3.91841200	-2.08524100	1.86554100
H	3.05098600	-2.60695300	0.43681500

CSST24

C	2.28481700	1.32535000	-0.69292800
C	1.98117900	0.20960700	-1.56522900
C	1.20856700	2.22599000	-0.44482800
C	0.70434300	-0.07821500	-1.93786000
H	2.80555100	-0.42891200	-1.87544100
C	-0.10939800	1.93623100	-0.74552100
H	1.40814300	3.13470900	0.11861700
C	-0.44425400	0.69448900	-1.46670300
O	-1.59686700	0.23663000	-1.59309300
H	0.46432800	-0.96114700	-2.52219600
C	-1.11460500	2.90701600	-0.24309300
O	-0.87027600	3.79183100	0.56249400
O	-2.35788800	2.72990200	-0.75263300
C	-3.34617500	3.64973000	-0.27337800
H	-3.45152300	3.57602900	0.81417700
H	-3.07736000	4.67951300	-0.52620500
H	-4.27410800	3.35969000	-0.76774900
H	2.02984300	0.66220900	0.61687000
C	-2.42599600	0.07659400	1.47416800
C	-1.55500400	-0.99318600	0.92055100
C	-1.75234400	0.91017400	2.51457600
C	-0.20285700	-1.00504400	1.07457400

H	-2.02182500	-1.77036800	0.32560200
C	-0.41180000	0.92525300	2.64228000
H	-2.37000000	1.59310600	3.09341000
C	0.42322700	0.09395300	1.79004200
O	1.67041500	0.38716100	1.71129100
H	-2.55992500	0.76221100	0.61469000
H	0.10645600	1.61793600	3.29691700
C	0.54213500	-2.12430500	0.41541700
O	0.00703000	-2.95655200	-0.28869700
O	1.85626300	-2.14712400	0.71441800
C	2.60213400	-3.19720200	0.07773300
H	2.59249900	-3.06078400	-1.00778400
H	3.61657800	-3.10798900	0.46579400
H	2.17658800	-4.17484100	0.31789500
C	6.43263700	-1.57852900	-0.15653300
C	6.69869900	-0.60426000	-1.31349600
C	5.64769700	0.47527400	-1.39846600
C	4.76786400	0.75711200	-0.42628300
C	4.76036900	0.00067800	0.88789900
C	6.04657200	-0.80827300	1.11235700
H	5.62419900	1.06090300	-2.31798000
H	4.60684200	0.70879800	1.71412400
H	3.88737200	-0.66439200	0.92346100
C	3.72728200	1.84113000	-0.59985500
H	3.78181300	2.54334800	0.24474800
H	3.95496500	2.42221500	-1.50395300
H	6.86633900	-0.12596200	1.37734800
H	5.91635300	-1.49183800	1.96042000
H	5.60847100	-2.25000000	-0.43617200
H	7.31157000	-2.21019500	0.02021400
H	6.74869300	-1.14834100	-2.26689900
H	7.68952500	-0.13848700	-1.18855400
C	-5.48978400	-1.91495600	-1.91408200
C	-5.55525700	-2.85442600	-0.70027400
C	-4.90067500	-2.24814500	0.51643700
C	-4.58312700	-0.95050400	0.63204400
C	-4.87481800	0.05163600	-0.46921600
C	-5.87368300	-0.48821500	-1.50329400
H	-4.67156600	-2.92572800	1.33992700
H	-5.25711400	0.98134800	-0.01986400
H	-3.93649500	0.32237600	-0.97394600
C	-3.85323000	-0.42237300	1.84434200
H	-4.39718300	0.43224700	2.27236100
H	-3.78221500	-1.18684900	2.62689100

H	-6.88588000	-0.49482700	-1.07396100
H	-5.89895100	0.17443500	-2.37637700
H	-4.46564500	-1.90598100	-2.31077100
H	-6.14459200	-2.28259600	-2.71331800
H	-5.07363100	-3.81393000	-0.93311000
H	-6.60461300	-3.09818700	-0.46771400

OSSTS25

N	-1.13978800	-1.79914200	-1.27200600
N	1.47262300	-0.58567700	-1.64188300
N	0.32617100	2.03274300	-1.16322500
N	-2.29867300	0.82620300	-0.82777200
C	-2.44422000	-2.17631300	-1.06614200
C	-2.53224700	-3.62802200	-1.03742700
C	-1.26322700	-4.10467400	-1.23931500
C	-0.40048600	-2.94489400	-1.39849600
C	0.97765500	-2.98785500	-1.59460600
C	1.84478300	-1.90643700	-1.69588400
C	3.28899500	-2.00027100	-1.83624700
C	3.76611900	-0.71748000	-1.89265500
C	2.61702400	0.16336100	-1.75008500
C	2.67947100	1.54977000	-1.64611100
C	1.62743200	2.41701200	-1.36666300
C	1.74249000	3.86012800	-1.21433500
C	0.48452900	4.32958800	-0.94449200
C	-0.40115700	3.17547500	-0.93197100
C	-1.77527300	3.22087500	-0.72518500
C	-2.65568900	2.14110000	-0.68229000
C	-4.09351200	2.23918800	-0.48799200
C	-4.58946600	0.96127900	-0.55821400
C	-3.45051800	0.08356600	-0.77660600
C	-3.51090000	-1.30338700	-0.87947000
H	3.65983900	1.99940800	-1.75602900
H	1.42604900	-3.97299700	-1.65834300
H	-4.49330500	-1.75347400	-0.78590500
H	-2.20970100	4.20454100	-0.58388800
C	-0.92585700	0.38609400	-3.24532200
H	-0.07163700	0.08779300	-3.86391400
H	-1.79419000	-0.23752500	-3.48352700
H	-1.16616700	1.43960200	-3.42519600
C	0.25182000	-0.30605400	0.97291900
C	0.03872700	-1.60866400	1.46389300
C	1.44377700	0.32291800	1.32289600
C	1.04972100	-2.31732300	2.10300600

H	-0.92080500	-2.09197700	1.30610500
C	2.49116800	-0.36045500	1.97096300
H	1.63531600	1.34936900	1.03154700
C	2.29592500	-1.72140800	2.33954400
O	3.23636300	-2.49696600	2.92892300
Ir	-0.40171900	0.11554200	-1.21134700
H	0.90513100	-3.34256000	2.43076400
C	3.73361700	0.40276500	2.19687600
O	3.89685100	1.58526600	1.96838800
O	4.75473200	-0.36085600	2.71652400
C	5.97929400	0.34157400	2.99659800
H	6.40324200	0.74368700	2.07414500
H	5.79470000	1.16095300	3.69577100
H	6.64687200	-0.40041500	3.43582300
C	4.06778900	-3.28088800	-1.76500000
C	4.19989600	-3.78553800	-0.31277600
H	5.06738900	-3.13377700	-2.19098300
H	3.58750700	-4.05625200	-2.37672700
H	4.76951900	-4.72131300	-0.26749500
H	4.70606300	-3.04137900	0.31207100
H	3.21505300	-3.95706100	0.13408100
C	5.19373200	-0.26154600	-1.98656800
C	5.79428100	0.11709800	-0.61919100
H	5.26683700	0.60033200	-2.66308700
H	5.80085300	-1.05388600	-2.44030300
H	6.84280200	0.42298200	-0.72079600
H	5.23722600	0.93966800	-0.16067900
H	5.74843400	-0.73467700	0.06901100
C	3.03450700	4.62287100	-1.25504000
C	3.77949300	4.58181300	0.09440400
H	2.84038500	5.66609500	-1.53275400
H	3.68342900	4.21768000	-2.04242100
H	4.74372500	5.10017600	0.02694000
H	3.18387100	5.07034600	0.87425600
H	3.95564000	3.55229700	0.42080500
C	0.06092200	5.73364100	-0.62454100
C	-0.14705200	5.95846100	0.88645200
H	-0.86810400	5.97817200	-1.15739200
H	0.81571700	6.43857900	-0.99232300
H	-0.45672500	6.98934900	1.09505000
H	-0.91527100	5.28323600	1.27988400
H	0.77966300	5.75851100	1.43579200
C	-4.82935200	3.51449100	-0.19490300
C	-4.66291700	3.96378800	1.27044000

H	-5.89611600	3.38636400	-0.41275900
H	-4.47816700	4.31397600	-0.86063300
H	-5.20157700	4.89895200	1.46329800
H	-5.04737100	3.19771700	1.95369200
H	-3.60574800	4.12084700	1.51276800
C	-6.01480600	0.50850700	-0.41445800
C	-6.33151000	-0.10247700	0.96401200
H	-6.25170500	-0.22657600	-1.19528000
H	-6.68458300	1.35880700	-0.58815700
H	-7.39354100	-0.36135200	1.04683200
H	-5.74957000	-1.01543500	1.13038600
H	-6.08500200	0.60125000	1.76725200
C	-3.78094100	-4.39827800	-0.72021400
C	-4.10511000	-4.39195300	0.78730500
H	-3.67481800	-5.43471500	-1.06159900
H	-4.63297900	-3.98225400	-1.27452100
H	-5.02974400	-4.94172400	0.99915500
H	-3.29074500	-4.85356900	1.35737300
H	-4.22141900	-3.36560400	1.15350900
C	-0.77889000	-5.52448200	-1.19213000
C	-0.14618800	-5.87827200	0.16912000
H	-0.04394000	-5.69888000	-1.98907700
H	-1.61157900	-6.20908900	-1.39274000
H	0.22318200	-6.91044400	0.18011800
H	0.69152800	-5.20908200	0.39485600
H	-0.88181900	-5.76780700	0.97427700
C	-2.35632400	-1.62817700	3.85133400
C	-3.02609600	-0.82357600	2.88243400
C	-2.49206400	0.39349600	2.45868300
C	-1.29063500	0.87623100	2.96698800
C	-0.60466900	0.13120100	4.07761800
C	-1.19347100	-1.20219400	4.41258500
H	-3.01722500	0.97360800	1.70995400
H	0.46848200	0.02454500	3.85330200
H	-0.62005700	0.77493900	4.98089200
C	-0.81514700	2.26864600	2.68048500
H	0.27645900	2.33634700	2.69539600
H	-1.16939500	2.62045800	1.71067700
H	-1.19239700	2.95295900	3.45721100
H	4.05449100	-1.96979300	3.01689900
H	-3.95844900	-1.17111400	2.45157300
H	-0.66530200	-1.81583400	5.13718500
H	-2.77642300	-2.59400600	4.11973600