Supporting Information

Involving Carbene or Not? Mechanism of Corey-Winter Reaction

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S1. Selected Total Syntheses of Natural Products Using Corey-Winter Reactions

Since discovered, the Corey-Winter reaction has been widely applied in total syntheses of natural products. Herein, several selected natural products listed in Figure S1 have been synthesized by using the Corey-Winter reaction in this century, including didehydrostemofoline,[1] isodidehydrostemofoline,[1] astellatol,[2] cortistain J,[3] trichodermamide A,[4] trichodermamide B[4] and pimara-15-en-3α,8α-diol.[5] These examples showcase that the Corey-Winter is a powerful and robust reaction to construct double bonds.

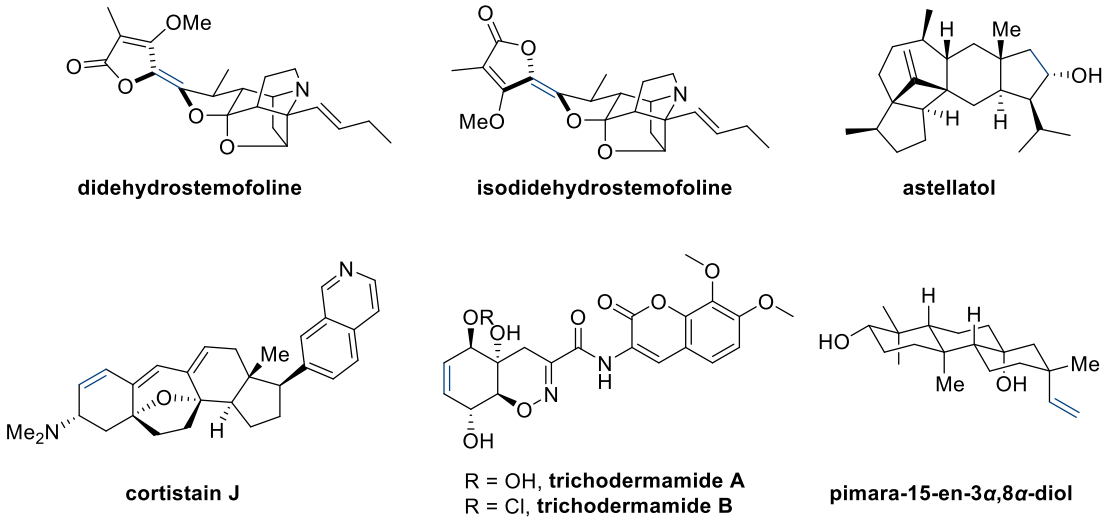


Figure S1. Selected total syntheses of natural products using the Corey-Winter reaction in the 21st century.

S2. More Details on Computational Methods

- **Example Commands for IRC calculations**

```
#p chkbas m062x irc=(lqa,rcfc,maxpoints=30,maxcycle=20) geom=allcheck
guess=tcheck int=ultrafine
```

- **Example Commands for IBO calculations**

```
! PBE0 def2-TZVP tightSCF nopop miniprint
%maxcore 2000
%pal nproc 16 end
%loc
LocMet IAOIBO
end
* xyz 0 1
Coordinates
*
```

- ***Ab initio* molecular dynamics**

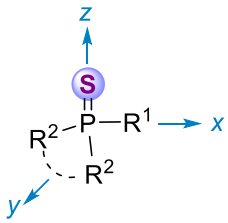
```
! wB97X-D3 def2-SVP def2/J RIJCOSX strongSCF noautostart miniprint
nopop
%maxcore  10000
%pal nprocs   10 end
%md
timestep 1.0_fs
 initvel 384.15_K no_overwrite
 thermostat berendsen 298.15_K timecon 30.0_fs
 dump position stride 1 format xyz filename "pos.xyz"
 constraint add center 0..25
 run 2000
end
* xyz 0 1
Coordinates
*
```

- **Example Commands for DLPNO-CCSD(T) Calculations**

```
! DLPNO-CCSD(T) def2-QZVPP def2-QZVPP/C tightSCF tightPNO nopop miniprint
%maxcore 5000
%pal nproc 16 end
* xyz 0 1
Coordinates
*
```

- **SambVca for Steric Map and %V_{Bur}**

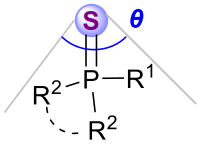
With the optimized structures of **[P]S**, the S atom was considered as a metal atom, while P−S and P−R^1 were considered as the *z* and *x* axis. Other settings are the same as the original paper.[6]



[P]S

- **Cone Angle**

Similar to steric map calculations, exact cone angles[7] were calculated based on the optimized structures of **[P]S**, using Allen's method with MORFEUS[8] module on Python. The S atom was considered as a metal atom.



[P]S

S3. Benchmark Study

To evaluate which functional is more propriate to study the mechanism of the Corey-Winter reaction, we did a benchmark study using DLPNO-CCSD(T)/def2-QZVPP single point energies as references (Figure S2). Eight functionals were tested, namely, B3LYP,[9] B3LYP-D3BJ,[9-10] BMK,[11] M06,[12] M06-2X, PBE0, TPSSh,[13] and ωB97X-D. Among these functionals, M06-2X showed the best performance (Table S1), with a mean absolute error (MAE) of only 2.0 kcal/mol. It performed extremely good in calculating the energies of **TS1**, **TS2**, and **TS3**, which are the most important transition states in determining the activation free energies of the Corey-Winter reactions. Other functionals like B3LYP-D3BJ, M06, PBE0, and ωB97X-D also have good performance, with MAEs of 3.0, 2.9, 2.3, and 2.8 kcal/mol, respectively. However, they overestimated the energies of **TS1**, **TS2**, or **TS3** significantly. Thus, M06-2X was selected as the functional for structure optimization.

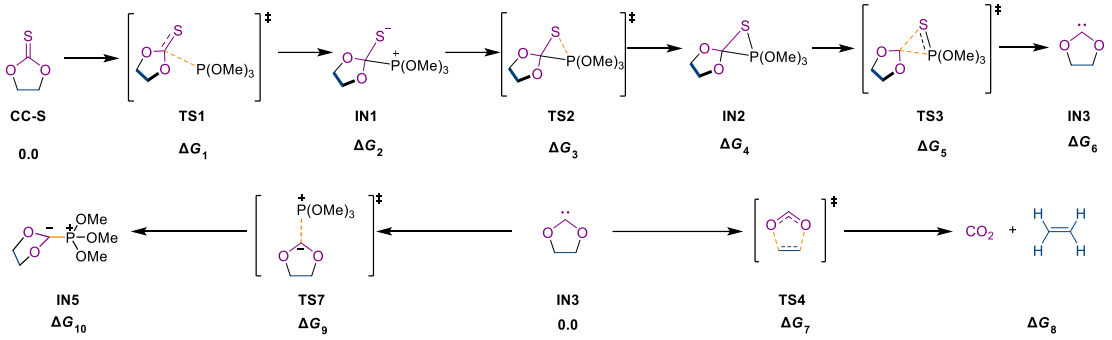


Figure S2. Key steps studied in the benchmark study.

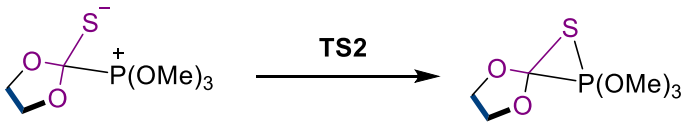
Table S1. Calculated Relative Gibbs Energy (with Solvation) for Structures in Figure S2.[a]

Method	DLPNO-CCSD(T)	B3LYP	B3LYP-D3BJ	BMK	M06	M06-2X	PBE0	TPSSh	ωB97X-D
ΔG_1	26.4	36.4	26.1	31.4	28.7	26.5	29.1	32.0	28.7
ΔG_2	20.2	33.8	23.2	27.1	25.2	22.5	24.4	28.8	24.2
ΔG_3	31.1	46.4	36.2	35.5	35.1	33.6	33.5	37.3	35.6
ΔG_4	27.7	43.2	33.1	32.2	31.7	30.3	30.2	33.8	32.6
ΔG_5	28.1	39.7	30.2	33.9	30.1	29.6	32.2	32.5	31.9
ΔG_6	1.2	6.5	4.3	5.2	3.7	3.9	4.5	4.1	3.8
ΔG_7	14.5	15.4	8.7	18.1	14.3	19.0	14.1	9.1	16.8
ΔG_8	-55.6	-55.1	-58.9	-54.9	-60.9	-52.5	-53.3	-55.4	-56.4
ΔG_9	21.7	27.6	21.0	24.7	21.1	21.3	20.9	23.2	22.9
ΔG_{10}	17.9	26.3	19.3	23.0	20.7	18.3	17.5	22.2	19.4
MAE	0.0	8.7	3.0	4.3	2.9	2.0	2.3	4.5	2.8

[a]MAE, mean absolute error. Calculated at Method/def2-QZVPP:SMD(TEP)//M06-2X/def2-TZVP level.

S4. Relative Stability of IN1 and IN2

To further support the relative stability between **IN1** and **IN2** mentioned in the main text, we applied other long-range-corrected functionals such as ωB97X-D and CAM-B3LYP to optimize these two structures. Based on the optimized structures, DLPNO-CCSD(T) single point calculations were used. The results indicated that both ωB97X-D and CAM-B3LYP gave results similar to those with M06-2X, further confirming that **IN1** is more stable than **IN2** in both the gas phase and solution phase (Figure S3).



	IN1	IN2
M06-2X	0.0 (0.0)	7.5 (3.4)
***ω*B97X-D**	0.0 (0.0)	7.3 (3.8)
CAM-B3LYP	0.0 (0.0)	7.2 (3.0)

Figure S3. Relative stability between **IN1** and **IN2** calculated by different functionals. **M06-2X**: calculated at DLPNO-CCSD(T)/def2-QZVPP: SMD(TEP)//M06-2X/def2-TZVP. ***ω*B97X-D**: DLPNO-CCSD(T)/def2-QZVPP: SMD(TEP)//ωB97X-D/def2-TZVP. **CAM-B3LYP**: calculated at DLPNO-CCSD(T)/def2-QZVPP: SMD(TEP)//CAM-B3LYP/def2-TZVP. Gas phase Gibbs energies are given in parentheses.

S5. Comparison of Gas Phase and Solution Phase Geometry Optimizations

In the main text, we mention that all geometry optimizations were carried out in the gas phase, since the structures optimized in gas phase and solution phase generally do not have much difference. To further support our conclusions, we also calculated the Gibbs energy profile of the Corey-Winter reaction of **CC-S** and trimethyl phosphite ($P(OMe)_3$, TMP) using structures optimized in the solution phase ($P(OEt)_3$, TEP), as shown in Figure S4. Compared to the gas phase optimization result, the solution phase optimization result showed neglectable difference. This comparison indicates that it's appropriate to do geometry optimization in the gas phase to reduce computational cost without decreasing computational accuracy.

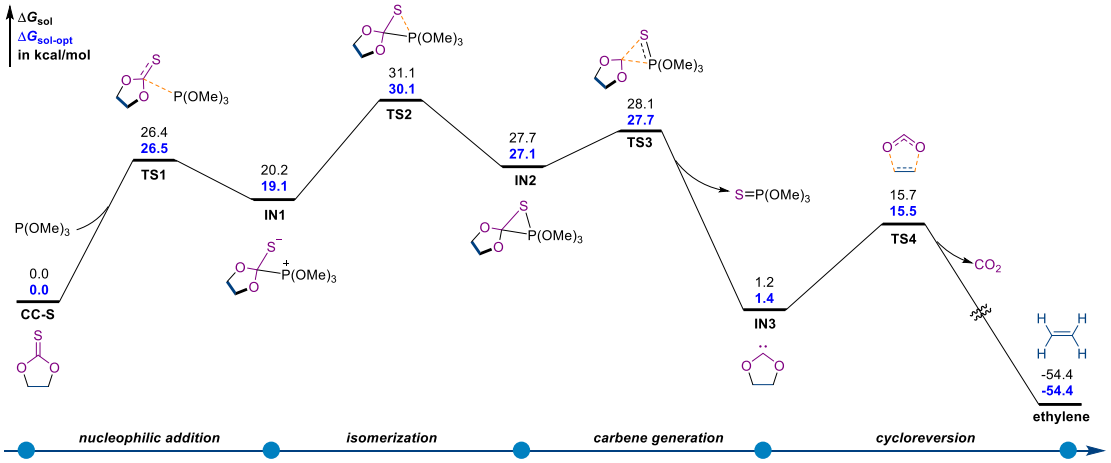
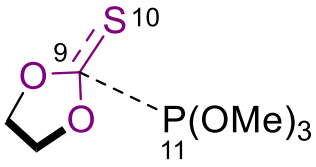


Figure S4. Gibbs energy profiles of the Corey-Winter reaction of **CC-S** with geometries optimized in the gas phase and solution.

S6. Relaxed Potential Energy Surface Scan for Carbene Generation

Table S2. Relaxed Potential Energy Surface Scan for Carbene IN3 Generation[a]



C9-C11 (Å)	C10-C11 (Å)	*E* (a.u.)	C9-C11 (Å)	C10-C11 (Å)	*E* (a.u.)	C9-C11 (Å)	C10-C11 (Å)	*E* (a.u.)
1.7	1.7	-1352.040128	1.8	1.7	-1352.052481	1.9	1.7	-1352.056800
1.7	1.8	-1352.080151	1.8	1.8	-1352.090550	1.9	1.8	-1352.095415
1.7	1.9	-1352.101690	1.8	1.9	-1352.110488	1.9	1.9	-1352.112069
1.7	2.0	-1352.111024	1.8	2.0	-1352.119121	1.9	2.0	-1352.119417
1.7	2.1	-1352.112981	1.8	2.1	-1352.120350	1.9	2.1	-1352.119680
1.7	2.2	-1352.114702	1.8	2.2	-1352.117601	1.9	2.2	-1352.115990
1.7	2.3	-1352.118768	1.8	2.3	-1352.122538	1.9	2.3	-1352.118605
1.7	2.4	-1352.120015	1.8	2.4	-1352.124082	1.9	2.4	-1352.120572
1.7	2.5	-1352.120653	1.8	2.5	-1352.125109	1.9	2.5	-1352.122133
1.7	2.6	-1352.120729	1.8	2.6	-1352.125655	1.9	2.6	-1352.123346
1.7	2.7	-1352.120286	1.8	2.7	-1352.125758	1.9	2.7	-1352.124114
1.7	2.8	-1352.119077	1.8	2.8	-1352.125269	1.9	2.8	-1352.124267
1.7	2.9	-1352.116675	1.8	2.9	-1352.123864	1.9	2.9	-1352.123549
1.7	3.0	-1352.112782	1.8	3.0	-1352.121208	1.9	3.0	-1352.121749
1.7	3.1	-1352.107256	1.8	3.1	-1352.117093	1.9	3.1	-1352.118703
1.7	3.2	-1352.100953	1.8	3.2	-1352.112188	1.9	3.2	-1352.114341
1.7	3.3	-1352.092345	1.8	3.3	-1352.105132	1.9	3.3	-1352.109209
1.7	3.4	-1352.082220	1.8	3.4	-1352.096356	1.9	3.4	-1352.102004
1.7	3.5	-1352.070860	1.8	3.5	-1352.085982	1.9	3.5	-1352.093002
2.0	1.7	-1352.062746	2.1	1.7	-1352.065614	2.2	1.7	-1352.068223
2.0	1.8	-1352.097608	2.1	1.8	-1352.098618	2.2	1.8	-1352.100129
2.0	1.9	-1352.112005	2.1	1.9	-1352.112562	2.2	1.9	-1352.113158
2.0	2.0	-1352.115822	2.1	2.0	-1352.114876	2.2	2.0	-1352.114492
2.0	2.1	-1352.114845	2.1	2.1	-1352.111379	2.2	2.1	-1352.108820
2.0	2.2	-1352.109882	2.1	2.2	-1352.102935	2.2	2.2	-1352.101322
2.0	2.3	-1352.102720	2.1	2.3	-1352.094084	2.2	2.3	-1352.089667
2.0	2.4	-1352.112956	2.1	2.4	-1352.103526	2.2	2.4	-1352.094782
2.0	2.5	-1352.115329	2.1	2.5	-1352.107322	2.2	2.5	-1352.100845
2.0	2.6	-1352.117551	2.1	2.6	-1352.111106	2.2	2.6	-1352.106744
2.0	2.7	-1352.119349	2.1	2.7	-1352.114440	2.2	2.7	-1352.111718
2.0	2.8	-1352.120418	2.1	2.8	-1352.116842	2.2	2.8	-1352.115353
2.0	2.9	-1352.120409	2.1	2.9	-1352.117924	2.2	2.9	-1352.117457
2.0	3.0	-1352.119189	2.1	3.0	-1352.117529	2.2	3.0	-1352.118021
2.0	3.1	-1352.116751	2.1	3.1	-1352.115408	2.2	3.1	-1352.117137
2.0	3.2	-1352.113205	2.1	3.2	-1352.112195	2.2	3.2	-1352.114967
2.0	3.3	-1352.108426	2.1	3.3	-1352.107317	2.2	3.3	-1352.110996
2.0	3.4	-1352.102205	2.1	3.4	-1352.102326	2.2	3.4	-1352.105792
2.0	3.5	-1352.095194	2.1	3.5	-1352.095478	2.2	3.5	-1352.098877
2.3	1.7	-1352.071136	2.4	1.7	-1352.074573	2.5	1.7	-1352.078573

2.3	1.8	-1352.102088	2.4	1.8	-1352.104707	2.5	1.8	-1352.108069
2.3	1.9	-1352.114257	2.4	1.9	-1352.116130	2.5	1.9	-1352.118906
2.3	2.0	-1352.114808	2.4	2.0	-1352.116004	2.5	2.0	-1352.118236
2.3	2.1	-1352.108442	2.4	2.1	-1352.109079	2.5	2.1	-1352.110801
2.3	2.2	-1352.098216	2.4	2.2	-1352.098396	2.5	2.2	-1352.099618
2.3	2.3	-1352.089464	2.4	2.3	-1352.090056	2.5	2.3	-1352.086705
2.3	2.4	-1352.089061	2.4	2.4	-1352.088556	2.5	2.4	-1352.090845
2.3	2.5	-1352.098138	2.4	2.5	-1352.099030	2.5	2.5	-1352.101528
2.3	2.6	-1352.105863	2.4	2.6	-1352.107483	2.5	2.6	-1352.110134
2.3	2.7	-1352.111956	2.4	2.7	-1352.114089	2.5	2.7	-1352.116933
2.3	2.8	-1352.116417	2.4	2.8	-1352.119044	2.5	2.8	-1352.122125
2.3	2.9	-1352.119261	2.4	2.9	-1352.122417	2.5	2.9	-1352.125890
2.3	3.0	-1352.120567	2.4	3.0	-1352.124315	2.5	3.0	-1352.128312
2.3	3.1	-1352.120785	2.4	3.1	-1352.125374	2.5	3.1	-1352.129965
2.3	3.2	-1352.119623	2.4	3.2	-1352.125098	2.5	3.2	-1352.130495
2.3	3.3	-1352.116809	2.4	3.3	-1352.123366	2.5	3.3	-1352.129761
2.3	3.4	-1352.112460	2.4	3.4	-1352.120183	2.5	3.4	-1352.127679
2.3	3.5	-1352.106481	2.4	3.5	-1352.115523	2.5	3.5	-1352.124323
2.6	1.7	-1352.083326	2.7	1.7	-1352.088312	2.8	1.7	-1352.093006
2.6	1.8	-1352.112283	2.7	1.8	-1352.116810	2.8	1.8	-1352.121225
2.6	1.9	-1352.122529	2.7	1.9	-1352.126588	2.8	1.9	-1352.130662
2.6	2.0	-1352.121263	2.7	2.0	-1352.124791	2.8	2.0	-1352.128494
2.6	2.1	-1352.113263	2.7	2.1	-1352.116248	2.8	2.1	-1352.119527
2.6	2.2	-1352.101927	2.7	2.2	-1352.104508	2.8	2.2	-1352.106906
2.6	2.3	-1352.088562	2.7	2.3	-1352.090715	2.8	2.3	-1352.093051
2.6	2.4	-1352.093733	2.7	2.4	-1352.096234	2.8	2.4	-1352.100083
2.6	2.5	-1352.104261	2.7	2.5	-1352.106513	2.8	2.5	-1352.109104
2.6	2.6	-1352.112817	2.7	2.6	-1352.114953	2.8	2.6	-1352.116834
2.6	2.7	-1352.119667	2.7	2.7	-1352.121804	2.8	2.7	-1352.123336
2.6	2.8	-1352.125008	2.7	2.8	-1352.127246	2.8	2.8	-1352.128701
2.6	2.9	-1352.129018	2.7	2.9	-1352.131454	2.8	2.9	-1352.133003
2.6	3.0	-1352.131856	2.7	3.0	-1352.134594	2.8	3.0	-1352.136343
2.6	3.1	-1352.134056	2.7	3.1	-1352.137184	2.8	3.1	-1352.139238
2.6	3.2	-1352.135267	2.7	3.2	-1352.138972	2.8	3.2	-1352.141471
2.6	3.3	-1352.135142	2.7	3.3	-1352.139843	2.8	3.3	-1352.142951
2.6	3.4	-1352.134341	2.7	3.4	-1352.139722	2.8	3.4	-1352.143606
2.6	3.5	-1352.132157	2.7	3.5	-1352.138603	2.8	3.5	-1352.143391
2.9	1.7	-1352.096961	3.0	1.7	-1352.100080			
2.9	1.8	-1352.125030	3.0	1.8	-1352.128060			
2.9	1.9	-1352.134277	3.0	1.9	-1352.137182			
2.9	2.0	-1352.131864	3.0	2.0	-1352.134613			
2.9	2.1	-1352.122611	3.0	2.1	-1352.125171			
2.9	2.2	-1352.109664	3.0	2.2	-1352.112003			
2.9	2.3	-1352.095077	3.0	2.3	-1352.097160			
2.9	2.4	-1352.102566	3.0	2.4	-1352.104152			
2.9	2.5	-1352.111101	3.0	2.5	-1352.112639			
2.9	2.6	-1352.118238	3.0	2.6	-1352.119474			
2.9	2.7	-1352.124363	3.0	2.7	-1352.125143			
2.9	2.8	-1352.129568	3.0	2.8	-1352.130023			

2.9	2.9	-1352.133903	3.0	2.9	-1352.134235			
2.9	3.0	-1352.137370	3.0	3.0	-1352.137753			
2.9	3.1	-1352.140310	3.0	3.1	-1352.140852			
2.9	3.2	-1352.142888	3.0	3.2	-1352.143460			
2.9	3.3	-1352.144790	3.0	3.3	-1352.145317			
2.9	3.4	-1352.146042	3.0	3.4	-1352.147235			
2.9	3.5	-1352.146544	3.0	3.5	-1352.148301			

[a]Computed at the M06-2X/def2-TZVP level.

S7. Site Preference for Addition of TMP to Different Thiocarbonates

As mentioned in the main text, we hypothesized that the P atom of TMP can attack the S atom of thiocarbonyl group when the thiocarbonyl is linked with an electron-withdrawing group in order to stabilize the formal carbanion after addition. To test our hypothesis, we scanned the potential energy surface of TMP attacking **TC1**, with an electron-withdrawing CO_2Me group attached to the thiocarbonyl group. Indeed, both **TS-X1** (P attacking C) and **TS-X2** (P attacking S) were located (Figure S5), and **TS-X2** has even a lower Gibbs energy in the gas phase (Figure S6). The solution phase Gibbs energy of **TS-X2** (20.6 kcal/mol) is also comparable with **TS-X1** (20.2 kcal/mol). As a comparison, there's only one transition state (**TS-X4**, P attacking C) found on the potential energy surface of **TC2** reacting with TMP (Figure S7). These two examples give a clear explanation on how the substitutions on thiocarbonyl controls the addition position when it is attacked by a phosphite.

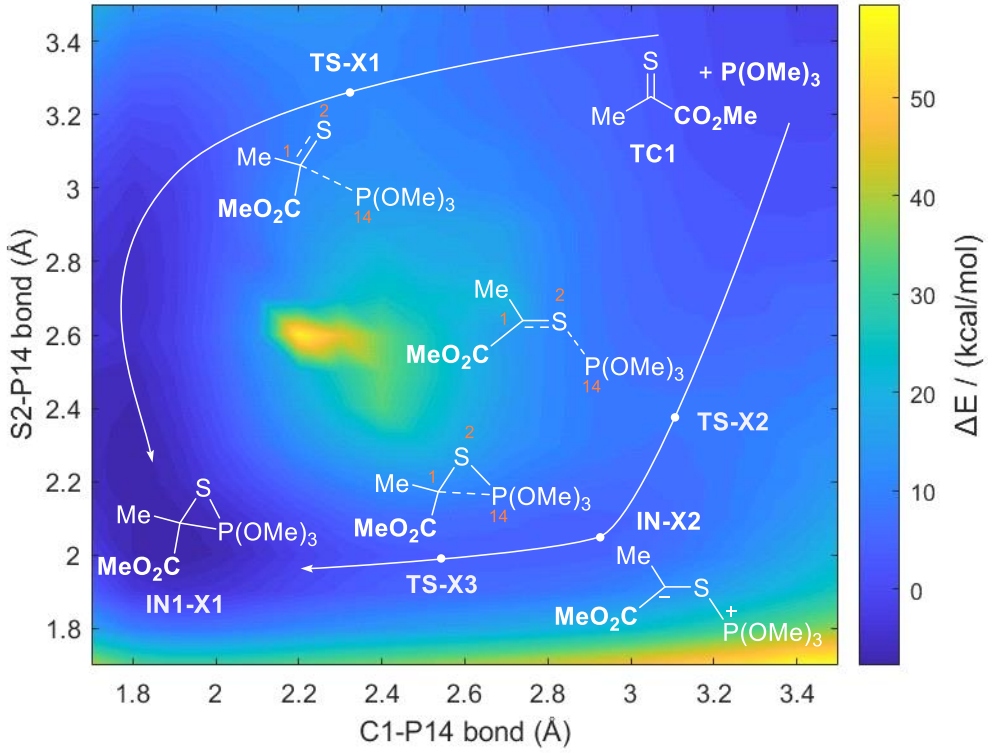


Figure S5. Potential energy surface for addition of TMP to **TC1**. Scanned at M06-2X/def2-TZVP level.

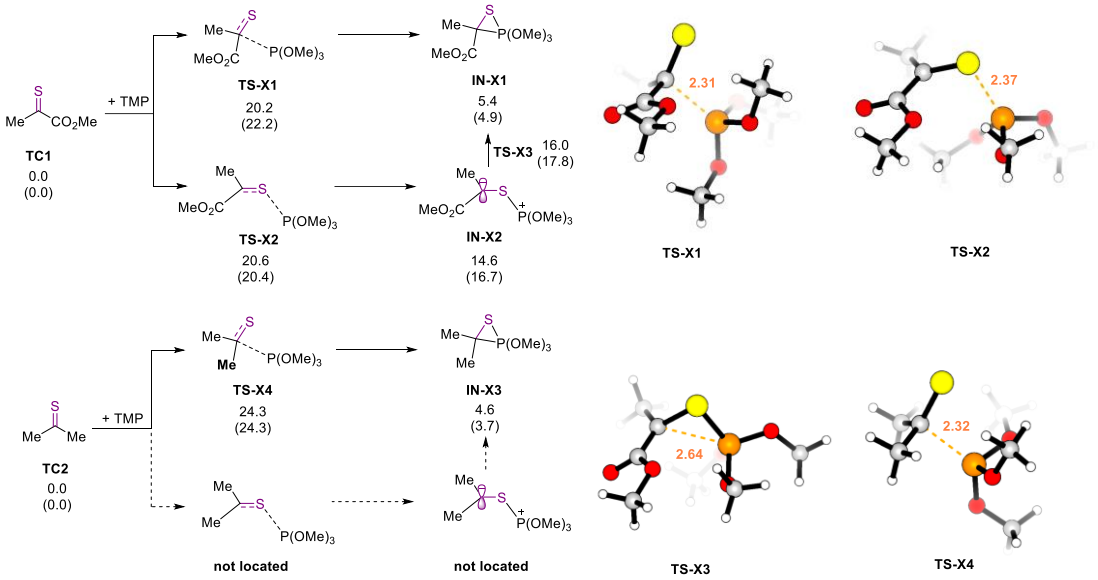


Figure S6. Gibbs energy profile of **TC1** and **TC2** attacked by TMP. Gas phase Gibbs energies are given in parentheses. Computed at DLPNO-CCSD(T)/def2-QZVPP:SMD(TEP)//M06-2X/def2-TZVP or DLPNO-CCSD(T)/def2-QZVPP//M06-2X/def2-TZVP (Gibbs energies shown in parentheses) level. Bond distances are reported in Å.

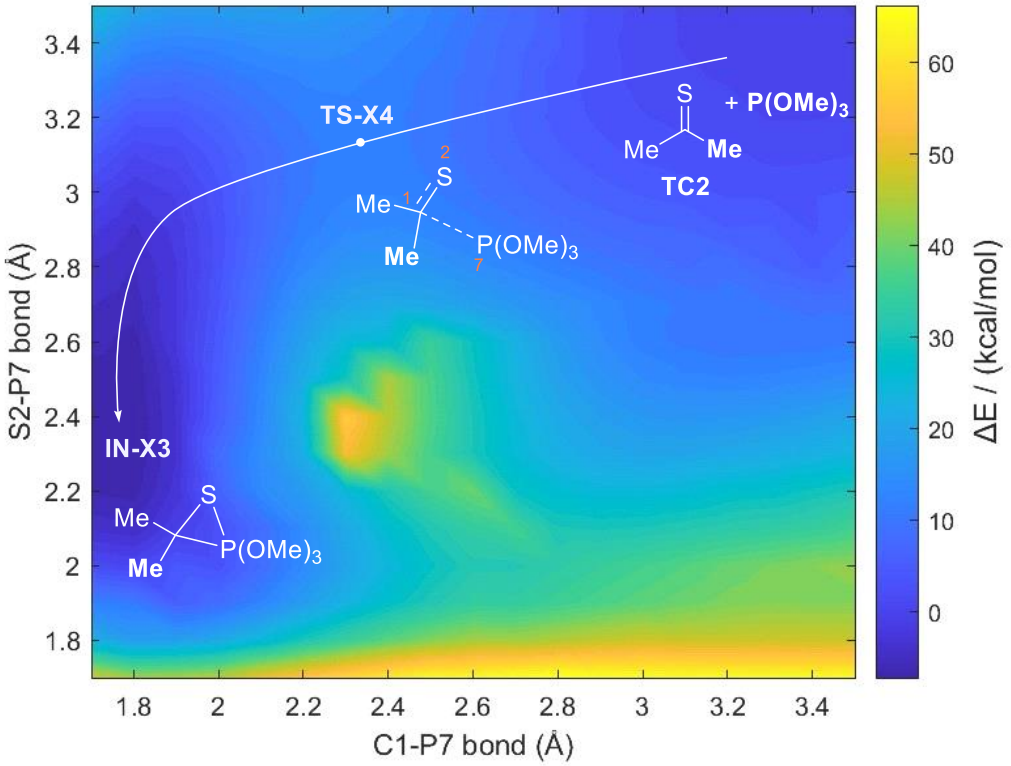
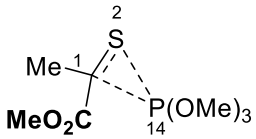


Figure S7. Potential energy surface for addition of TMP to **TC2**. Scanned at M06-2X/def2-TZVP level.

Table S3. Relaxed Potential Energy Surface Scan for Addition of TMP to TC1[a]



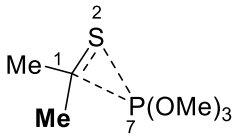
S2-P14 (Å)	C1-P14 (Å)	*E* (a.u.)	S2-P14 (Å)	C1-P14 (Å)	*E* (a.u.)	S2-P14 (Å)	C1-P14 (Å)	*E* (a.u.)
3.5	3.5	-1391.453623	3.4	3.5	-1391.453323	3.3	3.5	-1391.451681
3.5	3.4	-1391.453370	3.4	3.4	-1391.453207	3.3	3.4	-1391.452844
3.5	3.3	-1391.452623	3.4	3.3	-1391.452491	3.3	3.3	-1391.452254
3.5	3.2	-1391.451405	3.4	3.2	-1391.451188	3.3	3.2	-1391.450959
3.5	3.1	-1391.449775	3.4	3.1	-1391.449357	3.3	3.1	-1391.448950
3.5	3.0	-1391.447716	3.4	3.0	-1391.446990	3.3	3.0	-1391.446310
3.5	2.9	-1391.446896	3.4	2.9	-1391.445923	3.3	2.9	-1391.444386
3.5	2.8	-1391.444997	3.4	2.8	-1391.444290	3.3	2.8	-1391.442865
3.5	2.7	-1391.442585	3.4	2.7	-1391.442268	3.3	2.7	-1391.441120
3.5	2.6	-1391.439762	3.4	2.6	-1391.439982	3.3	2.6	-1391.439255
3.5	2.5	-1391.436548	3.4	2.5	-1391.437480	3.3	2.5	-1391.437376
3.5	2.4	-1391.433232	3.4	2.4	-1391.434976	3.3	2.4	-1391.435604
3.5	2.3	-1391.430852	3.4	2.3	-1391.433382	3.3	2.3	-1391.434645
3.5	2.2	-1391.429756	3.4	2.2	-1391.433504	3.3	2.2	-1391.435762
3.5	2.1	-1391.430227	3.4	2.1	-1391.435231	3.3	2.1	-1391.438684
3.5	2.0	-1391.431721	3.4	2.0	-1391.437906	3.3	2.0	-1391.442573
3.5	1.9	-1391.432579	3.4	1.9	-1391.439791	3.3	1.9	-1391.445608
3.5	1.8	-1391.423794	3.4	1.8	-1391.438437	3.3	1.8	-1391.445252
3.5	1.7	-1391.422043	3.4	1.7	-1391.430660	3.3	1.7	-1391.438264
3.2	3.5	-1391.451229	3.1	3.5	-1391.450538	3.0	3.5	-1391.449522
3.2	3.4	-1391.452208	3.1	3.4	-1391.450607	3.0	3.4	-1391.449769
3.2	3.3	-1391.451792	3.1	3.3	-1391.450158	3.0	3.3	-1391.449500
3.2	3.2	-1391.450619	3.1	3.2	-1391.450062	3.0	3.2	-1391.448530
3.2	3.1	-1391.448582	3.1	3.1	-1391.448146	3.0	3.1	-1391.446697
3.2	3.0	-1391.445721	3.1	3.0	-1391.445240	3.0	3.0	-1391.443840
3.2	2.9	-1391.443732	3.1	2.9	-1391.441653	3.0	2.9	-1391.440791
3.2	2.8	-1391.442122	3.1	2.8	-1391.440177	3.0	2.8	-1391.437285
3.2	2.7	-1391.440081	3.1	2.7	-1391.436090	3.0	2.7	-1391.435505
3.2	2.6	-1391.437789	3.1	2.6	-1391.434793	3.0	2.6	-1391.433823
3.2	2.5	-1391.435482	3.1	2.5	-1391.433842	3.0	2.5	-1391.432026
3.2	2.4	-1391.433495	3.1	2.4	-1391.433331	3.0	2.4	-1391.430561
3.2	2.3	-1391.434808	3.1	2.3	-1391.433762	3.0	2.3	-1391.430353
3.2	2.2	-1391.436714	3.1	2.2	-1391.436421	3.0	2.2	-1391.433233
3.2	2.1	-1391.440760	3.1	2.1	-1391.441583	3.0	2.1	-1391.439434
3.2	2.0	-1391.445858	3.1	2.0	-1391.447874	3.0	2.0	-1391.448697
3.2	1.9	-1391.450061	3.1	1.9	-1391.453242	3.0	1.9	-1391.455223
3.2	1.8	-1391.450780	3.1	1.8	-1391.455046	3.0	1.8	-1391.458101
3.2	1.7	-1391.444715	3.1	1.7	-1391.449941	3.0	1.7	-1391.453974
2.9	3.5	-1391.448142	2.8	3.5	-1391.446273	2.7	3.5	-1391.443078
2.9	3.4	-1391.448644	2.8	3.4	-1391.447098	2.7	3.4	-1391.442938
2.9	3.3	-1391.448609	2.8	3.3	-1391.447419	2.7	3.3	-1391.445738

2.9	3.2	-1391.447874	2.8	3.2	-1391.446991	2.7	3.2	-1391.445764
2.9	3.1	-1391.446257	2.8	3.1	-1391.445676	2.7	3.1	-1391.444841
2.9	3.0	-1391.443561	2.8	3.0	-1391.443238	2.7	3.0	-1391.442780
2.9	2.9	-1391.439535	2.8	2.9	-1391.439394	2.7	2.9	-1391.439271
2.9	2.8	-1391.434937	2.8	2.8	-1391.433891	2.7	2.8	-1391.434014
2.9	2.7	-1391.427739	2.8	2.7	-1391.426085	2.7	2.7	-1391.419359
2.9	2.6	-1391.426048	2.8	2.6	-1391.424369	2.7	2.6	-1391.417163
2.9	2.5	-1391.425308	2.8	2.5	-1391.422826	2.7	2.5	-1391.415500
2.9	2.4	-1391.425634	2.8	2.4	-1391.417766	2.7	2.4	-1391.411850
2.9	2.3	-1391.427492	2.8	2.3	-1391.422938	2.7	2.3	-1391.416957
2.9	2.2	-1391.432128	2.8	2.2	-1391.431328	2.7	2.2	-1391.428077
2.9	2.1	-1391.439657	2.8	2.1	-1391.442326	2.7	2.1	-1391.434456
2.9	2.0	-1391.448451	2.8	2.0	-1391.447396	2.7	2.0	-1391.446253
2.9	1.9	-1391.456131	2.8	1.9	-1391.456233	2.7	1.9	-1391.456072
2.9	1.8	-1391.460048	2.8	1.8	-1391.461094	2.7	1.8	-1391.461655
2.9	1.7	-1391.456854	2.8	1.7	-1391.458737	2.7	1.7	-1391.459922
2.6	3.5	-1391.441097	2.5	3.5	-1391.438120	2.4	3.5	-1391.434255
2.6	3.4	-1391.441991	2.5	3.4	-1391.439905	2.4	3.4	-1391.437243
2.6	3.3	-1391.443318	2.5	3.3	-1391.440130	2.4	3.3	-1391.439254
2.6	3.2	-1391.443950	2.5	3.2	-1391.441392	2.4	3.2	-1391.438820
2.6	3.1	-1391.443574	2.5	3.1	-1391.441744	2.4	3.1	-1391.439608
2.6	3.0	-1391.442023	2.5	3.0	-1391.440855	2.4	3.0	-1391.439464
2.6	2.9	-1391.439013	2.5	2.9	-1391.438517	2.4	2.9	-1391.437919
2.6	2.8	-1391.434212	2.5	2.8	-1391.434384	2.4	2.8	-1391.434658
2.6	2.7	-1391.429086	2.5	2.7	-1391.428140	2.4	2.7	-1391.429356
2.6	2.6	-1391.420574	2.5	2.6	-1391.419421	2.4	2.6	-1391.421754
2.6	2.5	-1391.409582	2.5	2.5	-1391.386692	2.4	2.5	-1391.411677
2.6	2.4	-1391.395914	2.5	2.4	-1391.396597	2.4	2.4	-1391.399375
2.6	2.3	-1391.379490	2.5	2.3	-1391.408706	2.4	2.3	-1391.414608
2.6	2.2	-1391.360316	2.5	2.2	-1391.421660	2.4	2.2	-1391.425855
2.6	2.1	-1391.431360	2.5	2.1	-1391.434739	2.4	2.1	-1391.437824
2.6	2.0	-1391.445366	2.5	2.0	-1391.447036	2.4	2.0	-1391.449298
2.6	1.9	-1391.455132	2.5	1.9	-1391.457179	2.4	1.9	-1391.458800
2.6	1.8	-1391.460369	2.5	1.8	-1391.463046	2.4	1.8	-1391.464190
2.6	1.7	-1391.458084	2.5	1.7	-1391.461554	2.4	1.7	-1391.462322
2.3	3.5	-1391.432970	2.2	3.5	-1391.429534	2.1	3.5	-1391.425027
2.3	3.4	-1391.434535	2.2	3.4	-1391.433827	2.1	3.4	-1391.430858
2.3	3.3	-1391.437738	2.2	3.3	-1391.436636	2.1	3.3	-1391.435216
2.3	3.2	-1391.439837	2.2	3.2	-1391.439925	2.1	3.2	-1391.439566
2.3	3.1	-1391.440669	2.2	3.1	-1391.441982	2.1	3.1	-1391.442816
2.3	3.0	-1391.440131	2.2	3.0	-1391.442700	2.1	3.0	-1391.444817
2.3	2.9	-1391.438200	2.2	2.9	-1391.442053	2.1	2.9	-1391.445526
2.3	2.8	-1391.435042	2.2	2.8	-1391.440154	2.1	2.8	-1391.445103
2.3	2.7	-1391.431752	2.2	2.7	-1391.437232	2.1	2.7	-1391.443899
2.3	2.6	-1391.425840	2.2	2.6	-1391.434282	2.1	2.6	-1391.442864
2.3	2.5	-1391.418913	2.2	2.5	-1391.431854	2.1	2.5	-1391.442240
2.3	2.4	-1391.419611	2.2	2.4	-1391.432707	2.1	2.4	-1391.443231
2.3	2.3	-1391.425299	2.2	2.3	-1391.436769	2.1	2.3	-1391.446286

2.3	2.2	-1391.432860	2.2	2.2	-1391.442769	2.1	2.2	-1391.451039
2.3	2.1	-1391.442122	2.2	2.1	-1391.449507	2.1	2.1	-1391.456556
2.3	2.0	-1391.452314	2.2	2.0	-1391.455814	2.1	2.0	-1391.461655
2.3	1.9	-1391.460835	2.2	1.9	-1391.462403	2.1	1.9	-1391.464832
2.3	1.8	-1391.465430	2.2	1.8	-1391.465996	2.1	1.8	-1391.464039
2.3	1.7	-1391.462895	2.2	1.7	-1391.462626	2.1	1.7	-1391.460145
2.0	3.5	-1391.418738	1.9	3.5	-1391.409945	1.8	3.5	-1391.391951
2.0	3.4	-1391.425385	1.9	3.4	-1391.415845	1.8	3.4	-1391.396515
2.0	3.3	-1391.431338	1.9	3.3	-1391.421648	1.8	3.3	-1391.401514
2.0	3.2	-1391.436443	1.9	3.2	-1391.427008	1.8	3.2	-1391.406519
2.0	3.1	-1391.440609	1.9	3.1	-1391.431708	1.8	3.1	-1391.411268
2.0	3.0	-1391.443683	1.9	3.0	-1391.435540	1.8	3.0	-1391.415455
2.0	2.9	-1391.445570	1.9	2.9	-1391.438352	1.8	2.9	-1391.418863
2.0	2.8	-1391.446448	1.9	2.8	-1391.440243	1.8	2.8	-1391.421462
2.0	2.7	-1391.446656	1.9	2.7	-1391.441851	1.8	2.7	-1391.424012
2.0	2.6	-1391.446619	1.9	2.6	-1391.443164	1.8	2.6	-1391.426142
2.0	2.5	-1391.447506	1.9	2.5	-1391.444389	1.8	2.5	-1391.428019
2.0	2.4	-1391.448751	1.9	2.4	-1391.445946	1.8	2.4	-1391.429930
2.0	2.3	-1391.451254	1.9	2.3	-1391.448194	1.8	2.3	-1391.432120
2.0	2.2	-1391.455065	1.9	2.2	-1391.451320	1.8	2.2	-1391.434783
2.0	2.1	-1391.459567	1.9	2.1	-1391.454999	1.8	2.1	-1391.437783
2.0	2.0	-1391.463660	1.9	2.0	-1391.458248	1.8	2.0	-1391.440329
2.0	1.9	-1391.465838	1.9	1.9	-1391.459597	1.8	1.9	-1391.440987
2.0	1.8	-1391.463973	1.9	1.8	-1391.456914	1.8	1.8	-1391.437652
2.0	1.7	-1391.454889	1.9	1.7	-1391.446980	1.8	1.7	-1391.427109
1.7	3.5	-1391.356716						
1.7	3.4	-1391.357655						
1.7	3.3	-1391.364097						
1.7	3.2	-1391.368213						
1.7	3.1	-1391.372438						
1.7	3.0	-1391.376482						
1.7	2.9	-1391.380058						
1.7	2.8	-1391.383006						
1.7	2.7	-1391.386092						
1.7	2.6	-1391.388818						
1.7	2.5	-1391.391211						
1.7	2.4	-1391.393455						
1.7	2.3	-1391.395695						
1.7	2.2	-1391.398070						
1.7	2.1	-1391.400527						
1.7	2.0	-1391.402458						
1.7	1.9	-1391.402543						
1.7	1.8	-1391.398696						
1.7	1.7	-1391.387726						

[a]Computed at the M06-2X/def2-TZVP level.

Table S4. Relaxed Potential Energy Surface Scan for Addition of TMP to TC2[a]



C1-P7 (Å)	S2-P7 (Å)	*E* (a.u.)	C1-P7 (Å)	S2-P7 (Å)	*E* (a.u.)	C1-P7 (Å)	S2-P7 (Å)	*E* (a.u.)
3.5	3.5	-1202.885225	3.4	3.5	-1202.884279	3.3	3.5	-1202.884324
3.5	3.4	-1202.884685	3.4	3.4	-1202.884804	3.3	3.4	-1202.883807
3.5	3.3	-1202.883763	3.4	3.3	-1202.88406	3.3	3.3	-1202.88294
3.5	3.2	-1202.882359	3.4	3.2	-1202.882792	3.3	3.2	-1202.88282
3.5	3.1	-1202.880375	3.4	3.1	-1202.880925	3.3	3.1	-1202.881121
3.5	3.0	-1202.877743	3.4	3.0	-1202.878359	3.3	3.0	-1202.878719
3.5	2.9	-1202.875192	3.4	2.9	-1202.878375	3.3	2.9	-1202.875161
3.5	2.8	-1202.872517	3.4	2.8	-1202.875996	3.3	2.8	-1202.873072
3.5	2.7	-1202.869433	3.4	2.7	-1202.869135	3.3	2.7	-1202.868527
3.5	2.6	-1202.866775	3.4	2.6	-1202.867736	3.3	2.6	-1202.867923
3.5	2.5	-1202.860741	3.4	2.5	-1202.862208	3.3	2.5	-1202.863295
3.5	2.4	-1202.852522	3.4	2.4	-1202.854672	3.3	2.4	-1202.856473
3.5	2.3	-1202.846085	3.4	2.3	-1202.848049	3.3	2.3	-1202.849541
3.5	2.2	-1202.835398	3.4	2.2	-1202.837698	3.3	2.2	-1202.840119
3.5	2.1	-1202.826586	3.4	2.1	-1202.829438	3.3	2.1	-1202.831029
3.5	2.0	-1202.816303	3.4	2.0	-1202.817185	3.3	2.0	-1202.819227
3.5	1.9	-1202.817785	3.4	1.9	-1202.817504	3.3	1.9	-1202.817339
3.5	1.8	-1202.808103	3.4	1.8	-1202.808265	3.3	1.8	-1202.807997
3.5	1.7	-1202.780654	3.4	1.7	-1202.780708	3.3	1.7	-1202.780685
3.2	3.5	-1202.883938	3.1	3.5	-1202.882998	3.0	3.5	-1202.881361
3.2	3.4	-1202.883597	3.1	3.4	-1202.882866	3.0	3.4	-1202.881518
3.2	3.3	-1202.88283	3.1	3.3	-1202.882272	3.0	3.3	-1202.881145
3.2	3.2	-1202.881556	3.1	3.2	-1202.881113	3.0	3.2	-1202.880158
3.2	3.1	-1202.879723	3.1	3.1	-1202.879329	3.0	3.1	-1202.878486
3.2	3.0	-1202.878584	3.1	3.0	-1202.876876	3.0	3.0	-1202.876053
3.2	2.9	-1202.875547	3.1	2.9	-1202.873335	3.0	2.9	-1202.872797
3.2	2.8	-1202.869637	3.1	2.8	-1202.871215	3.0	2.8	-1202.86879
3.2	2.7	-1202.866758	3.1	2.7	-1202.866455	3.0	2.7	-1202.86542
3.2	2.6	-1202.868067	3.1	2.6	-1202.867068	3.0	2.6	-1202.864874
3.2	2.5	-1202.863727	3.1	2.5	-1202.863271	3.0	2.5	-1202.861652
3.2	2.4	-1202.857697	3.1	2.4	-1202.858008	3.0	2.4	-1202.857144
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3.2	2.2	-1202.840745	3.1	2.2	-1202.843169	3.0	2.2	-1202.844505
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2.9	2.6	-1202.861219	2.8	2.6	-1202.855766	2.7	2.6	-1202.848009
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2.9	2.4	-1202.854813	2.8	2.4	-1202.850699	2.7	2.4	-1202.8445
2.9	2.3	-1202.851438	2.8	2.3	-1202.84842	2.7	2.3	-1202.843368
2.9	2.2	-1202.844386	2.8	2.2	-1202.842492	2.7	2.2	-1202.838655
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2.9	1.8	-1202.809456	2.8	1.8	-1202.811676	2.7	1.8	-1202.814179
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2.6	3.5	-1202.867538	2.5	3.5	-1202.863681	2.4	3.5	-1202.85999
2.6	3.4	-1202.869077	2.5	3.4	-1202.865074	2.4	3.4	-1202.862802
2.6	3.3	-1202.869858	2.5	3.3	-1202.867103	2.4	3.3	-1202.864712
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2.6	2.5	-1202.837312	2.5	2.5	-1202.825196	2.4	2.5	-1202.812262
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2.6	2.1	-1202.83007	2.5	2.1	-1202.834953	2.4	2.1	-1202.841848
2.6	2.0	-1202.834244	2.5	2.0	-1202.838797	2.4	2.0	-1202.844897
2.6	1.9	-1202.830314	2.5	1.9	-1202.83459	2.4	1.9	-1202.840142
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2.3	2.3	-1202.800344	2.2	2.3	-1202.84918	2.1	2.3	-1202.860768
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2.0	3.4	-1202.862344	1.9	3.4	-1202.863406	1.8	3.4	-1202.861548
2.0	3.3	-1202.868572	1.9	3.3	-1202.870755	1.8	3.3	-1202.869791
2.0	3.2	-1202.873228	1.9	3.2	-1202.876691	1.8	3.2	-1202.876763
2.0	3.1	-1202.876527	1.9	3.1	-1202.881219	1.8	3.1	-1202.882513
2.0	3.0	-1202.878583	1.9	3.0	-1202.884474	1.8	3.0	-1202.886947
2.0	2.9	-1202.879427	1.9	2.9	-1202.886513	1.8	2.9	-1202.890118
2.0	2.8	-1202.879199	1.9	2.8	-1202.887453	1.8	2.8	-1202.892127
2.0	2.7	-1202.878248	1.9	2.7	-1202.887578	1.8	2.7	-1202.893186
2.0	2.6	-1202.877083	1.9	2.6	-1202.887285	1.8	2.6	-1202.895358
2.0	2.5	-1202.876078	1.9	2.5	-1202.889348	1.8	2.5	-1202.896188
2.0	2.4	-1202.875424	1.9	2.4	-1202.8897	1.8	2.4	-1202.896676
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2.0	1.8	-1202.850977	1.9	1.8	-1202.85433	1.8	1.8	-1202.855474
2.0	1.7	-1202.81107	1.9	1.7	-1202.813453	1.8	1.7	-1202.814158
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1.7	3.4	-1202.853324						
1.7	3.3	-1202.862408						
1.7	3.2	-1202.870343						
1.7	3.1	-1202.87707						
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1.7	2.9	-1202.886825						
1.7	2.8	-1202.889867						
1.7	2.7	-1202.891848						
1.7	2.6	-1202.893349						
1.7	2.5	-1202.895704						
1.7	2.4	-1202.896291						
1.7	2.3	-1202.896114						
1.7	2.2	-1202.894567						
1.7	2.1	-1202.890373						
1.7	2.0	-1202.88147						
1.7	1.9	-1202.86463						
1.7	1.8	-1202.84875						
1.7	1.7	-1202.807316						

[a]Computed at the M06-2X/def2-TZVP level.

S8. Computational Details for IBO Analysis of Cycloreversion of IN3

The IBO change along the IRC of **TS4** was shown in Figure S8. During the cycloreversion process, Φ_1, Φ_2 and Φ_3 undergo significant orbital changes.

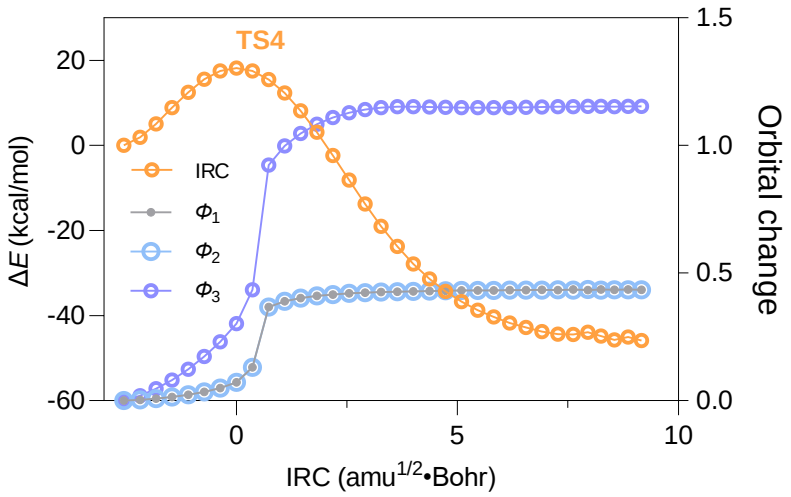

Figure S8. Change of IBOs Φ_1, Φ_2 and Φ_3 along the IRC of **TS4**.

Table S5. Orbital and Energy Change along the IRC of TS4

IRC/ (amu$^{1/2}$•Bohr)	E (a.u.)	Φ_1	Φ_2	Φ_3
-2.54727	-267.097526	0.000000	0.000000	0.000000
-2.18334	-267.094530	0.003472	0.003472	0.019839
-1.81944	-267.089422	0.008121	0.008122	0.046517
-1.45554	-267.083414	0.014392	0.014392	0.080817
-1.09166	-267.077572	0.022828	0.022828	0.122945
-0.72782	-267.072776	0.034100	0.034100	0.172743
-0.36399	-267.069661	0.049354	0.049353	0.230740
0.00000	-267.068589	0.072143	0.072142	0.302249
0.36399	-267.069674	0.130915	0.130915	0.434970
0.72781	-267.072839	0.366854	0.366854	0.923601
1.09165	-267.077894	0.389749	0.389750	0.998466
1.45552	-267.084564	0.402133	0.402133	1.047167
1.81940	-267.092514	0.410383	0.410382	1.083144
2.18330	-267.101326	0.416230	0.416230	1.109793
2.54720	-267.110468	0.420447	0.420447	1.128621
2.91112	-267.119434	0.423508	0.423508	1.140925
3.27504	-267.127831	0.425758	0.425758	1.148108
3.63895	-267.135390	0.427444	0.427445	1.151421
4.00286	-267.141982	0.428744	0.428743	1.151861
4.36674	-267.147587	0.429771	0.429772	1.150779
4.73060	-267.152248	0.430608	0.430606	1.149351
5.09444	-267.156075	0.431301	0.431305	1.148243
5.45828	-267.159220	0.431898	0.431890	1.147768
5.82209	-267.161825	0.432395	0.432413	1.147937

6.18586	-267.163985	0.432871	0.432826	1.148578
6.54955	-267.165765	0.433179	0.433299	1.149460
6.91300	-267.167209	0.433750	0.433413	1.150409
7.27395	-267.168253	0.433404	0.434362	1.151314
7.62269	-267.168345	0.435323	0.432976	1.152161
7.95527	-267.167499	0.432692	0.435883	1.152634
8.25216	-267.168983	0.435017	0.433593	1.152735
8.54887	-267.170338	0.434367	0.434603	1.152401
8.85913	-267.169344	0.435020	0.434033	1.152659
9.16746	-267.170604	0.434544	0.434551	1.152932

S9. More Details about Orbital Correlation Diagram of the Fragmentation Reaction of IN-S1

The original orbital correlation of the fragmentation reaction of **IN-S1** (forming benzene, ethylene and CO_2) proposed by Woodward and Hoffmann[14] is shown in Figure S9A. It was proposed that the π bonding orbital **B2** of CO_2 can be filled by symmetric **C1** bonding orbital of **IN-S**. The highest π bonding orbital **B3** is correlated with the antisymmetric O−C−O σ orbital **C2** and the symmetric π bonding orbital of ethylene (**B1**) is correlated with the symmetric O−C−O σ orbital **C3**. However, our computation of this process (Figure S9B) showed that the fragmentation reaction of **IN-S1** is stepwise, generating benzene and **IN3** as an intermediate, which subsequently undergoes cycloreversion to give ethylene and CO_2. Thus, the above orbital correlation diagram proposed by Woodward and Hoffmann should be revised, based on our analysis of **IN3**, which means **C1** should correlate with **B1**, while **C2** and **C3** correlate with **B3** and **B2**, respectively.

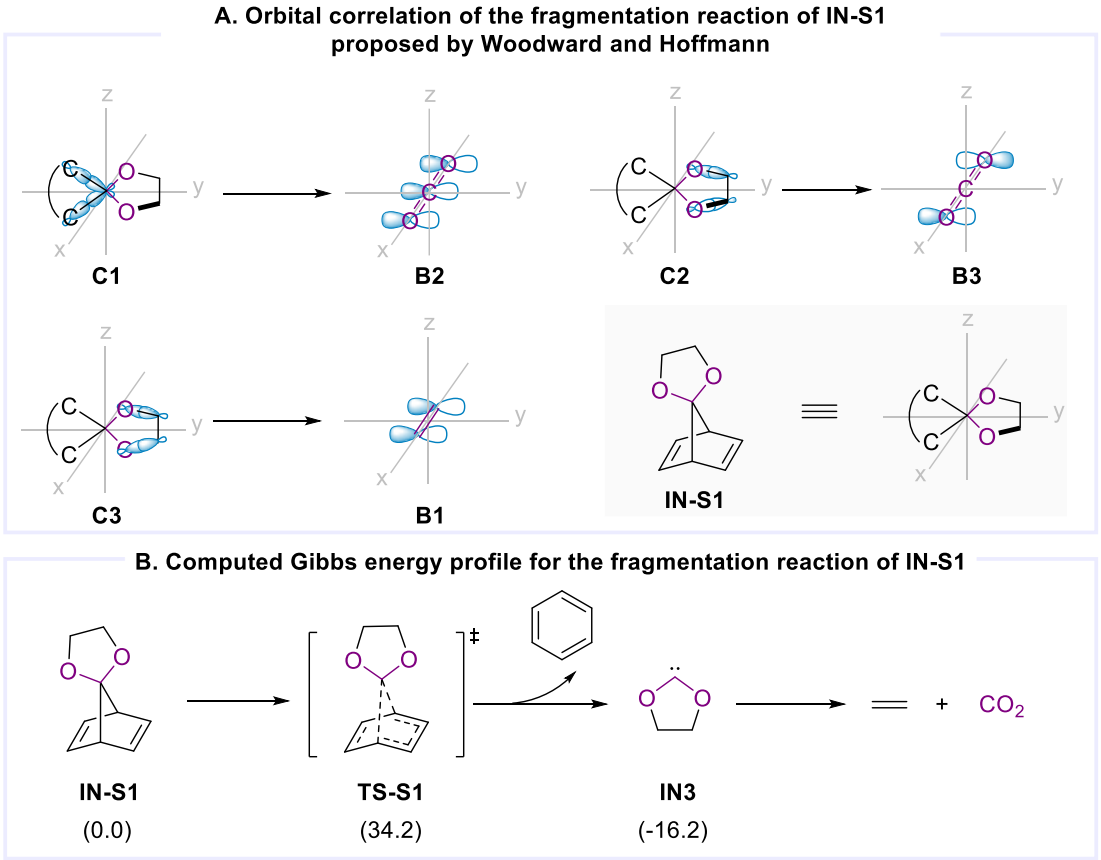

Figure S9. Computed energy profile of fragmentation reaction of **IN-S1** and orbital correlation of this process proposed by Woodward and Hoffmann. Computed at DLPNO-CCSD(T)/def2-QZVPP//M06-2X/def2-TZVP level. Adapted with permission from ref. 14. Copyright 2003 John Wiley and Sons.

In the main text, we have analyzed the molecular orbital changes along the IRC of **TS4**. However, due to page restrictions, we did not provide more detailed molecular orbital changes. Therefore, these are depicted in more details in Figure S10.

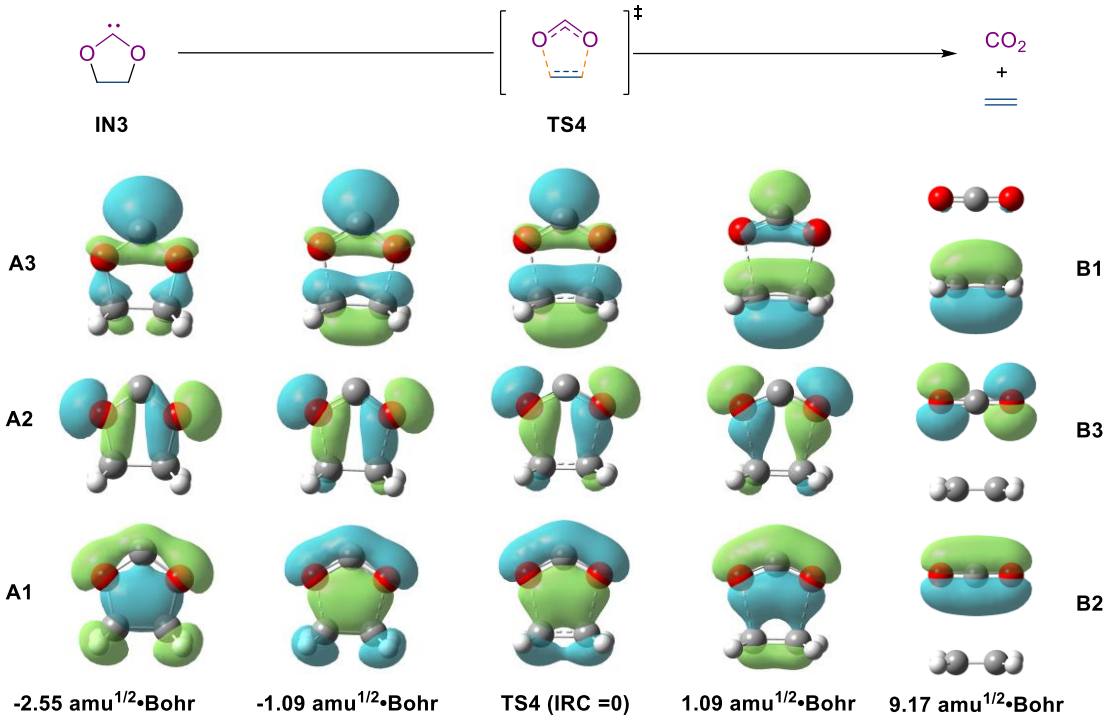

Figure S10. More detailed changes of molecular orbitals along the IRC of **TS4**.

Table S6. Change of Molecular Orbitals along the IRC of TS4.

IRC/ (amu$^{1/2}$•Bohr)	**A1** (a.u.)	**A2** (a.u.)	**A3** (a.u.)
-2.54727	-0.60678	-0.44917	-0.30710
-2.18334	-0.60041	-0.44312	-0.30290
-1.81944	-0.59467	-0.43820	-0.29897
-1.45554	-0.58950	-0.43402	-0.29599
-1.09166	-0.58504	-0.43040	-0.29428
-0.72782	-0.58168	-0.42746	-0.29381
-0.36399	-0.57990	-0.42546	-0.29430
0.00000	-0.58023	-0.42468	-0.29535
0.36399	-0.58252	-0.42489	-0.29697
0.72781	-0.58657	-0.42634	-0.29872
1.09165	-0.59163	-0.42876	-0.30055
1.45552	-0.59708	-0.43176	-0.30253
1.81940	-0.60226	-0.43501	-0.30474
2.18330	-0.60668	-0.43822	-0.30725
2.54720	-0.61000	-0.44113	-0.31010
2.91112	-0.61211	-0.44350	-0.31327
3.27504	-0.61314	-0.44527	-0.31665
3.63895	-0.61333	-0.44645	-0.32011
4.00286	-0.61289	-0.44701	-0.32358
4.36674	-0.61206	-0.44708	-0.32694
4.73060	-0.61109	-0.44681	-0.33001
5.09444	-0.61014	-0.44639	-0.33267
5.45828	-0.60928	-0.44594	-0.33489

5.82209	-0.60858	-0.44559	-0.33663
6.18586	-0.60801	-0.44537	-0.33797
6.54955	-0.60758	-0.44525	-0.33899
6.91300	-0.60772	-0.44517	-0.33979
7.27395	-0.60699	-0.44506	-0.34038
7.62269	-0.60688	-0.44454	-0.34055
7.95527	-0.60620	-0.44361	-0.34058
8.25216	-0.60504	-0.44389	-0.34116
8.54887	-0.60553	-0.44455	-0.34232
8.85913	-0.60829	-0.44611	-0.34227
9.16746	-0.60682	-0.44505	-0.34199

S10. Evaluation of the Non-Adiabatic Effect on TS4

To evaluate the non-adiabatic effect of the cycloreversion process of **IN3** via **TS4**, we calculated the S1 state of the points of the IRC along **IN3**→**TS4**→ethylene/CO_2 by using time-dependent density functional theory (TD-DFT), at TD-M06-2X/def2-TZVP level. The results (Figure S11) showed that the S1 state is much higher (more than 100 kcal/mol) than the S0 state, implying there's almost no non-adiabatic effect for **TS4**.

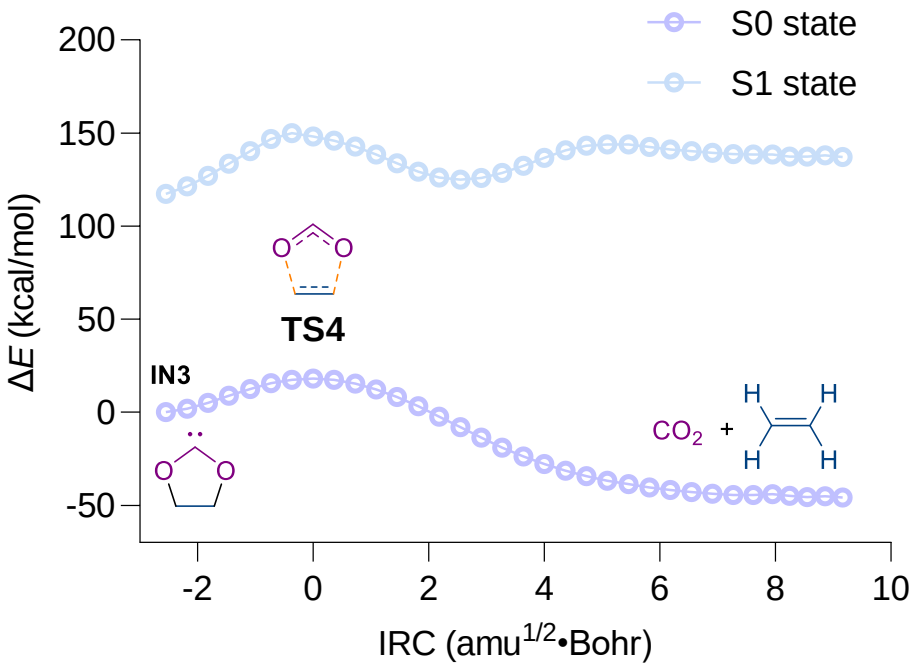

Figure S11. IRC along **IN3**→**TS4**→ethylene/CO_2 and computed energy of the first excited state (S1).

Table S7. Energies of S0 state and S1 state along the IRC of TS4.

IRC/ (amu$^{1/2}$•Bohr)	S0 state *E* (a.u.)	S1 state *E* (a.u.)[a]
-2.54727	-267.0975263	-266.910537
-2.18334	-267.0945302	-266.90414
-1.81944	-267.089422	-266.895277
-1.45554	-267.0834143	-266.884878
-1.09166	-267.0775721	-266.873944
-0.72782	-267.0727756	-266.863483
-0.36399	-267.0696609	-266.858502
0.00000	-267.0685887	-266.861357
0.36399	-267.0696741	-266.865099
0.72781	-267.0728389	-266.870213
1.09165	-267.0778937	-266.876843
1.45552	-267.0845637	-266.884437
1.81940	-267.0925144	-266.891643
2.18330	-267.1013258	-266.896623
2.54720	-267.1104677	-266.898351

2.91112	-267.1194345	-266.896815
3.27504	-267.1278308	-266.892598
3.63895	-267.1353899	-266.886528
4.00286	-267.1419824	-266.879566
4.36674	-267.147587	-266.873206
4.73060	-267.1522479	-266.869273
5.09444	-267.1560746	-266.8681
5.45828	-267.1592203	-266.868261
5.82209	-267.1618248	-266.870415
6.18586	-267.1639848	-266.872396
6.54955	-267.1657648	-266.87407
6.91300	-267.1672085	-266.875499
7.27395	-267.1682525	-266.876495
7.62269	-267.1683452	-266.876768
7.95527	-267.167499	-266.876759
8.25216	-267.1689834	-266.87849
8.54887	-267.1703376	-266.878744
8.85913	-267.1693439	-266.877557
9.16746	-267.1706045	-266.87896

[a]Computed at TD-M06-2X/def2-TZVP level (nstates=5).

S11. Spin States for the Cycloreversion Process of IN3

To further confirm the spin state during the cycloreversion process, we calculated both singlet and triplet state of **IN3**. Compared to the singlet **IN3**, the triplet **IN3-T** is 78.2 kcal/mol higher in terms of Gibbs energy (Figure S12), which means the whole cycloreversion process remains singlet state. **TS4-T**, which has a similar transition state structure with **TS4**, was also located (Figure S12B). However, it's not connecting **IN3** and **IN4** based on IRC calculations (Figure S12C). It's an isomerization transition state connected by two triplet diradicals.

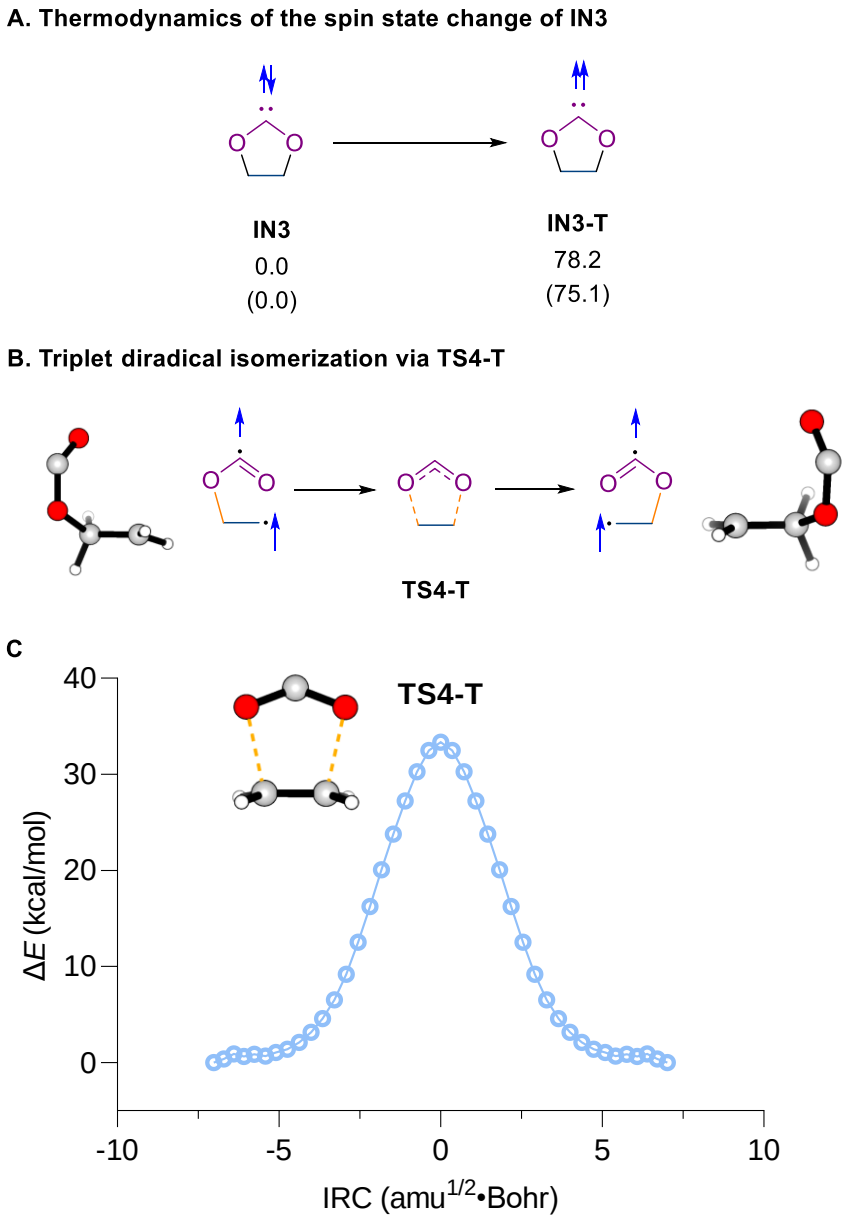

Figure S12. Spin states for the cycloreversion process of **IN3**. (A) Thermodynamics of **IN3** and **IN3-T**. Computed at DLPNO-CCSD(T)/def2-QZVPP:SMD(TEP)//M06-2X/def2-TZVP or DLPNO-CCSD(T)/def2-QZVPP//M06-2X/def2-TZVP (Gibbs energies shown in parentheses) level. (B) Triplet diradical isomerization via **TS4-T**. (C) IRC of **TS4-T**.

S12. Comparison of Dimerization between OHC and NHC

In addition to the dimerization of OHC **IN3** via **TS8**, we also calculated the dimerization process of NHC **IN3-N2** via **TS8-N**, yielding **IN6-N** (Figure S13). This process has an activation free energy of 29.5 kcal/mol, significantly higher than that of **IN3** dimerization. Previous studies[15] proposed that NHC dimerization proceeds via a proton-catalyzed pathway in the presence of a strong base and a proton source. However, under the conditions of the Corey-Winter reaction, no strong base or proton source is used, making it unlikely for OHCs like **IN3** to follow a proton-catalyzed pathway.

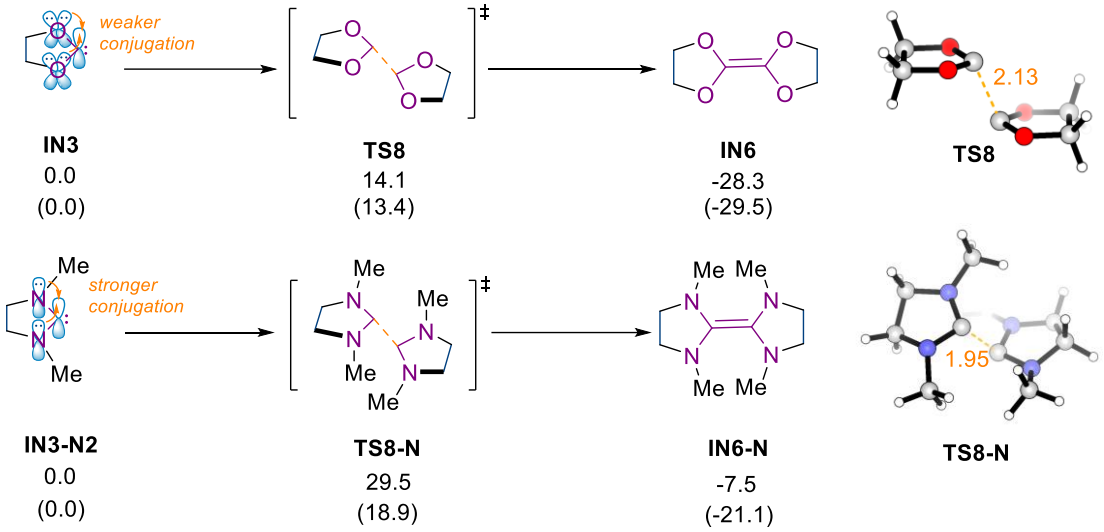

Figure S13. Dimerization of OHC and NHC. Computed at DLPNO-CCSD(T)/def2-QZVPP:SMD(TEP)//M06-2X/def2-TZVP or DLPNO-CCSD(T)/def2-QZVPP//M06-2X/def2-TZVP (Gibbs energies shown in parentheses) level. Bond distances are reported in Å.

S13. More Analysis, Data Sets, and Codes for Multivariable Linear Regression (MVLR)

S13.1. Construction of Data Sets

The phosphines and phosphates of the data sets are shown in Figure S14. Their parameters for the Corey-Winter reaction are given in Table S8 and Table S9.

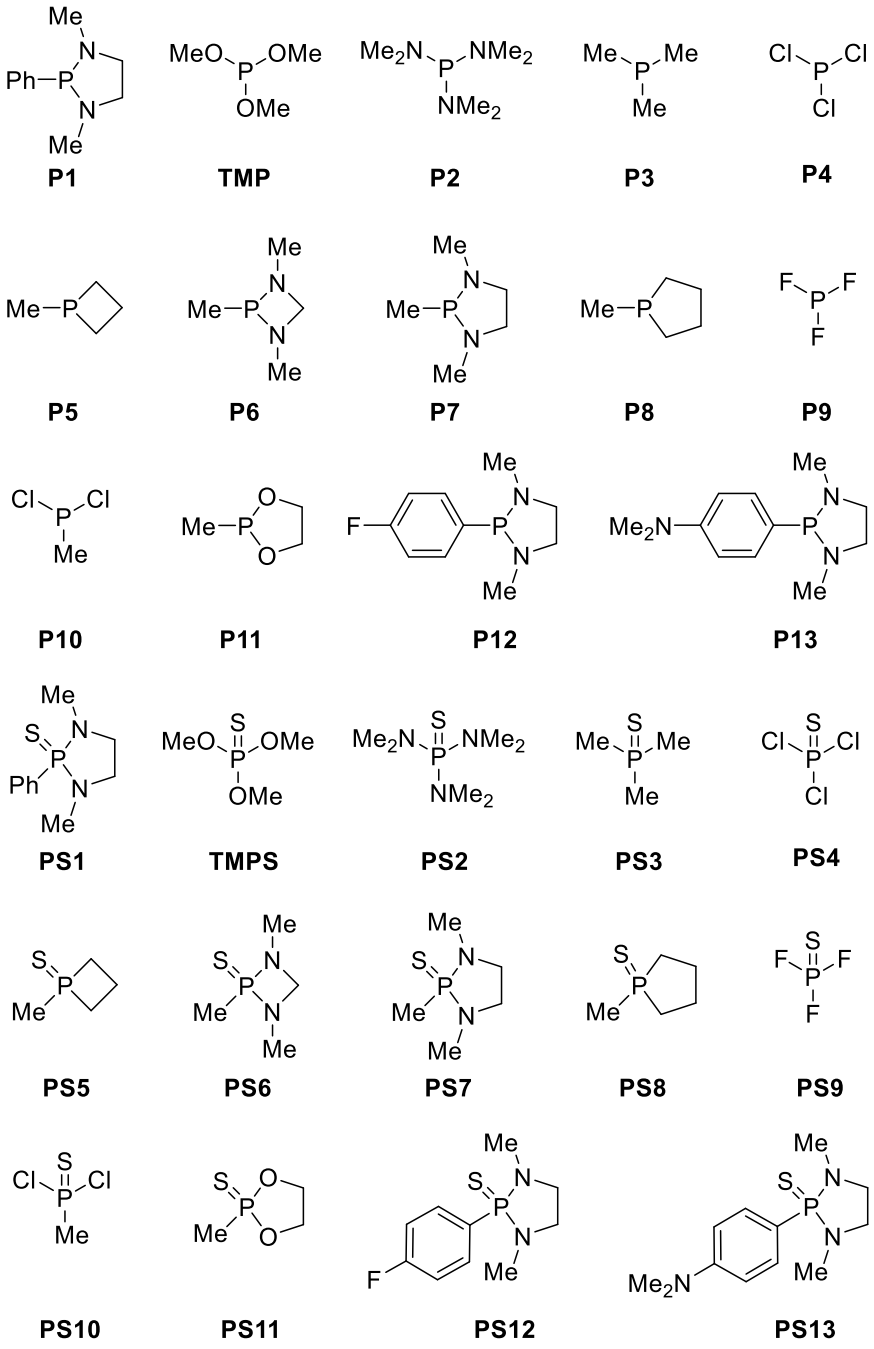

Figure S14. The phosphines and thiophosphates used in the MVLR study.

Table S8. ψ(R^2-P-C-S) of IN1-[P] and IN2-[P][a]

Phosphine	P1	TMP	P2	P3	P4	P5	P6
ψ(R^2-P-C-S) (IN1-[P])	58.9	61.9	42.6	60.5	77.1	70.7	73.7
ψ(R^2-P-C-S) (IN2-[P])	33.0	9.5	5.2	0.0	0.6	40.1	49.1
Phosphine	**P7**	**P8**	**P9**	**P10**	**P11**	**P12**	**P13**
ψ(R^2-P-C-S) (IN1-[P])	70.4	61.4	74.9	79.2	67.5	58.5	58.3
ψ(R^2-P-C-S) (IN2-[P])	30.8	12.6	1.3	10.9	24.4	33.0	35.6

[a]The unit for dihedrals reported is °.

Table S9. Parameters for Different Phosphines/Phosphate and Gibbs Energy of TS1-[P], TS2-[P] and TS3-[P]

Phosphine	P1	TMP	P2	P3	P4	P5*	P6
LUMO$_{[P]}$[a] (eV)	0.25	1.52	1.47	1.79	-0.38	1.42	0.70
HOMO$_{[P]}$[a] (eV)	-7.04	-8.21	-6.88	-7.46	-9.33	-7.31	-6.86
%V$_{Bur}$	34.4	34.8	37.6	28.2	28.9	26.6	32.4
Cone angle (◦)	171.8	179.2	182.1	136.1	145.4	137.7	159.2
dG[a] (kcal/mol)	15.9	22.5	15.8	17.0	37.8	19.8	7.9
GD	1	0	0	0	0	1	1
G(TS1)$_{Sol}$[b] (kcal/mol)	**21.8**	26.4	24.8	18.7	40.7	18.6	**18.8**
G(TS2)$_{Sol}$[b] (kcal/mol)	19.4	**31.1**	**35.5**	**33.2**	**41.5**	**25.3**	11.5
G(TS3)$_{Sol}$[b] (kcal/mol)	**21.9**	28.1	**36.0**	33.1	37.1	25.0	10.7
Phosphine	**P7***	**P8**	**P9**	**P10**	**P11**	**P12**	**P13**
LUMO$_{[P]}$[a] (eV)	1.46	1.53	0.74	0.04	1.39	0.26	0.68
HOMO$_{[P]}$[a] (eV)	-6.86	-7.47	-10.52	-8.67	-7.98	-7.16	-6.50
%V$_{Bur}$	31.7	27.4	25	28.6	26.6	34.5	34.4
Cone angle (◦)	159.4	136.6	149.8	143.1	143.1	171.9	171.4
dG[a] (kcal/mol)	13.2	16.9	34.8	28.3	18.4	16.1	13.4
GD	1	1	0	0	1	1	1
G(TS1)$_{Sol}$[b] (kcal/mol)	**20.4**	17.9	**43.8**	30.7	**23.3**	**21.9**	**21.1**
G(TS2)$_{Sol}$[b] (kcal/mol)	16.9	**31.7**	37.8	**44.5**	20.3	19.4	18.3
G(TS3)$_{Sol}$[b] (kcal/mol)	**20.9**	31.1	27.2	29.9	16.5	**21.8**	**22.1**

[a]Computed at M06-2X/def2-TZVP level. [b]Computed at DLPNO-CCSD(T)/def2-QZVPP:SMD(TEP)//M06-2X/def2-TZVP level. *Test set.

S13.2. Python Scripts for MVLR

MVLR was carried out using python script (see below for codes) with statsmodels[16] and Numpy,[17] visualized with Matplotlib.[18]

```
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.ticker as mtick
import statsmodels.api as sm
```

```
def train_and_evaluate_model(x_train, y_train, x_test, y_test,
color_label, m):
    x_train, y_train = np.array(x_train, dtype=float),
np.array(y_train, dtype=float)
    x_test = np.array(x_test, dtype=float)

    # Model training
    x_train_sm = sm.add_constant(x_train)
    model = sm.OLS(y_train, x_train_sm).fit()
    print(model.summary())

    # Predictions
    y_train_pred = model.predict(x_train_sm)
    x_test_sm = sm.add_constant(x_test, has_constant='add')
    y_test_pred = model.predict(x_test_sm)
    print(f"Prediction of test set: {y_test_pred}")

    # RMSE Calculation
    rmse_train = np.sqrt(np.mean((y_train_pred - y_train) ** 2))
    rmse_test = np.sqrt(np.mean((y_test_pred - y_test) ** 2))
    print(f"RMSE of training set: {rmse_train}")
    print(f"RMSE of test set: {rmse_test}")

    # Plot results
    font = {'family': 'Arial', 'weight': 'regular', 'size': 12}
    colors = [row[m] for row in x_train]
    sc = plt.scatter(y_train, y_train_pred, c=colors, cmap='viridis',
s=100, marker='o')
    colorbar = plt.colorbar(sc)
    colorbar.set_label(color_label, fontsize=12, fontweight='regular',
fontfamily='Arial')
    for label in colorbar.ax.get_yticklabels():
        label.set_fontname('Arial')  # Set font to Arial
        label.set_fontsize(12)

    plt.scatter(y_test, y_test_pred, c='m', s=100, marker='o')
    x_line = np.linspace(min(y_train) - 5, max(y_train) + 5, 100)
    plt.plot(x_line, x_line, 'g-')

    plt.xlabel('QC calculated ΔG$^‡$ (kcal/mol)', fontdict=font)
    plt.ylabel('MVLR predicted ΔG$^‡$ (kcal/mol)', fontdict=font)
    ax = plt.gca()
    ax.yaxis.set_major_formatter(mtick.FormatStrFormatter('%.1f'))
```

```
    ax.xaxis.set_major_formatter(mtick.FormatStrFormatter('%.1f'))
    plt.xticks(fontsize=12, fontfamily='Arial')
    plt.yticks(fontsize=12, fontfamily='Arial')
    plt.show()

# Data set for TS1
x_TS1 = [[0.25, -7.04, 34.4], [1.52, -8.21, 34.8], [1.47, -6.88, 37.6],
[1.79, -7.46, 28.2],
         [-0.38, -9.33, 28.9], [0.70, -6.86, 32.4], [1.53, -7.47,
27.4], [0.74, -10.52, 25.0],
         [0.04, -8.67, 28.6], [1.39, -7.98, 26.6], [0.26, -7.16, 34.5],
[0.68, -6.50, 34.4]]
y_TS1 = [21.8, 26.4, 24.8, 18.7, 40.7, 18.8, 17.9, 43.8, 30.7, 23.3,
21.9, 21.1]
x_TS1_noLUMO = np.delete(x_TS1, 0, axis=1)
x_TS1_noHOMO = np.delete(x_TS1, 1, axis=1)
x_TS1_noBV = np.delete(x_TS1, 2, axis=1)

x_test_TS1 = [[1.42, -7.31, 26.6], [1.46, -6.86, 31.7]]
y_test_TS1 = [18.6, 20.4]
x_test_TS1_noLUMO = np.delete(x_test_TS1, 0, axis=1)
x_test_TS1_noHOMO = np.delete(x_test_TS1, 1, axis=1)
x_test_TS1_noBV = np.delete(x_test_TS1, 2, axis=1)

# Data set for TS2
x_TS2 = [[1, 15.9], [0, 22.5], [0, 15.8], [0, 17.0], [0, 37.8], [1,
7.9], [1, 16.9], [0, 34.8],
         [0, 28.3], [1, 18.4], [1, 16.1], [1, 13.4]]
y_TS2 = [19.4, 31.1, 35.5, 33.2, 41.5, 11.5, 31.7, 37.8, 44.5, 20.3,
19.4, 18.3]
x_TS2_noGD = np.delete(x_TS2, 0, axis=1)
x_TS2_nodG = np.delete(x_TS2, 1, axis=1)

x_test_TS2 = [[1, 19.8], [1, 13.2]]
y_test_TS2 = [25.3, 16.9]
x_test_TS2_noGD = np.delete(x_test_TS2, 0, axis=1)
x_test_TS2_nodG = np.delete(x_test_TS2, 1, axis=1)

# Analysis
print("Please input the transition state (TS) you want to analysis.\n")
print("If you want to analyze TS1, please input 'TS1'.\n")
print("If you want to analyze TS2, please input 'TS2'.\n")
print("If you want to analyze TS1 without the LUMO descriptor, please
input 'TS1_noLUMO'.\n")
```

```
print("If you want to analyze TS1 without the HOMO descriptor, please
input 'TS1_noHOMO'.\n")
print("If you want to analyze TS1 without the BV descriptor, please
input 'TS1_noBV'.\n")
print("If you want to analyze TS2 without the GD descriptor, please
input 'TS2_noGD'.\n")
print("If you want to analyze TS2 without the dG descriptor, please
input 'TS2_nodG'.\n")
TS = input()

# MVLR analysis of TS1 with LUMO, HOMO, and %BV as descriptors
if TS == "TS1":
    print("MVLR result for TS1 is shown below.\n")
    train_and_evaluate_model(x_TS1, y_TS1, x_test_TS1, y_test_TS1,
"HOMO / eV", m=1)
# MVLR analysis of TS2 with GD and dG as descriptors
elif TS == "TS2":
    print("MVLR result for TS2 is shown below.\n")
    train_and_evaluate_model(x_TS2, y_TS2, x_test_TS2, y_test_TS2, "dG
/ (kcal/mol)", m=1)
# MVLR analysis of TS1 with HOMO and %BV as descriptors
elif TS == "TS1_noLUMO":
    print("MVLR result for TS1_noLUMO is shown below.\n")
    train_and_evaluate_model(x_TS1_noLUMO, y_TS1, x_test_TS1_noLUMO,
y_test_TS1, "HOMO / eV", m=0)
# MVLR analysis of TS1 with LUMO and %BV as descriptors
elif TS == "TS1_noHOMO":
    print("MVLR result for TS1_noHOMO is shown below.\n")
    train_and_evaluate_model(x_TS1_noHOMO, y_TS1, x_test_TS1_noHOMO,
y_test_TS1, "LUMO / eV", m=0)
# MVLR analysis of TS1 with LUMO and HOMO as descriptors
elif TS == "TS1_noBV":
    print("MVLR result for TS1_noBV is shown below.\n")
    train_and_evaluate_model(x_TS1_noBV, y_TS1, x_test_TS1_noBV,
y_test_TS1, "HOMO / eV", m=1)
# MVLR analysis of TS2 with dG as the descriptor
elif TS == "TS2_noGD":
    print("MVLR result for TS2_noGD is shown below.\n")
    train_and_evaluate_model(x_TS2_noGD, y_TS2, x_test_TS2_noGD,
y_test_TS2, "dG / (kcal/mol)", m=0)
# MVLR analysis of TS2 with GD as the descriptor
elif TS == "TS2_nodG":
    print("MVLR result for TS2_nodG is shown below.\n")
```

```
    train_and_evaluate_model(x_TS2_nodG, y_TS2, x_test_TS2_nodG,
y_test_TS2, "GD", m=0)
else:
    print('What you have inputted is wrong. Please try again.\n')
```

As for the MVLR for **TS1** with $\%V_{bur}$ replaced by cone angle as the steric descriptor, the above codes:

```
x_TS1 = [[0.25, -7.04, 34.4], [1.52, -8.21, 34.8], [1.47, -6.88, 37.6],
[1.79, -7.46, 28.2],
         [-0.38, -9.33, 28.9], [0.70, -6.86, 32.4], [1.53, -7.47,
27.4], [0.74, -10.52, 25.0],
         [0.04, -8.67, 28.6], [1.39, -7.98, 26.6], [0.26, -7.16, 34.5],
[0.68, -6.50, 34.4]]
```

and

```
x_test_TS1 = [[1.42, -7.31, 26.6], [1.46, -6.86, 31.7]]
```

were replaced by:

```
x_TS1 = [[0.25, -7.04, 171.8], [1.52, -8.21, 179.2], [1.47, -6.88,
182.1], [1.79, -7.46, 136.1], [-0.38, -9.33, 145.4], [0.70, -6.86,
159.2], [1.53, -7.47, 136.6], [0.74, -10.52, 149.8], [0.04, -8.67,
143.1], [1.39, -7.98, 143.1], [0.26, -7.16, 171.9], [0.68, -6.50,
171.4]]
```

and

```
x_test_TS1 = [[1.42, -7.31, 137.7], [1.46, -6.86, 159.4]]
```

S13.3. More Discussions on MVLR Results

As shown in Figure S17-22, HOMO descriptor is the most important one for **TS1-[P]** among the descriptors used, because R^2 decrease from 0.94 to 0.39 when HOMO was not used in MVLR model. LUMO and $\%V_{bur}$ was found to be less important since R^2 changes not so much when they were not used as a descriptor for MVLR of **TS1-[P]**.

As for MVLR of **TS2-[P]**, both descriptors dG and GD are important since the regression result become much worse if either of these two descriptors was not used (Figure S23-26).

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.938
Model:                            OLS   Adj. R-squared:                  0.915
Method:                 Least Squares   F-statistic:                     40.45
Date:                Sun, 23 Mar 2025   Prob (F-statistic):           3.51e-05
Time:                        21:46:19   Log-Likelihood:                -25.473
No. Observations:                  12   AIC:                             58.95
Df Residuals:                       8   BIC:                             60.89
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const        -54.2595     14.412     -3.765      0.006     -87.494     -21.025
x1            -2.2557      1.148     -1.965      0.085      -4.903       0.392
x2            -7.7501      0.920     -8.422      0.000      -9.872      -5.628
x3             0.6825      0.258      2.650      0.029       0.089       1.276
==============================================================================
Omnibus:                        0.694   Durbin-Watson:                   2.598
Prob(Omnibus):                  0.707   Jarque-Bera (JB):                0.620
Skew:                           0.219   Prob(JB):                        0.733
Kurtosis:                       1.976   Cond. No.                         652.
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
Prediction of test set: [17.34394128 17.24673114]
RMSE of training set: 2.021439521190314
RMSE of test set: 2.400082085749654
```

Figure S15. MVLR result for **TS1-[P]** with three descriptors.

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.812
Model:                            OLS   Adj. R-squared:                  0.770
Method:                 Least Squares   F-statistic:                     19.44
Date:                Sun, 23 Mar 2025   Prob (F-statistic):           0.000541
Time:                        21:48:32   Log-Likelihood:                -34.752
No. Observations:                  12   AIC:                             75.50
Df Residuals:                       9   BIC:                             76.96
Df Model:                           2
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         24.8779      6.302      3.948      0.003      10.622      39.134
x1           -11.8051      3.894     -3.031      0.014     -20.615      -2.995
x2             0.4759      0.229      2.081      0.067      -0.041       0.993
==============================================================================
Omnibus:                        5.684   Durbin-Watson:                   3.064
Prob(Omnibus):                  0.058   Jarque-Bera (JB):                2.715
Skew:                           1.137   Prob(JB):                        0.257
Kurtosis:                       3.505   Cond. No.                         108.
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
Prediction of test set: [22.49526373 19.35445433]
RMSE of training set: 4.380199769372771
RMSE of test set: 2.6354213704995684
```

Figure S16. MVLR result for **TS2-[P]** with two descriptors.

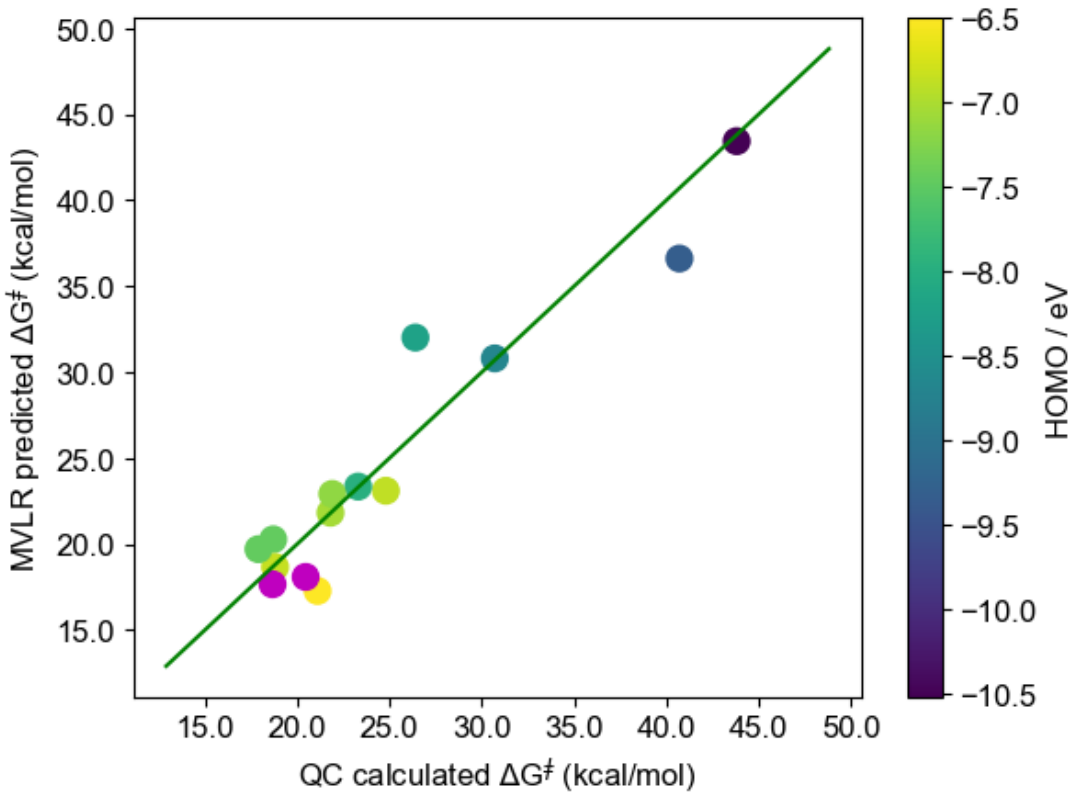

Figure S17. MVLR predicted $\Delta G^{\ddagger}$ vs QC calculated $\Delta G^{\ddagger}$ for **TS1-[P]** without the LUMO descriptor.

OLS Regression Results

Dep. Variable:	y	R-squared:	0.908
Model:	OLS	Adj. R-squared:	0.888
Method:	Least Squares	F-statistic:	44.57
Date:	Sun, 23 Mar 2025	Prob (F-statistic):	2.14e-05
Time:	21:49:42	Log-Likelihood:	-27.835
No. Observations:	12	AIC:	61.67
Df Residuals:	9	BIC:	63.13
Df Model:	2		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
const	-65.7295	15.126	-4.346	0.002	-99.947	-31.512
x1	-8.4264	0.980	-8.602	0.000	-10.642	-6.210
x2	0.8205	0.284	2.885	0.018	0.177	1.464

Omnibus:	1.804	Durbin-Watson:	2.425
Prob(Omnibus):	0.406	Jarque-Bera (JB):	0.295
Skew:	-0.318	Prob(JB):	0.863
Kurtosis:	3.432	Cond. No.	596.

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
Prediction of test set: [17.69390412 18.0868263]
RMSE of training set: 2.4612392499627536
RMSE of test set: 1.756670472707441

Figure S18. MVLR result for **TS1-[P]** without the LUMO descriptor.

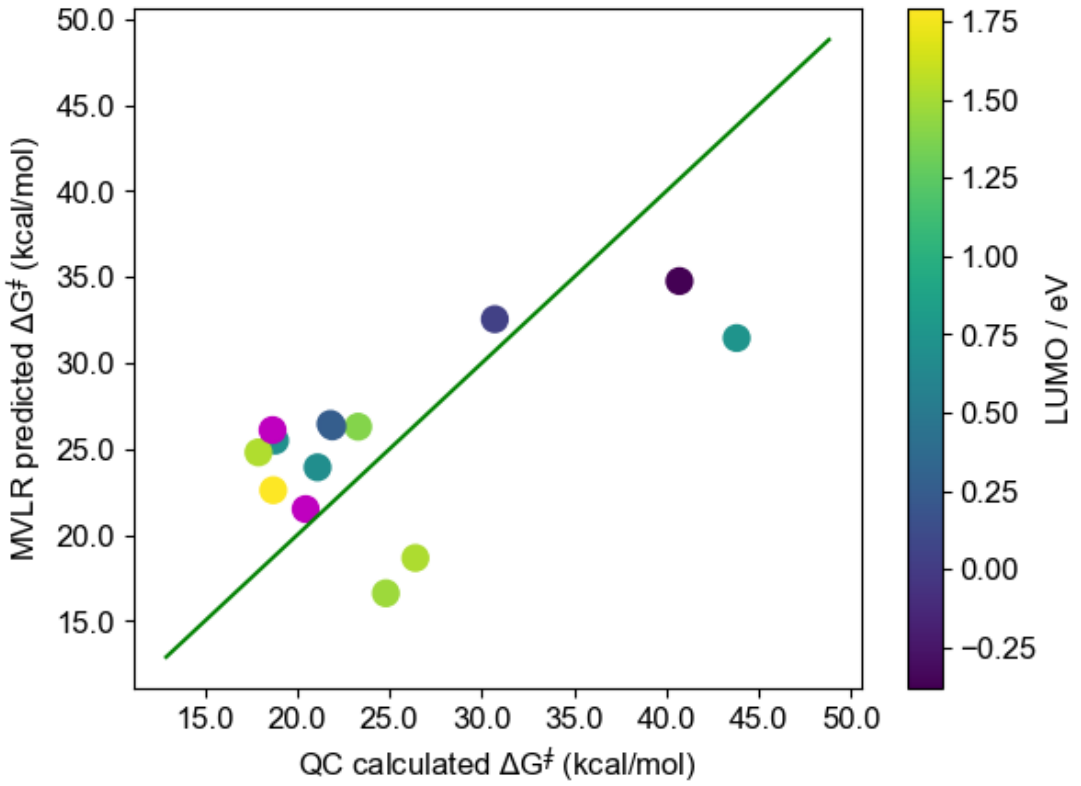

Figure S19. MVLR predicted $\Delta G^{\ddagger}$ vs QC calculated $\Delta G^{\ddagger}$ for **TS1-[P]** without the HOMO descriptor.

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.390
Model:                            OLS   Adj. R-squared:                  0.254
Method:                 Least Squares   F-statistic:                     2.873
Date:                Sun, 23 Mar 2025   Prob (F-statistic):              0.108
Time:                        21:50:46   Log-Likelihood:                -39.208
No. Observations:                  12   AIC:                             84.42
Df Residuals:                       9   BIC:                             85.87
Df Model:                           2
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         56.7328     17.280      3.283      0.009      17.643      95.822
x1            -5.8733      3.153     -1.863      0.095     -13.007       1.260
x2            -0.8375      0.544     -1.539      0.158      -2.068       0.393
==============================================================================
Omnibus:                        2.296   Durbin-Watson:                   2.344
Prob(Omnibus):                  0.317   Jarque-Bera (JB):                1.553
Skew:                           0.709   Prob(JB):                        0.460
Kurtosis:                       1.953   Cond. No.                         256.
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
Prediction of test set: [26.11525446 21.60907712]
RMSE of training set: 6.349753697681312
RMSE of test set: 5.3824212537682
```

Figure S20. MVLR result for **TS1-[P]** without the HOMO descriptor.

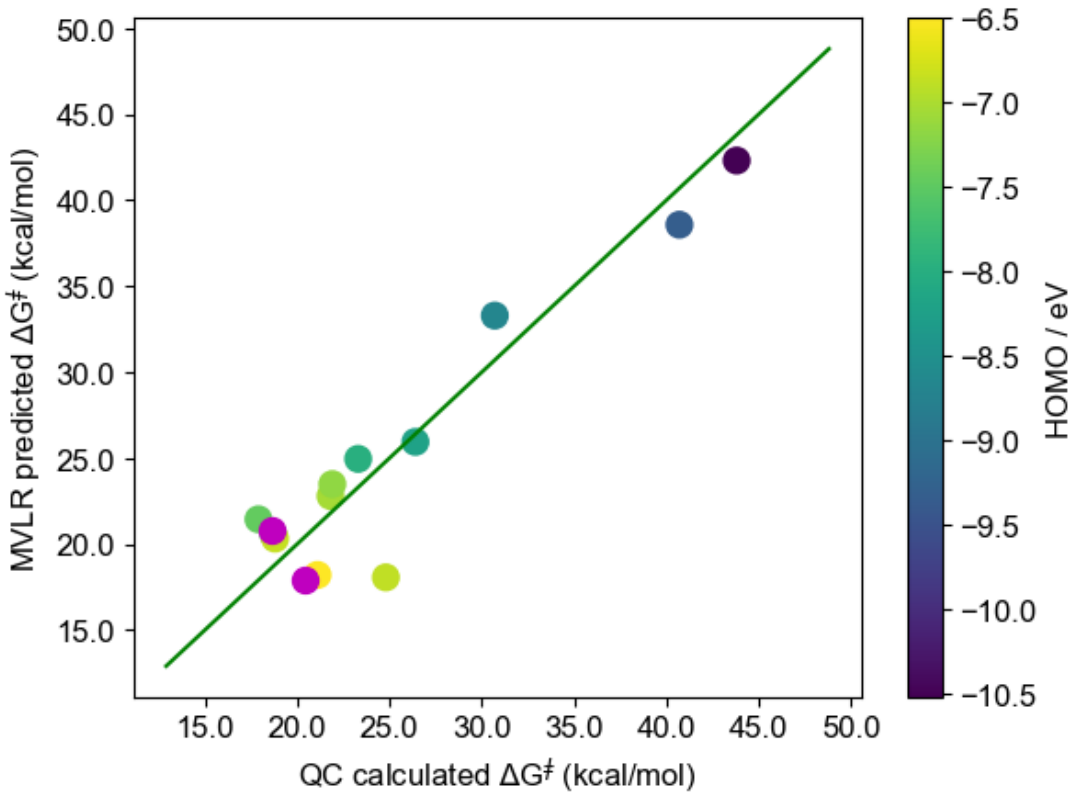

Figure S21. MVLR predicted $\Delta G^{\ddagger}$ vs QC calculated $\Delta G^{\ddagger}$ for **TS1-[P]** without the $\%V_{Bur}$ descriptor.

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.884
Model:                            OLS   Adj. R-squared:                  0.858
Method:                 Least Squares   F-statistic:                     34.24
Date:                Sun, 23 Mar 2025   Prob (F-statistic):           6.20e-05
Time:                        21:51:51   Log-Likelihood:                -29.253
No. Observations:                  12   AIC:                             64.51
Df Residuals:                       9   BIC:                             65.96
Df Model:                           2
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const        -18.9708      7.119     -2.665      0.026     -35.076      -2.865
x1            -3.0860      1.427     -2.163      0.059      -6.314       0.142
x2            -6.0414      0.848     -7.123      0.000      -7.960      -4.123
==============================================================================
Omnibus:                        4.780   Durbin-Watson:                   2.305
Prob(Omnibus):                  0.092   Jarque-Bera (JB):                2.203
Skew:                           1.031   Prob(JB):                        0.332
Kurtosis:                       3.392   Cond. No.                         62.5
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
Prediction of test set: [20.81001797 17.96792968]
RMSE of training set: 2.7700010490460256
RMSE of test set: 2.3236980714523656
```

Figure S22. MVLR result for **TS1-[P]** without the $\%V_{Bur}$ descriptor.

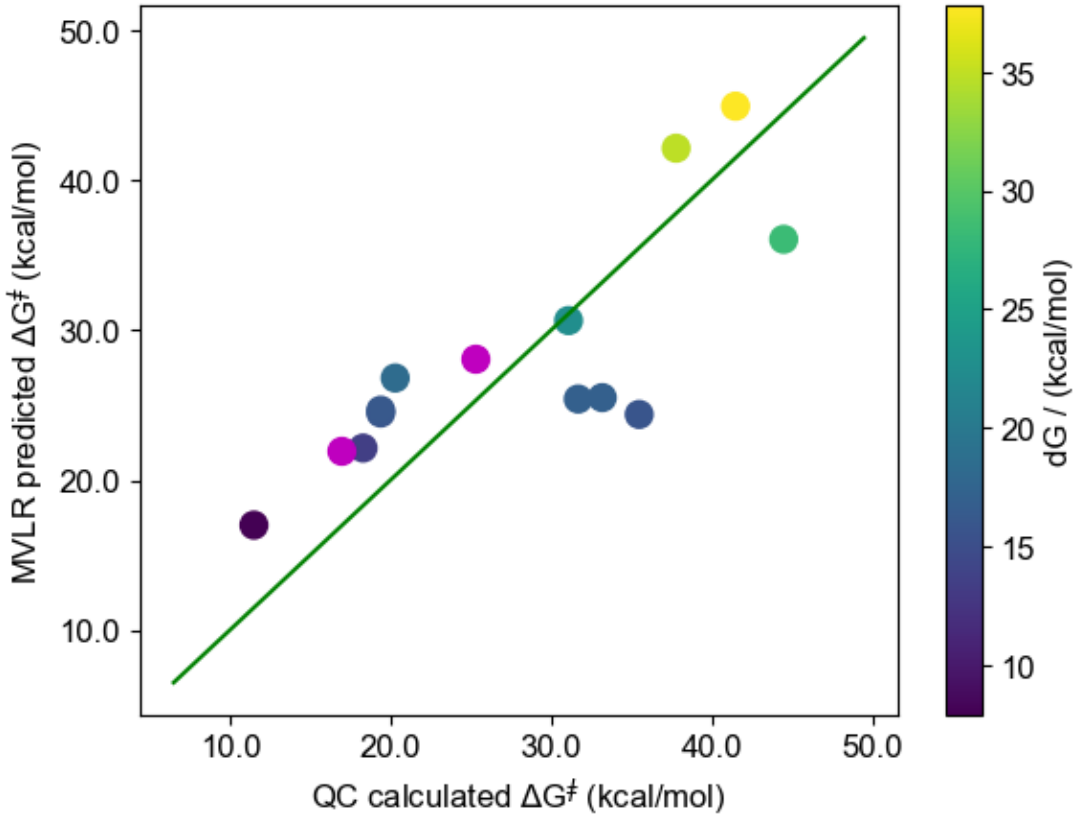

Figure S23. MVLR predicted $\Delta G^{\ddagger}$ vs QC calculated $\Delta G^{\ddagger}$ for **TS2-[P]** without the GD descriptor.

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.620
Model:                            OLS   Adj. R-squared:                  0.582
Method:                 Least Squares   F-statistic:                     16.33
Date:                Sun, 23 Mar 2025   Prob (F-statistic):           0.00236
Time:                        21:53:13   Log-Likelihood:                -38.974
No. Observations:                  12   AIC:                             81.95
Df Residuals:                      10   BIC:                             82.92
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const          9.6182      5.112      1.881      0.089      -1.773      21.009
x1             0.9346      0.231      4.041      0.002       0.419       1.450
==============================================================================
Omnibus:                        3.278   Durbin-Watson:                   1.991
Prob(Omnibus):                  0.194   Jarque-Bera (JB):                1.629
Skew:                           0.614   Prob(JB):                        0.443
Kurtosis:                       1.677   Cond. No.                         57.5
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
Prediction of test set: [28.12259302 21.95444955]
RMSE of training set: 6.226905539767967
RMSE of test set: 4.093561507845925
```

Figure S24. MVLR result for **TS2-[P]** without the GD descriptor.

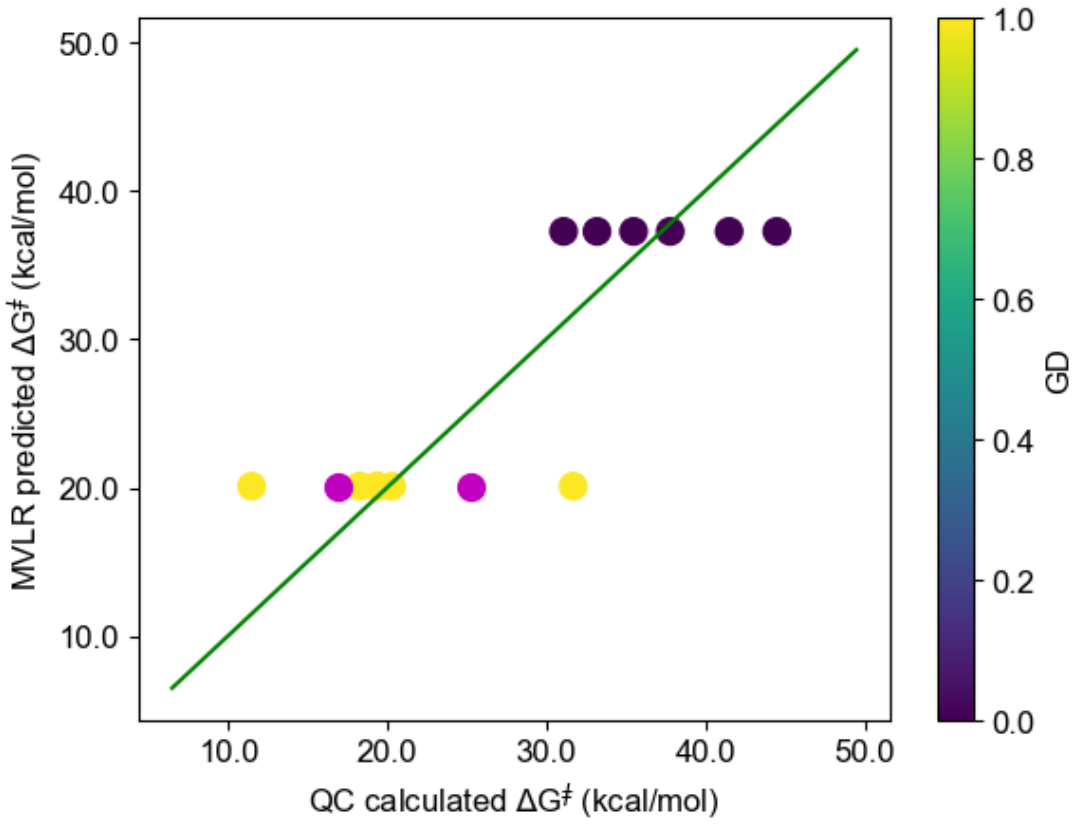

Figure S25. MVLR predicted $\Delta G^{\ddagger}$ vs QC calculated $\Delta G^{\ddagger}$ for **TS2-[P]** without the dG descriptor.

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.722
Model:                            OLS   Adj. R-squared:                  0.694
Method:                 Least Squares   F-statistic:                     25.93
Date:                Sun, 23 Mar 2025   Prob (F-statistic):           0.000470
Time:                        21:54:18   Log-Likelihood:                -37.109
No. Observations:                  12   AIC:                             78.22
Df Residuals:                      10   BIC:                             79.19
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         37.2667      2.384     15.632      0.000      31.955      42.578
x1           -17.1667      3.371     -5.092      0.000     -24.679      -9.655
==============================================================================
Omnibus:                        1.674   Durbin-Watson:                   2.683
Prob(Omnibus):                  0.433   Jarque-Bera (JB):                0.690
Skew:                           0.586   Prob(JB):                        0.708
Kurtosis:                       2.928   Cond. No.                         2.62
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
Prediction of test set: [20.1 20.1]
RMSE of training set: 5.33067642153518
RMSE of test set: 4.317406628984579
```

Figure S26. MVLR result for **TS2-[P]** without the dG descriptor.

S13.4. MVLR Analysis Using Cone Angle as the Steric Descriptor

We also tested MVLR analysis using cone angle as the steric descriptor to replace $\%V_{Bur}$ (Figure S27-28). It was found that similar regression result can be obtained with cone angle ($R^2 = 0.93$) as descriptor compared that with $\%V_{Bur}$ ($R^2 = 0.94$), which means that using $\%V_{Bur}$ as steric descriptor is reliable. Moreover, we found that the cone angle of **[P]S** have a good linear correlation with $\%V_{Bur}$ (Figure S29, $R^2 = 0.85$), which can explain why using cone angle as the steric descriptor has a similar performance with $\%V_{Bur}$ as the steric descriptor.

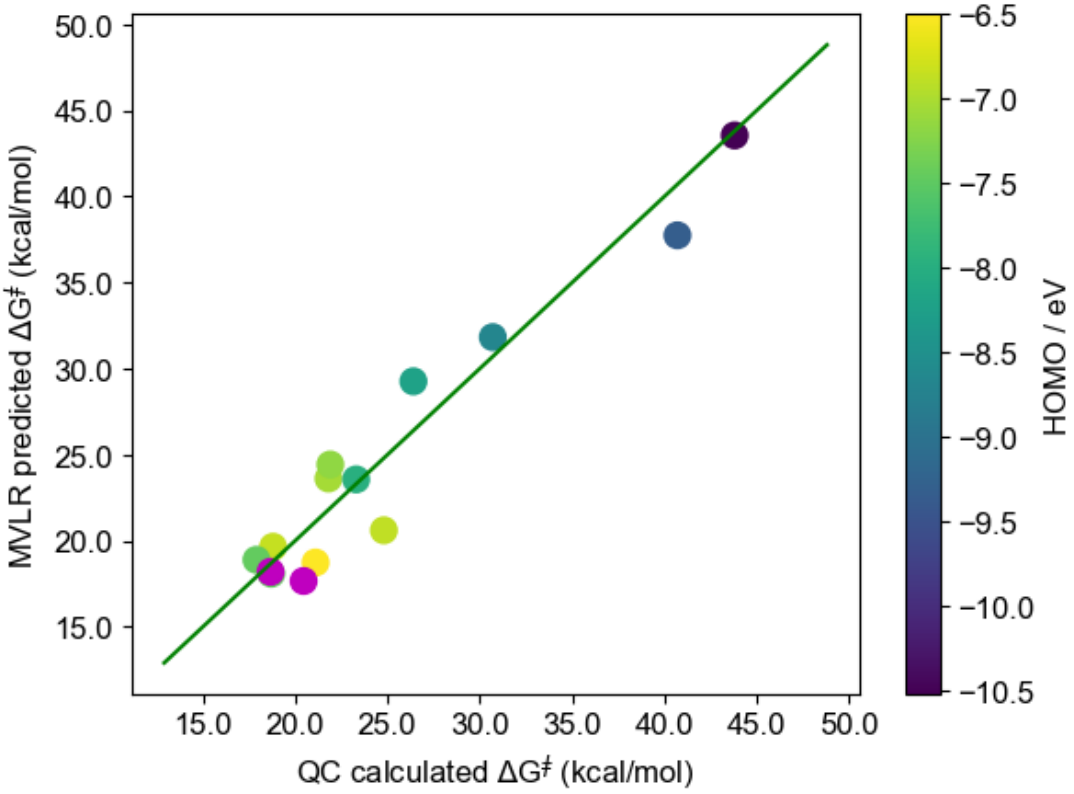

Figure S27. MVLR predicted $\Delta G^{\ddagger}$ vs QC calculated $\Delta G^{\ddagger}$ for **TS1-[P]** with $\%V_{Bur}$ replaced by cone angle.

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.933
Model:                            OLS   Adj. R-squared:                  0.908
Method:                 Least Squares   F-statistic:                     37.00
Date:                Sun, 23 Mar 2025   Prob (F-statistic):           4.89e-05
Time:                        22:04:31   Log-Likelihood:                -25.973
No. Observations:                  12   AIC:                             59.95
Df Residuals:                       8   BIC:                             61.88
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const        -45.3231     12.340     -3.673      0.006     -73.780     -16.866
x1            -2.6075      1.168     -2.232      0.056      -5.302       0.087
x2            -6.8738      0.766     -8.969      0.000      -8.641      -5.106
x3             0.1234      0.051      2.413      0.042       0.005       0.241
==============================================================================
Omnibus:                        1.191   Durbin-Watson:                   2.194
Prob(Omnibus):                  0.551   Jarque-Bera (JB):                0.932
Skew:                           0.581   Prob(JB):                        0.628
Kurtosis:                       2.282   Cond. No.                     2.63e+03
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 2.63e+03. This might indicate that there are
strong multicollinearity or other numerical problems.
Prediction of test set: [18.21026169 17.68999577]
RMSE of training set: 2.1073683276272375
RMSE of test set: 1.9359776407888662
```

Figure S28. MVLR result for **TS1-[P]** with %V_{Bur} replaced by cone angle.

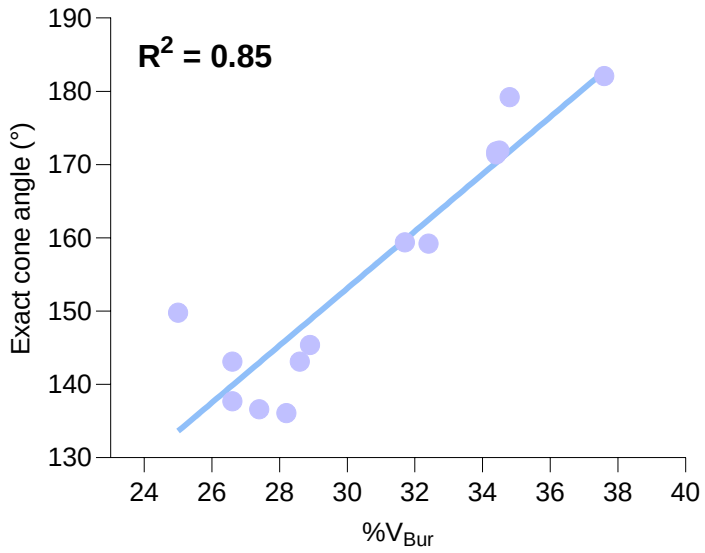

Figure S29. Linear regression of exact cone angle and %V_{Bur} of **[P]S**.

S14. Steric Map of Phosphines Used in MVLR

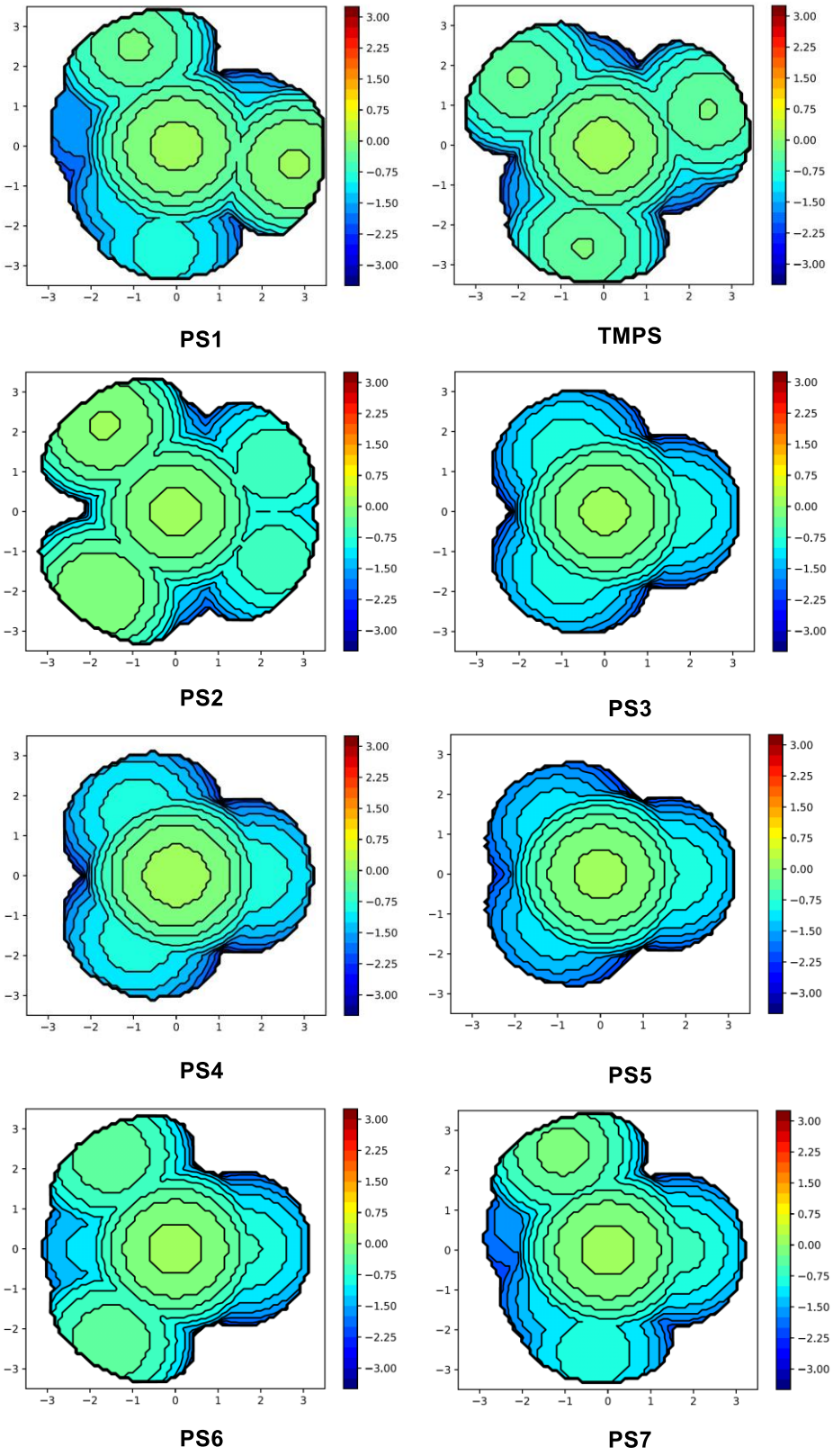

Figure S30. Steric maps of **PS1**, **TMPS**, **PS2**-**PS7**.

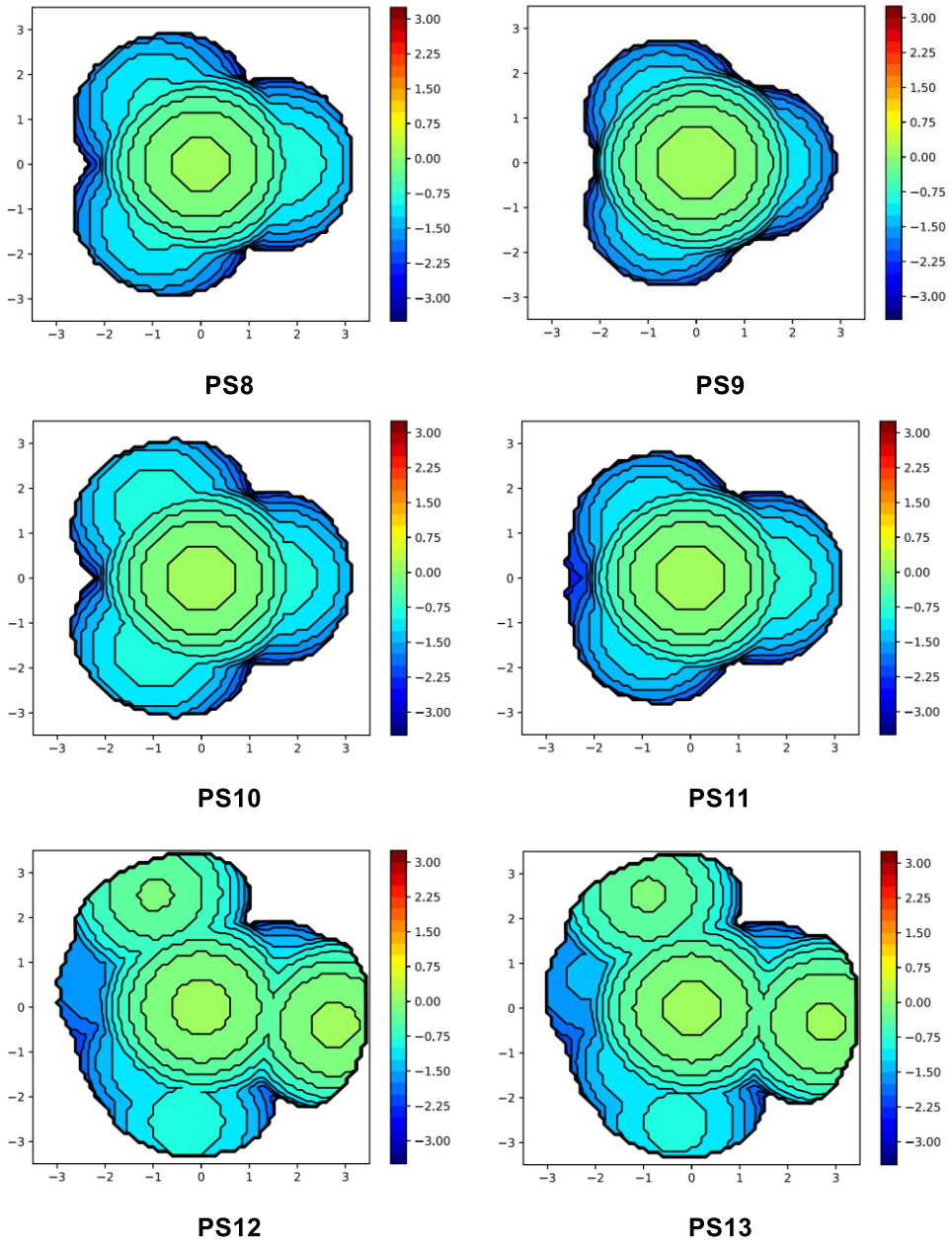

Figure S31. Steric maps of **PS8**-**PS13**.

S15. More Discussions on Standard States of Phosphines

For convenience and comparison, the standard state of 1.0 M was used for all species, as we mentioned in the main text. However, TMP and **P1** are used as both the reactant and solvent in the Corey-Winter reaction. Thus, the concentration is not 1.0 M in the real reaction system. As for TMP, its concentration is 8.48 M.[19] Once this concentration was considered as standard state, 1.27 kcal/mol (lower) correction will be applied (when TMP is involved), compared to the 1.0 M standard state. As shown in Figure S32, the activation free energy (from **CC-S** to **TS2**) decreased by 1.27 kcal/mol.

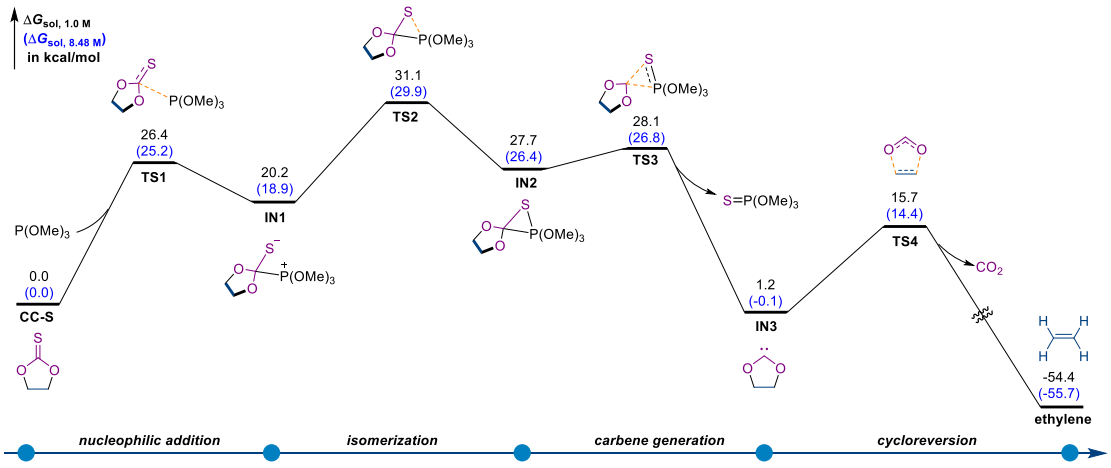

Figure S32. Comparison of the Gibbs energy profile of TMP mediated Corey-Winter reaction with different standard states considered.

Since the correction is small, it does not affect the conclusion on different pathways. For example, if 8.48 M standard state is used, the ring opening pathways of **IN2** is still disfavored over carbene generation pathway (Figure S33A). Similarly, the ylide formation pathway is still disfavored over cycloreversion process of **IN3** (Figure S33B).

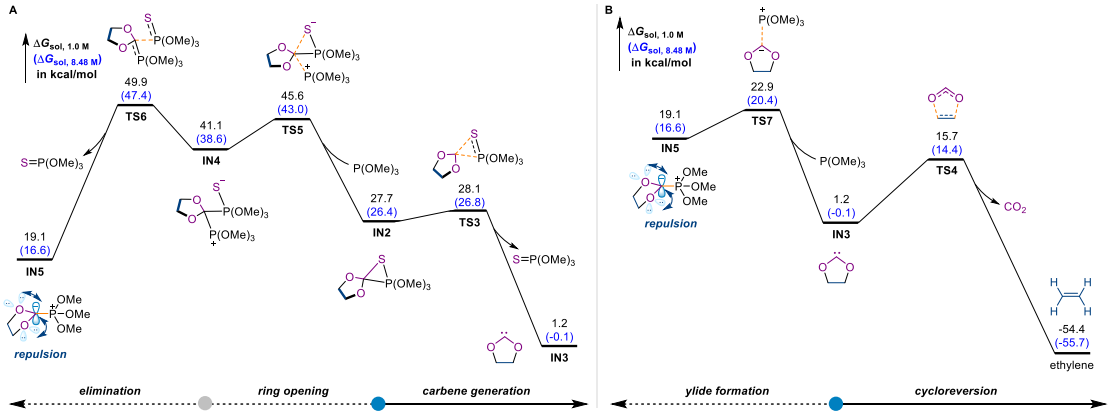

Figure S33. Comparison of competing pathways of TMP mediated Corey-Winter reaction with different standard states considered. (A) Comparison of the carbene generation process and the ylide formation process with assistance of TMP. (B) Comparison of the cycloreversion process and ylide formation process of carbene **IN3**.

As for **P1**, its concentration is 5.43 M[20] when used as a solvent for the Corey-Winter reaction. If 5.43 M is considered as the standard state for **P1**, and this will lead to 1.01 kcal/mol correction for reactions involving **P1** compared to the 1.0 M standard state, as shown in Figure S34.

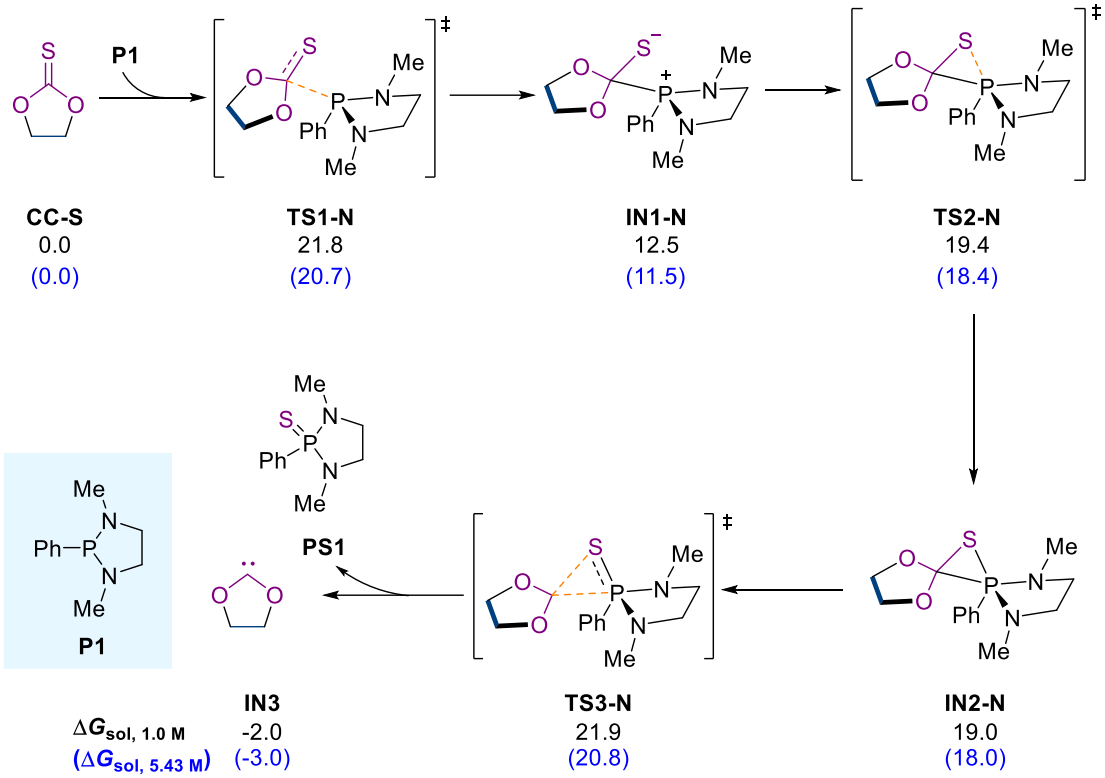

Figure S34. Comparison of the Gibbs energy profile of **P1** mediated Corey-Winter reaction with different standard states considered.

S16. Computed Energies of the Stationary Points

Table S10. Thermal Corrections to Enthalpies (TCHs), Thermal Corrections to Gibbs Energies (TCGs), and Single-Point Energies (SPEs)

Stationary point	**SPE**^{a,b} (a.u.)	**TCG**^{a,b} (a.u.)	**SPE**^{c} (a.u.)	**SPE**^{d} (a.u.)
$P(OMe)_3$ (TMP)	-686.792998	0.092721	-686.802094	-685.975343
$S=P(OMe)_3$ (TMPS)	-1085.035015	0.096199	-1085.048076	-1083.790313
CO_2	-188.596936	-0.008703	-188.598598	-188.383218
CC-S	-665.343671	0.044659	-665.360089	-664.582489
TS1	-1352.117627	0.159248	-1352.139376	-1350.538310
IN1	-1352.125856	0.162436	-1352.148644	-1350.550422
TS2	-1352.117115	0.164221	-1352.133215	-1350.541460
IN2	-1352.121103	0.163053	-1352.137369	-1350.545601
TS3	-1352.114412	0.159800	-1352.135233	-1350.537211
IN3	-267.097839	0.041980	-267.108538	-266.768164
IN3-T	-266.983855	0.040426	-266.989699	-266.646858
TS4	-267.068589	0.038794	-267.074690	-266.746518
TS4-T	-266.975367	0.033628	-266.986888	-266.646007
ethylene	-78.571977	0.030554	-78.575931	-78.461541
TS5	-2038.910495	0.281628	-2038.936153	-2036.514991
IN4	-2038.920183	0.286740	-2038.945635	-2036.527399
TS6	-2038.906794	0.282245	-2038.930913	-2036.510224
TS7	-953.884773	0.158522	-953.898098	-952.736149
IN5	-953.891475	0.160872	-953.904834	-952.744553
TS8	-534.195676	0.102867	-534.212880	-533.533938
IN6	-534.274343	0.110080	-534.290595	-533.609636
IN3-HS	-1069.061477	0.125331	-1069.078596	-1067.80285
TS4-HS	-1068.995903	0.119043	-1069.00896	-1067.738245
TS8-HS	-2138.121586	0.266827	-2138.153037	-2135.604933
trans-cyclohexene	-234.527526	0.118489	-234.539461	-234.1911505
IN6-HS	-2138.259139	0.275645	-2138.290191	-2135.739381
IN3-S	-913.025824	0.035047	-913.037291	-911.9939936
TS4-S	-913.004945	0.031567	-913.012667	-911.9726831
ethylene	-78.571977	0.030554	-78.575931	-78.46154085
TS7-S	-1599.816114	0.148513	-1599.832908	-1597.965558
IN5-S	-1599.867201	0.152217	-1599.885788	-1598.018173
IN7	-952.330598	0.061788	-952.34457	-951.2421197
TS9	-1639.120723	0.176865	-1639.139264	-1637.213069
IN8	-1639.183522	0.180826	-1639.203123	-1637.277713
cyclopropane	-117.878016	0.057771	-117.885888	-117.7048523
P1	-840.907462	0.199822	-840.926922	-839.769900

PS1	-1239.148164	0.200445	-1239.174624	-1237.584121
TS1-N	-1506.234066	0.264335	-1506.268451	-1504.336057
IN1-N	-1506.247596	0.266338	-1506.281959	-1504.352755
TS2-N	-1506.243383	0.268058	-1506.272051	-1504.349304
IN2-N	-1506.244940	0.267909	-1506.272429	-1504.350972
TS3-N	-1506.236137	0.265892	-1506.266797	-1504.341179
CC-O	-342.411219	0.048428	-342.424900	-342.003408
CC-Se	-2668.728157	0.042559	-2668.743162	-2667.270099
TS1-O	-1029.170818	0.167398	-1029.188005	-1027.948558
TS1-Se	-3355.507438	0.158323	-3355.529369	-3353.229653
IN3-yne	-265.881279	0.019473	-265.888867	-265.544746
TS4-yne	-265.820056	0.014217	-265.824551	-265.492268
acetylene	-77.325044	0.008519	-77.330313	-77.208666
IN3-N2	-305.971849	0.119578	-305.994496	-305.549427
TS4-N2	-305.896601	0.111925	-305.912792	-305.478855
TS8-N	-611.934087	0.261013	-611.959455	-611.090565
IN6-N	-612.002546	0.268215	-612.023210	-611.161546
CN2-Me	-227.377627	0.060676	-227.391192	-227.066922
CS_2	-834.478482	-0.015772	-834.482936	-833.556898
IN3-Ph	-419.526178	0.063236	-419.538604	-418.945520
TS4-Ph	-419.436137	0.056942	-419.446489	-418.867374
benzyne	-230.894066	0.048689	-230.906253	-230.538542
TC1	-704.648586	0.062689	-704.661088	-703.8341643
TS-X1	-1391.43485	0.181912	-1391.456522	-1389.800704
IN-X1	-1391.46607	0.187524	-1391.48392	-1389.833822
TS-X2	-1391.44025	0.182104	-1391.458428	-1389.803767
IN-X2	-1391.44669	0.18332	-1391.468569	-1389.810814
TS-X3	-1391.44664	0.185415	-1391.468178	-1389.8111
TC2	-516.082208	0.053443	-516.093603	-515.4860017
TS-X4	-1202.86516	0.172506	-1202.882609	-1201.448948
IN-X3	-1202.89771	0.175144	-1202.913647	-1201.484478
IN-S1	-499.313939	0.140051		-498.636363
TS-S1	-499.261028	0.136186		-498.578005
benzene	-232.224630	0.073777		-231.869763
P2	-745.036247	0.210081	-745.049498	-744.08216
TS1-P2	-1410.364982	0.278839	-1410.39263	-1408.648221
IN1-P2	-1410.381031	0.281036		
TS2-P2	-1410.351803	0.281749	-1410.373596	-1408.639871
TS3-P2	-1410.34939	0.279356	-1410.370867	-1408.637065
PS2	-1143.278043	0.211422	-1143.297357	-1141.89699

P3	-461.063089	0.083914	-461.069378	-460.4834675
TS1-P3	-1126.389695	0.147176	-1126.415324	-1125.048804
IN1-P3	-1126.400295	0.149141		
TS2-P3	-1126.374395	0.149902	-1126.39173	-1125.036764
TS3-P3	-1126.37413	0.148302	-1126.39048	-1125.036255
PS3	-859.295204	0.084686	-859.312368	-858.2883779
P4	-1722.017405	-0.025308	-1722.024885	-1720.27529
TS1-P4	-2387.315723	0.03847	-2387.335201	-2384.813424
IN1-P4	-2387.320678	0.039145		
TS2-P4	-2387.319127	0.042667	-2387.336198	-2384.818807
TS3-P4	-2387.31763	0.038482	-2387.339155	-2384.817144
PS4	-2120.224428	-0.024301	-2120.234692	-2118.055899
P5	-499.141403	0.092694	-499.149181	-498.4997201
TS1-P5	-1164.467818	0.155654	-1164.493996	-1163.065838
IN1-P5	-1164.473317	0.157096		
TS2-P5	-1164.465088	0.158294	-1164.483293	-1163.065853
TS3-P5	-1164.463609	0.157083	-1164.482782	-1163.064053
PS5	-897.373397	0.093398	-897.391067	-896.304448
P6	-609.841685	0.121508	-609.854173	-609.0653323
TS1-P6	-1275.173923	0.185171	-1275.200391	-1273.636259
IN1-P6	-1275.194002	0.187435		
TS2-P6	-1275.192759	0.189199	-1275.213	-1273.658136
TS3-P6	-1275.187609	0.186535	-1275.212158	-1273.65256
PS6	-1008.089209	0.12309	-1008.107897	-1006.885011
P7	-649.17662	0.15038	-649.188928	-648.3435037
TS1-P7	-1314.506319	0.215417	-1314.534534	-1312.911366
IN1-P7	-1314.520161	0.215913		
TS2-P7	-1314.517108	0.21882	-1314.538991	-1312.926673
TS3-P7	-1314.508089	0.216699	-1314.531422	-1312.916666
PS7	-1047.419599	0.151627	-1047.440051	-1046.159356
P8	-538.472751	0.120144	-538.482251	-537.7760005
TS1-P8	-1203.802275	0.185171	-1203.830757	-1202.344748
IN1-P8	-1203.810958	0.186346		
TS2-P8	-1203.787281	0.187063	-1203.807603	-1202.332866
TS3-P8	-1203.788981	0.186716	-1203.808016	-1202.334636
PS8	-936.70522	0.121472	-936.72509	-935.5811898
P9	-641.023995	-0.018241	-641.026555	-640.3506072
TS1-P9	-1306.31845	0.046398	-1306.335333	-1304.882382
IN1-P9	-1306.333366	0.047534		
TS2-P9	-1306.333289	0.04934	-1306.345326	-1304.899786
TS3P9	-1306.343356	0.045459	-1306.359371	-1304.908797
PS9	-1039.243179	-0.015571	-1039.248131	-1038.141374

P10	-1301.704123	0.011267	-1301.713136	-1300.349129
TS1-P10	-1967.018232	0.075882	-1967.039971	-1964.903405
IN1-P10	-1967.023869	0.077082		
TS2-P10	-1966.998006	0.077966	-1967.017059	-1964.886171
TS3-P10	-1967.015822	0.075075	-1967.039123	-1964.902196
PS10	-1699.922283	0.012284	-1699.936155	-1698.140488
P11	-610.347269	0.073756	-610.357061	-609.604116
TS1-P11	-1275.668122	0.137274	-1275.694967	-1274.164723
IN1-P11	-1275.683373	0.140187		
TS2-P11	-1275.681767	0.141885	-1275.700571	-1274.182186
TS3-P11	-1275.682106	0.139457	-1275.705291	-1274.181293
PS11	-1008.582401	0.07575	-1008.600744	-1007.412742
P12	-940.16195	0.190412	-940.180968	-938.9343123
TS1-P12	-1605.488601	0.254929	-1605.52237	-1603.500406
IN1-P12	-1605.502246	0.257421		
TS2-P12	-1605.497957	0.258616	-1605.526003	-1603.513764
TS3-P12	-1605.490749	0.256325	-1605.520801	-1603.505764
PS12	-1338.402555	0.190799	-1338.428436	-1336.74839
P13	-974.864338	0.267858	-974.888349	-973.5453336
TS1-P13	-1640.193112	0.332825	-1640.231913	-1638.113145
IN1-P13	-1640.20852	0.334346		
TS2-P13	-1640.201502	0.335535	-1640.23449	-1638.126059
TS3-P13	-1640.192845	0.333658	-1640.227852	-1638.116195
PS13	-1373.107025	0.267775	-1373.138383	-1371.361138

[a]Computed at the M06-2X/def2-TZVP level.

[b]A standard state at 1 atm and 298.15 K was used.

[c]Computed at SMD(TEP)/M06-2X/def2-TZVP level.

[d]Computed at the DLPNO-CCSD(T)/def2-QZVPP//M06-2X/def2-TZVP level.

Table S11. Orbital Energies of Cyclic Carbonates

	HOMO (a.u.) [a]	**LUMO** (a.u.) [a,b]
CC-O	-0.38267	0.07464
CC-S	-0.28554	0.00669
CC-Se	-0.26318	-0.00418

[a]Computed at the M06-2X/def2-TZVP level. [b]LUMO+2 for **CC-O**.

Table S12. Orbital Energies of IN3, Ethylene and CO_2

Orbital	M06-2X (a.u.)[a]	HF (a.u.)[b]	**Orbital**	M06-2X (a.u.)[a]	HF (a.u.)[b]
A3	-0.30788	-0.38522	**B1**	-0.33641	-0.37737
A2	-0.45260	-0.54833	**B3**	-0.45223	-0.54128
A1	-0.60968	-0.71794	**B2**	-0.61315	-0.71520

[a]Computed at the M06-2X/def2-TZVP level.

[b]Computed at the HF/6-311G(d)[21]//M06-2X/def2-TZVP level.

Table S13. Energy Data for Solution Phase Geometry Optimization

Stationary point	SPE[a,b] (a.u.)	TCG[a,b] (a.u.)	SPE[c] (a.u.)	SPE[d] (a.u.)
TMP (Sol)	-686.802215	0.093006	-686.792873	-685.9753679
TMPS (Sol)	-1085.048362	0.09609	-1085.034708	-1083.790009
CO_2 (Sol)	-188.598598	-0.0088	-188.596936	-188.3832159
CC-S (Sol)	-665.360635	0.044736	-665.343089	-664.5820588
TS1 (Sol)	-1352.139901	0.158893	-1352.117068	-1350.537352
IN1 (Sol)	-1352.150549	0.161908	-1352.124081	-1350.548606
TS2 (Sol)	-1352.13434	0.163606	-1352.116461	-1350.541252
IN2 (Sol)	-1352.137676	0.161957	-1352.120774	-1350.545409
TS3 (Sol)	-1352.135895	0.159521	-1352.113829	-1350.53683
IN3 (Sol)	-267.108639	0.042201	-267.097738	-266.7680989
TS4 (Sol)	-267.074464	0.038598	-267.068783	-266.7472725
ethylene (Sol)	-78.575937	0.030425	-78.571971	-78.46156319

[a]Computed at the SMD(TEP)/M06-2X/def2-TZVP level.

[b]A standard state at 1 atm and 298.15 K was used.

[c]Computed at M06-2X/def2-TZVP level.

[d]Computed at the DLPNO-CCSD(T)/def2-QZVPP//SMD(TEP)/M06-2X/def2-TZVP level.

Table S14. Single Point Energy Data for Benchmark Study[a]

Stationary point	B3LYP	B3LYP-D3BJ	BMK	M06
TMP	-687.015932	-687.038507	-686.713739	-686.786420
TMPS	-1085.297949	-1085.328376	-1084.875225	-1085.042544
CO_2	-188.680369	-188.682014	-188.593973	-188.595917
CC-S	-665.514853	-665.528987	-665.246834	-665.328109
TS1	-1352.495417	-1352.548483	-1351.933095	-1352.091464
IN1	-1352.501755	-1352.555248	-1351.942146	-1352.099104
TS2	-1352.490072	-1352.543074	-1351.937221	-1352.091814
IN2	-1352.493804	-1352.546602	-1351.941231	-1352.095937
TS3	-1352.491661	-1352.543394	-1351.930728	-1352.090693
IN3	-267.224988	-267.234894	-267.079615	-267.068640
TS4	-267.212201	-267.222506	-267.052225	-267.047214
ethylene	-78.630764	-78.634712	-78.561023	-78.557800
TS7	-954.224247	-954.267237	-953.781346	-953.848644
IN5	-954.228560	-954.272253	-953.786305	-953.851638
Stationary point	**M06-2X**	**PBE0**	**TPSSh**	**ωB97XD**
TMP	-686.836748	-686.467917	-687.013608	-686.877064
TMPS	-1085.092143	-1084.603001	-1085.299454	-1085.145093
CO_2	-188.610505	-188.476125	-188.677517	-188.615597
CC-S	-665.378541	-665.061170	-665.521385	-665.405006
TS1	-1352.195620	-1351.505359	-1352.506557	-1352.258885
IN1	-1352.204177	-1351.514903	-1352.513919	-1352.268331
TS2	-1352.194986	-1351.508978	-1352.508749	-1352.258513
IN2	-1352.198895	-1351.512823	-1352.513003	-1352.262040
TS3	-1352.192228	-1351.501951	-1352.507314	-1352.255320
IN3	-267.119494	-266.921471	-267.231559	-267.133437

TS4	-267.090574	-266.900474	-267.218535	-267.108028
ethylene	-78.580670	-78.518186	-78.630232	-78.595608
TS7	-953.949657	-953.383287	-954.235513	-954.001240
IN5	-953.956630	-953.391165	-954.239408	-954.009154

[a]Computed at the Method/def2-QZVPP//M06-2X/def2-TZVP level. Here, method is the functional used. Unit is a.u.

S17. Cartesian Coordinates of the Stationary Points

CO_2

O	0.000000	0.000000	1.154580
O	0.000000	0.000000	-1.154580
C	0.000000	0.000000	0.000000

CO_2 (Sol)

O	0.000000	0.000000	1.154580
O	0.000000	0.000000	-1.154580
C	0.000000	0.000000	0.000000

TMP

P	0.002690	-0.441438	-0.548265
O	-1.177443	-0.673225	0.546620
O	0.001100	1.172502	-0.711899
O	1.182797	-0.672778	0.546689
C	-2.510862	-0.620040	0.063888
H	-2.798638	0.407306	-0.173214
H	-2.634613	-1.236415	-0.830436
H	-3.155246	-1.000634	0.852789
C	2.516595	-0.605579	0.066704
H	3.161080	-1.005015	0.846165
H	2.642115	-1.198907	-0.842941
H	2.802173	0.427977	-0.144057
C	-0.014559	2.032078	0.425468
H	0.059228	3.052132	0.055956
H	-0.941461	1.909301	0.986893
H	0.826324	1.815079	1.085185

TMP (Sol)

P	0.000943	-0.445772	-0.544379
O	-1.180806	-0.673874	0.546585
O	0.018618	1.165874	-0.710912
O	1.180317	-0.703806	0.542851
C	-2.517616	-0.603844	0.058615
H	-2.788225	0.424206	-0.194281
H	-2.651191	-1.234775	-0.824175
H	-3.169984	-0.959810	0.853331
C	2.518077	-0.587251	0.067407
H	3.168560	-1.031623	0.818004
H	2.651155	-1.116788	-0.880172
H	2.790998	0.461726	-0.070081
C	-0.015455	2.032274	0.425839
H	0.225445	3.033404	0.073643
H	-1.009837	2.034439	0.874350
H	0.713867	1.723163	1.175711

TMPS

P	-0.000134	-0.000183	-0.094154
O	0.386070	-1.361593	-0.796377
O	0.986101	1.013986	-0.797322
O	-1.371334	0.345767	-0.798248
C	1.518477	-2.108951	-0.350864
H	2.431746	-1.533763	-0.505715
H	1.411570	-2.357223	0.704707
H	1.545472	-3.013114	-0.952331
C	-2.585663	-0.259548	-0.352814
H	-3.381376	0.169173	-0.955338
H	-2.545091	-1.338300	-0.506169
H	-2.747667	-0.041282	0.702350
C	1.068736	2.368466	-0.352361
H	1.337653	2.400077	0.703083
H	1.838564	2.842832	-0.954317
H	0.114452	2.872774	-0.506926
S	-0.001206	0.001031	1.822173

TMPS (Sol)

P	-0.000179	0.000474	-0.099949
O	1.375660	0.330780	-0.795446
O	-0.974676	1.027684	-0.793438
O	-0.402602	-1.355887	-0.795732
C	2.179583	1.431521	-0.352184
H	1.615944	2.363164	-0.411809
H	2.514233	1.263226	0.670931
H	3.033979	1.475727	-1.022565
C	0.150750	-2.601944	-0.353282
H	-0.229711	-3.362869	-1.029675
H	1.239799	-2.574998	-0.404155
H	-0.169376	-2.812887	0.666556
C	-2.330582	1.170206	-0.351012
H	-2.353766	1.547415	0.670885
H	-2.798175	1.884291	-1.023853
H	-2.852587	0.214368	-0.407709
S	0.001049	-0.001492	1.825401

CC-S

C	0.193924	0.735315	-1.721327
H	1.241547	0.894999	-1.979167
H	-0.442875	1.361417	-2.340147
C	-0.193924	-0.735315	-1.721327
H	-1.241547	-0.894999	-1.979167
H	0.442875	-1.361417	-2.340147
O	0.000000	1.098322	-0.352629
O	0.000000	-1.098322	-0.352629
C	0.000000	0.000000	0.413370
S	0.000000	0.000000	2.028524

CC-S (Sol)

C	0.190242	0.734258	-1.730403
H	1.236559	0.902579	-1.983895
H	-0.455671	1.358305	-2.340744
C	-0.190242	-0.734258	-1.730403
H	-1.236559	-0.902579	-1.983895
H	0.455671	-1.358305	-2.340744
O	0.000000	1.093856	-0.346488
O	0.000000	-1.093856	-0.346488
C	0.000000	0.000000	0.401887
S	0.000000	0.000000	2.034162

TS1

C	-2.184365	1.633560	0.452579
H	-1.425912	2.328961	0.818594
H	-3.164283	1.932106	0.818153
C	-2.118419	1.475351	-1.075939
H	-3.065678	1.669075	-1.574280
H	-1.336321	2.098250	-1.513804
O	-1.913415	0.325400	0.941718
O	-1.798573	0.101693	-1.262892
C	-1.356222	-0.414467	-0.073912
S	-1.193907	-2.094620	0.105966
P	0.713906	0.156324	-0.051600
O	1.163709	1.687450	-0.155238
O	1.543811	-0.478127	-1.234017
O	1.469739	-0.425204	1.221845
C	2.547783	2.058693	-0.235471
H	2.592179	3.134603	-0.090333
H	3.119328	1.553801	0.543196
H	2.942517	1.794401	-1.214762
C	0.829931	-0.407627	2.507210
H	1.564415	-0.778390	3.216598
H	0.542806	0.610425	2.774954
H	-0.046358	-1.054116	2.487622
C	1.823705	-1.875544	-1.398994
H	2.743279	-1.933872	-1.977177
H	1.951704	-2.348862	-0.427415
H	0.999596	-2.346812	-1.926961

TS1 (Sol)

C	2.124646	-1.708701	0.442195
H	1.313071	-2.356645	0.777373
H	3.072998	-2.075884	0.826612
C	2.113975	-1.511280	-1.078953
H	3.076209	-1.706092	-1.547224
H	1.338795	-2.103145	-1.566749
O	1.922232	-0.388857	0.953945
O	1.822620	-0.118580	-1.238517
C	1.416318	0.387251	-0.043333
S	1.329169	2.076186	0.167860
P	-0.736664	-0.131011	-0.058067
O	-1.212615	-1.646931	-0.173440
O	-1.513244	0.532798	-1.264863
O	-1.513481	0.486390	1.187802
C	-2.603587	-2.003452	-0.283722
H	-2.664622	-3.074925	-0.110495
H	-3.193098	-1.474181	0.464903
H	-2.966951	-1.765350	-1.281983
C	-0.957087	0.339901	2.504690
H	-1.687195	0.755120	3.194872
H	-0.796029	-0.714050	2.738666
H	-0.020036	0.891268	2.575370
C	-1.785600	1.934434	-1.412725
H	-2.713642	2.010097	-1.976401
H	-1.900628	2.407502	-0.439154
H	-0.971703	2.405009	-1.958879

IN1

C	-2.889001	0.679090	0.419250
H	-3.102400	1.551698	1.034753
H	-3.744759	0.000547	0.422652
C	-2.455810	1.022348	-0.994838
H	-3.272919	1.052684	-1.712157
H	-1.891736	1.958259	-1.026781
O	-1.750085	0.010606	0.943857

O	-1.621561	-0.078420	-1.322960
C	-0.977019	-0.498437	-0.145820
S	-0.512347	-2.190653	-0.083296
P	0.688806	0.216010	-0.026289
O	0.562767	1.786617	-0.151729
O	1.702673	-0.112556	-1.158930
O	1.444099	-0.067991	1.313660
C	1.715892	2.635868	-0.161084
H	1.351694	3.656950	-0.093617
H	2.355230	2.413025	0.693266
H	2.269298	2.495087	-1.087948
C	0.792316	-0.373925	2.562203
H	1.593091	-0.544306	3.275517
H	0.174870	0.467014	2.871940
H	0.181754	-1.265645	2.432698
C	2.402277	-1.356017	-1.335086
H	3.302634	-1.109369	-1.892178
H	2.648523	-1.783472	-0.365714
H	1.765107	-2.041791	-1.884303

IN1 (Sol)

C	-2.838708	0.813100	0.402698
H	-3.065420	1.703521	0.985919
H	-3.684864	0.122019	0.425843
C	-2.398654	1.104444	-1.015437
H	-3.215128	1.121480	-1.734656
H	-1.823068	2.031201	-1.078709
O	-1.686311	0.183969	0.957629
O	-1.574468	-0.022327	-1.304839
C	-0.980578	-0.462297	-0.099899
S	-0.777019	-2.209530	0.031365
P	0.728640	0.187157	-0.041186
O	0.652371	1.741862	-0.194221
O	1.651032	-0.266660	-1.200360
O	1.502424	-0.163783	1.264379
C	1.837843	2.560978	-0.267732
H	1.502144	3.591230	-0.194235
H	2.507832	2.328589	0.559737
H	2.337985	2.395198	-1.220084
C	0.884751	-0.200478	2.570795
H	1.686171	-0.424678	3.268715
H	0.442373	0.767561	2.800772
H	0.128833	-0.983087	2.585740
C	2.312113	-1.544113	-1.321800
H	3.217200	-1.356702	-1.894186
H	2.556125	-1.936378	-0.337062
H	1.651547	-2.229142	-1.844307

IN1 (*ω*B97X-D)

C	-2.887811	0.655757	0.452352
H	-3.019653	1.562993	1.042900
H	-3.787746	0.039667	0.521436
C	-2.504154	0.935630	-0.992329
H	-3.348419	0.919850	-1.678997
H	-1.963330	1.881173	-1.092390
O	-1.781093	-0.076248	0.954086
O	-1.662564	-0.160134	-1.305090
C	-0.986306	-0.526395	-0.135211
S	-0.406878	-2.186261	-0.068385
P	0.673512	0.214356	-0.029174
O	0.486599	1.785841	-0.141000
O	1.682307	-0.044426	-1.187874
O	1.470887	-0.021929	1.298503
C	1.580594	2.701349	-0.129463
H	1.152583	3.700226	-0.090779
H	2.208275	2.537015	0.747654
H	2.174856	2.588510	-1.036243
C	0.899380	-0.404608	2.558894
H	1.738223	-0.515882	3.241003
H	0.220915	0.370531	2.912815
H	0.364752	-1.345770	2.436202
C	2.436241	-1.240883	-1.418203
H	3.257238	-0.948456	-2.069430
H	2.815520	-1.633465	-0.476297
H	1.797381	-1.981505	-1.891361

IN1 (CAM-B3LYP)

C	-2.896737	0.655958	0.476812
H	-3.128744	1.498026	1.127112
H	-3.732623	-0.047278	0.471076
C	-2.498270	1.061944	-0.925667
H	-3.326938	1.085140	-1.630238
H	-1.975003	2.021672	-0.936474
O	-1.728806	0.009055	0.961929
O	-1.626103	0.008494	-1.307467
C	-0.975170	-0.474749	-0.154985
S	-0.569726	-2.181030	-0.169076
P	0.699895	0.224488	-0.016566

O	0.579011	1.795492	-0.085279
O	1.693396	-0.069635	-1.175921
O	1.463693	-0.117017	1.302119
C	1.707556	2.675631	-0.070886
H	1.312425	3.686677	-0.036266
H	2.321912	2.489556	0.809358
H	2.298695	2.537922	-0.974304
C	0.894335	-0.599589	2.535855
H	1.739273	-0.811751	3.183958
H	0.259404	0.166913	2.973448
H	0.317997	-1.498328	2.328939
C	2.396924	-1.297021	-1.433138
H	3.197275	-1.036450	-2.120491
H	2.802307	-1.692315	-0.504838
H	1.709843	-2.014786	-1.868565

TS2

C	-3.249781	-0.029771	0.453800
H	-3.755617	0.589015	1.193991
H	-3.791165	-0.967022	0.324331
C	-3.016563	0.700926	-0.875559
H	-3.140074	0.030057	-1.730183
H	-3.630721	1.587677	-1.006817
O	-1.926735	-0.291995	0.930433
O	-1.660041	1.106838	-0.774129
C	-1.047401	0.088717	-0.074445
S	-0.377964	-1.294812	-1.140224
P	0.762894	0.100188	0.035382
O	0.879750	1.678834	0.267604
O	2.167053	0.023582	-0.762373
O	1.221038	-0.619370	1.376309
C	2.103915	2.398526	0.353406
H	1.853486	3.384492	0.738831
H	2.797787	1.901576	1.031945
H	2.562506	2.487456	-0.629353
C	0.372726	-1.287921	2.304246
H	1.033312	-1.765742	3.023637
H	-0.282283	-0.579106	2.806636
H	-0.229360	-2.037600	1.791736
C	2.701306	-1.210928	-1.194744
H	3.718751	-1.012324	-1.524474
H	2.712877	-1.937208	-0.380361
H	2.120792	-1.607520	-2.030051

TS2(Sol)

C	-3.213180	0.459881	0.365751
H	-3.565341	1.488216	0.282139
H	-3.848850	-0.095016	1.054829
C	-3.077856	-0.223212	-0.993112
H	-3.282061	-1.295559	-0.930730
H	-3.683107	0.226108	-1.775877
O	-1.865771	0.486189	0.861474
O	-1.702430	-0.009532	-1.305082
C	-1.055575	-0.113418	-0.094086
S	-0.425156	-1.811057	0.343656
P	0.745537	-0.005541	-0.037096
O	0.894186	1.183550	-1.104528
O	2.121134	-0.714910	-0.471625
O	1.149321	0.589424	1.376757
C	2.146143	1.746556	-1.494493
H	1.922432	2.691312	-1.987100
H	2.779919	1.930196	-0.625081
H	2.663624	1.083922	-2.186259
C	0.580186	1.798034	1.892912
H	1.382061	2.329770	2.402286
H	0.181765	2.418974	1.090401
H	-0.213391	1.555491	2.596033
C	2.642818	-1.854110	0.194196
H	3.663879	-1.976808	-0.162194
H	2.647044	-1.712443	1.275759
H	2.064732	-2.744304	-0.059249

IN2

C	3.181928	-0.596872	0.098316
H	3.927694	-0.923568	-0.622566
H	3.343660	-1.099548	1.053855
C	3.102335	0.934761	0.266583
H	3.237232	1.231693	1.308467
H	3.795568	1.483644	-0.366519
O	1.895011	-0.940611	-0.410771
O	1.777232	1.249305	-0.154190
C	1.063090	0.089644	-0.045115
S	0.288613	-0.186780	1.712241
P	-0.776841	0.005626	-0.044828
O	-0.997033	-1.238286	-1.027482
O	-0.952486	1.411555	-0.764467
O	-2.304512	-0.047280	0.530886
C	-0.226465	-1.447042	-2.206023

H	0.486619	-2.250908	-2.041172
H	-0.925171	-1.717183	-2.995771
H	0.311937	-0.542638	-2.491631
C	-2.764660	-1.163983	1.262539
H	-3.793911	-0.956635	1.548643
H	-2.728106	-2.067951	0.652095
H	-2.166203	-1.313347	2.164859
C	-2.120975	2.226657	-0.731762
H	-1.879110	3.116802	-1.307688
H	-2.966677	1.706838	-1.177606
H	-2.365929	2.500438	0.292581

IN2 (Sol)

C	-3.191828	-0.575882	0.188997
H	-3.923099	-0.539928	0.993000
H	-3.366259	-1.455197	-0.433419
C	-3.122974	0.713055	-0.646946
H	-3.290006	0.518410	-1.707441
H	-3.797428	1.494068	-0.303530
O	-1.889114	-0.658328	0.778694
O	-1.779414	1.170992	-0.449022
C	-1.068865	0.100032	-0.006043
S	-0.267315	-0.963749	-1.456368
P	0.774412	0.022048	0.034300
O	0.976727	-0.633082	1.480337
O	0.945414	1.602578	0.029691
O	2.308186	-0.285116	-0.437368
C	0.224515	-0.241791	2.627756
H	-0.461153	-1.039185	2.905643
H	0.938293	-0.067329	3.431962
H	-0.339361	0.673771	2.444981
C	2.770772	-1.611164	-0.602286
H	3.827740	-1.552245	-0.858356
H	2.653795	-2.187316	0.317957
H	2.239324	-2.115298	-1.413776
C	2.128598	2.321011	-0.324205
H	1.881043	3.375213	-0.215404
H	2.952567	2.062853	0.338730
H	2.409716	2.113545	-1.355264

IN2 (*ω*B97X-D)

C	-3.200943	-0.601509	-0.060611
H	-3.921555	-0.903085	0.697339
H	-3.405062	-1.132497	-0.993405
C	-3.122757	0.921160	-0.273757
H	-3.301580	1.193988	-1.316413
H	-3.789991	1.489244	0.372010
O	-1.900642	-0.937346	0.409237
O	-1.784079	1.242002	0.086365
C	-1.074651	0.081864	0.019682
S	-0.257894	-0.252002	-1.734602
P	0.771803	0.004546	0.038997
O	0.996480	-1.206680	1.064385
O	0.924773	1.434513	0.719749
O	2.312475	-0.047243	-0.506700
C	0.238759	-1.393200	2.250499
H	-0.482004	-2.196316	2.109266
H	0.944172	-1.658174	3.037564
H	-0.290890	-0.483010	2.535776
C	2.818095	-1.161821	-1.203047
H	3.825448	-0.905851	-1.529269
H	2.856943	-2.042173	-0.556969
H	2.208356	-1.390536	-2.082630
C	2.079573	2.262643	0.700466
H	1.809385	3.163256	1.249233
H	2.922537	1.770260	1.183953
H	2.352978	2.521925	-0.321459

IN2 (CAM-B3LYP)

C	-3.206597	-0.590026	-0.091144
H	-3.920775	-0.936985	0.652177
H	-3.419917	-1.063293	-1.051257
C	-3.127654	0.940022	-0.210657
H	-3.320498	1.278398	-1.230210
H	-3.784199	1.468018	0.477381
O	-1.900643	-0.958038	0.348414
O	-1.781340	1.238220	0.152467
C	-1.069769	0.081206	0.009825
S	-0.258232	-0.145090	-1.742705
P	0.772152	0.004490	0.041356
O	0.995621	-1.273001	0.980151
O	0.926299	1.387562	0.810038
O	2.313259	-0.008689	-0.507370
C	0.233120	-1.562679	2.146228
H	-0.487006	-2.348406	1.933050
H	0.936637	-1.895634	2.907261
H	-0.295424	-0.680743	2.505826
C	2.827098	-1.079802	-1.268573

H	3.830487	-0.798298	-1.582556
H	2.873601	-1.992609	-0.672433
H	2.216046	-1.262483	-2.155898
C	2.079662	2.222289	0.849031
H	1.804852	3.082180	1.455705
H	2.922409	1.701196	1.298299
H	2.352490	2.548263	-0.152266

TS3

C	-3.559588	0.690449	0.237867
H	-4.288758	1.092788	-0.461562
H	-3.696312	1.133351	1.221149
C	-3.493110	-0.830522	0.257421
H	-3.493586	-1.249865	1.261557
H	-4.245555	-1.317538	-0.356799
O	-2.240761	1.054575	-0.231046
O	-2.195351	-1.093922	-0.322318
C	-1.501001	0.003701	-0.466394
S	0.204939	-0.071365	1.698735
P	0.815856	0.043789	-0.159079
O	0.637685	1.358416	-1.039377
O	0.692161	-1.197891	-1.154170
O	2.445498	0.108447	-0.083677
C	1.377679	2.528992	-0.703003
H	2.410615	2.434337	-1.032751
H	0.889895	3.353162	-1.217526
H	1.350177	2.706156	0.374247
C	3.229323	-0.187223	1.056051
H	3.040716	-1.198372	1.420992
H	4.269402	-0.099450	0.744673
H	3.022429	0.512676	1.865585
C	1.512069	-2.339870	-0.933218
H	2.554964	-2.114928	-1.154255
H	1.416862	-2.685835	0.099000
H	1.146203	-3.111633	-1.605528

TS3 (Sol)

C	-3.643571	0.677367	0.218582
H	-4.331967	1.134296	-0.487324
H	-3.805680	1.074147	1.217798
C	-3.615966	-0.840248	0.161217
H	-3.778661	-1.317258	1.124339
H	-4.276654	-1.266368	-0.589167
O	-2.289530	1.030859	-0.182832
O	-2.244169	-1.114356	-0.242508
C	-1.547018	-0.022115	-0.374214
S	0.336655	-0.035997	1.767002
P	0.839900	0.048362	-0.128253
O	0.583883	1.341563	-1.019914
O	0.663016	-1.214024	-1.087547
O	2.464328	0.145576	-0.156123
C	1.320575	2.538449	-0.759512
H	2.324444	2.468127	-1.174828
H	0.771202	3.343487	-1.243040
H	1.378933	2.736617	0.312618
C	3.337604	-0.202576	0.904200
H	3.151717	-1.214132	1.268691
H	4.348852	-0.145093	0.501903
H	3.235805	0.493782	1.737052
C	1.538548	-2.332831	-0.942595
H	2.554356	-2.074847	-1.240906
H	1.532844	-2.698129	0.086875
H	1.148573	-3.109343	-1.596915

IN3

C	0.896527	-0.758002	-0.000234
H	1.334806	-1.200668	-0.890961
H	1.335349	-1.201420	0.889840
C	0.896439	0.758105	0.000352
H	1.334554	1.200852	0.891118
H	1.335320	1.201548	-0.889682
O	-0.524128	-1.069536	0.000044
O	-0.524253	1.069475	-0.000115
C	-1.285129	-0.000074	-0.000076

IN3 (Sol)

C	0.899731	-0.756890	-0.000239
H	1.335069	-1.198586	-0.892608
H	1.335454	-1.199287	0.891590
C	0.899018	0.757731	0.000349
H	1.333836	1.199828	0.892773
H	1.334439	1.200531	-0.891427
O	-0.527953	-1.069841	-0.000078
O	-0.528958	1.069350	0.000013
C	-1.279335	-0.000600	-0.000078

IN3-T

C	0.771206	0.862042	-0.000691

H	1.183862	1.334345	-0.891369
H	1.185438	1.336247	0.888223
C	-0.771206	0.862043	0.000695
H	-1.183861	1.334336	0.891378
H	-1.185439	1.336256	-0.888215
O	1.150049	-0.517606	0.000596
O	-1.150049	-0.517606	-0.000609
C	0.000000	-1.233999	0.000011

TS4

C	-1.099146	-0.706868	0.000064
H	-1.352143	-1.227762	0.912543
H	-1.352293	-1.227939	-0.912271
C	-1.099142	0.706871	-0.000064
H	-1.352138	1.227765	-0.912544
H	-1.352290	1.227945	0.912270
O	0.693515	-1.086436	-0.000051
O	0.693519	1.086433	0.000051
C	1.250387	-0.000001	-0.000001

TS4 (Sol)

C	-1.114203	0.705072	-0.000053
H	-1.359068	1.226660	-0.915289
H	-1.359053	1.226797	0.915109
C	-1.114203	-0.705072	0.000053
H	-1.359067	-1.226660	0.915289
H	-1.359053	-1.226797	-0.915109
O	0.705865	1.088881	-0.000095
O	0.705865	-1.088881	0.000095
C	1.252139	0.000000	0.000000

TS4-T

C	-1.202057	0.706145	0.018627
H	-1.391566	1.245745	-0.895403
H	-1.316125	1.249619	0.943487
C	-1.202044	-0.706164	0.018600
H	-1.316114	-1.249675	0.943437
H	-1.391525	-1.245733	-0.895454
O	0.781243	1.129171	-0.091997
O	0.781268	-1.129160	-0.091977
C	1.223308	0.000011	0.192062

ethylene

C	0.000000	0.000000	0.661074
H	0.000000	0.922128	1.228746
H	0.000000	-0.922128	1.228746
C	0.000000	0.000000	-0.661074
H	0.000000	-0.922128	-1.228746
H	0.000000	0.922128	-1.228746

ethylene (Sol)

C	0.000000	0.000000	0.661667
H	0.000000	0.923312	1.229937
H	0.000000	-0.923312	1.229937
C	0.000000	0.000000	-0.661667
H	0.000000	-0.923312	-1.229937
H	0.000000	0.923312	-1.229937

TS5

C	0.866956	3.138386	0.450653
H	1.705806	3.468416	1.058933
H	0.020626	3.820022	0.546239
C	1.223761	2.860284	-0.997810
H	0.979867	3.668589	-1.681179
H	2.265979	2.553878	-1.122253
O	0.444448	1.849244	0.903855
O	0.376901	1.749301	-1.297918
C	0.104613	1.092891	-0.164319
S	-2.615825	1.692792	0.040569
P	-1.554090	0.034450	-0.060960
O	-0.787529	-0.614797	1.245499
O	-0.971486	-0.584964	-1.455848
O	-2.734568	-1.160173	0.007168
C	-1.506136	-1.201605	2.316375
H	-2.354353	-0.575600	2.600336
H	-1.864862	-2.195556	2.052168
H	-0.815127	-1.265972	3.157014
C	-4.117565	-0.961152	0.171042
H	-4.540187	-0.376679	-0.648468
H	-4.577372	-1.950864	0.189084
H	-4.345660	-0.437076	1.101680
C	-1.796183	-1.212791	-2.420524
H	-1.233253	-1.213486	-3.353350
H	-2.038229	-2.234207	-2.125546
H	-2.723217	-0.655086	-2.562347
P	1.756088	-0.433182	-0.013197
O	1.638667	-2.019714	0.147614
O	2.819023	-0.199361	-1.173558

O	2.646503	-0.119843	1.276051	O	1.980228	-1.376214	1.355470
C	0.725873	-2.839297	-0.587995	C	0.382901	-2.871730	-0.853826
H	-0.282862	-2.719955	-0.195390	H	0.693537	-3.663716	-1.529340
H	0.735533	-2.580015	-1.646323	H	0.386036	-3.228839	0.174434
H	1.067514	-3.862981	-0.454422	H	-0.598921	-2.490882	-1.121921
C	4.101779	-0.837452	-1.163820	C	3.337557	0.070064	-1.893072
H	3.989692	-1.909429	-1.003320	H	4.270616	0.624819	-1.929461
H	4.549627	-0.652307	-2.136196	H	3.451996	-0.889026	-2.393891
H	4.720938	-0.411112	-0.376189	H	2.534131	0.644547	-2.350793
C	2.095203	-0.318202	2.582383	C	1.745931	-0.921533	2.699160
H	2.871593	-0.038464	3.289483	H	0.723957	-0.569904	2.798303
H	1.213922	0.307825	2.717166	H	1.932968	-1.785589	3.330772
H	1.831764	-1.367551	2.717307	H	2.440345	-0.119681	2.935961

IN4

				TS6			
C	1.126753	2.718186	1.070373	C	-1.078148	3.011734	-0.688808
H	1.897281	3.030137	1.773848	H	-1.909723	3.442184	-1.247125
H	0.215952	3.301259	1.198568	H	-0.185551	3.631655	-0.794561
C	1.593190	2.712139	-0.374419	C	-1.403577	2.751830	0.773020
H	1.340280	3.621400	-0.915856	H	-1.135008	3.569951	1.437689
H	2.667738	2.514316	-0.452782	H	-2.457366	2.483044	0.907502
O	0.841048	1.344036	1.303934	O	-0.794711	1.713527	-1.191650
O	0.851554	1.642162	-0.943096	O	-0.570972	1.638408	1.069622
C	0.483450	0.746698	0.069809	C	-0.506305	0.859368	-0.095734
S	-2.136439	1.936045	0.471901	S	2.258283	1.659914	-0.751205
P	-1.403097	0.185518	-0.066145	P	1.739387	-0.057491	-0.001093
O	-0.828473	-0.973697	0.994800	O	1.066314	-1.233566	-0.876631
O	-0.972483	-0.170317	-1.606812	O	1.243377	-0.296444	1.509765
O	-2.817975	-0.720889	-0.268014	O	3.168427	-0.833172	0.279096
C	-1.653653	-1.825319	1.766420	C	1.311705	-2.603510	-0.572506
H	-2.417000	-1.251728	2.294472	H	1.264145	-2.774912	0.502565
H	-2.140388	-2.576592	1.145345	H	0.521715	-3.167578	-1.066184
H	-1.005485	-2.312551	2.497798	H	2.286808	-2.916770	-0.945039
C	-4.117363	-0.338443	0.106451	C	4.171147	-0.858299	-0.715076
H	-4.170714	-0.021827	1.150553	H	4.637639	0.121667	-0.817964
H	-4.482669	0.489482	-0.504720	H	4.911391	-1.595163	-0.403772
H	-4.757820	-1.210701	-0.041199	H	3.762435	-1.146764	-1.688856
C	-1.917460	-0.165077	-2.662950	C	1.937282	0.348188	2.571424
H	-1.354181	-0.026481	-3.585082	H	1.968731	1.424604	2.399283
H	-2.470909	-1.103440	-2.697763	H	1.375690	0.139445	3.480923
H	-2.622119	0.660357	-2.544382	H	2.949624	-0.046333	2.657768
P	1.669075	-0.684012	0.000422	P	-1.730531	-0.444136	-0.105709
O	1.357079	-1.826939	-1.007423	O	-3.241741	-0.071855	0.235360
O	3.060380	-0.153717	-0.499499	O	-1.769418	-1.206417	-1.465861

O	-1.359570	-1.595605	0.897727
C	-4.280637	-1.058952	0.166518
H	-5.174469	-0.603180	0.582879
H	-4.452536	-1.343262	-0.870588
H	-4.007352	-1.941322	0.746363
C	-1.259066	-0.707912	-2.719958
H	-1.940592	0.042175	-3.114173
H	-0.270129	-0.282232	-2.580705
H	-1.217985	-1.571135	-3.378212
C	-1.387636	-1.335817	2.311148
H	-1.075760	-0.314250	2.522013
H	-2.394842	-1.516316	2.687772
H	-0.684492	-2.028511	2.764138

IN5

C	-2.725697	0.767713	0.759179
H	-3.695938	1.204965	0.530400
H	-2.356695	1.156231	1.712112
C	-2.725469	-0.778184	0.749060
H	-2.356575	-1.179048	1.696899
H	-3.695547	-1.212667	0.514392
O	-1.818659	1.116213	-0.285445
O	-1.818138	-1.112745	-0.299854
C	-1.013122	0.003070	-0.463592
P	0.576614	-0.000825	0.159316
O	1.278450	-1.301926	-0.417021
O	1.215940	-0.010302	1.622406
O	1.278415	1.307580	-0.400259
C	0.938473	-1.899468	-1.667766
H	-0.082002	-2.275614	-1.640186
H	1.036758	-1.179771	-2.479387
H	1.639904	-2.718208	-1.812989
C	0.937952	1.921733	-1.642805
H	1.639263	2.742408	-1.777284
H	1.036053	1.212959	-2.463997
H	-0.082542	2.297385	-1.609901
C	2.629143	-0.012670	1.841512
H	3.075744	-0.903272	1.399863
H	3.077184	0.882165	1.409986
H	2.779460	-0.018874	2.918203

TS7

C	2.921427	-0.918892	0.625684
H	3.859229	-1.198125	0.147351
H	2.738585	-1.556711	1.489550
C	2.823779	0.568094	0.952208
H	2.312295	0.745520	1.901969
H	3.774024	1.094918	0.927759
O	1.859416	-1.103518	-0.323129
O	1.990036	1.064480	-0.099371
C	1.211895	0.058331	-0.551944
P	-0.644260	-0.004920	0.283801
O	-1.359297	1.187505	-0.532944
O	-1.635157	-0.121097	1.553000
O	-1.165662	-1.309591	-0.495761
C	-0.654878	2.285602	-1.095160
H	-0.087983	1.964458	-1.969338
H	-1.402710	3.022393	-1.381195
H	0.032281	2.727320	-0.373488
C	-0.948255	-1.520890	-1.882725
H	-1.041945	-0.583384	-2.432610
H	0.042029	-1.942021	-2.050330
H	-1.711578	-2.220691	-2.220658
C	-3.047016	-0.271793	1.408010
H	-3.475347	-0.219143	2.406597
H	-3.453158	0.530097	0.790688
H	-3.278222	-1.235766	0.955887

TS8

C	2.714618	0.788453	0.303882
H	2.533099	1.155646	1.313530
H	3.553034	1.314677	-0.144377
C	2.816482	-0.725852	0.231116
H	3.611048	-1.081755	-0.422493
H	2.890604	-1.205128	1.204298
O	1.533363	1.057797	-0.478437
O	1.550185	-1.094178	-0.357175
C	0.822325	-0.038615	-0.673924
C	-2.816569	0.725897	-0.230835
H	-2.891009	1.205355	-1.203900
H	-3.610943	1.081653	0.423090
C	-2.714679	-0.788387	-0.303891
H	-3.553038	-1.314721	0.144340
H	-2.533223	-1.155383	-1.313622
O	-1.550105	1.094146	0.357156
O	-1.533341	-1.057835	0.478274
C	-0.822243	0.038540	0.673750

IN6

C	-0.275513	-0.708433	-2.758788
H	-1.353944	-0.718124	-2.939699
H	0.227028	-1.382933	-3.447690
C	0.275513	0.708433	-2.758788
H	1.353944	0.718124	-2.939699
H	-0.227028	1.382933	-3.447690
O	0.000000	-1.132861	-1.429427
O	0.000000	1.132861	-1.429427
C	0.000000	0.000000	-0.660866
C	-0.275513	-0.708433	2.758788
H	0.227028	-1.382933	3.447690
H	-1.353944	-0.718124	2.939699
C	0.275513	0.708433	2.758788
H	-0.227028	1.382933	3.447690
H	1.353944	0.718124	2.939699
O	0.000000	-1.132861	1.429427
O	0.000000	1.132861	1.429427
C	0.000000	0.000000	0.660866

IN3-HS

C	-0.068500	0.762052	-2.571829
C	-0.755639	1.286675	-1.303200
C	0.000000	0.755070	-0.096730
C	0.000000	-0.755070	-0.096730
C	0.755639	-1.286675	-1.303200
C	0.068500	-0.762052	-2.571829
H	1.037835	1.107172	-0.139113
H	-0.771685	2.377721	-1.304562
H	-1.793411	0.942869	-1.264176
H	-0.622927	1.085042	-3.454305
H	0.926611	1.212333	-2.642190
H	-1.037835	-1.107172	-0.139113
C	0.000000	0.000000	2.487887
S	0.588623	-1.264769	1.573203
S	-0.588623	1.264769	1.573203
H	0.622927	-1.085042	-3.454305
H	-0.926611	-1.212333	-2.642190
H	1.793411	-0.942869	-1.264176
H	0.771685	-2.377721	-1.304562

TS4-HS

C	2.838973	-0.764539	-0.100440
C	1.533627	-1.494420	0.384392
C	0.492423	-0.634329	-0.267508
C	0.492425	0.634326	0.267528
C	1.533616	1.494421	-0.384386
C	2.838971	0.764541	0.100426
H	0.538176	-0.677141	-1.356942
H	0.538189	0.677142	1.356961
H	1.465231	1.452781	-1.473104
H	1.548353	2.538713	-0.068097
H	3.707186	1.191890	-0.406934
H	2.958629	0.982415	1.165344
C	-2.396910	0.000000	-0.000004
S	-2.013560	1.496317	0.112861
S	-2.013562	-1.496318	-0.112863
H	3.707199	-1.191885	0.406902
H	2.958612	-0.982412	-1.165360
H	1.465258	-1.452780	1.473111
H	1.548363	-2.538712	0.068105

trans-cyclohexene

C	-0.134987	0.761686	1.115668
C	0.306979	1.533020	-0.197754
C	-0.306979	0.597265	-1.189144
C	0.306979	-0.597265	-1.189144
C	-0.306979	-1.533020	-0.197754
C	0.134987	-0.761686	1.115668
H	-1.396796	0.586430	-1.153326
H	-0.072690	2.555385	-0.181155
H	1.395775	1.548901	-0.264638
H	1.396796	-0.586430	-1.153326
H	-1.395775	-1.548901	-0.264638
H	0.072690	-2.555385	-0.181155
H	-0.361236	-1.209093	1.980553
H	1.206947	-0.931201	1.245945
H	-1.206947	0.931201	1.245945
H	0.361236	1.209093	1.980553

TS8-HS

C	-5.644922	0.662594	-0.755244
C	-4.547868	1.465410	-0.043161
C	-3.252263	0.674126	-0.106815
C	-3.421453	-0.674539	0.555685
C	-4.446924	-1.510154	-0.193963
C	-5.782425	-0.754551	-0.194834
H	-2.970856	0.516914	-1.155497

H	-4.428723	2.443573	-0.512002
H	-4.821219	1.633497	1.002927
H	-6.598390	1.187780	-0.678071
H	-5.400905	0.605015	-1.820653
H	-3.765261	-0.520390	1.585066
C	-0.832795	0.041657	0.837729
S	-1.730478	-1.376142	0.707370
S	-1.764902	1.431216	0.653646
C	5.782436	-0.754558	0.194776
C	4.446938	-1.510156	0.193912
C	3.421444	-0.674535	-0.555700
C	3.252281	0.674131	0.106805
C	4.547885	1.465410	0.043106
C	5.644946	0.662587	0.755188
H	3.765218	-0.520386	-1.585092
H	4.565581	-2.490388	-0.270939
H	4.102405	-1.672969	1.219305
H	6.524091	-1.311845	0.769421
H	6.155457	-0.699707	-0.832956
H	2.970913	0.516920	1.155498
C	0.832778	0.041664	-0.837655
S	1.764888	1.431221	-0.653595
S	1.730461	-1.376136	-0.707325
H	-6.155450	-0.699702	0.832896
H	-6.524082	-1.311831	-0.769483
H	-4.565572	-2.490395	0.270870
H	-4.102373	-1.672950	-1.219352
H	6.598418	1.187766	0.678010
H	5.400932	0.605014	1.820598
H	4.821220	1.633477	-1.002989
H	4.428754	2.443582	0.511931

IN6-HS

C	-0.310440	-0.698593	-5.668479
C	0.057024	-1.484763	-4.406853
C	-0.345775	-0.677992	-3.180293
C	0.345775	0.677992	-3.180293
C	-0.057024	1.484763	-4.406853
C	0.310440	0.698593	-5.668479
H	-1.427445	-0.515130	-3.187889
H	-0.438664	-2.457060	-4.402833
H	1.135290	-1.668418	-4.377008
H	0.008278	-1.250878	-6.553925
H	-1.399749	-0.608113	-5.727158
H	1.427445	0.515130	-3.187889
C	0.000000	0.000000	-0.667564
S	-0.088308	1.486199	-1.617988
S	0.088308	-1.486199	-1.617988
C	-0.310440	0.698593	5.668479
C	0.057024	1.484763	4.406853
C	-0.345775	0.677992	3.180293
C	0.345775	-0.677992	3.180293
C	-0.057024	-1.484763	4.406853
C	0.310440	-0.698593	5.668479
H	-1.427445	0.515130	3.187889
H	-0.438664	2.457060	4.402833
H	1.135290	1.668418	4.377008
H	0.008278	1.250878	6.553925
H	-1.399749	0.608113	5.727158
H	1.427445	-0.515130	3.187889
C	0.000000	0.000000	0.667564
S	-0.088308	-1.486199	1.617988
S	0.088308	1.486199	1.617988
H	1.399749	-0.608113	5.727158
H	-0.008278	-1.250878	6.553925
H	-1.135290	-1.668418	4.377008
H	0.438664	-2.457060	4.402833
H	-0.008278	1.250878	-6.553925
H	1.399749	0.608113	-5.727158
H	-1.135290	1.668418	-4.377008
H	0.438664	2.457060	-4.402833

IN3-S

C	0.000000	0.760202	-1.296999
H	0.884673	1.169640	-1.779067
H	-0.884673	1.169640	-1.779067
C	0.000000	-0.760202	-1.296999
H	-0.884673	-1.169640	-1.779067
H	0.884673	-1.169640	-1.779067
C	0.000000	0.000000	1.331463
S	0.000000	-1.392601	0.459109
S	0.000000	1.392601	0.459109

TS4-S

C	-0.701995	1.576363	-0.000154
H	-1.215212	1.848609	0.912696
H	-1.214630	1.848414	-0.913397
C	0.702057	1.576320	0.000164

H	1.215197	1.848580	-0.912723
H	1.214742	1.848333	0.913385
C	-0.000018	-1.207215	-0.000002
S	1.443681	-0.595853	-0.000045
S	-1.443704	-0.595819	0.000044

CS_2

C	0.000000	0.000000	0.000000
S	0.000000	0.000000	1.546609
S	0.000000	0.000000	-1.546609

TS7-S

C	-3.076862	-0.956309	-0.642890
H	-3.972743	-1.546103	-0.455571
H	-2.560871	-1.344111	-1.522187
C	-3.382308	0.518568	-0.785931
H	-3.624916	0.783928	-1.813750
H	-4.196267	0.826535	-0.130492
C	-1.061449	0.291200	0.620165
P	1.086555	-0.067403	-0.270853
O	1.454003	1.488666	-0.132577
O	2.305052	-0.483883	-1.284812
O	1.748819	-0.746794	1.049624
C	2.801803	1.925122	0.014164
H	2.763667	2.954146	0.364628
H	3.330644	1.306519	0.741070
H	3.320984	1.874474	-0.941811
C	1.348491	-0.445109	2.378173
H	1.110402	0.614096	2.481182
H	0.473470	-1.029984	2.661535
H	2.184629	-0.704232	3.027370
C	2.432532	-1.852300	-1.626469
H	3.090394	-1.915209	-2.490779
H	2.862709	-2.415266	-0.796508
H	1.461461	-2.286490	-1.885324
S	-1.879912	1.458838	-0.276558
S	-1.931220	-1.149975	0.777950

IN5-S

C	2.480734	-0.792084	0.906976
H	3.379523	-1.391278	1.049769
H	1.819266	-0.926434	1.761468
C	2.820000	0.692053	0.727936
H	2.759128	1.207723	1.685145
H	3.818947	0.822049	0.316080
C	0.622925	0.055426	-0.662899
P	-0.845222	0.030506	0.131734
O	-0.910665	-0.132629	1.700373
O	-1.779640	-1.143545	-0.366173
O	-1.661717	1.370563	-0.054337
C	-2.153057	-0.181395	2.409589
H	-1.905785	-0.320885	3.458176
H	-2.694972	0.753948	2.275578
H	-2.753717	-1.017953	2.053994
C	-1.907277	1.895712	-1.358642
H	-2.579171	2.740159	-1.230743
H	-0.973535	2.222319	-1.813467
H	-2.382621	1.142427	-1.989524
C	-1.599758	-1.892010	-1.570848
H	-1.082982	-1.296735	-2.322119
H	-1.013254	-2.782301	-1.352463
H	-2.592477	-2.169822	-1.918125
S	1.654903	1.468194	-0.476596
S	1.602270	-1.397077	-0.579740

IN7

C	-0.000162	-1.458803	0.119131
S	1.469590	-0.733218	0.002478
S	-1.469780	-0.732855	0.002440
C	-1.263850	1.073438	-0.240300
H	-1.268769	1.281294	-1.311113
H	-2.155086	1.523768	0.196967
C	1.264138	1.073515	-0.240392
H	1.268918	1.280915	-1.311265
H	2.155563	1.523447	0.196807
C	0.000214	1.610416	0.415908
H	0.000081	2.700332	0.345292
H	0.000299	1.356026	1.478546

TS9

C	0.849076	0.182278	-0.671111
P	-1.316152	-0.006983	0.309039
O	-1.734455	1.466918	-0.169523
O	-2.517080	-0.225067	1.404154
O	-1.967721	-0.978683	-0.823626
C	-3.095071	1.813892	-0.406237
H	-3.090136	2.738811	-0.978793
H	-3.600709	1.030716	-0.973630

H	-3.616327	1.961832	0.538520
C	-1.605261	-0.931670	-2.195381
H	-1.400505	0.092468	-2.509513
H	-0.720466	-1.540260	-2.384328
H	-2.446930	-1.332316	-2.760180
C	-2.594394	-1.486059	2.043246
H	-3.241303	-1.376172	2.911218
H	-3.012976	-2.233032	1.366620
H	-1.606419	-1.821380	2.375286
S	1.554955	1.590517	-0.115190
S	1.591321	-1.319429	-0.698415
C	3.032113	-1.305740	0.418674
H	2.679853	-1.512458	1.431163
H	3.648110	-2.144737	0.094266
C	3.007209	1.171226	0.907413
H	2.658840	0.971958	1.922837
H	3.606845	2.081574	0.927793
C	3.814591	-0.001627	0.371804
H	4.718483	-0.112054	0.975971
H	4.129967	0.203247	-0.653641

IN8

C	0.472263	0.262753	0.663075
P	-1.046085	0.028490	0.035394
O	-2.063069	1.200729	0.321339
O	-1.793667	-1.243114	0.605516
O	-1.179417	-0.081090	-1.544182
C	-2.166687	1.768420	1.629735
H	-1.220544	2.226418	1.912957
H	-2.949673	2.519675	1.574731
H	-2.437102	1.000735	2.354674
C	-2.457644	-0.035169	-2.185423
H	-3.156182	-0.717128	-1.697479
H	-2.852987	0.978290	-2.150330
H	-2.301759	-0.342306	-3.216171
C	-1.470954	-2.575383	0.198982
H	-0.758782	-3.003491	0.899518
H	-2.400766	-3.140362	0.201303
H	-1.041765	-2.579011	-0.804422
S	1.282707	1.736181	0.166842
S	1.446471	-1.071706	1.228276
C	2.310023	1.056010	-1.171376
H	1.648322	0.722713	-1.974499
H	2.913080	1.885256	-1.543848
C	2.462111	-1.339450	-0.258230
H	1.815578	-1.702970	-1.062032
H	3.169778	-2.130198	-0.004075
C	3.212601	-0.086032	-0.706691
H	3.871027	-0.360964	-1.536948
H	3.845137	0.265290	0.112020

cyclopropane

C	0.000000	0.864855	0.000000
C	0.748990	-0.432435	0.000000
C	-0.748992	-0.432438	0.000000
H	0.000005	1.448376	0.909167
H	0.000005	1.448376	-0.909167
H	1.254332	-0.724154	0.909174
H	1.254332	-0.724154	-0.909174
H	-1.254330	-0.724166	-0.909174
H	-1.254330	-0.724166	0.909174

P1

C	-2.277432	-0.509988	1.087164
C	-1.530480	0.773565	1.423411
H	-2.168813	-1.262570	1.873985
H	-3.346988	-0.295320	0.965828
H	-0.580063	0.554457	1.932681
H	-2.120758	1.425766	2.071042
N	-1.311468	1.412215	0.133285
N	-1.726422	-0.984450	-0.181169
P	-0.822934	0.208399	-0.997696
C	-2.593096	-1.874628	-0.926969
H	-2.763359	-2.792162	-0.358462
H	-3.569569	-1.419899	-1.141290
H	-2.125380	-2.148940	-1.871173
C	-0.578514	2.659527	0.185058
H	-1.136953	3.385939	0.779105
H	0.420518	2.545514	0.628946
H	-0.462651	3.060461	-0.822963
C	0.893278	-0.169425	-0.412323
C	1.928002	0.598735	-0.945916
C	1.203892	-1.148910	0.528508
C	3.239745	0.414341	-0.531319
H	1.703699	1.346323	-1.701130
C	2.515956	-1.342932	0.939605
H	0.407965	-1.768744	0.924293
C	3.534634	-0.558561	0.414310

H	4.032204	1.019989	-0.952372
H	2.746074	-2.109384	1.669129
H	4.557419	-0.712113	0.733848

PS1

S	-1.072189	-2.350802	0.023685
C	-1.790577	1.693460	0.968573
C	-2.417334	1.426817	-0.392950
H	-1.022184	2.476781	0.898142
H	-2.534936	2.009446	1.702384
H	-2.550323	2.345044	-0.968315
H	-3.395022	0.942156	-0.275183
N	-1.474753	0.543196	-1.069884
N	-1.219077	0.416035	1.355185
P	-0.691229	-0.460338	0.026306
C	-0.503736	0.343951	2.610372
H	0.377768	0.997644	2.622521
H	-1.167397	0.632249	3.427053
H	-0.180453	-0.683125	2.782777
C	-1.896129	0.011885	-2.353033
H	-2.807181	-0.590082	-2.266089
H	-2.076801	0.838288	-3.042255
H	-1.110799	-0.618848	-2.767162
C	1.082095	-0.109716	-0.168917
C	2.034596	-1.074732	0.146430
C	1.498802	1.164327	-0.555902
C	3.386637	-0.768002	0.082046
H	1.704768	-2.066588	0.429464
C	2.850599	1.467520	-0.622618
H	0.760141	1.907964	-0.827655
C	3.795567	0.501765	-0.301160
H	4.121635	-1.524066	0.325846
H	3.167381	2.454999	-0.932642
H	4.850548	0.737762	-0.356595

TS1-N

C	3.325578	-0.189147	0.731520
H	3.219714	0.885221	0.891333
H	4.380425	-0.451120	0.668897
C	2.560406	-0.999635	1.787851
H	3.198832	-1.636504	2.396056
H	1.966340	-0.350541	2.435480
O	2.707620	-0.557263	-0.495961
O	1.704879	-1.834058	1.022924
C	1.575507	-1.298453	-0.234596
S	0.847884	-2.196257	-1.460798
C	0.687680	2.792890	-0.813303
C	0.049104	2.926660	0.557378
H	0.317654	3.547267	-1.510970
H	1.779290	2.892668	-0.744592
H	1.019386	3.168070	0.462517
H	0.526698	3.699539	1.162999
N	0.240281	1.617285	1.167474
N	0.301980	1.466351	-1.277560
P	0.142348	0.378408	-0.006063
C	0.760587	1.087221	-2.605591
H	0.274220	0.166256	-2.916796
H	0.494756	1.886823	-3.299841
H	1.842039	0.923726	-2.638289
C	0.419026	1.410191	2.442407
H	0.248328	0.389726	2.790195
H	0.010972	2.098572	3.184581
H	1.503752	1.563119	2.374231
C	1.579482	-0.202139	-0.025535
C	1.882613	-1.394649	0.629383
C	2.600128	0.568323	-0.575079
C	3.201967	-1.805583	0.741325
H	1.079578	-2.009088	1.021355
C	3.920059	0.152661	-0.462630
H	2.353037	1.479804	-1.105859
C	4.219536	-1.031411	0.197309
H	3.436418	-2.736660	1.240414
H	4.713512	0.748202	-0.895525
H	5.248473	-1.357546	0.279793

IN1-N

C	2.462157	-2.313793	0.885002
H	2.627314	-2.551584	1.934697
H	2.523170	-3.220579	0.282128
C	3.408262	-1.217968	0.346382
H	3.911592	-1.544300	-0.564664
H	4.138684	-0.875639	1.077159
O	1.167562	-1.733860	0.770099
O	2.536024	-0.133406	0.058113
C	1.292632	-0.750328	-0.251008
S	1.055205	-1.292474	-1.916166
C	1.006095	2.646507	0.963845
C	0.519052	3.016504	-0.435176

H	0.827928	3.450466	1.679593
H	2.076051	2.410374	0.950434
H	0.336664	3.699618	-0.390661
H	1.311229	3.491852	-1.016910
N	0.117216	1.763899	-1.064627
N	0.225051	1.467545	1.338662
P	0.013380	0.513923	-0.018989
C	0.581165	0.839252	2.602275
H	0.035501	-0.045281	2.758821
H	0.393044	1.543644	3.413773
H	1.633040	0.536151	2.620657
C	0.269265	1.781626	-2.462102
H	0.789783	0.861233	-2.713056
H	0.609698	1.851854	-3.104747
H	0.926734	2.637456	-2.640211
C	1.610238	-0.234488	0.075216
C	1.836718	-1.599108	-0.089306
C	2.669678	0.627157	0.361601
C	3.127563	-2.091020	0.037290
H	1.011066	-2.253624	-0.333454
C	3.956587	0.127600	0.475128
H	2.479185	1.684722	0.502043
C	4.183498	-1.233318	0.314062
H	3.308613	-3.150000	-0.090154
H	4.779208	0.796400	0.691002
H	5.188436	-1.625739	0.403853

TS2-N

C	3.567031	-1.167862	0.455594
H	4.229920	-1.086128	1.314172
H	4.147995	-1.126355	-0.467901
C	2.655237	-2.414535	0.490897
H	2.788185	-3.031221	-0.399813
H	2.781854	-3.023771	1.383335
O	2.649646	-0.082138	0.503977
O	1.338742	-1.868981	0.518378
C	1.469053	-0.589443	-0.030168
S	1.270971	-0.460296	-1.839053
C	0.051977	3.165096	-0.179888
C	-0.163229	2.783404	1.278740
H	-0.583869	3.998788	-0.480865
H	1.098024	3.441435	-0.362186
H	-1.205900	2.962448	1.579568
H	0.483740	3.357676	1.946745
N	0.179362	1.385494	1.318074
N	-0.318990	1.973685	-0.927993
P	0.063515	0.538562	-0.134146
C	-0.396537	2.098141	-2.365473
H	-1.025138	2.957571	-2.604271
H	0.588949	2.231464	-2.823456
H	-0.855179	1.208547	-2.791859
C	0.263861	0.711408	2.589450
H	0.990116	1.208725	3.236902
H	-0.706617	0.687801	3.101257
H	0.591965	-0.317447	2.436938
C	-1.440874	-0.472380	-0.080849
C	-1.539188	-1.769202	-0.574950
C	-2.546086	0.110132	0.539718
C	-2.730003	-2.470252	-0.446470
H	-0.686251	-2.220389	-1.061749
C	-3.735903	-0.590754	0.660949
H	-2.474898	1.121830	0.921103
C	-3.828178	-1.885193	0.167938
H	-2.799241	-3.478765	-0.832983
H	-4.589027	-0.126885	1.138783
H	-4.755584	-2.435675	0.260978

IN2-N

C	-2.588452	-2.541264	0.068555
H	-2.683980	-3.369519	0.767052
H	-2.727174	-2.901199	-0.953022
C	-3.519873	-1.350441	0.380123
H	-4.138891	-1.090179	-0.481024
H	-4.149436	-1.502914	1.254042
O	-1.281981	-1.990605	0.215521
O	-2.617298	-0.286900	0.665318
C	-1.431220	-0.629459	0.046970
S	-1.321138	-0.037814	-1.746575
C	0.005471	2.890316	1.178954
C	0.166244	3.197160	-0.301696
H	0.951024	3.055780	1.712895
H	-0.766496	3.506557	1.646673
H	0.842089	4.037063	-0.473513
H	-0.806913	3.438752	-0.756426
N	0.724069	1.974903	-0.840742
N	-0.370042	1.494172	1.217488
P	-0.054350	0.588663	-0.152770
C	-0.684173	0.924319	2.506875

H	0.128667	1.121687	3.215120
H	-1.610229	1.344051	2.906856
H	-0.806633	-0.153973	2.423520
C	0.997479	1.983197	-2.256750
H	0.089444	2.130699	-2.858698
H	1.699998	2.786949	-2.485793
H	1.454391	1.037992	-2.552284
C	1.392479	-0.503217	-0.007373
C	2.371673	-0.136263	0.914551
C	1.554626	-1.667816	-0.749291
C	3.492834	-0.929523	1.101161
H	2.257195	0.782551	1.478191
C	2.684559	-2.454712	-0.569713
H	0.795756	-1.956569	-1.464473
C	3.651365	-2.091063	0.356279
H	4.246032	-0.638304	1.821910
H	2.807415	-3.356335	-1.155836
H	4.529168	-2.708877	0.495754

TS3-N

C	-3.281938	-1.827878	-0.372195
H	-3.658765	-2.756895	0.047293
H	-3.362834	-1.834523	-1.458252
C	-3.873705	-0.566768	0.253675
H	-4.329621	0.095287	-0.480029
H	-4.559379	-0.756289	1.076127
O	-1.883852	-1.718119	-0.045055
O	-2.710587	0.100182	0.780007
C	-1.608674	-0.510746	0.397142
S	-1.089163	0.711602	-1.757426
C	0.648370	2.831989	1.228103
C	1.129678	3.077850	-0.192312
H	1.501697	2.793656	1.917187
H	-0.036015	3.611947	1.572014
H	2.005555	3.729394	-0.213970
H	0.339007	3.539795	-0.802914
N	1.467088	1.751460	-0.667914
N	-0.020182	1.538164	1.204701
P	0.189308	0.683157	-0.220092
C	-0.449273	1.044488	2.493815
H	0.284819	1.340964	3.250214
H	-1.424455	1.446095	2.781546
H	-0.506337	-0.041826	2.496721
C	1.971422	1.701343	-2.023931
H	1.258658	2.111319	-2.749697
H	2.904587	2.266737	-2.078506
H	2.181018	0.667574	-2.301410
C	1.166091	-0.829440	0.000270
C	1.044310	-1.909678	-0.864684
C	2.082245	-0.881236	1.048055
C	1.829002	-3.040169	-0.675684
H	0.335341	-1.856084	-1.681535
C	2.855158	-2.015555	1.241777
H	2.195239	-0.023793	1.701710
C	2.728762	-3.097327	0.378743
H	1.737200	-3.877307	-1.355738
H	3.562687	-2.053502	2.060154
H	3.337053	-3.980631	0.525525

CC-O

C	0.182333	0.741437	-1.291116
H	1.223038	0.915054	-1.567262
H	-0.470907	1.350366	-1.910415
C	-0.182333	-0.741437	-1.291116
H	-1.223038	-0.915054	-1.567262
H	0.470907	-1.350366	-1.910415
O	0.000000	1.107369	0.071932
O	0.000000	-1.107369	0.071932
C	0.000000	0.000000	0.845838
O	0.000000	0.000000	2.027851

CC-Se

C	-0.185524	-0.737356	-2.304626
H	-1.228732	-0.912623	-2.568431
H	0.464868	-1.358881	-2.913495
C	0.185524	0.737356	-2.304626
H	1.228732	0.912623	-2.568431
H	-0.464868	1.358881	-2.913495
O	0.000000	-1.094974	-0.929788
O	0.000000	1.094974	-0.929788
C	0.000000	0.000000	-0.173208
Se	0.000000	0.000000	1.603977

TS1-O

C	3.003552	0.462879	-0.770023
H	3.185266	1.380803	-1.328189
H	3.841518	-0.223356	-0.909953
C	2.718384	0.707962	0.707915

H	3.594921	0.623158	1.346256
H	2.240049	1.680567	0.865206
O	1.811527	-0.150344	-1.230519
O	1.821847	-0.339467	1.019216
C	1.020527	-0.543785	-0.127503
P	-0.624730	0.205342	-0.029640
O	-0.742878	1.781854	0.040409
O	-1.394226	-0.243462	1.264529
O	-1.511014	-0.093087	-1.288913
C	-2.001538	2.454649	0.125188
H	-2.598976	2.239958	-0.760009
H	-2.534270	2.139801	1.022238
H	-1.784694	3.517940	0.177439
C	-1.941878	-1.399887	-1.681798
H	-2.695860	-1.246419	-2.449543
H	-1.096272	-1.966138	-2.059843
H	-2.377070	-1.921830	-0.830149
C	-1.155346	-1.419256	2.051964
H	-1.793724	-1.315767	2.925764
H	-1.411328	-2.308795	1.483983
H	-0.107784	-1.469764	2.337315
O	0.395615	-1.678701	-0.206020

TS1-Se

C	-0.655649	2.723276	0.479400
H	0.356058	2.864774	0.864187
H	-1.310594	3.503961	0.858723
C	-0.669882	2.591191	-1.051221
H	-1.352923	3.279642	-1.543369
H	0.329463	2.688321	-1.477899
O	-1.162860	1.468733	0.930011
O	-1.151504	1.266494	-1.271248
C	-1.104535	0.581927	-0.101051
P	1.002695	-0.089653	-0.054774
O	2.200397	0.973068	-0.103885
O	1.401611	-1.036672	-1.255364
O	1.318224	-1.022047	1.198894
C	3.571724	0.554143	-0.163294
H	4.177500	1.438021	0.017175
H	3.770529	-0.196019	0.601964
H	3.788576	0.144188	-1.148010
C	0.781183	-0.687378	2.487208
H	1.193167	-1.410232	3.185775
H	1.088909	0.318435	2.778273
H	-0.305739	-0.758514	2.461766
C	0.927718	-2.376400	-1.453410
H	1.698674	-2.889470	-2.024294
H	0.773508	-2.865388	-0.493422
H	-0.010150	-2.348431	-2.001067
Se	-1.976109	-1.057107	0.046140

IN3-yne

C	-0.661318	-0.897897	-0.000032
C	0.661317	-0.897898	0.000004
O	-1.058408	0.419226	0.000002
O	1.058408	0.419225	0.000029
C	0.000001	1.231520	-0.000022
H	1.415946	-1.660984	-0.000103
H	-1.415948	-1.660983	0.000158

TS4-yne

C	1.152904	0.622563	0.000062
C	1.152598	-0.623097	-0.000057
O	-0.629005	1.084006	0.000095
O	-0.629675	-1.083703	-0.000098
C	-1.172285	0.000303	-0.000002
H	1.634400	-1.575570	-0.000105
H	1.635735	1.574535	0.000111

acetylene

C	0.000000	0.000000	0.597242
H	0.000000	0.000000	1.661167
C	0.000000	0.000000	-0.597242
H	0.000000	0.000000	-1.661167

IN3-N2

C	0.765845	-1.225103	0.000108
H	1.189937	-1.708462	0.883925
H	1.190161	-1.708920	-0.883342
C	-0.765845	-1.225104	-0.000067
H	-1.189941	-1.708538	-0.883839
H	-1.190157	-1.708845	0.883427
C	0.000000	1.017417	-0.000049
N	1.067897	0.209131	-0.000169
N	-1.067897	0.209131	0.000084
C	2.434160	0.654235	-0.000487
H	2.965515	0.292476	0.885271
H	2.964955	0.293124	-0.886848

H	2.436596	1.740824	-0.000099
C	-2.434160	0.654235	0.000531
H	-2.965700	0.292086	-0.884954
H	-2.964769	0.293514	0.887165
H	-2.436596	1.740824	-0.000325

TS4-N2

C	-0.688432	-1.595191	-0.087014
H	-1.110450	-1.823097	-1.055701
H	-1.331473	-1.798680	0.760533
C	0.688120	-1.595379	0.087033
H	1.110138	-1.823238	1.055727
H	1.331108	-1.798998	-0.760515
C	0.000064	0.931281	-0.000075
N	1.104198	0.401375	0.232938
N	-1.104133	0.401480	-0.233107
C	2.447099	0.809827	-0.086324
H	3.140383	0.127011	0.403496
H	2.633022	0.785540	-1.162684
H	2.636011	1.817575	0.281965
C	-2.446915	0.809999	0.086458
H	-3.140346	0.127074	-0.403004
H	-2.632527	0.785936	1.162879
H	-2.635941	1.817669	-0.281982

CN2-Me

C	-0.000002	-0.335785	0.000006
N	1.148502	-0.405689	0.386118
N	-1.148501	-0.405692	-0.386113
C	2.269268	0.364324	-0.121863
H	2.703821	0.941443	0.693460
H	3.031503	-0.322490	-0.487753
H	1.984215	1.042275	-0.928018
C	-2.269261	0.364351	0.121833
H	-2.707431	0.936824	-0.694797
H	-3.029019	-0.322289	0.493221
H	-1.983128	1.046562	0.924002

IN3-Ph

O	1.593852	1.073470	-0.000104
O	1.593864	-1.073455	-0.000108
C	2.395811	-0.000018	-0.000068
C	-0.883917	-1.431439	0.000047
C	-2.066052	-0.698197	0.000118
C	-2.066050	0.698188	0.000115
C	-0.883920	1.431436	0.000040
C	0.273886	0.685364	-0.000017
C	0.273872	-0.685351	-0.000013
H	-0.870733	-2.511603	0.000033
H	-3.011009	-1.224032	0.000149
H	-3.011008	1.224023	0.000145
H	-0.870751	2.511600	0.000024

TS4-Ph

O	2.233722	1.057865	-0.000090
O	1.784468	-1.120610	-0.000077
C	2.433112	-0.099364	-0.000102
C	-0.953983	-1.400672	0.000037
C	-2.186463	-0.745619	0.000089
C	-2.272847	0.650261	0.000096
C	-1.133664	1.459081	0.000050
C	0.061476	0.765023	-0.000001
C	0.098495	-0.518862	-0.000005
H	-0.863632	-2.478035	0.000031
H	-3.095426	-1.333246	0.000126
H	-3.250795	1.115852	0.000137
H	-1.212420	2.538301	0.000056

benzyne

C	-1.456578	-0.133139	-0.000013
C	-0.701026	1.048644	0.000040
C	0.700223	1.049100	0.000046
C	1.456564	-0.132020	0.000002
C	0.618673	-1.227237	-0.000048
C	-0.617592	-1.227230	-0.000054
H	-2.536720	-0.133858	-0.000017
H	-1.222292	1.998386	0.000077
H	1.220713	1.999286	0.000088
H	2.536716	-0.132523	0.000007

TC1

C	0.941197	0.209445	0.000012
S	1.604785	-1.253114	-0.000008
C	-0.565160	0.418284	-0.000001
O	-1.049958	1.518711	-0.000018
O	-1.268315	-0.704549	0.000014
C	1.701425	1.495028	0.000009
H	1.418240	2.089094	-0.871653

H	1.418230	2.089106	0.871660
H	2.770321	1.307615	0.000017
C	-2.684299	-0.531722	0.000002
H	-2.996358	0.018578	-0.886535
H	-3.103411	-1.532682	0.000013
H	-2.996370	0.018604	0.886518

TS-X1

C	0.877619	-1.069517	-0.601497
S	0.891692	-2.328939	0.505484
C	1.902690	0.030460	-0.425965
O	2.642909	0.382618	-1.304093
O	1.911072	0.566635	0.799075
C	0.580357	-1.352444	-2.057514
H	0.444437	-0.437694	-2.636252
H	1.437443	-1.889358	-2.466681
H	-0.298162	-1.988541	-2.132209
C	2.908957	1.559272	1.020596
H	2.774638	2.395165	0.334246
H	2.782407	1.883960	2.048984
H	3.900709	1.135678	0.871064
P	-0.978916	0.234867	-0.153938
O	-1.174911	0.691162	1.363940
O	-2.116400	-0.826001	-0.436815
O	-1.574451	1.534886	-0.886558
C	-0.787902	-0.117372	2.485145
H	-1.170908	0.389643	3.367775
H	-1.225753	-1.112545	2.400477
H	0.294339	-0.207214	2.527196
C	-0.783346	2.723586	-0.878757
H	0.226693	2.516986	-1.242868
H	-1.268277	3.430443	-1.546063
H	-0.735144	3.137049	0.128945
C	-3.490920	-0.567586	-0.131887
H	-3.892325	0.164938	-0.830328
H	-4.013688	-1.513933	-0.236471
H	-3.590222	-0.197339	0.888389

IN-X1

C	0.430184	-0.852925	0.647297
S	-0.096599	0.275934	2.020799
C	1.827625	-0.621902	0.146674
O	2.632373	-1.501291	-0.007027
O	2.089646	0.661838	-0.132506
C	0.136904	-2.325828	0.858030
H	0.312796	-2.888608	-0.060014
H	0.796970	-2.716813	1.632533
H	-0.894945	-2.461350	1.177541
C	3.402956	0.919781	-0.621299
H	3.578131	0.370811	-1.546149
H	3.449634	1.990454	-0.796499
H	4.146606	0.618474	0.114660
P	-0.907256	0.114466	-0.036712
O	-0.668802	1.584716	-0.569333
O	-2.380838	-0.166411	0.467281
O	-1.138149	-0.527538	-1.518841
C	-0.404111	2.746568	0.210089
H	-0.500528	3.586147	-0.474746
H	-1.126396	2.838014	1.019674
H	0.600595	2.695156	0.622494
C	-0.055020	-0.589313	-2.429381
H	0.707692	-1.293391	-2.085007
H	-0.452223	-0.943640	-3.377964
H	0.393555	0.396238	-2.568838
C	-3.480134	-0.464147	-0.402787
H	-3.348663	-1.441618	-0.860459
H	-4.361516	-0.457312	0.233053
H	-3.571560	0.291579	-1.180715

TS-X2

C	-1.532588	-1.130982	-0.604350
S	-0.350796	-0.739064	-1.676733
C	-2.315907	-0.103730	0.070579
O	-3.199940	-0.335946	0.865795
O	-1.957752	1.174019	-0.227103
C	-1.763959	-2.539287	-0.132758
H	-1.373040	-2.704026	0.877572
H	-2.832828	-2.752212	-0.093765
H	-1.280965	-3.247305	-0.802868
C	-2.735240	2.172745	0.417159
H	-2.657417	2.084595	1.501236
H	-2.334132	3.126751	0.083777
H	-3.784843	2.084448	0.138943
P	1.433811	-0.156669	-0.223201
O	2.960886	-0.557669	-0.379769
O	1.081038	-0.762249	1.199714
O	1.423006	1.409554	0.118802
C	3.923056	-0.288831	0.651625

H	4.899766	-0.501829	0.226755
H	3.867621	0.756251	0.955767
H	3.734157	-0.936777	1.505600
C	1.117377	2.366531	-0.902764
H	1.133158	3.341320	-0.422597
H	1.871014	2.338555	-1.690744
H	0.130288	2.162997	-1.316243
C	0.092926	-0.247402	2.100085
H	0.561725	-0.152035	3.077597
H	-0.263160	0.726599	1.767810
H	-0.737670	-0.948196	2.149924

IN-X2

C	-1.296036	-1.059970	-0.653681
S	0.004696	-0.520376	-1.672416
C	-2.166941	-0.153922	-0.016992
O	-3.056301	-0.444678	0.773083
O	-1.936658	1.177196	-0.320443
C	-1.427084	-2.538597	-0.436299
H	-0.540504	-2.983446	0.033190
H	-2.283743	-2.712782	0.215511
H	-1.598275	-3.085412	-1.367600
C	-2.814781	2.084536	0.318613
H	-2.729155	2.018576	1.404096
H	-2.524038	3.077435	-0.021804
H	-3.851139	1.886225	0.046437
P	1.222609	-0.112204	-0.121303
O	2.723019	-0.131241	-0.586466
O	1.157127	-1.084873	1.091191
O	0.952647	1.282711	0.555166
C	3.793161	0.159909	0.326977
H	4.698983	0.210585	-0.269156
H	3.616401	1.113659	0.823888
H	3.870211	-0.637154	1.064151
C	0.791282	2.472941	-0.233091
H	0.500094	3.255254	0.461494
H	1.738778	2.728541	-0.709068
H	0.009499	2.317905	-0.973291
C	0.152863	-1.042413	2.130998
H	0.656984	-1.349807	3.043372
H	-0.240110	-0.033336	2.231569
H	-0.651722	-1.725012	1.876010

TS-X3

C	-1.223187	-1.041880	-0.599738
S	0.001541	-0.454429	-1.704002
C	-2.152686	-0.174337	0.010363
O	-3.031820	-0.503499	0.795567
O	-1.992555	1.159753	-0.314250
C	-1.352760	-2.530518	-0.465669
H	-0.419799	-3.009082	-0.145881
H	-2.123355	-2.741806	0.276687
H	-1.652047	-3.015540	-1.400001
C	-2.897725	2.033607	0.333568
H	-2.779878	1.990149	1.417412
H	-2.665848	3.033464	-0.030734
H	-3.929615	1.779436	0.093233
P	1.198126	-0.092256	-0.148140
O	2.677671	0.080652	-0.658516
O	1.293662	-1.172172	0.969053
O	0.829367	1.204529	0.661236
C	3.753875	0.346992	0.252545
H	4.621732	0.581433	-0.356374
H	3.507512	1.193122	0.894503
H	3.946015	-0.536144	0.859056
C	0.655127	2.465830	-0.002607
H	0.191806	3.127629	0.722968
H	1.629144	2.855080	-0.301108
H	0.000171	2.345887	-0.862724
C	0.377612	-1.289275	2.079600
H	0.966081	-1.673321	2.908777
H	-0.041334	-0.316335	2.323688
H	-0.419272	-1.975895	1.813531

TC2

C	0.247160	-0.000016	0.000020
S	-1.367545	-0.000016	-0.000001
C	1.058154	1.261565	0.000012
C	1.058197	-1.261536	-0.000003
H	1.712108	-1.278129	-0.876523
H	1.711878	-1.278292	0.876684
H	0.426004	-2.144275	-0.000166
H	1.711376	1.278578	-0.877004
H	0.425874	2.144245	0.000613
H	1.712425	1.278047	0.876248

TS-X4

C	1.658988	-0.169386	-0.608849

S	2.280923	0.289335	0.885808
C	1.828642	-1.599862	-1.073053
H	1.164476	-1.841635	-1.904682
H	2.863183	-1.702517	-1.413833
H	1.679598	-2.304437	-0.258472
P	-0.630287	-0.065104	-0.219555
O	-0.969430	-0.588422	1.261381
O	-1.860027	-0.550880	-1.118719
O	-1.001293	1.475959	-0.039516
C	-0.483070	-1.865374	1.682030
H	-0.982833	-2.095465	2.619446
H	-0.728936	-2.635839	0.947991
H	0.595026	-1.814800	1.835917
C	-0.515342	2.316976	1.011863
H	0.464697	2.710050	0.749994
H	-1.235814	3.125493	1.117894
H	-0.438517	1.754329	1.940765
C	-3.215818	-0.228686	-0.784337
H	-3.406129	0.823241	-0.989727
H	-3.849366	-0.852933	-1.408858
H	-3.406878	-0.439194	0.268017
C	1.681970	0.829858	-1.747389
H	2.717194	0.891895	-2.093960
H	1.054984	0.513661	-2.583528
H	1.382636	1.820950	-1.413336

IN-X3

C	1.361759	-0.630266	0.010455
S	1.607808	1.200450	0.039072
C	1.829560	-1.343738	1.267770
H	1.535212	-2.395492	1.247468
H	2.918834	-1.277877	1.315157
H	1.425977	-0.878169	2.166098
P	-0.325235	-0.156084	0.001800
O	-0.993058	0.403030	1.320352
O	-1.100890	-1.559224	-0.021662
O	-0.971608	0.437848	-1.312223
C	-0.878444	1.702026	1.895110
H	-1.023480	2.474669	1.142508
H	-1.663923	1.760867	2.645350
H	0.102371	1.826135	2.345524
C	-0.770759	1.707011	-1.929015
H	0.199620	1.735100	-2.417109
H	-1.574954	1.809447	-2.654495
H	-0.817562	2.510484	-1.197579
C	-2.518240	-1.657552	-0.036015
H	-2.923343	-1.181788	-0.929688
H	-2.763509	-2.716940	-0.043976
H	-2.940875	-1.191239	0.854520
C	1.850423	-1.307229	-1.259209
H	2.940211	-1.239423	-1.287556
H	1.556722	-2.359248	-1.273798
H	1.460963	-0.817221	-2.150899

IN-S1

C	1.626126	-1.277958	0.574042
C	0.857093	-0.081658	1.125170
C	0.857993	0.081669	-1.125172
C	1.624081	-1.184267	-0.750548
H	2.074326	-2.048463	1.182486
H	2.070071	-1.860976	-1.463246
C	-0.232968	-0.000012	-0.000454
C	1.623404	1.184337	0.751166
H	2.068785	1.861087	1.464207
C	1.626499	1.278026	-0.573420
H	2.075143	2.048543	-1.181520
H	0.493252	-0.153614	2.146376
H	0.494887	0.153626	-2.146635
O	-1.072182	-1.116225	-0.128422
O	-1.072250	1.116395	0.126786
C	-2.391540	-0.728861	0.205272
H	-3.087848	-1.354279	-0.349620
C	-2.392039	0.728607	-0.204612
H	-3.087641	1.353808	0.351427
H	-2.567515	-0.841098	1.279887
H	-2.569893	0.840702	-1.278929

TS-S1

C	1.720949	-1.242434	0.643304
C	1.267137	-0.035110	1.276539
C	1.266951	0.035110	-1.276560
C	1.719635	-1.205577	-0.710143
H	1.911408	-2.139663	1.215721
H	1.908779	-2.070257	-1.331006
C	-0.463445	0.000000	0.000072
C	1.719741	1.205573	0.710064
H	1.908961	2.070256	1.330898
C	1.720852	1.242438	-0.643384

H	1.911240	2.139664	-1.215828
H	1.059439	-0.063848	2.341611
H	1.059111	0.063848	-2.341605
O	-1.233429	-1.079094	-0.077719
O	-1.233434	1.079093	0.077836
C	-2.623040	-0.753577	0.094894
H	-3.200086	-1.294500	-0.650343
C	-2.623031	0.753578	-0.094894
H	-3.200139	1.294506	0.650292
H	-2.929193	-1.059508	1.095273
H	-2.929100	1.059506	-1.095301

benzene

C	-0.331118	-1.348459	0.000001
C	1.002321	-0.960928	0.000009
C	1.333400	0.387469	-0.000001
C	0.331055	1.348475	0.000001
C	-1.002276	0.960975	0.000003
C	-1.333382	-0.387532	-0.000007
H	-0.589157	-2.399636	-0.000007
H	1.783560	-1.710083	-0.000008
H	2.372757	0.689632	-0.000024
H	0.589234	2.399617	-0.000005
H	-1.783612	1.710028	0.000007
H	-2.372779	-0.689558	0.000000

TS8-N

C	2.662761	-1.050704	0.182586
H	2.825054	-1.944466	-0.424804
H	3.346431	-1.082439	1.040981
C	2.803635	0.243612	-0.600608
H	3.805211	0.671813	-0.573532
H	2.498070	0.103508	-1.649479
C	0.788789	0.331405	0.553989
C	-2.654539	-1.066249	-0.178859
H	-2.783471	-1.959983	0.437188
H	-3.358823	-1.118988	-1.018869
C	-2.800275	0.228451	0.604626
H	-3.806901	0.645367	0.587979
H	-2.482824	0.091907	1.650418
C	-0.798926	0.337192	-0.571032
N	-1.288493	-0.928545	-0.661136
N	-1.842678	1.089400	-0.086724
C	-0.699096	-1.952190	-1.474582
H	-0.620312	-2.895015	-0.924460
H	-1.294234	-2.133124	-2.377625
H	0.296778	-1.630091	-1.770679
C	-1.594396	2.375389	0.502047
H	-2.542489	2.830201	0.789845
H	-0.948926	2.277889	1.387709
H	-1.107929	3.025028	-0.221876
N	1.829962	1.092367	0.082867
N	1.281488	-0.938174	0.627209
C	1.580151	2.383355	-0.494140
H	2.527506	2.842796	-0.776639
H	0.935594	2.291477	-1.381061
H	1.090648	3.025144	0.234702
C	0.721215	-1.937702	1.492384
H	0.822102	-2.930476	1.045908
H	1.215928	-1.950974	2.471332
H	-0.335279	-1.720259	1.638981

IN6-N

C	-2.846558	0.646007	0.391687
H	-3.592088	1.362396	0.046776
H	-3.019319	0.441478	1.458102
C	-2.846584	-0.645801	-0.391818
H	-3.592277	-1.362059	-0.046965
H	-3.019218	-0.441293	-1.458260
C	-0.672935	-0.000004	-0.000013
C	2.846560	0.645891	-0.391771
H	3.592173	1.362193	-0.046847
H	3.019263	0.441431	-1.458207
C	2.846586	-0.645959	0.391674
H	3.592176	-1.362259	0.046686
H	3.019362	-0.441524	1.458101
C	0.672931	-0.000031	-0.000034
N	1.490549	1.151212	-0.181746
N	1.490564	-1.151232	0.181714
C	1.079228	2.045148	-1.252227
H	1.793486	2.866899	-1.315864
H	1.051675	1.518528	-2.217207
H	0.087748	2.451675	-1.066303
C	1.079208	-2.045093	1.252228
H	1.793278	-2.867021	1.315767
H	1.051866	-1.518491	2.217234
H	0.087600	-2.451372	1.066419
N	-1.490631	-1.151190	-0.181716

N	-1.490486	1.151230	0.181763
C	-1.079316	-2.045183	-1.252119
H	-1.793552	-2.866961	-1.315700
H	-1.051749	-1.518640	-2.217156
H	-0.087817	-2.451668	-1.066197
C	-1.079129	2.045023	1.252347
H	-1.793242	2.866899	1.315942
H	-1.051748	1.518327	2.217299
H	-0.087538	2.451330	1.066534

P2

P	-0.000409	-0.026417	-0.742482
N	0.005855	1.507132	0.068647
N	-1.392786	-0.656656	-0.006776
N	1.385966	-0.668628	-0.006093
C	1.658973	-0.619648	1.415846
H	1.326251	-1.530927	1.929207
H	2.735876	-0.516255	1.585586
H	1.158098	0.237951	1.861431
C	-1.664326	-0.606427	1.415441
H	-1.335005	-1.519056	1.928651
H	-1.159393	0.249071	1.860506
H	-2.740616	-0.498464	1.585991
C	1.205603	2.298399	-0.169968
H	1.181146	3.182226	0.470798
H	2.096238	1.721440	0.068824
H	1.283974	2.638283	-1.213280
C	-1.186872	2.308787	-0.170587
H	-2.082583	1.739321	0.067163
H	-1.155385	3.192068	0.470629
H	-1.261426	2.649802	-1.213803
C	-2.101662	-1.716342	-0.693444
H	-1.840725	-2.708784	-0.303075
H	-3.182363	-1.586773	-0.577627
H	-1.863991	-1.692436	-1.756737
C	2.089417	-1.731252	-0.693704
H	3.170846	-1.606744	-0.578849
H	1.824256	-2.722556	-0.303362
H	1.850894	-1.705945	-1.756771

TS1-P2

P	-0.517261	0.110895	-0.054248
N	-1.382161	-0.589106	-1.282270
N	-1.235100	-0.466912	1.345952
N	-0.915964	1.758504	0.067393
C	-0.397230	2.567697	-1.023845
H	-0.191064	3.584158	-0.678124
H	0.527194	2.136097	-1.410588
H	-1.109815	2.625992	-1.856580
C	-1.660587	-1.855908	1.462871
H	-1.823166	-2.292038	0.480956
H	-0.898871	-2.455859	1.966228
H	-2.592641	-1.896610	2.035540
C	-2.831510	-0.655329	-1.294276
H	-3.166079	-1.690104	-1.425455
H	-3.236831	-0.285868	-0.353237
H	-3.242368	-0.059007	-2.115530
C	3.000705	1.130812	-0.678810
H	2.832450	1.960477	-1.364793
H	4.058468	0.862730	-0.682202
C	2.478326	1.387873	0.727827
H	3.245116	1.707433	1.429067
H	1.642563	2.093342	0.740006
O	2.242510	0.002272	-1.100818
O	2.025471	0.100119	1.117662
C	1.624501	-0.578576	-0.011465
S	1.418418	-2.251010	0.062629
C	-2.212949	2.231046	0.528797
H	-2.110316	3.247152	0.918430
H	-2.950041	2.253618	-0.284358
H	-2.587907	1.588693	1.322075
C	-0.776683	0.072151	2.621156
H	0.074603	-0.498292	3.005655
H	-0.475505	1.112633	2.510131
H	-1.594020	0.020629	3.345704
C	-0.733338	-1.191313	-2.435073
H	-1.132748	-0.752160	-3.354648
H	0.340740	-1.025908	-2.398131
H	-0.904219	-2.271612	-2.453862

IN1-P2

P	0.621222	0.085620	0.062050
N	1.176696	-0.570916	1.455280
N	1.455039	-0.493858	-1.228093
N	0.937243	1.697597	0.031152
C	0.085515	2.609571	0.782888
H	-0.399800	3.315150	0.104118
H	-0.684214	2.057051	1.316627

H	0.687489	3.167377	1.506195
C	1.977837	-1.856296	-1.226077
H	2.204142	-2.174954	-0.210872
H	1.244282	-2.546668	-1.646496
H	2.897733	-1.875541	-1.815052
C	2.541535	-0.272140	1.861657
H	3.213231	-1.110693	1.648930
H	2.914822	0.610422	1.344109
H	2.563898	-0.077388	2.935856
C	-3.160771	0.349321	0.867699
H	-3.510677	1.110086	1.564019
H	-3.770613	-0.550234	0.954400
C	-3.092847	0.838916	-0.596313
H	-3.649241	0.174838	-1.258520
H	-3.424527	1.867721	-0.726705
O	-1.807317	0.054442	1.192424
O	-1.706563	0.788107	-0.903205
C	-1.190765	-0.237494	-0.059928
S	-1.403193	-1.894366	-0.647277
C	2.052029	2.340200	-0.639015
H	1.686023	3.051429	-1.385637
H	2.659949	2.891446	0.085777
H	2.677695	1.602329	-1.133614
C	1.026022	-0.057790	-2.558317
H	0.244325	-0.724042	-2.933294
H	0.622633	0.952881	-2.517039
H	1.886899	-0.072105	-3.230086
C	0.577685	-1.694101	2.171086
H	0.623630	-1.479861	3.240937
H	-0.454216	-1.837847	1.869493
H	1.130036	-2.617126	1.968328

TS2-P2

C	3.302680	0.209950	-1.051064
H	3.927213	1.081018	-1.239003
H	3.514827	-0.565117	-1.789899
C	3.421681	-0.338906	0.388972
H	3.681691	-1.398975	0.390267
H	4.121536	0.213729	1.012162
O	1.943092	0.616709	-1.144220
O	2.115235	-0.154183	0.926740
C	1.271498	-0.151201	-0.193361
S	0.712994	-1.781665	-0.769408
P	-0.524589	0.040846	-0.023682
C	0.382116	2.604831	0.285830
H	-0.052656	3.292451	1.020389
H	1.190300	2.059131	0.763946
H	0.805064	3.194972	-0.530961
C	-2.044223	-1.307660	-1.957204
H	-2.152298	-2.351776	-1.637440
H	-2.928599	-1.032456	-2.537046
H	-1.173595	-1.238693	-2.600077
C	-1.251740	-1.741603	1.869388
H	-1.956295	-1.746267	2.705566
H	-1.717552	-2.218241	1.009420
H	-0.367898	-2.329765	2.137743
N	-0.901693	-0.367424	1.553077
N	-0.644503	1.705681	-0.225946
N	-1.940528	-0.401958	-0.831161
C	-3.217005	-0.162545	-0.172944
H	-3.935152	0.251005	-0.887682
H	-3.634932	-1.092900	0.230120
H	-3.106720	0.540186	0.648718
C	-1.750252	2.444885	-0.808322
H	-1.345648	3.267406	-1.403290
H	-2.337377	1.812245	-1.465094
H	-2.405519	2.876280	-0.042340
C	-0.314116	0.345330	2.675614
H	-0.175508	1.395461	2.431040
H	-1.002936	0.288013	3.522068
H	0.649597	-0.076548	2.973747

IN2-P2

C	3.432606	0.733118	-0.592033
H	4.190703	1.323383	-0.081790
H	3.515238	0.878259	-1.671451
C	3.452954	-0.765489	-0.220187
H	3.550293	-1.396041	-1.106628
H	4.219781	-1.028737	0.505173
O	2.154180	1.169160	-0.143459
O	2.180474	-0.975310	0.383559
C	1.368520	0.034514	-0.093743
S	0.585773	-0.372810	-1.776934
P	-0.509677	0.012033	-0.036470
C	0.175573	2.082237	1.669241
H	-0.409840	2.259033	2.578547
H	0.993761	1.411505	1.903461
H	0.616248	3.030622	1.350785

C	-2.503271	-0.236810	-2.045411
H	-2.996236	-1.202339	-2.223682
H	-3.218674	0.551237	-2.315678
H	-1.657762	-0.158147	-2.721913
C	-1.282659	-2.520954	0.647909
H	-2.005586	-2.853316	1.400730
H	-1.793088	-2.417879	-0.306150
H	-0.514819	-3.295729	0.544021
N	-0.678365	-1.264549	1.045968
N	-0.679920	1.546759	0.623627
N	-2.100521	-0.101477	-0.669802
C	-3.228520	-0.100365	0.236552
H	-3.945021	0.685732	-0.031625
H	-3.761392	-1.059763	0.206361
H	-2.899234	0.071055	1.259931
C	-1.689042	2.514370	0.228498
H	-1.205358	3.477767	0.046368
H	-2.190335	2.208086	-0.683704
H	-2.439118	2.656823	1.015170
C	0.090006	-1.390415	2.268465
H	0.592605	-0.460862	2.515135
H	-0.583484	-1.642719	3.093986
H	0.851523	-2.170671	2.185856

TS3-P2

C	3.518290	-0.805851	0.634568
H	4.355380	-1.320670	0.169170
H	3.436237	-1.083813	1.685688
C	3.526291	0.713803	0.438004
H	3.477602	1.252112	1.384599
H	4.353797	1.080558	-0.164994
O	2.313165	-1.210104	-0.027765
O	2.306225	0.952003	-0.276727
C	1.532606	-0.140578	-0.218012
S	0.431006	0.091554	1.779743
P	-0.632718	0.037689	0.066643
C	0.043281	-1.989446	-1.754488
H	-0.541528	-2.501236	-2.523918
H	0.678887	-1.254386	-2.232743
H	0.687858	-2.723780	-1.262020
C	-2.702752	0.091557	1.987670
H	-3.350448	0.927204	2.272879
H	-3.300519	-0.827700	2.074139
H	-1.882080	0.035377	2.694758
C	-0.547550	2.665525	-0.364013
H	-1.044916	3.392470	-1.010463
H	-1.059260	2.649264	0.596523
H	0.488536	2.982372	-0.201962
N	-0.621616	1.350879	-0.982853
N	-0.883388	-1.378871	-0.811204
N	-2.219115	0.292362	0.639565
C	-3.309001	0.373734	-0.313199
H	-3.895934	-0.555294	-0.335891
H	-3.987563	1.186804	-0.035469
H	-2.930297	0.567405	-1.312982
C	-1.696884	-2.420895	-0.192294
H	-1.061831	-3.159673	0.309337
H	-2.384123	-2.010947	0.538754
H	-2.275513	-2.934184	-0.964362
C	-0.068476	1.284884	-2.317638
H	-0.455076	0.412222	-2.841575
H	-0.402804	2.168979	-2.864294
H	1.027154	1.264535	-2.336905

PS2

P	-0.006714	-0.286309	-0.030171
N	1.530595	0.393350	-0.000310
N	-0.611879	0.365783	-1.448309
N	-0.701577	0.412349	1.316380
C	-0.559898	1.824749	1.625707
H	-1.471191	2.383788	1.386166
H	-0.365891	1.944810	2.696282
H	0.274219	2.256935	1.078630
C	-0.575381	1.805477	-1.654993
H	-1.444039	2.308181	-1.211870
H	0.332301	2.229584	-1.231045
H	-0.580599	2.009706	-2.728199
C	2.290577	0.159651	1.225251
H	3.162732	0.815141	1.225245
H	1.683562	0.383781	2.099386
H	2.629349	-0.880639	1.294350
C	2.355591	0.145594	-1.180826
H	1.798179	0.369288	-2.086786
H	3.232459	0.793142	-1.134226
H	2.688730	-0.897957	-1.224415
C	-1.735677	-0.267880	-2.120257
H	-2.697245	0.086893	-1.728589
H	-1.692115	-0.026025	-3.184439

H	-1.680553	-1.345979	-2.000642
C	-1.734572	-0.244127	2.097429
H	-1.518627	-0.122328	3.162821
H	-2.719163	0.193002	1.897479
H	-1.761694	-1.304629	1.864860
S	-0.105057	-2.221578	-0.004909

P3

P	-0.000013	0.000139	-0.607464
C	1.419172	0.771285	0.280856
H	2.345196	0.272061	-0.006712
H	1.504025	1.820066	-0.006015
H	1.303597	0.707979	1.365117
C	-0.041417	-1.614484	0.280750
H	-0.936803	-2.166977	-0.006402
H	0.824472	-2.212183	-0.006350
H	-0.038060	-1.482524	1.364987
C	-1.377734	0.843014	0.280876
H	-1.408785	1.894724	-0.006179
H	-2.328144	0.391808	-0.006517
H	-1.265427	0.774072	1.365136

TS1-P3

P	1.158612	-0.300988	-0.003414
C	1.918060	0.321062	-1.523465
H	1.450421	-0.169917	-2.376990
H	1.726155	1.390982	-1.585198
H	2.990550	0.124070	-1.529432
C	1.618895	-2.077417	0.000356
H	1.324194	-2.532407	0.945825
H	1.102376	-2.588630	-0.812480
H	2.695426	-2.202900	-0.130921
C	2.107316	0.391886	1.373473
H	1.913519	1.462724	1.410449
H	1.765527	-0.060800	2.304340
H	3.173490	0.201705	1.245120
C	-2.197692	-1.146234	-0.715529
H	-1.912197	-2.016125	-1.307769
H	-3.247287	-0.911742	-0.896619
C	-1.886959	-1.308048	0.770572
H	-2.754213	-1.551455	1.379133
H	-1.101882	-2.051806	0.942763
O	-1.410884	-0.024403	-1.096134
O	-1.426683	-0.021702	1.137983
C	-0.839845	0.551910	0.029534
S	-0.507711	2.211938	0.032410

IN1-P3

P	1.282381	-0.222534	-0.000042
C	2.048791	0.447764	-1.473527
H	1.534165	0.034194	-2.340764
H	1.908112	1.527080	-1.458768
H	3.106417	0.186240	-1.502334
C	1.509272	-2.010550	-0.000265
H	1.025143	-2.416473	0.887030
H	1.022519	-2.416442	-0.886150
H	2.566647	-2.273884	-0.001850
C	2.048144	0.447343	1.473977
H	1.908368	1.526767	1.459042
H	1.532275	0.034287	2.340727
H	3.105509	0.184894	1.503811
C	-2.417360	-0.679229	-0.772942
H	-2.742718	-1.622550	-1.207740
H	-3.014749	0.143707	-1.166737
C	-2.417168	-0.679693	0.772900
H	-3.014703	0.142830	1.167332
H	-2.742190	-1.623375	1.207177
O	-1.048940	-0.491365	-1.111284
O	-1.048718	-0.491709	1.111022
C	-0.496863	0.210643	-0.000153
S	-0.643635	1.959854	0.000125

TS2-P3

P	1.203757	-0.156935	0.020172
C	2.792352	0.716236	-0.358554
H	2.757378	1.076621	-1.385572
H	2.891063	1.567462	0.312601
H	3.637221	0.034656	-0.233751
C	1.444331	-1.603132	-1.074664
H	0.745575	-2.389538	-0.792672
H	1.214478	-1.299357	-2.097073
H	2.471128	-1.964201	-1.032078
C	1.512005	-0.701653	1.723701
H	1.356881	0.146152	2.390193
H	0.807806	-1.487543	1.989601
H	2.537837	-1.055864	1.819227
C	-2.687404	-0.262607	-0.776196
H	-3.312444	-1.081461	-1.125374

H	-2.958634	0.658300	-1.296023
C	-2.710599	-0.072658	0.757278
H	-3.010094	0.940971	1.029645
H	-3.336732	-0.794290	1.277419
O	-1.330458	-0.596930	-1.050909
O	-1.358484	-0.304735	1.145368
C	-0.606607	-0.055133	0.003294
S	-0.050672	1.693070	-0.222722

IN2-P3

P	-1.215037	-0.135287	-0.000122
C	-2.890630	0.698302	0.000589
H	-2.973872	1.328920	0.886466
H	-2.973858	1.330395	-0.884240
H	-3.702035	-0.032661	-0.000033
C	-1.450761	-1.150559	1.495893
H	-0.756045	-1.988286	1.491828
H	-1.232774	-0.527828	2.364212
H	-2.480659	-1.499596	1.558013
C	-1.450835	-1.147979	-1.497888
H	-1.232613	-0.523810	-2.365107
H	-0.756231	-1.985810	-1.495194
H	-2.480774	-1.496741	-1.560691
C	2.745755	-0.066201	0.771776
H	3.432515	-0.786726	1.210183
H	2.946030	0.928776	1.174140
C	2.745593	-0.064277	-0.771967
H	2.945210	0.931828	-1.171874
H	3.432648	-0.783312	-1.212347
O	1.416323	-0.462630	1.104811
O	1.416306	-0.460564	-1.105694
C	0.650119	-0.169131	-0.000169
S	-0.043654	1.619923	0.001509

TS3-P3

P	-1.258262	-0.113034	0.000064
C	-2.973676	0.624034	-0.000398
H	-3.101387	1.250642	0.883124
H	-3.101351	1.249660	-0.884620
H	-3.740426	-0.154082	0.000022
C	-1.421116	-1.126295	1.508004
H	-0.883881	-2.064736	1.384129
H	-0.964675	-0.576355	2.330921
H	-2.469062	-1.312542	1.736836
C	-1.421077	-1.128119	-1.506662
H	-0.964298	-0.579331	-2.330160
H	-0.884114	-2.066546	-1.381473
H	-2.469010	-1.314400	-1.735509
C	2.799999	0.036168	0.768292
H	3.545716	-0.618286	1.212999
H	2.889812	1.043804	1.175518
C	2.800008	0.035292	-0.768319
H	2.889811	1.042462	-1.176696
H	3.545729	-0.619666	-1.212278
O	1.502991	-0.476474	1.095372
O	1.503007	-0.477735	-1.094822
C	0.727131	-0.368135	0.000209
S	-0.158408	1.600680	-0.000933

PS3

P	0.165640	0.000043	-0.000013
C	0.914914	-1.613271	0.354065
H	0.573597	-1.946915	1.333157
H	0.572960	-2.326525	-0.394767
H	2.004078	-1.555299	0.340912
C	0.914966	1.113287	1.219983
H	0.572880	2.127849	1.019891
H	0.573717	0.820787	2.212142
H	2.004113	1.073535	1.175650
C	0.914889	0.499948	-1.574075
H	0.573384	-0.181047	-2.352560
H	0.573000	1.505146	-1.817216
H	2.004034	0.482158	-1.517308
S	1.775311	-0.000008	0.000028

P4

P	-0.000070	0.000030	0.737925
Cl	1.547631	0.943378	-0.217023
Cl	-1.590860	0.868440	-0.217060
Cl	0.043290	-1.811843	-0.217027

TS1-P4

C	2.621108	0.811451	-0.768386
H	2.171643	1.714673	-1.179775
H	3.604994	0.653549	-1.203142
C	2.621888	0.810932	0.768181
H	3.606079	0.651750	1.201806
H	2.173784	1.714325	1.180656

O	1.812552	-0.319235	-1.109052
O	1.812541	-0.319171	1.108957
C	1.135981	-0.721639	-0.000039
S	0.285123	-2.233155	-0.000021
P	-0.668606	0.073929	-0.000006
Cl	-0.715403	2.206909	-0.000061
Cl	-1.799932	-0.233035	1.619582
Cl	-1.800193	-0.233285	-1.619338

IN1-P4

C	-2.750480	0.529851	0.769341
H	-2.457000	1.498210	1.172802
H	-3.697186	0.214715	1.201959
C	-2.752440	0.527730	-0.769385
H	-3.699343	0.208460	-1.198594
H	-2.463147	1.495872	-1.176348
O	-1.771354	-0.452917	1.116979
O	-1.771175	-0.452919	-1.117077
C	-1.008664	-0.689917	0.000026
S	0.068443	-2.120854	0.000214
P	0.694034	-0.032505	0.000011
Cl	0.327061	2.110537	-0.001029
Cl	1.843637	0.004360	-1.646612
Cl	1.842290	0.005379	1.647493

TS2-P4

C	3.087958	0.077560	-0.619155
H	3.368108	0.695317	-1.469180
H	3.851874	-0.679216	-0.435185
C	2.757544	0.875841	0.632914
H	3.581887	0.962389	1.335412
H	2.351708	1.860359	0.394181
O	1.849952	-0.574814	-0.914192
O	1.746626	0.068679	1.236403
C	1.041622	-0.502741	0.202034
S	0.022091	-1.940333	0.627913
P	-0.712788	-0.050324	-0.001969
Cl	-0.546119	2.084452	0.041302
Cl	-2.463315	-0.007498	1.063288
Cl	-1.279423	-0.294221	-1.911339

IN2-P4

C	-3.222353	0.751504	-0.133205
H	-3.645926	1.056024	-1.089004
H	-3.737299	1.256279	0.681852
C	-3.166613	-0.766580	0.040705
H	-3.303292	-1.065503	1.082789
H	-3.846923	-1.317403	-0.601634
O	-1.837576	1.128831	-0.124086
O	-1.828580	-1.070052	-0.357475
C	-1.093423	0.006501	-0.011114
S	-0.211087	-0.184609	1.790401
P	0.742408	-0.002568	0.036521
Cl	1.003510	-1.537098	-1.274773
Cl	2.751037	-0.085495	0.724861
Cl	1.010058	1.778127	-0.908561

TS3-P4

C	-3.498458	0.761293	0.146106
H	-4.185492	1.206248	-0.568596
H	-3.641469	1.198726	1.131014
C	-3.498176	-0.761475	0.146232
H	-3.640135	-1.198752	1.131375
H	-4.185663	-1.206834	-0.567764
O	-2.147574	1.074289	-0.278119
O	-2.147535	-1.074044	-0.279056
C	-1.426938	0.000204	-0.432453
S	0.168803	-0.001121	1.895375
P	0.960776	-0.000079	0.140863
Cl	0.952435	-1.633734	-1.063384
Cl	3.003612	-0.000212	0.462093
Cl	0.952341	1.634984	-1.061466

PS4

P	-0.190261	-0.000053	-0.000147
Cl	0.706877	0.508938	1.732485
Cl	0.707351	1.246122	-1.306714
Cl	0.707222	-1.755023	-0.425407
S	-2.075671	0.000010	-0.000248

P5

C	1.080495	1.135674	0.000000
C	0.134208	0.748658	1.154554
C	0.134208	0.748658	-1.154554
H	1.966607	0.502499	0.000000
P	-0.900636	-0.308768	0.000000
C	0.134208	-1.839363	0.000000
H	-0.113287	-2.432733	0.880868

H	-0.113287	-2.432733	-0.880868
H	1.205167	-1.634998	0.000000
H	-0.458099	1.594186	-1.504245
H	0.580309	0.253481	-2.015642
H	1.421203	2.172387	0.000000
H	0.580309	0.253481	2.015642
H	-0.458099	1.594186	1.504245

TS1-P5

C	1.880850	-1.417997	0.980295
H	1.121437	-1.769631	1.685899
H	2.864476	-1.722798	1.330046
C	1.567580	-1.866706	-0.458497
H	2.412127	-2.337908	-0.957820
H	0.705761	-2.538449	-0.495846
O	1.853378	-0.004168	0.907462
O	1.271019	-0.656605	-1.138515
C	1.108615	0.347347	-0.199706
S	1.087349	1.965813	-0.714959
C	-2.405090	-1.045955	-0.970672
H	-3.443149	-1.220331	-1.247537
H	-1.771878	-1.683435	-1.587344
P	-0.899245	0.178354	0.396243
C	-1.184713	1.330107	1.763003
H	-0.963539	0.812596	2.697338
H	-0.516350	2.180667	1.643647
H	-2.222745	1.661705	1.773093
C	-2.089023	-1.254157	0.529531
H	-2.934599	-0.986121	1.165460
H	-1.704644	-2.225536	0.830506
C	-1.933614	0.428135	-1.082294
H	-2.736437	1.140191	-0.891521
H	-1.382173	0.722274	-1.971750

IN1-P5

C	2.615727	-0.503921	0.911254
H	2.901982	-1.080078	1.788965
H	3.375534	0.246152	0.688796
C	2.311196	-1.376415	-0.327712
H	2.905914	-1.063803	-1.186775
H	2.437041	-2.442723	-0.150826
O	1.373395	0.130016	1.192693
O	0.931275	-1.135634	-0.578203
C	0.697730	0.162451	-0.053041
S	0.999751	1.534890	-1.117954
C	-2.271452	-1.520902	-0.582916
H	-3.274690	-1.917397	-0.720526
H	-1.548413	-2.211090	-1.010521
P	-1.082091	0.309058	0.285185
C	-1.406039	1.793779	1.236895
H	-0.814843	1.731090	2.151372
H	-1.082531	2.653112	0.655135
H	-2.466827	1.850578	1.478311
C	-1.905545	-1.207519	0.895632
H	-2.777941	-0.981882	1.508793
H	-1.265230	-1.922843	1.404525
C	-2.059122	-0.096401	-1.177430
H	-2.977148	0.489187	-1.219241
H	-1.509829	-0.005897	-2.110525

TS2-P5

P	-0.917557	0.043205	-0.124189
C	-2.488697	-0.289054	-1.099887
H	-3.038992	0.576618	-1.466846
H	-2.252016	-0.953360	-1.930346
C	-1.335955	1.528458	0.831303
H	-0.740134	1.552664	1.741719
H	-1.106115	2.406986	0.231731
H	-2.397566	1.520568	1.074550
C	-1.687316	-1.386654	0.774566
C	2.969149	0.445484	0.695610
H	3.477320	0.575228	1.648627
H	3.434477	1.079406	-0.061262
C	2.887921	-1.025687	0.231205
H	3.283714	-1.147937	-0.779039
H	3.374728	-1.725914	0.906146
O	1.603737	0.819354	0.871479
O	1.490666	-1.301843	0.241439
C	0.877497	-0.071159	0.100132
S	0.560199	0.468321	-1.665073
C	-3.042142	-1.061995	0.110139
H	-3.650541	-0.423351	0.749292
H	-3.631909	-1.938989	-0.151156
H	-1.622644	-1.400368	1.861689
H	-1.264360	-2.312266	0.380104

IN2-P5

C	-3.048392	-0.275710	0.520947

H	-3.691726	-0.157082	1.389869
H	-3.417510	-1.089664	-0.105678
C	-2.852393	1.022557	-0.290816
H	-3.102201	0.878514	-1.343871
H	-3.398530	1.875377	0.105539
O	-1.733419	-0.582818	0.983574
O	-1.457812	1.289802	-0.159607
C	-0.874564	0.083742	0.142839
S	-0.357639	-0.934294	-1.409069
C	3.092011	0.898679	0.118865
H	3.544492	0.634820	1.074363
H	3.773644	1.569347	-0.401943
P	0.946872	-0.191995	0.062471
C	1.160115	-1.190811	1.569207
H	0.474286	-0.857979	2.345435
H	0.937709	-2.228292	1.322040
H	2.191611	-1.120546	1.911666
C	1.675466	1.478598	0.323579
H	1.437379	1.981444	1.259769
H	1.377246	2.116592	-0.509972
C	2.686409	-0.352799	-0.680053
H	3.250740	-1.268737	-0.508943
H	2.639960	-0.146583	-1.749369

TS3-P5

C	-3.113826	-0.244201	0.467458
H	-3.827203	-0.031282	1.259573
H	-3.374569	-1.172330	-0.040990
C	-2.902464	0.914710	-0.516929
H	-3.049603	0.606068	-1.551849
H	-3.494191	1.799565	-0.296498
O	-1.818783	-0.405068	1.063823
O	-1.518686	1.245540	-0.337246
C	-0.925287	0.235391	0.304191
S	-0.206157	-1.203181	-1.251250
C	3.061909	0.970593	0.024569
H	3.415913	0.922801	1.055280
H	3.776160	1.557351	-0.551663
P	0.978373	-0.217675	0.064456
C	1.118936	-0.842112	1.773870
H	0.952370	-0.021101	2.471352
H	0.342766	-1.589614	1.928578
H	2.095923	-1.288379	1.946843
C	1.613042	1.502817	-0.022137
H	1.277372	2.185735	0.757192
H	1.364736	1.917741	-0.999903
C	2.763736	-0.435700	-0.526079
H	3.367546	-1.260118	-0.150847
H	2.779171	-0.443185	-1.616196

PS5

C	-0.484277	-2.100493	0.000000
C	-0.023490	-1.189034	1.166841
C	-0.023490	-1.189034	-1.166841
H	-1.566676	-2.218374	0.000000
P	-0.023490	0.228796	0.000000
C	-1.734399	0.833658	0.000000
H	-1.881177	1.450839	0.885202
H	-1.881177	1.450839	-0.885202
H	-2.446361	0.008078	0.000000
H	1.003003	-1.398218	-1.464741
H	-0.658970	-1.128872	-2.047073
H	-0.036765	-3.092263	0.000000
H	-0.658970	-1.128872	2.047073
H	1.003003	-1.398218	1.464741
S	1.316898	1.618284	0.000000

P6

C	0.000136	-1.235532	0.639077
H	0.000157	-1.597541	1.672713
H	0.000251	-2.105926	-0.041232
P	-0.000047	0.711706	-0.567130
C	-0.000275	2.245950	0.425559
H	0.883012	2.835245	0.170506
H	-0.883579	2.835090	0.170101
H	-0.000584	2.005141	1.487373
N	1.093336	-0.305052	0.330531
N	-1.093219	-0.305258	0.330452
C	-2.279323	-0.865604	-0.280520
H	-2.059981	-1.466385	-1.174190
H	-2.800437	-1.499440	0.439931
H	-2.957629	-0.061361	-0.566165
C	2.279476	-0.865207	-0.280530
H	2.800436	-1.499424	0.439706
H	2.060257	-1.465579	-1.174512
H	2.957903	-0.060890	-0.565683

TS1-P6

C	-2.559856	0.677394	-0.593679
H	-3.547761	0.482167	-0.154932
H	-2.686567	1.166142	-1.567372
P	-0.593588	0.080895	0.423742
C	-0.850557	-0.543116	2.117236
H	-0.182216	-1.373775	2.327032
H	-0.637920	0.288973	2.790631
H	-1.890190	-0.841976	2.253767
N	-1.736570	-0.531542	-0.664632
N	-1.682374	1.424125	0.310231
C	-1.264898	2.755941	-0.068808
H	-2.083011	3.464699	0.070357
H	-0.443617	3.073844	0.575523
H	-0.932109	2.816062	-1.113978
C	-2.381208	-1.824332	-0.721241
H	-1.629214	-2.604765	-0.783845
H	-3.024415	-2.005100	0.150228
H	-2.999994	-1.872166	-1.619126
C	2.218022	1.360041	-0.990018
H	1.452304	2.112904	-1.189678
H	3.087400	1.548027	-1.616473
C	2.545477	1.261369	0.509771
H	3.593813	1.431238	0.744374
H	1.924133	1.935513	1.105663
O	1.712318	0.072590	-1.312033
O	2.230831	-0.083433	0.834933
C	1.437998	-0.589181	-0.155660
S	1.026296	-2.224078	-0.163518

IN1-P6

C	-2.315012	0.841025	-0.841092
H	-3.387165	1.049010	-0.776453
H	-1.943108	1.090909	-1.845404
P	-0.757013	-0.070705	0.569265
C	-0.869391	-0.267269	2.357577
H	0.137474	-0.345156	2.762499
H	-1.399760	0.587693	2.773020
H	-1.406220	-1.188484	2.574434
N	-1.982721	-0.531593	-0.453270
N	-1.527546	1.443102	0.227271
C	-0.799479	2.671211	-0.014560
H	-1.483367	3.521692	-0.037758
H	-0.096021	2.831551	0.803935
H	-0.228931	2.646005	-0.949927
C	-2.204117	-1.676609	-1.298700
H	-1.900282	-2.578252	-0.774326
H	-3.268347	-1.746575	-1.530947
H	-1.631878	-1.612274	-2.228855
C	2.640707	0.283676	-1.352928
H	2.965447	1.113368	-1.976872
H	2.926357	-0.663721	-1.813301
C	3.138405	0.373324	0.107618
H	3.685437	-0.525333	0.397464
H	3.740460	1.256190	0.310416
O	1.223236	0.355875	-1.229575
O	1.937136	0.479743	0.868155
C	0.957666	-0.097017	0.062729
S	0.665083	-1.888225	0.257661

TS2-P6

C	-2.445407	0.973248	-0.613371
H	-3.423208	1.344696	-0.290503
H	-2.322787	1.143035	-1.693846
P	-0.712602	-0.086147	0.494628
C	-0.764554	-0.396043	2.272408
H	0.248386	-0.431796	2.668577
H	-1.332637	0.403465	2.745784
H	-1.254234	-1.352070	2.445280
N	-2.217580	-0.416340	-0.227257
N	-1.332458	1.476610	0.168428
C	-0.627777	2.692127	-0.148625
H	-1.186366	3.569734	0.185453
H	0.331609	2.685316	0.369931
H	-0.425521	2.784858	-1.220941
C	-2.626360	-1.520108	-1.054940
H	-2.257823	-2.448416	-0.622182
H	-3.716159	-1.572667	-1.089568
H	-2.237884	-1.441771	-2.076320
C	2.820160	0.361419	-1.222663
H	3.290084	1.247021	-1.644479
H	2.982032	-0.494682	-1.880523
C	3.261906	0.051924	0.225481
H	3.666532	-0.957999	0.312210
H	3.971359	0.770556	0.629574
O	1.425280	0.620011	-1.097756
O	2.054159	0.158837	0.976464
C	1.038402	-0.048072	0.054366
S	0.496179	-1.805117	-0.190505

IN2-P6

C	-2.539586	1.005648	-0.425331
H	-3.312008	1.559811	0.120876
H	-2.717160	1.098663	-1.506173
P	-0.692103	-0.136375	0.412336
C	-0.697322	-0.613214	2.162298
H	0.311327	-0.723947	2.551356
H	-1.235553	0.158684	2.714054
H	-1.246083	-1.548655	2.257539
N	-2.392978	-0.371314	0.023278
N	-1.192655	1.385523	-0.040194
C	-0.653818	2.714113	0.035625
H	-1.243723	3.344147	0.708560
H	0.365339	2.659116	0.414536
H	-0.619716	3.185922	-0.949709
C	-2.882365	-1.432829	-0.822949
H	-2.581407	-2.393634	-0.404129
H	-3.973586	-1.415315	-0.859588
H	-2.495460	-1.372631	-1.849160
C	3.008022	0.449564	-0.991229
H	3.629706	1.332294	-1.122025
H	3.067613	-0.182303	-1.879589
C	3.317566	-0.347967	0.293726
H	3.546563	-1.392133	0.072441
H	4.109991	0.084466	0.900267
O	1.662861	0.879674	-0.799484
O	2.101788	-0.270043	1.034868
C	1.119840	0.007446	0.113553
S	0.357745	-1.563871	-0.707070

TS3-P6

C	-3.471652	-0.560186	-0.273696
H	-4.359561	-0.282012	-0.834545
H	-3.418838	-1.639444	-0.140549
C	-3.282386	0.208431	1.029446
H	-3.231008	-0.436216	1.903698
H	-4.003371	1.007586	1.184917
O	-2.310476	-0.170348	-1.037348
O	-1.978642	0.805726	0.854188
C	-1.431688	0.434187	-0.275425
S	-0.066362	-1.727817	0.577066
C	2.544673	1.052501	0.517000
H	3.160476	1.768237	-0.044099
H	2.867570	1.041591	1.566428
P	0.795353	-0.192036	-0.318801
C	0.664336	-0.208905	-2.127672
H	0.966170	0.765925	-2.515371
H	-0.340822	-0.451166	-2.458281
H	1.367940	-0.960930	-2.483557
N	1.114595	1.317385	0.368699
N	2.503751	-0.271307	-0.083808
C	0.651034	2.642141	0.043952
H	1.014219	3.342125	0.799168
H	-0.434841	2.678226	0.056366
H	1.005130	2.984413	-0.937597
C	3.212439	-1.358254	0.552211
H	4.289598	-1.201155	0.464564
H	2.961708	-2.292225	0.051972
H	2.951108	-1.464409	1.612005

PS6

S	0.001872	-1.679258	-1.120766
C	-0.002308	1.801398	-0.050633
H	-0.003415	2.729144	0.526008
H	-0.002705	2.025481	-1.127963
P	0.000527	-0.415143	0.332247
C	0.002153	-1.175572	1.961703
H	-0.881294	-1.806559	2.054405
H	0.888021	-1.803350	2.053540
H	0.001262	-0.399706	2.724591
N	-1.090968	0.882200	0.324031
N	1.088753	0.884949	0.323743
C	2.312111	0.902879	-0.452389
H	2.130425	0.725445	-1.518343
H	2.804030	1.868113	-0.326759
H	2.985609	0.129522	-0.085676
C	-2.314666	0.896984	-0.451616
H	-2.808435	1.861361	-0.326645
H	-2.133086	0.718993	-1.517496
H	-2.986494	0.122644	-0.083911

P7

C	0.946772	-1.368913	0.522050
C	-0.571470	-1.415454	0.610324
H	1.419817	-1.654623	1.465651
H	1.288542	-2.065608	-0.254905
H	-0.920127	-1.070870	1.595335

H	-0.951765	-2.428508	0.459478
N	-1.023705	-0.543731	-0.463784
N	1.298884	-0.000721	0.145642
P	-0.031415	0.862373	-0.505788
C	-0.598364	1.798845	0.988030
H	0.141707	2.574853	1.190417
H	-1.549497	2.291745	0.774325
H	-0.697577	1.174104	1.876081
C	-2.457123	-0.372390	-0.556883
H	-2.933464	-1.335691	-0.751382
H	-2.896273	0.043789	0.361668
H	-2.695273	0.297080	-1.384673
C	2.596190	0.120982	-0.490602
H	3.380101	-0.186623	0.205557
H	2.679031	-0.499723	-1.393552
H	2.783733	1.157233	-0.767704

TS1-P7

C	-1.674655	2.129461	-0.656118
H	-0.805560	2.741057	-0.405093
H	-2.532560	2.773594	-0.840445
C	-1.373091	1.167113	-1.815371
H	-1.989738	1.336198	-2.695199
H	-0.316110	1.192737	-2.093258
O	-1.994340	1.270999	0.431160
O	-1.699303	-0.108274	-1.284771
C	-1.689292	-0.023307	0.087091
S	-2.274388	-1.306739	1.012896
C	2.903491	0.363044	-0.337069
C	2.420374	-0.810125	-1.173928
H	3.494621	0.008203	0.520171
H	3.520017	1.053627	-0.915578
H	3.177130	-1.594972	-1.247270
H	2.171302	-0.478811	-2.190961
N	1.233467	-1.314085	-0.494829
N	1.679292	1.024684	0.102780
P	0.495464	-0.150514	0.466121
C	0.776844	-0.638409	2.198783
H	0.275800	0.065582	2.864649
H	0.348385	-1.624096	2.360793
H	1.849475	-0.658674	2.397582
C	1.856294	2.124899	1.031096
H	2.401497	2.935414	0.544521
H	0.882973	2.507482	1.343618
H	2.411097	1.827512	1.930809
C	0.497597	-2.360869	-1.186149
H	-0.404936	-2.611325	-0.631014
H	0.202309	-2.044972	-2.192316
H	1.127010	-3.249839	-1.265931

IN1-P7

C	-2.844957	1.162187	-0.292288
H	-3.114772	2.158450	0.054241
H	-3.744528	0.561304	-0.448713
C	-1.953793	1.152028	-1.518790
H	-2.495516	1.151167	-2.463064
H	-1.238604	1.981141	-1.495093
O	-2.011987	0.551019	0.678727
O	-1.286278	-0.091177	-1.385302
C	-1.182007	-0.399168	-0.000333
S	-1.354879	-2.095051	0.415564
C	2.313160	1.423212	-0.550547
C	2.324418	0.101203	-1.302961
H	3.163384	1.481333	0.142890
H	2.360554	2.277521	-1.228956
H	3.338521	-0.221047	-1.541475
H	1.747081	0.174356	-2.231410
N	1.716926	-0.864778	-0.385386
N	1.049212	1.414585	0.166404
P	0.535744	-0.143681	0.521103
C	0.723439	-0.462004	2.279269
H	-0.207252	-0.194067	2.779352
H	0.909481	-1.519191	2.442272
H	1.554468	0.137710	2.654374
C	0.758293	2.527930	1.045519
H	0.719282	3.453668	0.467940
H	-0.215375	2.380648	1.513167
H	1.516537	2.644477	1.830295
C	1.724309	-2.254462	-0.821617
H	1.389852	-2.899009	-0.014792
H	1.056634	-2.413294	-1.671755
H	2.748126	-2.512072	-1.098855

TS2-P7

C	2.974808	0.267658	1.287731
H	3.407971	1.119499	1.807461
H	3.208168	-0.653623	1.825101
C	3.386500	0.170721	-0.198891

H	3.843375	-0.794604	-0.424084
H	4.042915	0.974888	-0.524507
O	1.565735	0.457144	1.232830
O	2.151712	0.302436	-0.897886
C	1.178190	-0.102793	0.022154
S	0.780768	-1.888700	0.035824
C	-2.764263	0.210292	1.020433
C	-2.421181	1.587391	0.475192
H	-3.833483	0.002032	0.958368
H	-2.450668	0.115938	2.067697
H	-3.068623	1.837468	-0.378487
H	-2.536307	2.366488	1.232697
N	-1.041000	1.455069	0.085080
N	-2.035703	-0.712367	0.162980
P	-0.572747	-0.091374	-0.412206
C	-0.620570	-0.202338	-2.216825
H	-1.010168	-1.173693	-2.512250
H	0.382850	-0.078209	-2.619404
H	-1.279248	0.583506	-2.591136
C	-2.291031	-2.119827	0.374269
H	-3.370800	-2.278432	0.374559
H	-1.873967	-2.479084	1.320687
H	-1.859907	-2.709266	-0.431457
C	-0.327842	2.630737	-0.351368
H	-0.317409	3.382202	0.441515
H	-0.781079	3.078802	-1.245552
H	0.704956	2.369285	-0.583453

IN2-P7

C	-3.446604	-0.346718	0.263485
H	-4.232036	0.108956	0.862423
H	-3.692015	-1.391791	0.064420
C	-3.131651	0.419361	-1.039898
H	-3.200613	-0.232903	-1.913088
H	-3.747901	1.303097	-1.189931
O	-2.228241	-0.267131	0.998829
O	-1.784973	0.844193	-0.859794
C	-1.241529	-0.031815	0.058287
S	-0.519006	-1.592499	-0.724841
C	2.305844	1.694662	-0.443986
C	2.805733	0.338575	-0.908554
H	2.927063	2.075141	0.377732
H	2.308053	2.432952	-1.249922
H	3.895475	0.274640	-0.888509
H	2.467060	0.133141	-1.935960
N	2.221936	-0.586895	0.041247
N	0.955304	1.441767	0.005835
P	0.573808	-0.142995	0.389862
C	0.552635	-0.575378	2.153468
H	1.067846	0.222962	2.690043
H	-0.465864	-0.677386	2.517977
H	1.100290	-1.502157	2.311645
C	0.188003	2.584196	0.445176
H	0.748727	3.152746	1.196089
H	-0.042642	3.245450	-0.393592
H	-0.752367	2.263376	0.888648
C	2.524930	-1.973851	-0.222575
H	2.165164	-2.299130	-1.209134
H	3.605999	-2.123008	-0.182246
H	2.065598	-2.615979	0.528670

TS3-P7

C	-3.575740	-0.700520	0.101315
H	-4.473972	-0.560851	0.697220
H	-3.527467	-1.714341	-0.293007
C	-3.363112	0.360371	-0.977160
H	-3.226271	-0.069083	-1.968032
H	-4.123785	1.136997	-0.996751
O	-2.431518	-0.515774	0.956160
O	-2.112851	0.961124	-0.589219
C	-1.545732	0.270622	0.377479
S	-0.232724	-1.432276	-0.975829
C	2.233359	1.726828	-0.525850
C	2.860635	0.391756	-0.884032
H	2.838328	2.243084	0.230003
H	2.140429	2.381688	-1.396466
H	3.951257	0.437531	-0.859995
H	2.549294	0.068251	-1.888735
N	2.364644	-0.509248	0.139061
N	0.921491	1.416797	0.023635
P	0.671517	-0.213224	0.327412
C	0.494214	-0.640601	2.082652
H	0.565503	0.276573	2.668767
H	-0.462825	-1.120229	2.264282
H	1.309850	-1.302339	2.368185
C	0.190722	2.558349	0.523982
H	0.894173	3.258092	0.986637
H	-0.342838	3.082141	-0.274082

H	-0.532394	2.262663	1.279737
C	2.812232	-1.877268	-0.030318
H	2.535562	-2.285852	-1.009650
H	3.898617	-1.912978	0.079636
H	2.369911	-2.519439	0.731536

PS7

S	-1.208002	-1.718657	0.806649
C	1.573947	1.423763	0.189879
C	0.212607	2.084032	0.357636
H	1.976130	1.613597	-0.816275
H	2.295672	1.792041	0.921485
H	0.172054	3.062318	-0.125201
H	-0.018010	2.209595	1.423325
N	-0.734468	1.169967	-0.271583
N	1.314936	0.011722	0.410468
P	-0.189684	-0.421936	-0.192258
C	0.049704	-0.934306	-1.913664
H	0.685886	-0.216668	-2.433634
H	0.496670	-1.927771	-1.937195
H	-0.921969	-0.981078	-2.404344
C	2.430562	-0.904301	0.323487
H	2.902916	-0.897132	-0.667840
H	3.184444	-0.636868	1.065655
H	2.083757	-1.914701	0.542798
C	-2.138043	1.467113	-0.050917
H	-2.391748	1.468129	1.014942
H	-2.369405	2.446071	-0.474000
H	-2.759045	0.720385	-0.542941

P8

C	1.419880	0.775156	0.449745
C	0.336423	1.296524	-0.510109
C	0.336405	-1.296478	-0.510212
C	1.419790	-0.775230	0.449778
H	2.397923	1.166431	0.167710
H	1.222658	1.144532	1.456384
H	0.741106	1.441855	-1.514090
H	-0.082404	2.252240	-0.193418
H	-0.082412	-2.252256	-0.193686
H	0.741151	-1.441657	-1.514192
H	1.222349	-1.144540	1.456400
H	2.397827	-1.166643	0.167919
P	-0.978887	0.000026	-0.658248
C	-1.609917	-0.000018	1.079711
H	-2.235984	0.880307	1.228765
H	-2.235832	-0.880449	1.228782
H	-0.818569	0.000060	1.829674

TS1-P8

C	2.012353	-1.668055	0.746682
H	1.283327	-2.013753	1.485889
H	2.985220	-2.097312	0.976180
C	1.540013	-1.944209	-0.692176
H	2.269069	-2.487233	-1.290446
H	0.587440	-2.481449	-0.711552
O	2.125356	-0.257724	0.803454
O	1.380431	-0.652346	-1.254810
C	1.388666	0.277829	-0.232110
S	1.554260	1.921404	-0.609510
C	-2.649467	-1.244131	-0.473610
C	-2.970472	0.200407	-0.859871
H	-3.546828	-1.847012	-0.331793
H	-2.062928	-1.708707	-1.271893
H	-3.651506	0.625488	-0.117343
H	-3.464378	0.264809	-1.829490
P	-0.633305	0.238401	0.480328
C	-0.714286	1.295213	1.949527
H	-0.398825	0.721125	2.820754
H	-0.032106	2.130789	1.798289
H	-1.730581	1.659148	2.104384
C	-1.809533	-1.167395	0.805847
H	-2.437520	-0.911612	1.663023
H	-1.285076	-2.093895	1.035269
C	-1.646292	0.972255	-0.857322
H	-1.754336	2.044910	-0.714029
H	-1.081743	0.825318	-1.780950

IN1-P8

P	0.801300	-0.452095	0.388002
C	0.889680	-1.857078	1.497531
C	1.828147	-0.593160	-1.098465
H	0.361935	-1.600940	2.416048
H	1.931408	-2.091407	1.715993
H	0.389801	-2.692803	1.011226
C	1.634936	1.004167	1.101872
C	2.976166	0.403697	-0.874482
H	2.141893	-1.620937	-1.266903

H	1.177436	-0.305320	-1.926727
C	2.398897	1.590355	-0.095354
H	0.893416	1.678581	1.527773
H	2.318376	0.684373	1.891336
H	3.412431	0.712713	-1.823605
H	3.769476	-0.066322	-0.286907
H	3.172958	2.285843	0.227347
H	1.696873	2.134271	-0.730617
C	-0.939710	-0.154257	-0.067582
O	-1.633220	0.115792	1.143130
O	-0.963864	1.108081	-0.727567
S	-1.442747	-1.558855	-1.000997
C	-2.764089	0.880277	0.743623
C	-2.297364	1.573871	-0.556682
H	-3.612132	0.220824	0.555603
H	-2.998113	1.575148	1.547883
H	-2.909781	1.271544	-1.406796
H	-2.264847	2.659313	-0.482993

TS2-P8

P	0.694325	0.448061	0.104875
C	2.295856	0.262003	1.071471
H	2.833342	1.213594	1.032840
H	2.092824	0.003623	2.106148
C	0.626265	2.276308	-0.022412
H	-0.145572	2.563762	-0.734383
H	0.362453	2.685386	0.954100
H	1.595763	2.674514	-0.320585
C	1.394808	-0.252183	-1.438506
H	0.882997	-1.201269	-1.600379
H	1.159991	0.400268	-2.279351
C	-3.266130	0.327947	0.178814
H	-3.990693	1.066770	-0.156313
H	-3.588044	-0.102939	1.128757
C	-2.968439	-0.770102	-0.866950
H	-3.149068	-1.767028	-0.460864
H	-3.516296	-0.646351	-1.798550
O	-2.012270	0.983668	0.340399
O	-1.581334	-0.599806	-1.148511
C	-1.062535	0.038882	-0.027446
S	-0.467871	-1.066373	1.326193
C	3.058807	-0.804687	0.291841
C	2.891682	-0.451370	-1.190705
H	3.432814	0.475144	-1.401561
H	3.300858	-1.222459	-1.843325
H	4.108916	-0.848189	0.582634
H	2.617727	-1.785453	0.486873

IN2-P8

C	2.982305	-1.211488	-0.150591
H	3.549116	-1.933854	0.432202
H	3.091369	-1.425445	-1.215597
C	3.325068	0.257850	0.171047
H	3.621005	0.807213	-0.724619
H	4.081489	0.374289	0.943811
O	1.609022	-1.321375	0.221480
O	2.095991	0.783898	0.670810
C	1.107648	-0.044780	0.204264
S	0.457499	0.485757	-1.558293
C	-3.121476	-0.532571	-0.708409
C	-2.846652	-1.263188	0.611391
H	-4.190538	-0.439964	-0.904028
H	-2.684530	-1.101736	-1.534585
H	-3.382122	-0.754417	1.417875
H	-3.195919	-2.295814	0.590141
P	-0.722330	0.407851	0.160218
C	-0.659733	1.752001	1.394512
H	-0.695988	2.705568	0.867710
H	0.243808	1.702418	1.996423
H	-1.545993	1.674075	2.025733
C	-2.424179	0.816451	-0.584922
H	-2.980929	1.456201	0.106274
H	-2.314074	1.343676	-1.530680
C	-1.341920	-1.187309	0.848570
H	-1.038838	-1.250421	1.894534
H	-0.809367	-1.973641	0.310719

TS3-P8

C	-3.011851	-1.200885	0.203742
H	-3.617032	-1.929391	-0.330508
H	-3.036530	-1.402413	1.275835
C	-3.364727	0.262121	-0.111636
H	-3.612959	0.825136	0.788881
H	-4.149800	0.378227	-0.855278
O	-1.662233	-1.317810	-0.255923
O	-2.149731	0.780881	-0.662965
C	-1.152332	-0.069784	-0.336794
S	-0.374708	0.480603	1.557747

C	3.127382	-0.564516	0.688492
C	2.818765	-1.315739	-0.611092
H	4.200356	-0.505094	0.876010
H	2.673462	-1.093161	1.532356
H	3.378119	-0.852585	-1.428841
H	3.118487	-2.363242	-0.565061
P	0.746622	0.426131	-0.147022
C	0.646256	1.810253	-1.331028
H	0.900141	2.727405	-0.800058
H	-0.338594	1.902210	-1.779744
H	1.398842	1.642362	-2.104196
C	2.475296	0.803151	0.527495
H	3.035768	1.388273	-0.209026
H	2.419449	1.376665	1.451100
C	1.318338	-1.177240	-0.857779
H	1.026778	-1.212183	-1.908353
H	0.752456	-1.952571	-0.339029

PS8

C	-2.141751	0.123260	0.658497
C	-0.769697	0.218015	1.332661
C	-0.756659	-0.408809	-1.307106
C	-1.983516	-0.860423	-0.505072
H	-2.912961	-0.193893	1.360753
H	-2.438450	1.102195	0.270707
H	-0.568802	-0.664007	1.941848
H	-0.637617	1.102479	1.955053
H	-1.010863	0.417784	-1.974097
H	-0.299547	-1.202412	-1.893462
H	-2.876752	-0.908427	-1.127788
H	-1.805884	-1.861845	-0.105470
P	0.444556	0.192440	-0.045016
C	0.733926	1.938553	-0.449905
H	1.362623	2.375174	0.324700
H	1.259663	1.995397	-1.402288
H	-0.209943	2.482167	-0.516273
S	2.061024	-0.849674	0.216694

P9

P	-0.000025	0.000226	0.503260
F	1.162116	0.703579	-0.279612
F	-1.190826	0.653832	-0.279684
F	0.028753	-1.357788	-0.279471

TS1-P9

C	-2.471599	-0.642170	-0.734856
H	-2.391413	-1.535870	-1.350835
H	-3.424994	-0.148840	-0.916683
C	-2.211952	-0.909863	0.747123
H	-3.105841	-0.906356	1.363760
H	-1.653669	-1.836100	0.905891
O	-1.428936	0.274629	-1.087172
O	-1.402720	0.201241	1.128128
C	-0.706231	0.589139	0.024918
S	0.253413	2.022255	0.055869
P	1.042556	-0.392235	-0.018807
F	1.194093	-1.964120	-0.061850
F	1.922311	-0.102349	-1.244973
F	1.980809	-0.164084	1.177415

IN1-P9

C	2.676974	-0.199856	0.704089
H	2.988751	-0.973432	1.402704
H	3.395045	0.621305	0.707708
C	2.413507	-0.719338	-0.701379
H	3.255778	-0.619954	-1.380445
H	2.054488	-1.751690	-0.689994
O	1.397789	0.295957	1.103470
O	1.378103	0.153095	-1.146478
C	0.595305	0.398364	-0.029401
S	-0.558322	1.790948	-0.136654
P	-1.064157	-0.268092	0.031062
F	-0.830513	-1.839826	0.104988
F	-1.931597	-0.246049	1.306318
F	-2.029045	-0.400509	-1.168553

TS2-P9

C	2.696068	-0.168226	0.684202
H	3.035176	-0.911868	1.402216
H	3.394469	0.669316	0.651993
C	2.425150	-0.735401	-0.700697
H	3.258767	-0.647213	-1.391907
H	2.078725	-1.771045	-0.652459
O	1.410090	0.307552	1.085738
O	1.374509	0.110153	-1.160486
C	0.599844	0.379128	-0.043073
S	-0.552107	1.776846	-0.183832
P	-1.071672	-0.259172	0.034775

F	-0.850927	-1.828044	-0.088739
F	-1.722202	-0.310728	1.429723
F	-2.255928	-0.314093	-0.967068

IN2-P9

C	-2.849275	-0.214281	-0.725097
H	-3.405516	-1.134837	-0.887261
H	-3.198075	0.564770	-1.397352
C	-2.787710	0.222548	0.736232
H	-2.850830	1.303222	0.859024
H	-3.495142	-0.281671	1.386804
O	-1.462756	-0.481124	-1.029537
O	-1.457062	-0.177147	1.121577
C	-0.736708	-0.335770	0.044547
S	0.612007	1.716043	-0.229131
P	1.178522	-0.133263	0.015446
F	1.236212	-1.211322	-1.116460
F	2.756717	0.015358	-0.005692
F	1.238217	-0.879374	1.389127

TS3-P9

C	-3.076793	0.111863	-0.760602
H	-3.778838	-0.588246	-1.205324
H	-3.199434	1.098680	-1.199416
C	-3.076657	0.111122	0.760874
H	-3.198959	1.097541	1.200681
H	-3.778786	-0.589231	1.205065
O	-1.734799	-0.342976	-1.073515
O	-1.734708	-0.344303	1.073105
C	-1.020584	-0.535071	-0.000354
S	0.831792	1.706875	0.000580
P	1.423110	-0.099370	-0.000039
F	1.291081	-1.030105	1.222450
F	2.984379	-0.103703	0.000098
F	1.291312	-1.029242	-1.223208

PS9

P	0.000000	0.000000	-0.175066
F	0.000000	1.353466	-0.903764
F	-1.172136	-0.676733	-0.903764
F	1.172136	-0.676733	-0.903764
S	0.000000	0.000000	1.689227

P10

P	-0.000164	0.338697	0.683278
Cl	-1.591944	-0.654184	-0.177392
Cl	1.592249	-0.653839	-0.177339
C	-0.000305	1.806913	-0.402982
H	-0.889232	2.395637	-0.173242
H	0.889068	2.395310	-0.173990
H	-0.000734	1.523517	-1.453622

TS1-P10

C	-2.482846	1.149868	0.402041
H	-2.136278	2.074823	0.860975
H	-3.549368	1.022705	0.580382
C	-2.108705	1.053510	-1.080581
H	-2.958005	1.136946	-1.753150
H	-1.342177	1.779571	-1.357780
O	-1.805546	0.037748	0.994703
O	-1.581714	-0.265901	-1.198265
C	-1.095788	-0.629125	0.022827
S	-0.585449	-2.245011	0.295061
P	0.794872	0.017647	0.215718
Cl	1.168728	2.101844	0.269448
Cl	1.990870	-0.548962	-1.293500
C	1.613349	-0.459359	1.754212
H	0.883897	-0.314302	2.552152
H	1.904211	-1.502769	1.709044
H	2.470690	0.195354	1.898028

IN1-P10

C	-2.709168	0.525623	0.461675
H	-2.542031	1.503270	0.912283
H	-3.706332	0.165257	0.706829
C	-2.425514	0.537045	-1.049872
H	-3.292877	0.278506	-1.652645
H	-2.012711	1.491456	-1.375327
O	-1.770070	-0.415391	0.988089
O	-1.456250	-0.496778	-1.226088
C	-0.854483	-0.703249	-0.006562
S	0.164727	-2.154582	0.190145
P	0.813243	-0.025368	0.251825
Cl	0.414693	2.142303	0.231684
Cl	2.130763	0.012922	-1.263162
C	1.643623	-0.010398	1.851941
H	0.849276	-0.024713	2.599634
H	2.258333	-0.900709	1.945567

H	2.223124	0.905173	1.940006

TS2-P10

C	3.067223	0.600807	0.233514
H	3.507940	1.256421	0.981061
H	3.678066	0.598184	-0.671964
C	2.792756	-0.807274	0.725647
H	3.604723	-1.509988	0.555548
H	2.505872	-0.814337	1.781813
O	1.756475	1.071391	-0.064490
O	1.694515	-1.190153	-0.092325
C	0.953615	-0.035308	-0.357387
S	-0.003338	-0.045549	-1.879847
P	-0.763698	0.004641	0.213053
Cl	-2.114168	-1.536160	-0.014077
Cl	-1.658360	1.827471	0.158828
C	-0.694416	-0.147182	2.040453
H	-0.246303	-1.115240	2.271505
H	-0.052115	0.655256	2.407163
H	-1.679315	-0.079570	2.497012

IN2-P10

C	3.063290	0.460855	-0.666530
H	3.748859	1.301488	-0.719236
H	3.140715	-0.146112	-1.572038
C	3.203824	-0.387823	0.602711
H	3.663315	-1.356696	0.412468
H	3.734624	0.124761	1.403258
O	1.735658	0.969774	-0.557558
O	1.845466	-0.575602	1.023316
C	1.035394	0.010451	0.093957
S	0.148397	-1.277596	-1.110864
P	-0.801671	-0.067555	0.196795
Cl	-2.848513	-0.586361	-0.329421
Cl	-1.135966	1.925726	-0.083648
C	-1.021630	-0.512130	1.937178
H	-1.205961	-1.584209	1.982805
H	-0.130383	-0.251483	2.502776
H	-1.898586	0.016405	2.304086

TS3-P10

C	3.300633	0.445233	-0.670908
H	4.021448	1.254406	-0.599410
H	3.293521	0.026740	-1.675374
C	3.429019	-0.608477	0.421601
H	3.622483	-1.608633	0.043185
H	4.140580	-0.353364	1.203142
O	1.983271	0.991068	-0.425615
O	2.103593	-0.608357	1.007741
C	1.322982	0.267992	0.431286
S	-0.192744	-1.296393	-1.248652
P	-0.968899	-0.151386	0.114488
Cl	-3.046837	-0.390831	-0.137097
Cl	-1.045785	1.884976	-0.121580
C	-0.980799	-0.573081	1.881306
H	-1.673999	-1.402520	2.001331
H	0.012468	-0.847553	2.218291
H	-1.350476	0.291838	2.430738

PS10

P	-0.166783	-0.000004	0.188655
Cl	0.959222	1.572840	-0.449443
Cl	0.959288	-1.572793	-0.449464
C	0.148759	-0.000020	1.959699
H	-0.317052	0.891044	2.378374
H	-0.316856	-0.891214	2.378318
H	1.220042	0.000088	2.149427
S	-1.974475	-0.000032	-0.388295

P11

C	-1.345942	-0.774960	0.399436
C	-1.346233	0.774701	0.399428
H	-1.194058	-1.171038	1.405246
H	-2.271270	-1.183098	-0.003552
H	-1.194968	1.170819	1.405310
H	-2.271519	1.182487	-0.004013
P	0.818869	0.000151	-0.673772
C	1.641993	-0.000129	0.972190
H	2.277015	-0.884481	1.042980
H	2.277240	0.884051	1.043108
H	0.937386	-0.000075	1.805088
O	-0.283880	1.196085	-0.450618
O	-0.283840	-1.195911	-0.451121

TS1-P11

C	1.851031	1.904365	-0.536615
H	1.066243	2.644379	-0.695840
H	2.776311	2.245364	-0.999134

C	2.017410	1.539727	0.942902
H	2.938042	1.908788	1.387283
H	1.160989	1.867458	1.538733
O	1.479862	0.671107	-1.147763
O	2.068527	0.121227	0.922404
C	1.384972	-0.301944	-0.185527
S	1.376349	-1.938413	-0.611730
C	-2.498240	0.438487	-1.245389
C	-2.848553	1.033625	0.111218
H	-3.350350	-0.020767	-1.742074
H	-2.044520	1.184733	-1.901232
H	-3.578048	0.412682	0.638987
H	-3.213547	2.056921	0.051204
P	-0.680692	-0.256179	0.367549
C	-1.103025	-1.583861	1.526720
H	-0.285316	-1.707211	2.235744
H	-2.017011	-1.301428	2.050150
H	-1.243618	-2.514827	0.985592
O	-1.609257	1.028729	0.820785
O	-1.544378	-0.583712	-0.964778

IN1-P11

C	-2.276982	-1.563651	-0.606420
H	-1.808184	-2.540549	-0.726972
H	-3.246778	-1.556710	-1.104460
C	-2.372963	-1.144113	0.864511
H	-3.370206	-1.244654	1.285630
H	-1.649375	-1.686176	1.479132
O	-1.463345	-0.555593	-1.198662
O	-2.042204	0.237112	0.824466
C	-1.094598	0.349215	-0.194010
S	-0.620835	1.992744	-0.702601
C	2.559662	-0.771902	-1.000447
C	2.314962	-1.549386	0.286832
H	3.608145	-0.535112	-1.168470
H	2.150652	-1.293687	-1.866602
H	3.017971	-1.244300	1.069954
H	2.380265	-2.627426	0.148626
P	0.645650	0.387470	0.241442
C	1.054470	1.231605	1.776012
H	0.127473	1.365773	2.332960
H	1.747791	0.621669	2.355131
H	1.480972	2.206459	1.557803
O	0.995525	-1.195727	0.645384
O	1.847846	0.455225	-0.833891

TS2-P11

C	-2.412973	-1.525316	-0.346697
H	-1.836466	-2.239220	0.249777
H	-3.073528	-2.050384	-1.032100
C	-3.111187	-0.499135	0.533798
H	-3.958540	-0.039050	0.020919
H	-3.430542	-0.893721	1.497243
O	-1.539503	-0.703680	-1.102267
O	-2.093242	0.474223	0.742882
C	-1.078205	0.253751	-0.204730
S	-0.325007	1.718801	-0.979392
C	2.946688	-0.505292	-0.660166
C	2.331629	-1.653206	0.130318
H	4.006574	-0.368620	-0.451323
H	2.801742	-0.644266	-1.735159
H	2.779725	-1.730869	1.125380
H	2.405414	-2.612831	-0.378531
P	0.678455	0.324484	0.256143
C	0.736275	0.949706	1.943695
H	-0.274820	1.072523	2.324554
H	1.281886	0.230887	2.556750
H	1.261316	1.901857	1.954307
O	0.967427	-1.296467	0.249023
O	2.238715	0.636243	-0.224763

IN2-P11

C	2.901821	-1.228941	0.068865
H	3.448967	-1.939580	-0.545704
H	3.015247	-1.484066	1.124449
C	3.267480	0.244202	-0.201435
H	3.613573	0.748596	0.702183
H	3.991699	0.378324	-1.001625
O	1.524441	-1.301026	-0.290719
O	2.031341	0.819966	-0.624221
C	1.045937	-0.031633	-0.210698
S	0.356660	0.422207	1.591176
C	-2.978417	-0.571715	0.585396
C	-2.550585	-1.348354	-0.654155
H	-4.051402	-0.390715	0.622596
H	-2.665133	-1.088470	1.499217
H	-3.147315	-1.066996	-1.524582
H	-2.579177	-2.428362	-0.520906

P	-0.742605	0.414620	-0.131560
C	-0.743741	1.924453	-1.119760
H	0.269591	2.234705	-1.356559
H	-1.289480	1.707777	-2.039754
H	-1.271694	2.703124	-0.574791
O	-1.201327	-0.957289	-0.873852
O	-2.299121	0.653720	0.453891

TS3-P11

C	-3.456601	0.321900	-0.040623
H	-4.325336	0.511079	0.583361
H	-3.497648	0.919218	-0.949889
C	-3.180329	-1.151501	-0.304045
H	-3.227525	-1.421456	-1.355759
H	-3.788836	-1.829955	0.289905
O	-2.275385	0.730609	0.684981
O	-1.805730	-1.292415	0.123936
C	-1.330557	-0.174346	0.597761
S	0.054798	0.804502	-1.598065
C	2.422637	-1.604103	0.370397
C	3.118484	-0.548508	-0.485538
H	2.911640	-1.715198	1.340048
H	2.355443	-2.573524	-0.120679
H	4.191113	-0.500063	-0.308673
H	2.925602	-0.708052	-1.550378
P	0.900836	0.433421	0.125283
C	0.704354	1.590499	1.493849
H	0.866954	1.051429	2.427083
H	-0.290753	2.023107	1.483896
H	1.459932	2.365970	1.380693
O	2.525793	0.662619	-0.061517
O	1.100593	-1.113255	0.587520

PS11

C	-1.960310	-0.352080	0.775882
C	-1.960163	-0.355859	-0.775143
H	-2.507771	0.504185	1.172055
H	-2.385827	-1.265933	1.185307
H	-2.509627	0.497135	-1.175529
H	-2.383362	-1.272748	-1.180181
P	0.392306	0.140234	-0.000157
C	0.353854	1.939884	-0.002044
H	0.869538	2.304165	0.884725
H	0.869338	2.302280	-0.889703
H	-0.676608	2.299570	-0.002340
O	-0.603189	-0.281968	-1.196697
O	-0.603227	-0.279473	1.197236
S	2.118173	-0.648269	0.000721

P12

C	-2.535975	-0.656394	1.142232
C	-1.858956	0.662451	1.488471
H	-2.346175	-1.423551	1.898897
H	-3.621147	-0.508296	1.071342
H	-0.873154	0.491561	1.946748
H	-2.458371	1.253869	2.184083
N	-1.743094	1.353355	0.212092
N	-2.008842	-1.056055	-0.161757
P	-1.233823	0.222422	-0.981586
C	-2.842492	-1.986973	-0.896359
H	-2.924978	-2.927130	-0.345765
H	-3.855924	-1.596875	-1.059577
H	-2.396344	-2.205519	-1.865223
C	-1.089679	2.643832	0.271301
H	-1.662400	3.313392	0.916131
H	-0.064504	2.581409	0.662976
H	-1.050493	3.082907	-0.726689
C	0.532069	-0.060689	-0.499310
C	1.490770	0.775012	-1.072126
C	0.952567	-1.036736	0.402045
C	2.833607	0.667333	-0.740526
H	1.184423	1.521937	-1.798050
C	2.291691	-1.168493	0.741504
H	0.219094	-1.710598	0.828182
C	3.205744	-0.307391	0.165027
H	3.587871	1.308686	-1.175795
H	2.636466	-1.923167	1.435641
F	4.502275	-0.429751	0.487221

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C	-3.548158	-0.577149	-0.778559
H	-3.614355	0.498183	-0.950623
H	-4.548014	-1.004889	-0.723668
C	-2.651209	-1.267740	-1.814743
H	-3.180872	-1.974450	-2.449288
H	-2.125145	-0.538823	-2.435648
O	-2.893767	-0.827048	0.460519
O	-1.720603	-1.992879	-1.026337

C	-1.679200	-1.435190	0.227152
S	-0.875074	-2.230385	1.476417
C	-1.329648	2.716356	0.798789
C	-0.705295	2.937284	-0.567148
H	-1.082803	3.520177	1.495380
H	-2.423147	2.651232	0.720079
H	0.315003	3.334045	-0.464410
H	-1.285541	3.629129	-1.180976
N	-0.696724	1.611552	-1.171337
N	-0.752074	1.464793	1.273536
P	-0.451173	0.399646	0.007477
C	-1.154418	1.030326	2.603475
H	-0.527443	0.203941	2.928562
H	-1.026102	1.870220	3.288925
H	-2.195010	0.693618	2.632078
C	-0.001839	1.493150	-2.438186
H	-0.023738	0.457104	-2.781383
H	-0.494176	2.113355	-3.189242
H	1.049813	1.797697	-2.360616
C	1.325432	0.031480	0.054769
C	1.777306	-1.139714	-0.553030
C	2.242823	0.933000	0.587313
C	3.133855	-1.404630	-0.640731
H	1.059202	-1.858444	-0.931449
C	3.604365	0.680164	0.507746
H	1.885567	1.826904	1.083707
C	4.019415	-0.484797	-0.109120
H	3.512556	-2.309386	-1.095624
H	4.340051	1.358370	0.917801
F	5.332101	-0.736306	-0.188183

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C	-2.295492	-2.637898	-0.905887
H	-2.378357	-2.918372	-1.954665
H	-2.234363	-3.531127	-0.283199
C	-3.425118	-1.698701	-0.428292
H	-3.911490	-2.089690	0.466235
H	-4.166594	-1.484194	-1.195691
O	-1.115777	-1.855208	-0.758051
O	-2.748165	-0.486137	-0.123417
C	-1.435625	-0.892628	0.240356
S	-1.178944	-1.372262	1.922141
C	-1.646437	2.493681	-1.016552
C	-1.267837	2.950370	0.390547
H	-1.575446	3.308156	-1.738897
H	-2.665235	2.090734	-1.030765
H	-0.531562	3.761309	0.361312
H	-2.143426	3.297916	0.942205
N	-0.690377	1.784188	1.049465
N	-0.677437	1.449336	-1.351332
P	-0.363966	0.554470	0.026407
C	-0.893667	0.758164	-2.614403
H	-0.140138	-0.018559	-2.741167
H	-0.797324	1.474768	-3.431168
H	-1.882928	0.291005	-2.654976
C	-0.362359	1.874068	2.459268
H	0.289796	1.051291	2.739882
H	-1.263560	1.806558	3.070546
H	0.142144	2.825852	2.648256
C	1.353766	0.060171	-0.014285
C	1.783390	-1.246258	0.217355
C	2.278405	1.057531	-0.326940
C	3.132122	-1.550128	0.134336
H	1.062380	-2.008509	0.480637
C	3.628544	0.763887	-0.402339
H	1.935569	2.066804	-0.520719
C	4.025761	-0.540432	-0.169973
H	3.498445	-2.552063	0.309381
H	4.367882	1.516316	-0.638272
F	5.327813	-0.833768	-0.243737

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C	-3.363756	-2.049024	-0.481562
H	-4.017195	-2.156656	-1.344367
H	-3.940223	-2.164468	0.438456
C	-2.143724	-2.996350	-0.503337
H	-2.116085	-3.632310	0.383155
H	-2.083602	-3.610351	-1.399474
O	-2.779976	-0.752963	-0.531391
O	-1.027110	-2.109558	-0.506937
C	-1.515571	-0.912044	0.025962
S	-1.390062	-0.722404	1.835670
C	-1.184924	3.085877	0.141116
C	-0.843137	2.765888	-1.308106
H	-0.809207	4.064728	0.441805
H	-2.270022	3.065014	0.301369
H	0.115182	3.223939	-1.593932
H	-1.609848	3.132963	-1.994970

N	-0.785352	1.327249	-1.333907
N	-0.515645	2.048919	0.912453
P	-0.474704	0.557842	0.132305
C	-0.504231	2.203398	2.349424
H	-0.143662	3.205762	2.585751
H	-1.496872	2.062044	2.788774
H	0.174541	1.480178	2.796278
C	-0.664986	0.643314	-2.597238
H	-1.492565	0.913450	-3.257524
H	0.279921	0.884343	-3.100574
H	-0.697386	-0.434565	-2.434359
C	1.246779	-0.005984	0.117780
C	1.685607	-1.222229	0.633810
C	2.165632	0.846553	-0.494152
C	3.020827	-1.582891	0.539893
H	0.978822	-1.883602	1.114464
C	3.504121	0.502566	-0.589407
H	1.832182	1.796519	-0.894044
C	3.904339	-0.712959	-0.068556
H	3.383284	-2.522472	0.933545
H	4.231567	1.153259	-1.054549
F	5.196062	-1.057405	-0.155784

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C	-1.806272	-3.231489	-0.065841
H	-1.587477	-4.045862	-0.752814
H	-1.842983	-3.610841	0.957367
C	-3.082110	-2.439129	-0.422098
H	-3.774721	-2.395286	0.421027
H	-3.598000	-2.811674	-1.304234
O	-0.766689	-2.262976	-0.187203
O	-2.593271	-1.134034	-0.713543
C	-1.383470	-1.035602	-0.056030
S	-1.544531	-0.417025	1.724346
C	-1.220992	2.745313	-1.240090
C	-1.225966	3.109981	0.236243
H	-0.377385	3.225108	-1.754433
H	-2.144719	3.043886	-1.741999
H	-0.891921	4.135393	0.404842
H	-2.236389	3.002096	0.659816
N	-0.294068	2.167600	0.819497
N	-1.081237	1.305695	-1.253721
P	-0.521526	0.586823	0.148213
C	-1.143392	0.641924	-2.535103
H	-0.434165	1.101776	-3.232662
H	-2.147416	0.703308	-2.961427
H	-0.881827	-0.409272	-2.429134
C	-0.088315	2.291236	2.241783
H	-1.010886	2.123131	2.815396
H	0.284058	3.292080	2.468757
H	0.657454	1.567767	2.573419
C	1.217037	0.061740	0.075077
C	2.052233	0.748679	-0.804467
C	1.737600	-0.982630	0.831915
C	3.384825	0.395849	-0.942093
H	1.656808	1.577406	-1.379961
C	3.072956	-1.340706	0.714407
H	1.095229	-1.519303	1.517059
C	3.868789	-0.646789	-0.174577
H	4.048163	0.914248	-1.620643
H	3.499582	-2.145282	1.297394
F	5.159030	-0.991764	-0.295523

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C	1.668591	3.458166	0.305565
H	1.382881	4.366940	-0.218878
H	1.713991	3.634737	1.378348
C	2.927293	2.787733	-0.239760
H	3.628244	2.507610	0.545366
H	3.430274	3.348789	-1.022756
O	0.651701	2.464191	0.067196
O	2.412565	1.570885	-0.811217
C	1.181909	1.354068	-0.396188
S	1.613596	0.044951	1.727264
C	1.473980	-2.646840	-1.305910
C	1.307092	-3.163958	0.113325
H	0.760169	-3.140466	-1.977593
H	2.482560	-2.818559	-1.690819
H	1.032266	-4.220473	0.127897
H	2.235900	-3.039749	0.690517
N	0.233411	-2.348863	0.644911
N	1.184642	-1.220377	-1.246836
P	0.546130	-0.707914	0.213835
C	1.171189	-0.541016	-2.522876
H	0.773929	-1.221934	-3.282433
H	2.171696	-0.225587	-2.830051
H	0.525232	0.334012	-2.493429
C	0.137810	-2.649784	2.011568

H	0.702736	-2.536958	2.706809
H	0.510424	-3.675407	2.062235
H	0.935786	-1.979576	2.333472
C	1.168645	-0.136461	0.073398
C	1.708352	0.783591	0.963987
C	1.966535	-0.666283	-0.937677
C	3.032028	1.183944	0.844106
H	1.085405	1.183481	1.754180
C	3.286092	-0.267538	-1.077469
H	1.552873	-1.406747	-1.612343
C	3.791794	0.653918	-0.179222
H	3.477982	1.892902	1.528104
H	3.924908	-0.661377	-1.856027
F	5.070586	1.040520	-0.304199

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C	-2.653766	-1.512789	-0.489017
C	-2.078448	-1.773945	0.896024
H	-2.729992	-2.427692	-1.079447
H	-3.651462	-1.062333	-0.409828
H	-1.283292	-2.531992	0.852247
H	-2.843318	-2.121485	1.593520
N	-1.565754	-0.483394	1.318991
N	-1.711313	-0.590958	-1.114210
P	-1.035668	0.441801	0.026714
C	-2.090774	-0.064688	-2.413023
H	-2.214337	-0.892191	-3.113175
H	-3.022651	0.508863	-2.364524
H	-1.306961	0.591918	-2.788290
C	-0.915538	-0.394095	2.607517
H	-1.604985	-0.716253	3.389422
H	-0.010044	-1.012046	2.658098
H	-0.643092	0.643491	2.803256
C	0.759824	0.203316	-0.109037
C	1.642289	1.235962	0.197240
C	1.268379	-1.050531	-0.450644
C	3.012710	1.026328	0.170635
H	1.243863	2.211431	0.446384
C	2.635033	-1.275485	-0.483909
H	0.587297	-1.849403	-0.715317
C	3.480998	-0.228060	-0.168765
H	3.715869	1.814869	0.400805
H	3.051960	-2.235759	-0.754746
F	4.802868	-0.437545	-0.201762
S	-1.525276	2.307116	0.032572

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C	-3.166001	-0.959417	1.033285
C	-2.545839	0.304272	1.611505
H	-2.917777	-1.844772	1.626874
H	-4.259185	-0.858228	1.012912
H	-1.535685	0.105047	2.000412
H	-3.148464	0.714210	2.425441
N	-2.513939	1.232644	0.491068
N	-2.655811	-1.076142	-0.330699
P	-1.976782	0.381391	-0.911619
C	-3.464074	-1.893408	-1.212041
H	-3.492208	-2.922303	-0.844532
H	-4.498172	-1.529676	-1.285919
H	-3.031549	-1.907904	-2.211265
C	-1.908293	2.514581	0.783069
H	-2.480142	3.019862	1.564364
H	-0.866287	2.422148	1.121352
H	-1.923866	3.141076	-0.110171
C	-0.191447	0.119687	-0.551239
C	0.712215	1.070149	-1.023142
C	0.330839	-0.951553	0.170489
C	2.068900	0.987397	-0.763395
H	0.347521	1.900118	-1.621788
C	1.684625	-1.060725	0.434860
H	-0.340571	-1.730727	0.513039
C	2.589459	-0.079992	-0.010783
H	2.723525	1.749023	-1.160146
H	2.038894	-1.918791	0.986896
N	3.936852	-0.165649	0.274616
C	4.853332	0.722289	-0.404321
H	4.632724	1.764668	-0.166854
H	5.865243	0.514305	-0.066141
H	4.819621	0.606663	-1.494983
C	4.458123	-1.394601	0.829096
H	4.007015	-1.605744	1.800443
H	4.280758	-2.258238	0.175884
H	5.529589	-1.289651	0.979284

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C	4.046195	-0.823155	0.741300
H	4.182033	0.236358	0.963106
H	5.015881	-1.313736	0.668289

C	3.101632	-1.499561	1.743274
H	3.583971	-2.260508	2.352597
H	2.613528	-0.765495	2.388471
O	3.381916	-0.972184	-0.508409
O	2.138156	-2.136977	0.920642
C	2.134903	-1.524698	-0.306921
S	1.294734	-2.215395	-1.590338
C	2.154113	2.645893	-0.673836
C	1.567938	2.870661	0.708353
H	2.003483	3.508665	-1.326497
H	3.232694	2.445567	-0.610438
H	0.598173	3.383859	0.633341
H	2.225533	3.464690	1.346718
N	1.414177	1.527807	1.250900
N	1.423889	1.501773	-1.199631
P	1.025333	0.403789	0.016200
C	1.753171	1.087670	-2.554376
H	1.035190	0.346770	-2.898307
H	1.702063	1.965035	-3.202583
H	2.750899	0.643013	-2.622492
C	0.700892	1.431578	2.508770
H	0.607033	0.385362	2.806205
H	1.251516	1.962044	3.288093
H	0.311697	1.850120	2.441281
C	0.762965	0.203942	-0.040760
C	1.325555	-0.969911	0.460750
C	1.616734	1.207763	-0.492254
C	2.694212	-1.132993	0.527651
H	0.675903	-1.779947	0.774475
C	2.989185	1.060261	-0.433555
H	1.195519	2.111096	-0.918083
C	3.564324	-0.115108	0.089167
H	3.088343	-2.064832	0.903833
H	3.615729	1.856186	-0.807320
N	4.926232	-0.266536	0.162184
C	5.480731	-1.549735	0.533891
H	5.165232	-1.836551	1.539360
H	6.565192	-1.481521	0.532543
H	5.181793	-2.345536	-0.157625
C	5.786490	0.718712	-0.453536
H	5.639842	1.703245	-0.003718
H	5.610733	0.806513	-1.531967
H	6.823050	0.433146	-0.296441

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C	-2.596549	-2.737857	-1.034757
H	-2.627270	-2.989977	-2.093787
H	-2.481798	-3.643123	-0.437187
C	-3.812130	-1.908549	-0.563893
H	-4.296556	-2.372975	0.296078
H	-4.541649	-1.721568	-1.350274
O	-1.490345	-1.869247	-0.826975
O	-3.244140	-0.661696	-0.188829
C	-1.910748	-0.978457	0.203515
S	-1.683563	-1.525818	1.867581
C	-2.438412	2.393305	-0.949844
C	-2.131627	2.835117	0.480416
H	-2.444080	3.237914	-1.640804
H	-3.408276	1.886026	-0.996760
H	-1.493032	3.725857	0.493327
H	-3.049072	3.060377	1.028222
N	-1.433356	1.718999	1.103373
N	-1.360304	1.471040	-1.305420
P	-0.962086	0.565897	0.043954
C	-1.483590	0.810771	-2.595734
H	-0.652801	0.119306	-2.733007
H	-1.447080	1.563479	-3.384842
H	-2.419512	0.247778	-2.673847
C	-1.124681	1.788019	2.517172
H	-0.408609	1.011766	2.775027
H	-2.021190	1.623439	3.117331
H	-0.701868	2.770802	2.746642
C	0.777824	0.233988	0.024053
C	1.332020	-1.028122	0.248500
C	1.631712	1.303436	-0.255112
C	2.696900	-1.211689	0.193311
H	0.682374	-1.860153	0.486704
C	2.997984	1.132560	-0.306590
H	1.214181	2.286019	-0.443712
C	3.568843	-0.138300	-0.082711
H	3.090163	-2.200161	0.375911
H	3.623624	1.985243	-0.522608
N	4.921038	-0.321392	-0.131979
C	5.794291	0.802002	-0.387338
H	6.825310	0.460213	-0.382045
H	5.591371	1.254186	-1.362565
H	5.687890	1.578064	0.376953
C	5.482953	-1.629869	0.122870

H	5.236438	-1.985924	1.127566
H	5.120827	-2.367794	-0.598333
H	6.564406	-1.575278	0.036876

TS2-P13

C	-3.593575	-2.424956	-0.635768
H	-4.167843	-2.614872	-1.540147
H	-4.211429	-2.619544	0.243286
C	-2.261389	-3.204816	-0.571098
H	-2.195851	-3.806003	0.337946
H	-2.077872	-3.831624	-1.441242
O	-3.183564	-1.063470	-0.653144
O	-1.272560	-2.180006	-0.553728
C	-1.930538	-1.056781	-0.048597
S	-1.916544	-0.865270	1.773218
C	-2.115732	2.958993	0.289910
C	-1.781604	2.736903	-1.178832
H	-1.873940	3.972254	0.614575
H	-3.182079	2.778032	0.480122
H	-0.895821	3.321346	-1.468373
H	-2.608178	3.027773	-1.832374
N	-1.542525	1.319495	-1.262759
N	-1.277460	2.004251	0.993386
P	-1.097847	0.537016	0.162698
C	-1.257234	2.086313	2.433975
H	-1.020907	3.112208	2.721922
H	-2.215341	1.797901	2.880986
H	-0.482915	1.432104	2.831088
C	-1.366411	0.710105	-2.556611
H	-2.248167	0.873721	-3.181352
H	-0.487070	1.113165	-3.074826
H	-1.226294	-0.364839	-2.439778
C	0.669659	0.191098	0.136807
C	1.269791	-0.951495	0.657680
C	1.488856	1.136617	-0.478258
C	2.634379	-1.147365	0.563612
H	0.658757	-1.694909	1.151078
C	2.854595	0.957122	-0.579768
H	1.049896	2.043286	-0.879230
C	3.464361	-0.202811	-0.067148
H	3.055405	-2.045515	0.989861
H	3.446029	1.723791	-1.057321
N	4.819713	-0.404913	-0.180129
C	5.658539	0.669740	-0.659294
H	6.692190	0.334503	-0.674225
H	5.386547	0.954787	-1.678048
H	5.592663	1.563047	-0.026606
C	5.431110	-1.513557	0.517439
H	6.499106	-1.514287	0.316225
H	5.281888	-1.455947	1.602199
H	5.025697	-2.465972	0.169448

IN2-P13

C	-2.051526	3.350236	0.265341
H	-1.751595	4.108027	0.985848
H	-2.067681	3.780565	-0.738377
C	-3.389933	2.659774	0.605119
H	-4.100496	2.736385	-0.220676
H	-3.849915	3.023403	1.521576
O	-1.103958	2.288161	0.323598
O	-3.022654	1.299599	0.804194
C	-1.832857	1.131460	0.118566
S	-2.064438	0.647458	-1.685365
C	-2.031858	-2.686747	1.134828
C	-2.128367	-2.967657	-0.356743
H	-1.229066	-3.284028	1.588986
H	-2.965080	-2.910545	1.658196
H	-1.921436	-4.013974	-0.589874
H	-3.133056	-2.721842	-0.734296
N	-1.112303	-2.108575	-0.925984
N	-1.734608	-1.274959	1.212056
P	-1.126300	-0.549162	-0.170534
C	-1.672737	-0.673596	2.522593
H	-0.971746	-1.223552	3.161358
H	-2.656141	-0.669736	2.999219
H	-1.326305	0.355736	2.447632
C	-0.954945	-2.183259	-2.356832
H	-1.864103	-1.880619	-2.895766
H	-0.707205	-3.207916	-2.641534
H	-0.137342	-1.534338	-2.672939
C	0.650089	-0.221702	-0.118227
C	1.443919	-1.077469	0.642363
C	1.274150	0.829602	-0.780574
C	2.807131	-0.886645	0.760569
H	0.986444	-1.923292	1.143468
C	2.639540	1.028141	-0.683146
H	0.684117	1.501914	-1.389453
C	3.441347	0.184572	0.105092

H	3.378801	-1.580101	1.358907
H	3.080471	1.849438	-1.227794
N	4.796892	0.397319	0.231593
C	5.612092	-0.616447	0.861172
H	5.309381	-0.771864	1.898675
H	6.647912	-0.287151	0.865509
H	5.555899	-1.581067	0.341644
C	5.439145	1.366912	-0.626644
H	5.032834	2.366136	-0.458092
H	5.322147	1.126538	-1.690562
H	6.500579	1.398363	-0.394648

TS3-P13

C	1.714005	3.629639	0.156421
H	1.279419	4.491732	-0.343964
H	1.798092	3.810585	1.226683
C	3.020511	3.135978	-0.462556
H	3.808048	2.996918	0.276850
H	3.376856	3.737619	-1.294844
O	0.829968	2.508470	-0.029582
O	2.661816	1.835998	-0.962124
C	1.495663	1.461181	-0.471294
S	2.197178	0.346319	1.658216
C	2.371176	-2.459972	-1.261088
C	2.360805	-2.929459	0.184564
H	1.718831	-3.097544	-1.871915
H	3.374836	-2.481132	-1.694328
H	2.274800	-4.015816	0.254941
H	3.279541	-2.620556	0.706470
N	1.187107	-2.286057	0.737057
N	1.850197	-1.101263	-1.240838
P	1.190581	-0.635038	0.228733
C	1.636828	-0.502404	-2.538257
H	1.283953	-1.271234	-3.233875
H	2.553970	-0.064952	-2.942193
H	0.875349	0.273040	-2.487719
C	0.927996	-2.582048	2.129450
H	1.764538	-2.298532	2.779971
H	0.736780	-3.652384	2.238065
H	0.041605	-2.039915	2.461251
C	0.589942	-0.357329	0.159440
C	1.241634	0.530370	1.005823
C	1.351701	-1.076960	-0.756259
C	2.613351	0.702062	0.941745
H	0.662593	1.093907	1.727148
C	2.720737	-0.908190	-0.841947
H	0.863740	-1.790643	-1.411053
C	3.390060	-0.017012	0.017127
H	3.078954	1.400720	1.620589
H	3.270151	-1.480255	-1.574548
N	4.759770	0.135551	-0.039293
C	5.375942	1.213003	0.700916
H	5.210759	1.094328	1.773658
H	6.448953	1.194538	0.528297
H	4.992094	2.197135	0.404493
C	5.486480	-0.448976	-1.143108
H	5.143720	-0.073967	-2.115625
H	6.542700	-0.215492	-1.036519
H	5.386349	-1.536283	-1.144979

PS13

C	-3.268519	-1.578302	-0.464639
C	-2.742839	-1.759384	0.952176
H	-3.329431	-2.525980	-1.003140
H	-4.266435	-1.120435	-0.446199
H	-1.945558	-2.516459	0.976972
H	-3.531486	-2.071145	1.640652
N	-2.246991	-0.446466	1.318659
N	-2.297348	-0.700508	-1.105937
P	-1.694507	0.424877	-0.005695
C	-2.618137	-0.262369	-2.451330
H	-2.718256	-1.135038	-3.098769
H	-3.546431	0.318894	-2.482708
H	-1.813000	0.362913	-2.835637
C	-1.628369	-0.286095	2.614642
H	-2.333251	-0.572900	3.397068
H	-0.718889	-0.891976	2.717606
H	-1.366699	0.762141	2.762658
C	0.098754	0.264671	-0.073882
C	0.939179	1.358801	0.113195
C	0.685975	-0.988998	-0.250495
C	2.313151	1.215078	0.133335
H	0.498968	2.341007	0.234555
C	2.056764	-1.151868	-0.234332
H	0.055235	-1.851842	-0.429214
C	2.910205	-0.048957	-0.030747
H	2.924316	2.094288	0.271445
H	2.466076	-2.138668	-0.390998

N	4.273084	-0.202358	0.002394	H	4.519144	-2.256458	0.375790
C	5.120848	0.967662	0.054462	H	4.604456	-1.809799	-1.336880
H	4.933650	1.548712	0.960378	H	5.937154	-1.414418	-0.240856
H	6.160710	0.652901	0.069801	S	-2.282584	2.262451	-0.125266
H	4.970494	1.625383	-0.809158				
C	4.855817	-1.484932	-0.320633				

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