

Supporting Information

Dynamically or Kinetically Controlled? Computational Study of the Mechanisms of Electrophilic Aminoalkenylation of Heteroaromatics with Keteniminium Ions

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S1. Detailed Molecular Dynamics Simulation Methods

Molecular dynamics simulations were performed at the SMD(DCM)¹/ ω B97X-D²/def2-SVP³ or SMD(Et₂O)/ ω B97X-D/def2-SVP level of theory and the temperature was set to be 238.15 K or 298.15 K (as indicated in Table S1). As shown in Figure S1, QCTs were initiated from the region of corresponding transition states and propagated forward and backward until either one of the products (the forming bond *Bond1* or *Bond2* is less than 1.6 Å, the other bond is larger than 2.2 Å) is formed or the reactants (both distance of *Bond1* and *Bond2* is larger than 3.0 Å) are generated. The classical equations of motion were integrated with a velocity-Verlet algorithm using Singleton's program ProgDyn,⁴ with the energies and derivatives computed on the fly with SMD(DCM)/ ω B97X-D/def2-SVP or SMD(Et₂O)/ ω B97X-D/def2-SVP (as indicated in Table S1) using Gaussian 09.⁵ A QM-like gaussian distribution of displacements of normal modes was used. The step length for integration was 1 fs.

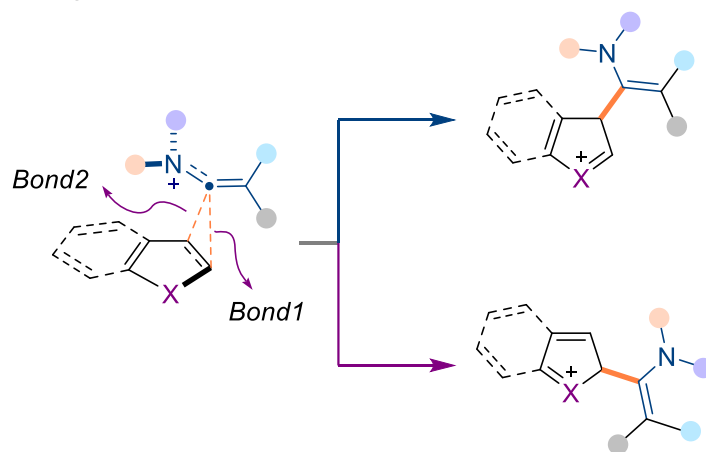


Figure S1. Molecular dynamic simulations of electrophilic addition reactions.

S2. More Discussions

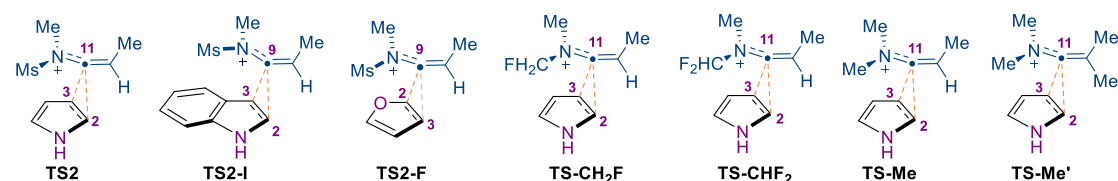
S2.1. Temperature Effects in Dynamically Controlled Electrophilic Additions

Temperature was also found to have an influence on the reaction selectivity for dynamically controlled electrophilic addition of keteniminium ions to pyrrole. For example, the ratio of **C2-Pro**/**C3-Pro** was predicted to be 3.5 for addition of **IN1** to pyrrole at 238.15 K by quasi-classical trajectories (QCT) molecular dynamics simulations (Table S1). While it becomes 2.8 at 298.15 K (Table S1), a little smaller than that at 238.15 K, which means lower temperature can make the regio-selectivity better, just similar to other kinetic controlled reactions.

S2.2. Solvent Effects in Dynamically Controlled Electrophilic Additions

It was also discovered that solvent plays a role in controlling reaction selectivity for dynamically controlled electrophilic addition of keteniminium ions to pyrrole. As indicated in Table S1, QCTs initiated from **TS-Me'** in DCM shows better regio-selectivity than that in ethyl ether.

Table S1. Molecular Dynamics Simulation Trajectories Initiated from Different Transition States^a



TS	Temperature	Solvent	Total	C2P	C3P	Recross	Ratio
TS2	238.15 K	DCM	331	199	57	75	3.5
TS2	298.15 K	DCM	183	111	39	33	2.8
TS2-I	238.15 K	DCM	102	2	90	10	0.02
TS2-F	238.15 K	DCM	150	130	0	20	-
TS-CHF₂	298.15 K	DCM	310	157	54	99	2.9
TS-CH₂F	298.15 K	DCM	283	197	71	15	2.8
TS-Me	298.15 K	DCM	245	218	14	14	15.6
TS-Me'	298.15 K	DCM	192	183	5	4	36.6
TS-Me'	298.15 K	Et ₂ O	144	132	7	5	18.9

^aTS, transition state initiated from; Temperature, simulation temperature; Solvent, simulation solvent; Total, total trajectories simulated; **C2P**, trajectories leading to C2 functionalized product; **C3P**, trajectories leading to C3 functionalized product; Recross, trajectories recross to give starting materials or products; Ratio, **C2P/C3P**.

S2.3. [2 + 2] Cycloaddition Pathways

After electrophilic addition, the generated **IN2** and **IN3** may undergo [2 + 2] cycloaddition to give 5/4 fused bicycles. To test the possibility, we also calculated these pathways, as shown in Figure S1. As for **IN2**, the [2 + 2] cycloaddition pathway via **TS8-endo** and **TS8-exo** has an activation free energy of 41.2 and 44.9 kcal/mol, respectively, which indicate these pathways are impossible under experimental conditions. Besides, these pathways generating **IN7-trans** and **IN7-cis** are endergonic

by 24.5 and 21.8 kcal/mol, respectively, as a result of dearomatization. Similar result was found in the [2 + 2] pathways of **IN3**, which are both kinetically and thermodynamically disfavored. Thus, by considering the kinetics and thermodynamics, we can conclude [2 + 2] pathways are disfavored.

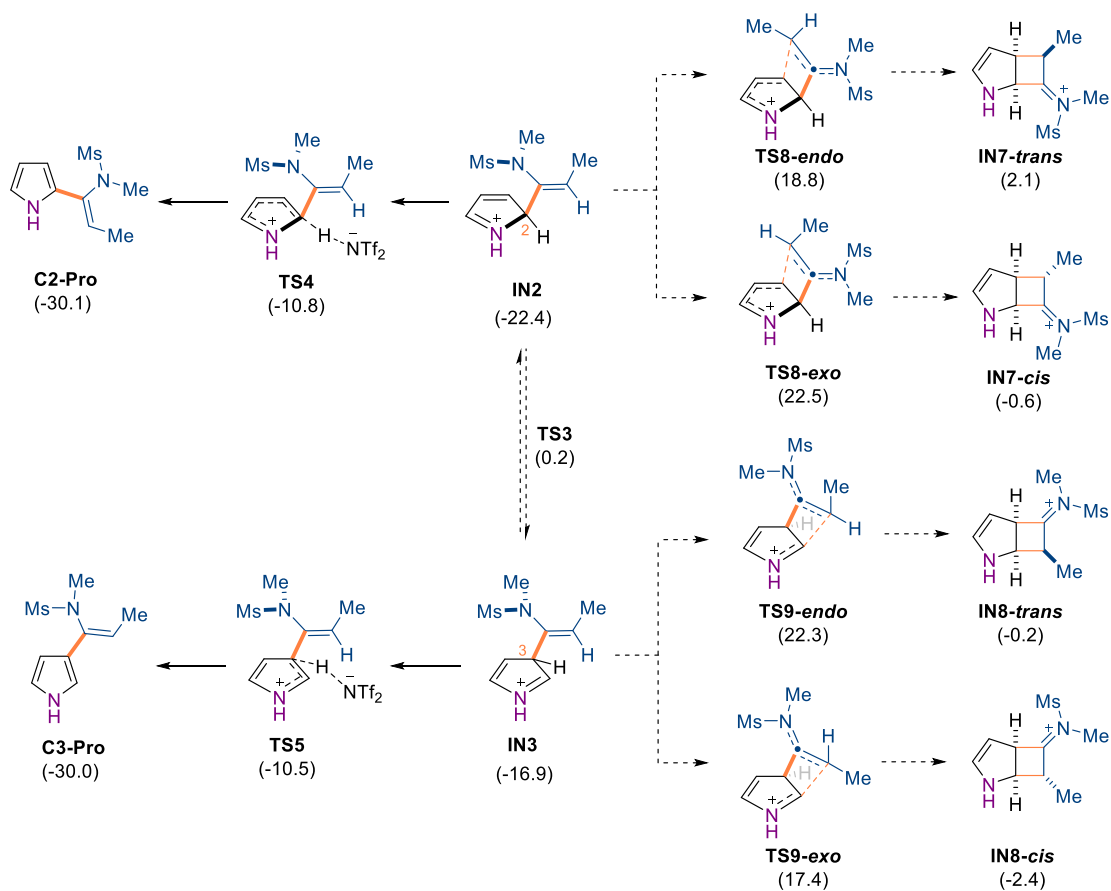


Figure S2. [2 + 2] cycloaddition pathways of **IN2** and **IN3**.

S2.4. IRC of Key Transition States

Intrinsic reaction coordinate (IRC) for different electrophilic transition states have been calculated and given in Figure S3. IRC along **TS2** (electrophilic addition of **Ket3** to pyrrole) leading to **IN2** is the very flat. IRC along **TS2-F** (electrophilic addition of **Ket3** to furan) leading to **IN2-F** is steeper than the other two.

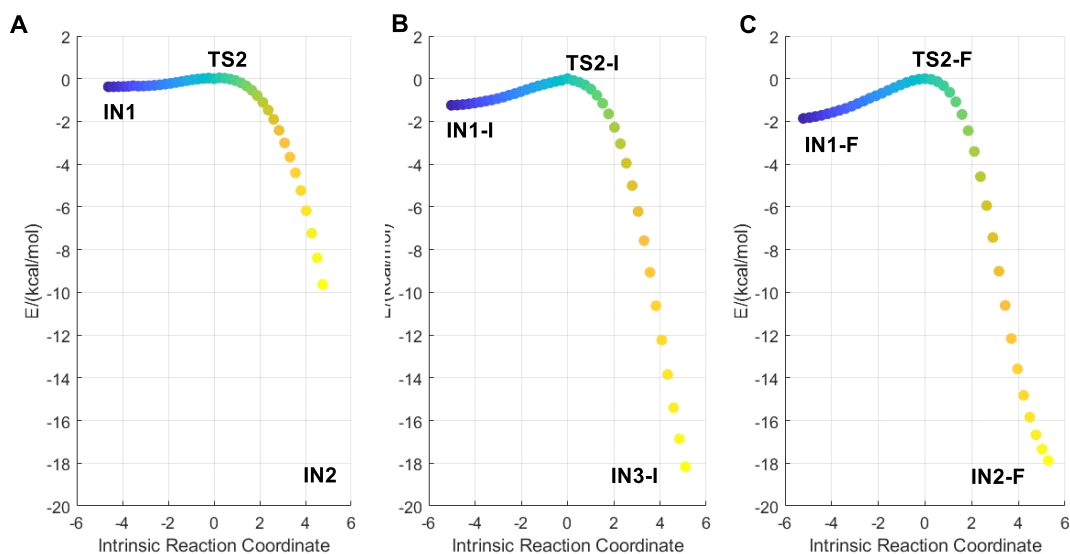


Figure S3. Intrinsic reaction coordinate (IRC) along **TS2** (A), **TS2-I** (B), and **TS2-F** (C).

S2.5. Comparison on Gibbs Free Energies Calculated by DLPNO-CCSD(T) and ω B97X-D Methods

Previously, our benchmark study⁶ has found that ω B97X-D is a good functional for calculating both the kinetics and thermodynamics data of keteniminium ions related reactions. We further evaluated the accuracy of ω B97X-D for geometry optimization and molecular dynamics study in the present work. As indicated in Figure S4, ω B97X-D and DLPNO-CCSD(T) show very negligible difference. For example, DLPNO-CCSD(T) and ω B97X-D have only 0.4 kcal/mol difference for **TS2** (def2-TZVPP basis set was used). The computed thermodynamics is also quite close. Besides, the Gibbs energy profile computed at SMD(DCM)/ ω B97X-D/def2-SVP level is also like those computed by ω B97X-D and DLPNO-CCSD(T) with a larger basis set. Thus, we can conclude ω B97X-D is a good functional for computational study of the present work.

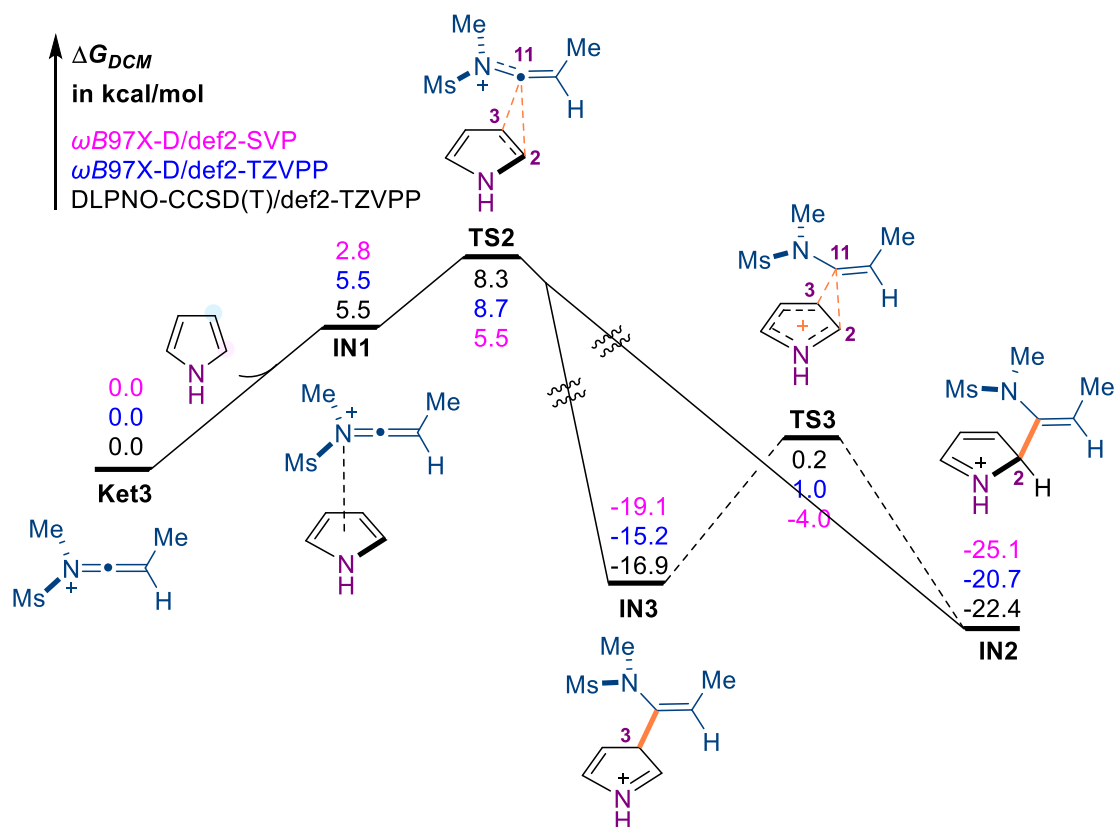


Figure S4. Comparison of Gibbs free energies calculated by DLPNO-CCSD(T) and $\omega B97X-D$ methods using electrophilic addition of **Ket3** to pyrroles as an example. Computed at SMD(DCM)/ $\omega B97X-D/def2-SVP$ (labelled in magenta), SMD(DCM)/ $\omega B97X-D/def2-TZVPP$ //SMD(DCM)/ $\omega B97X-D/def2-SVP$ (labelled in blue) and DLPNO-CCSD(T)/def2-TZVPP:SMD(DCM)//SMD(DCM)/ $\omega B97X-D/def2-SVP$ level (labelled in black).

S3. Computed Energies of Potential Energy Surface Scan

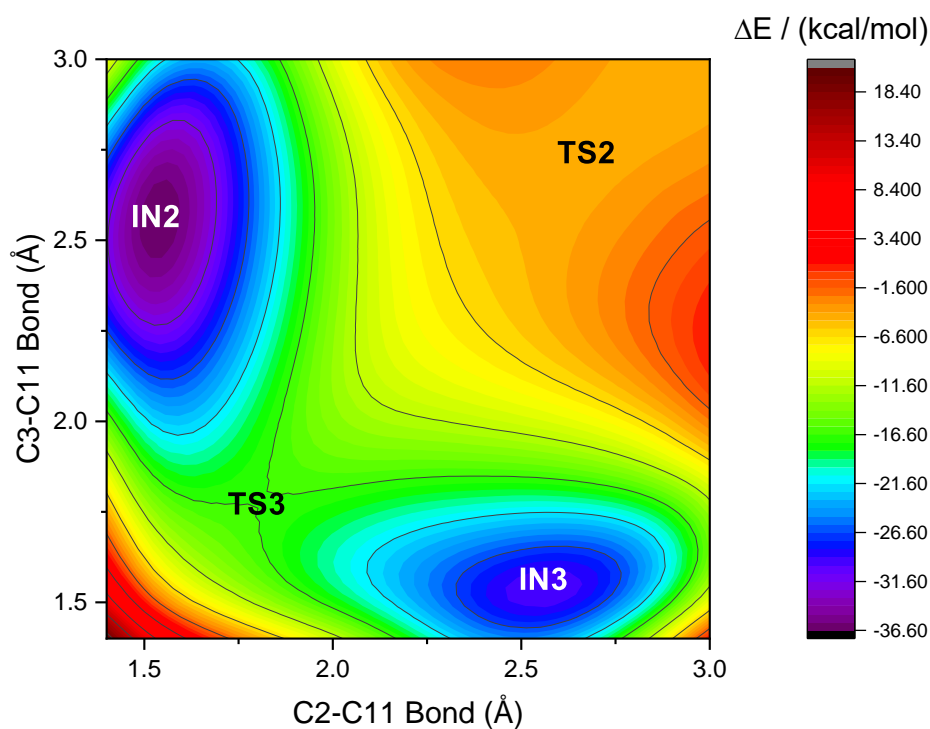
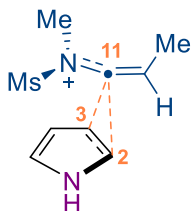


Figure S5. Potential energy surface of electrophilic addition of **Ket3** to pyrrole.

Table S2. Relaxed Potential Energy Surface Scan for Electrophilic Addition of Ket3 to Pyrrole



C2-C11 (Å)	C3-C11 (Å)	<i>E</i> (a.u.)	C2-C11 (Å)	C3-C11 (Å)	<i>E</i> (a.u.)	C2-C11 (Å)	C3-C11 (Å)	<i>E</i> (a.u.)
3.0	3.0	-1009.070489	2.9	3.0	-1009.070373	2.8	3.0	-1009.069862
3.0	2.9	-1009.070077	2.9	2.9	-1009.070255	2.8	2.9	-1009.070109
3.0	2.8	-1009.069255	2.9	2.8	-1009.069725	2.8	2.8	-1009.069999
3.0	2.7	-1009.067961	2.9	2.7	-1009.068853	2.8	2.7	-1009.069528
3.0	2.6	-1009.066308	2.9	2.6	-1009.067002	2.8	2.6	-1009.068616
3.0	2.5	-1009.064434	2.9	2.5	-1009.066125	2.8	2.5	-1009.067470
3.0	2.4	-1009.062937	2.9	2.4	-1009.064790	2.8	2.4	-1009.066644
3.0	2.3	-1009.062045	2.9	2.3	-1009.064037	2.8	2.3	-1009.066233
3.0	2.2	-1009.061690	2.9	2.2	-1009.064507	2.8	2.2	-1009.067085
3.0	2.1	-1009.062905	2.9	2.1	-1009.066593	2.8	2.1	-1009.069558
3.0	2.0	-1009.066590	2.9	2.0	-1009.071142	2.8	2.0	-1009.074038

3.0	1.9	-1009.072470	2.9	1.9	-1009.076744	2.8	1.9	-1009.080799
3.0	1.8	-1009.080651	2.9	1.8	-1009.086335	2.8	1.8	-1009.089775
3.0	1.7	-1009.085666	2.9	1.7	-1009.093329	2.8	1.7	-1009.098359
3.0	1.6	-1009.085757	2.9	1.6	-1009.096200	2.8	1.6	-1009.103411
3.0	1.5	-1009.077684	2.9	1.5	-1009.090682	2.8	1.5	-1009.100881
3.0	1.4	-1009.058116	2.9	1.4	-1009.072431	2.8	1.4	-1009.085063
2.7	3.0	-1009.069155	2.6	3.0	-1009.068163	2.5	3.0	-1009.067250
2.7	2.9	-1009.069667	2.6	2.9	-1009.069080	2.5	2.9	-1009.068445
2.7	2.8	-1009.069955	2.6	2.8	-1009.069639	2.5	2.8	-1009.069402
2.7	2.7	-1009.069943	2.6	2.7	-1009.069979	2.5	2.7	-1009.070003
2.7	2.6	-1009.069515	2.6	2.6	-1009.070087	2.5	2.6	-1009.070434
2.7	2.5	-1009.068805	2.6	2.5	-1009.069911	2.5	2.5	-1009.070724
2.7	2.4	-1009.068276	2.6	2.4	-1009.069720	2.5	2.4	-1009.070975
2.7	2.3	-1009.068209	2.6	2.3	-1009.069941	2.5	2.3	-1009.071464
2.7	2.2	-1009.069239	2.6	2.2	-1009.071077	2.5	2.2	-1009.072704
2.7	2.1	-1009.071851	2.6	2.1	-1009.073668	2.5	2.1	-1009.075207
2.7	2.0	-1009.076493	2.6	2.0	-1009.078222	2.5	2.0	-1009.079467
2.7	1.9	-1009.083122	2.6	1.9	-1009.084640	2.5	1.9	-1009.085498
2.7	1.8	-1009.091493	2.6	1.8	-1009.092592	2.5	1.8	-1009.092904
2.7	1.7	-1009.100798	2.6	1.7	-1009.101291	2.5	1.7	-1009.100923
2.7	1.6	-1009.107572	2.6	1.6	-1009.108761	2.5	1.6	-1009.107943
2.7	1.5	-1009.107368	2.6	1.5	-1009.110526	2.5	1.5	-1009.110577
2.7	1.4	-1009.094706	2.6	1.4	-1009.100576	2.5	1.4	-1009.102223
2.4	3.0	-1009.067116	2.3	3.0	-1009.067382	2.2	3.0	-1009.068988
2.4	2.9	-1009.068468	2.3	2.9	-1009.069290	2.2	2.9	-1009.071351
2.4	2.8	-1009.069594	2.3	2.8	-1009.070713	2.2	2.8	-1009.073080
2.4	2.7	-1009.070469	2.3	2.7	-1009.071706	2.2	2.7	-1009.074314
2.4	2.6	-1009.071049	2.3	2.6	-1009.072439	2.2	2.6	-1009.074972
2.4	2.5	-1009.071611	2.3	2.5	-1009.073025	2.2	2.5	-1009.075511
2.4	2.4	-1009.072173	2.3	2.4	-1009.073629	2.2	2.4	-1009.075941
2.4	2.3	-1009.072888	2.3	2.3	-1009.074391	2.2	2.3	-1009.076379
2.4	2.2	-1009.074173	2.3	2.2	-1009.075646	2.2	2.2	-1009.077354
2.4	2.1	-1009.076538	2.3	2.1	-1009.077760	2.2	2.1	-1009.079091
2.4	2.0	-1009.080466	2.3	2.0	-1009.081353	2.2	2.0	-1009.082067
2.4	1.9	-1009.085985	2.3	1.9	-1009.086283	2.2	1.9	-1009.086413
2.4	1.8	-1009.092646	2.3	1.8	-1009.092258	2.2	1.8	-1009.091633
2.4	1.7	-1009.099794	2.3	1.7	-1009.098379	2.2	1.7	-1009.096846
2.4	1.6	-1009.105921	2.3	1.6	-1009.103228	2.2	1.6	-1009.100467
2.4	1.5	-1009.108051	2.3	1.5	-1009.104233	2.2	1.5	-1009.099883
2.4	1.4	-1009.100924	2.3	1.4	-1009.096511	2.2	1.4	-1009.090800
2.1	3.0	-1009.072490	2.0	3.0	-1009.078191	1.9	3.0	-1009.085968
2.1	2.9	-1009.075264	2.0	2.9	-1009.081331	1.9	2.9	-1009.089185
2.1	2.8	-1009.077235	2.0	2.8	-1009.083550	1.9	2.8	-1009.091667

2.1	2.7	-1009.078609	2.0	2.7	-1009.085026	1.9	2.7	-1009.093237
2.1	2.6	-1009.079326	2.0	2.6	-1009.085613	1.9	2.6	-1009.093705
2.1	2.5	-1009.079502	2.0	2.5	-1009.085552	1.9	2.5	-1009.093430
2.1	2.4	-1009.079627	2.0	2.4	-1009.085145	1.9	2.4	-1009.092459
2.1	2.3	-1009.079631	2.0	2.3	-1009.084580	1.9	2.3	-1009.091202
2.1	2.2	-1009.079852	2.0	2.2	-1009.084009	1.9	2.2	-1009.089759
2.1	2.1	-1009.080809	2.0	2.1	-1009.083825	1.9	2.1	-1009.088370
2.1	2.0	-1009.082990	2.0	2.0	-1009.084659	1.9	2.0	-1009.087611
2.1	1.9	-1009.086366	2.0	1.9	-1009.086765	1.9	1.9	-1009.087918
2.1	1.8	-1009.090662	2.0	1.8	-1009.089773	1.9	1.8	-1009.089217
2.1	1.7	-1009.095008	2.0	1.7	-1009.092980	1.9	1.7	-1009.090922
2.1	1.6	-1009.097657	2.0	1.6	-1009.094669	1.9	1.6	-1009.091456
2.1	1.5	-1009.095719	2.0	1.5	-1009.091662	1.9	1.5	-1009.087569
2.1	1.4	-1009.084714	2.0	1.4	-1009.079142	1.9	1.4	-1009.074136
1.8	3.0	-1009.094105	1.7	3.0	-1009.099797	1.6	3.0	-1009.100313
1.8	2.9	-1009.098251	1.7	2.9	-1009.105987	1.6	2.9	-1009.109154
1.8	2.8	-1009.100876	1.7	2.8	-1009.109727	1.6	2.8	-1009.115037
1.8	2.7	-1009.102497	1.7	2.7	-1009.111753	1.6	2.7	-1009.118385
1.8	2.6	-1009.103057	1.7	2.6	-1009.112332	1.6	2.6	-1009.119583
1.8	2.5	-1009.102417	1.7	2.5	-1009.111589	1.6	2.5	-1009.118987
1.8	2.4	-1009.100983	1.7	2.4	-1009.109692	1.6	2.4	-1009.116738
1.8	2.3	-1009.098946	1.7	2.3	-1009.106829	1.6	2.3	-1009.113289
1.8	2.2	-1009.096582	1.7	2.2	-1009.103511	1.6	2.2	-1009.108867
1.8	2.1	-1009.094029	1.7	2.1	-1009.099833	1.6	2.1	-1009.104043
1.8	2.0	-1009.091717	1.7	2.0	-1009.096210	1.6	2.0	-1009.099249
1.8	1.9	-1009.090096	1.7	1.9	-1009.092717	1.6	1.9	-1009.094383
1.8	1.8	-1009.089306	1.7	1.8	-1009.089680	1.6	1.8	-1009.089578
1.8	1.7	-1009.089009	1.7	1.7	-1009.087336	1.6	1.7	-1009.084845
1.8	1.6	-1009.087900	1.7	1.6	-1009.084243	1.6	1.6	-1009.079819
1.8	1.5	-1009.083075	1.7	1.5	-1009.077985	1.6	1.5	-1009.071837
1.8	1.4	-1009.069086	1.7	1.4	-1009.063336	1.6	1.4	-1009.056336
1.5	3.0	-1009.093036	1.4	3.0	-1009.073947			
1.5	2.9	-1009.104429	1.4	2.9	-1009.087103			
1.5	2.8	-1009.112995	1.4	2.8	-1009.098151			
1.5	2.7	-1009.118440	1.4	2.7	-1009.106251			
1.5	2.6	-1009.120961	1.4	2.6	-1009.111059			
1.5	2.5	-1009.120998	1.4	2.5	-1009.112711			
1.5	2.4	-1009.119010	1.4	2.4	-1009.111488			
1.5	2.3	-1009.115211	1.4	2.3	-1009.107820			
1.5	2.2	-1009.109805	1.4	2.2	-1009.101837			
1.5	2.1	-1009.103675	1.4	2.1	-1009.094159			
1.5	2.0	-1009.097621	1.4	2.0	-1009.086382			
1.5	1.9	-1009.091693	1.4	1.9	-1009.079400			

1.5	1.8	-1009.085677	1.4	1.8	-1009.072626			
1.5	1.7	-1009.079490	1.4	1.7	-1009.065680			
1.5	1.6	-1009.072430	1.4	1.6	-1009.057613			
1.5	1.5	-1009.062897	1.4	1.5	-1009.046685			
1.5	1.4	-1009.046180	1.4	1.4	-1009.028875			

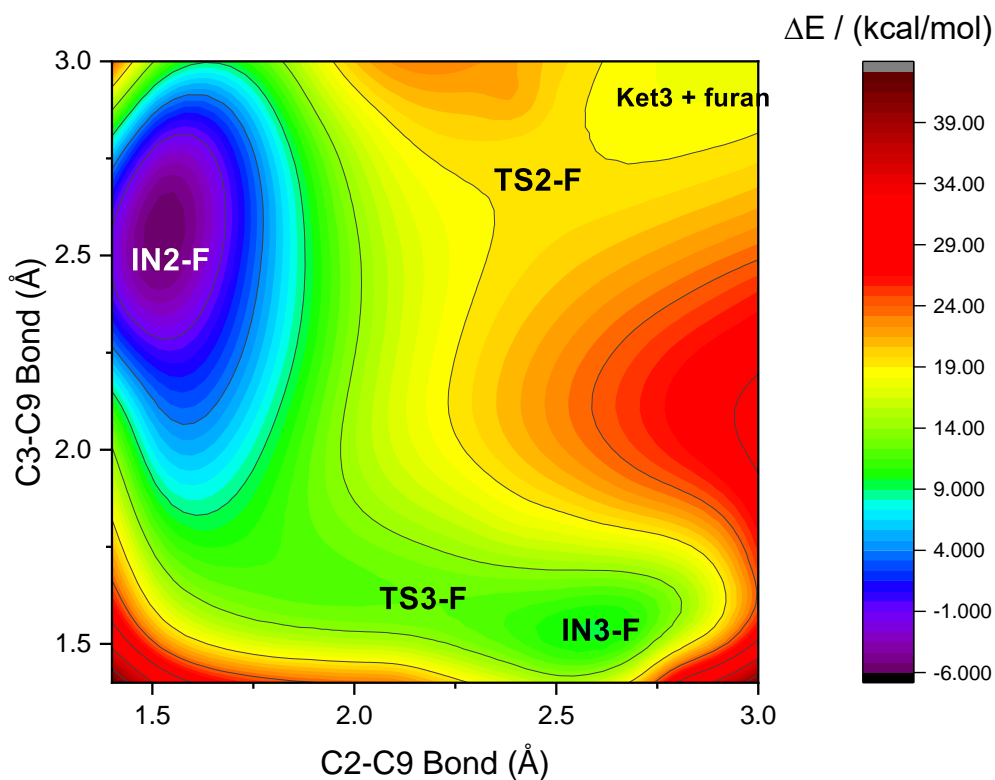
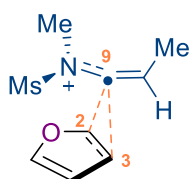


Figure S6. Potential energy surface of electrophilic addition of **Ket3** to furan.

Table S3. Relaxed Potential Energy Surface Scan for Electrophilic Addition of Ket3 to Furan



C2-C9 (Å)	C3-C9 (Å)	<i>E</i> (a.u.)	C2-C9 (Å)	C3-C9 (Å)	<i>E</i> (a.u.)	C2-C9 (Å)	C3-C9 (Å)	<i>E</i> (a.u.)
3.0	3.0	-1028.888387	2.9	3.0	-1028.888356	2.8	3.0	-1028.888053
3.0	2.9	-1028.887536	2.9	2.9	-1028.887747	2.8	2.9	-1028.887731
3.0	2.8	-1028.886164	2.9	2.8	-1028.886642	2.8	2.8	-1028.886911
3.0	2.7	-1028.884261	2.9	2.7	-1028.885038	2.8	2.7	-1028.885620
3.0	2.6	-1028.881855	2.9	2.6	-1028.882860	2.8	2.6	-1028.883782
3.0	2.5	-1028.878811	2.9	2.5	-1028.880173	2.8	2.5	-1028.881473
3.0	2.4	-1028.875375	2.9	2.4	-1028.877135	2.8	2.4	-1028.878795
3.0	2.3	-1028.873228	2.9	2.3	-1028.874614	2.8	2.3	-1028.876260

3.0	2.2	-1028.870511	2.9	2.2	-1028.872472	2.8	2.2	-1028.874375
3.0	2.1	-1028.868959	2.9	2.1	-1028.871414	2.8	2.1	-1028.873770
3.0	2.0	-1028.869165	2.9	2.0	-1028.872440	2.8	2.0	-1028.874840
3.0	1.9	-1028.871568	2.9	1.9	-1028.875617	2.8	1.9	-1028.878337
3.0	1.8	-1028.873867	2.9	1.8	-1028.880739	2.8	1.8	-1028.884053
3.0	1.7	-1028.875711	2.9	1.7	-1028.886069	2.8	1.7	-1028.890838
3.0	1.6	-1028.878360	2.9	1.6	-1028.888435	2.8	1.6	-1028.895088
3.0	1.5	-1028.869452	2.9	1.5	-1028.882315	2.8	1.5	-1028.889382
3.0	1.4	-1028.849668	2.9	1.4	-1028.861180	2.8	1.4	-1028.867406
2.7	3.0	-1028.887323	2.6	3.0	-1028.886193	2.5	3.0	-1028.884498
2.7	2.9	-1028.887379	2.6	2.9	-1028.886631	2.5	2.9	-1028.885647
2.7	2.8	-1028.886979	2.6	2.8	-1028.886216	2.5	2.8	-1028.886141
2.7	2.7	-1028.886020	2.6	2.7	-1028.886178	2.5	2.7	-1028.886165
2.7	2.6	-1028.884554	2.6	2.6	-1028.885157	2.5	2.6	-1028.885550
2.7	2.5	-1028.882612	2.6	2.5	-1028.883692	2.5	2.5	-1028.884624
2.7	2.4	-1028.880382	2.6	2.4	-1028.881865	2.5	2.4	-1028.883368
2.7	2.3	-1028.878081	2.6	2.3	-1028.880066	2.5	2.3	-1028.881953
2.7	2.2	-1028.876482	2.6	2.2	-1028.878608	2.5	2.2	-1028.880823
2.7	2.1	-1028.875876	2.6	2.1	-1028.878110	2.5	2.1	-1028.880418
2.7	2.0	-1028.877088	2.6	2.0	-1028.879333	2.5	2.0	-1028.881488
2.7	1.9	-1028.880155	2.6	1.9	-1028.882301	2.5	1.9	-1028.884206
2.7	1.8	-1028.885759	2.6	1.8	-1028.886937	2.5	1.8	-1028.888577
2.7	1.7	-1028.892920	2.6	1.7	-1028.893508	2.5	1.7	-1028.893673
2.7	1.6	-1028.898745	2.6	1.6	-1028.899581	2.5	1.6	-1028.898555
2.7	1.5	-1028.898346	2.6	1.5	-1028.901013	2.5	1.5	-1028.900664
2.7	1.4	-1028.885430	2.6	1.4	-1028.891005	2.5	1.4	-1028.892585
2.4	3.0	-1028.882581	2.3	3.0	-1028.880918	2.2	3.0	-1028.879982
2.4	2.9	-1028.881224	2.3	2.9	-1028.883195	2.2	2.9	-1028.883095
2.4	2.8	-1028.885551	2.3	2.8	-1028.885067	2.2	2.8	-1028.885336
2.4	2.7	-1028.886069	2.3	2.7	-1028.886183	2.2	2.7	-1028.886965
2.4	2.6	-1028.886108	2.3	2.6	-1028.886719	2.2	2.6	-1028.887939
2.4	2.5	-1028.885650	2.3	2.5	-1028.886766	2.2	2.5	-1028.888394
2.4	2.4	-1028.884818	2.3	2.4	-1028.886343	2.2	2.4	-1028.888321
2.4	2.3	-1028.883788	2.3	2.3	-1028.885681	2.2	2.3	-1028.887902
2.4	2.2	-1028.882957	2.3	2.2	-1028.885070	2.2	2.2	-1028.887403
2.4	2.1	-1028.882673	2.3	2.1	-1028.884880	2.2	2.1	-1028.887134
2.4	2.0	-1028.883578	2.3	2.0	-1028.885766	2.2	2.0	-1028.887940
2.4	1.9	-1028.886018	2.3	1.9	-1028.887993	2.2	1.9	-1028.889901
2.4	1.8	-1028.889059	2.3	1.8	-1028.891213	2.2	1.8	-1028.892706
2.4	1.7	-1028.894297	2.3	1.7	-1028.894785	2.2	1.7	-1028.895545
2.4	1.6	-1028.897917	2.3	1.6	-1028.897305	2.2	1.6	-1028.896907
2.4	1.5	-1028.898135	2.3	1.5	-1028.896162	2.2	1.5	-1028.894243
2.4	1.4	-1028.889633	2.3	1.4	-1028.886898	2.2	1.4	-1028.883159

2.1	3.0	-1028.880514	2.0	3.0	-1028.883495	1.9	3.0	-1028.889160
2.1	2.9	-1028.884408	2.0	2.9	-1028.887811	1.9	2.9	-1028.893126
2.1	2.8	-1028.887150	2.0	2.8	-1028.891105	1.9	2.8	-1028.897095
2.1	2.7	-1028.889034	2.0	2.7	-1028.893134	1.9	2.7	-1028.899370
2.1	2.6	-1028.890265	2.0	2.6	-1028.894382	1.9	2.6	-1028.900368
2.1	2.5	-1028.890933	2.0	2.5	-1028.895067	1.9	2.5	-1028.900832
2.1	2.4	-1028.891072	2.0	2.4	-1028.895153	1.9	2.4	-1028.900763
2.1	2.3	-1028.890744	2.0	2.3	-1028.894783	1.9	2.3	-1028.900076
2.1	2.2	-1028.890221	2.0	2.2	-1028.894059	1.9	2.2	-1028.899034
2.1	2.1	-1028.889833	2.0	2.1	-1028.893342	1.9	2.1	-1028.897787
2.1	2.0	-1028.890261	2.0	2.0	-1028.893140	1.9	2.0	-1028.896795
2.1	1.9	-1028.891745	2.0	1.9	-1028.893933	1.9	1.9	-1028.896514
2.1	1.8	-1028.893973	2.0	1.8	-1028.895400	1.9	1.8	-1028.896998
2.1	1.7	-1028.896271	2.0	1.7	-1028.897083	1.9	1.7	-1028.897711
2.1	1.6	-1028.896926	2.0	1.6	-1028.897093	1.9	1.6	-1028.896962
2.1	1.5	-1028.892967	2.0	1.5	-1028.892469	1.9	1.5	-1028.891596
2.1	1.4	-1028.878671	2.0	1.4	-1028.878835	1.9	1.4	-1028.877895
1.8	3.0	-1028.895835	1.7	3.0	-1028.901108	1.6	3.0	-1028.901605
1.8	2.9	-1028.901256	1.7	2.9	-1028.908490	1.6	2.9	-1028.911809
1.8	2.8	-1028.905023	1.7	2.8	-1028.913343	1.6	2.8	-1028.918747
1.8	2.7	-1028.907219	1.7	2.7	-1028.915935	1.6	2.7	-1028.922698
1.8	2.6	-1028.908106	1.7	2.6	-1028.916663	1.6	2.6	-1028.924075
1.8	2.5	-1028.907924	1.7	2.5	-1028.915824	1.6	2.5	-1028.923173
1.8	2.4	-1028.907350	1.7	2.4	-1028.914317	1.6	2.4	-1028.920589
1.8	2.3	-1028.906331	1.7	2.3	-1028.912575	1.6	2.3	-1028.917365
1.8	2.2	-1028.904815	1.7	2.2	-1028.910507	1.6	2.2	-1028.914279
1.8	2.1	-1028.902922	1.7	2.1	-1028.908068	1.6	2.1	-1028.911318
1.8	2.0	-1028.901113	1.7	2.0	-1028.905422	1.6	2.0	-1028.908099
1.8	1.9	-1028.899592	1.7	1.9	-1028.902813	1.6	1.9	-1028.904634
1.8	1.8	-1028.898689	1.7	1.8	-1028.900423	1.6	1.8	-1028.901060
1.8	1.7	-1028.898123	1.7	1.7	-1028.898256	1.6	1.7	-1028.897425
1.8	1.6	-1028.896398	1.7	1.6	-1028.895309	1.6	1.6	-1028.892857
1.8	1.5	-1028.890855	1.7	1.5	-1028.888835	1.6	1.5	-1028.885280
1.8	1.4	-1028.876668	1.7	1.4	-1028.874400	1.6	1.4	-1028.870399
1.5	3.0	-1028.894671	1.4	3.0	-1028.875962			
1.5	2.9	-1028.907314	1.4	2.9	-1028.890528			
1.5	2.8	-1028.916983	1.4	2.8	-1028.902788			
1.5	2.7	-1028.923265	1.4	2.7	-1028.911895			
1.5	2.6	-1028.925810	1.4	2.6	-1028.917249			
1.5	2.5	-1028.926139	1.4	2.5	-1028.918940			
1.5	2.4	-1028.923482	1.4	2.4	-1028.917177			
1.5	2.3	-1028.918913	1.4	2.3	-1028.912490			
1.5	2.2	-1028.913702	1.4	2.2	-1028.905683			

1.5	2.1	-1028.909588	1.4	2.1	-1028.898244			
1.5	2.0	-1028.905827	1.4	2.0	-1028.893573			
1.5	1.9	-1028.901958	1.4	1.9	-1028.889403			
1.5	1.8	-1028.897680	1.4	1.8	-1028.885090			
1.5	1.7	-1028.892965	1.4	1.7	-1028.880137			
1.5	1.6	-1028.887286	1.4	1.6	-1028.873789			
1.5	1.5	-1028.878426	1.4	1.5	-1028.864468			
1.5	1.4	-1028.862635	1.4	1.4	-1028.847534			

S4. Substitution Effects of Keteniminium Ions

The Figure 6B-E in the main text were drawn based on Table S4.

Table S4. Substitution Effects of Keteniminium Ions for Electrophilic Aminoalkenylation

Ket-R	σ_p of R	LUMO	$\Delta Bond$	P1/P2
Ket-Me	-0.17	-1.84	0.21	15.6
Ket-CH ₂ F	0.11	-2.23	0.09	2.8
Ket-CHF ₂	0.32	-2.36	0.04	2.9
Ket-Ms (Ket3)	0.72	-2.28	0.04	2.8

S5. Computed Energies of the Stationary Points

Table S5. Gibbs Energies, Thermal Corrections to Gibbs Energies (TCGs), and Single-Point Energies (SPEs)

Stationary Point	$G^{a,b}$ (a.u.)	TCG ^{a,b} (a.u.)	SPE ^a (a.u.)	SPE ^c (a.u.)	SPE ^d (a.u.)	SPE ^e (a.u.)
pyrrole	-209.906371	0.057037	-209.963408	-210.191405	-209.951121	-209.795671
Tf ₂ NH	-1826.361306	0.023024	-1826.38433	-1828.02166	-1826.37538	-1825.712948
Tf ₂ N ⁺	-1825.927423	0.012226	-1825.939649	-1827.586427	-1825.878825	-1825.228522
yne-N		0.102569	-798.657688	-799.310227	-798.640419	-798.156088
TS1		0.144938	-2625.049523	-2627.331354	-2625.030233	-2623.87348
Ket3	-798.978909	0.115388	-799.094297	-799.744815	-799.003751	-798.512101
IN1	-1008.877864	0.192784	-1009.070648	-1009.944837	-1008.980895	-1008.329368
TS2	-1008.873512	0.19648	-1009.069992	-1009.943455	-1008.98275	-1008.331115
TS2'		0.195652	-1009.069201	-1009.942301	-1008.981813	-1008.329128
TS3	-1008.888708	0.200484	-1009.089192	-1009.959657	-1008.999941	-1008.346134
IN2	-1008.922259	0.199428	-1009.121687	-1009.993197	-1009.03207	-1008.380647
IN3	-1008.912723	0.198348	-1009.111072	-1009.983303	-1009.019154	-1008.36852
IN4		0.233296	-2835.094924		-2835.056285	-2833.742407
IN5		0.232643	-2835.080933		-2835.034959	-2833.721386
TS4		0.230746	-2835.080186		-2835.050584	-2833.727633
TS5		0.229781	-2835.077321		-2835.042044	-2833.720563
C2-Pro		0.187461	-1008.699297		-1008.677156	-1008.026696
C3-Pro		0.186299	-1008.697063		-1008.672127	-1008.022531
TS6		0.232212	-2835.086209		-2835.063198	-2833.737659
IN6		0.236613	-2835.11784		-2835.08695	-2833.767107
TS7		0.230643	-2835.082784		-2835.06031	-2833.734245
C2-Pro-trans		0.186756	-1008.697039		-1008.672682	-1008.024585
C3-Pro-trans		0.185834	-1008.694199		-1008.669663	-1008.021211
TS8-exo		0.20149	-1009.054528		-1008.966555	-1008.312902
TS8-endo		0.200999	-1009.062235		-1008.974585	-1008.318613
TS9-exo		0.199956	-1009.059268		-1008.970971	-1008.319119
TS9-endo		0.201255	-1009.055535		-1008.967458	-1008.312762
IN7-cis		0.201619	-1009.09209		-1009.003782	-1008.349447
IN7-trans		0.201457	-1009.089376		-1008.998377	-1008.342241
IN8-cis		0.20115	-1009.096652		-1009.007582	-1008.350997
IN8-trans		0.201325	-1009.094203		-1009.004813	-1008.347429
indole		0.101272	-363.45645		-363.439424	-363.15319
IN1-I		0.238397	-1162.565949		-1162.474197	-1161.692268
TS2-I		0.241902	-1162.563986		-1162.476056	-1161.693973

IN2-I		0.242457	-1162.59847		-1162.512675	-1161.731098
IN3-I		0.244529	-1162.615342		-1162.52407	-1161.741652
TS3-I		0.244617	-1162.582956		-1162.493759	-1161.708713
IN4-I		0.276639	-2988.571655		-2988.530922	-2987.086832
IN5-I		0.277411	-2988.588159		-2988.549018	-2987.104117
TS4-I		0.274244	-2988.563742		-2988.530378	-2987.078945
TS5-I		0.275394	-2988.57307		-2988.535425	-2987.083138
C2-Pro-I		0.230987	-1162.191932		-1162.162213	-1161.382337
C3-Pro-I		0.231627	-1162.190219		-1162.161608	-1161.381579
furan		0.044645	-229.784064		-229.778056	-229.637932
IN1-F		0.179081	-1028.88921		-1028.80032	-1028.165196
TS2-F		0.183944	-1028.886084		-1028.800187	-1028.164981
IN2-F		0.187465	-1028.926678		-1028.836677	-1028.200044
IN3-F		0.185837	-1028.901508		-1028.80714	-1028.170542
TS3-F		0.187906	-1028.897685		-1028.805752	-1028.170412
IN4-F		0.218933	-2854.897101		-2854.856034	-2853.557799
IN5-F		0.219046	-2854.874796		-2854.837617	-2853.538508
TS4-F		0.217113	-2854.888373		-2854.855971	-2853.550398
TS5-F		0.220622	-2854.872207		-2854.828178	-2853.528518
C2-Pro-F		0.173427	-1028.520706		-1028.500794	-1027.866211
C3-Pro-F		0.17284	-1028.516929		-1028.49706	-1027.863049
Ket-CHF₂		0.093493	-449.090609			
TS-CHF₂		0.172281	-659.064653			
Ket-CH₂F		0.102345	-349.953015			
TS-CH₂F		0.181462	-559.924705			
Ket-Me		0.111403	-250.830067			
TS-Me		0.191351	-460.795239			
TS-Me' (DCM)		0.218043	-500.075813			
TS-Me' (Et₂O)^f		0.218503	-500.064793			

^aComputed at the SMD(DCM)/ ω B97X-D/def2-SVP level unless otherwise specified.

^bA standard state at 1 atm and 298.15 K was used.

^cComputed at the SMD(DCM)/ ω B97X-D/def2-TZVPP//SMD(DCM)/ ω B97X-D/def2-SVP level.

^dComputed at the ω B97X-D/def2-SVP//SMD(DCM)/ ω B97X-D/def2-SVP level.

^eComputed at the DLPNO-CCSD(T)/def2-TZVPP//SMD(DCM)/ ω B97X-D/def2-SVP level.

^fComputed at SMD(Et₂O)/ ω B97X-D/def2-SVP level.

Table S6. Thermal Corrections to Gibbs Energies (TCGs) and Single-Point Energies (SPEs) for Full Model

Stationary Point	TCG^{a,b} (a.u.)	SPE^a (a.u.)	SPE^c (a.u.)	SPE^d (a.u.)
TS2-Full	0.483024	-1555.544441	-1555.457249	-1552.895273
TS2'-Full	0.481934	-1555.541147	-1555.454392	-1552.892917

^aComputed at the SMD(DCM)/ ω B97X-D/def2-TZVP level.

^bA standard state at 1 atm and 298.15 K was used.

^cComputed at the ω B97X-D/def2-TZVP//SMD(DCM)/ ω B97X-D/def2-TZVP level.

^dComputed at the DLPNO-CCSD(T)/def2-TZVPP//SMD(DCM)/ ω B97X-D/def2-TZVP level.

S6. Cartesian Coordinates of the Stationary Points

pyrrole			F	-2.898613	0.810758	-1.144251	
C	0.335153	-1.119274	-0.000031	O	-0.845332	-1.249008	1.264615
C	-0.984543	-0.712991	-0.000139	O	-1.654357	-1.837619	-1.034476
C	-0.984518	0.713027	0.000092	O	1.653461	1.837490	-1.034477
C	0.335193	1.119263	-0.000008	O	0.844818	1.248361	1.264621
N	1.116964	-0.000021	0.000066				
H	2.130115	-0.000041	0.000193	yne-N			
H	0.776035	-2.114002	-0.000064	C	-2.465505	-0.012239	0.033889
H	-1.854391	-1.368295	-0.000254	C	-1.312337	0.351977	0.117984
H	-1.854340	1.368365	0.000160	N	-0.034279	0.787959	0.206086
H	0.776123	2.113969	0.000012	C	0.279288	2.172077	-0.150625
			H	1.307750	2.392006	0.157148	
Tf ₂ NH			H	0.166478	2.350180	-1.232355	
N	0.000035	0.000450	0.826687	H	-0.400749	2.835955	0.399226
H	0.000222	0.000714	1.852588	S	1.192106	-0.379971	0.169187
S	-1.220618	0.883511	0.093521	C	1.306143	-0.855747	-1.535551
S	1.220403	-0.883263	0.093575	H	2.091933	-1.620994	-1.598632
C	-2.552360	-0.409631	-0.093529	H	0.340212	-1.270284	-1.851542
C	2.552588	0.409417	-0.093588	H	1.578973	0.024536	-2.131655
F	-2.822373	-0.919923	1.090896	O	2.416551	0.307279	0.545704
F	-3.621147	0.181815	-0.583849	O	0.716082	-1.515459	0.937620
F	-2.145968	-1.357697	-0.907968	C	-3.855013	-0.453412	-0.051823
F	2.147288	1.356641	-0.909507	H	-4.497224	0.377603	-0.381508
F	3.621730	-0.182829	-0.582144	H	-3.967575	-1.270018	-0.781215
F	2.821395	0.920860	1.090637	H	-4.230063	-0.805650	0.921105
O	0.800130	-1.261463	-1.229556				
O	1.696118	-1.812305	1.086435	TS1			
O	-1.696565	1.812638	1.086209	C	-0.975666	-0.085711	2.138067
O	-0.800523	1.261586	-1.229688	C	-1.930782	-0.493435	1.444235
			N	-2.780731	-0.917065	0.560636	
Tf ₂ N ⁻			C	-3.045217	-2.338005	0.297380	
N	0.000056	-0.000531	-0.844844	H	-2.911371	-2.551910	-0.770713
S	1.134121	0.848636	-0.104733	H	-2.320448	-2.926246	0.870399
S	-1.134415	-0.849093	-0.104702	H	-4.066778	-2.590477	0.607660
C	2.517904	-0.382208	0.051403	S	-3.624547	0.269578	-0.407423
C	-2.517624	0.382543	0.051434	C	-2.547100	0.458327	-1.795297
F	2.899068	-0.810431	-1.144252	H	-3.059225	1.148624	-2.480673
F	3.555750	0.198307	0.643601	H	-1.603267	0.891929	-1.446859
F	2.146477	-1.427081	0.776490	H	-2.395550	-0.518662	-2.269644
F	-2.145460	1.427384	0.776283	O	-4.850610	-0.385170	-0.816165
F	-3.555676	-0.197246	0.643860	O	-3.639242	1.488955	0.372464

C	-0.531592	0.383204	3.469820	C	-2.721234	0.971463	0.047210
H	0.389034	-0.140287	3.763619	C	-2.839593	-0.139679	0.931330
H	-0.284126	1.452542	3.406559	C	-2.410891	-1.254699	0.240495
H	-1.304174	0.232654	4.235499	N	-2.045328	-0.856500	-1.013393
N	0.973752	0.019720	0.297132	H	-1.693857	-1.471017	-1.738707
H	0.023880	-0.068133	1.136648	H	-2.004782	0.991917	-2.089215
S	1.996822	1.295524	0.446300	H	-2.983597	2.007225	0.257802
S	1.059579	-1.153150	-0.842267	H	-3.197807	-0.124283	1.959284
C	1.100742	2.588457	-0.546487	H	-2.331737	-2.296018	0.543480
C	2.143576	-2.415591	-0.011183	C	0.396574	1.318858	0.297584
F	-0.097316	2.785605	-0.021571	C	0.366304	2.520320	-0.195646
F	1.790653	3.711384	-0.507893	H	-0.565328	2.840978	-0.673948
F	0.966782	2.192847	-1.798806	C	0.349857	-0.217893	2.175448
F	3.350483	-1.924374	0.184596	H	1.321973	-0.340801	2.672317
F	2.216797	-3.481957	-0.785090	H	-0.226717	0.576366	2.661142
F	1.609059	-2.748621	1.150875	H	-0.213014	-1.157064	2.189860
O	1.746362	-0.730785	-2.040492	N	0.584036	0.172161	0.774664
O	-0.251399	-1.770239	-0.897568	C	1.525927	3.467394	-0.134940
O	1.912917	1.747240	1.817798	H	1.800118	3.751562	-1.161517
O	3.264387	1.070338	-0.208643	H	1.212013	4.379506	0.393283
				H	2.396386	3.031779	0.370344
Ket3				S	1.274292	-1.107271	-0.347320
C	1.312379	0.432420	-0.281138	O	0.683895	-2.343681	0.107489
C	2.499808	-0.019026	-0.538648	O	1.058923	-0.581950	-1.674231
H	2.779071	0.008591	-1.601858	C	2.976672	-1.021904	0.100964
C	-0.250307	2.212399	0.238821	H	3.478081	-1.785976	-0.511351
H	-0.741626	2.249053	1.219751	H	3.352762	-0.019908	-0.140529
H	0.652451	2.832282	0.249090	H	3.072422	-1.260145	1.168173
H	-0.938000	2.547064	-0.547049				
N	0.145588	0.823171	-0.047261	TS2			
C	3.471310	-0.552086	0.466455	C	-2.109325	0.397871	-1.130732
H	3.712567	-1.592213	0.202388	C	-2.629433	0.839811	0.082273
H	4.400984	0.032094	0.407858	C	-2.742727	-0.297199	0.928186
H	3.075363	-0.514240	1.488063	C	-2.272991	-1.379656	0.213767
S	-1.208407	-0.430814	-0.165965	N	-1.907666	-0.942789	-1.027654
O	-2.290117	0.298741	-0.781204	H	-1.526025	-1.529145	-1.761723
O	-0.576550	-1.566144	-0.791050	H	-1.908308	0.928834	-2.058127
C	-1.518768	-0.725184	1.542966	H	-2.931144	1.860318	0.311184
H	-2.329714	-1.468560	1.567186	H	-3.111250	-0.318377	1.951771
H	-0.604919	-1.127931	1.997435	H	-2.170166	-2.425982	0.491297
H	-1.843974	0.212777	2.010701	C	0.069265	1.270333	0.173804
				C	0.097038	2.498597	-0.267501
IN1				H	-0.780558	2.913926	-0.767858
C	-2.230131	0.487413	-1.152156	C	0.330056	-0.116404	2.149883

H	1.306236	0.053697	2.626864	H	-2.085967	3.307620	-1.240567
H	-0.421230	0.554052	2.580042	H	-2.955021	1.923930	-0.509295
H	0.016597	-1.158462	2.274383				
N	0.447996	0.184460	0.713678	TS3			
C	1.315402	3.357384	-0.100601	C	-1.811850	0.268807	-1.104673
H	1.675675	3.659580	-1.095346	C	-2.319880	0.743104	0.154974
H	1.036807	4.270264	0.446205	C	-2.564904	-0.429434	0.956744
H	2.120556	2.841268	0.437709	C	-2.156688	-1.503838	0.220931
S	1.314227	-1.020745	-0.318159	N	-1.745983	-1.084186	-1.015929
O	0.883426	-2.312861	0.164891	H	-1.326391	-1.678241	-1.725331
O	1.083440	-0.589329	-1.677951	H	-1.761293	0.772674	-2.065927
C	2.982192	-0.705424	0.158889	H	-2.784049	1.714033	0.310972
H	3.591186	-1.422297	-0.410878	H	-2.958388	-0.444127	1.969224
H	3.235700	0.325737	-0.116710	H	-2.113065	-2.558516	0.485455
H	3.084202	-0.887541	1.236231	C	-0.571703	1.042642	-0.023085
				C	-0.269783	2.308645	-0.373178
TS2'				H	-1.038081	2.889513	-0.894275
C	-1.983027	-0.528135	-1.014160	C	0.376797	0.152991	2.086056
C	-2.567419	-0.656972	0.241506	H	-0.610048	0.366263	2.515362
C	-1.984326	-1.796447	0.859265	H	0.687576	-0.841608	2.432638
C	-1.061167	-2.309806	-0.028457	H	1.092528	0.911145	2.441478
N	-1.082018	-1.537373	-1.153847	N	0.271625	0.152903	0.629261
H	-0.500508	-1.684042	-1.971303	C	1.027013	2.981000	-0.126112
H	-2.167942	0.173497	-1.824282	H	1.573820	3.068906	-1.080869
H	-3.355063	-0.025450	0.649391	H	0.854617	4.007296	0.230601
H	-2.206443	-2.190023	1.849174	H	1.654890	2.442582	0.594733
H	-0.391649	-3.162723	0.052680	S	1.325236	-0.837158	-0.243334
C	-0.410067	1.185063	0.478615	O	1.196590	-2.187069	0.284749
C	-0.980858	2.338954	0.276787	O	1.065285	-0.582122	-1.653779
C	0.605043	-0.243825	2.160433	C	2.947834	-0.250739	0.154449
H	1.403262	0.288196	2.697110	H	3.644203	-0.944093	-0.337063
H	-0.348765	-0.117283	2.683036	H	3.070141	0.763469	-0.242663
H	0.844361	-1.308465	2.072209	H	3.094253	-0.281323	1.241291
N	0.472490	0.335504	0.813052				
S	1.759988	-0.063953	-0.393901	IN2			
O	2.098940	-1.445798	-0.141830	C	-1.684714	0.770673	-0.601484
O	1.239684	0.382697	-1.666178	C	-2.667204	0.807424	0.524602
C	3.050037	1.005237	0.156482	C	-3.255332	-0.401682	0.660171
H	3.894476	0.820350	-0.523526	C	-2.676338	-1.258617	-0.343445
H	2.703919	2.043032	0.072745	N	-1.820875	-0.599438	-1.060440
H	3.320263	0.739073	1.185895	H	-1.174843	-1.009631	-1.740901
H	-0.305647	3.139970	0.622694	H	-2.027687	1.450707	-1.401553
C	-2.281941	2.760877	-0.305344	H	-2.858689	1.709559	1.105430
H	-2.769034	3.463795	0.385324	H	-4.017432	-0.708051	1.373170

H	-2.879099	-2.315727	-0.525135	S	0.998940	-1.245004	-0.096577
C	-0.247222	1.124350	-0.232084	O	1.120174	-2.255479	0.941709
C	0.276456	2.307040	-0.577105	O	0.033743	-1.429586	-1.182637
H	-0.347454	2.966329	-1.189426	C	2.591226	-1.026796	-0.844131
C	0.453051	0.358986	2.038175	H	2.842485	-1.979753	-1.330074
H	1.079975	1.218141	2.324676	H	2.528154	-0.221694	-1.586947
H	-0.567761	0.518845	2.414433	H	3.323689	-0.795658	-0.060303
H	0.844350	-0.550325	2.511371				
N	0.420023	0.173474	0.590793	IN4			
C	1.617257	2.831877	-0.198344	C	-1.184678	-1.044473	0.873941
H	2.225691	2.999949	-1.101583	C	-2.025689	-2.240995	1.162073
H	1.506679	3.812394	0.290994	C	-1.640886	-2.786213	2.338816
H	2.164950	2.162913	0.477203	C	-0.576207	-1.962021	2.849513
S	1.296854	-1.057689	-0.105828	N	-0.331133	-0.981884	2.036310
O	1.208473	-2.216733	0.768693	H	0.386793	-0.244085	2.153265
O	0.832234	-1.162062	-1.491462	H	-0.531859	-1.267038	0.006443
C	2.988510	-0.535291	-0.151048	H	-2.806293	-2.593560	0.487953
H	3.564785	-1.382341	-0.548107	H	-2.035661	-3.670641	2.833916
H	3.075671	0.333174	-0.814494	H	-0.008432	-2.091000	3.772621
H	3.314726	-0.299354	0.870216	C	-1.937176	0.245582	0.577773
				C	-2.002081	1.276575	1.425423
IN3				H	-1.506625	1.179482	2.394816
C	-2.030673	0.036628	-1.200988	C	-1.768650	0.087321	-1.891139
C	-1.533392	1.077159	-0.258037	H	-0.833576	0.644215	-1.753667
C	-2.290403	0.745422	0.998623	H	-1.524078	-0.966236	-2.095962
C	-3.108781	-0.281607	0.748010	H	-2.289634	0.506463	-2.763487
N	-2.935958	-0.669103	-0.607839	N	-2.581261	0.267653	-0.688790
H	-3.459260	-1.424565	-1.053466	C	-2.725845	2.553482	1.168935
H	-1.780422	-0.086422	-2.252780	H	-3.674280	2.571844	1.731274
H	-1.932864	2.025102	-0.675629	H	-2.128405	3.409748	1.514850
H	-2.182256	1.275651	1.942323	H	-2.955423	2.683102	0.102610
H	-3.830696	-0.807865	1.367884	S	-4.169602	-0.274355	-0.766982
C	-0.026204	1.217693	-0.111806	O	-4.221096	-1.474877	-1.598172
C	0.631679	2.295537	-0.558967	O	-4.670763	-0.339575	0.599864
H	0.039035	3.072765	-1.052367	C	-5.015866	1.021221	-1.626973
C	1.086573	0.419260	2.003655	H	-6.054151	0.683507	-1.748070
H	2.185370	0.487410	2.061598	H	-4.970635	1.932883	-1.019552
H	0.666276	1.373402	2.343918	H	-4.552286	1.172391	-2.609867
H	0.738498	-0.377802	2.674109	N	1.490590	0.116310	-0.188340
N	0.615207	0.185946	0.638789	S	2.162171	1.219650	0.740141
C	2.091560	2.562647	-0.428262	S	2.222719	-0.752710	-1.316696
H	2.535058	2.728660	-1.423000	C	1.645920	2.800447	-0.086546
H	2.253840	3.489683	0.144885	C	2.853313	-2.195524	-0.327110
H	2.634463	1.748105	0.067272	F	0.326157	2.896681	-0.132375

F	2.129591	3.827946	0.591907	F	1.814300	2.825639	-1.326471
F	2.120578	2.829078	-1.320796	F	4.006476	-1.488057	0.444073
F	3.689573	-1.786059	0.614073	F	3.691459	-2.759517	-1.268210
F	3.482333	-3.039132	-1.128879	F	2.261570	-2.746732	0.345428
F	1.840506	-2.828912	0.253523	O	3.138504	0.080773	-2.007935
O	3.399139	-0.147440	-1.913921	O	1.086000	-1.365368	-1.921441
O	1.199169	-1.333718	-2.169966	O	1.507769	1.363048	2.133439
O	1.427322	1.219263	2.011605	O	3.574617	1.484789	0.712953
O	3.611353	1.266871	0.781827	C	-0.266702	-1.511711	1.816476
				H	0.506339	-0.844416	2.201134
				N	-0.477549	-2.702281	2.278899
IN5							
C	-1.184005	-1.273492	0.690483				
C	-2.006948	-2.526437	0.661948	TS4			
C	-1.534575	-3.358380	1.600352	C	-1.036543	-0.728168	1.174189
H	-0.487961	-1.329112	-0.184827	C	-1.101840	-2.100610	0.770250
H	-2.818877	-2.717944	-0.037648	C	-0.480558	-2.874556	1.733333
H	-1.812783	-4.369338	1.887706	C	-0.087939	-2.001310	2.761945
H	0.065903	-3.128241	3.031687	N	-0.465591	-0.765251	2.462874
C	-1.900030	0.062629	0.627749	H	-0.169810	0.063727	2.974193
C	-1.903029	0.947774	1.630181	H	0.057545	-0.413552	0.499222
H	-1.374890	0.685543	2.550987	H	-1.528812	-2.439732	-0.172020
C	-1.832177	0.253473	-1.837964	H	-0.294778	-3.945424	1.704161
H	-0.875744	0.765827	-1.676500	H	0.479575	-2.212469	3.667586
H	-1.630052	-0.775432	-2.174415	C	-2.004543	0.338033	0.770487
H	-2.371338	0.785541	-2.633940	C	-2.268158	1.428966	1.500640
N	-2.591325	0.312280	-0.590730	H	-1.798926	1.519675	2.484256
C	-2.596338	2.266562	1.614512	C	-1.800924	0.504176	-1.716414
H	-3.517833	2.219327	2.218370	H	-1.399495	1.518856	-1.598828
H	-1.955494	3.041257	2.060743	H	-0.973183	-0.198922	-1.895585
H	-2.868880	2.569847	0.594747	H	-2.454484	0.497953	-2.598708
S	-4.206310	-0.144816	-0.679648	N	-2.572125	0.160036	-0.525171
O	-4.346306	-1.220571	-1.659493	C	-3.160114	2.552713	1.093659
O	-4.672254	-0.365438	0.682736	H	-4.058765	2.584976	1.731945
C	-5.008610	1.291513	-1.334777	H	-2.642618	3.515118	1.229630
H	-6.067359	1.024920	-1.455433	H	-3.478856	2.468210	0.046245
H	-4.892510	2.115237	-0.620611	S	-3.904993	-0.822693	-0.697873
H	-4.570446	1.543918	-2.308338	O	-3.672376	-1.724260	-1.822217
N	1.484432	0.140228	-0.012557	O	-4.211995	-1.374206	0.615635
S	2.132355	1.341946	0.816496	C	-5.215636	0.280386	-1.157469
S	2.149738	-0.645118	-1.231463	H	-6.102347	-0.339971	-1.346696
C	1.449049	2.834923	-0.054207	H	-5.396312	0.972001	-0.325767
C	3.094218	-1.994225	-0.368801	H	-4.930330	0.821990	-2.068350
F	0.125355	2.856698	0.006822	N	1.255593	0.079854	0.001979
F	1.920699	3.929261	0.524258	S	1.869830	1.417615	0.697318

S	1.982737	-0.782815	-1.178847	C	1.187707	2.822696	-0.330230
C	1.226820	2.805150	-0.373990	C	3.152740	-1.877250	-0.255110
C	3.146032	-1.906759	-0.248060	F	-0.096569	3.001174	-0.066935
F	-0.056467	3.010819	-0.129760	F	1.843105	3.934817	-0.046200
F	1.904274	3.899845	-0.080166	F	1.330173	2.544681	-1.612705
F	1.384823	2.516835	-1.650773	F	4.124133	-1.215984	0.343358
F	4.216059	-1.247882	0.146446	F	3.671031	-2.726207	-1.126052
F	3.506191	-2.882006	-1.063667	F	2.468636	-2.553726	0.655604
F	2.536751	-2.421901	0.806637	O	2.901088	0.105273	-1.989766
O	2.818871	0.016784	-2.046992	O	1.032605	-1.574091	-1.783375
O	0.971502	-1.673443	-1.716357	O	1.218285	1.588090	2.008030
O	1.192208	1.588078	1.970617	O	3.319651	1.577110	0.617445
O	3.311914	1.492282	0.605752	C	-0.412985	-1.024216	2.408648
				H	-0.135761	-0.288428	3.160556
				N	-0.051125	-2.292026	2.501715
TS5							
C	-1.061221	-0.837569	1.148782				
C	-1.135594	-2.179274	0.567876	C2-Pro			
C	-0.480212	-3.023367	1.401414	C	-1.657270	0.320159	0.018040
H	0.060034	-0.457102	0.637375	C	-2.950303	0.820487	0.059808
H	-1.591096	-2.432027	-0.386651	C	-3.836832	-0.274236	-0.132732
H	-0.247244	-4.081377	1.315908	C	-3.058554	-1.406444	-0.276624
H	0.519806	-2.668582	3.255344	N	-1.751026	-1.035352	-0.179854
C	-1.996666	0.279961	0.795157	H	-0.954048	-1.665448	-0.272611
C	-2.205328	1.347540	1.575141	H	-3.218079	1.862316	0.228630
H	-1.700862	1.376473	2.544968	H	-4.924963	-0.239791	-0.150995
C	-1.818879	0.522851	-1.679256	H	-3.334581	-2.446444	-0.436862
H	-1.475174	1.562746	-1.599740	C	-0.353927	0.996969	0.136929
H	-0.949433	-0.140668	-1.805490	C	-0.141053	2.265848	-0.246891
H	-2.446969	0.433419	-2.574752	H	-0.980086	2.787697	-0.717760
N	-2.598964	0.179335	-0.494134	C	0.487753	-0.334153	2.043086
C	-3.068263	2.516879	1.242204	H	-0.255085	-1.148107	2.051636
H	-3.952575	2.543626	1.900705	H	1.428945	-0.711438	2.465064
H	-2.519300	3.455519	1.414499	H	0.135097	0.477339	2.693258
H	-3.411081	2.492979	0.199172	N	0.717538	0.227066	0.712083
S	-3.967802	-0.748398	-0.677237	C	1.142618	3.013319	-0.126015
O	-3.789592	-1.622330	-1.833724	H	0.971310	4.016056	0.296583
O	-4.275585	-1.330451	0.622938	H	1.867841	2.478946	0.502445
C	-5.245560	0.413359	-1.081488	H	1.594325	3.161192	-1.121233
H	-6.156977	-0.169093	-1.274017	S	1.592618	-0.727806	-0.353950
H	-5.387975	1.085942	-0.227112	O	1.105556	-2.111687	-0.268756
H	-4.954613	0.971563	-1.980428	O	1.578349	-0.068589	-1.650367
N	1.290573	0.104680	0.025073	C	3.242047	-0.692372	0.287001
S	1.881264	1.446917	0.724313	H	3.592236	0.346621	0.287084
S	2.027487	-0.711655	-1.173562	H	3.271972	-1.127615	1.292647

H	3.839530	-1.303674	-0.402918	H	0.455299	-1.563336	1.789030
				C	2.790379	1.158772	-1.040305
C3-Pro				H	1.880971	1.745857	-0.885735
C	-1.650242	0.284077	0.029894	H	3.664299	1.745435	-0.731363
C	-2.946852	0.870185	-0.128683	H	2.863484	0.934542	-2.114081
C	-3.854911	-0.162156	-0.217064	N	2.661366	-0.098013	-0.294042
H	-3.183166	1.932395	-0.164230	C	0.905561	-2.529967	-0.153086
H	-4.936072	-0.150235	-0.336894	H	1.707860	-3.242044	0.090419
H	-3.583569	-2.260767	-0.148043	H	0.051330	-3.066222	-0.099592
C	-0.347574	0.963505	0.136383	H	1.034232	-2.185422	-1.189462
C	-0.133835	2.244813	-0.204710	S	3.988507	-1.156284	-0.420143
H	-0.982125	2.798599	-0.619561	O	5.169867	-0.308941	-0.470858
C	0.686712	-0.194798	2.079419	O	3.855119	-2.142857	0.637697
H	0.447400	0.701772	2.667754	C	3.832797	-1.934671	-2.002117
H	-0.064128	-0.973128	2.291834	H	4.760995	-2.506141	-2.139518
H	1.669843	-0.558948	2.409095	H	2.964702	-2.601411	-2.007426
N	0.734213	0.182519	0.671605	H	3.750901	-1.160649	-2.775463
C	1.161737	2.978933	-0.102163	N	1.316886	-0.149884	-0.159660
H	1.895436	2.429898	0.504253	H	0.186509	-0.635080	0.296223
H	1.597408	3.141601	-1.103127	S	2.618049	-0.223085	0.817985
H	1.012032	3.976197	0.341057	S	1.296488	0.444725	-1.687171
S	1.600353	-0.803528	-0.353467	C	3.301360	-1.925820	0.501711
O	1.531228	-2.180370	0.135981	C	1.178581	2.291346	-1.412085
O	1.182386	-0.507238	-1.716560	F	2.403001	-2.829864	0.849691
C	3.278098	-0.261232	-0.155913	F	4.387744	-2.079016	1.232780
H	3.565278	-0.335752	0.900476	F	3.596967	-2.065341	-0.773400
H	3.900237	-0.931173	-0.764781	F	2.366823	2.798023	-1.167140
H	3.353984	0.772095	-0.514667	F	0.679952	2.834594	-2.506565
C	-1.837082	-1.090259	0.034906	F	0.374565	2.543904	-0.391348
H	-1.112236	-1.897699	0.119364	O	2.532826	0.220393	-2.399834
N	-3.167240	-1.337654	-0.116583	O	0.013608	0.063154	-2.241456
				O	2.097400	-0.287473	2.176606
				O	3.653332	0.715428	0.451760
TS6				IN6			
C	1.616408	0.838333	1.662673	C	-2.307045	0.653513	1.013924
C	2.572483	1.797453	2.007578	C	-3.624180	1.018988	0.672344
C	2.022767	2.593497	3.028283	C	-3.792614	2.355457	1.033017
C	0.743934	2.108106	3.274568	C	-2.574083	2.788202	1.564749
N	0.516361	1.054955	2.462262	N	-1.713058	1.762995	1.584207
H	0.366910	0.543409	2.429137	H	-0.705337	1.868889	1.755600
H	3.570866	1.872094	1.581896	H	-4.377345	0.349477	0.261491
H	2.498767	3.429340	3.536555	H	-4.695037	2.954146	0.932742
H	0.019540	2.450979	3.970060	H	-2.275143	3.774447	1.915280
C	1.733877	-0.258963	0.733150				
C	0.881970	-1.363881	0.798160				

C	-1.718327	-0.633368	1.036075	H	-5.119242	3.544506	0.272579
C	-0.788230	-0.991490	2.158182	H	-2.602009	4.500694	-0.208475
H	-0.178614	-1.856431	1.874399	C	-1.983511	0.131746	1.027673
C	-1.893247	-3.002220	0.411769	C	-0.789616	0.069265	1.745926
H	-2.678390	-3.552360	-0.121778	H	-0.485545	-0.943462	2.031893
H	-0.900119	-3.334879	0.081847	C	-2.553691	-2.245902	1.454954
H	-2.028563	-3.204093	1.478652	H	-2.506622	-1.966103	2.514531
N	-2.077231	-1.569204	0.156218	H	-3.477100	-2.821564	1.305386
C	-1.525602	-1.227243	3.479234	H	-1.683401	-2.867408	1.198386
H	-0.794634	-1.472193	4.262273	N	-2.623032	-1.026259	0.652251
H	-2.073561	-0.325800	3.790023	C	-0.274280	1.152363	2.665899
H	-2.242584	-2.058590	3.409394	H	0.822566	1.219941	2.606055
S	-2.674122	-1.194561	-1.473090	H	-0.683116	2.143814	2.435271
O	-4.072005	-1.582639	-1.486011	H	-0.529795	0.917745	3.711707
O	-2.274925	0.158485	-1.793229	S	-3.389409	-1.179261	-0.886348
C	-1.713863	-2.297333	-2.465099	O	-4.812926	-1.366211	-0.656494
H	-1.933013	-1.973920	-3.492704	O	-2.917444	-0.098141	-1.733141
H	-0.654343	-2.144820	-2.218584	C	-2.709454	-2.690478	-1.513977
H	-2.032582	-3.334314	-2.317791	H	-3.098550	-2.754105	-2.539879
N	1.182474	0.176009	0.100343	H	-1.615839	-2.608673	-1.514155
S	1.940876	-1.017673	-0.639828	H	-3.058058	-3.547754	-0.927917
S	1.738958	1.658996	0.279962	N	1.105426	0.035894	-0.153527
C	3.062446	-1.715186	0.671447	H	0.123968	0.106714	0.627968
C	0.978074	2.566924	-1.154179	S	1.500685	-1.497732	-0.590052
F	3.977218	-0.832834	1.029946	S	1.595663	1.422129	-0.878230
F	2.362142	-2.063127	1.743166	C	2.580979	-2.024139	0.837671
F	3.662726	-2.790930	0.185897	C	3.315502	1.694673	-0.215069
F	-0.338183	2.601037	-1.032731	F	1.987932	-1.734036	1.982309
F	1.293225	1.968896	-2.289577	F	2.763071	-3.326267	0.751542
F	1.441582	3.807139	-1.171626	F	3.744328	-1.407577	0.777890
O	3.170671	1.841545	0.131840	F	3.319728	1.533720	1.094953
O	1.082257	2.236256	1.456184	F	3.675048	2.926673	-0.512248
O	0.974439	-2.091108	-0.849827	F	4.149000	0.839940	-0.771943
O	2.821184	-0.635370	-1.728801	O	0.805214	2.476097	-0.261610
H	-0.088741	-0.152786	2.275388	O	1.720262	1.316293	-2.310264
				O	0.310322	-2.312025	-0.444406
				O	2.324992	-1.540887	-1.774129
TS7							
C	-2.652810	1.369850	0.667843				
C	-4.019574	1.636054	0.689318	C2-Pro-trans			
C	-4.182811	2.994861	0.343942	C	1.541222	-0.031086	0.092660
C	-2.916439	3.508027	0.107017	C	2.770527	0.181221	-0.526158
N	-2.007492	2.527817	0.323464	C	3.527190	-1.012473	-0.387290
H	-1.006982	2.603610	0.136991	C	2.742628	-1.914537	0.306677
H	-4.796708	0.916737	0.939064	N	1.559579	-1.308550	0.587308

H	0.767426	-1.733814	1.055064	H	-3.525761	0.952449	-0.728735
H	3.083959	1.083755	-1.043383	C	1.601939	-1.394303	0.238076
H	4.534193	-1.193127	-0.759623	H	0.777166	-2.086194	0.389519
H	2.937518	-2.938772	0.617108	N	2.897383	-1.790441	0.345413
C	0.353561	0.808234	0.276605	C	1.219529	3.052040	0.346310
C	0.283439	2.142905	0.112222	H	1.777500	3.513477	-0.486732
C	-1.408735	0.501315	2.016705	H	0.721392	3.871224	0.886218
H	-2.092339	-0.283395	2.362940	H	1.951888	2.588725	1.022592
H	-0.608029	0.618616	2.759059	H	-0.769669	2.479369	-0.432324
H	-1.962198	1.453632	1.940872				
N	-0.801345	0.088426	0.754779	TS8-exo			
S	-1.804122	-0.602457	-0.389808	C	-1.725989	-0.216572	0.923589
O	-0.953417	-1.132742	-1.444602	C	-1.681719	0.992911	0.009411
O	-2.710650	-1.490995	0.325415	C	-3.800690	0.129269	0.092559
C	-2.768147	0.722872	-1.076949	H	-3.499123	-1.456885	1.582819
H	-3.444129	0.267053	-1.813131	H	-0.998245	-0.342976	1.727128
H	-3.346998	1.200823	-0.276175	H	-1.377512	1.966677	0.408511
H	-2.096322	1.437701	-1.567655	H	-3.345701	1.833531	-1.021167
C	1.405086	3.058532	-0.259483	H	-4.865687	0.106570	-0.139150
H	1.627214	3.009223	-1.339440	C	-0.496834	0.206251	-0.575994
H	1.149567	4.101101	-0.025187	C	-0.930647	-1.118300	-0.664909
H	2.335118	2.801777	0.272358	H	-1.932485	-1.149366	-1.098922
H	-0.694755	2.603606	0.283074	N	0.726280	0.762279	-0.386191
				C	-0.205859	-2.418298	-0.781582
C3-Pro-trans				H	-0.916700	-3.236062	-0.602016
C	1.585951	-0.040275	-0.067398	H	0.629655	-2.518438	-0.082680
C	2.957001	0.370849	-0.153476	H	0.164761	-2.535932	-1.813647
C	3.733734	-0.736411	0.109197	C	-3.115803	-0.633320	0.986384
H	3.332577	1.359732	-0.405582	N	-2.980595	0.992687	-0.585680
H	4.814441	-0.856648	0.137675	C	0.886330	2.210721	-0.593404
H	3.196966	-2.733104	0.565718	H	0.163963	2.540578	-1.348749
C	0.356144	0.740015	-0.280929	H	0.751310	2.775831	0.339337
C	0.206606	2.070404	-0.151114	H	1.892004	2.403561	-0.983653
C	-0.897433	-0.369514	-2.120641	S	2.077008	-0.022992	0.362532
H	-1.166851	0.518224	-2.717552	O	1.527434	-1.020565	1.263406
H	0.059789	-0.767312	-2.490668	O	2.891486	1.053894	0.888167
H	-1.662354	-1.143840	-2.254855	C	2.935245	-0.783591	-0.979168
N	-0.769105	-0.046682	-0.708849	H	3.240476	0.007086	-1.676119
S	-1.960794	-0.457515	0.358892	H	3.816492	-1.269774	-0.537078
O	-2.605531	-1.663338	-0.151693	H	2.289305	-1.522351	-1.465933
O	-1.377333	-0.465644	1.693966				
C	-3.172141	0.841844	0.304650	TS8-endo			
H	-3.999292	0.537232	0.960110	C	-2.335086	-0.620465	-0.206829
H	-2.718082	1.770734	0.670168	C	-1.157787	-1.008297	-1.091710

C	-0.990638	-2.057433	0.917312	H	0.716822	2.384004	1.316918
H	-2.673317	-1.129717	1.974846	H	2.355015	1.885361	0.892783
H	-1.288221	-1.162239	-2.165572	N	0.849330	0.634119	0.158841
H	0.319078	-2.509175	-0.675920	C	-1.463376	2.773802	-0.561880
H	-0.526495	-2.710869	1.656051	H	-2.503857	3.110629	-0.664133
C	-0.750460	0.440445	-0.656388	H	-1.039809	3.253474	0.327877
C	-1.914485	1.205370	-0.747759	H	-0.915840	3.138179	-1.445548
N	0.251713	0.619414	0.231536	S	2.079319	-0.592076	0.092936
C	-2.237036	2.511660	-0.089630	O	2.806777	-0.518742	1.343617
H	-3.155479	2.926369	-0.522001	O	1.436764	-1.827165	-0.316508
H	-1.423452	3.234682	-0.251275	C	3.102256	-0.015710	-1.229931
H	-2.386462	2.407216	0.992705	H	3.898171	-0.768475	-1.324645
C	-2.064416	-1.229933	1.080529	H	2.498263	0.026638	-2.144514
N	-0.522429	-2.042246	-0.362068	H	3.534381	0.960018	-0.977633
C	0.172094	1.424130	1.454974				
H	-0.804356	1.262267	1.922702				
H	0.930692	1.053338	2.156173	TS9-endo			
H	0.336707	2.492361	1.261206	C	-2.190822	0.826435	-0.256628
S	1.800694	-0.071337	-0.114698	C	-2.104323	-0.133894	0.925050
O	1.702362	-0.679370	-1.431707	C	-2.187420	-1.475506	0.272057
O	2.201072	-0.861499	1.034211	C	-2.063581	-1.290830	-1.057341
C	2.820013	1.367910	-0.226764	N	-2.044829	0.058570	-1.379444
H	3.819025	0.990563	-0.487188	H	-2.033152	0.428689	-2.321945
H	2.429061	2.012403	-1.023724	H	-2.701409	0.080436	1.816876
H	2.852791	1.882775	0.740597	H	-2.255489	-2.428783	0.787692
H	-2.475545	1.000852	-1.661631	H	-2.003661	-2.032776	-1.852775
H	-3.350785	-0.522980	-0.590518	C	-0.642317	0.431266	0.961752
				C	-0.778490	1.788111	0.654486
				C	0.442688	-1.651844	1.583096
TS9-exo				H	-0.286160	-1.572548	2.397756
C	-2.089272	0.003348	0.936670	H	0.221600	-2.525410	0.959641
C	-1.130190	-0.911152	0.218113	H	1.436775	-1.765713	2.036442
C	-2.050441	-1.693377	-0.675742	N	0.416919	-0.401467	0.811317
C	-3.316486	-1.375920	-0.356561	C	0.218683	2.809373	0.209585
N	-3.353700	-0.410503	0.655069	H	-0.299482	3.753628	-0.002497
H	-4.185612	0.114702	0.904115	H	0.928840	3.005525	1.030221
H	-1.857986	0.515282	1.872150	H	0.777734	2.503192	-0.679882
H	-0.492266	-1.550160	0.835198	S	1.617678	-0.298443	-0.428391
H	-1.725789	-2.470641	-1.363400	O	2.011264	-1.670760	-0.679407
H	-4.248129	-1.774198	-0.755370	O	1.053382	0.497886	-1.502424
C	-0.413316	0.371277	-0.239122	C	2.965369	0.546170	0.338071
C	-1.443653	1.276109	-0.500482	H	3.765941	0.583726	-0.414142
H	-2.217322	0.798005	-1.111689	H	2.654089	1.556712	0.624191
C	1.332382	1.973227	0.508584	H	3.286353	-0.038240	1.209612
H	1.329685	2.642715	-0.361222	H	-1.604375	2.222017	1.223526

H	-2.850976	1.692236	-0.309687	C	-2.201601	2.207757	0.467747
				H	-3.223468	2.505955	0.193255
IN7-cis				H	-1.594620	3.118500	0.550486
C	-2.327528	0.864536	0.120249	H	-2.242261	1.713063	1.447942
C	-1.896385	-0.238624	-0.913849	C	-3.220735	-0.637465	0.263603
C	-2.729834	-1.295191	0.924867	N	-1.310320	-1.885524	0.177304
H	-3.040603	0.379964	2.257646	C	1.078042	2.169413	0.407102
H	-3.090091	1.596352	-0.184873	H	0.762853	2.347341	1.442717
H	-2.155266	-0.078814	-1.969274	H	2.161354	2.312503	0.332766
H	-2.797924	-2.145948	-0.972101	H	0.576542	2.861902	-0.278420
H	-3.028015	-2.153220	1.529853	S	2.088117	-0.400783	0.165046
C	-0.470329	0.168249	-0.573023	O	1.479427	-1.710465	0.099349
C	-0.878130	1.438386	0.117453	O	2.819518	0.034460	1.329462
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N	0.613250	-0.524108	-0.618488	H	3.851526	-0.729304	-1.286102
C	-0.716600	2.687201	-0.751273	H	2.333768	-0.306760	-2.173949
H	-1.250049	3.516647	-0.266113	H	3.293518	0.986339	-1.321227
H	-1.147902	2.540908	-1.752620	H	-1.490105	1.818347	-1.546025
H	0.342695	2.953172	-0.853360	H	-2.970007	-0.078233	-1.853806
C	-2.736570	-0.001110	1.283453				
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C	0.722981	-1.823757	-1.287860	C	-2.507553	0.071915	0.533045
H	-0.201816	-2.021892	-1.836657	C	-1.144873	-0.642965	0.829055
H	1.572495	-1.787339	-1.979320	C	-1.208640	-1.855706	-0.084999
H	0.882361	-2.611260	-0.538969	C	-2.424354	-1.880806	-0.675939
S	2.115027	0.049945	0.215170	N	-3.249008	-0.869681	-0.267278
O	2.052327	1.492592	0.204588	H	-4.088696	-0.606259	-0.767863
O	3.176982	-0.667861	-0.447887	H	-3.080750	0.444203	1.392368
C	1.830362	-0.589060	1.832916	H	-0.820878	-0.828812	1.860944
H	1.724089	-1.679459	1.763818	H	-0.422092	-2.601579	-0.172618
H	2.723578	-0.322502	2.416990	H	-2.797539	-2.630166	-1.375975
H	0.933824	-0.111750	2.248760	C	-0.466778	0.471446	0.082739
				C	-1.744147	1.201465	-0.225332
				H	-1.948382	1.241751	-1.309108
				C	1.112608	1.851336	-1.149522
				H	1.823937	1.514911	-1.913461
				H	0.211575	2.224361	-1.647669
				H	1.568821	2.643088	-0.543148
				N	0.748311	0.721240	-0.287156
				C	-1.860131	2.586245	0.407618
				H	-2.895954	2.936598	0.295628
				H	-1.621185	2.552559	1.480623
				H	-1.192788	3.311855	-0.076705
				S	2.120133	-0.280832	0.282417
IN7-trans							
C	-2.437067	-0.065768	-0.893772				
C	-1.092750	-0.865081	-0.814599				
C	-2.505719	-1.618537	0.836194				
H	-4.221465	-0.321912	0.552092				
H	-0.648364	-1.236944	-1.750846				
H	-0.512574	-2.280936	0.660934				
H	-2.779083	-2.236451	1.692917				
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N	0.737985	0.789546	0.027186				

O	3.195665	0.666765	0.457871	C	0.930882	-1.419018	0.000002
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C	2.405009	-1.301010	-1.126591	C	-1.625747	1.169278	0.000002
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H	1.491052	-1.867380	-1.344717	H	3.123180	1.203151	-0.000001
H	2.713027	-0.672539	-1.971026	H	3.072565	-1.277263	-0.000001
				H	0.905790	-2.511019	0.000002
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				H	-3.464040	-0.095992	-0.000003
				N	-1.563419	-1.074957	0.000000
				H	-1.879027	-2.037085	-0.000001
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C	2.357443	0.418670	-0.929180				
C	1.698448	-0.996218	-0.749181				
C	2.260246	-1.416442	0.599009				
C	3.195355	-0.521360	0.985766				
N	3.318294	0.548271	0.136702	IN1-I			
H	4.215076	0.994134	-0.014731	C	0.658380	1.137006	2.048244
H	1.717914	-1.762584	-1.539688	C	1.249343	1.942712	1.105535
H	1.959533	-2.314997	1.133802	C	2.083000	1.091678	0.299481
H	3.826948	-0.582644	1.873873	C	1.943862	-0.221668	0.817773
C	0.399572	-0.307408	-0.485512	N	1.066705	-0.158287	1.871571
C	0.970239	1.081639	-0.643088	H	0.775496	-0.944403	2.439958
C	-1.010358	-2.268080	-0.303168	H	-0.037888	1.389523	2.845598
H	-0.156687	-2.753988	-0.785538	H	1.122870	3.019219	1.009552
H	-1.131181	-2.649727	0.718903	C	-1.412056	1.151652	-0.481195
H	-1.918089	-2.468777	-0.882797	C	-1.933381	2.302658	-0.183339
N	-0.770261	-0.820069	-0.262968	H	-1.378364	2.919490	0.532986
C	0.882179	2.158806	0.423196	C	-0.158880	-0.332962	-1.937272
H	1.588061	2.959299	0.159879	H	-0.741368	-0.924029	-2.657306
H	-0.123080	2.590874	0.488170	H	0.173270	0.602666	-2.399359
H	1.156537	1.764722	1.410408	H	0.702190	-0.908131	-1.576177
S	-2.172655	0.168166	0.283662	N	-1.024497	-0.000239	-0.793112
O	-3.232925	-0.803427	0.423213	C	-3.219902	2.808944	-0.760059
O	-1.707825	0.934209	1.416495	H	-3.919378	3.008432	0.064908
C	-2.476956	1.196471	-1.115487	H	-3.027694	3.761560	-1.274887
H	-3.407640	1.731919	-0.875923	H	-3.670953	2.096552	-1.461248
H	-1.654571	1.909369	-1.246388	S	-1.624874	-1.396058	0.244065
H	-2.616966	0.552568	-1.993147	O	-0.535063	-2.342468	0.238646
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C	-0.253711	-0.668286	0.000002	H	-2.562208	-2.285623	-1.725383
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H	3.963427	-1.916005	-1.297094	C	-2.308631	1.020702	0.173308
H	4.231721	0.364595	-2.234412	C	-1.995277	-0.037800	-0.774732
H	3.044708	2.303961	-1.230907	N	-0.872322	0.251043	-1.404190
TS2-I				H	-0.340987	-0.402213	-1.981260
C	0.457411	1.193585	1.893701	H	-0.211783	2.225051	-1.689878
C	1.055586	1.945007	0.895662	H	-1.184357	2.847649	0.678618
C	1.991324	1.077117	0.232150	C	1.114887	1.241613	-0.306465
C	1.870531	-0.191226	0.847295	C	2.112547	2.096781	-0.559423
N	0.932649	-0.079530	1.850795	H	1.899340	2.924095	-1.244345
H	0.648738	-0.826613	2.474309	C	1.084903	0.344723	2.021513
H	-0.277082	1.487329	2.640502	H	1.920561	0.933353	2.431656
H	0.919413	3.010759	0.727933	H	0.139846	0.866343	2.234641
C	-1.140678	1.203791	-0.263047	H	1.045478	-0.629209	2.525414
C	-1.835348	2.297448	-0.083949	N	1.232082	0.140440	0.584914
H	-1.475170	3.064826	0.604097	C	3.488428	2.041938	0.007355
C	-0.105915	-0.272946	-1.901764	H	4.222703	1.880500	-0.798461
H	-0.772070	-0.703232	-2.663099	H	3.739999	3.008576	0.471226
H	0.319113	0.664497	-2.274284	H	3.608860	1.250087	0.757618
H	0.696189	-0.978678	-1.652468	S	1.605790	-1.374017	0.004295
N	-0.891032	0.029336	-0.694368	O	0.849463	-2.350639	0.774151
C	-3.127327	2.525438	-0.808972	O	1.438207	-1.315722	-1.448911
H	-3.935018	2.628446	-0.068436	C	3.326695	-1.632623	0.336233
H	-3.064408	3.470698	-1.367771	H	3.554135	-2.661395	0.024480
H	-3.369756	1.709370	-1.501033	H	3.912106	-0.913601	-0.248974
S	-1.604427	-1.364928	0.197902	H	3.504690	-1.513823	1.412981
O	-0.586489	-2.391165	0.175779	C	-2.842889	-1.169296	-0.911409
O	-2.107739	-0.805918	1.432211	C	-3.957827	-1.198817	-0.120904
C	-2.936622	-1.797960	-0.872597	C	-4.299164	-0.152013	0.813907
H	-3.441188	-2.642471	-0.381342	C	-3.505421	0.939952	0.967566
H	-3.612390	-0.938146	-0.958216	H	-2.600160	-1.969401	-1.610621
H	-2.529519	-2.110211	-1.842069	H	-4.632005	-2.055589	-0.193996
C	2.606974	-1.303323	0.419397	H	-5.213442	-0.259225	1.399618
C	3.476806	-1.114903	-0.643631	H	-3.746050	1.738354	1.670989
C	3.621905	0.146155	-1.264749	IN3-I			
C	2.889333	1.241669	-0.838870	C	0.626567	-0.476653	2.053636
H	2.489466	-2.276612	0.898031	C	0.527171	0.793395	1.266824
H	4.068212	-1.958874	-1.006262	C	1.713070	0.663115	0.340998
H	4.324603	0.252849	-2.094231	C	2.388390	-0.515254	0.656921
H	3.000323	2.213806	-1.324753	N	1.686565	-1.136186	1.722754
IN2-I				H	1.975542	-2.011297	2.163101
C	-0.283639	1.466958	-0.888701	H	-0.017499	-0.787289	2.874341
				H	0.716636	1.589373	2.012950

C	-0.810408	1.079867	0.604063	N	-0.808494	0.067061	-0.529141
C	-1.611238	2.063585	1.035701	C	-2.838120	2.288170	-0.793997
H	-1.264781	2.649705	1.893085	H	-3.763020	2.297992	-0.192777
C	-1.023079	0.897078	-1.906474	H	-2.831671	3.233227	-1.359610
H	-1.960889	0.760105	-2.466648	H	-2.867605	1.441914	-1.491090
H	-0.850291	1.974443	-1.798960	S	-1.542315	-1.321624	0.082866
H	-0.195308	0.456942	-2.480961	O	-0.716069	-2.449046	-0.316639
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C	-2.920624	2.460369	0.446818	C	-3.092960	-1.438020	-0.764525
H	-3.709027	2.415394	1.215087	H	-3.548331	-2.380026	-0.429316
H	-2.878228	3.506739	0.103857	H	-3.718127	-0.584732	-0.476177
H	-3.216691	1.828125	-0.399886	H	-2.922356	-1.467800	-1.847798
S	-1.668268	-1.229286	-0.415977	C	3.651908	0.026962	-1.156003
O	-1.325826	-1.946201	-1.633156	C	2.862314	1.127091	-0.884217
O	-1.189703	-1.723039	0.878821	C	2.552022	-1.312368	0.578802
C	-3.434142	-1.117782	-0.314179	C	3.484548	-1.179815	-0.434831
H	-3.812267	-2.145036	-0.220373	H	4.408235	0.077368	-1.941392
H	-3.700501	-0.526016	0.570353	H	2.966816	2.056593	-1.446968
H	-3.814062	-0.656116	-1.234539	H	2.420537	-2.248505	1.121989
C	3.534847	-0.942558	0.007255	H	4.114273	-2.035693	-0.688570
C	4.003602	-0.122577	-1.021299				
C	3.341915	1.062795	-1.360415				
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H	4.040492	-1.869360	0.281700	C	-1.254587	0.581365	-0.005112
H	4.900993	-0.414475	-1.570275	C	-2.366908	1.460958	0.439598
H	3.733807	1.680392	-2.171045	C	-2.305799	2.634205	-0.252246
H	1.678135	2.396717	-0.951916	C	-1.182501	2.529284	-1.169748
				N	-0.604064	1.353770	-1.028604
TS3-I				H	0.219698	1.003186	-1.538430
C	0.172781	1.201681	1.648390	H	-0.545144	0.474355	0.842064
C	0.898121	1.912932	0.629616	H	-3.083442	1.179486	1.212090
C	1.904668	1.015323	0.139221	C	-1.673735	-0.820743	-0.436398
C	1.769885	-0.185707	0.871684	C	-1.635193	-1.242039	-1.703572
N	0.791818	-0.021115	1.815556	H	-1.303435	-0.536054	-2.468539
H	0.380324	-0.771947	2.360328	C	-1.221173	-1.893895	1.751348
H	-0.393229	1.634689	2.470957	H	-0.203333	-1.993135	1.355012
H	0.859200	2.985034	0.456173	H	-1.231862	-1.083269	2.495907
C	-0.783080	1.239410	0.223281	H	-1.485780	-2.836983	2.250534
C	-1.670420	2.253721	0.112644	N	-2.121674	-1.652254	0.624882
H	-1.516902	3.128948	0.752818	C	-2.038048	-2.599879	-2.166115
C	-0.265832	-0.001990	-1.888602	H	-3.033304	-2.559522	-2.639287
H	0.062286	1.004383	-2.174243	H	-1.333832	-2.973623	-2.923767
H	0.590777	-0.688306	-1.941011	H	-2.082524	-3.314868	-1.333197
H	-1.034633	-0.323363	-2.607829	S	-3.767440	-1.662022	0.964735
				O	-3.983634	-1.083485	2.289816

O	-4.447752	-1.070785	-0.180145	H	3.208677	-3.812015	0.244313
C	-4.171369	-3.383039	1.050363	H	2.290729	-4.523057	-1.110618
H	-5.239070	-3.435139	1.303259	H	4.036421	-4.295032	-1.261151
H	-3.979957	-3.838369	0.071470	S	1.936767	-0.953694	1.669693
H	-3.574260	-3.860211	1.837394	O	2.561277	-0.553947	2.920813
N	1.716645	-0.296085	0.226254	O	0.975017	-0.060961	1.023603
S	2.440197	-0.541378	-1.170482	C	1.125379	-2.509317	1.907037
S	2.435983	0.024471	1.620179	H	0.290541	-2.320455	2.595660
C	2.387711	-2.391141	-1.318711	H	0.737058	-2.848802	0.938776
C	2.570335	1.878429	1.554105	H	1.838288	-3.219383	2.344514
F	1.141897	-2.834346	-1.247632	N	-1.861511	0.233407	-0.434596
F	2.907481	-2.752599	-2.480777	S	-1.909210	-1.316279	-0.052430
F	3.091446	-2.933283	-0.338296	S	-1.996157	1.486023	0.533696
F	3.258629	2.257285	0.487875	C	-3.386555	-1.858238	-1.040108
F	3.181779	2.316590	2.642650	C	-3.785065	1.963262	0.387652
F	1.361430	2.424171	1.492851	F	-3.555674	-3.162243	-0.876399
O	3.799213	-0.456748	1.752305	F	-4.477644	-1.229618	-0.630842
O	1.480421	-0.221349	2.687917	F	-3.202512	-1.606984	-2.326609
O	1.535859	-0.069050	-2.224465	F	-4.149494	2.036255	-0.882183
O	3.845949	-0.193495	-1.261057	F	-3.969688	3.144130	0.957752
C	-2.761732	4.840848	-1.073574	F	-4.538538	1.065932	1.003980
C	-1.637554	4.717529	-1.971009	O	-1.306273	2.606930	-0.117504
C	-0.847847	3.604032	-2.039016	O	-1.790142	1.262030	1.949742
C	-3.099729	3.832362	-0.226937	O	-0.807590	-2.013439	-0.710910
H	-3.337365	5.767693	-1.087972	O	-2.226672	-1.641183	1.327648
H	-1.412370	5.563065	-2.625518	C	1.139374	0.448667	-1.447160
H	-0.001117	3.528307	-2.721575	H	0.236910	-0.147048	-1.591749
H	-3.944724	3.909195	0.459062	N	1.096535	1.709764	-1.181604
				C	5.060075	2.740480	-0.612064
				C	4.119216	3.758589	-0.422716
IN5-I				C	2.754024	3.521506	-0.597558
C	2.548991	-0.034963	-1.554075	C	4.668137	1.450827	-0.985127
C	3.314026	1.202778	-1.158820	H	6.119929	2.957070	-0.462654
C	2.393416	2.234106	-0.961202	H	4.455335	4.754990	-0.128657
H	2.691582	-0.230770	-2.635141	H	2.007597	4.302704	-0.447559
H	0.209934	2.209148	-0.973049	H	5.407699	0.660520	-1.127714
C	2.851555	-1.329218	-0.809294				
C	2.880108	-2.504227	-1.453028				
H	2.718423	-2.483564	-2.535468	TS4-I			
C	4.491640	-1.526370	1.094740	C	0.961566	0.845899	0.716888
H	4.496508	-2.420028	1.739204	C	0.835024	1.938085	-0.194474
H	5.144512	-1.722570	0.235759	C	-0.026414	2.877241	0.371860
H	4.897202	-0.676013	1.660039	C	-0.372232	2.389687	1.670532
N	3.157736	-1.220482	0.579459	N	0.279288	1.235327	1.894057
C	3.118672	-3.845219	-0.848462	H	0.019424	0.572617	2.621240

H	0.046290	0.172820	0.159558				
H	1.288509	1.972405	-1.183600	TS5-I			
C	2.127852	-0.092857	0.763464	C	0.378169	-1.705750	0.055335
C	2.491170	-0.761117	1.864372	C	-0.634580	-2.470381	0.822290
H	1.946874	-0.558908	2.791138	C	-1.497237	-3.057192	-0.119813
C	2.191787	-1.240211	-1.453821	H	-0.197588	-0.533348	-0.009242
H	2.082163	-2.226131	-0.983288	H	-1.451406	-3.025445	-2.263447
H	1.213122	-0.897847	-1.823690	C	1.759799	-1.316740	0.490618
H	2.862867	-1.339774	-2.316231	C	2.065434	-0.966255	1.747339
N	2.765384	-0.303758	-0.491477	H	1.244100	-0.898595	2.464141
C	3.585678	-1.769343	1.946241	C	3.315521	-2.592400	-0.954811
H	4.404565	-1.399970	2.585433	H	3.807459	-2.501609	-1.932631
H	3.211936	-2.692587	2.415709	H	4.055097	-2.950842	-0.220648
H	3.995809	-2.016221	0.957933	H	2.518315	-3.346470	-1.046323
S	3.930945	0.771864	-0.997284	N	2.727168	-1.322593	-0.553297
O	3.693541	1.076381	-2.404576	C	3.423024	-0.616381	2.255637
O	3.967192	1.855306	-0.022693	H	3.464637	0.447455	2.534999
C	5.457452	-0.122990	-0.888447	H	3.648273	-1.197108	3.164213
H	6.243791	0.540951	-1.272856	H	4.211525	-0.799925	1.513235
H	5.640688	-0.371296	0.163978	S	3.445927	0.087959	-1.083663
H	5.388778	-1.028657	-1.504555	O	2.908979	1.188183	-0.297754
N	-1.125170	-0.721208	-0.123466	O	4.887658	-0.133339	-1.140217
S	-1.552992	-1.820081	0.989769	C	2.861065	0.274852	-2.747550
S	-1.862899	-0.500189	-1.554203	H	3.379938	1.148670	-3.165009
C	-0.561544	-3.329384	0.511381	H	3.109654	-0.621720	-3.329614
C	-3.246926	0.675944	-1.144103	H	1.777942	0.450841	-2.710710
F	0.696921	-3.187266	0.894394	N	-0.773569	0.776507	0.013852
F	-1.081285	-4.380384	1.119734	S	-1.215289	1.373656	-1.428953
F	-0.596667	-3.515488	-0.794716	S	-1.087776	1.503060	1.441168
F	-4.152107	0.086272	-0.387892	C	-2.960390	0.758317	-1.655275
F	-3.806792	1.063670	-2.277540	C	0.351374	2.673910	1.685905
F	-2.773831	1.734470	-0.508233	F	-3.794585	1.386876	-0.854981
O	-2.504840	-1.686531	-2.079986	F	-3.310467	0.974081	-2.912478
O	-0.953283	0.281909	-2.373142	F	-3.015865	-0.542496	-1.408909
O	-0.983845	-1.394899	2.258131	F	1.389764	2.023309	2.168709
O	-2.939219	-2.229041	0.905651	F	-0.027641	3.590890	2.563529
C	-1.470884	4.759552	0.703544	F	0.679049	3.263793	0.555533
C	-1.823295	4.244900	1.988634	O	-0.940605	0.500907	2.477814
C	-1.301992	3.074265	2.486373	O	-2.261527	2.350769	1.386456
C	-0.591307	4.091183	-0.107371	O	-1.297483	2.816441	-1.481555
H	-1.923706	5.694881	0.369439	O	-0.464620	0.634022	-2.432994
H	-2.538833	4.805446	2.595010	C	0.096148	-2.034580	-1.304674
H	-1.582683	2.686730	3.466556	H	0.636068	-1.720770	-2.195322
H	-0.325124	4.465925	-1.097316	N	-1.003615	-2.758673	-1.389969

C	-2.015097	-3.411852	2.544189				
C	-2.872411	-3.968635	1.580335	C3-Pro-I			
C	-2.626694	-3.796797	0.223880	C	-0.737418	-0.128441	-0.010813
C	-0.904485	-2.656374	2.182103	C	-2.146077	0.203519	0.005117
H	-2.229325	-3.570012	3.603329	C	-2.853336	-1.017328	-0.154477
H	-3.742367	-4.545413	1.901249	H	-2.138529	-3.007796	-0.371087
H	-3.279923	-4.221433	-0.540198	C	0.432070	0.760885	0.090625
H	-0.267436	-2.222188	2.951368	C	0.456426	2.034439	-0.336985
				H	-0.441623	2.412060	-0.834208
C2-Pro-I				C	1.517176	-0.311952	2.053506
C	-0.619928	0.519407	0.130664	H	0.995230	0.442316	2.657732
C	-1.116023	-0.755679	0.307699	H	0.977552	-1.269212	2.131675
C	-2.539850	-0.681727	0.150356	H	2.522575	-0.441069	2.478507
C	-2.846888	0.677411	-0.121363	N	1.608525	0.188789	0.685824
N	-1.666961	1.375857	-0.125382	C	1.621282	2.963425	-0.250579
H	-1.588836	2.373535	-0.277702	H	2.129598	3.041044	-1.227121
H	-0.521325	-1.639116	0.527961	H	1.294040	3.979348	0.019439
C	0.781020	0.958403	0.200410	H	2.359062	2.620570	0.488323
C	1.199435	2.205796	-0.076018	S	2.725310	-0.557891	-0.308312
H	0.455571	2.933648	-0.416060	O	2.814380	-1.973786	0.050411
C	1.866684	-0.267251	2.067988	O	2.414611	-0.192794	-1.683175
H	0.880210	-0.262587	2.553070	C	4.268206	0.194398	0.138148
H	2.331048	-1.244633	2.255927	H	5.041846	-0.307489	-0.458636
H	2.495426	0.513738	2.526526	H	4.223032	1.262422	-0.105519
N	1.689294	-0.051269	0.638057	H	4.458842	0.039237	1.207491
C	2.603338	2.699279	0.004781	C	-0.671296	-1.497540	-0.162925
H	3.288319	1.951816	0.426656	H	0.208203	-2.138170	-0.216494
H	2.970875	2.968074	-0.998838	N	-1.927403	-2.024292	-0.253972
H	2.651839	3.614299	0.616767	C	-4.253190	-1.077176	-0.176022
S	2.770890	-0.744906	-0.415026	C	-2.882714	1.392550	0.168943
O	2.657446	-0.057805	-1.693937	C	-4.268839	1.336583	0.151898
O	4.065397	-0.824112	0.255114	C	-4.948858	0.113000	-0.025099
C	2.183236	-2.405537	-0.635512	H	-4.772766	-2.029307	-0.303578
H	1.203566	-2.364496	-1.127032	H	-2.374290	2.347598	0.316064
H	2.915173	-2.920281	-1.272926	H	-4.846662	2.255136	0.279452
H	2.117391	-2.900851	0.341674	H	-6.041448	0.102557	-0.037908
C	-5.172342	0.170962	-0.263775				
C	-4.160333	1.118365	-0.330979	furan			
C	-3.588281	-1.619446	0.211241	C	1.088686	-0.352435	-0.000355
C	-4.889672	-1.185991	0.004534	C	0.717584	0.957594	0.000206
H	-6.208127	0.481050	-0.422168	C	-0.717624	0.957566	-0.000165
H	-4.376376	2.168568	-0.538870	C	-1.088672	-0.352478	-0.000194
H	-3.377630	-2.671731	0.418069	O	0.000024	-1.149313	0.000470
H	-5.712817	-1.903245	0.049080	H	2.054401	-0.852764	-0.000514

H	1.382099	1.819342	0.000366	C	-0.001814	2.461345	0.268725
H	-1.382174	1.819287	-0.000292	H	0.867984	2.916773	0.746992
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IN1-F				C	-1.258716	3.267458	0.141284
C	-2.739113	0.843394	0.187222	H	-1.028460	4.215333	-0.366947
C	-2.464511	0.533915	-1.111683	H	-1.627155	3.510861	1.149611
C	-2.192403	-0.873264	-1.131525	H	-2.042821	2.738195	-0.415254
C	-2.328329	-1.296351	0.154910	O	2.441905	-0.315140	-0.973520
H	-3.015220	1.766395	0.692212	C	-0.355626	-0.135893	-2.148390
H	-2.460097	1.221348	-1.955220	H	-1.313381	0.162634	-2.598534
H	-1.921043	-1.485556	-1.988209	H	-0.185300	-1.209130	-2.291100
H	-2.226301	-2.267563	0.632663	H	0.462921	0.433039	-2.601775
C	0.419486	1.322681	0.306712	S	-1.309980	-0.976750	0.347989
C	0.344884	2.514924	-0.201439	O	-1.041332	-0.544561	1.699913
H	-0.604854	2.781558	-0.680656	O	-0.971680	-2.299760	-0.126320
N	0.605395	0.172358	0.771033	C	-2.965020	-0.572310	-0.110905
C	1.461857	3.512188	-0.164215	H	-3.603582	-1.261720	0.460731
H	1.108934	4.422022	0.342697	H	-3.089570	-0.742599	-1.187800
H	1.721804	3.783942	-1.197895	H	-3.164183	0.467479	0.175356
H	2.351137	3.126957	0.349324	IN2-F			
O	-2.660578	-0.262227	0.957888	C	-1.632908	0.962556	-0.477143
C	0.365637	-0.236220	2.165670	C	-1.993167	-0.247720	-1.252042
H	1.335277	-0.361588	2.666547	C	-2.764103	-1.061393	-0.481084
H	-0.185470	-1.182796	2.166681	C	-2.910589	-0.385025	0.749485
H	-0.216326	0.548253	2.660895	H	-2.079218	1.861111	-0.935038
S	1.316795	-1.094969	-0.369457	H	-1.693338	-0.396360	-2.287270
O	1.056191	-0.577358	-1.689809	H	-3.200569	-2.026045	-0.728429
O	0.779292	-2.344963	0.110325	H	-3.460725	-0.693286	1.643314
C	3.024861	-0.947132	0.041596	C	-0.164739	1.190834	-0.174283
H	3.537557	-1.697587	-0.578418	C	0.431998	2.335148	-0.532666
H	3.153666	-1.176339	1.106906	H	-0.184718	3.072480	-1.056218
H	3.360990	0.065528	-0.214160	N	0.445279	0.168249	0.603683
TS2-F				C	1.848129	2.716411	-0.286421
C	2.456425	0.764701	-0.166156	H	1.883275	3.666689	0.269326
C	2.231333	0.374790	1.136603	H	2.357060	2.896483	-1.246976
C	2.029438	-1.031984	1.098365	H	2.409149	1.959503	0.274653
C	2.149084	-1.387411	-0.213959	O	-2.324309	0.752662	0.788362
H	2.772802	1.702949	-0.615628	C	0.698780	0.388263	2.026696
H	2.213967	1.024982	2.008640	H	1.602132	0.993952	2.204180
H	1.790483	-1.692024	1.927898	H	0.808084	-0.581944	2.527312
H	2.069662	-2.340564	-0.731297	H	-0.165265	0.904683	2.465011
C	0.071293	1.235116	-0.186324	S	1.109875	-1.167769	-0.139548
				O	0.492981	-1.240219	-1.461937

O	0.987615	-2.288242	0.779551	H	2.346140	-2.576762	-0.602407
C	2.834967	-0.831616	-0.362184	C	0.466994	0.992896	0.336229
H	3.270985	-1.737945	-0.804577	C	0.282340	2.308550	0.546096
H	3.291596	-0.631018	0.615864	H	1.051677	2.838607	1.117285
H	2.946108	0.019904	-1.044114	N	-0.323708	0.198699	-0.504000
				C	-0.879625	3.115882	0.095484
				H	-0.531486	3.912047	-0.582870
IN3-F				H	-1.331216	3.622551	0.962828
C	2.660199	0.686040	0.605339	H	-1.649655	2.525336	-0.414878
C	1.623183	0.754307	-0.426574	O	2.682235	-0.513806	-0.903184
C	1.852284	-0.536380	-1.151819	C	-0.384667	0.429960	-1.947119
C	2.909921	-1.129130	-0.604101	H	-1.136465	1.187009	-2.221693
H	2.908825	1.404816	1.391454	H	-0.618335	-0.515437	-2.454073
H	2.028188	1.583419	-1.061314	H	0.597178	0.771905	-2.299725
H	1.256491	-0.898810	-1.986837	S	-1.416812	-0.890407	0.170062
H	3.475218	-2.040154	-0.780838	C	-3.001543	-0.121353	-0.016018
C	0.203502	1.154342	-0.030994	H	-3.012813	0.808126	0.566382
C	-0.315821	2.338136	-0.378165	H	-3.736685	-0.835270	0.380773
H	0.312300	3.014087	-0.966462	H	-3.193725	0.063876	-1.080543
N	-0.541171	0.180482	0.681789	O	-1.397865	-2.095764	-0.642663
C	-1.699323	2.792458	-0.071778	O	-1.099418	-0.955557	1.590403
H	-1.699637	3.850011	0.230692				
H	-2.323685	2.718204	-0.977884				
H	-2.164466	2.187821	0.718286	IN4-F			
O	3.394478	-0.337168	0.467833	C	-1.154885	-0.625354	0.238153
C	-0.008937	-0.302950	1.948024	C	-1.372721	-0.554009	1.693538
H	0.266208	0.561511	2.566794	C	-1.371865	-1.813986	2.208968
H	-0.775493	-0.871352	2.491952	C	-1.189527	-2.668134	1.101910
H	0.863861	-0.969673	1.820664	H	-0.118590	-0.262567	0.035087
S	-1.442637	-0.929363	-0.221642	H	-1.437398	0.389184	2.231474
O	-1.461270	-0.440518	-1.594004	H	-1.463555	-2.130210	3.244897
O	-0.940937	-2.269617	0.057016	H	-1.111031	-3.757973	1.078950
C	-3.068192	-0.793271	0.463170	C	-2.130252	0.018871	-0.711956
H	-3.680743	-1.553034	-0.041343	C	-1.722008	0.972813	-1.560100
H	-3.024403	-0.997506	1.540590	H	-0.668714	1.269346	-1.518337
H	-3.451355	0.214207	0.262620	N	-3.445380	-0.528358	-0.717883
				C	-2.561955	1.661779	-2.575942
				H	-2.101187	1.550184	-3.570209
				H	-2.592238	2.743547	-2.367883
				H	-3.588962	1.276803	-2.617243
				N	1.808477	0.124607	-0.254130
				S	2.314178	1.613561	-0.565980
				S	2.629088	-0.992386	0.551030
				C	1.668763	2.548641	0.905684
				C	3.465573	-1.924127	-0.819799
TS3-F							
C	2.533250	0.561949	-0.224326				
C	1.773321	0.315963	0.985754				
C	1.727406	-1.168595	1.024938				
C	2.221366	-1.605761	-0.131179				
H	2.902591	1.498590	-0.647333				
H	2.040855	0.870301	1.890411				
H	1.294226	-1.771192	1.817244				

F	0.345688	2.436460	0.972166	O	-3.686033	-1.159052	-2.341282
F	1.982455	3.828684	0.787366	C	-2.752881	1.300099	-2.144264
F	2.188393	2.076184	2.026830	H	-2.329750	1.261251	-3.157596
F	4.254086	-1.117761	-1.511179	H	-3.783564	1.674861	-2.169630
F	4.193514	-2.901446	-0.299806	H	-2.102475	1.894637	-1.489924
F	2.563496	-2.447690	-1.635480	N	1.453962	0.081018	0.352241
O	3.704213	-0.508954	1.398478	S	1.311634	1.281951	-0.698923
O	1.667256	-1.943798	1.093069	S	2.530603	-1.112326	0.298485
O	1.536639	2.133044	-1.680311	C	2.499312	2.557035	-0.046185
O	3.752463	1.807913	-0.546928	C	1.681734	-2.417117	-0.719261
O	-1.098074	-2.052936	-0.016317	F	2.425362	3.639191	-0.806262
C	-3.853215	-1.504821	-1.728489	F	2.173002	2.885427	1.198257
H	-4.769243	-1.186874	-2.249878	F	3.739575	2.104775	-0.055743
H	-4.020280	-2.498447	-1.288284	F	0.539226	-2.774897	-0.149929
H	-3.049530	-1.575547	-2.471614	F	2.474172	-3.479582	-0.779627
O	-5.520538	-1.101655	0.571573	F	1.444767	-1.987851	-1.943056
O	-3.845945	0.533265	1.523057	O	2.601911	-1.695646	1.627187
C	-5.440749	1.333762	-0.384311	O	3.749589	-0.807679	-0.430000
H	-6.213390	1.652646	0.328716	O	1.749944	1.008718	-2.053601
H	-5.905791	0.981223	-1.313735	O	0.010517	1.900131	-0.462087
H	-4.733595	2.150759	-0.572453	C	-0.344293	0.317294	2.135877
S	-4.575012	-0.012008	0.380489	H	-0.006804	1.347710	2.028543
				O	0.165468	-0.398925	3.054128

IN5-F

C	-1.395591	-0.394499	1.419258
C	-1.427991	-1.698266	2.151270
C	-0.460816	-1.665047	3.064233
H	-0.885492	-0.610658	0.442289
H	-2.077202	-2.537784	1.913624
H	-0.054859	-2.362906	3.790663
C	-2.657800	0.340874	1.029468
C	-3.060580	1.465203	1.638114
H	-2.489054	1.796235	2.511307
C	-4.809766	-0.637302	0.181276
H	-5.014872	-1.623424	-0.253452
H	-4.998164	-0.686446	1.261056
H	-5.497229	0.099555	-0.262836
N	-3.399591	-0.294123	-0.003466
C	-4.229955	2.307845	1.250459
H	-4.531412	2.148764	0.206601
H	-5.100297	2.099225	1.894896
H	-3.983169	3.371758	1.381129
S	-2.762479	-0.365912	-1.547139
O	-1.368338	-0.795140	-1.433232

TS4-F

C	-0.870756	-1.452807	-0.924273
C	-0.645793	-2.553311	-0.041503
C	0.182126	-3.457458	-0.687230
C	0.373613	-2.936498	-1.960204
H	-0.001689	-0.695330	-0.451676
H	-0.993444	-2.594235	0.989512
H	0.626013	-4.365808	-0.288835
H	0.977533	-3.301029	-2.792370
C	-2.130196	-0.641557	-1.041728
C	-2.301645	0.244043	-2.029717
H	-1.472701	0.376435	-2.730553
C	-4.000499	-2.043594	-0.236995
H	-3.436161	-2.992838	-0.244025
H	-4.539035	-1.941373	-1.189922
H	-4.730432	-2.083306	0.579923
N	-3.122281	-0.895675	-0.055892
C	-3.519346	1.068989	-2.258842
H	-3.902604	0.904494	-3.278458
H	-3.265181	2.139100	-2.189993

H	-4.316994	0.846396	-1.537966	S	-2.578712	-0.303655	1.608664
S	-2.918314	-0.213366	1.454126	O	-1.285820	0.316260	1.350531
O	-1.503106	0.109996	1.596114	O	-2.724664	-1.312904	2.645049
O	-3.557833	-1.093711	2.423327	C	-3.725919	1.006487	1.950913
C	-3.825255	1.306551	1.402417	H	-3.405910	1.460957	2.898760
H	-3.704674	1.779126	2.387012	H	-4.734859	0.586510	2.051837
H	-4.881026	1.078029	1.210419	H	-3.672826	1.743305	1.139723
H	-3.404330	1.946587	0.618797	N	1.333557	0.103202	-0.254107
N	1.182804	0.187099	-0.135604	S	1.866341	1.569652	-0.617019
S	1.336290	1.599974	-0.914528	S	1.807238	-0.784110	1.002716
S	2.095783	-0.286016	1.119238	C	0.691701	2.721062	0.252976
C	0.203422	2.750151	0.019951	C	3.308330	-1.654249	0.330009
C	3.547103	-1.090459	0.274672	F	-0.532746	2.582767	-0.238668
F	-1.062447	2.467893	-0.241587	F	1.093333	3.967380	0.029767
F	0.453911	3.986750	-0.385207	F	0.673346	2.505579	1.552492
F	0.412845	2.668408	1.318098	F	4.253612	-0.796643	-0.014055
F	4.228193	-0.217465	-0.442466	F	3.783977	-2.467245	1.263368
F	4.338571	-1.606835	1.201144	F	2.981009	-2.375649	-0.734996
F	3.124992	-2.064283	-0.521475	O	2.286625	-0.030446	2.147132
O	2.651537	0.798746	1.900950	O	0.853621	-1.863983	1.184231
O	1.411907	-1.391760	1.762508	O	1.566373	1.799880	-2.025604
O	0.719877	1.449756	-2.219066	O	3.178371	1.912979	-0.098955
O	2.653018	2.192339	-0.786882	C	-0.583329	-0.116263	-2.573034
O	-0.267938	-1.817891	-2.144277	H	-0.612128	0.906634	-2.950606
				O	0.274497	-0.919890	-3.076515

TS5-F

C	-1.275188	-0.727260	-1.472742
C	-0.757634	-2.117375	-1.495665
C	0.187427	-2.159561	-2.438693
H	-0.514206	-0.248763	-0.723336
H	-1.040104	-2.909248	-0.807330
H	0.885850	-2.909644	-2.797261
C	-2.676301	-0.381510	-1.048919
C	-3.504092	0.350950	-1.806779
H	-3.137213	0.684368	-2.782627
C	-4.068351	-2.056326	0.191231
H	-5.099280	-1.680710	0.300826
H	-3.849586	-2.750015	1.012479
H	-3.995316	-2.606313	-0.756303
N	-3.071467	-0.990015	0.175444
C	-4.900742	0.746606	-1.468134
H	-5.606882	0.294467	-2.183373
H	-5.013432	1.838232	-1.562848
H	-5.196812	0.451486	-0.454168

C2-Pro-F

C	-1.612310	0.108318	0.049707
C	-1.837220	-1.231478	0.217043
C	-3.238100	-1.428173	-0.002109
C	-3.748771	-0.197868	-0.283125
H	-1.084049	-1.981573	0.449399
H	-3.791260	-2.363891	0.042365
H	-4.749065	0.159743	-0.515143
C	-0.384371	0.902286	0.128906
C	-0.316032	2.203412	-0.197571
H	-1.234220	2.674125	-0.561646
C	0.846058	0.005060	2.088884
H	0.701495	0.972234	2.590367
H	0.095829	-0.710348	2.463660
H	1.844086	-0.368983	2.353481
N	0.752349	0.208720	0.647759
C	0.900706	3.059025	-0.111491
H	1.215136	3.382206	-1.118206

H	0.687143	3.977317	0.458722	H	-1.294796	2.081455	1.174771
H	1.740029	2.533170	0.363502	H	0.004230	2.631343	0.055867
S	1.610416	-0.812928	-0.349852	H	-1.596497	2.127119	-0.599807
O	1.739807	-2.110520	0.308034	N	-0.361038	0.565440	0.067912
O	1.017677	-0.731888	-1.677279	C	3.176950	-0.223546	0.325550
C	3.227736	-0.086896	-0.419165	H	3.571030	-1.242130	0.197975
H	3.853713	-0.760542	-1.020102	H	3.974438	0.481671	0.050798
H	3.146177	0.896443	-0.898036	H	2.890835	-0.068008	1.372337
H	3.631146	-0.000758	0.597774	C	-1.351977	-0.498124	0.382007
O	-2.771913	0.734225	-0.251917	H	-1.683108	-0.389373	1.425227
C3-Pro-F				H	2.179689	-0.162875	-1.692210
C	-1.638702	0.264420	0.017439	F	-2.373592	-0.345992	-0.455739
C	-2.949607	0.806092	-0.236244	F	-0.783774	-1.675587	0.176375
C	-3.798731	-0.254850	-0.242397	TS-CHF₂			
H	-3.218983	1.849118	-0.388298	C	-1.662062	1.208815	-1.014092
H	-4.872762	-0.344408	-0.388284	C	-1.824641	1.635855	0.298774
C	-0.349140	0.967776	0.116807	C	-2.351498	0.538730	1.033900
C	-0.175453	2.258566	-0.208588	C	-2.477037	-0.515119	0.152913
H	-1.045027	2.800586	-0.593532	N	-2.062953	-0.091381	-1.077892
C	0.774965	-0.048851	2.084709	H	-2.078716	-0.655306	-1.920859
H	1.738028	-0.492977	2.369963	H	-1.338629	1.745172	-1.903409
H	0.672018	0.908672	2.614407	H	-1.619709	2.637345	0.672880
H	-0.029877	-0.727859	2.411398	H	-2.597572	0.517700	2.093715
N	0.744222	0.206831	0.649341	H	-2.827622	-1.533182	0.305757
C	1.099847	3.024672	-0.108203	C	0.827423	0.826910	0.058590
H	0.938584	3.977312	0.421047	C	1.344062	1.989244	-0.220934
H	1.879903	2.455652	0.415434	C	0.613412	-0.796412	1.834513
H	1.474176	3.283854	-1.113094	H	1.583537	-1.213583	2.135512
S	1.577838	-0.833162	-0.347713	H	0.375503	0.088817	2.431564
O	1.588093	-2.162476	0.260205	H	-0.175268	-1.548029	1.940695
O	1.056373	-0.664393	-1.696801	N	0.705205	-0.388470	0.418704
C	3.243853	-0.223914	-0.316478	C	2.824671	2.223716	-0.136392
H	3.847943	-0.922512	-0.911284	H	3.185539	2.579206	-1.112480
H	3.256156	0.777367	-0.763673	H	3.013649	3.018013	0.600848
H	3.603962	-0.199266	0.719762	H	3.376091	1.319344	0.150041
C	-1.825761	-1.085014	0.142811	C	0.860032	-1.442348	-0.589208
H	-1.138328	-1.908766	0.323657	H	0.692848	2.813502	-0.521543
O	-3.125513	-1.401553	-0.013233	F	2.071280	-1.984973	-0.428229
Ket-CHF₂				F	-0.045287	-2.393570	-0.368352
C	0.813682	0.265718	-0.268848	H	0.754479	-1.019500	-1.597574
C	2.024015	-0.035825	-0.610939	Ket-CH₂F			
C	-0.846381	1.954598	0.181219	C	0.682294	0.058200	-0.238614

C	1.902598	-0.210551	-0.575495	Ket-Me			
C	-1.072620	1.673768	0.029193	C	0.300951	-0.000131	-0.288099
H	-1.391566	1.954307	1.041189	C	1.568004	0.000007	-0.560851
H	-0.307697	2.363811	-0.340719	C	-1.689160	1.250283	0.114981
H	-1.934759	1.658888	-0.648484	H	-2.133305	1.262106	1.118617
N	-0.505998	0.313390	0.086527	H	-1.017746	2.104685	-0.017199
C	3.086779	-0.221295	0.341816	H	-2.483541	1.264200	-0.642802
H	3.547505	-1.219312	0.314856	N	-0.928625	-0.000016	-0.037766
H	3.829366	0.500563	-0.027551	C	2.681117	-0.000033	0.442753
H	2.814793	0.028319	1.374428	H	3.309474	-0.887949	0.281049
C	-1.405092	-0.767685	0.536473	H	3.309522	0.887849	0.281062
H	-1.824943	-0.469080	1.507172	H	2.308775	-0.000038	1.474292
H	2.043316	-0.449027	-1.639644	C	-1.689386	-1.250172	0.114991
F	-2.397137	-0.895716	-0.372855	H	-2.133410	-1.261970	1.118680
H	-0.823547	-1.695383	0.608517	H	-2.483849	-1.263871	-0.642711
				H	-1.018159	-2.104697	-0.017343
				H	1.813450	0.000063	-1.631929
TS-CH₂F							
C	0.862918	-1.549208	-0.908463				
C	0.836359	-1.944835	0.431244	TS-Me			
C	1.786938	-1.149002	1.120974	C	1.037899	-1.287593	-0.733387
C	2.343332	-0.292758	0.192937	C	1.169508	-1.459770	0.656203
N	1.792028	-0.563072	-1.024884	C	2.010577	-0.430771	1.127960
H	2.021226	-0.076575	-1.884666	C	2.373945	0.326079	0.026734
H	0.358856	-1.957561	-1.781042	N	1.826391	-0.229870	-1.083413
H	0.232403	-2.750359	0.843940	H	1.935892	0.124452	-2.027528
H	2.022023	-1.182210	2.182642	H	0.618990	-1.948616	-1.487872
H	3.090462	0.489056	0.307433	H	0.713395	-2.257110	1.239230
C	-1.078893	-0.254516	-0.004804	H	2.297440	-0.238031	2.159160
C	-2.073552	-1.072231	-0.241144	H	2.994136	1.217802	-0.040713
C	-0.408135	1.299748	1.707020	C	-0.844660	-0.248996	-0.079535
H	-1.217446	2.002117	1.955163	C	-1.773410	-1.182752	-0.075394
H	-0.463171	0.417510	2.352450	C	-0.558339	1.665891	1.343395
H	0.563582	1.790855	1.829597	H	-1.490039	2.238469	1.474726
N	-0.567058	0.879828	0.307366	H	-0.479365	0.908469	2.130994
C	-3.499740	-0.608101	-0.198747	H	0.297965	2.350275	1.402915
H	-3.972920	-0.797651	-1.173832	N	-0.577625	1.012362	0.034790
H	-4.047121	-1.193975	0.554842	C	-3.233059	-0.854593	0.012599
H	-3.583837	0.459205	0.042322	H	-3.758273	-1.251733	-0.869455
C	-0.296525	1.872917	-0.728058	H	-3.666283	-1.344338	0.898336
H	-0.966527	2.730273	-0.563199	H	-3.413063	0.226649	0.078844
H	-1.873542	-2.119331	-0.477435	C	-0.493918	1.877864	-1.140090
F	0.988244	2.305163	-0.631300	H	-1.374969	2.537695	-1.163436
H	-0.469183	1.412815	-1.709644	H	0.414173	2.493692	-1.089317
				H	-0.478042	1.266383	-2.049384

H -1.484580 -2.233656 -0.147045

TS-Me' (DCM)

C 0.874598 -1.390543 -0.679012
C 0.995951 -1.529402 0.715355
C 2.076157 -0.720266 1.123846
C 2.585954 -0.125052 -0.017411
N 1.887429 -0.574945 -1.090340
H 2.055859 -0.301470 -2.052474
H 0.289809 -1.955887 -1.400562
H 0.378996 -2.164768 1.347583
H 2.429254 -0.561728 2.140213
H 3.407536 0.578390 -0.137903
C -0.690401 0.139552 -0.052674
C -1.880335 -0.438803 -0.019462
C 0.147314 1.936530 1.304510
H -0.597178 2.739783 1.425335
H 0.036020 1.209463 2.116251
H 1.154786 2.371623 1.336630
N -0.065507 1.272723 0.019269
C -3.071563 0.490836 0.042663
H -3.731653 0.297502 -0.817046
H -3.649591 0.279733 0.955826
H -2.787180 1.550723 0.039698
C 0.227008 2.055174 -1.179529
H -0.457884 2.916795 -1.223009
H 1.261436 2.422937 -1.147058
H 0.080191 1.435576 -2.071436
C -2.206218 -1.898514 -0.047822
H -2.831858 -2.113277 -0.928158
H -1.334545 -2.558842 -0.068742
H -2.808243 -2.148072 0.839577

TS-Me' (Et₂O)

C 0.882653 -1.396742 -0.675721
C 0.996975 -1.520614 0.719756
C 2.076192 -0.707992 1.125256
C 2.591226 -0.124237 -0.018206
N 1.893897 -0.581270 -1.090455
H 2.076438 -0.329717 -2.055463
H 0.299203 -1.968095 -1.393687
H 0.381219 -2.153010 1.356003
H 2.428517 -0.545212 2.141109
H 3.417882 0.572763 -0.141447
C -0.697173 0.143865 -0.050187
C -1.883647 -0.440924 -0.018419
C 0.147288 1.940951 1.301801
H -0.594810 2.746040 1.424988
H 0.037957 1.214689 2.114448
H 1.155848 2.373604 1.330891
N -0.071344 1.276156 0.017602
C -3.079768 0.483210 0.036661
H -3.737721 0.282502 -0.822896
H -3.658698 0.274927 0.949809
H -2.801933 1.544768 0.028375
C 0.222193 2.055529 -1.183007
H -0.461990 2.917494 -1.230697
H 1.256464 2.423782 -1.150980
H 0.075527 1.433854 -2.073522
C -2.201876 -1.902451 -0.042577
H -2.814231 -2.126783 -0.929877
H -1.326924 -2.558762 -0.046714
H -2.815010 -2.150606 0.837489

S7. References

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