

Revisiting Oxime-Nitrone Tautomerism. Evidences of Nitrone Tautomer Participation in Oxime Nucleophilic Addition Reactions

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Starting materials

Table S1. Calculated (M06-2X/cc-pVTZ) absolute (hartrees) and relative (kcal/mol) energies of the oximes **1a-c** and nitrones **2a-c** in different environments (PCM model used when needed).

		E_0	ΔE_0^a	G	ΔG^a
gas	1a	-169.763099	0.0	-169.787344	0.0
	2a	-169.741257	13.7	-169.765342	13.8
	1b	-456.078061	0.0	-456.111587	0.0
	2b	-456.057214	13.1	-456.090581	13.2
	1c	-456.069386	5.4	-456.103024	5.4
	2c	-456.044733	20.9	-456.078203	20.9
MeCN	1a	-169.768618	0.0	-169.792893	0.0
	2a	-169.753081	9.8	-169.777172	9.9
	1b	-456.087815	0.0	-456.121499	0.0
	2b	-456.073455	9.0	-456.106908	9.2
	1c	-456.079226	6.2	-456.113043	5.8
	2c	-456.062667	15.8	-456.096074	16.0
EtOH	1a	-169.768505	0.0	-169.792780	0.0
	2a	-169.752826	9.8	-169.776916	10.0
	1b	-456.087600	0.0	-456.121283	0.0
	2b	-456.073111	9.1	-456.106562	9.2
	1c	-456.077768	6.2	-456.112000	5.8
	2c	-456.062242	15.9	-456.095633	16.1

^a Referred to **1a** or **1b**.

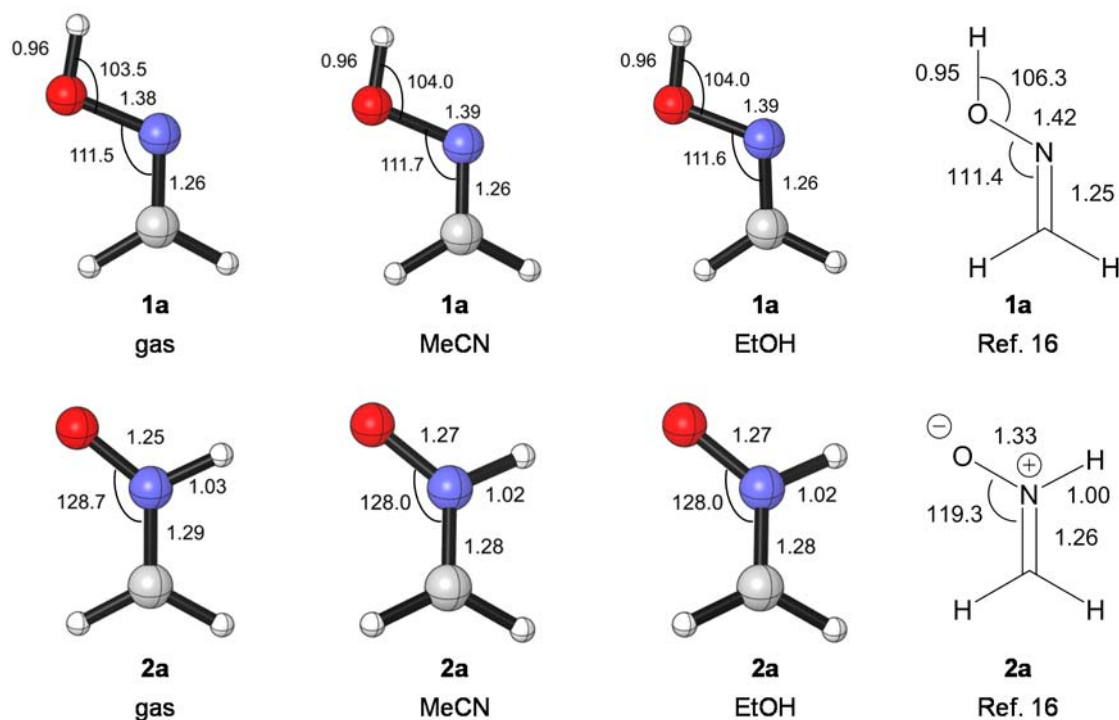


Figure S1. Optimized geometries (M06-2X/cc-pVTZ) in gas phase, MeCN and EtOH of oxime **1a** and nitrone **2a**. Data from ref. 16 (Radom and co-workers) of the manuscript are also included for comparison. Distances are given in angstroms, angles in degrees.

Oxime-Nitrone tautomerism

Unimolecular direct 1,2-H shift

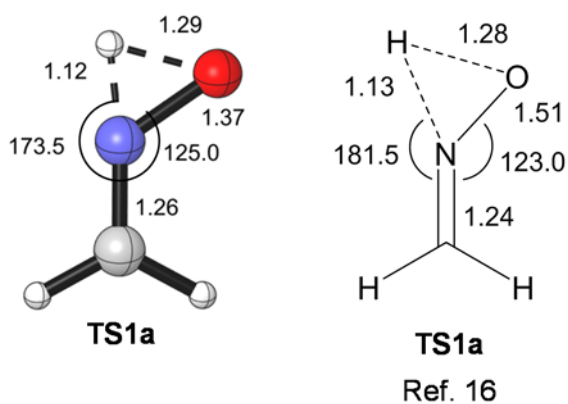


Figure S2. Optimized transition structure (M06-2X/cc-pVTZ) in gas phase for isomerization of oxime **1a** into nitrone **2a** through 1,2H-shift. Data from ref. 16 (Radom and co-workers) of the manuscript are also included for comparison. Distances are given in angstroms. Angles are given in degrees.

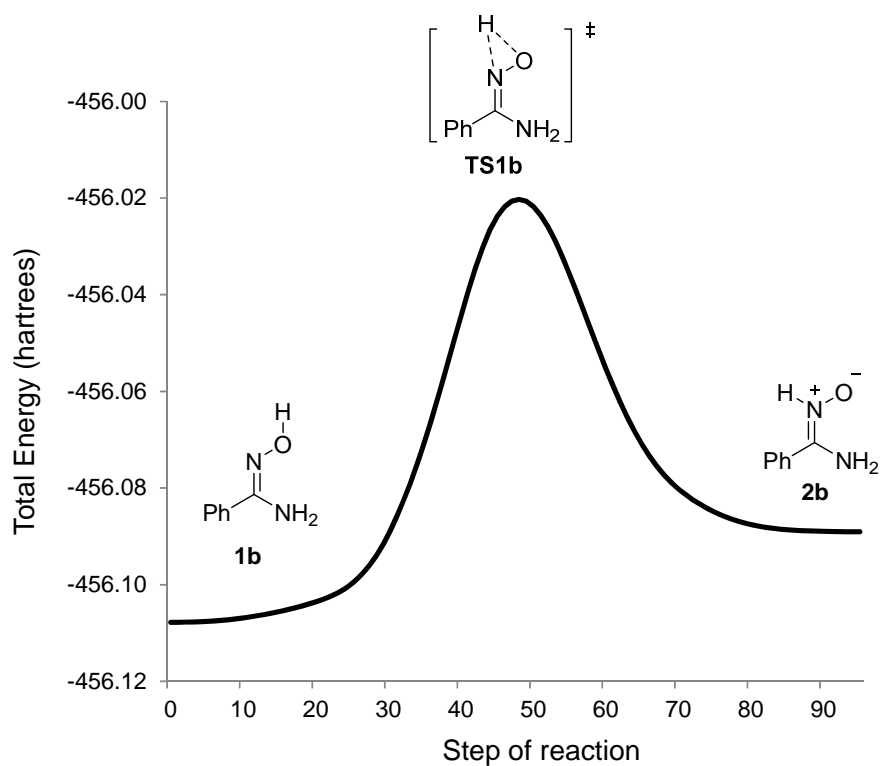
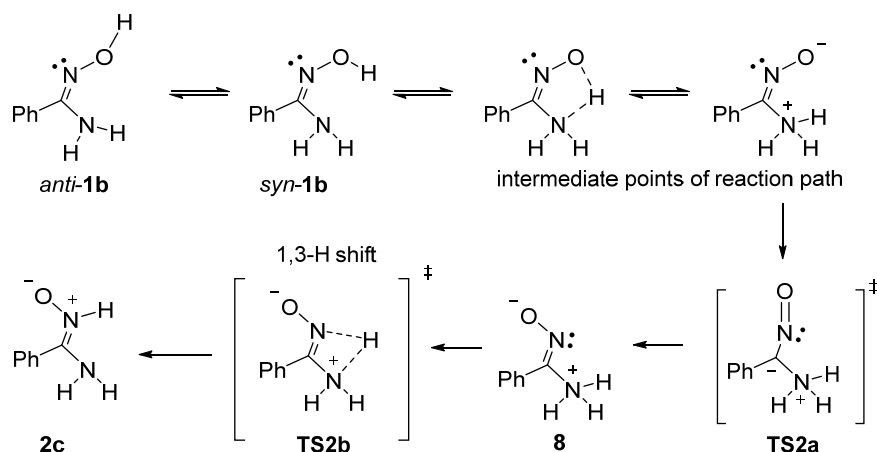


Figure S3. Calculated IRC (M06-2X/cc-pVTZ/PCM=EtOH) for isomerization of oxime **1b** into nitrone **2b** through 1,2H-shift.

Unimolecular 1,2-H shift promoted by neighboring groups



Scheme S1. 1,2-H shift promoted by neighboring groups.

Merged IRCs of the two steps of the reaction is shown in Figure S4. Point 101 is the final point of the first IRC connecting **1b** with **8**. Actually, the first point of the IRC corresponds to the *syn* conformer of oxime **1b**. However, any attempt of minimizing such a conformer led to the more stable *anti* isomer and no stationary point could be found for *syn-1b*. Point 102 is the initial point of the second IRC connecting **8** with **2c**. At this point, intermediate **8** is found as a stationary point (minimum).

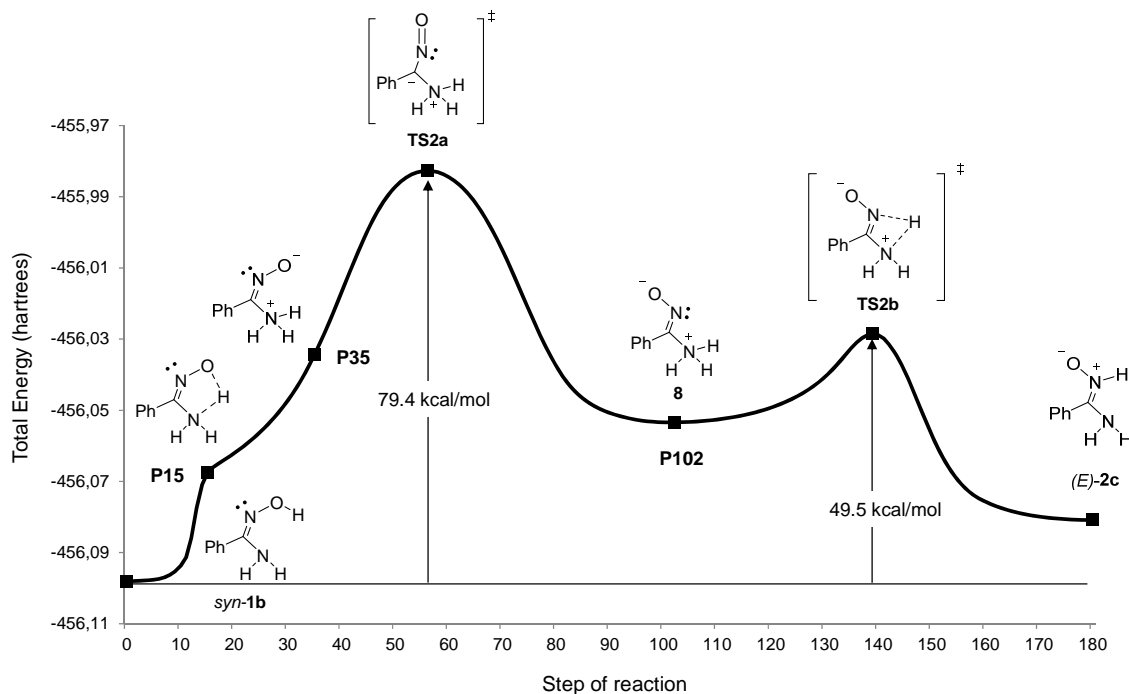


Figure S4. Merged IRCs (M06-2X/cc-pVTZ/PCM=EtOH) corresponding to the isomerization of **1b** into **2c** promoted by neighboring amino group.

The initial proton transfer from oxime to amino group takes place at the start of the reaction and it does not correspond with any stationary point. At point 15 the proton is at middle distance of oxygen and nitrogen atoms. It could be possible to consider the presence of a hidden intermediate in the first stage of the reaction. Admittedly, point 15 might be considered to be close to a hidden transition state. At point 35 the proton is completely transferred. The presence of hidden intermediates has been observed in several situations¹ and also in this case we observed how the RMS gradient norm dips, approaching but not reaching 0, leading to a so-called hidden intermediate (Figure S5).

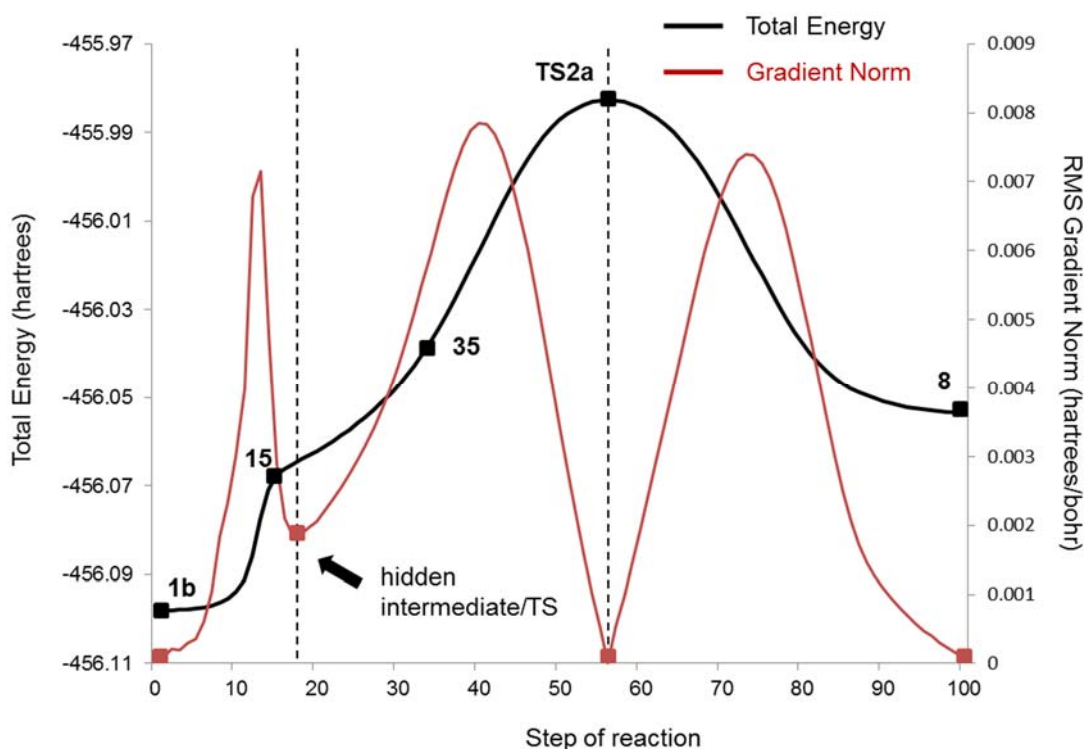


Figure S5. Computed (M06-2X/cc-pVTZ/PCM=EtOH) intrinsic reaction coordinate (IRC) for the transformation of **1b** into **8** showing the total energy (left axis, black line) and the gradient norm showing a prominent hidden intermediate (right axis, red line).

TS2a (point 57) corresponds to the required C-N rotation for orienting adequately the nitrogen lone pair. Such a rotation can take place because there is a rearrangement of the electronic distribution of the C=N-O⁻ system which temporary evolves to ⁻C-N=O. At point 103 the C=N-O⁻ system is recovered and intermediate **8** is formed, and it corresponds with a minimum. The change of the electronic distribution in the C-N-O

¹ (a) Armstrong, A.; Boto, R. A.; Dingwall, P.; Contreras-Garcia, J.; Harvey, M. J.; Masona, N. J.; Rzepa, H. S., *Chem. Sci.* **2014**, *4*, 2057-2071. (b) Roca-López, D.; Polo, V.; Tejero, T.; Merino, P., *J. Org. Chem.* **2015**, *80*, 4076-4083. (c) Roca-López, D.; Polo, V.; Tejero, T.; Merino, P., *Eur. J. Org. Chem.* **2015**, 4143-4152.

system is evidenced by monitoring the distance of the N-O bond which goes from 1.35 Å at the start of the reaction (oxime) to 1.19 Å in **TS2a** more in agreement with a typical distance of a nitroso group. After the transition structure, in **8**, the N-O bond has a distance of 1.27 Å (Figure S6).

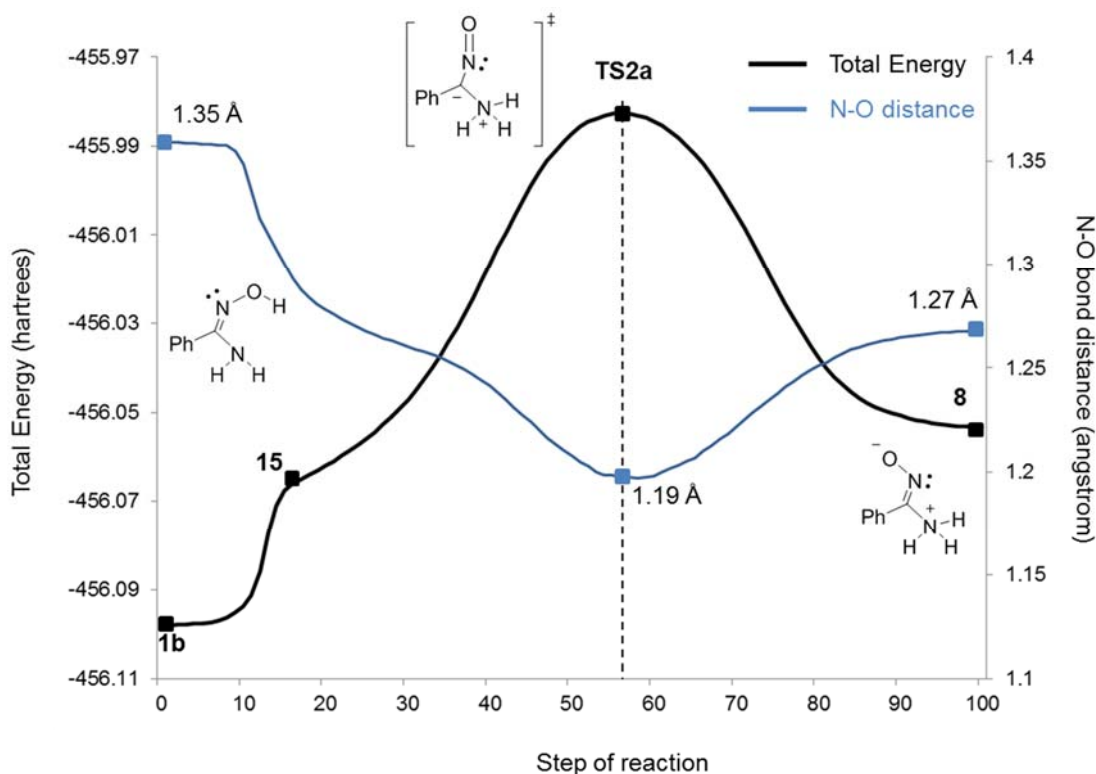


Figure S6. Computed (M06-2X/cc-pVTZ/PCM=EtOH) intrinsic reaction coordinate (IRC) for the transformation of **1b** into **8** showing the total energy (left axis, black line) and the evolution of the distance corresponding to N-O bond (right axis, red line).

Finally, **TS2b** (point 140) corresponds to the proton transfer from the amino group to the nitrogen atom to form the (*E*)-nitron **2c**.

A deeper analysis, including topological analyses (ELF), should be required to ascertain if we are in front of a typical one step two stage process as defined by Domingo and co-workers.² However, the observed barrier is so high that we did not consider further studies on this mechanism.

² Domingo, L. R.; Saez, J. A.; Zaragoza, R. J.; Arno, M. *J. Org. Chem.* **2008**, *73*, 8791–8799.

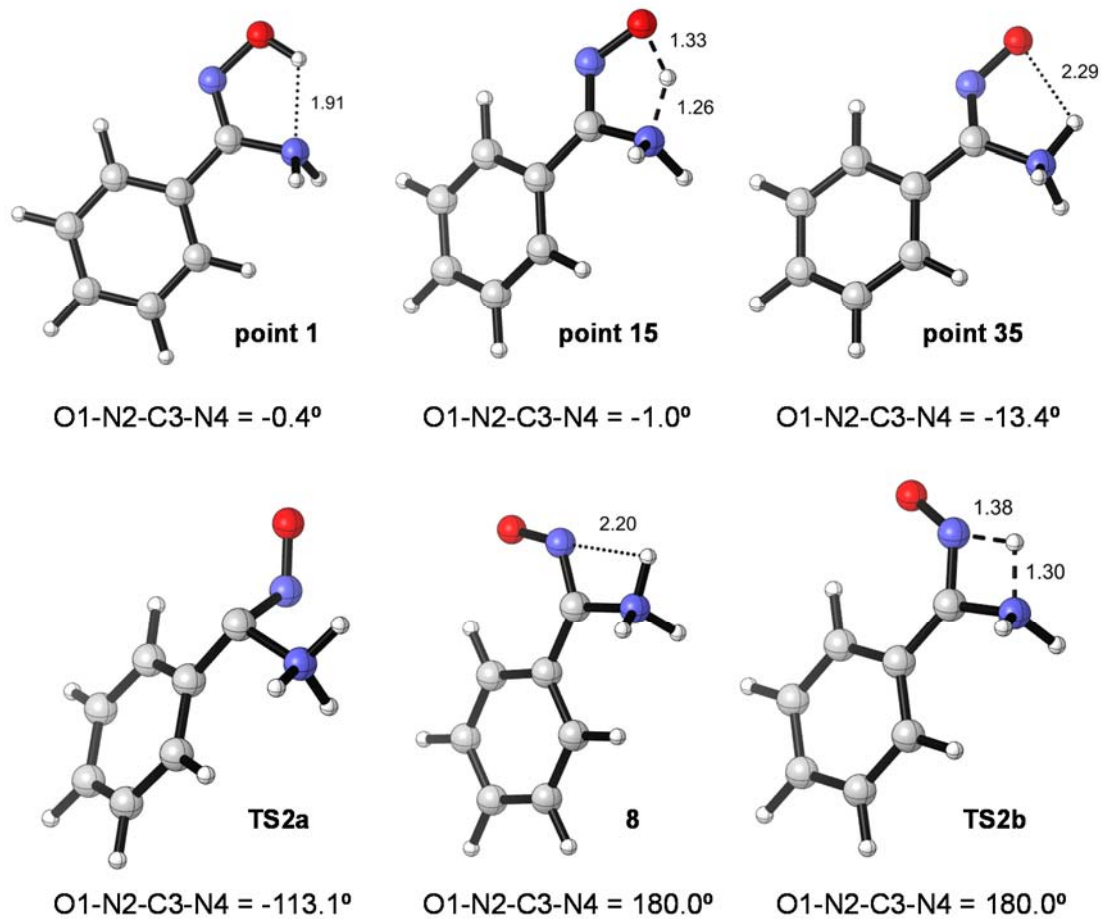


Figure S7. Optimized geometries (M06-2X/cc-pVTZ/PCM=EtOH) of non-stationary points 1, 15 and 35 of the IRC, transition structures **TS2a,b** and intermediate **8**; all of them corresponding to isomerization of oxime **1b** into nitrone **2c** through neighboring amino group participation. Distances are given in angstroms.

Bimolecular mechanism promoted by a discrete molecule of EtOH

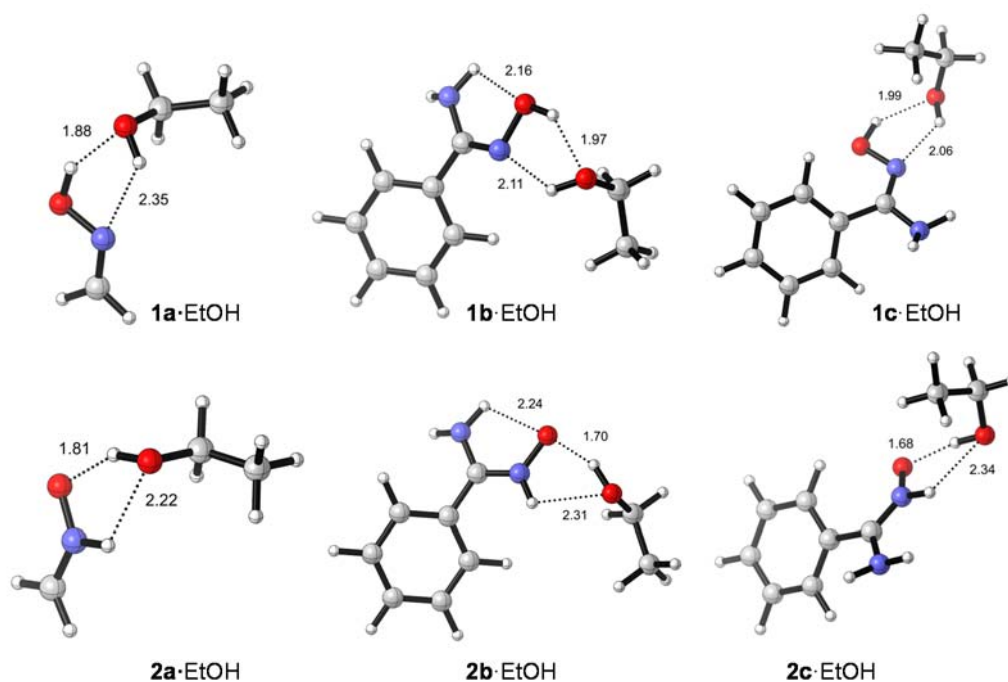


Figure S8. Optimized geometries (M06-2X/cc-pVTZ/PCM=EtOH) of initial and final complexes with EtOH. Distances are given in angstroms.

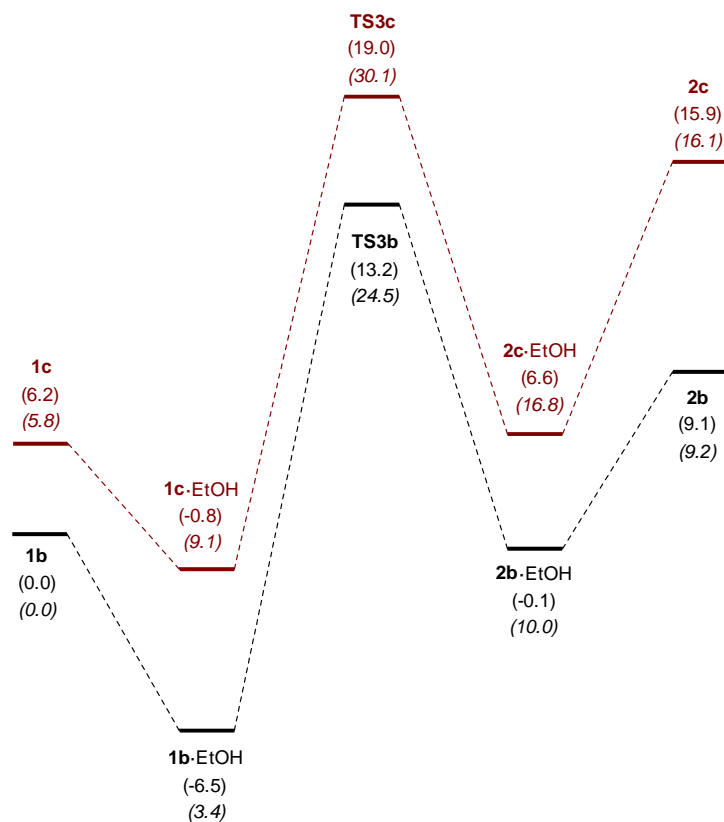


Figure S9. Energy diagram (M06-2X/cc-pVTZ/PCM=EtOH) for isomerization of **1b,c** into **2b,c** promoted by a discrete molecule of ethanol. Relative energies are referred to the most stable **1b** and correspond to E_0 in order to compare adequately unimolecular entities with bimolecular complexes. Free energy barriers (ΔG) are given in italic font. Energies are given in kcal/mol.

Bimolecular mechanism via oxime dimer complexes

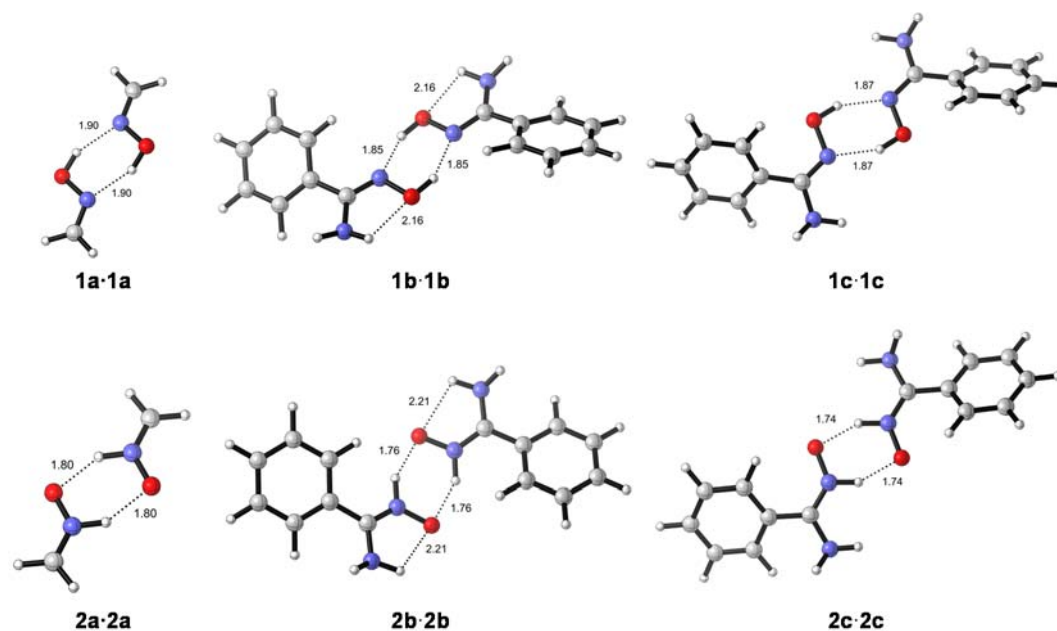


Figure S10. Optimized geometries (M06-2X/cc-pVTZ/PCM=EtOH) of initial and final dimer complexes. Distances are given in angstroms.

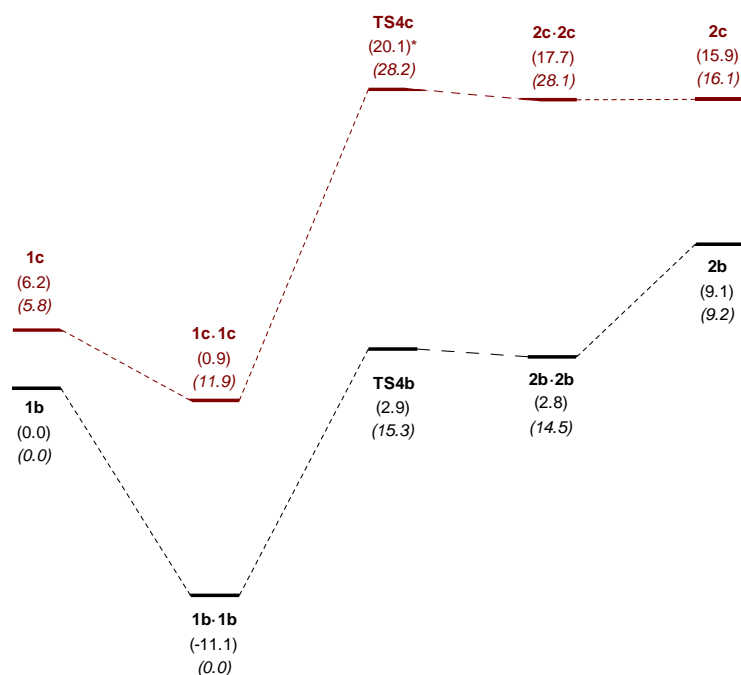
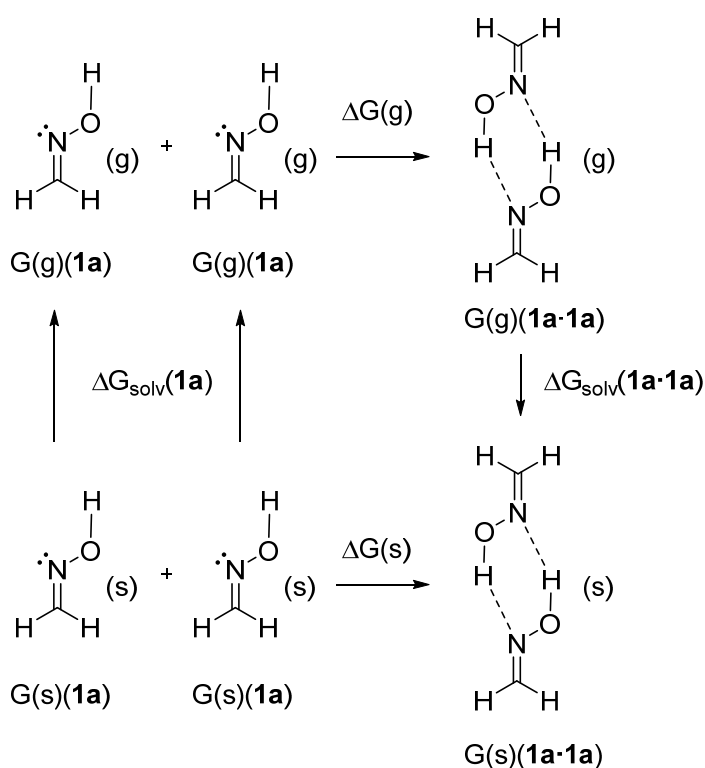


Figure S11. Energy diagram (M06-2X/cc-pVTZ/PCM=EtOH) for isomerization of **1b** and **1c** into **2b** and **2c**, respectively, through a bimolecular mechanism involving two oxime molecules. Relative energies (kcal/mol) are referred to the most stable **1b** and correspond to E_0 in order to compare adequately unimolecular entities with bimolecular complexes. Free energy barriers (ΔG) are given in italic font. *: Values corresponding to E without ZPVE correction. After ZPVE correction the value for **TS4c** is 16.7 kcal/mol indicating a close proximity to **2c·2c**, within the experimental error, already revealed when ZPVE correction is applied.³

³ In fact, even though the error in the electronic energy can be narrowed down to 1 kcal/mol, the error in the ZPE can reach 3 kcal/mol. See: *Computational Organic Chemistry* 2nd. Ed. Steven M. Baruch. Wiley. Hoboken. USA. 2014, p. 50

Solvation considerations

In the case of the reactions carried out in ethanol as a solvent, the formation of the oxime pair **1•1** requires desolvation of two molecules of oxime which is not necessary in the ethanol-assisted mechanism. However, it is also necessary to consider the additional solvation energy of the newly formed oxime dimer, which compensate desolvation of oximes **1**. We have calculated the solvation energy for oxime **1a** ($\Delta G_{\text{solv}} = -3.4$ kcal/mol) but it is also necessary to consider the solvation energy of the formed complex **1a•1a** ($\Delta G_{\text{solv}} = -4.2$ kcal/mol). The corresponding difference is already included in the formation of the dimer by including the solvent model. The thermodynamic cycle illustrated in Scheme S2 should be considered.



Scheme S2. Thermodynamic cycle considering solvation of species.

where

$$\Delta G_{\text{solv}}(\mathbf{1a}) = G(s)(\mathbf{1a}) - G(g)(\mathbf{1a})$$

$$\Delta G_{\text{solv}}(\mathbf{1a}\cdot\mathbf{1a}) = G(s)(\mathbf{1a}\cdot\mathbf{1a}) - G(g)(\mathbf{1a}\cdot\mathbf{1a})$$

$$\Delta G(g) = G(g)(\mathbf{1a}\cdot\mathbf{1a}) - 2 \cdot G(g)(\mathbf{1a})$$

From the cycle,

$$\Delta G(s) = -[2 \cdot \Delta G_{\text{solv}}(\mathbf{1a})] + \Delta G(g) + \Delta G_{\text{solv}}(\mathbf{1a} \cdot \mathbf{1a})$$

by substitution:

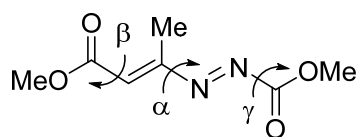
$$\begin{aligned} \Delta G(s) &= -[2 \cdot [G(s)(\mathbf{1a}) - G(g)(\mathbf{1a})]] + [G(g)(\mathbf{1a} \cdot \mathbf{1a}) - 2 \cdot G(g)(\mathbf{1a})] + [G(s)(\mathbf{1a} \cdot \mathbf{1a}) - \\ &G(g)(\mathbf{1a} \cdot \mathbf{1a})] = \\ &= -2 \cdot G(s)(\mathbf{1a}) + 2 \cdot G(g)(\mathbf{1a}) + G(g)(\mathbf{1a} \cdot \mathbf{1a}) - 2 \cdot G(g)(\mathbf{1a}) + G(s)(\mathbf{1a} \cdot \mathbf{1a}) - G(g)(\mathbf{1a} \cdot \mathbf{1a}) = \\ &= -2 \cdot G(s)(\mathbf{1a}) + G(s)(\mathbf{1a} \cdot \mathbf{1a}) \end{aligned}$$

Thus,

$$\Delta G(s) = G(s)(\mathbf{1a} \cdot \mathbf{1a}) - 2 \cdot G(s)(\mathbf{1a})$$

that corresponds to the calculation of $\Delta G(s)$ in a direct way considering solvent effects.

Conformational analysis of 1,2-diaza-1,3-diene **6**



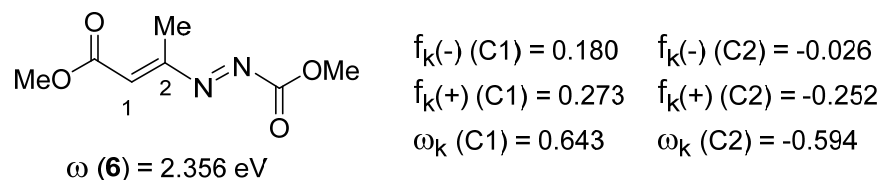
α -(*s-trans*)- β -(*s-cis*)- γ -(*s-cis*)-**6**

Table S2. Calculated (M06-2X/cc-pVTZ) absolute (hartrees) and relative (kcal/mol) energies for the eight main conformations of 1,2-diaza-1,3-diene **6** in different environments.

	α	β	γ	E_0	ΔE_0^a	G	ΔG^a	rel.ab. (%) ^b
gas	<i>s-cis</i>	<i>s-cis</i>	<i>s-cis</i>	-682.915647	2.6	-682.958840	2.7	0.5
	<i>s-cis</i>	<i>s-cis</i>	<i>s-trans</i>	-682.915942	2.4	-682.958982	2.6	0.6
	<i>s-cis</i>	<i>s-trans</i>	<i>s-cis</i>	-682.912891	4.3	-682.957403	3.6	0.1
	<i>s-cis</i>	<i>s-trans</i>	<i>s-trans</i>	-682.912902	4.3	-682.956452	4.2	0.0
	<i>s-trans</i>	<i>s-cis</i>	<i>s-cis</i>	-682.919818	0.0	-682.963159	0.0	50.6
	<i>s-trans</i>	<i>s-cis</i>	<i>s-trans</i>	-682.919746	0.0	-682.963039	0.1	44.6
	<i>s-trans</i>	<i>s-trans</i>	<i>s-cis</i>	-682.916570	2.0	-682.959731	2.2	1.3
	<i>s-trans</i>	<i>s-trans</i>	<i>s-trans</i>	-682.916710	2.0	-682.960207	1.9	2.2
MeCN	<i>s-cis</i>	<i>s-cis</i>	<i>s-cis</i>	-682.926498	2.3	-682.970204	2.5	1.2
	<i>s-cis</i>	<i>s-cis</i>	<i>s-trans</i>	-682.926628	2.2	-682.970969	2.0	2.7
	<i>s-cis</i>	<i>s-trans</i>	<i>s-cis</i>	-682.924497	3.5	-682.967869	3.9	0.1
	<i>s-cis</i>	<i>s-trans</i>	<i>s-trans</i>	-682.924520	3.5	-682.967915	3.9	0.1
	<i>s-trans</i>	<i>s-cis</i>	<i>s-cis</i>	-682.930092	0.0	-682.974129	0.0	76.2
	<i>s-trans</i>	<i>s-cis</i>	<i>s-trans</i>	-682.929675	0.3	-682.972357	1.1	11.7
	<i>s-trans</i>	<i>s-trans</i>	<i>s-cis</i>	-682.927966	1.3	-682.971609	1.6	5.3
	<i>s-trans</i>	<i>s-trans</i>	<i>s-trans</i>	-682.927701	1.5	-682.971000	2.0	2.8
EtOH	<i>s-cis</i>	<i>s-cis</i>	<i>s-cis</i>	-682.926270	2.8	-682.969994	2.5	0.6
	<i>s-cis</i>	<i>s-cis</i>	<i>s-trans</i>	-682.926271	2.4	-682.969995	1.3	4.1
	<i>s-cis</i>	<i>s-trans</i>	<i>s-cis</i>	-682.924221	3.7	-682.966374	3.6	0.1
	<i>s-cis</i>	<i>s-trans</i>	<i>s-trans</i>	-682.924201	3.7	-682.967219	3.1	0.2
	<i>s-trans</i>	<i>s-cis</i>	<i>s-cis</i>	-682.929583	0.4	-682.972606	0.0	40.2
	<i>s-trans</i>	<i>s-cis</i>	<i>s-trans</i>	-682.930114	0.0	-682.972089	0.0	38.0
	<i>s-trans</i>	<i>s-trans</i>	<i>s-cis</i>	-682.927384	1.7	-682.970531	1.0	7.3
	<i>s-trans</i>	<i>s-trans</i>	<i>s-trans</i>	-682.927474	1.7	-682.970774	0.9	9.4

^a Referred to the most stable conformer. ^b According to Boltzmann's distribution

Reactivity indices of 1,2-diaza-1,3-diene **6**.



The reactivity indices⁴ of **6** clearly indicate that the more electrophilic carbon is C1 in agreement with experimental findings on nucleophilic additions to 1,2-diaza-1,3-dienes.⁵

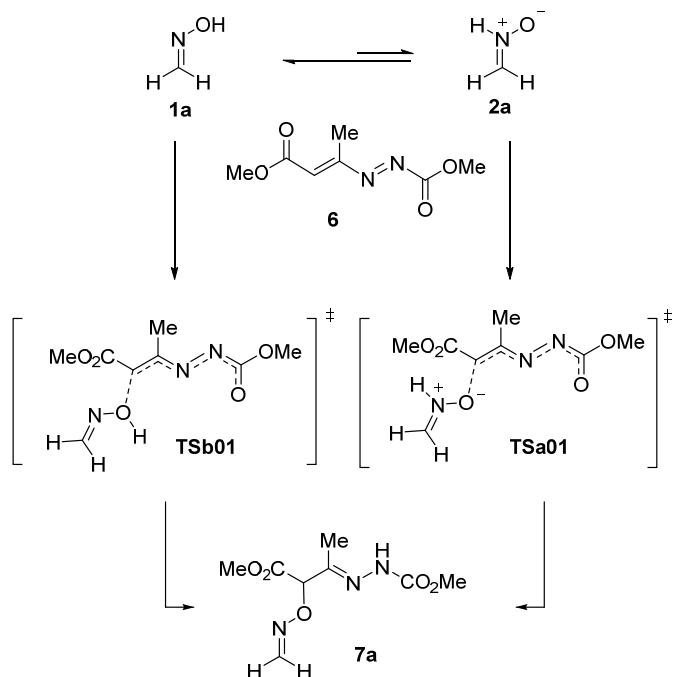
⁴ Chattaraj, P.K.; Sarkar, U.; Roy, D. R. *Chem. Rev.* **2006**, *106*, 2065-2091.

⁵ For recent examples see: (a) Mantenuto, S.; Mantellini, F.; Favi, G.; Attanasi, O. A., *Org. Lett.* **2015**, *17*, 2014-2017. (b) De Crescentini, L.; Attanasi, O. A.; Campisi, L. A.; Favi, G.; Lillini, S.; Ursini, F.; Mantellini, F., *Tetrahedron* **2015**, *71*, 7282-7292

Michael addition of arylamidoximes to 1,2-diaza-1,3-dienes

Model system. Addition of 1a to 6.

The addition of oxime **1a** to **6** was studied as a model system (Scheme S3).



Scheme S3. Reaction paths for the addition of oxime **1a** to 1,2-diaza-1,3-diene **6**.

The most stable $\beta(s\text{-cis}),\gamma(s\text{-cis})$ -**6** was used for the initial systematic study. We have considered oxime and nitronium tautomers. For each tautomer of oxime and nitronium and conformer of **6**, three staggered approaches of two face-oriented nucleophile (oxime or nitronium) have been considered making a total of 12 initial transition structures. Once these approaches have been studied, variability conformational of 1,2-diaza-1,3-diene **6** at β and γ dihedral angles ($s\text{-cis}$ and $s\text{-trans}$ conformations) has been checked, covering a complete PES of 96 transition structures (Figure S12).

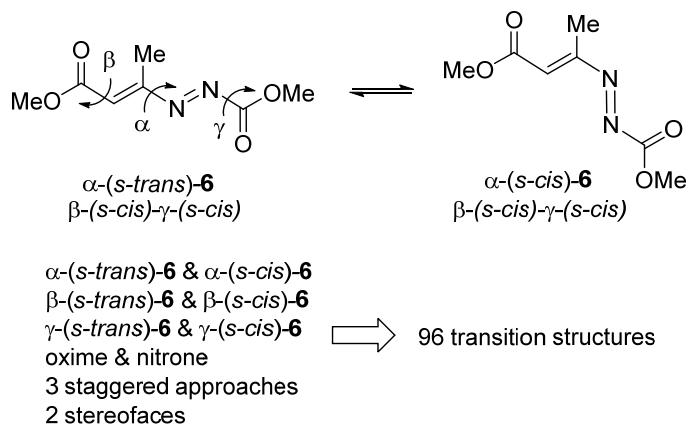


Figure S12. Computational approach to study the reaction between oxime **1a** and 1,2-diaza-1,3-diene **6**. Definition of PES.

After optimization (M06-2X/cc-pVTZ/PCM=EtOH) of the 96 approaches illustrated in Figure S12, 37 independent TSs were located (Table S3). In Table S3, TSs are ordered by relative abundance according to Boltzmann's distribution. Notably, 22 TSs account for 100% of probability and from those 22, 12 contribute for more than 1%, accounting for 95.6% of probability. Note that all attacks of the nitron isomer are lower in energy than those corresponding to the oxime isomer, the first entry corresponding to an oxime attack being #30 with a relative free energy of 7.4 kcal/mol.

Table S3. Calculated (M06-2X/cc-pVTZ/PCM=EtOH) absolute (hartrees) and relative (kcal/mol) energies for transition structures of the reaction of oxime **1a** and nitron **2a** with 1,2-diaza-1,3-diene **6**.

entry	TS	O/N ^a	face ^b	stag. ^c	α^d	β^d	γ^d	G	$\Delta\Delta G^e$	rel.ab. ^f	im. freq.
1	TSa01	N	Re	g	t	c	c	-852.716990	0.0	20.5	-376.6
2	TSa02	N	Re	d	t	c	t	-852.716831	0.1	17.3	-370.2
3	TSa03	N	Si	g	t	t	c	-852.716665	0.2	14.5	-354.7
4	TSa04	N	Si	g	t	c	c	-852.716432	0.4	11.4	-361.8
5	TSa05	N	Si	g	t	c	t	-852.716040	0.6	7.5	-363.1
6	TSa06	N	Si	g	c	c	t	-852.715798	0.7	5.8	-352.2
7	TSa07	N	Re	g	t	t	t	-852.715604	0.9	4.7	-366.8
8	TSa08	N	Si	d	t	t	c	-852.715466	1.0	4.1	-384.2
9	TSa09	N	Re	d	t	t	c	-852.715384	1.0	3.8	-369.9
10	TSa10	N	Si	d	t	c	c	-852.715085	1.2	2.7	-399.9
11	TSa11	N	Si	g	t	t	t	-852.714861	1.3	2.2	-363.5
12	TSa12	N	Si	g	c	c	c	-852.714193	1.8	1.1	-357.8
13	TSa13	N	Si	g	c	t	c	-852.713899	1.9	0.8	-341.7
14	TSa14	N	Si	d	t	t	t	-852.713844	2.0	0.7	-390.5
15	TSa15	N	Re	g	c	t	c	-852.713756	2.0	0.7	-438.8
16	TSa16	N	Re	d	c	c	c	-852.713695	2.1	0.6	-376.2
17	TSa17	N	Re	d	c	t	c	-852.713325	2.3	0.4	-360.8
18	TSa18	N	Re	a	c	c	c	-852.713156	2.4	0.4	-454.7
19	TSa19	N	Si	g	c	t	t	-852.712937	2.5	0.3	-339.2
20	TSa20	N	Re	d	c	c	t	-852.712405	2.9	0.2	-370.3
21	TSa21	N	Re	d	c	t	t	-852.712308	2.9	0.1	-358.2
22	TSa22	N	Re	g	c	t	t	-852.712035	3.1	0.1	-435.1
23	TSa23	N	Re	g	c	c	t	-852.711266	3.6	0.0	-452.0
24	TSa24	N	Si	a	t	t	t	-852.710910	3.8	0.0	-384.7
25	TSa25	N	Re	a	t	c	c	-852.709377	4.8	0.0	-397.6
26	TSa26	N	Si	a	c	c	c	-852.709058	5.0	0.0	-437.0
27	TSa27	N	Si	a	c	c	t	-852.708372	5.4	0.0	-435.3
28	TSa28	N	Si	a	c	t	c	-852.706934	6.3	0.0	-432.8
29	TSa29	N	Si	a	c	t	t	-852.706262	6.7	0.0	-433.5
30	TSb01	O	Re	a	c	t	c	-852.705177	7.4	0.0	-691.9
31	TSb02	O	Re	a	c	c	c	-852.704795	7.7	0.0	-734.2
32	TSb03	O	Re	a	c	c	t	-852.703476	8.5	0.0	-765.5
33	TSb04	O	Re	a	c	t	t	-852.702990	8.8	0.0	-566.3
34	TSb05	O	Si	a	c	c	c	-852.701874	9.5	0.0	-449.9
35	TSb06	O	Si	a	c	c	t	-852.699489	11.0	0.0	-443.6
36	TSb07	O	Si	a	c	t	c	-852.697934	12.0	0.0	-422.7
37	TSb08	O	Si	a	c	t	t	-852.696194	13.0	0.0	-421.8

^a O and N correspond to oxime and nitron attacks, respectively. ^b Face indicates the two faces of the oxime/nitron considering the nitrogen atom. ^c Three staggered orientations of the oxime/nitron attack to **6**, defined as d (droite), g (gauche) and a (anti). See Figures S14 and S15. ^d c and t correspond to *s-cis* and *s-trans* conformations of **6**, respectively. ^e With respect to the most stable. ^f According to Boltzmann's distribution

The geometry of the most stable and representative transition structures corresponding to nitron (entry 1) and oxime (entry 30) nucleophilic attacks and the corresponding barriers of the reaction are given in Figure S13. Energy data are given in Table S4.

Table S4. Calculated (M06-2X/cc-pVTZ/PCM=EtOH) absolute (hartrees) and relative (kcal/mol) energies of the stationary points corresponding to addition of **1a** to **6**. Transition structure **TS4a** corresponding o isomerization of **1a** into **2a** has also been included for the purpose of comparison

	ΔE_0	$\Delta\Delta E_0^a$	ΔG	$\Delta\Delta G^a$
1a	-169.768505	0.0	-169.792780	0.0
2a	-169.752826	9.8	-169.776916	10.0
TS4a	-339.524943	7.6	-339.555692	18.7
TSa01	-852.670737	17.5	-852.716990	30.1
TSb01	-852.658219	25.4	-852.705177	37.5
7a	-852.741815	-27.1	-852.789231	-15.3

^a Referred to **1a**

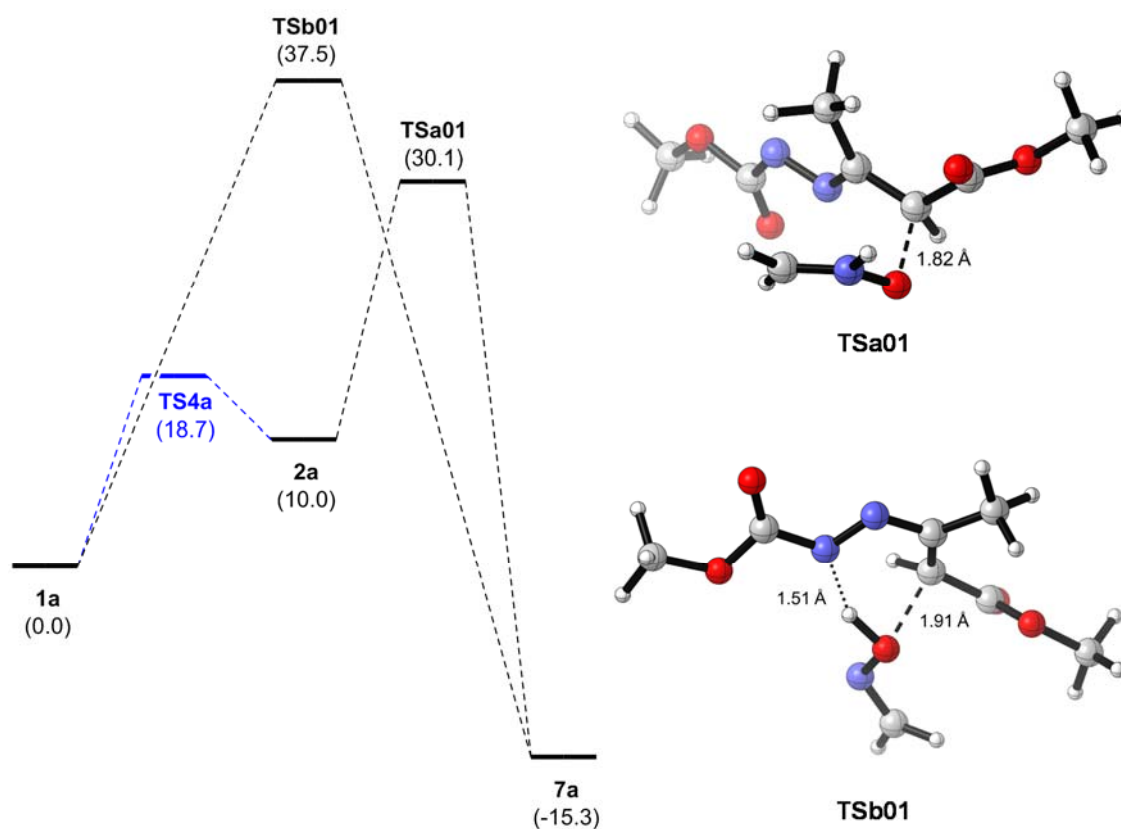


Figure S13. Optimized geometries (M06-2X/cc-pVTZ/PCM=EtOH) of the most stable transition structures corresponding to the attack of oxime **1a** (**TSb01**) and nitron **2a** (**TSa01**) to **6**. The transition state **TS4a** corresponding to isomerization (blue) of **1a** into **2a** has also been included for comparison. Relative free energies are given in kcal/mol.

Real system. Addition of **1b,c/2b,c** to **6**.

The most stable $\beta(s\text{-cis}),\gamma(s\text{-cis})$ -**6** was used for the first systematic study. We have also considered both *E* and *Z* configurations for oxime and nitron tautomers. For each isomer of oxime and nitron and conformer of **6**, three staggered approaches of two face-oriented nucleophile (oxime or nitron) have been considered making a total of 48 initial transition structures. Once these approaches have been studied, variability conformational of 1,2-diaza-1,3-diene **6** at β and γ dihedral angles (*s-cis* and *s-trans* conformations) has been checked, covering a complete PES of 192 (Figure S14).

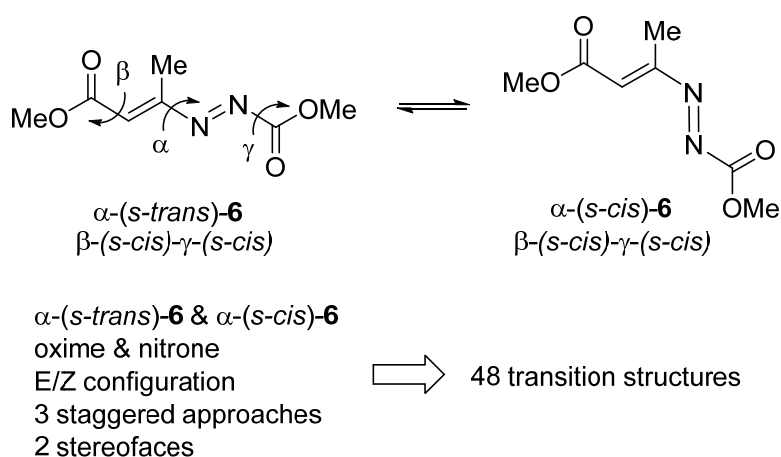


Figure S14. Computational approach to study the reaction between oxime **1b** and 1,2-diaza-1,3-diene **6**. Definition of PES.

In summary the following variability was initially considered:

- i) α -(*s-trans*)/ α -(*s-cis*),
- ii) oxime/nitron;
- iii) *E/Z* isomerism;
- iv) *Re/Si* faces of oxime/nitron and
- v) 3 staggered orientations (*droite*, *gauche*, *anti*) for the attack.

48 approaches were generated:

24 for of oximes **1b,c** (Figure S15) and

24 for nitrones **2b,c** (Figure S16)

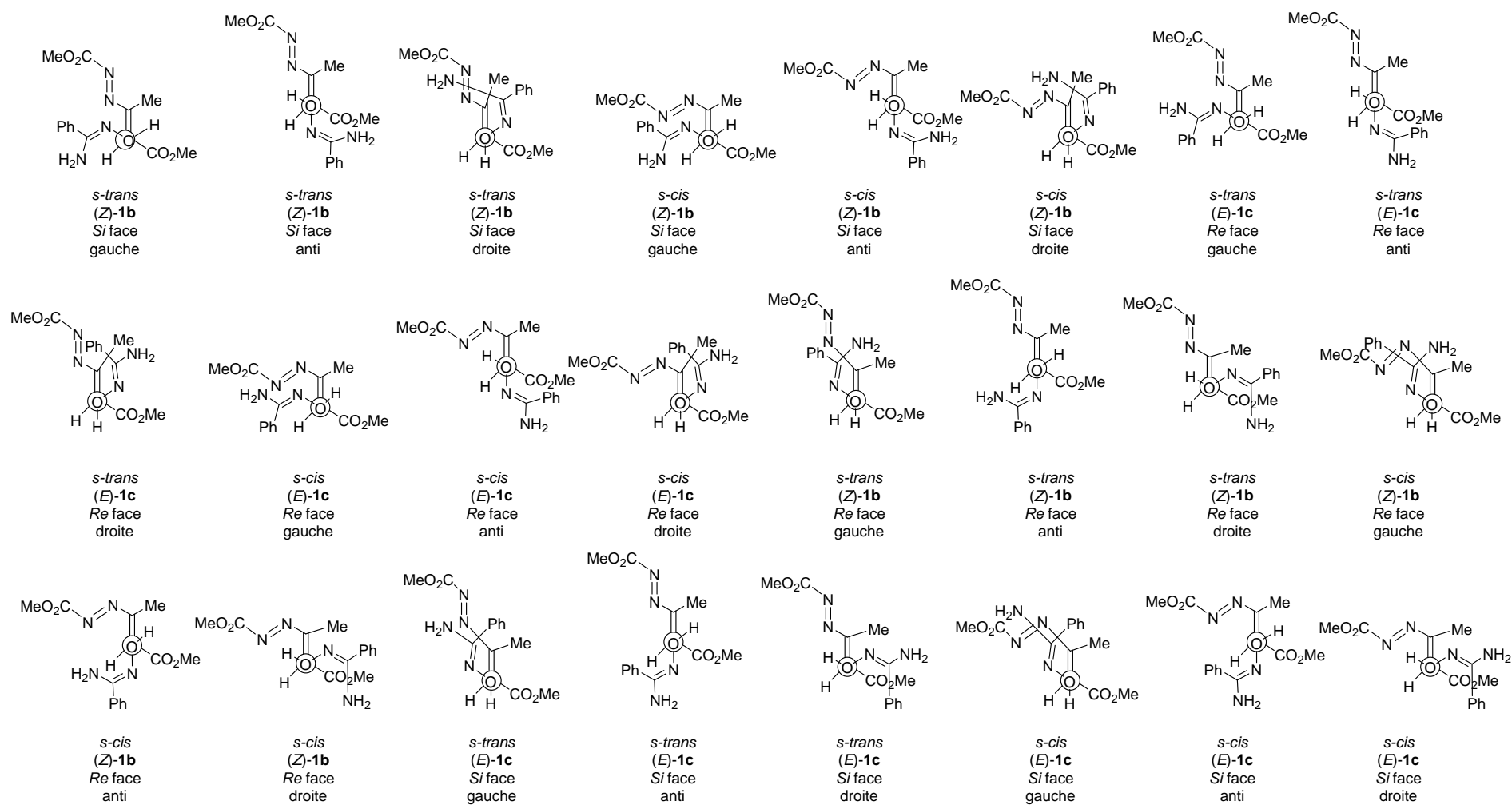


Figure S15. Approaches corresponding to the attack of oximes **1b** and **1c** to **6** (leading to TSS's).

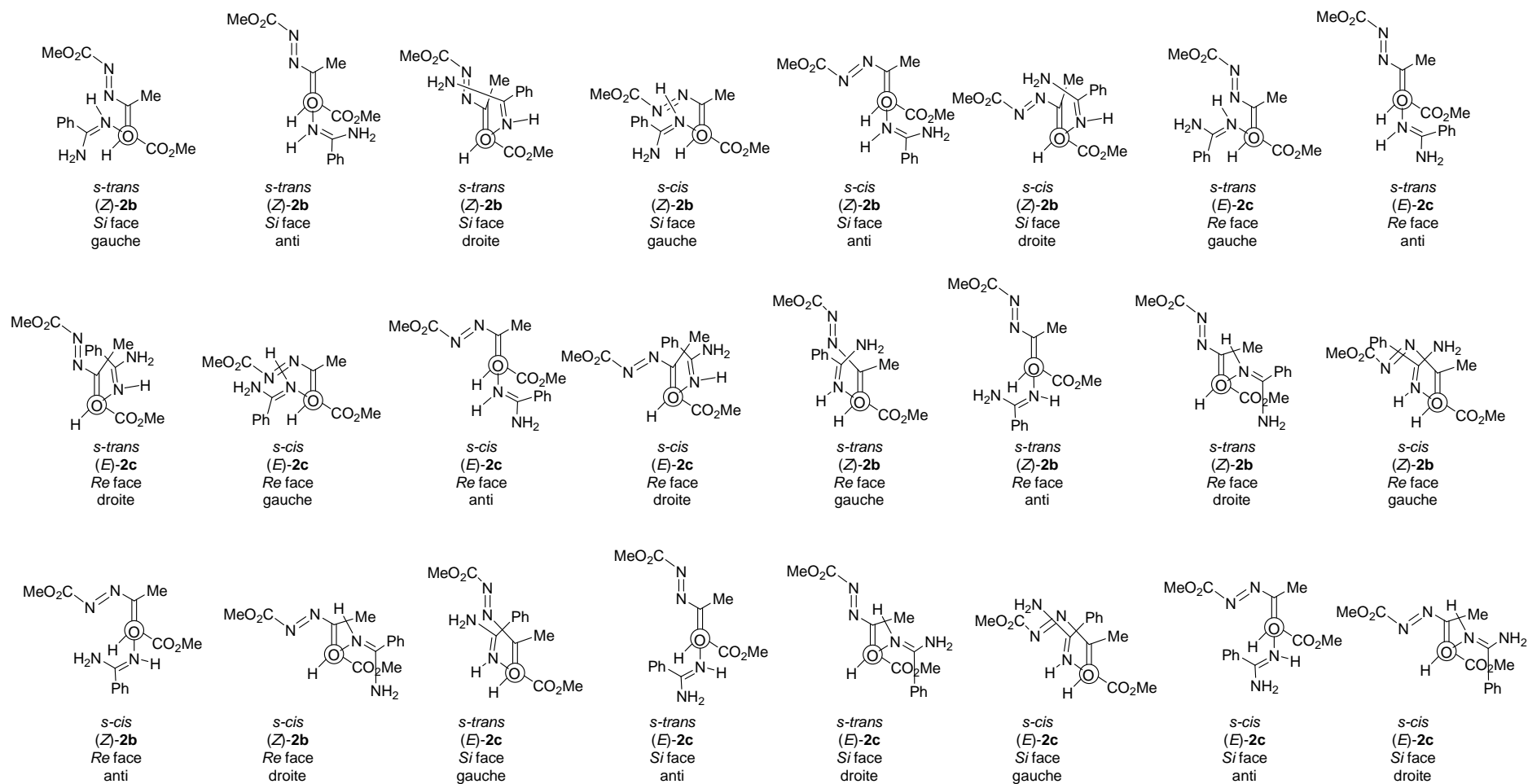


Figure S16. Approaches corresponding to the attack of nitrones **2b** and **2c** to **6** (leading to TS's).

After optimization of the 48 approaches illustrated in Figures S14 and S15, 38 independent TSs were obtained from which those with a relative energy above 15 kcal/mol with respect to the most stable were discarded. It remained 26 TSs which were checked for conformational variability (*s-cis/s-trans*) at β and γ dihedral angles of 6. 78 new TSs were calculated which were joined to the previous 26 (making a total of 104 structures). After full optimization at M06-2x/cc-pVDZ/PCM=EtOH level of theory, the 99 TSs collected in Table S5 were located as independent transition structures. In that table, those having β and γ as "c" are a part of the initial 48 approaches. In Table S4, TSs are ordered by relative abundance according to Boltzmann's distribution. Notably, 27 TSs account for 100% of probability and from those 27, only 8 contribute for more than 1%, accounting for 97.4% of probability. The line in the table marks the end of TS's accounting for 100% of abundance. Note that the first entry corresponding to an oxime attack is #55 with a relative free energy of 10.9 kcal/mol.

Table S5. Calculated (M06-2X/cc-pVDZ/PCM=EtOH) absolute (hartrees) and relative (kcal/mol) energies for transition structures of the reaction of oximes **1b,c** and nitrones **2b,c** with 1,2-diaza-1,3-diene **6**.

entry	O/N ^a	E/Z ^b	face ^c	stag. ^d	α^e	β^e	γ^e	G	$\Delta\Delta G^f$	rel.ab. ^g	im. freq.
1	N	Z	Si	g	t	t	c	-1138.742775	0.0	43.28	-275.3
2	N	Z	Si	g	t	c	c	-1138.742267	0.3	25.28	-277.0
3	N	Z	Re	d	t	t	c	-1138.740988	1.1	6.53	-291.9
4	N	Z	Re	g	t	c	c	-1138.740967	1.1	6.39	-287.3
5	N	Z	Si	g	t	c	t	-1138.740923	1.2	6.10	-266.7
6	N	Z	Re	d	t	c	c	-1138.740790	1.2	5.30	-293.7
7	N	Z	Re	d	t	c	t	-1138.740108	1.7	2.57	-297.8
8	N	Z	Si	g	t	t	t	-1138.739840	1.8	1.94	-265.9
9	N	Z	Si	a	t	c	c	-1138.738958	2.4	0.76	-220.1
10	N	Z	Re	d	c	c	c	-1138.738466	2.7	0.45	-286.6
11	N	Z	Re	g	t	c	t	-1138.737982	3.0	0.27	-281.8
12	N	Z	Re	d	c	t	c	-1138.737754	3.2	0.21	-264.5
13	N	Z	Re	d	t	t	t	-1138.737719	3.2	0.21	-280.2
14	N	Z	Re	d	c	c	t	-1138.737447	3.3	0.15	-293.9
15	N	Z	Si	g	c	c	t	-1138.737174	3.5	0.12	-251.1
16	N	Z	Re	g	t	t	t	-1138.736775	3.8	0.08	-286.2
17	N	Z	Si	g	c	c	c	-1138.736744	3.8	0.07	-262.1
18	N	E	Si	g	t	c	c	-1138.736614	3.9	0.06	-238.1
19	N	Z	Si	a	t	t	c	-1138.736544	3.9	0.06	-220.0
20	N	Z	Re	g	t	t	c	-1138.736168	4.1	0.04	-290.9
21	N	Z	Si	g	c	t	c	-1138.736025	4.2	0.03	-259.8
22	N	Z	Re	d	c	t	t	-1138.735524	4.6	0.02	-265.0
23	N	Z	Si	a	t	c	t	-1138.735137	4.8	0.01	-234.2
24	N	E	Si	g	t	t	c	-1138.734966	4.9	0.01	-235.7
25	N	E	Si	g	t	c	t	-1138.734586	5.1	0.01	-271.5
26	N	Z	Si	a	c	c	c	-1138.734437	5.2	0.01	-233.2
27	N	Z	Si	d	t	c	c	-1138.734365	5.3	0.01	-295.3
28	N	Z	Si	g	c	t	t	-1138.733613	5.7	0.00	-254.2
29	N	Z	Si	a	c	c	t	-1138.733599	5.8	0.00	-225.5
30	N	Z	Si	d	t	t	c	-1138.733580	5.8	0.00	-296.9
31	N	Z	Si	a	t	t	t	-1138.733538	5.8	0.00	-226.5

32	N	Z	Si	a	c	t	c	-1138.732982	6.1	0.00	-217.6
33	N	Z	Re	g	c	c	c	-1138.732899	6.2	0.00	-307.3
34	N	Z	Si	a	c	t	t	-1138.732779	6.3	0.00	-231.5
35	N	Z	Re	a	t	c	c	-1138.732766	6.3	0.00	-273.7
36	N	Z	Si	d	t	c	t	-1138.732398	6.5	0.00	-295.4
37	N	Z	Si	d	t	t	t	-1138.731290	7.2	0.00	-292.8
38	N	Z	Re	g	c	c	t	-1138.730939	7.4	0.00	-317.1
39	N	Z	Re	g	c	t	c	-1138.730678	7.6	0.00	-298.8
40	N	E	Si	g	t	t	t	-1138.730548	7.7	0.00	-283.0
41	N	E	Re	d	t	c	c	-1138.730342	7.8	0.00	-311.5
42	N	Z	Re	g	c	t	t	-1138.729656	8.2	0.00	-313.6
43	N	E	Re	g	t	c	c	-1138.729042	8.6	0.00	-310.3
44	N	E	Re	d	c	c	c	-1138.728592	8.9	0.00	-297.9
45	N	E	Si	d	t	c	c	-1138.728579	8.9	0.00	-290.4
46	N	Z	Si	d	c	c	c	-1138.727513	9.6	0.00	-314.4
47	N	E	Si	g	c	c	c	-1138.727377	9.7	0.00	-319.9
48	N	E	Si	a	t	c	c	-1138.727215	9.8	0.00	-275.9
49	N	E	Si	g	c	c	t	-1138.726968	9.9	0.00	-313.0
50	N	Z	Re	a	c	c	c	-1138.726763	10.0	0.00	-299.7
51	N	E	Re	g	t	t	c	-1138.725978	10.5	0.00	-303.8
52	N	E	Si	g	c	t	c	-1138.725968	10.5	0.00	-313.7
53	N	E	Si	g	c	t	t	-1138.725544	10.8	0.00	-311.4
54	N	E	Si	a	t	t	c	-1138.725469	10.9	0.00	-273.7
55	O	Z	Re	a	c	c	c	-1138.725404	10.9	0.00	-321.6
56	N	E	Si	a	t	c	t	-1138.725165	11.1	0.00	-276.5
57	N	E	Si	a	t	t	t	-1138.724150	11.7	0.00	-277.8
58	N	E	Re	g	c	c	c	-1138.723890	11.9	0.00	-331.2
59	O	Z	Re	a	c	t	c	-1138.723621	12.0	0.00	-586.5
60	N	E	Re	g	t	c	t	-1138.723518	12.1	0.00	-332.7
61	O	Z	Si	a	t	c	c	-1138.723505	12.1	0.00	-340.7
62	N	E	Re	g	c	c	t	-1138.723448	12.1	0.00	-340.0
63	O	Z	Re	a	c	c	t	-1138.723344	12.2	0.00	-584.5
64	N	E	Re	a	t	c	c	-1138.722072	13.0	0.00	-273.8
65	N	E	Re	g	c	t	c	-1138.721784	13.2	0.00	-321.2
66	O	Z	Re	a	c	t	t	-1138.721514	13.3	0.00	-554.2
67	N	E	Re	g	t	t	t	-1138.721375	13.4	0.00	-325.7
68	O	Z	Si	a	c	t	c	-1138.720934	13.7	0.00	-404.5
69	O	Z	Si	a	c	c	c	-1138.720866	13.7	0.00	-401.3
70	N	E	Re	g	c	t	t	-1138.720535	14.0	0.00	-337.3
71	O	Z	Si	a	c	c	t	-1138.720313	14.1	0.00	-397.1
72	O	Z	Re	d	t	c	c	-1138.720085	14.2	0.00	-198.9
73	N	E	Si	a	c	c	c	-1138.720057	14.3	0.00	-297.5
74	N	E	Si	a	c	t	c	-1138.719563	14.6	0.00	-298.6
75	O	Z	Si	a	t	c	t	-1138.719447	14.6	0.00	-328.9
76	O	Z	Si	a	t	t	c	-1138.719349	14.7	0.00	-282.2
77	O	Z	Si	a	c	t	t	-1138.718235	15.4	0.00	-403.0
78	N	E	Si	a	c	t	t	-1138.717854	15.6	0.00	-298.6
79	N	E	Si	a	c	c	t	-1138.717313	16.0	0.00	-291.8
80	O	E	Re	a	c	t	c	-1138.717215	16.0	0.00	-568.0
81	N	E	Si	d	c	c	c	-1138.717169	16.1	0.00	-327.4
82	O	E	Re	a	c	c	c	-1138.716969	16.2	0.00	-563.2
83	O	Z	Re	d	c	c	c	-1138.716449	16.5	0.00	-394.4
84	O	Z	Si	a	t	t	t	-1138.716067	16.8	0.00	-225.3
85	O	E	Re	a	c	c	t	-1138.716033	16.8	0.00	-558.3
86	O	E	Re	a	c	t	t	-1138.715258	17.3	0.00	-568.3
87	O	E	Si	d	c	c	c	-1138.715050	17.4	0.00	-614.7
88	O	Z	Re	a	t	c	c	-1138.714694	17.6	0.00	-226.1
89	O	E	Si	a	t	c	c	-1138.712525	19.0	0.00	-258.6
90	O	Z	Re	a	t	c	t	-1138.708924	21.2	0.00	-407.5
91	O	E	Re	d	c	c	c	-1138.708453	21.5	0.00	-333.5

92	O	Z	Re	a	t	t	t	-1138.707871	21.9	0.00	-290.1
93	O	E	Si	a	c	c	c	-1138.707865	21.9	0.00	-370.4
94	O	E	Si	g	t	c	c	-1138.707605	22.1	0.00	-214.2
95	O	E	Re	a	t	c	c	-1138.706129	23.0	0.00	-193.1
96	O	E	Si	g	c	c	c	-1138.705830	23.2	0.00	-411.5
97	O	E	Si	d	t	c	c	-1138.705566	23.3	0.00	-196.7
98	O	E	Re	a	t	t	t	-1138.700564	26.5	0.00	-330.2
99	O	E	Re	a	t	c	t	-1138.700255	26.7	0.00	-432.8

^a O and N correspond to oxime (TS5) and nitron (TS6) attacks, respectively. ^b E and Z correspond to the configuration of the attacking nitron/oxime; O/Z, O/E, N/Z and N/E correspond to **1b**, **1c**, **2b** and **2c**, respectively. ^c Face indicates the two faces of the oxime/nitron. ^d Three staggered orientations of the oxime/nitron attack to **6**, defined as d (droite), g (gauche) and a (anti); see above for definition of d/g/a. ^e c and t correspond to *s-cis* and *s-trans* conformations of **6**, respectively. ^f With respect to the most stable. ^g According to Boltzmann's distribution

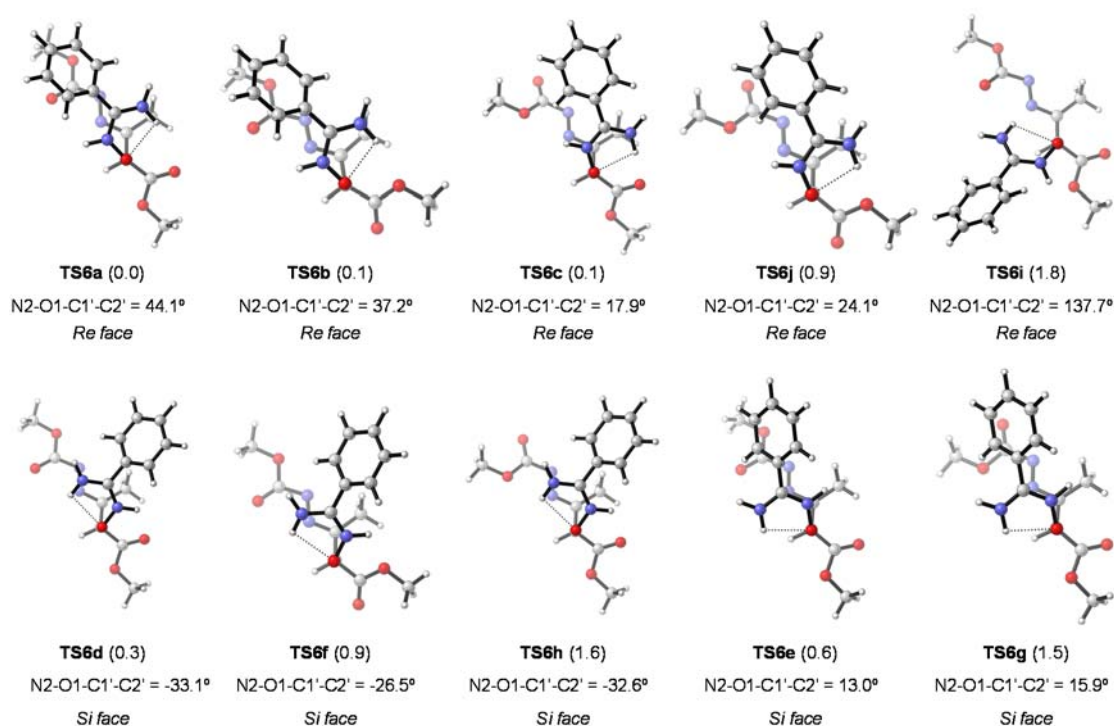


Figure S17. Optimized geometries (M06-2X/cc-pVTZ/PCM=EtOH) of the most stable transition structures **TS6a-j**. Illustrations are oriented as Newmann projections with the forming bond perpendicular to the paper.

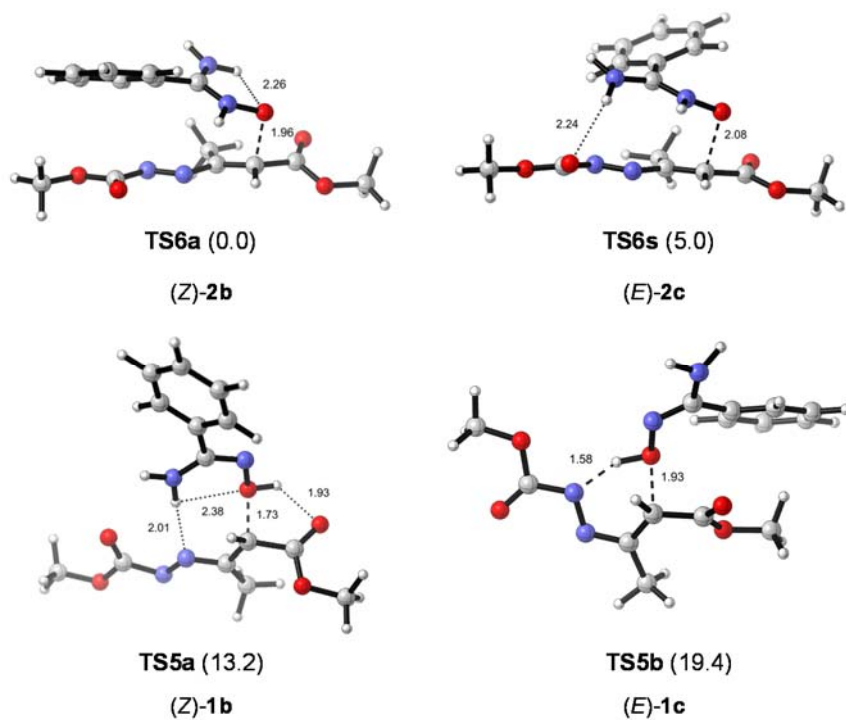
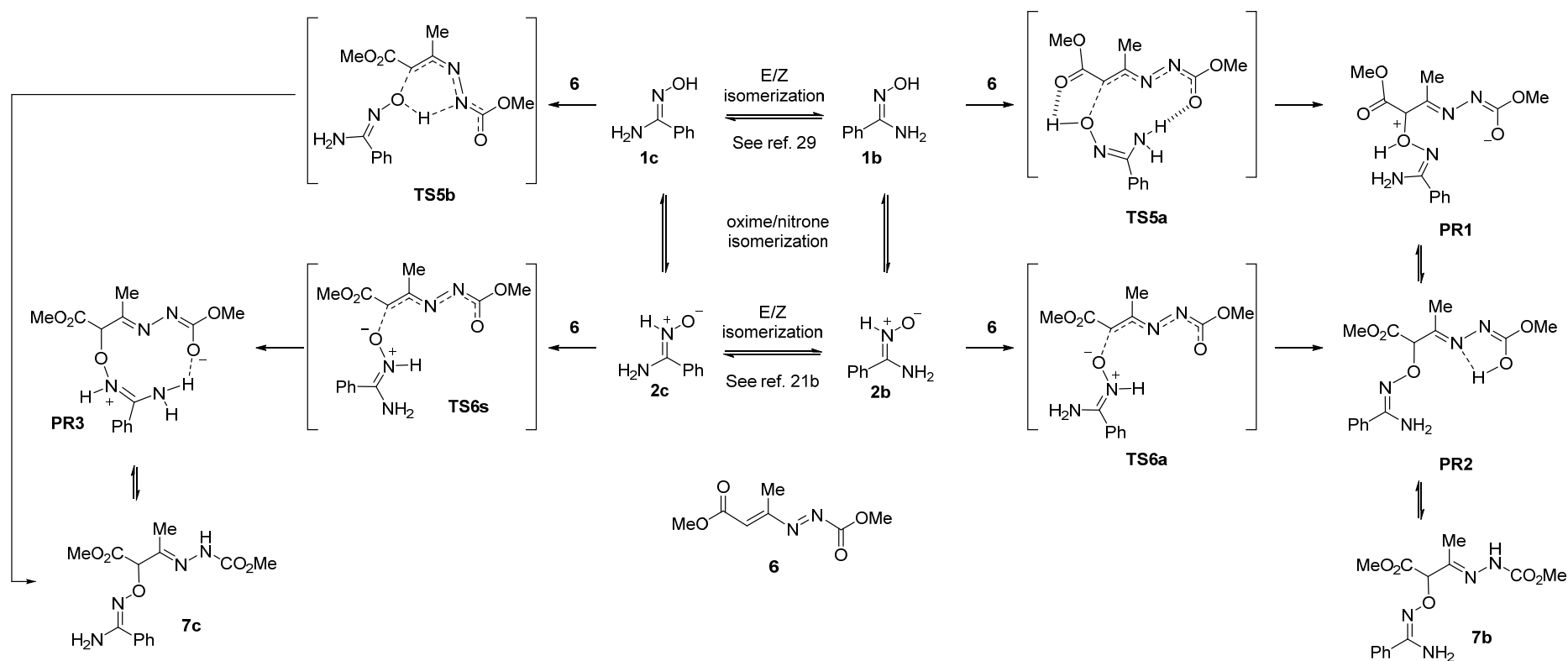


Figure S18. Optimized geometries (M06-2X/cc-pVTZ/PCM=EtOH) of the most stable transition structures for attacks of each tautomer. Relative free energies are given in kcal/mol. Distances are given in angstroms.



Scheme S4. Full reaction paths for each isomer corresponding to the reaction of oxime **1b** with 1,2-diaza-1,3-diene **6**. The most stable TS is indicated in each case. For energy values see Table S4. For geometries of the TSs see Figure S18

TableS6. Calculated (M06-2X/cc-pVTZ/PCM=EtOH) absolute (hartrees) and relative (kcal/mol) energies for the reaction between nitrone **1b** and 1,2-diaza-1,3-diene **6** by considering all possible paths and the most stable TS in each case. Points corresponding to nitrone/oxime isomerization have also been included

	E_0	ΔE_0	G	ΔG	im. freq.
1b	-456.087600	0.0	-456.121283	0.0	
1c	-456.077768	6.2 ^a	-456.112000	5.8 ^a	
2b	-456.073111	9.1 ^a	-456.106562	9.2 ^a	
2c	-456.062242	15.9 ^a	-456.095633	16.1 ^a	
6	-682.930114		-682.972089		
1b·1b	-912.192958	-11.1 ^a	-912.242615	0.0 ^a	
1c·1c	-912.173703	0.9 ^a	-912.223666	11.9 ^a	
2b·2b	-912.170715	2.8 ^a	-912.219528	14.5 ^a	
2c·2c	-912.146933	17.7 ^a	-912.196835	28.7 ^a	
TS4b	-912.170593	2.9 ^a	-912.218246	15.3 ^a	-1042.4
TS4c	-912.148562	20.1 ^{a,b}	-912.197549	28.2 ^a	-1031.7
TS5a	-1138.986698	19.5 ^c	-1139.040766	33.0 ^c	-386.4
TS5b	-1138.978251	24.8 ^c	-1139.030866	39.1 ^c	-552.8
TS6a	-1139.009383	5.2 ^c	-1139.061812	19.8 ^c	-317.1
TS6s	-1139.001261	10.3 ^c	-1139.053822	24.9 ^c	-254.6
PR1	-1138.988292	18.5	-1139.044554	30.7	
PR2	-1139.040053	-14 ^c	-1139.095583	-1.4 ^c	
PR3	-1139.018382	-0.4	-1139.068967	15.3	
7b	-1139.062854	-32.2	-1139.118922	-20.6	
7c	-1139.055485	-23.7	-1139.111165	-11.1	

^a Referred to **1b**. ^b Barrier calculated from E values, without ZPVE correction. After ZPVE correction the value of the barrier is 16.7 kcal/mol revealing the introduction of an experimental error that situates **2c·2c** above **TS4**. This error only affected to **TS4c** since the rest of energy barrier values are similar after ZPVE correction. ^c Referred to **1b** + **6**.

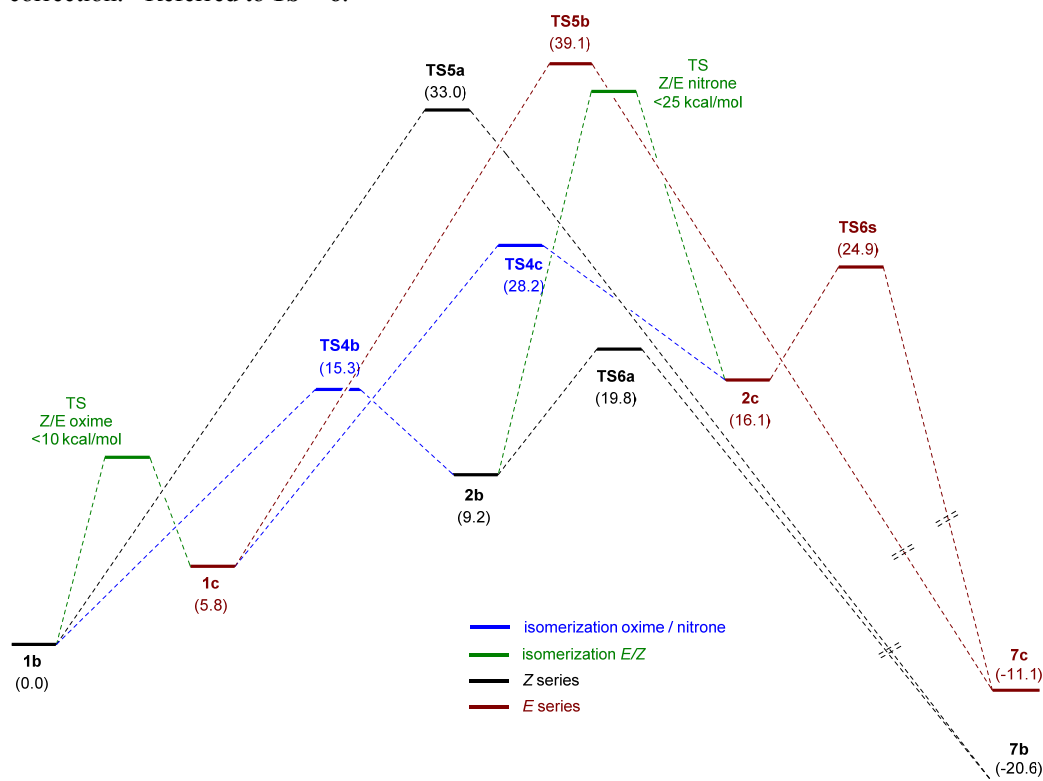


Figure S19. Complete free energy (M06-2X/cc-pVTZ/PCM=EtOH) diagram for the nucleophilic addition of oxime and nitron isomers **1** and **2** to 1,2-diaza-1,3-diene **6**. Dimers involved in oxime-nitron isomerization and tautomers of the final products **7b,c** have been omitted for clarity. Relative free energies are given in kcal/mol.

Ene-like reactions and related processes

*Ene-like between nitronne **1b** and methyl-2-methylfumarate (model system).*

Methyl 2-methylfumarate is a simple model in which the diazo moiety has been replaced by an ester moiety (Figure S20). By using this model, the ene-like TS_A was located and the IRC confirmed the transfer of the proton with the presence of a typical hidden intermediate (Figure S21)

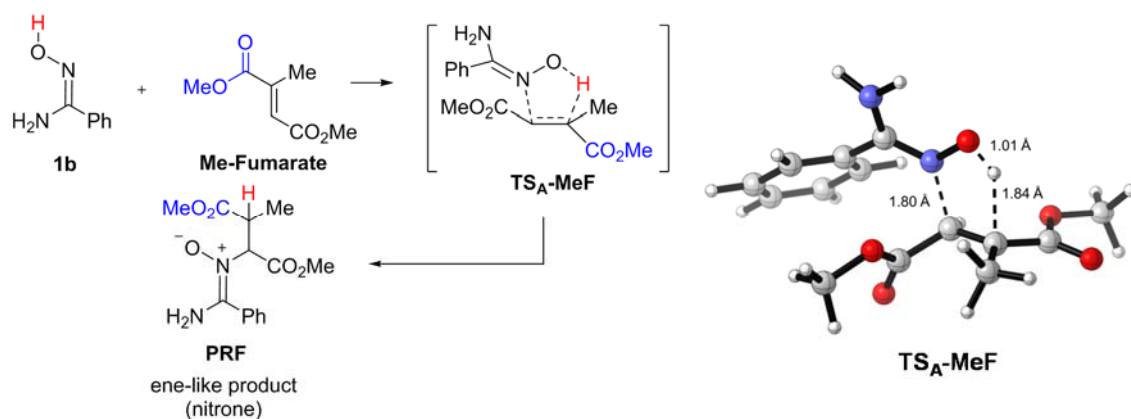


Figure S20. Reaction scheme and optimized geometry (M06-2X/cc-pVTZ/PCM=EtOH) of the ene-like transition structure TS_A -MeF.

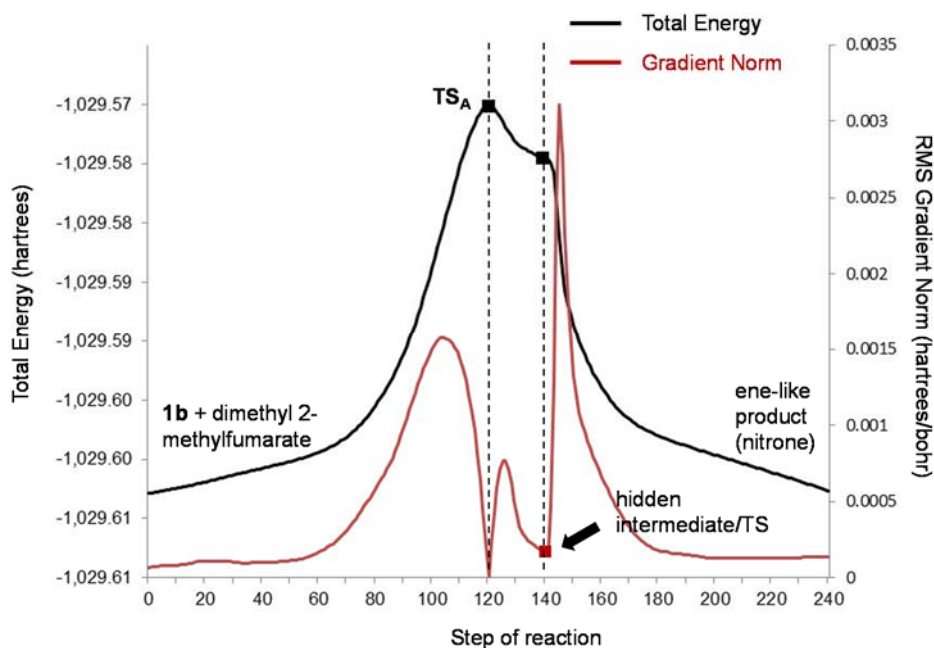
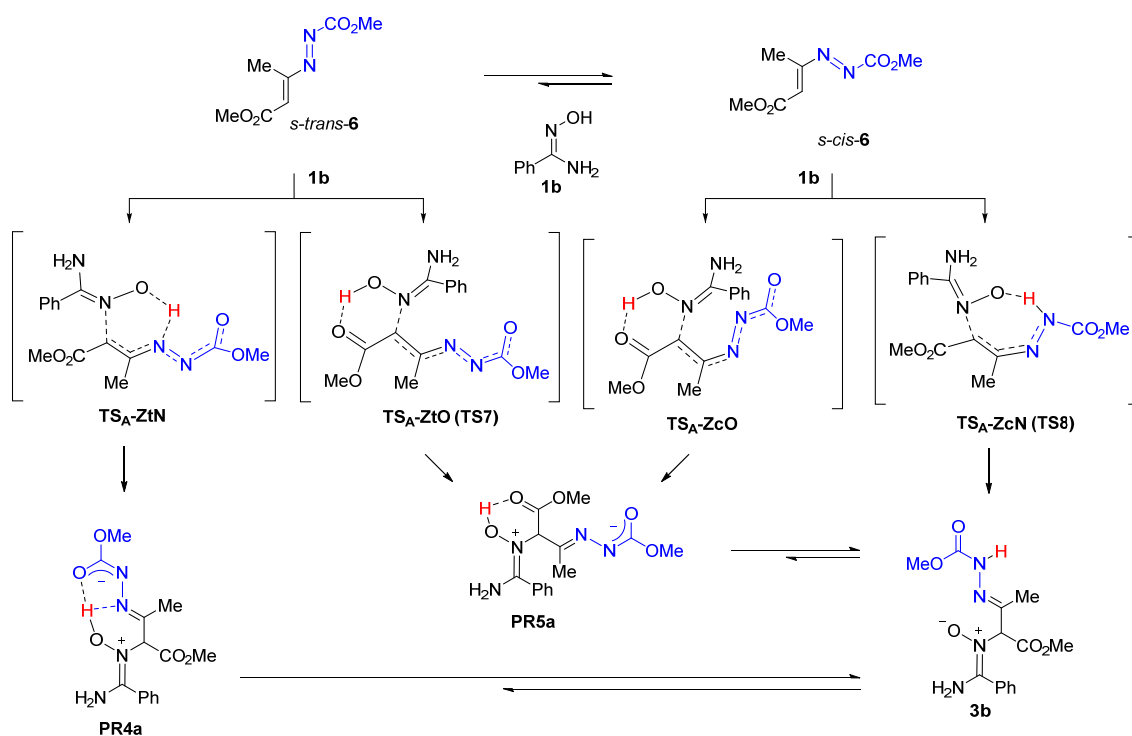


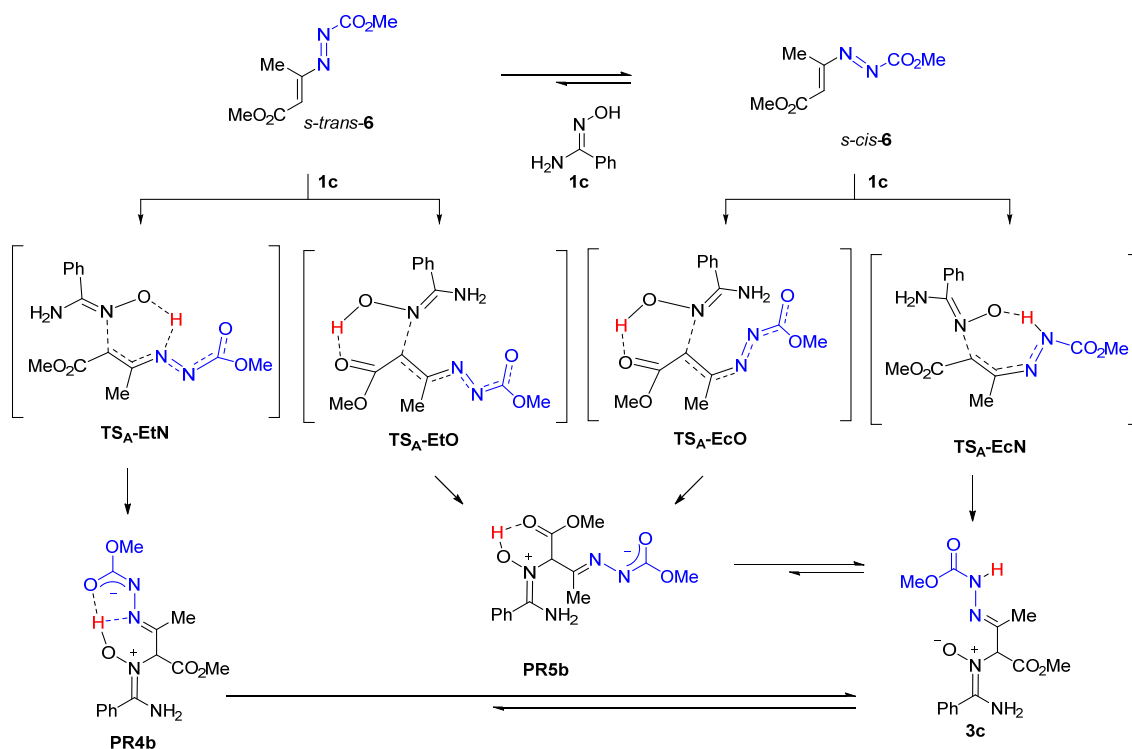
Figure S21. Computed (M06-2X/cc-pVTZ/PCM=EtOH) intrinsic reaction coordinate (IRC) for the transformation of **1b** into ene-like product showing the total energy (left axis, black line) and the gradient norm showing a prominent hidden intermediate (right axis, red line).

Ene-like between nitron **1b** and 1,2-diaza-1,3-diene **6**.

Both α -(*s-trans*)-**6** and α -(*s-cis*)-**6** conformers have been considered in the study since they could lead to different interactions during the course of the reaction. Since the interconversion barrier between (*Z*) and (*E*) oximes is known to be low, we have also considered for oxime isomers **1b** and **1c**. Contrary to that observed for the reaction with dimethyl 2-methylfumarate any attempt of locating ene-like transition structures led to two types of transition structures in which the oxime hydrogen interacts with either the diazo group or the ester group linked to the double bond. The exhaustive exploration of the PES for this reaction included staggered approaches between the reagents and conformations of the 1,2-diaza-1,3-diene **6** as mentioned above. No stereofaces were considered because the attack of the nitrogen takes place in a perpendicular way with respect to the unsaturated system of **6**. According to this analysis the processes illustrated in Scheme S5 and S6 corresponding to addition to **1b** and **1c**, respectively have been studied. The corresponding energy values are given in Table S7. The geometries of transition structures are given in Figure S22.



Scheme S5. Ene-like processes corresponding to *Z*-isomers

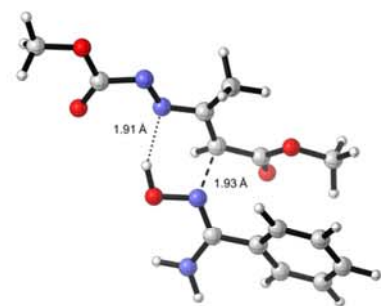


Scheme S6. Ene-like processes corresponding to *E*-isomers

Table S7. Calculated (M06-2X/cc-pVTZ) absolute (hartrees) and relative (kcal/mol) energies for ene-like processes between oximes **1b** and **1c**, and 1,2-diaza-1,3-diene **6** (Schemes S4 and S5).^a

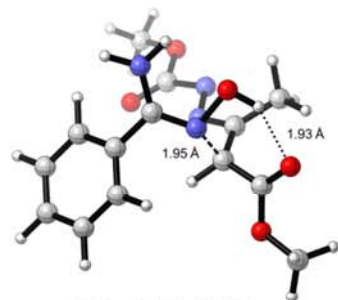
	E_0	ΔE_0^b	G	ΔG^b	im. freq.
α -(<i>s-trans</i> - 6)	-682.929583		-682.972606		
α -(<i>s-cis</i> - 6)	-682.926270		-682.969994		
1b	-456.087600		-456.121283		
1c	-456.077768		-456.112000		
TS_A-ZtN	-1138.999365	11.1	-1139.053989	24.7	-446.1
TS_A-ZtO	-1139.006343	6.7	-1139.060524	20.6	-435.9
TS_A-ZcO	-1139.000023	10.7	-1139.053204	25.2	-436.8
TS_A-ZcN	-1139.003864	8.3	-1139.059717	21.2	-429.4
TS_A-EtN	-1138.991031	16.3	-1139.043944	31.1	-457.4
TS_A-EtO	-1138.996820	12.7	-1139.051737	26.2	-443.3
TS_A-EcO	-1138.990704	16.5	-1139.046479	29.5	-400.7
TS_A-EcN	-1138.998110	11.9	-1139.050529	26.9	-414.8
PR4a	-1139.031262	-8.9	-1139.084735	5.5	
PR5a	-1139.034257	-10.8	-1139.08755	3.7	
PR4b	-1139.024558	-4.7	-1139.079465	8.8	
PR5b	-1139.031847	-9.3	-1139.085279	5.1	
3b	-1139.050441	-21.0	-1139.103760	-6.5	
3c	-1139.040427	-14.7	-1139.093785	-0.2	

^a TS_A-ZtO and TS_A-ZcN are **TS7b** and **TS8** in the main text. ^b Referred to **1b** + *s-trans*-**6**.



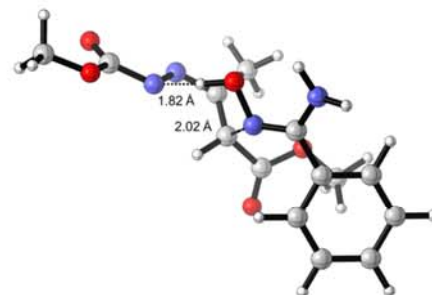
TS_A-ZtN (4.1)

$$O_{OX}-N_{OX}-C_{DD}-C_{DD} = 72.3^\circ$$



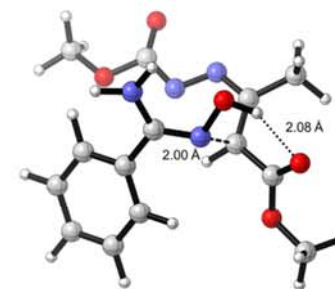
TS_A-ZtO (0.0)

$$O_{OX}-N_{OX}-C_{DD}-C_{DD} = -49.4^\circ$$



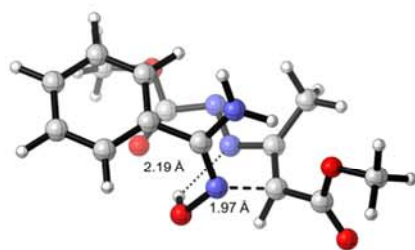
TS_A-ZcN (0.6)

$$O_{OX}-N_{OX}-C_{DD}-C_{DD} = 27.3^\circ$$



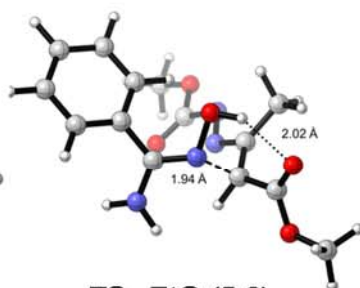
TS_A-ZcO (4.6)

$$O_{OX}-N_{OX}-C_{DD}-C_{DD} = -40.0^\circ$$



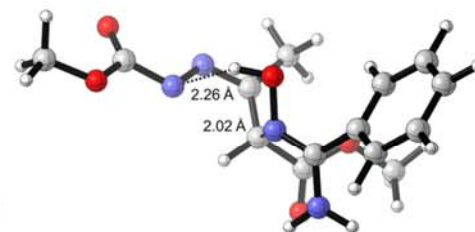
TS_A-EtN (10.5)

$$O_{OX}-N_{OX}-C_{DD}-C_{DD} = 92.1^\circ$$



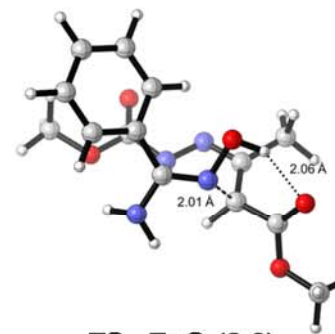
TS_A-EtO (5.6)

$$O_{OX}-N_{OX}-C_{DD}-C_{DD} = -45.6^\circ$$



TS_A-EcN (6.3)

$$O_{OX}-N_{OX}-C_{DD}-C_{DD} = -0.1^\circ$$



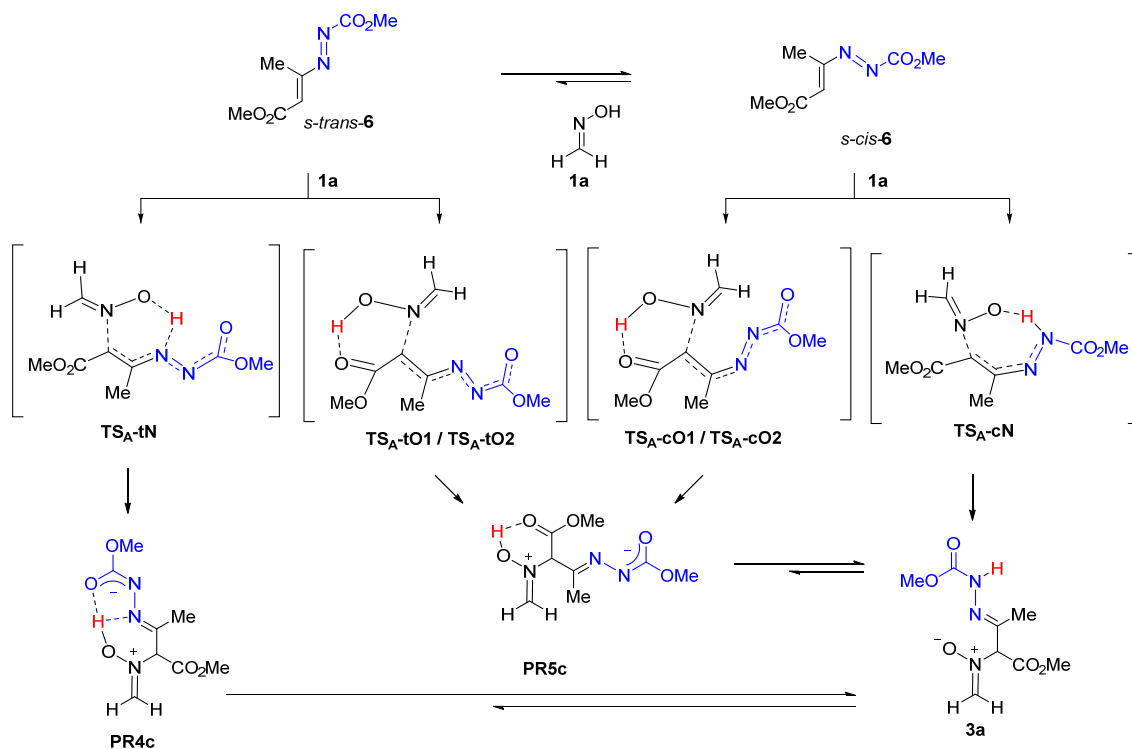
TS_A-EcO (8.9)

$$O_{OX}-N_{OX}-C_{DD}-C_{DD} = -44.1^\circ$$

Figure S22. Optimized geometries (M06-2X/cc-pVTZ/PCM=EtOH) of the transition structures corresponding to ene-like processes between **1b,c** and **6**. Relative energies are given in kcal/mol. **TS_A-ZtO** and **TS_A-ZcN** are **TS7b** and **TS8** in the main text.

Ene-like between nitronne **1a** and 1,2-diaza-1,3-diene **6**.

The same study of an ene-like process for oxime **1a** lead to three different staggered transition structures for both α -(*s-trans*) and α -(*s-cis*) conformers of 1,2-diaza-1,3-diene **6** (Scheme S7). Energy data are given in Table S8 and geometries of transition structures illustrated in Figure S23. A comparative energy diagram is given in Figure S24.



Scheme S7. Ene-like processes corresponding to oxime **1a**.

Table S8. Calculated (M06-2X/cc-pVTZ) absolute (hartrees) and relative (kcal/mol) energies for ene-like processes between oximes **1b** and **1c**, and 1,2-diaza-1,3-diene **6** (Schemes S4 and S5).

	E_0	ΔE_0^b	G	ΔG^b	im. freq.
α -(<i>s-trans</i> - 6)	-682.929583		-682.972606		
α -(<i>s-cis</i> - 6)	-682.926270		-682.969994		
1a	-169.768505		-169.792780		
TSA-tN	-852.675778	13.9	-852.723253	26.1	
TSA-tO1	-852.678901	12.0	-852.725704	24.6	
TSA-tO2	-852.676865	13.2	-852.723629	25.9	
TSA-cN	-852.676146	13.7	-852.722262	26.5	
TSA-cO1	-852.672790	15.8	-852.718798	28.9	
TSA-cO2	-852.674654	14.6	-852.721876	27.0	
PR4c	-852.713509	-9.8	-852.759972	3.1	
PR5c	-852.691945	3.8	-852.737967	16.9	
3a	-852.729045	-19.5	-852.775633	-6.7	

^a **TSA-tO1** is **TS7a** in the main text. ^b Referred to **1b** + *s-trans*-**6**.

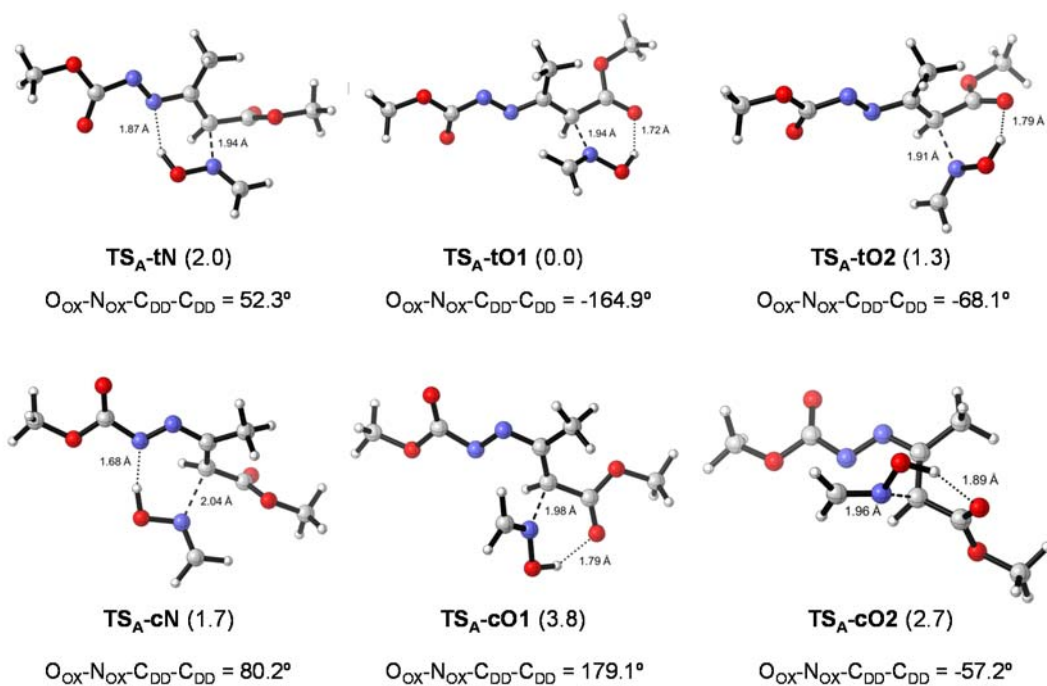


Figure S23. Optimized geometries (M06-2X/cc-pVTZ/PCM=EtOH) of the transition structures corresponding to ene-like processes between **1a** and **6**. **TS_A-tO1** corresponds to **TS7a** in the main text. Relative energies are given in kcal/mol.

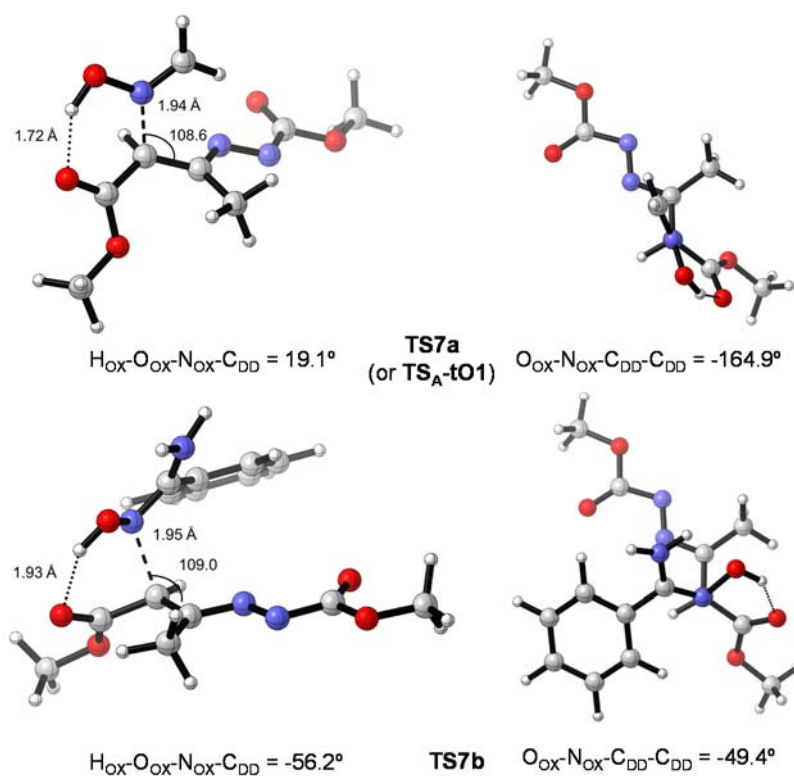


Figure S24. Comparison of the optimized (M06-2X/cc-pVTZ/PCM=EtOH) geometries for the most stable transition structures corresponding to the nucleophilic attack of oxime nitrogen of oximes **1a** and **1b** to 1,2-diaza-1,3-diene **6**. On the right, Newman projection is represented with the forming bond perpendicular to the observer.

Cartesian Coordinates

From the main text

1a (gas phase)

0 1

N	0.0758996336	0.3694989625	0.3176762970
O	-0.8563109115	-0.6523494520	0.3656117856
C	1.2110526936	-0.0566861306	-0.0300917158
H	-1.6622861551	-0.2073865090	0.6381682654
H	2.0060994184	0.6721406449	-0.0953104800
H	1.3909973310	-1.1041228458	-0.2553367323

1a

0 1

N	0.0767314378	0.3703924679	0.3168696752
O	-0.8591240219	-0.6509744724	0.3674145640
C	1.2127211824	-0.0560500755	-0.0303276246
H	-1.6696109954	-0.2100111923	0.6385798121
H	2.0092993594	0.6707932453	-0.0977997098
H	1.3954350477	-1.1030553032	-0.2540192968

1a·1a

0 1

N	1.4851421320	-0.1741503044	-0.0000016258
O	1.1403939656	1.1584985882	-0.0000008133
C	2.7318304989	-0.3722702933	-0.0000033792
H	-0.1631316384	-1.1252688169	0.0000001871
H	3.0685835040	-1.3987674376	-0.0000040899
H	3.4414520736	0.4493759796	-0.0000041591
N	-1.4851421320	0.1741503045	0.0000022020
O	-1.1403939656	-1.1584985881	0.0000013895
C	-2.7318304989	0.3722702934	0.0000039554
H	0.1631316384	1.1252688170	0.0000003891
H	-3.0685835040	1.3987674377	0.0000046661
H	-3.4414520736	-0.4493759795	0.0000047353

1a·EtOH

0 1

N	-1.5424627569	0.3973575436	-0.1015890148
O	-1.4982243089	-0.9400274947	0.2373631931

C	-2.6278417685	0.9487266629	0.2342257028
H	-0.6229853299	-1.2102401794	-0.0916984864
H	-2.7384423032	1.9982771117	0.0021582434
H	-3.4232137574	0.4022997696	0.7328409761
H	0.5669028509	0.0989813688	-1.0951192314
O	1.0390118328	-0.6836547650	-0.7823645600
C	1.7573663689	-0.3038065690	0.3929867180
H	1.0533429787	0.0102250144	1.1694638822
H	2.2568018574	-1.2071558218	0.7391679345
C	2.7607729845	0.7933758352	0.1094113046
H	2.2532059699	1.6939921023	-0.2398676900
H	3.3140808887	1.0458297835	1.0136472813
H	3.4678354933	0.4752726377	-0.6558582531

1b

0 1

N	-1.9358703243	-0.8331827871	0.2816994350
O	-3.3073343706	-0.5386044234	0.1843366576
C	-1.2431984747	0.1934599347	-0.0512294349
H	-3.7292004989	-1.3655766215	0.4295810650
N	-1.7814702784	1.4132764552	-0.3658134928
C	0.2333430772	0.0682503645	-0.0260378860
H	-1.2373672238	1.9959626113	-0.9809165175
H	-2.7704864886	1.4052238823	-0.5592655305
C	1.0306102286	1.1885419620	0.1951977124
C	0.8370043998	-1.1731670538	-0.2205871984
C	2.4132941240	1.0686841069	0.2238814609
H	0.5718062735	2.1533148675	0.3658791396
C	2.2168201863	-1.2900114618	-0.1898921336
H	0.2145111839	-2.0374407608	-0.4032843002
C	3.0091929511	-0.1693139642	0.0313868302
H	3.0231352051	1.9435687839	0.4030541487
H	2.6769788154	-2.2563660051	-0.3454939036
H	4.0864312142	-0.2624128908	0.0522969479

1b·1b

0 1

N	-1.3208908932	-0.6610982507	-0.1766070617
O	-0.2783879820	-1.5880201492	-0.2702983029
C	-2.4622699070	-1.2406426628	-0.0930878844
H	-0.5055598822	1.0005728088	-0.2731053034
N	-2.6244747165	-2.5938382641	-0.1741863746
C	-3.6680320127	-0.3896598707	0.0301697950
H	-3.4381132611	-2.9825818642	0.2728254654
H	-1.7786932782	-3.1331040370	-0.0765849828
C	-4.8953567320	-0.8367323751	-0.4531269009

C	-3.5842532332	0.8672028754	0.6275849676
C	-6.0233816307	-0.0356154977	-0.3444655166
H	-4.9678295188	-1.8029072746	-0.9343543578
C	-4.7115156378	1.6653815776	0.7324755269
H	-2.6349346024	1.2077189026	1.0177797030
C	-5.9344328551	1.2160799208	0.2474452666
H	-6.9705004841	-0.3897884287	-0.7277122972
H	-4.6376899142	2.6375550586	1.2003976635
H	-6.8138477681	1.8398235224	0.3317299381
N	1.3208947332	0.6611319852	-0.1766251090
O	0.2783913704	1.5880535920	-0.2703138844
C	2.4622747797	1.2406765063	-0.0931203861
H	0.5055629907	-1.0005389514	-0.2731019064
N	2.6244793492	2.5938714937	-0.1742304841
C	3.6680376031	0.3896940895	0.0301329241
H	3.4381217391	2.9826179152	0.2727719473
H	1.7786988400	3.1331379337	-0.0766246247
C	4.8953588375	0.8367635912	-0.4531753962
C	3.5842630301	-0.8671653186	0.6275557183
C	6.0233844181	0.0356471394	-0.3445177883
H	4.9678282598	1.8029356848	-0.9344089650
C	4.7115260271	-1.6653436914	0.7324423376
H	2.6349472479	-1.2076790860	1.0177593609
C	5.9344397795	-1.2160449453	0.2474006229
H	6.9705005403	0.3898178761	-0.7277733397
H	4.6377035558	-2.6375145828	1.2003703557
H	6.8138552080	-1.8397882230	0.3316822729

1b·EtOH

0 1

H	-2.9539172250	0.7239575684	-0.6608309912
N	-0.8060112279	0.9929603808	-0.1975412619
O	-1.8042868113	1.8635163398	-0.1340442953
C	0.4060179263	1.2869804994	0.1535295036
H	-1.0182799071	0.0768161001	-0.5886270102
N	0.6688517806	2.5528297828	0.5271757142
C	1.4701258119	0.2732305679	0.0859830421
H	1.4758753423	2.7314771588	1.0994948398
H	-0.1432615736	3.1404261481	0.6485716441
C	2.7636209296	0.6551496356	-0.2646498481
C	1.1951686778	-1.0633366175	0.3715595250
C	3.7696747019	-0.2952820070	-0.3397659792
H	2.9749319965	1.6904675372	-0.4968197826
C	2.2043564126	-2.0097358821	0.2898049258
H	0.2020465642	-1.3600079565	0.6837236024
C	3.4913675144	-1.6279403122	-0.0661337786
H	4.7705028670	0.0044601921	-0.6177501037
H	1.9882125183	-3.0443570825	0.5171292947

H	4.2776274618	-2.3678124196	-0.1261954324
C	-3.6492569718	-0.7978146649	0.3440672434
H	-2.8744065672	-0.6215129247	1.0995845385
H	-4.5811802925	-0.3733540135	0.7331118714
O	-3.2934099950	-0.1759605019	-0.8778356638
C	-3.8179373656	-2.2828352163	0.1101167725
H	-2.8824016510	-2.7209182876	-0.2388400570
H	-4.1166722978	-2.7877441010	1.0283822506
H	-4.5826216196	-2.4602629239	-0.6461605641

1c

0 1

N	-2.3673955384	-0.3800153232	-0.2239761702
O	-1.8455645801	-1.5733315455	-0.7520040497
C	-1.4512875561	0.4292690665	0.1497817901
H	-2.6384683524	-2.0559483584	-0.9991457065
N	-1.8373330715	1.6258569627	0.7198188771
C	0.0148125815	0.1869398923	0.0754129007
H	-1.1561824110	2.3662629405	0.6907220691
H	-2.7765209818	1.9233405657	0.5025846685
C	0.8356496038	1.1247314014	-0.5446233423
C	0.5787389384	-0.9527158677	0.6425785937
C	2.2076025097	0.9222375888	-0.6042919171
H	0.4018006591	2.0084393020	-0.9959449844
C	1.9504840471	-1.1457960688	0.5943498825
H	-0.0613786554	-1.6823838567	1.1169098781
C	2.7665978667	-0.2112493992	-0.0316078492
H	2.8373194697	1.6504404864	-1.0965745118
H	2.3841754982	-2.0287756021	1.0435702889
H	3.8359269724	-0.3676101847	-0.0726674176

1c·1c

0 1

N	-1.3945490434	0.5608551948	0.1161152468
O	-1.3824102399	-0.8331287267	0.0505984465
C	-2.5625281753	1.0818738724	0.1489577626
H	0.4225735475	1.0197445799	0.0853786601
N	-2.6596988640	2.4395107298	0.3911798160
C	-3.8528093159	0.3596420266	0.0168432462
H	-3.3978631223	2.9080394177	-0.1125239514
H	-1.7794672389	2.9328759881	0.3519373470
C	-4.9197870494	0.7112767749	0.8409955454
C	-4.0283927685	-0.6275996036	-0.9517299000
C	-6.1441577282	0.0712798281	0.7103222090
H	-4.7837284510	1.4802838722	1.5892289494
C	-5.2572588525	-1.2530971296	-1.0897497485

H	-3.2014381995	-0.8984902490	-1.5907144481
C	-6.3150338468	-0.9098013935	-0.2562648440
H	-6.9643748078	0.3419559549	1.3608824189
H	-5.3902386874	-2.0117777314	-1.8488811548
H	-7.2710372406	-1.4043380368	-0.3628990423
N	1.3945424858	-0.5608714220	0.1160428814
O	1.3824013409	0.8331177872	0.0506371489
C	2.5625226451	-1.0818922139	0.1488232496
H	-0.4225820222	-1.0197591993	0.0853069261
N	2.6596987570	-2.4395482073	0.3909354369
C	3.8528007339	-0.3596488089	0.0167423040
H	3.3978556526	-2.9080359988	-0.1128169542
H	1.7794672430	-2.9329117409	0.3516686008
C	4.9197945041	-0.7113459636	0.8408473867
C	4.0283640869	0.6276686327	-0.9517569297
C	6.1441610524	-0.0713354061	0.7102015872
H	4.7837507217	-1.4804106523	1.5890242083
C	5.2572256023	1.2531806657	-1.0897502599
H	3.2013971351	0.8986051576	-1.5907059593
C	6.3150163997	0.9098231559	-0.2563106272
H	6.9643910846	-0.3420602087	1.3607252501
H	5.3901903222	2.0119188983	-1.8488267011
H	7.2710163389	1.4043711552	-0.3629231072

1c·EtOH

0 1

H	-1.8032231847	-0.7421528264	-1.0758187305
N	-0.9031792064	0.6388081302	-0.2249245548
O	-0.8744065300	-0.6247362735	-0.8247070216
C	0.2444220080	1.0707541118	0.1388550742
H	-2.9287248491	0.7745816958	-0.5600828818
N	0.3243464771	2.3798491505	0.5800732436
C	1.5339730749	0.3369558513	0.0772411241
H	0.9708263363	2.5308772054	1.3399623472
H	-0.5737193938	2.8151980273	0.7349352277
C	2.6810457823	1.0141645011	-0.3324302961
C	1.6278913847	-0.9974795546	0.4692024273
C	3.9048127955	0.3614417153	-0.3659683580
H	2.6081687575	2.0507681337	-0.6318863845
C	2.8549900553	-1.6414910126	0.4492725523
H	0.7411329103	-1.5230843845	0.7902260320
C	3.9940274614	-0.9665964578	0.0267906091
H	4.7875878269	0.8919121886	-0.6956075020
H	2.9225659470	-2.6740971287	0.7634378413
H	4.9484420951	-1.4750514394	0.0063094201
C	-4.4629771660	-0.3018080374	0.0120307722
H	-5.1878029881	-0.9252883741	-0.5101529288
H	-5.0072988606	0.5350920048	0.4571556106

O	-3.5650557952	0.1781146066	-0.9834299600
C	-3.7505316146	-1.0998473541	1.0866486319
H	-4.4612956165	-1.4578959545	1.8313787713
H	-3.2427234944	-1.9609575428	0.6514061180
H	-3.0059672126	-0.4823339820	1.5912108149

2a (gas phase)

0 1			
N	0.0559410725	0.3422075587	-0.0000049847
O	1.1710045237	-0.2244523405	-0.0000071225
C	-1.1205016128	-0.1906370655	0.0000120914
H	0.0784180894	1.3695234081	-0.0000187801
H	-1.9729599734	0.4658632548	0.0000108571
H	-1.1889220994	-1.2655668155	0.0000269388

2a

0 1			
N	0.0486603694	0.3481334901	-0.0000050154
O	1.1761794008	-0.2342101529	-0.0000070506
C	-1.1180423073	-0.1883923173	0.0000120418
H	0.0770799476	1.3723155527	-0.0000187803
H	-1.9744907473	0.4634291657	0.0000108835
H	-1.1864066634	-1.2643377383	0.0000269209

2a·2a

0 1			
N	-1.4981608333	0.0412385200	-0.0000013201
O	-0.9963738895	-1.1483254954	-0.0000029795
C	-2.7401228911	0.3399935238	-0.0000026313
H	-0.7710617782	0.7864281161	0.0000012355
H	-3.0088025248	1.3833523944	-0.0000009884
H	-3.4662247458	-0.4586187830	-0.0000054753
N	1.4981608333	-0.0412385200	0.0000027959
O	0.9963738895	1.1483254954	0.0000044553
C	2.7401228910	-0.3399935239	0.0000041071
H	0.7710617781	-0.7864281161	0.0000002403
H	3.0088025247	-1.3833523944	0.0000024642
H	3.4662247458	0.4586187829	0.0000069511

2a·EtOH

0 1			
N	-1.6600763389	0.2632965109	-0.0784417988

O	-1.4902535789	-0.9842671276	0.1651487838
C	-2.7097336169	0.9607587232	0.1396942807
H	0.2168792746	-0.9962386671	-0.4498206684
H	-2.6867072366	2.0044355008	-0.1250107550
H	-3.5681472022	0.4760704389	0.5775552723
H	-0.8424613308	0.7277487081	-0.4956304607
O	0.9988760341	-0.4821698274	-0.7254269764
C	1.7911525022	-0.2527091108	0.4313176140
H	1.1748320688	0.1643688931	1.2351389696
H	2.2099944724	-1.1957581999	0.7953073353
C	2.9030620096	0.7066888468	0.0731633282
H	2.4909364272	1.6555981057	-0.2699277987
H	3.5382310150	0.8971471543	0.9375407301
H	3.5189015002	0.2902380511	-0.7237498562

2b

0 1

N	-2.0191068211	-0.7138158396	0.3041571953
O	-3.3259745442	-0.6222724926	0.2758759567
C	-1.2279431155	0.2354529248	-0.0926080078
H	-1.6046595508	-1.5517633657	0.7025443471
N	-1.7973443057	1.4026501301	-0.4799682842
C	0.2321019162	0.0767092416	-0.0475385757
H	-1.2951752458	1.9663808741	-1.1453286151
H	-2.7994452902	1.3357398775	-0.5982761590
C	1.0349122236	1.1833985221	0.2267865403
C	0.8258778614	-1.1635806082	-0.2806459076
C	2.4129561530	1.0458241422	0.2825239016
H	0.5764031264	2.1452131224	0.4135170044
C	2.2037037456	-1.2969012463	-0.2154695710
H	0.2159301812	-2.0184513714	-0.5412733266
C	2.9997305907	-0.1939483940	0.0658424722
H	3.0284210322	1.9071094944	0.5024453941
H	2.6573437474	-2.2609667056	-0.3990555353
H	4.0748742959	-0.2999803057	0.1098741707

2b·2b

0 1

N	-1.1561902747	-0.8126834771	-0.5715454080
O	-0.0861464234	-1.5778143893	-0.7879855095
C	-2.2870770412	-1.3027373703	-0.1834213623
H	-1.0130469735	0.2062091590	-0.7180822004
N	-2.4028187046	-2.6473829455	-0.0787679498
C	-3.4318637929	-0.4152347955	0.0793183268
H	-3.0856949771	-3.0116023438	0.5640934767
H	-1.5193242479	-3.1350103270	-0.1352760572

C	-4.7292527896	-0.9095556465	-0.0366100096
C	-3.2312451248	0.9166253145	0.4456650127
C	-5.8148389347	-0.0817644516	0.2074666811
H	-4.8914933038	-1.9357074638	-0.3379524082
C	-4.3198159081	1.7399387093	0.6809835776
H	-2.2271219493	1.3079591203	0.5545601217
C	-5.6129810446	1.2435032699	0.5654917413
H	-6.8181854813	-0.4729108730	0.1118105346
H	-4.1581125847	2.7702273888	0.9662856453
H	-6.4592899269	1.8887361855	0.7571484035
N	1.1561588642	0.8126998048	-0.5713485175
O	0.0861184583	1.5778738420	-0.7876546314
C	2.2870383612	1.3026760531	-0.1831067130
H	1.0130211216	-0.2061631931	-0.7180967433
N	2.4027819349	2.6473010513	-0.0781849005
C	3.4318199472	0.4151206607	0.0794770948
H	3.0856423450	3.0113860704	0.5647701522
H	1.5192883581	3.1349397424	-0.1346075358
C	4.7292106629	0.9094597230	-0.0363541152
C	3.2311953642	-0.9168060501	0.4455781943
C	5.8147933206	0.0816211764	0.2075759416
H	4.8914550847	1.9356672738	-0.3375044070
C	4.3197629983	-1.7401647299	0.6807535135
H	2.2270701627	-1.3081566653	0.5543941491
C	5.6129299834	-1.2437114231	0.5653584926
H	6.8181415540	0.4727816757	0.1119951530
H	4.1580546172	-2.7705052518	0.9658655005
H	6.4592353448	-1.8889828243	0.7569007560

2b·EtOH

0 1

H	-2.5741892079	1.5467373671	-0.5015996136
N	-0.8325059342	0.9039003678	-0.3360920492
O	-1.7505852554	1.9547201209	-0.1939342885
C	0.3294900243	1.2543869065	0.0799122810
H	-2.3559317259	-0.3481507204	-1.0776995319
N	0.6315648952	2.5151621422	0.5125469257
C	1.4171498511	0.2496332914	0.0247344087
H	1.3943789487	2.6013886539	1.1635514758
H	-0.1626791630	3.1052898122	0.7031040768
C	2.7457572592	0.6525630930	-0.0835042529
C	1.1176998168	-1.1107680462	0.0788854984
C	3.7610078798	-0.2926249786	-0.1388262469
H	2.9893855845	1.7047002510	-0.1469198710
C	2.1322217808	-2.0516152772	0.0199282809
H	0.0865301027	-1.4196498151	0.1764589587
C	3.4572715298	-1.6452577667	-0.0880728490
H	4.7890363831	0.0306878002	-0.2277516994

H	1.8907617692	-3.1048179110	0.0658556775
H	4.2486518080	-2.3810609409	-0.1319780149
C	-3.6566618591	-0.7404209664	0.3112602412
H	-3.0235256428	-0.2809124578	1.0770845222
H	-4.6837586435	-0.4282332922	0.4962527111
O	-3.3107688879	-0.2238575476	-0.9717339145
C	-3.5397280397	-2.2499418197	0.3640364543
H	-2.5113592211	-2.5619942878	0.1759307661
H	-3.8335728216	-2.6221454493	1.3454918942
H	-4.1816102311	-2.7069615292	-0.3884188405

2c

0 1

N	2.2939773905	-0.4478332484	-0.1349739717
O	2.1392489526	-1.6844947925	-0.5174394040
C	1.3870464052	0.4589704308	0.0668686190
H	3.2607276356	-0.1414745747	-0.0161310550
N	1.7781397589	1.7660014207	0.2858348735
C	-0.0539495096	0.1754268812	0.0113768203
H	1.2579797549	2.2399250653	1.0104000438
H	2.7722348011	1.9195377193	0.3765718687
C	-0.9382187460	1.2222152217	-0.2603513123
C	-0.5616920004	-1.0988386776	0.2767751304
C	-2.3057233731	0.9989786100	-0.2715797687
H	-0.5513071199	2.2077219296	-0.4786244058
C	-1.9313071157	-1.3105365920	0.2758948588
H	0.1244128193	-1.9063372121	0.4743691648
C	-2.8059139376	-0.2675395303	-0.0011969680
H	-2.9799077531	1.8148693662	-0.4924987512
H	-2.3178528380	-2.2978761543	0.4888993244
H	-3.8732091245	-0.4421378629	-0.0086090673

2c·2c

0 1

N	-1.4079966477	0.3759563311	0.0493294499
O	-1.2325488285	-0.9413898995	0.0286814935
C	-2.5328708391	1.0077270410	0.1131618170
H	-0.5048187149	0.9036036204	0.0516398098
N	-2.5211269494	2.3716826169	0.3139108587
C	-3.8438934937	0.3404378909	0.0466878253
H	-3.2248045196	2.8801164699	-0.2009175150
H	-1.6152819663	2.8159542640	0.2712755576
C	-4.9410561114	0.9343805283	0.6727465857
C	-4.0199230520	-0.8439907338	-0.6710145459
C	-6.1947441765	0.3488633243	0.5897813243
H	-4.8077338804	1.8471933955	1.2367182862

C	-5.2787238216	-1.4164356480	-0.7602274307
H	-3.1673795443	-1.3041634190	-1.1443632554
C	-6.3665397330	-0.8265023953	-0.1284078150
H	-7.0364694114	0.8117591784	1.0861052207
H	-5.4107162946	-2.3305399924	-1.3228110594
H	-7.3450455880	-1.2824046183	-0.1961541396
N	1.4079382898	-0.3759838673	0.0492977348
O	1.2325030028	0.9413652800	0.0287749991
C	2.5328034591	-1.0077739513	0.1130930021
H	0.5047540326	-0.9036237508	0.0515429044
N	2.5210344147	-2.3717496483	0.3137120589
C	3.8438368764	-0.3404969163	0.0467117836
H	3.2247067940	-2.8801465434	-0.2011602162
H	1.6151805334	-2.8159979455	0.2710200077
C	4.9409774758	-0.9345192081	0.6727341172
C	4.0198997432	0.8440014033	-0.6708679521
C	6.1946760090	-0.3490132300	0.5898547194
H	4.8076294071	-1.8473868829	1.2366105640
C	5.2787112600	1.4164357735	-0.7599961999
H	3.1673733104	1.3042343028	-1.1441892783
C	6.3665049306	0.8264221428	-0.1282127673
H	7.0363833169	-0.8119711535	1.0861511615
H	5.4107306586	2.3305948173	-1.3224844836
H	7.3450190581	1.2823164235	-0.1958926229

2c·EtOH

0 1

H	-2.7034471673	-0.3763068694	-1.1289901609
N	-0.8808087980	0.4838061730	-0.2014370549
O	-1.0641234723	-0.6478169924	-0.8621508261
C	0.2420227555	0.9950860447	0.1932725026
H	-1.7349690129	1.0235061730	-0.0412250867
N	0.2636530969	2.2678459887	0.6958858366
C	1.5249426184	0.2841291218	0.0663409988
H	0.9281795494	2.4343482246	1.4357698457
H	-0.6237661059	2.7253164607	0.8421727621
C	2.6934362450	1.0261487966	-0.1086370461
C	1.5957636310	-1.1062957055	0.1628069809
C	3.9190685049	0.3849895475	-0.1944384168
H	2.6393400443	2.1023758182	-0.1971034865
C	2.8264266823	-1.7384763406	0.0915580424
H	0.6873653225	-1.6750588296	0.2855662045
C	3.9876681623	-0.9976005102	-0.0920142029
H	4.8188931235	0.9653034790	-0.3436357623
H	2.8789987516	-2.8152503049	0.1751536734
H	4.9440511268	-1.4984133839	-0.1569460074
C	-4.3616313202	-0.6566027057	-0.1211775658
H	-4.4471635548	-1.7129804396	-0.3978107891

H	-5.3672151413	-0.2344445948	-0.1472997015
O	-3.5953913305	0.0469535809	-1.0810388337
C	-3.7846600696	-0.5389900817	1.2789711675
H	-4.4093313708	-1.0646211450	2.0017805922
H	-2.7828965320	-0.9700718279	1.3143217918
H	-3.7235787388	0.5088173225	1.5779325421

6-s-cis

0 1

N	-0.3251404389	-2.6386005720	0.3378485206
N	0.6143577416	-1.8745312790	0.1269401107
C	-1.5709275239	-2.0000744009	0.6267278747
C	1.8337452164	-2.5993870301	-0.1728727611
C	-1.9905591921	-1.0308642694	-0.1884771077
C	-2.2911670023	-2.6139919739	1.7831719117
O	2.3618049939	-2.0867998884	-1.2626593586
O	2.2893615945	-3.4651230152	0.5146502360
H	-1.3681536621	-0.7104009147	-1.0111044673
C	-3.3051946952	-0.3829574670	-0.0427595170
H	-1.7033713645	-3.4317860628	2.1920915232
H	-2.4551068087	-1.8638429966	2.5550981790
H	-3.2701655650	-2.9797366532	1.4801123291
C	3.6085265470	-2.6706857547	-1.6760678674
O	-3.4797171612	0.5494599339	-0.9836764949
O	-4.1312802949	-0.6350543699	0.8021738506
H	3.8811206113	-2.1605220583	-2.5921270685
H	4.3596127285	-2.5109087979	-0.9063446353
H	3.4774841041	-3.7355895512	-1.8505252237
C	-4.7213836090	1.2569284303	-0.9316426414
H	-4.6963427792	1.9613072538	-1.7554500904
H	-5.5533478632	0.5653032632	-1.0451305788
H	-4.8154995773	1.7818851741	0.0167072765

6-s-trans

0 1

N	0.6595834108	-2.4652076520	-0.0143932174
N	-0.3194405851	-1.9072967416	0.4752420194
C	1.7587019622	-1.6043456896	-0.3317594824
C	-1.3438473535	-2.8642286531	0.8506043571
C	2.1909967888	-0.7796832960	0.6239651787
C	2.3096773422	-1.8788188609	-1.6927029622
O	-2.4981175443	-2.4433716158	0.3829125129
O	-1.1460734668	-3.8274827269	1.5308155678
H	1.6458656898	-0.7269700231	1.5559625800
C	3.3689730169	0.1059541614	0.5755024845
H	1.5209265941	-2.2701724258	-2.3323029226

H	2.7282534474	-0.9799204710	-2.1304485485
H	3.1001565259	-2.6284267033	-1.6326721522
C	-3.6315571701	-3.2638362658	0.7111251296
O	4.1972599772	-0.1320394156	-0.4412373208
O	3.5638311281	0.9664792250	1.4011357451
H	-4.4837192032	-2.7860583147	0.2428001553
H	-3.4872069377	-4.2670131266	0.3180892725
H	-3.7539928652	-3.3031121891	1.7906966926
C	5.3469894201	0.7178743703	-0.5146931887
H	5.9095607808	0.3799595191	-1.3777309051
H	5.0392942803	1.7537916992	-0.6386266722
H	5.9410537614	0.6224191958	0.3913566768

7a

0 1

N	-1.7031387902	2.4453092596	-0.1728428404
O	-1.4078813546	1.6286480730	-1.2606455011
C	-1.9062805253	3.6359415416	-0.5373064008
N	1.0040543901	-0.2955096138	-0.4070140818
N	2.0826508193	-0.4531641194	0.3957800158
C	-0.0758015580	0.1161666468	0.1308297621
C	3.2554862155	-0.9224235330	-0.1334001266
C	-1.2216692304	0.2947935063	-0.8396250862
C	-0.2423003678	0.4091750946	1.5921032863
O	4.1774506987	-0.9735986950	0.8350064725
O	3.4371309083	-1.2424834209	-1.2800509461
H	-0.9660326484	-0.2472106270	-1.7506191645
C	-2.5291506729	-0.2972538232	-0.3225574665
H	-1.2661291598	0.6821618719	1.8255281359
H	0.3975787212	1.2423381315	1.8916870112
H	0.0322073064	-0.4655488855	2.1862101018
C	5.4596601409	-1.4590418958	0.4285574123
O	-2.3063999889	-1.4729588415	0.2559609556
O	-3.6104313643	0.2056374431	-0.4528814886
H	5.3761262758	-2.4783194894	0.0580815904
H	6.0802414790	-1.4285215235	1.3170659895
H	5.8760784497	-0.8214643223	-0.3479288002
C	-3.4666862431	-2.1621758749	0.7401686478
H	-3.1014695162	-3.0789770478	1.1881803910
H	-4.1412394078	-2.3799235206	-0.0847440592
H	-3.9790777556	-1.5513102402	1.4796996312
H	-1.8547433116	3.9417626842	-1.5781147929
H	-2.1393775627	4.3497940520	0.2401261098
H	2.0615828327	-0.2114589007	1.3769712815

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0 1

N	1.2233063304	0.0188336022	1.1222457068
O	0.8944329559	-0.0365579782	-0.2472198736
C	2.1767440107	-0.8052685063	1.3713516956
N	-2.2995309921	-0.0655384558	-0.4456629463
N	-3.4571269827	-0.4018611686	0.1729764285
C	-1.4248788425	0.5616966946	0.2374461856
C	-4.4300911816	-1.0599648642	-0.5299546704
C	-0.1504901076	0.8608101877	-0.5214526603
C	-1.6006036906	0.9761126858	1.6676472195
O	-5.4581253922	-1.3157024944	0.2882361882
O	-4.3814398697	-1.3619626940	-1.6950314558
H	-0.3676305541	0.7221801908	-1.5817401483
C	0.3169893540	2.3054407724	-0.3629515451
H	-1.6786039903	0.0967710801	2.3117571541
H	-0.7570678922	1.5631370333	2.0142777996
H	-2.5127598071	1.5665697270	1.7816475426
C	-6.5584213790	-2.0014914197	-0.3150691700
O	-0.7239777844	3.1344952901	-0.3493753191
O	1.4633844884	2.6552603060	-0.3156796910
H	-7.2908865266	-2.1324274422	0.4735987272
H	-6.9745954479	-1.4071692435	-1.1252644608
H	-6.2355309461	-2.9663137175	-0.6994934245
C	-0.4075283033	4.5311524940	-0.2906591752
H	-1.3576810195	5.0525794656	-0.3045606096
H	0.1380513732	4.7504921007	0.6243032107
H	0.1965956771	4.8108356307	-1.1505922010
H	-3.6139930300	-0.2207604254	1.1549122747
C	2.6436259623	-0.9009718322	2.7751323432
C	3.9571896403	-1.2681413112	3.0561245769
C	1.7718296390	-0.6154849701	3.8244369137
C	4.3940447564	-1.3485039960	4.3711356539
H	4.6483860614	-1.4700205136	2.2488610106
C	2.2111916589	-0.6958086854	5.1355796573
H	0.7513959395	-0.3374820729	3.6007374348
C	3.5230735659	-1.0633660033	5.4125569428
H	5.4172579300	-1.6294221411	4.5791617286
H	1.5277559617	-0.4770999866	5.9446618814
H	3.8630654822	-1.1272798580	6.4372092261
N	2.8208694080	-1.5466093188	0.4260849950
H	3.2665208264	-2.3949929477	0.7325615481
H	2.3821474179	-1.5894828543	-0.4794502245

7c

0 1

N	0.3626289329	-1.5518465685	-0.3012052878
O	1.4625057809	-1.1847618246	-1.1021368063
C	-0.0643859617	-2.7260288934	-0.5834545923

N	1.2926750753	1.9865334556	-1.2604734963
N	0.4950366782	3.0790097931	-1.1753864668
C	1.2123580172	1.1231489307	-0.3261852593
C	0.5639075775	4.0395731983	-2.1476430255
C	2.1086317084	-0.0821353134	-0.5233683586
C	0.3211598042	1.2509196624	0.8727188271
O	-0.3336058795	4.9957572416	-1.8781913371
O	1.3086891469	4.0372511420	-3.0945869478
H	2.8775406573	0.2007174498	-1.2440348807
C	2.8363385389	-0.4914270439	0.7538832449
H	-0.7280141625	1.2389250556	0.5691913025
H	0.4704028037	0.4285005898	1.5639661262
H	0.5200861740	2.1900481761	1.3943632894
C	-0.3715405701	6.0751752571	-2.8150089867
O	3.2651785559	0.5805507966	1.4135134587
O	3.0356276078	-1.6248096751	1.0973687041
H	-1.1465323466	6.7455799028	-2.4606665628
H	0.5883822637	6.5860066832	-2.8417299817
H	-0.6143893062	5.7044107085	-3.8081216399
C	4.0092925585	0.3237411693	2.6116119660
H	4.2876506077	1.2960117990	3.0016918520
H	3.3879419254	-0.2126301525	3.3253518408
H	4.8937355981	-0.2655826855	2.3814735492
H	-0.1821026273	3.1935804602	-0.4338258325
N	-1.2624433860	-3.1183553694	-0.0282366226
H	-1.6149211104	-2.5041418561	0.6915324598
H	-1.3311822022	-4.0974555814	0.2031752804
C	0.5662647419	-3.7063729733	-1.5039456257
C	-0.2324189317	-4.3989668877	-2.4099490035
C	1.9307713248	-3.9817223906	-1.4294823820
C	0.3298248254	-5.3497916086	-3.2497983456
H	-1.2915544764	-4.1848761031	-2.4579181458
C	2.4839873848	-4.9450130307	-2.2583222791
H	2.5419362487	-3.4437859298	-0.7175782724
C	1.6875177279	-5.6254696203	-3.1727009205
H	-0.2933273334	-5.8757259211	-3.9600370945
H	3.5407282312	-5.1656955180	-2.1933253582
H	2.1260289970	-6.3710992745	-3.8220917890

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0 1

N	-2.7161955228	-0.9807405886	0.1342150688
O	-2.1038153631	-2.1008312426	0.1096337872
C	-2.0537882660	0.1385032463	0.1141898654
H	-3.9312037805	0.8526977117	0.1818654756
N	-2.9993189560	1.2751566498	0.1504016953
C	-0.6391305277	0.4632519249	0.0654559596
H	-2.8901514499	1.8701458000	0.9743846122

H	-2.9479059195	1.8746361302	-0.6759544822
C	-0.2040172845	1.7975403315	0.0539676700
C	0.3344238867	-0.5486769318	0.0284257495
C	1.1453454483	2.1089975294	0.0074898195
H	-0.9088603009	2.6180107660	0.0810631961
C	1.6810305373	-0.2243106740	-0.0179329866
H	0.0081901188	-1.5749098343	0.0369729966
C	2.0981926062	1.1004832472	-0.0288213050
H	1.4500870132	3.1468175341	-0.0002531132
H	2.4137227533	-1.0201019827	-0.0459122077
H	3.1510563672	1.3437907828	-0.0650880310

9a

0 1

C	0.1839557129	0.6881008620	-0.0070867797
C	1.3328817899	1.6595722422	-0.2775676043
H	0.3660631616	0.2845925910	0.9934498758
N	0.1306200284	-0.4236731086	-0.9762207343
O	1.0896310227	-0.4757202121	-1.8848094021
H	2.3731277738	-0.6137685871	-0.4614037985
C	-0.8032241255	-1.3253461380	-0.8557130417
C	1.0213982073	3.0525891497	-0.7211014159
H	0.5650941040	3.0292444631	-1.7122136291
H	0.3175333815	3.5391024225	-0.0439109361
H	1.9390543543	3.6313031232	-0.7623814032
C	-1.1431921019	1.4427526086	0.0462407989
O	-1.5908366438	1.8932013709	1.0665217194
O	-1.6840919537	1.5850664584	-1.1509703884
C	-2.9186535573	2.3156290668	-1.1930231826
H	-3.2105906415	2.3403699105	-2.2362097288
H	-3.6680607925	1.8035523702	-0.5936523688
H	-2.7654625243	3.3220793164	-0.8101367753
C	4.0517959095	-0.2787835531	0.6756297205
O	4.8334251053	0.4957230942	1.1682294472
O	4.2656069211	-1.5936442930	0.5366506884
C	5.5162534309	-2.0636197747	1.0434533913
H	5.5818020961	-1.8833051569	2.1143166443
H	5.5369146501	-3.1281063586	0.8371542975
H	6.3400854505	-1.5635386771	0.5395723537
N	2.5478759373	1.3546701738	-0.0646813104
N	2.7944723537	0.0264644303	0.2178698877
C	-0.9783785281	-2.3914174218	-1.8591148217
C	-0.8357842298	-2.1235818095	-3.2203357764
C	-1.3531462317	-3.6661928358	-1.4393330787
C	-1.0788094476	-3.1228003857	-4.1469772334
H	-0.5322936241	-1.1372791610	-3.5361430081
C	-1.5752252019	-4.6688015428	-2.3717753824
H	-1.4503396819	-3.8844633918	-0.3836650770

C	-1.4433150632	-4.3968217844	-3.7256416529
H	-0.9796961640	-2.9094719651	-5.2023487387
H	-1.8503307338	-5.6597181214	-2.0386274742
H	-1.6219038752	-5.1760688162	-4.4540056188
N	-1.6979460162	-1.2555154089	0.17144440050
H	-2.4227092779	-1.9529040567	0.1806103962
H	-1.4091613249	-0.9419911935	1.0854010855

9b

0 1

C	-0.0073895157	0.7943500867	-0.0898341908
C	1.1781183883	1.7191654481	-0.3750898264
H	0.1340115375	0.4417504419	0.9328298967
N	-0.0521919321	-0.3607138095	-1.0032579610
O	0.8896165607	-0.4654591074	-1.9388906166
H	2.1454081770	-0.5904184017	-0.5351222246
C	-1.0002299698	-1.2542696810	-0.9487765444
C	0.9156282402	3.1154558778	-0.8397178913
H	0.4561769972	3.0923146815	-1.8297523381
H	0.2299625609	3.6361959218	-0.1696960823
H	1.8524804621	3.6615589322	-0.8931130914
C	-1.3101516004	1.5853135269	-0.0970458015
O	-1.7547192903	2.1091763285	0.8892650675
O	-1.8529257564	1.6604223871	-1.3028836786
C	-3.0776773527	2.4024948669	-1.3843074766
H	-3.3784123753	2.3628766898	-2.4246943100
H	-3.8277890154	1.9380742478	-0.7465733472
H	-2.9109028952	3.4295852995	-1.0677945026
C	3.8234431864	-0.2997462727	0.6145177657
O	4.6328542403	0.4526546637	1.0968930989
O	3.9893575880	-1.6246318072	0.4999544827
C	5.2227461354	-2.1297028669	1.0149096044
H	5.3110554244	-1.9034999741	2.0753760399
H	5.1911055741	-3.2022995019	0.8577677076
H	6.0629810526	-1.6930377680	0.4796008395
N	2.3816957591	1.3749940774	-0.1571146743
N	2.5798768377	0.0415986818	0.1468638405
N	-1.0127252446	-2.2081158507	-1.8841802589
H	-1.6311020427	-2.9942757000	-1.7978156914
H	-0.2431937982	-2.2171651153	-2.5363632232
C	-2.0740743844	-1.2108432275	0.0683508301
C	-1.7868053319	-1.4051671870	1.4159357467
C	-3.3840296388	-0.9761133243	-0.3423640479
C	-2.8069557910	-1.3424039948	2.3528135879
H	-0.7705666471	-1.6095327517	1.7282318616
C	-4.3994536102	-0.9091615621	0.5993470425
H	-3.5975870669	-0.8313926655	-1.3935825296
C	-4.1100228294	-1.0873182257	1.9460964709

H	-2.5840241669	-1.4939444393	3.3995639928
H	-5.4147562372	-0.7156226848	0.2820046890
H	-4.9024642293	-1.0315842404	2.6796837438

P4a

0 1

C	-1.3660605547	0.5695821347	-0.3218147839
C	-0.1790974267	0.1115337422	0.4535150842
H	-1.1006957079	0.6734384304	-1.3754101819
N	-1.8217613244	1.9437759912	0.1023581342
O	-2.9727033453	2.4005589956	-0.4473160144
H	-3.5902822022	1.6282497490	-0.3563886486
C	-1.1455490514	2.7342744870	0.8232158918
C	-0.3486660560	-0.3864041656	1.8577116287
H	0.3076343846	0.1602135446	2.5362761719
H	-1.3774344587	-0.2840913009	2.2048581758
H	-0.0616124320	-1.4372886383	1.9247682597
C	-2.5631887386	-0.3744441005	-0.2241176562
O	-3.7071883301	-0.0151615070	-0.0388067457
O	-2.1931447212	-1.6143593058	-0.3908302873
C	-3.2438594923	-2.6020587916	-0.3681970856
H	-2.7520149375	-3.5498469046	-0.5475026275
H	-3.7277819564	-2.5914182715	0.6046999408
H	-3.9675330082	-2.3827390249	-1.1483998341
C	3.1452027538	-0.0794387176	-0.2418933650
O	3.2968656950	0.2825368333	-1.4005004583
O	4.2217492998	-0.4604645181	0.5082132558
C	5.4751557256	-0.3974759843	-0.1521956115
H	5.6775850506	0.6098586018	-0.5137100413
H	6.2205181944	-0.6832339492	0.5848321082
H	5.5087932358	-1.0844155983	-0.9975101331
N	0.9436248308	0.1991074869	-0.1711903426
N	2.0249357197	-0.1914182987	0.5132715634
H	-0.1863883193	2.4001580981	1.1887175748
H	-1.5532743375	3.7144419022	1.0220063178

P4b

0 1

C	-1.2287712294	-0.6690549939	-0.1077622953
C	-0.0395180999	-1.5591468939	-0.4541663512
H	-1.2217666354	0.2168904698	-0.7391536913
N	-1.1393692707	-0.2036652389	1.2765816206
O	-1.1457774250	-1.2017796651	2.2264397882
H	-2.0493795461	-1.5640200291	2.1630452174
C	-0.6605141541	0.9550790772	1.6706670068
C	-0.2196470167	-3.0314932988	-0.6690537592

H	0.6952544058	-3.5437614102	-0.3818425765
H	-1.0501055261	-3.4235516258	-0.0795349630
H	-0.4182221243	-3.2638555024	-1.7179511333
C	-2.5631468142	-1.3662150272	-0.2823533757
O	-3.2848100093	-1.6874678831	0.6331846021
O	-2.8140338487	-1.5963161802	-1.5527018336
C	-4.0151339968	-2.3338083725	-1.8373741107
H	-4.0636752155	-2.4075451633	-2.9169985617
H	-3.9524940761	-3.3206436071	-1.3846978871
H	-4.8773551151	-1.8008885896	-1.4453898072
C	3.2696061762	-0.8090990867	-0.6539178247
O	3.3674816121	0.3802322077	-0.3501611196
O	4.3971048580	-1.5267099467	-0.9595414014
C	5.6183543731	-0.8143170385	-0.8711449394
H	5.7978449331	-0.4639128472	0.1452815719
H	6.3977882966	-1.5140422305	-1.1609558719
H	5.6255986638	0.0446145661	-1.5413133300
N	1.0653493929	-0.9204706444	-0.4744254960
N	2.1960340884	-1.6109479870	-0.7503433545
C	-0.5297285208	2.0854997027	0.7178961896
C	-1.6034265311	2.9599597543	0.5847461020
C	0.6563454962	2.2785397094	0.0167812414
C	-1.4913511399	4.0451261717	-0.2710880655
H	-2.5150643909	2.7893371110	1.1422376827
C	0.7523925201	3.3716691995	-0.8338270194
H	1.4728011369	1.5706061578	0.1068231469
C	-0.3138432298	4.2495978544	-0.9784097811
H	-2.3220280084	4.7273460835	-0.3838093804
H	1.6667473839	3.5324155809	-1.3883490153
H	-0.2285050215	5.0969149526	-1.6450169145
N	-0.3359867625	1.1387304759	2.9294574529
H	-0.4185531513	0.3878872337	3.5987305165
H	-0.0102104775	2.0420519538	3.2313987208

TS1a (gas phase)

0 1			
N	0.0258816403	0.4024096386	0.0000028949
O	-1.1714009916	-0.2602094940	0.0000361307
C	1.1593312448	-0.1515777715	0.0002243960
H	-0.9185356293	1.0052875775	0.0006557907
H	2.0445085237	0.4649532659	0.0003181620
H	1.1942712120	-1.2362172166	0.0001956256

TS1a

0 1			
N	0.0350077712	0.4127733036	0.0000664252

O	-1.1742876401	-0.2592360652	0.0000747913
C	1.1604870579	-0.1511037171	0.0002167503
H	-0.9323364377	0.9993761762	0.0005851593
H	2.0506557580	0.4590131830	0.0003284502
H	1.1945294907	-1.2361768805	0.0001614237

TS1b

0 1

N	-1.9917367506	-0.8398308306	0.1758460309
O	-3.4168191703	-0.5598727867	0.2269027259
C	-1.2446105795	0.1995983938	-0.0705553198
H	-2.6117918228	-1.2210784960	1.0194328978
N	-1.8239447133	1.3596237697	-0.3807866100
C	0.2223863366	0.0676107745	-0.0374219816
H	-1.3232820512	2.0742283734	-0.8787454028
H	-2.8350598753	1.3431798736	-0.3902054794
C	1.0215651694	1.1857810964	0.1907438155
C	0.8146401420	-1.1810897409	-0.2201824053
C	2.4013629972	1.0554115686	0.2336331827
H	0.5677689804	2.1533592922	0.3592436491
C	2.1930626161	-1.3063650571	-0.1744177365
H	0.1885288388	-2.0412549883	-0.4105557189
C	2.9885739194	-0.1891134631	0.0504457063
H	3.0165986833	1.9250987002	0.4178066309
H	2.6489626651	-2.2757346158	-0.3214470802
H	4.0648176148	-0.2894008640	0.0828490954

TS1c

0 1

N	2.2857600586	-0.3833954243	-0.2004723859
O	1.9948732311	-1.7031454700	-0.6619975684
C	1.4129062283	0.4883937761	0.1322341186
H	3.1133472391	-1.1109491499	-0.3867327279
N	1.8123181034	1.7091887707	0.5845745295
C	-0.0407822902	0.2107176952	0.0660241577
H	2.7539717965	2.0065184568	0.3888615959
H	1.1213318510	2.4327854413	0.6718777619
C	-0.9062376000	1.1768310773	-0.4424516925
C	-0.5476271828	-1.0030902536	0.5252082215
C	-2.2701627637	0.9311373284	-0.4923604746
H	-0.5161645076	2.1142779081	-0.8178971627
C	-1.9131435050	-1.2383494591	0.4843328140
H	0.1323540808	-1.7498895327	0.9048581815
C	-2.7746609118	-0.2751396854	-0.0259812514
H	-2.9373680132	1.6806153897	-0.8947793089
H	-2.3060411126	-2.1769486588	0.8504920660

H	-3.8387097018	-0.4652852098	-0.0609818742
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TS2a

0 1

N	-2.0755917459	0.5214056020	0.5115596167
O	-2.9292700222	1.2160493895	0.0521626672
C	-1.3973011935	-0.3799169028	-0.4936466137
H	-1.5116695721	-2.4499057600	-0.6523910364
N	-1.8529885222	-1.7330089530	-0.0153486357
C	0.0450289457	-0.2454284851	-0.2981812909
H	-1.5431218114	-1.9859735654	0.9344090086
H	-2.8692706060	-1.7948535331	-0.0432065837
C	0.9394336982	-1.3267744292	-0.2428196864
C	0.5955587629	1.0464022811	-0.1946361893
C	2.3064545079	-1.1240331374	-0.1071003628
H	0.5873049436	-2.3478625572	-0.3195945176
C	1.9560691929	1.2406562578	-0.0414944793
H	-0.0618206330	1.9049240030	-0.2507642392
C	2.8283393826	0.1566931501	0.0000365119
H	2.9669673942	-1.9810767958	-0.0786507797
H	2.3427500440	2.2484042775	0.0395130110
H	3.8927521343	0.3103626981	0.1095161095

TS2b

0 1

N	-2.1095613015	-0.7973095621	-0.1496242202
O	-1.9932044016	-2.0506396587	-0.1557661244
C	-1.1632268814	0.1063571105	-0.1046542108
H	-2.8380552888	0.3689652048	-0.1671376071
N	-1.9557120508	1.3199388618	-0.1243197258
C	0.2780230431	0.0176421037	-0.0491872836
H	-1.9135961870	1.8900994092	0.7156771400
H	-1.8489849534	1.9055048069	-0.9478357425
C	1.0598366916	1.1773945315	-0.0092009860
C	0.9107947032	-1.2328194785	-0.0356438782
C	2.4412383384	1.0905373135	0.0438271987
H	0.5849919834	2.1497734097	-0.0196113698
C	2.2936158599	-1.3068970538	0.0176579779
H	0.3042027445	-2.1250076440	-0.0672088990
C	3.0640739833	-0.1512998175	0.0577338787
H	3.0327963155	1.9953899729	0.0740784753
H	2.7739379226	-2.2760761621	0.0276327258
H	4.1425238892	-0.2177113778	0.0996159511

TS3a

0 1

N	-1.4612990891	0.2267119671	-0.1023354706
O	-1.4559359372	-1.0752095058	0.1798416543
C	-2.4783355494	0.9626203551	0.0589950946
H	-0.2368928312	-1.1558820579	-0.1931731760
H	-2.3887115473	2.0071969862	-0.1965473881
H	-3.4005678193	0.5437680800	0.4419189757
H	-0.2598410797	0.2804093323	-0.4960906000
O	0.6767083862	-0.5495208115	-0.6058319027
C	1.6381261156	-0.3486342184	0.4262288818
H	1.1274264212	-0.0736983272	1.3557142528
H	2.1552045381	-1.2933026390	0.6027349920
C	2.6187725785	0.7293609403	0.0209538294
H	2.1018855440	1.6756513663	-0.1406114958
H	3.3680192990	0.8756637497	0.7983671383
H	3.1262929706	0.4510007827	-0.9019737855

TS3b

0 1

H	-2.6224562276	1.2904061773	-0.3532730168
N	-0.8776921425	1.0403775243	-0.0978101585
O	-1.8612564533	1.9892354252	-0.0093138416
C	0.3451834054	1.3516143935	0.1528619724
H	-1.4687109463	0.1658170881	-0.4793376812
N	0.6788665305	2.6172240166	0.4435952304
C	1.3802517788	0.3025113044	0.0788379338
H	1.5630888792	2.8100254605	0.8805430676
H	-0.0644917909	3.2887494447	0.5512220472
C	2.6703048188	0.6283093967	-0.3309785153
C	1.0665646263	-1.0127360698	0.4139059688
C	3.6398917306	-0.3597388088	-0.4091047409
H	2.9107350958	1.6454721485	-0.6102088174
C	2.0391377415	-1.9959773791	0.3323715313
H	0.0704457241	-1.2585636407	0.7573187901
C	3.3256714488	-1.6710011916	-0.0789727517
H	4.6390680308	-0.1053971303	-0.7337761057
H	1.7949809905	-3.0151648834	0.5976697261
H	4.0834010529	-2.4399303509	-0.1413832615
C	-3.4649285781	-0.7556048788	0.2716601157
H	-2.9568671273	-0.5439051005	1.2285583031
H	-4.5128124692	-0.4583383752	0.4146167834
O	-2.8875936638	-0.0292483263	-0.7752780380
C	-3.4081355533	-2.2524408543	0.0094896446
H	-2.3718848144	-2.5804593255	-0.0904519962
H	-3.8718324870	-2.8163176742	0.8205744384
H	-3.9286056005	-2.4896073903	-0.9190686282

TS3c

0 1

H	-1.9996891561	-0.5547709492	-1.1666715710
N	-0.8386999997	0.3348784155	-0.1498928441
O	-0.9213084644	-0.6541222529	-1.0939527537
C	0.2680277628	0.7709451104	0.3376944206
H	-1.9235683778	0.6144099798	-0.0665314311
N	0.2533378551	1.8726572475	1.1276570483
C	1.5791342301	0.1563752776	0.0425989495
H	0.9875554891	1.9592100065	1.8110195761
H	-0.6379691714	2.2599201105	1.3952541228
C	2.7020614887	0.9737245748	-0.0736370223
C	1.7072608852	-1.2260673426	-0.0788535479
C	3.9450356657	0.4112453354	-0.3199679015
H	2.5987105069	2.0471016138	0.0088760870
C	2.9546424588	-1.7820301312	-0.3106283349
H	0.8336667252	-1.8538387266	0.0091316219
C	4.0724131030	-0.9659679495	-0.4357238811
H	4.8123008046	1.0485404358	-0.4214026669
H	3.0548051561	-2.8551177037	-0.3950430285
H	5.0427398184	-1.4048924519	-0.6237607098
C	-3.8267333276	-0.6997469957	0.2233386715
H	-3.1166989678	-1.2780175381	0.8392722298
H	-4.4457519787	-1.4417384734	-0.2993805428
O	-3.1533519729	0.1107963128	-0.6957720240
C	-4.7143616439	0.1225771809	1.1451143745
H	-5.2509590364	-0.5102994127	1.8539464774
H	-4.1118265077	0.8367595598	1.7094270665
H	-5.4439463452	0.6831657664	0.5595156137

TS4a

0 1

N	1.3500667206	-0.0739701344	0.0000150429
O	0.8559510153	1.1600312847	0.0000289010
C	2.5961101899	-0.3085973549	0.0000208444
H	0.4360944318	-0.8324156454	-0.0000022499
H	2.9156428772	-1.3391116418	0.0000087859
H	3.2979444002	0.5151759379	0.0000378278
N	-1.3500680657	0.0739690838	-0.0000025515
O	-0.8559524723	-1.1600323735	-0.0000164256
C	-2.5961115227	0.3085964024	-0.0000083319
H	-0.4360956381	0.8324145617	0.0000147278
H	-2.9156441350	1.3391107134	0.0000037381
H	-3.2979458013	-0.5151768339	-0.0000253091

TS4b

0 1

N	-1.1488246058	-0.6640149007	-0.1471541949
O	-0.0186245202	-1.4230023516	-0.2089127960
C	-2.2984295114	-1.2342262826	-0.0342608399
H	-0.9069136018	0.4088342261	-0.2035227079
N	-2.3857938068	-2.5764070102	-0.0572987387
C	-3.5092538151	-0.3987949082	0.0727726505
H	-3.2020453344	-3.0183769478	0.3281791736
H	-1.5121575347	-3.0787509159	-0.0139675238
C	-4.7334689644	-0.8843148703	-0.3791796438
C	-3.4302092466	0.8797709692	0.6236807138
C	-5.8703966572	-0.0962579101	-0.2814923845
H	-4.7968765355	-1.8669368201	-0.8271771444
C	-4.5686601731	1.6632598427	0.7156966487
H	-2.4828381710	1.2558369275	0.9884352363
C	-5.7900670981	1.1767525413	0.2653343269
H	-6.8173864048	-0.4757195034	-0.6392328197
H	-4.5034647919	2.6525035044	1.1468247117
H	-6.6776125972	1.7898934349	0.3401052199
N	1.1479036528	0.7202709411	-0.1229962680
O	0.0655442452	1.5350783187	-0.2106184548
C	2.3132472625	1.2574136178	-0.0454345963
H	0.7716071702	-0.4860747994	-0.1756960321
N	2.4511193723	2.6163231216	-0.1354053993
C	3.5091389896	0.4019885980	0.0687347202
H	3.2235945947	3.0219510402	0.3680421868
H	1.5664628762	3.0939232191	-0.0274218774
C	4.7451383823	0.8634101881	-0.3799420695
C	3.4180793028	-0.8747945866	0.6252562001
C	5.8713142796	0.0586841565	-0.2806386722
H	4.8234509977	1.8458726480	-0.8258929376
C	4.5435112603	-1.6767226388	0.7180442409
H	2.4668811962	-1.2324688695	0.9972180969
C	5.7738932309	-1.2127148342	0.2663805793
H	6.8242528956	0.4251337982	-0.6371693731
H	4.4626445484	-2.6633876977	1.1533601220
H	6.6518021125	-1.8395132464	0.3428426462

TS4c

0 1

N	-1.3014741753	0.5301230325	-0.0500419737
O	-1.1231086855	-0.8186852030	-0.0591821608
C	-2.4516693177	1.0999798016	0.0437924814
H	-0.3179107491	1.0252368505	-0.0806701758
N	-2.5131442093	2.4505327718	0.2314262429
C	-3.7288666932	0.3598916503	0.0123401133

H	-3.3121693914	2.9192544367	-0.1648125462
H	-1.6506151508	2.9695543865	0.1662144991
C	-4.7947078729	0.8051902993	0.7923364212
C	-3.8931446464	-0.7435202332	-0.8237694015
C	-6.0131574923	0.1446634948	0.7446064327
H	-4.6629921045	1.6567227007	1.4459343161
C	-5.1174483756	-1.3892873264	-0.8781796558
H	-3.0623401707	-1.0847036884	-1.4217554152
C	-6.1761126716	-0.9507087078	-0.0919770286
H	-6.8338676720	0.4859642467	1.3599952526
H	-5.2458736003	-2.2381936040	-1.5353145173
H	-7.1277290663	-1.4630979181	-0.1325131079
N	1.2811588945	-0.3441441598	-0.0048058758
O	1.1819866637	0.9976963695	-0.1216047023
C	2.3983906206	-0.9643537729	0.1211547630
H	0.1251673643	-0.8105778314	-0.0130658513
N	2.3686777720	-2.3251837986	0.4135592300
C	3.7335243082	-0.3359604157	0.0485707989
H	3.0478528984	-2.8688816823	-0.1001027876
H	1.4473786076	-2.7359730277	0.3568241418
C	4.7969227933	-0.9061789167	0.7507466246
C	3.9673766588	0.7863658268	-0.7485757270
C	6.0686336209	-0.3593586661	0.6673079865
H	4.6213864044	-1.7728673962	1.3728388610
C	5.2431133302	1.3209798831	-0.8379252431
H	3.1431498063	1.2297358434	-1.2837908109
C	6.2953057110	0.7548171343	-0.1286620388
H	6.8819354244	-0.8058646574	1.2230147059
H	5.4175159339	2.1860405329	-1.4634510882
H	7.2873622324	1.1803277445	-0.1979487629

TS5a

0 1

N	1.5108772320	0.9449968234	0.9535389699
O	0.1045382482	1.0868152114	1.2486046921
C	1.7251389733	-0.2279088494	0.4326681340
H	0.0716618955	1.9187788947	1.7665419890
N	-2.0705556943	-0.4731296572	-0.1859696170
N	-3.1149276724	-1.2172253585	0.0059868428
C	-2.1603761065	0.8138905212	0.0785487856
C	-2.7861525665	-2.5468031930	-0.2140756321
C	-0.9087472263	1.4792254773	-0.0959745703
C	-3.3859948497	1.4554366899	0.6502991290
O	-3.9011220232	-3.2937601878	-0.1345241088
O	-1.6915502943	-3.0336168713	-0.4228891768
H	-0.2510077788	1.0821062124	-0.8618240494
C	-0.8994818844	2.9872867143	0.0014803871
H	-3.6850938810	0.9471456691	1.5686560626

H	-3.2314252947	2.5105748606	0.8703413907
H	-4.2205237412	1.3663814908	-0.0465377864
C	-3.7108193145	-4.6940387615	-0.3104568825
O	-1.4067716735	3.5340760207	-1.0764138508
O	-0.4964871205	3.5828030653	0.9711525863
H	-4.6894640295	-5.1478269907	-0.1928429833
H	-3.3147584284	-4.9047652179	-1.3024699321
H	-3.0214968408	-5.0833118612	0.4365911221
C	-1.4974422249	4.9726133152	-1.0715401718
H	-1.9410782002	5.2383498429	-2.0231162528
H	-2.1271935554	5.2927323642	-0.2453930646
H	-0.5041127461	5.4015762316	-0.9710691454
N	0.8231663812	-1.1824472724	0.1825680431
H	1.1164563771	-1.9842884344	-0.3498562284
H	-0.1848117046	-1.0343564586	0.2142118480
C	3.1498488808	-0.5150959896	0.1209057039
C	3.6466685167	-1.8056064876	0.2825054675
C	3.9912952814	0.5021515994	-0.3216695323
C	4.9773876908	-2.0765897721	0.0009769847
H	3.0046483802	-2.5947831499	0.6509165633
C	5.3192762068	0.2249698750	-0.6063157091
H	3.5964016566	1.4998342888	-0.4491935577
C	5.8139312938	-1.0630100379	-0.4456225253
H	5.3604215318	-3.0785841620	0.1350034040
H	5.9678973805	1.0146615775	-0.9594364335
H	6.8505149250	-1.2756440330	-0.6688208954

TS5b

0 1

N	-0.1192436099	-1.5481495555	-0.5603157640
O	-0.3533408025	-0.4203411855	0.2429047153
C	1.1256594147	-1.8900389720	-0.6102253717
H	-1.3907828535	-0.4021328193	0.2720863269
N	-2.6869239820	1.5268732358	0.1529697428
N	-2.8158003208	0.2414316884	0.0198677088
C	-1.4717104311	1.9963049638	-0.1341454502
C	-4.1087666276	-0.2172344154	0.2769070939
C	-0.6027724369	1.1490606698	-0.8505040536
C	-1.1443031447	3.3886526769	0.3257275950
O	-4.0925980416	-1.5540393006	0.2322000695
O	-5.0975303994	0.4369104495	0.4995625371
H	-1.0411391892	0.5139145108	-1.6119639878
C	0.8411240251	1.4502047273	-1.0982671639
H	-2.0822399724	3.9020388282	0.5268468254
H	-0.5535585854	3.3786127599	1.2414588506
H	-0.5876661873	3.9486346492	-0.4224128914
C	-5.3516132951	-2.1859198693	0.4629045038
O	1.3929918813	2.1292237136	-0.1076857597

O	1.4214434848	1.0617955532	-2.0796271336
H	-5.7120831414	-1.9576805934	1.4640159205
H	-6.0831498839	-1.8482276084	-0.2683378754
H	-5.1741780439	-3.2507364024	0.3583052220
C	2.7982223362	2.3864264800	-0.2318744579
H	3.0730945664	2.9524877929	0.6507077535
H	3.3376814407	1.4426154317	-0.2686769903
H	2.9927881351	2.9598538354	-1.1354699789
N	1.4366223406	-2.8806286610	-1.4949358902
H	2.2076807485	-3.4835799504	-1.2582736038
H	0.6544388671	-3.3352214024	-1.9410507273
C	2.2714699942	-1.3305571040	0.1543526453
C	2.1443116248	-0.9287692033	1.4835663498
C	3.5253073157	-1.2867968096	-0.4572490102
C	3.2583187047	-0.4924053853	2.1850442229
H	1.1828295756	-0.9740413828	1.9709145737
C	4.6361079600	-0.8520810452	0.2490884679
H	3.6249559281	-1.5818240129	-1.4927835326
C	4.5042790571	-0.4548940401	1.5728252501
H	3.1525482761	-0.1896366947	3.2175631134
H	5.6014456694	-0.8184518156	-0.2366225469
H	5.3697596021	-0.1171457373	2.1264187012

TS6a

0 1

N	0.7522038287	-1.6416248913	-0.5768035902
O	2.0580512275	-1.5122566661	-0.4274208843
C	-0.0473889036	-1.6545180543	0.4653427950
H	0.3579129815	-1.4707360395	-1.4953122046
N	0.2396328286	1.2652751453	-0.3609835160
N	-0.7310443525	1.7443550382	0.3217806929
C	1.3986060749	1.0754452598	0.3109838173
C	-1.8955528471	1.8386971218	-0.4573761483
C	2.3509782794	0.4250945817	-0.4658115101
C	1.5250484411	1.4510299950	1.7530247943
O	-2.8640513373	2.3714658983	0.3023035687
O	-2.0692972574	1.5065241381	-1.6065793501
H	2.1879784571	0.4478733864	-1.5327531539
C	3.7740418090	0.2466562892	-0.0578742826
H	0.8037564135	0.8945805521	2.3555622961
H	2.5244251029	1.2597606587	2.1271441266
H	1.2807473667	2.5065586941	1.8784421082
C	-4.1299620096	2.5149397771	-0.3359835991
O	4.5780018659	0.3431425282	-1.1147842455
O	4.1643988000	0.0138279202	1.0581293393
H	-4.7953314602	2.9386838194	0.4090940433
H	-4.0515312316	3.1795298765	-1.1945646700
H	-4.5007098302	1.5456929866	-0.6665611927

C	5.9725089851	0.1502900362	-0.8539529573
H	6.4701245635	0.2586298007	-1.8108884384
H	6.3290831186	0.8981986178	-0.1491813309
H	6.1402304790	-0.8430055150	-0.4434998146
N	0.4848691913	-1.6689213975	1.6757239028
H	-0.0849125694	-1.8096985477	2.4913419871
H	1.4893363019	-1.6057584852	1.7609143391
C	-1.5011040236	-1.6425208450	0.2563430922
C	-2.0671827122	-2.3211811896	-0.8217529400
C	-2.3035899239	-0.8961155827	1.1166390046
C	-3.4319641167	-2.2419914235	-1.0414864448
H	-1.4488877040	-2.9276304020	-1.4703751169
C	-3.6687679078	-0.8201800873	0.8878160814
H	-1.8581634288	-0.3411538026	1.9312653193
C	-4.2320472229	-1.4894183516	-0.1901439216
H	-3.8732309636	-2.7723252417	-1.8734137894
H	-4.2890865644	-0.2267414554	1.5451719233
H	-5.2970787495	-1.4265521434	-0.3669651304

TS6b

0 1

N	0.7424345782	-1.4007976541	-1.0990553525
O	2.0482341376	-1.2218257082	-1.1388048444
C	0.1355459944	-1.6511262646	0.0379631317
H	0.1914144582	-1.0904148020	-1.8920236191
N	0.1522001975	1.3817993417	-0.3694655267
N	-0.7763925554	1.6818262814	0.4544876781
C	1.3744297889	1.1574134703	0.1731739829
C	-2.0164341457	1.7937965504	-0.1993240219
C	2.2923502931	0.7129363718	-0.7689680674
C	1.5998862906	1.3134617615	1.6446402997
O	-2.9277111838	2.1863164421	0.7011029843
O	-2.2854611525	1.5703432130	-1.3561681913
H	2.0685952637	0.9316145223	-1.8018068937
C	3.7516269077	0.5577263178	-0.5070810710
H	0.9773856800	0.6165023010	2.2093918655
H	2.6383524193	1.1533239775	1.9139201645
H	1.2987469990	2.3157674055	1.9510457357
C	-4.2599286938	2.3008480699	0.2075850054
O	4.0224476590	-0.1909392644	0.5588431023
O	4.5965618407	1.0530698596	-1.2094716059
H	-4.8680209457	2.6042728963	1.0534196158
H	-4.3111538840	3.0468245509	-0.5834030370
H	-4.6015584861	1.3424708199	-0.1809099596
C	5.4131638519	-0.3688713162	0.8553069222
H	5.4490570621	-1.0068785297	1.7309230664
H	5.9158002445	-0.8416690893	0.0148532037
H	5.8766385969	0.5931260370	1.0622208436

N	0.8733808590	-1.8379267741	1.1212523057
H	0.4614581771	-2.1534307598	1.9816650900
H	1.8729525547	-1.7009872379	1.0508837207
C	-1.3319957351	-1.7026545931	0.0718186672
C	-2.0452526840	-2.2471958325	-0.9950591881
C	-2.0066903902	-1.1450685245	1.1559362790
C	-3.4297343413	-2.2242556045	-0.9779551235
H	-1.5209531304	-2.7060446497	-1.8228656974
C	-3.3929068584	-1.1202470037	1.1621460441
H	-1.4532666032	-0.6953119382	1.9689454246
C	-4.1035967582	-1.6572983663	0.0973173112
H	-3.9826523990	-2.6537616747	-1.8013133917
H	-3.9160567508	-0.6719395648	1.9953457835
H	-5.1847771564	-1.6368230375	0.1057163633

TS6c

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N	0.4817744136	-1.0134483459	-1.4473209946
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C	0.0358215269	-1.7400324547	-0.4518702841
H	-0.1669036638	-0.5529906596	-2.0744808896
N	0.1194015060	1.5758274663	0.2322888578
N	-0.8305278132	1.7234901465	1.0697810737
C	1.1778152601	0.8436743447	0.6656412712
C	-1.9257583366	2.4406085887	0.5607550064
C	2.1674262369	0.7137072221	-0.2992214758
C	1.1896328764	0.2659575893	2.0476524104
O	-1.9549731178	2.5961360826	-0.7676766855
O	-2.8000681941	2.8468843438	1.2907562204
H	2.1521715479	1.4206501373	-1.1135283862
C	3.4994144154	0.1217618865	0.0160480643
H	2.0850563641	-0.3185683306	2.2307815133
H	0.3119610347	-0.3622275199	2.2108321728
H	1.1292965827	1.0726172338	2.7800657124
C	-3.0870316846	3.3049061034	-1.2743321680
O	4.4860202379	0.8953185367	-0.4173473899
O	3.6747946905	-0.9341822962	0.5775674941
H	-2.9520809698	3.3490535445	-2.3498082599
H	-3.1251244368	4.3079543720	-0.8546109059
H	-4.0063181542	2.7771826867	-1.0278029195
C	5.8129900932	0.4140614756	-0.1664431400
H	6.4813648301	1.1554815166	-0.5884224650
H	5.9547370887	-0.5511550488	-0.6469300002
H	5.9759221368	0.3146583841	0.9043047319
N	0.9188458911	-2.3548150780	0.3281390101
H	1.8985541779	-2.1011125397	0.2397937981
H	0.6087896546	-2.7646201584	1.1925443141
C	-1.4118730479	-1.8921660784	-0.2497030474

C	-1.9232642806	-3.0837823311	0.2620587976
C	-2.2709637471	-0.8345702470	-0.5482841274
C	-3.2865417961	-3.2165690458	0.4663105152
H	-1.2613890767	-3.9121666124	0.4772166468
C	-3.6344901329	-0.9761695267	-0.3422580127
H	-1.8789847990	0.1060122165	-0.9128224191
C	-4.1425243739	-2.1640258981	0.1655642536
H	-3.6817191133	-4.1439535080	0.8563669281
H	-4.2974762314	-0.1525560772	-0.5684717733
H	-5.2059518914	-2.2702692392	0.3297914942

TS6d

0 1

N	1.1466872815	1.1485086452	1.0563755483
O	1.8923404332	0.1644576751	1.5430973851
C	-0.1572890784	1.1420083419	1.1925498419
H	1.5877206406	1.7754234388	0.3886713576
N	-0.0635527442	-1.9267363233	-0.1745577397
N	-1.2134497911	-1.8737635997	-0.7202564151
C	0.8819268420	-1.1144810784	-0.7003892339
C	-2.1243963731	-2.7249643672	-0.0607644396
C	2.0440400118	-1.1195091394	0.0615979370
C	0.5952756084	-0.2778824102	-1.9111073231
O	-3.3186738257	-2.5867308948	-0.6488648629
O	-1.9279312946	-3.4641803366	0.8728998789
H	2.1745234971	-1.9381606686	0.7527733143
C	3.2926961702	-0.4221553899	-0.3552363388
H	1.4730061418	0.2724484573	-2.2303621154
H	-0.2158556182	0.4282785283	-1.7178593328
H	0.2518521614	-0.9200320052	-2.7237148529
C	-4.3646935446	-3.3880269060	-0.1025020903
O	4.3699210086	-1.1068583630	0.0136982323
O	3.3393672659	0.6441417438	-0.9224906739
H	-5.2517205311	-3.1588925873	-0.6831530330
H	-4.5232963380	-3.1424986307	0.9458292065
H	-4.1175046377	-4.4444028046	-0.1891838580
C	5.6295788057	-0.4980137493	-0.2933101052
H	6.3860838013	-1.1766567988	0.0835214978
H	5.7038249431	0.4703814569	0.1962930100
H	5.7305680018	-0.3695765104	-1.3686581622
N	-0.7348362522	0.1995065082	1.9201237802
H	-0.1849630853	-0.5917267024	2.2202013456
H	-1.7255008724	0.2141965040	2.0863288191
C	-0.9568587892	2.1952524095	0.5481447226
C	-2.1704760735	1.8523819756	-0.0457631526
C	-0.4968775774	3.5090911980	0.5018082983
C	-2.9193216386	2.8269735537	-0.6862996975
H	-2.5075218590	0.8230091702	-0.0372676887

C	-1.2533333215	4.4775379301	-0.1385473651
H	0.4325639577	3.7772952389	0.9863532409
C	-2.4624727882	4.1375958326	-0.7314611636
H	-3.8563103782	2.5617295030	-1.1553109547
H	-0.9022153133	5.4993041533	-0.1678674668
H	-3.0499438467	4.8965540014	-1.2294593503

TS6e

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N	-1.0384697812	1.6849222918	-0.1078769581
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C	0.0119813043	1.5353874517	-0.8817478799
H	-0.9105328809	1.9013983259	0.8738181756
N	-0.1336994003	-1.4366472345	-0.0437582360
N	0.9122229893	-1.7181404831	0.6383818888
C	-1.1896491445	-0.9685888084	0.6543771298
C	1.9443072573	-2.1807320342	-0.1916790057
C	-2.2737248472	-0.6553956447	-0.1585770334
C	-1.0963676138	-0.7020728659	2.1245728189
O	3.0032054300	-2.4681732317	0.5767743461
O	1.9534590372	-2.3090729510	-1.3951709955
H	-2.1880539957	-0.9577332242	-1.1920487834
C	-3.6766620581	-0.5105531069	0.3260456796
H	-1.9485333747	-0.1278373615	2.4720221012
H	-0.1690291926	-0.1648321623	2.3343456691
H	-1.0483057713	-1.6330707352	2.6928475356
C	4.1519526495	-2.9474366030	-0.1182545766
O	-4.5062279443	-0.3744274490	-0.7075725676
O	-4.0418864862	-0.5181696995	1.4745638217
H	4.9125232856	-3.1102415501	0.6378820577
H	4.4920437251	-2.2116764387	-0.8450159509
H	3.9245971680	-3.8785928478	-0.6339049650
C	-5.8842565596	-0.1795650350	-0.3769500637
H	-6.4032964092	-0.0726807059	-1.3227822176
H	-6.0002942765	0.7180961931	0.2266806724
H	-6.2640938122	-1.0379220221	0.1729903740
N	-0.1667746748	1.1186633008	-2.1219745703
H	-1.0996938840	0.8894481855	-2.4286759731
H	0.6027292307	1.0665911183	-2.7660820434
C	1.3511420053	1.8253377704	-0.3507165798
C	2.4155318211	1.0050155018	-0.7200271652
C	1.5497138400	2.8765451805	0.5420385565
C	3.6742294455	1.2347808403	-0.1871328767
H	2.2542104756	0.1746220974	-1.3958602715
C	2.8118295619	3.0999173817	1.0676901678
H	0.7309593127	3.5337900196	0.8033322546
C	3.8723456012	2.2786977119	0.7065850337
H	4.4997405305	0.5954063427	-0.4667698714

H	2.9683785874	3.9192202777	1.7548792068
H	4.8553133564	2.4543038486	1.1214414931

TS6f

0 1

N	1.3217222076	0.8599773861	1.1695001733
O	1.9510686145	-0.2013279482	1.6559739426
C	0.0268297316	1.0061563027	1.3104245925
H	1.8266147860	1.4341222251	0.5015445473
N	-0.2810569270	-1.9096037869	-0.1778498890
N	-1.3681008422	-1.6301202916	-0.7787692383
C	0.8317544421	-1.2904216896	-0.6397658626
C	-2.4567221935	-2.3152557395	-0.2008265742
C	1.9230457762	-1.5210903043	0.1897360200
C	0.7689880939	-0.4145607661	-1.8555307273
O	-3.5825033279	-1.8255037401	-0.7345614516
O	-2.4422386430	-3.1983198089	0.6213795120
H	1.8309668981	-2.3406552291	0.8861992290
C	3.3400385178	-1.1965365394	-0.1394407917
H	1.7498621443	-0.0581926392	-2.1473716482
H	0.1157502678	0.4448561283	-1.6832568411
H	0.3272110424	-0.9712244200	-2.6830976374
C	-4.7906194206	-2.4255321240	-0.2702319268
O	3.5046436330	0.0207730123	-0.6590884216
O	4.2492123243	-1.9591248454	0.0684224032
H	-5.5954935861	-1.9226574372	-0.7953546345
H	-4.8951790844	-2.2878500657	0.8042350055
H	-4.7966903752	-3.4897938122	-0.4975534081
C	4.8577367074	0.3946662015	-0.9469449623
H	4.8052452720	1.3950438277	-1.3615619890
H	5.2919339415	-0.2961558898	-1.6655947484
H	5.4475761393	0.3884834180	-0.0331300545
N	-0.6478515430	0.1491508100	2.0599190304
H	-0.1822568999	-0.6855198405	2.3830803926
H	-1.6312528011	0.2732926497	2.2236052237
C	-0.6540593947	2.1223442500	0.6358729045
C	-1.8944030810	1.8899357069	0.0433068197
C	-0.0572306234	3.3780928618	0.5494663582
C	-2.5333859860	2.9162298621	-0.6343408489
H	-2.3376516163	0.9026232530	0.0793625155
C	-0.7047128870	4.3988679706	-0.1281198711
H	0.8935905140	3.5638713155	1.0313537657
C	-1.9408806752	4.1689784000	-0.7190743293
H	-3.4912535228	2.7348539304	-1.1012727159
H	-0.2480755681	5.3767566080	-0.1875006676
H	-2.4439970554	4.9687647983	-1.2447901962

TS6g

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N	0.8752821771	-1.7132518966	-0.2677925108
O	2.0829505908	-1.3191162583	-0.6440175230
C	-0.1817587091	-1.4064771098	-0.9847920813
H	0.7562894817	-2.0432257097	0.6828408141
N	0.1247445458	1.3690204738	0.3259459553
N	-0.8628049555	1.5673604391	1.1172227532
C	1.2077385272	0.7785821344	0.8726246047
C	-1.9579567967	2.1849943651	0.5063301705
C	2.2200834136	0.5451277067	-0.0535710172
C	1.2054407112	0.3107963111	2.2948484280
O	-1.8042812653	2.5392496707	-0.7780803398
O	-2.9848726726	2.3860507498	1.1169956674
H	2.0739408019	0.9898211752	-1.0272990638
C	3.6493239555	0.3087365567	0.3029884279
H	2.0718651116	-0.3070095657	2.5051353250
H	0.2875790919	-0.2487675237	2.4899853711
H	1.2001709091	1.1551701991	2.9868558847
C	-2.9364050086	3.1725712795	-1.3722000669
O	4.3995746431	0.2959492921	-0.7982219053
O	4.0949890060	0.1564311774	1.4121220047
H	-2.6447623327	3.4103600727	-2.3899540881
H	-3.1949183524	4.0795581344	-0.8296454937
H	-3.7936113686	2.5008334431	-1.3717006260
C	5.7931516140	0.0436136770	-0.5965319205
H	6.2468067735	0.0803368412	-1.5805661986
H	5.9344265530	-0.9366639812	-0.1462780489
H	6.2226943211	0.8045332754	0.0513909127
N	-0.0047496846	-0.8332682011	-2.1610238174
H	0.9349281235	-0.6282459207	-2.4642374285
H	-0.7800597458	-0.6736752446	-2.7799622713
C	-1.5248801982	-1.6906542267	-0.4615459280
C	-2.5468433561	-0.7752290749	-0.7056801358
C	-1.7692125661	-2.8298675064	0.3024620536
C	-3.8087430768	-0.9965492666	-0.1780806648
H	-2.3432405903	0.1211347720	-1.2777153732
C	-3.0348147534	-3.0451228312	0.8233716297
H	-0.9864463578	-3.5589567303	0.4654747863
C	-4.0523140038	-2.1293778660	0.5864871737
H	-4.5971258686	-0.2786145355	-0.3549719188
H	-3.2293903030	-3.9328003281	1.4084222622
H	-5.0370983853	-2.3001579691	0.9989411967

TS6h

0 1

N	0.9774960311	-1.1447341098	-1.1048005393
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O	1.6982777157	-0.1311586916	-1.5673719371
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H	1.4576765426	-1.8301284622	-0.5284118546
N	-0.1273406507	1.8282892408	0.4125792556
N	-1.2342319144	1.7423898501	1.0380785347
C	0.8533358496	0.9903285843	0.8204373449
C	-2.2345427846	2.5869805017	0.5263606829
C	1.9575125274	1.0477311173	-0.0228990462
C	0.6512798455	0.0740559637	1.9900986548
O	-1.9252012706	3.2677592649	-0.5806304801
O	-3.3171154854	2.6593088937	1.0627584721
H	2.0391045153	1.9114705531	-0.6651087941
C	3.2346286565	0.3339613541	0.2582385823
H	1.5468042845	-0.4974419862	2.2065948296
H	-0.1759855151	-0.6161614542	1.8073055523
H	0.3711490400	0.6584353148	2.8679408307
C	-2.9606068391	4.1128397295	-1.0827288372
O	4.2796122984	1.0471943606	-0.1482268348
O	3.3257693122	-0.7639959358	0.7545477088
H	-2.5576353750	4.5770667783	-1.9767144469
H	-3.2214186346	4.8704905767	-0.3464595516
H	-3.8453264938	3.5272228627	-1.3240008302
C	5.5600872298	0.4280095091	0.0201405142
H	6.2834422782	1.1361859766	-0.3674311515
H	5.5980379575	-0.5045694975	-0.5383232045
H	5.7444807339	0.2291458819	1.0733853099
N	-0.9533039154	-0.1240266781	-1.7544293718
H	-0.4222787378	0.6909956464	-2.0238293151
H	-1.9547410307	-0.1191033291	-1.8362552590
C	-1.0945403986	-2.2142069613	-0.5198991019
C	-2.2429069795	-1.9027948984	0.2063218494
C	-0.6623274543	-3.5341038504	-0.6226677010
C	-2.9547458759	-2.9149865882	0.8300171397
H	-2.5544459757	-0.8706393711	0.3106501448
C	-1.3824030175	-4.5402769113	0.0011794922
H	0.2148350362	-3.7757390507	-1.2080929627
C	-2.5266220422	-4.2319360597	0.7259217808
H	-3.8393550907	-2.6742431715	1.4025101672
H	-1.0546581454	-5.5665580790	-0.0855419861
H	-3.0857884525	-5.0203223846	1.2105815969

TS6i

0 1

N	1.4202732284	0.5902356352	0.9335861600
O	0.2929165524	1.1978394199	1.2765972425
C	1.4604186136	-0.6374319738	0.4758853092
H	2.2764064806	1.1323139357	0.9591033306
N	-2.3171280468	0.1307866790	-0.2871491825

N	-3.4761677601	-0.3041360184	-0.0153399277
C	-2.0938594140	1.4638671304	-0.1378525751
C	-3.4899902916	-1.7171657959	-0.0967996958
C	-0.7720363806	1.7592186182	-0.3871562068
C	-3.1584235154	2.3671076246	0.3931666680
O	-4.7531532158	-2.1342417423	-0.0478734342
O	-2.5371500106	-2.4574614774	-0.1617486280
H	-0.2017113844	1.0386194228	-0.9546787595
C	-0.1548428738	3.1093249844	-0.3068963920
H	-3.4807968957	2.0252137894	1.3788763474
H	-2.8065689217	3.3892194387	0.4623210903
H	-4.0359833777	2.3227822542	-0.2531926259
C	-4.9342786936	-3.5504344946	-0.0845142551
O	1.0471391299	3.0974886719	-0.8896745669
O	-0.6276936931	4.0863181145	0.2162390152
H	-6.0046373261	-3.7150612281	-0.0278643664
H	-4.5351720699	-3.9579757695	-1.0110756827
H	-4.4319492571	-4.0168218683	0.7604780751
C	1.7792315593	4.3245814538	-0.8204605038
H	2.7184717138	4.1389021589	-1.3292338836
H	1.2275754045	5.1209301517	-1.3150907287
H	1.9542993511	4.5963821327	0.2185069970
N	0.3415827720	-1.3165881293	0.2631727462
H	0.3883283095	-2.2893006780	0.0134793247
H	-0.5761609915	-0.8778488764	0.2776659590
C	2.7749184191	-1.2511798492	0.2084398038
C	3.8553375875	-0.9926184234	1.0497799950
C	2.9343370986	-2.0927508310	-0.8903720207
C	5.0894455226	-1.5640432214	0.7839531317
H	3.7260242904	-0.3716103091	1.9261487829
C	4.1701449602	-2.6638114352	-1.1486724305
H	2.1015992722	-2.2815056476	-1.5547706369
C	5.2481088062	-2.3987546975	-0.3139400210
H	5.9235385656	-1.3664015441	1.4424052231
H	4.2922656909	-3.3114872619	-2.0054065821
H	6.2111557914	-2.8468913438	-0.5163050959

TS6j

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N	-0.6054854630	0.8970413158	-1.5026557816
O	-1.8579484527	0.5150058894	-1.6419362188
C	-0.2408949530	1.6449462224	-0.4903663608
H	0.0887283469	0.5174031195	-2.1351227955
N	0.0340879210	-1.6190792642	0.1917362248
N	0.9477534572	-1.6412841327	1.0810795025
C	-1.1489219094	-1.0720697924	0.5727939164
C	2.1581423179	-2.1948002944	0.6324346143
C	-2.0779887723	-1.0663262349	-0.4593216812

C	-1.3292620890	-0.5543012242	1.9666535834
O	2.2473643738	-2.4282604197	-0.6820558566
O	3.0649407986	-2.4147239268	1.4019979550
H	-1.8673984767	-1.7206838047	-1.2906054635
C	-3.5350157442	-0.8000116277	-0.2883489903
H	-2.3128362654	-0.1228059133	2.1149429580
H	-0.5708613367	0.1959807732	2.1972478267
H	-1.1814179331	-1.3673152881	2.6791737628
C	3.4828085833	-2.9967267119	-1.1182893321
O	-3.8048220037	0.3215010090	0.3808962561
O	-4.3852714485	-1.5271377934	-0.7342932925
H	3.3944915248	-3.1079311899	-2.1938909839
H	3.6396353747	-3.9656497263	-0.6486132174
H	4.3141274288	-2.3398380625	-0.8704908699
C	-5.1958957447	0.6192681385	0.5613255429
H	-5.2284561432	1.5378287777	1.1361191387
H	-5.6837223091	-0.1891364870	1.1003578541
H	-5.6739825101	0.7543447680	-0.4060390474
N	-1.1907814360	2.1561555487	0.2853645863
H	-2.1399821551	1.8326881675	0.1431989978
H	-0.9452759272	2.5827010700	1.1617625727
C	1.1807425285	1.9381026440	-0.2658222353
C	1.5600813626	3.1671454491	0.2719530129
C	2.1469132280	0.9803270907	-0.5722373435
C	2.8999427006	3.4363111029	0.4952523650
H	0.8135223319	3.9191263552	0.4904630418
C	3.4861770079	1.2583496318	-0.3466228266
H	1.8556319860	0.0117460012	-0.9569138094
C	3.8627513590	2.4830531689	0.1875589487
H	3.1943012237	4.3923722899	0.9045613008
H	4.2342036780	0.5126290503	-0.5772574583
H	4.9076955400	2.6952163106	0.3669986030

TS6k

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N	0.2330221314	-0.5227798892	-1.3819563237
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C	-0.0500656699	-1.6308117396	-0.7451060458
H	-0.4831846036	0.1918779361	-1.4774345350
N	-0.0396042236	1.2268298998	1.2250747236
N	-0.3643057957	1.9056890310	0.2092676009
C	1.1331550119	0.5089670577	1.1548143540
C	-1.5561765264	2.6429091793	0.4401131470
C	2.0372174571	0.7896695520	0.1582282464
C	1.3386637626	-0.4781505517	2.2691317425
O	-1.9776808690	3.1122858995	-0.7340904377
O	-2.1106512034	2.8471298272	1.4883917146
H	1.9386700399	1.7177855680	-0.3809509277

C	3.3628253194	0.1280641530	0.0890061879
H	1.2850796996	-1.5087493410	1.9177333571
H	2.3110994032	-0.3558341889	2.7437733818
H	0.5602576944	-0.3242552038	3.0135682647
C	-3.1655009069	3.9042042862	-0.6850843761
O	4.2741782985	0.9287360796	-0.4536636816
O	3.5975960184	-1.0042054019	0.4442121584
H	-3.3799482058	4.1833571882	-1.7107935440
H	-3.9878279168	3.3271096637	-0.2672654687
H	-2.9999005500	4.7902839074	-0.0755853634
C	5.5828921705	0.3689658954	-0.6103656347
H	6.1894074805	1.1520812188	-1.0506233476
H	5.9819974928	0.0731399567	0.3571593076
H	5.5409623562	-0.4981956363	-1.2658141917
N	0.9392717851	-2.4456720090	-0.3950182029
H	0.7409494675	-3.3414921268	0.0135006821
H	1.8945897904	-2.1142436263	-0.4462793690
C	-1.4554272625	-1.9494773278	-0.4446497210
C	-2.4689468455	-1.5943141456	-1.3330074336
C	-1.7715250383	-2.5841557659	0.7549153386
C	-3.7901631445	-1.8664298223	-1.0151072950
H	-2.2252418102	-1.1327013083	-2.2805882686
C	-3.0943645168	-2.8552867710	1.0652292737
H	-0.9888808613	-2.8421769004	1.4563090329
C	-4.1040099438	-2.4961924542	0.1820431999
H	-4.5739698049	-1.5956041443	-1.7084411065
H	-3.3368181438	-3.3409472947	1.9999533216
H	-5.1356464320	-2.7099492079	0.4251441635

TS61

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N	1.2534745949	0.6595784781	1.1999700988
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C	-0.0170705644	0.9769120996	1.2541240768
H	1.8864862103	1.2047286167	0.6228478226
N	-0.5866924842	-1.7529976959	-0.4478742723
N	-1.5719943849	-1.2737516772	-1.0976659495
C	0.6363771983	-1.2851564296	-0.7940058500
C	-2.8187072147	-1.7549993261	-0.6625662256
C	1.6148375952	-1.7139228628	0.0962656787
C	0.7938384653	-0.3472861333	-1.9537891891
O	-2.7918239034	-2.8303968218	0.1268185647
O	-3.8452247353	-1.2159639879	-1.0111460718
H	1.3575725923	-2.5547510748	0.7225434618
C	3.0845652408	-1.5727954912	-0.1072245447
H	1.8355455122	-0.1314533987	-2.1607634681
H	0.2669639331	0.5928903145	-1.7708991898
H	0.3349468583	-0.7864170742	-2.8406105052

C	-4.0691530078	-3.3074535966	0.5509603721
O	3.4532459370	-0.3612888178	-0.5255802471
O	3.8626032957	-2.4659976728	0.1123569167
H	-3.8699115605	-4.1678832939	1.1808841610
H	-4.6697889179	-3.5968718434	-0.3088900528
H	-4.5946549071	-2.5380469980	1.1129871160
C	4.8634217699	-0.1619143896	-0.6843169042
H	4.9790469121	0.8541652704	-1.0442499242
H	5.2636805584	-0.8715550404	-1.4043710789
H	5.3656152103	-0.2902544402	0.2720115453
N	-0.8669110021	0.1786031776	1.8794578615
H	-0.5540013084	-0.7345981062	2.1725098925
H	-1.8322492300	0.4382188485	1.9805584304
C	-0.4772742179	2.2240486491	0.6232262514
C	-1.6561288564	2.2054146741	-0.1208578197
C	0.2705301438	3.3939935473	0.7321141047
C	-2.0820290256	3.3627035318	-0.7539277618
H	-2.2127161941	1.2829428567	-0.2369221221
C	-0.1655546258	4.5464907789	0.0983841090
H	1.1719272655	3.4087761998	1.3303934454
C	-1.3401927291	4.5313846994	-0.6428549176
H	-2.9898793793	3.3490248759	-1.3403267800
H	0.4076182184	5.4583759266	0.1890716110
H	-1.6774149946	5.4328611358	-1.1356139958

TS6m

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N	-0.8734470604	-1.6959308895	0.5490069307
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C	0.2516604852	-1.3787414101	1.1475712600
H	-0.8496683996	-2.0613300950	-0.3957247765
N	-0.1433609964	1.3447981859	-0.2597631731
N	0.7580831505	1.4957602778	-1.1556191027
C	-1.2875623566	0.7486615079	-0.6617035723
C	1.9209951111	2.1139262289	-0.6842846038
C	-2.1915169175	0.5875146290	0.3849912966
C	-1.4314168828	0.2078068619	-2.0512120841
O	1.9018279419	2.5288257105	0.5905845502
O	2.8851273728	2.2628249388	-1.4022966361
H	-1.9053170869	1.0665014013	1.3102520814
C	-3.6698228354	0.4062672892	0.3027233335
H	-2.2582501708	-0.4904362884	-2.1196830975
H	-0.5021838300	-0.2881929891	-2.3371237644
H	-1.5909655600	1.0070522478	-2.7778107775
C	3.1031771472	3.1513218404	1.0440289326
O	-4.1279334608	0.1163866336	-0.9096635007
O	-4.3784285400	0.5229100156	1.2719122630
H	2.9182118882	3.4384492634	2.0739492660

H	3.3317840934	4.0272938880	0.4405614472
H	3.9377747192	2.4537513508	0.9895533886
C	-5.5430002151	-0.0795656370	-1.0070786139
H	-5.7378225244	-0.3089168575	-2.0486501676
H	-6.0673854966	0.8257143730	-0.7097060608
H	-5.8505982603	-0.9044148938	-0.3684140282
N	0.1959430768	-0.7640591283	2.3153467350
H	-0.7080777025	-0.5463964185	2.7061189560
H	1.0289294925	-0.6001936497	2.8528485307
C	1.5344141618	-1.6929260626	0.5037423116
C	2.5863673920	-0.7874934769	0.6296588193
C	1.6902299033	-2.8492993440	-0.2575420819
C	3.7884904460	-1.0360761793	-0.0128823803
H	2.4512854770	0.1221036655	1.2010250423
C	2.8967658354	-3.0916855372	-0.8941036560
H	0.8868216659	-3.5703869667	-0.3316507024
C	3.9437215076	-2.1861738684	-0.7744060924
H	4.5990711935	-0.3264297631	0.0744238656
H	3.0219736927	-3.9925003228	-1.4780955257
H	4.8828594338	-2.3792473023	-1.2741345289

TS6n

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N	-1.4240390808	0.7818011709	-0.8139589425
O	-0.2259713965	1.2539397986	-1.1312788601
C	-1.6236966500	-0.4542661495	-0.4262579050
H	-2.2036443338	1.4298475032	-0.8048868595
N	2.2119321833	-0.2251200733	0.3577628781
N	3.3056928731	-0.7881986590	0.0534381477
C	2.1673004343	1.1341144493	0.3166444794
C	3.1294016675	-2.1923470288	0.0212748318
C	0.8844504298	1.5692946691	0.5718380921
C	3.3623625542	1.9234885369	-0.1099844995
O	4.3245296007	-2.7696113487	-0.0791686176
O	2.0859331287	-2.8014193909	0.0403345821
H	0.2287217110	0.8812639568	1.0851977932
C	0.3658906119	2.9606198320	0.6180541049
H	3.6036043289	1.7134366701	-1.1544705647
H	3.2039066913	2.9880117248	0.0103347314
H	4.2267358317	1.6146452497	0.4780458431
C	4.3112409133	-4.1956290607	-0.1622901480
O	1.0577484890	3.8301163749	-0.1088964991
O	-0.6261437176	3.2504015349	1.2437842194
H	5.3488389844	-4.4985841224	-0.2490371666
H	3.8643718937	-4.6216597135	0.7337018919
H	3.7457184514	-4.5159217987	-1.0348998933
C	0.5344505661	5.1621934585	-0.1430239569
H	1.2191241394	5.7336037514	-0.7594753931

H	-0.4618773276	5.1585272777	-0.5802006159
H	0.4878274308	5.5738591143	0.8624392453
N	-0.6044165865	-1.2870995038	-0.2689611794
H	-0.7808033298	-2.2557229990	-0.0659733279
H	0.3634600884	-0.9739952220	-0.2697056245
C	-3.0052636711	-0.9038651695	-0.1709022697
C	-4.0449219064	-0.4964580101	-1.0042002185
C	-3.2660937522	-1.7407483921	0.9123336261
C	-5.3398298532	-0.9183668210	-0.7467082206
H	-3.8383471884	0.1227973318	-1.8669820849
C	-4.5627291243	-2.1585249191	1.1640980140
H	-2.4610275251	-2.0439544562	1.5686841907
C	-5.5995476617	-1.7474933895	0.3363048844
H	-6.1441238417	-0.6080200995	-1.3987214802
H	-4.7651053298	-2.8005500197	2.0097994448
H	-6.6104337268	-2.0767010578	0.5335263272

TS6o

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N	-0.8218369774	1.1780301144	-1.0778118811
O	-1.7016581194	0.2421761903	-1.3709351424
C	0.4699279655	0.9374943047	-1.1387637312
H	-1.1551190473	2.0113186217	-0.6045366169
N	0.1751034583	-1.1287034380	1.2086619115
N	0.3264324134	-2.0810380511	0.3774791388
C	-1.0117703449	-0.4646816337	1.2265883670
C	1.6440771469	-2.5678552778	0.3966123042
C	-2.0086506283	-0.7801529996	0.3149504110
C	-1.0970741166	0.6402890353	2.2442172665
O	1.6678489606	-3.7580612992	-0.2097711833
O	2.6347793532	-2.0167284387	0.8185178706
H	-1.9416370840	-1.7223004905	-0.2062905157
C	-3.3635633655	-0.1792293967	0.3948643690
H	-1.9629694214	0.5273240102	2.8950806807
H	-1.1802907524	1.6254973195	1.7830810222
H	-0.1923900427	0.6177646802	2.8481694766
C	2.9563262409	-4.3612406225	-0.3251709335
O	-4.2625077414	-0.9526634013	-0.2140554278
O	-3.6330879816	0.8784054204	0.9096194152
H	2.8029570303	-5.2939737182	-0.8570443139
H	3.3753473023	-4.5519468589	0.6607659454
H	3.6295181698	-3.7121536284	-0.8815617166
C	-5.5977768763	-0.4410043945	-0.2513500749
H	-6.1808454789	-1.1738190663	-0.7977151958
H	-5.6162674195	0.5201243730	-0.7606848031
H	-5.9838479377	-0.3224203355	0.7588733646
N	0.8845056802	-0.1931769961	-1.6817211133
H	0.2096995900	-0.9245409445	-1.8559638095

H	1.8673502074	-0.4013448539	-1.7286337988
C	1.4247819919	1.9340235830	-0.6289624418
C	2.4937460748	1.4933449098	0.1499490787
C	1.2497344240	3.2902221524	-0.8905312585
C	3.3871752988	2.4194911060	0.6645584681
H	2.5988367527	0.4378963025	0.3779358449
C	2.1502118666	4.2077209955	-0.3717002570
H	0.4319997266	3.6237186494	-1.5156428079
C	3.2169927292	3.7734200430	0.4039093553
H	4.2130155666	2.0842581233	1.2761833071
H	2.0228369050	5.2606385003	-0.5801978951
H	3.9175404800	4.4915764106	0.8073643205

TS6p

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N	0.3166709632	-0.8029076793	-1.3399004620
O	1.5747170967	-0.4788466205	-1.5503769947
C	-0.0245528329	-1.7580008455	-0.5121130838
H	-0.3860648046	-0.1355543813	-1.6457030741
N	-0.0818443995	1.4829559303	0.8094046574
N	-0.3245063049	1.9286251291	-0.3496054941
C	1.0737971599	0.7547521009	0.9741881410
C	-1.5100370908	2.6956475396	-0.4264105275
C	2.0440001378	0.7999881876	0.0001348791
C	1.1817654196	0.0272196663	2.2845488586
O	-1.9313230196	3.2154106291	0.7218939125
O	-2.0567801759	2.8732868631	-1.4882226802
H	2.0090243224	1.5975123555	-0.7245646037
C	3.3529709627	0.1210522649	0.1658543947
H	1.0471368609	-1.0490533935	2.1693658678
H	2.1530632216	0.1768343903	2.7526863447
H	0.4067538935	0.4017291816	2.9502008764
C	-3.1257534375	3.9964116145	0.6345843497
O	4.3224177640	0.7779604766	-0.4610800473
O	3.5285826248	-0.9175108519	0.7613463990
H	-3.3030093348	4.3796723385	1.6334620460
H	-2.9905013142	4.8138919155	-0.0702151112
H	-3.9582562584	3.3750496045	0.3110165737
C	5.6203235429	0.1739995766	-0.4104806577
H	6.2696357046	0.8209776320	-0.9890633338
H	5.9628370133	0.1088228585	0.6197875363
H	5.5833111579	-0.8221803786	-0.8453994688
N	0.9246867860	-2.4675441567	0.0878379555
H	0.6863036120	-3.2691099949	0.6444766157
H	1.8840236671	-2.1435090505	0.0573320160
C	-1.4531837584	-2.0316236173	-0.2838744404
C	-2.3733843156	-1.8925354547	-1.3215115936
C	-1.8861990638	-2.4094708683	0.9855739793

C	-3.7190295797	-2.1239479058	-1.0845827523
H	-2.0363586615	-1.6318147643	-2.3158062501
C	-3.2328346646	-2.6418554016	1.2147296667
H	-1.1768779633	-2.4973279283	1.7979038267
C	-4.1494750141	-2.4988561770	0.1813314816
H	-4.4306272889	-2.0217541749	-1.8916852490
H	-3.5667993208	-2.9285004766	2.2019313075
H	-5.1995893072	-2.6824351336	0.3620011387

TS6q

0 1

N	1.2211125467	0.4107633113	1.2773808499
O	1.3757332174	-0.8534347945	1.6174367266
C	0.0241894955	0.9504261653	1.2185013726
H	2.0046206279	0.8725567299	0.8264432918
N	-0.8004197004	-0.9976236004	-1.0837739782
N	-1.4669799824	-1.7177613118	-0.2783871076
C	0.5619715040	-1.0681479223	-1.0474204837
C	-2.8408386876	-1.4193605475	-0.3420492386
C	1.1947055506	-1.8698160424	-0.1115677155
C	1.2516356989	-0.1763699979	-2.0466985518
O	-3.5304396837	-2.4635003677	0.1185499839
O	-3.3510687083	-0.3762288620	-0.6799243588
H	0.6155004878	-2.6431127075	0.3691322899
C	2.6566829312	-2.1281620394	-0.0987007560
H	2.0031548721	-0.7127637927	-2.6239744725
H	1.7553963853	0.6703124805	-1.5762948788
H	0.4995932347	0.2144900910	-2.7288252746
C	-4.9457600993	-2.2835909601	0.1857337736
O	3.3815551379	-1.0521844615	-0.4062294676
O	3.1381596270	-3.1969626753	0.1849821350
H	-5.3451127806	-3.2136003558	0.5753301125
H	-5.3496148552	-2.0804833366	-0.8038362326
H	-5.1885919461	-1.4569757728	0.8505331617
C	4.8016057246	-1.2287969389	-0.3713593408
H	5.2261695217	-0.2684909244	-0.6420892553
H	5.1011135553	-1.9941179569	-1.0836527668
H	5.1181788313	-1.5190939038	0.6281637096
N	-1.0007180741	0.2855561505	1.7260683556
H	-0.8742729640	-0.6921406161	1.9478639551
H	-1.9315512524	0.6576671472	1.6415215174
C	-0.1527445618	2.2786566825	0.6110808887
C	-1.2297953157	2.4726420060	-0.2529512427
C	0.7531272929	3.3072289901	0.8561153148
C	-1.3960052072	3.7037484346	-0.8674219860
H	-1.9064992211	1.6518574133	-0.4670876575
C	0.5769014766	4.5347186776	0.2362280297
H	1.5737775163	3.1588934521	1.5456279590

C	-0.4954411582	4.7330214812	-0.6234997183
H	-2.2253689041	3.8573692768	-1.5434930064
H	1.2722579232	5.3388170680	0.4318213257
H	-0.6298280565	5.6924373303	-1.1038712628

TS6r

0 1

N	0.8234963209	1.1508061032	1.1660908527
O	1.7110120936	0.2334475806	1.4999104543
C	-0.4631296483	0.8845237512	1.2121792051
H	1.1566747684	1.9484470071	0.6317408950
N	-0.1157683249	-1.4428389526	-0.9447821508
N	-0.1115672040	-2.3092446622	-0.0154375610
C	0.9642421034	-0.6185873224	-1.0566678943
C	-1.3001883402	-3.0528859216	0.0660409817
C	2.0467453872	-0.7600160299	-0.2022715278
C	0.8457736559	0.4279735043	-2.1328027382
O	-2.3837342828	-2.4490533738	-0.4328150538
O	-1.3342554269	-4.1280681312	0.6165007714
H	2.1643300911	-1.6896483964	0.3327157606
C	3.2689160219	0.0631828359	-0.3748598296
H	1.7251820315	0.4563853765	-2.7739283429
H	0.7203735183	1.4322915444	-1.7234673808
H	-0.0283088133	0.1975096645	-2.7385545967
C	-3.6020263061	-3.1857425411	-0.3097723209
O	4.3528784950	-0.5765239584	0.0581217367
O	3.2867524505	1.1874774716	-0.8170013448
H	-4.3703494645	-2.5668560508	-0.7609283328
H	-3.8277850267	-3.3698722779	0.7386215160
H	-3.5238789108	-4.1364275655	-0.8327790419
C	5.5783644721	0.1592331655	-0.0133746462
H	6.3428286903	-0.4990285718	0.3835857588
H	5.5054065178	1.0659176684	0.5833352276
H	5.7985231668	0.4217905872	-1.0458178667
N	-0.8668921128	-0.2228059058	1.8114072793
H	-0.1818219656	-0.9369952340	2.0176418178
H	-1.8458019764	-0.4519940416	1.8401209514
C	-1.4241899859	1.8300967252	0.6236198106
C	-2.4481007433	1.3253965244	-0.1766299783
C	-1.2941620836	3.2009169401	0.8262502654
C	-3.3430475900	2.2005485311	-0.7708655829
H	-2.5158180870	0.2580387398	-0.3562816883
C	-2.1959578523	4.0681635294	0.2287612069
H	-0.5107072473	3.5839098815	1.4666253164
C	-3.2187184539	3.5693374764	-0.5668994774
H	-4.1331184568	1.8149398124	-1.3997891060
H	-2.1040480853	5.1326875549	0.3917123392
H	-3.9204563962	4.2490649614	-1.0302296848

TS6s

0 1

N	0.4416853306	-0.1954766797	1.9799731141
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H	0.0488209948	-0.9179522386	2.5800235248
N	-0.9261655873	-1.3736552226	-0.3812704209
N	-1.9501962588	-0.8220934074	-0.8913336471
C	0.2975627722	-1.0100111263	-0.8681339850
C	-3.1261149607	-1.2353523211	-0.2299078517
C	1.3141976595	-1.5977940324	-0.1504230989
C	0.4848131713	-0.0310646648	-1.9889614997
O	-4.1738436493	-0.8871454813	-0.9749868591
O	-3.2255337885	-1.7745592688	0.8498692429
H	1.0576837667	-2.4114115599	0.5094409913
C	2.7483940669	-1.4834868263	-0.5088036479
H	1.0943622598	0.8131364110	-1.6676530957
H	1.0036121080	-0.5011332715	-2.8242447152
H	-0.4809065950	0.3330825769	-2.3257540007
C	-5.4539844257	-1.1940547890	-0.4206475183
O	3.4627329206	-2.4297790737	0.1034178846
O	3.2315705898	-0.6531943966	-1.2376523492
H	-6.1828060254	-0.8212732465	-1.1318639461
H	-5.5621898786	-2.2691299695	-0.2927642970
H	-5.5752999365	-0.7031237293	0.5427566012
C	4.8711489251	-2.3976874248	-0.1407465513
H	5.2883360422	-3.2296947940	0.4154910385
H	5.0717612019	-2.5104578406	-1.2040939714
H	5.2904194108	-1.4564937372	0.2086873667
N	-1.6781060731	0.6388869555	1.8664648780
H	-2.1070944292	-0.2564711643	2.0563720971
H	-2.2793150762	1.4361564474	1.7567937377
C	0.0771621951	1.8713770402	0.7373856097
C	-0.8068309094	2.4413925255	-0.1787018671
C	1.3667596862	2.3874493386	0.8744534458
C	-0.4037043835	3.5160229425	-0.9560355598
H	-1.7915763136	2.0156146923	-0.3175745127
C	1.7581251251	3.4672439604	0.1016042086
H	2.0512773892	1.9379310177	1.5769774258
C	0.8773093557	4.0298604277	-0.8161777063
H	-1.0880570626	3.9444495141	-1.6747913572
H	2.7546386854	3.8713482110	0.2127390346
H	1.1924902289	4.8678748457	-1.4227494327

TS7a

0 1

C	-1.2154165387	0.1283759811	-0.4629980773
C	-0.1336870318	-0.3109596440	0.3042297887
H	-0.9723177942	0.4512485424	-1.4695097253
N	-1.7018789651	1.9089572193	0.1208898558
O	-2.8713014249	2.5116197169	-0.1951499124
H	-3.4366391560	1.7512458169	-0.4569237345
C	-0.8186453139	2.5973808851	0.6949037971
C	-0.2583612582	-0.9221481991	1.6652011597
H	0.3192980724	-0.3454831801	2.3896405553
H	-1.2953930525	-0.9573344196	1.9908642746
H	0.1463667825	-1.9352838838	1.6733132611
C	-2.5730805396	-0.5261157084	-0.3863062184
O	-3.6265010730	0.0475873104	-0.5608774000
O	-2.4756402428	-1.8198831983	-0.1872210138
C	-3.7126600946	-2.5557926850	-0.1819220766
H	-3.4351627270	-3.5867658568	0.0006124684
H	-4.3586652968	-2.1811489892	0.6077896956
H	-4.2046208555	-2.4498230863	-1.1453228603
C	3.2649667388	-0.0982700024	-0.2937694208
O	3.3947135033	0.4266067340	-1.3751574642
O	4.3062410682	-0.4952540548	0.4524158102
C	5.5904904340	-0.2553632223	-0.1168934999
H	5.7431543413	0.8105182523	-0.2765367580
H	6.3114085874	-0.6365271806	0.5986195449
H	5.6890993729	-0.7755134839	-1.0679017000
N	1.0531541741	-0.0450445731	-0.2623951930
N	2.0872017312	-0.4026492136	0.4042432636
H	0.1252593081	2.1110132050	0.9004883050
H	-1.0044847494	3.6314229181	0.9556952742

TS7b

0 1

C	-1.1350693449	-0.8550166198	-0.3209409228
C	0.0003585539	-1.6689690776	-0.2547562320
H	-1.0184571382	0.0721370221	-0.8643411164
N	-1.4354364586	-0.0440411724	1.4234940690
O	-1.3804782260	-1.0609813489	2.3713899642
H	-2.0560433463	-1.6831942459	2.0533778463
C	-0.6304027527	0.9377641638	1.7312572127
C	0.0360697491	-3.0892221182	0.2151504514
H	0.6028472414	-3.1627746282	1.1457147535
H	-0.9624121481	-3.4819446384	0.3834039643
H	0.5513318043	-3.7133591917	-0.5157732195
C	-2.5040466911	-1.4579120327	-0.4085310403
O	-3.0106811064	-2.1557955737	0.4407571272
O	-3.0931846032	-1.1334954293	-1.5443685484
C	-4.4043384720	-1.6823354306	-1.7535409169

H	-4.7198644826	-1.3237131479	-2.7260640464
H	-4.3567444869	-2.7683921200	-1.7391733706
H	-5.0773669659	-1.3331531910	-0.9745540697
C	3.3110991315	-0.8476781751	-0.8388118141
O	3.3227632194	0.3081561672	-1.1936591922
O	4.4256340515	-1.5829729256	-0.7164198097
C	5.6401022400	-0.9060828701	-1.0297006030
H	5.7740606081	-0.0443912770	-0.3784042622
H	6.4350278451	-1.6270435312	-0.8703700893
H	5.6342589774	-0.5722495743	-2.0657638853
N	1.1206249845	-0.9971773020	-0.5741989331
N	2.2168368101	-1.6519356205	-0.4852519103
C	-0.5497530712	2.0818655845	0.8066851507
C	-1.6818861714	2.4938783808	0.1058016095
C	0.6641258846	2.7396453930	0.6184667980
C	-1.5974203343	3.5592875205	-0.7759782492
H	-2.6232601308	1.9865517780	0.2684128168
C	0.7422049791	3.8041467889	-0.2657736920
H	1.5517560375	2.4008579808	1.1358448875
C	-0.3867874509	4.2150653769	-0.9619074887
H	-2.4781640499	3.8821532514	-1.3131788116
H	1.6878185511	4.3049932731	-0.4185765081
H	-0.3225257797	5.0457295246	-1.6512226667
N	0.1388830550	0.9114035447	2.8199184734
H	0.0688481603	0.1287810634	3.4498780065
H	0.5925713273	1.7495984281	3.1400662675

TS8

0 1

C	1.1777517629	-0.0401848871	0.6195150778
C	0.0426196993	-0.5902973129	0.0168032145
H	1.0376755104	0.3815530394	1.6038295327
N	1.5210889741	1.7954048465	-0.1413346196
O	0.2631513251	2.2333779501	-0.5340412339
H	-0.3196119659	1.9711700110	0.2130252713
C	2.4506929526	2.2553352463	-0.9269017492
C	0.0725194471	-1.5777889848	-1.1151757020
H	0.3755710706	-1.0927917882	-2.0446221099
H	0.7618174959	-2.4015258422	-0.9373697791
H	-0.9295744611	-1.9783240402	-1.2491128286
C	2.5107808229	-0.7021057243	0.4688512504
O	3.1617825617	-1.0430533845	1.4236755509
O	2.8750702008	-0.8893450766	-0.7901903235
C	4.1625442622	-1.4927072040	-0.9758854084
H	4.3270165105	-1.5129779890	-2.0473415661
H	4.9235388416	-0.8918742584	-0.4803824523
H	4.1625475161	-2.5001043963	-0.5655225786
C	-2.5602097072	0.9330341706	1.7644217900

O	-3.4703966927	0.1422334428	1.7647381208
O	-2.6229925102	2.1391498099	2.3370187295
C	-3.8634513853	2.4477606172	2.9723731022
H	-4.0768844023	1.7231969438	3.7555991286
H	-3.7434246381	3.4392588036	3.3950824743
H	-4.6730061488	2.4404698414	2.2452810603
N	-1.1779355887	-0.2844891123	0.5039797160
N	-1.2799152975	0.7831217371	1.2052131868
N	2.1679617299	3.0312758000	-1.9840772195
H	2.8956701836	3.5900269532	-2.3950164296
H	1.2120780604	3.3128030568	-2.1276549304
C	3.8659978007	1.9425572824	-0.6439221387
C	4.3030770332	1.8123166819	0.6715103857
C	4.7753669567	1.8180186921	-1.6935295748
C	5.6409561702	1.5558668350	0.9338634831
H	3.5966189028	1.9300759204	1.4818531277
C	6.1114354997	1.5673752536	-1.4259397570
H	4.4348414040	1.8975124512	-2.7174958554
C	6.5460508225	1.4376005866	-0.1122960785
H	5.9766410964	1.4581625507	1.9567248189
H	6.8130825992	1.4668701710	-2.2421723205
H	7.5895587447	1.2434998064	0.0942360742

From supporting information

Me-fumarate

0 1

C	-0.2098743761	-0.4369877394	-0.7534192322
C	0.5530363786	-0.8623848125	0.2542799312
H	0.2517199714	0.0461273403	-1.6023592195
C	0.1308934737	-1.5995181407	1.4848886734
H	-0.8657746374	-2.0108689128	1.3900194545
H	0.8452700094	-2.3940800241	1.6912344102
H	0.1519411862	-0.9254307110	2.3433074873
C	-1.6765707941	-0.5860176108	-0.9158538210
O	-2.2014426029	-0.5767423662	-2.0033017334
O	-2.3563553392	-0.6940173643	0.2230721563
C	-3.7763191528	-0.8237704666	0.0866598487
H	-4.1655307144	-0.8869996976	1.0964580055
H	-4.1818056410	0.0447728919	-0.4274149629
H	-4.0183061584	-1.7229151392	-0.4754628781
C	2.0304212582	-0.5879908995	0.1941823169
O	2.7807156416	-0.8777638337	1.0929221865
O	2.4291936966	0.0061763834	-0.9267188724
C	3.8284893381	0.2938559411	-1.0128512753

H	3.9758116481	0.7567657004	-1.9819707283
H	4.1205244470	0.9735643049	-0.2153677279
H	4.4040843572	-0.6257818536	-0.9350180094

PR1

0 1

N	1.3513707445	1.0817399824	0.6628687690
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C	1.5907494259	-0.1575370661	0.3174147134
H	-0.1604153165	2.0331032025	1.4539342334
N	-2.0955700513	-0.4801230952	-0.1660390772
N	-3.1604832033	-1.2704843088	-0.0247467381
C	-2.2498425633	0.7960755304	-0.1767718844
C	-2.7549923299	-2.5633236528	0.0552063851
C	-0.9424572490	1.5118352340	-0.3104348296
C	-3.5479635271	1.5233154069	-0.0082615484
O	-3.8404746650	-3.3731033824	0.1672233628
O	-1.6212673163	-3.0320467005	0.0448496704
H	-0.3349290876	1.1543232891	-1.1380098525
C	-1.0432471969	3.0230299190	-0.3113891895
H	-4.2074011618	0.9238859430	0.6159276579
H	-3.4090389239	2.4992193847	0.4573814272
H	-4.0474692655	1.6784117781	-0.9670621488
C	-3.5568667163	-4.7595050446	0.2833334743
O	-1.5450077875	3.4914821830	-1.4218191891
O	-0.7067380181	3.6657809201	0.6552177623
H	-4.5182228737	-5.2582076681	0.3657381655
H	-3.0219730326	-5.1231987367	-0.5928706660
H	-2.9561064216	-4.9605439552	1.1693787355
C	-1.7378548402	4.9202435256	-1.4777289730
H	-2.1627657335	5.1173043619	-2.4540156185
H	-2.4191199197	5.2243939926	-0.6871866957
H	-0.7803371724	5.4203101134	-1.3606796576
N	0.7208075616	-1.1485600572	0.1864040208
H	1.0514341173	-2.0270550187	-0.1774164050
H	-0.3035433770	-1.0342118933	0.2025700356
C	3.0317413140	-0.4305026283	0.0746183400
C	3.5816561016	-1.6360114691	0.5013716328
C	3.8287874112	0.5153057181	-0.5635324941
C	4.9270000239	-1.8938841998	0.2873376204
H	2.9676305177	-2.3615682082	1.0183440631
C	5.1718499211	0.2484832356	-0.7801897642
H	3.3909381567	1.4463612279	-0.8942502220
C	5.7216636555	-0.9536942319	-0.3547633294
H	5.3543744311	-2.8274514308	0.6255781280
H	5.7891786257	0.9789618794	-1.2842034203
H	6.7700018488	-1.1580108286	-0.5239784836

PR2

0 1

N	0.5640795134	-1.7111420090	0.1191095822
O	1.7469267131	-1.3545539524	-0.5549337745
C	0.0374096401	-2.7752859122	-0.3605481933
H	2.0903837141	2.4209832148	-2.7374642260
N	1.3853477738	1.7435229333	-1.0479744714
N	0.4762669398	2.7903328893	-1.1154745950
C	1.2833407006	0.9878084442	-0.0272713667
C	0.6946812350	3.4734581855	-2.1866359813
C	2.2608881737	-0.1717426269	-0.0004725814
C	0.2834546541	1.1886292589	1.0693326549
O	-0.0670071462	4.5187385931	-2.4358106954
O	1.6343457273	3.2164575767	-3.0810792271
H	3.1016221582	0.0930630780	-0.6436098609
C	2.8370896425	-0.4138422660	1.3907270799
H	-0.7253242756	1.1123082070	0.6637672364
H	0.4009907376	0.4448260997	1.8515402838
H	0.3911075357	2.1891502907	1.4880296078
C	0.1875015175	5.2726573247	-3.6288116625
O	3.2079240046	0.7416384557	1.9393406222
O	2.9828841968	-1.4865704818	1.9075009983
H	-0.5416633162	6.0746484430	-3.6201707186
H	1.1957674099	5.6790526428	-3.6130235666
H	0.0516349081	4.6489177299	-4.5089238969
C	3.8084292755	0.6528508491	3.2371113715
H	4.0516037953	1.6698638934	3.5226975723
H	3.1051018027	0.2150837091	3.9421177657
H	4.7068636195	0.0417082121	3.1912703516
N	-1.0213736537	-3.3280413043	0.3286222861
H	-1.3924191583	-2.7436682250	1.0637887063
H	-1.7321609325	-3.7549568504	-0.2456690350
C	0.4840905453	-3.5287369413	-1.5605024755
C	0.5627681910	-4.9179607243	-1.5021856876
C	0.7761528379	-2.8709955450	-2.7541144761
C	0.9488527483	-5.6423554473	-2.6211947120
H	0.3305969833	-5.4260715512	-0.5760102693
C	1.1456585889	-3.5990568537	-3.8737459040
H	0.7082297755	-1.7937040492	-2.8005693495
C	1.2394569350	-4.9842682857	-3.8078283917
H	1.0203502479	-6.7199333300	-2.5652847636
H	1.3621450944	-3.0847403498	-4.8001003931
H	1.5359837561	-5.5490785153	-4.6812348542

PR3

0 1

N	0.5180706761	-0.1593025238	1.7821678524
O	1.6394271808	-0.3815249674	1.0292283961
C	-0.3706838742	0.7563555906	1.3834467021
H	0.1781099468	-0.9828626891	2.2699690068
N	-0.9065366840	-1.4015473533	-0.3972952236
N	-2.0446792429	-1.0509764007	-1.0338022061
C	0.2234839276	-1.0163462513	-0.8817737991
C	-3.1106897046	-1.2840887197	-0.2525291352
C	1.3594522149	-1.4137281980	0.0079844180
C	0.4109626461	-0.1371113929	-2.0809354867
O	-4.2579795461	-1.1167198815	-0.9638164452
O	-3.1725151479	-1.5715902292	0.9525130746
H	1.0882073642	-2.3184918376	0.5501284609
C	2.7270263247	-1.6191589825	-0.6281111305
H	1.1553654903	0.6339985388	-1.8796619323
H	0.7686114578	-0.7095885462	-2.9379188340
H	-0.5390360824	0.3242174667	-2.3366038419
C	-5.4678082836	-1.2435233162	-0.2323358927
O	3.4740745125	-2.4050772814	0.1386625353
O	3.0982516996	-1.1381473158	-1.6643313985
H	-6.2675670260	-1.0541067758	-0.9425276606
H	-5.5724128649	-2.2443204016	0.1840734702
H	-5.5134245835	-0.5183809740	0.5793472411
C	4.8070950905	-2.6465137975	-0.3303768957
H	5.2767599046	-3.2706730843	0.4209496845
H	4.7759345719	-3.1575897925	-1.2899021915
H	5.3398267887	-1.7044071728	-0.4366034139
N	-1.6280966432	0.6030691423	1.7119418609
H	-2.0574167645	-0.3306923538	1.7788500256
H	-2.2561993612	1.3817507939	1.5845120590
C	0.0725833037	1.9438937496	0.6493503585
C	-0.7695603754	2.4615929700	-0.3326344565
C	1.3061905752	2.5378753165	0.9130248106
C	-0.3785236212	3.5805908914	-1.0495178729
H	-1.6998096044	1.9583410026	-0.5651410788
C	1.6827938315	3.6629940783	0.2015836979
H	1.9519619688	2.1266719921	1.6759151464
C	0.8428120284	4.1819674142	-0.7784420936
H	-1.0217879990	3.9763135472	-1.8223211738
H	2.6316060959	4.1370018182	0.4088090442
H	1.1458798085	5.0579129263	-1.3354696824

PR4a

0 1

C	0.1792412816	0.7206856676	-1.4953265729
C	-0.9189471499	1.3032362028	-0.6174557004
H	-0.0759831683	0.9317591156	-2.5407438289
N	0.1566076332	-0.7375217314	-1.4098625011

O	-0.9532796801	-1.2961429512	-2.0021107212
H	-1.6627058334	-1.0489325774	-1.3451010524
C	0.8355163444	-1.5409870975	-0.6141865532
C	-1.1405674450	2.7807159854	-0.5563007303
H	-0.6637310926	3.2862799350	-1.3944052623
H	-2.2117941912	2.9755366134	-0.5636106105
H	-0.7270755751	3.2021771690	0.3611812587
C	1.6086258195	1.2556750456	-1.3751404535
O	2.5228648769	0.7894687011	-1.9996452717
O	1.6951261017	2.2997079514	-0.5725637637
C	3.0096551047	2.8552485632	-0.4179457187
H	2.8949268525	3.7000880238	0.2510462042
H	3.6698940192	2.1061258996	0.0159259991
H	3.3956635289	3.1737781349	-1.3828582715
C	-3.5884394785	-0.2816795503	0.7129928970
O	-3.5243515225	-1.3829510115	0.1609899467
O	-4.6298822687	0.0080078782	1.5478283258
C	-5.6073599104	-1.0102757697	1.6831488027
H	-5.1786591321	-1.9138664193	2.1153330380
H	-6.3694161073	-0.6106344275	2.3467051815
H	-6.0498802781	-1.2602154218	0.7195042619
N	-1.6938870748	0.4166711688	-0.1277332075
N	-2.7675974963	0.7782705746	0.6136203331
C	1.8971442575	-1.0599987421	0.2943001465
C	3.1749495365	-1.6051707003	0.1993781906
C	1.5899630221	-0.1252822706	1.2772432685
C	4.1573452556	-1.1894714253	1.0818475019
H	3.3994968256	-2.3284020481	-0.5731770092
C	2.5787581999	0.2754827973	2.1639908997
H	0.5851851924	0.2691373899	1.3548987243
C	3.8590941814	-0.2508562965	2.0630991183
H	5.1555690389	-1.5962224452	1.0040157316
H	2.3449697230	0.9965834522	2.9343590735
H	4.6280955368	0.0695737829	2.7524310610
N	0.5675308551	-2.8282871399	-0.6243162405
H	1.0523600155	-3.4436014203	0.0073753607
H	-0.1554687986	-3.1944846064	-1.2253948557

PR4b

0 1

C	0.0566750607	0.4952859628	-1.6188011115
C	-1.0725964624	1.1998257754	-0.9163604183
H	-0.0593694994	0.6756639690	-2.6897968279
N	-0.0302266065	-0.9635440434	-1.5058275545
O	-0.7853337057	-1.5156092707	-2.4326329773
H	-1.8660117987	-0.5340884320	-0.2711687860
C	0.4984746942	-1.6151686322	-0.5015193588
C	-1.2531908788	2.6681715860	-1.0246855251

H	-0.5233438101	3.1023517270	-1.7011421815
H	-2.2644877605	2.8770101735	-1.3753480717
H	-1.1464391561	3.1280573924	-0.0414323204
C	1.4672667761	1.0049814815	-1.2831607008
O	2.4340753083	0.6076400569	-1.8679515779
O	1.4699723566	1.9274763824	-0.3347369994
C	2.7626171528	2.4405099510	0.0272728177
H	2.5802122915	3.1806359677	0.7970756186
H	3.3795681694	1.6291226433	0.4070805267
H	3.2371629036	2.8908940347	-0.8407115218
C	-3.6854339218	-0.0513448116	0.9086169751
O	-3.3774011811	-1.2397995444	0.8612338200
O	-4.7778074025	0.3868024111	1.5522149268
C	-5.5636829931	-0.6227328135	2.1810512719
H	-4.9900093085	-1.1291614384	2.9552035446
H	-6.4118222853	-0.1080722075	2.6205124849
H	-5.9037477819	-1.3543778622	1.4510252536
N	-1.9390318853	0.4928640811	-0.2861499150
N	-3.0134588835	0.9884149382	0.3518944440
C	0.5503383779	-3.0871186787	-0.5019211394
C	0.3973722892	-3.7831035004	0.6950895138
C	0.8166325124	-3.7825731988	-1.6816575511
C	0.5031607755	-5.1667919523	0.7117497615
H	0.1735608193	-3.2492722450	1.6095955451
C	0.9413895278	-5.1598000577	-1.6547610777
H	0.9172929383	-3.2353591218	-2.6065189195
C	0.7802194854	-5.8544902726	-0.4603527475
H	0.3697580608	-5.7042328404	1.6401057210
H	1.1615183116	-5.6956213889	-2.5676518182
H	0.8696050104	-6.9321217002	-0.4461382449
N	1.0574821491	-0.9384065720	0.5413952797
H	0.6239993852	-0.1010905820	0.9009808537
H	1.5434083548	-1.4888634275	1.2291961175

PR4c

0 1

C	0.0941548985	0.4955995726	-1.5970048639
C	-1.1396842240	1.1382239323	-1.0165565075
H	0.0428523395	0.5298498581	-2.6862168186
N	0.1845879905	-0.9489751614	-1.2596046434
O	-0.7944948104	-1.6315574309	-1.7299149274
H	-1.9912676493	-0.6030981531	-0.5163112420
C	1.1452132884	-1.4414558921	-0.5656844048
C	-1.2909421636	2.6137220676	-1.0949487536
H	-0.5320261798	3.0563816437	-1.7364577903
H	-2.2833477691	2.8528771779	-1.4754796095
H	-1.2106791414	3.0462327310	-0.0961464099
C	1.3534180844	1.2645809048	-1.1877167874

O	2.2509311651	1.4967282423	-1.9471863915
O	1.3142872661	1.6164367323	0.0866168857
C	2.4534316159	2.3481587892	0.5733203699
H	2.2487037656	2.5444211644	1.6187369381
H	3.3526360212	1.7471389990	0.4597055363
H	2.5551497750	3.2757626443	0.0157664650
C	-3.9513354638	-0.0878612365	0.5000643582
O	-3.7224765840	-1.2886551222	0.3947867107
O	-5.0684407914	0.3854275546	1.0787266258
C	-5.9717179418	-0.6043918961	1.5630322696
H	-5.4892312552	-1.2335533666	2.3085259406
H	-6.7973176519	-0.0598726476	2.0099636752
H	-6.3314829291	-1.2286641923	0.7470679867
N	-2.0602263624	0.4265613239	-0.4789476535
N	-3.1685307354	0.9394593637	0.0827082228
H	1.1175696655	-2.5035384653	-0.3828847892
H	1.9319464767	-0.8105819876	-0.1911972222

PR5a

0 1

C	-1.2287712294	-0.6690549939	-0.1077622953
C	-0.0395180999	-1.5591468939	-0.4541663512
H	-1.2217666354	0.2168904698	-0.7391536913
N	-1.1393692707	-0.2036652389	1.2765816206
O	-1.1457774250	-1.2017796651	2.2264397882
H	-2.0493795461	-1.5640200291	2.1630452174
C	-0.6605141541	0.9550790772	1.6706670068
C	-0.2196470167	-3.0314932988	-0.6690537592
H	0.6952544058	-3.5437614102	-0.3818425765
H	-1.0501055261	-3.4235516258	-0.0795349630
H	-0.4182221243	-3.2638555024	-1.7179511333
C	-2.5631468142	-1.3662150272	-0.2823533757
O	-3.2848100093	-1.6874678831	0.6331846021
O	-2.8140338487	-1.5963161802	-1.5527018336
C	-4.0151339968	-2.3338083725	-1.8373741107
H	-4.0636752155	-2.4075451633	-2.9169985617
H	-3.9524940761	-3.3206436071	-1.3846978871
H	-4.8773551151	-1.8008885896	-1.4453898072
C	3.2696061762	-0.8090990867	-0.6539178247
O	3.3674816121	0.3802322077	-0.3501611196
O	4.3971048580	-1.5267099467	-0.9595414014
C	5.6183543731	-0.8143170385	-0.8711449394
H	5.7978449331	-0.4639128472	0.1452815719
H	6.3977882966	-1.5140422305	-1.1609558719
H	5.6255986638	0.0446145661	-1.5413133300
N	1.0653493929	-0.9204706444	-0.4744254960
N	2.1960340884	-1.6109479870	-0.7503433545
C	-0.5297285208	2.0854997027	0.7178961896

C	-1.6034265311	2.9599597543	0.5847461020
C	0.6563454962	2.2785397094	0.0167812414
C	-1.4913511399	4.0451261717	-0.2710880655
H	-2.5150643909	2.7893371110	1.1422376827
C	0.7523925201	3.3716691995	-0.8338270194
H	1.4728011369	1.5706061578	0.1068231469
C	-0.3138432298	4.2495978544	-0.9784097811
H	-2.3220280084	4.7273460835	-0.3838093804
H	1.6667473839	3.5324155809	-1.3883490153
H	-0.2285050215	5.0969149526	-1.6450169145
N	-0.3359867625	1.1387304759	2.9294574529
H	-0.4185531513	0.3878872337	3.5987305165
H	-0.0102104775	2.0420519538	3.2313987208

PR5b

0 1

C	-0.9835291400	-0.7239892944	0.1129862071
C	0.0547408883	-1.5532789937	-0.6100196008
H	-0.9838216225	0.2741481619	-0.3296388346
N	-0.6716677215	-0.5189720917	1.5333129645
O	-0.9904074771	-1.5527099143	2.3925357143
H	-1.9641598363	-1.5733730078	2.3750845687
C	0.2458424821	0.3469810367	1.9567819518
C	-0.0842259937	-3.0357177004	-0.7525257078
H	0.8943828305	-3.5023062201	-0.6572783362
H	-0.7552668098	-3.4418450458	0.0048954309
H	-0.4852588154	-3.3002975251	-1.7332216202
C	-2.4155068283	-1.2137733122	-0.0082737133
O	-3.1909231511	-1.3062240305	0.9139141103
O	-2.7069087587	-1.4870380374	-1.2614699266
C	-4.0527359395	-1.9237821222	-1.5181754354
H	-4.0971262159	-2.1211576307	-2.5823854210
H	-4.2616292498	-2.8254242947	-0.9481205053
H	-4.7522200658	-1.1395091164	-1.2399868475
C	3.1301213571	-0.5605658057	-1.6368095295
O	3.2241431910	0.5712974482	-1.1610965286
O	4.1740993327	-1.1072142114	-2.3246779225
C	5.3307230712	-0.2931930203	-2.4281829531
H	5.7175076102	-0.0328616613	-1.4436942064
H	6.0658484551	-0.8811059920	-2.9707567567
H	5.1168856276	0.6255565570	-2.9734455425
N	1.0614478389	-0.8495526177	-0.9706435144
N	2.1098938510	-1.4383600673	-1.5804048881
C	0.4057370285	0.6032156081	3.3991652714
C	1.6873343950	0.7515059737	3.9206673917
C	-0.7121460805	0.7448374105	4.2190110591
C	1.8515412042	1.0337242839	5.2683667564
H	2.5497108097	0.6229025084	3.2799620661

C	-0.5411644609	1.0419931999	5.5591020837
H	-1.7048673106	0.6424192399	3.8025292679
C	0.7391804573	1.1814123035	6.0843136080
H	2.8462194670	1.1362174998	5.6783448518
H	-1.4049857957	1.1661773460	6.1966436097
H	0.8670889431	1.4063263972	7.1342536509
N	0.9903671492	0.9900016538	1.0864315001
H	1.1530232197	0.6047860637	0.1304583350
H	1.5649149135	1.7481933608	1.4195081516

PR5c

0 1

C	-1.3660605547	0.5695821347	-0.3218147839
C	-0.1790974267	0.1115337422	0.4535150842
H	-1.1006957079	0.6734384304	-1.3754101819
N	-1.8217613244	1.9437759912	0.1023581342
O	-2.9727033453	2.4005589956	-0.4473160144
H	-3.5902822022	1.6282497490	-0.3563886486
C	-1.1455490514	2.7342744870	0.8232158918
C	-0.3486660560	-0.3864041656	1.8577116287
H	0.3076343846	0.1602135446	2.5362761719
H	-1.3774344587	-0.2840913009	2.2048581758
H	-0.0616124320	-1.4372886383	1.9247682597
C	-2.5631887386	-0.3744441005	-0.2241176562
O	-3.7071883301	-0.0151615070	-0.0388067457
O	-2.1931447212	-1.6143593058	-0.3908302873
C	-3.2438594923	-2.6020587916	-0.3681970856
H	-2.7520149375	-3.5498469046	-0.5475026275
H	-3.7277819564	-2.5914182715	0.6046999408
H	-3.9675330082	-2.3827390249	-1.1483998341
C	3.1452027538	-0.0794387176	-0.2418933650
O	3.2968656950	0.2825368333	-1.4005004583
O	4.2217492998	-0.4604645181	0.5082132558
C	5.4751557256	-0.3974759843	-0.1521956115
H	5.6775850506	0.6098586018	-0.5137100413
H	6.2205181944	-0.6832339492	0.5848321082
H	5.5087932358	-1.0844155983	-0.9975101331
N	0.9436248308	0.1991074869	-0.1711903426
N	2.0249357197	-0.1914182987	0.5132715634
H	-0.1863883193	2.4001580981	1.1887175748
H	-1.5532743375	3.7144419022	1.0220063178

PRF

0 1

C	-0.6482194295	-0.2477649662	0.5236953558
C	-2.1491968185	-0.0854824249	0.8084514314

H	-0.4572142214	-1.2684788157	0.2053664294
N	0.1583322997	0.0520931805	1.7051234779
O	0.4343007946	1.3312487440	1.9000834896
C	0.4686319126	-0.8299792173	2.6128000549
C	-2.5418161333	1.1907225322	1.5367170021
H	-2.3045614349	2.0649634668	0.9340764152
H	-3.6120857638	1.1799343609	1.7307273120
H	-2.0057399204	1.2657056290	2.4792614623
C	-0.1516599979	0.6620484791	-0.5907782426
O	-0.8453535281	1.4369778824	-1.1949034868
O	1.1290403445	0.4404198491	-0.8490737814
C	1.7150280989	1.2751243927	-1.8545059088
H	2.7500166203	0.9626329944	-1.9328184615
H	1.2001387855	1.1384401964	-2.8024919805
H	1.6511333060	2.3178159764	-1.5506143475
C	-2.9514555961	-0.2549320425	-0.4677515621
O	-3.9591641075	0.3447421582	-0.7335562092
O	-2.4312303666	-1.1995414105	-1.2574919543
C	-3.1111240830	-1.4205263141	-2.4968349060
H	-2.5596753383	-2.2049417313	-3.0030630428
H	-4.1373745747	-1.7305697937	-2.3142160176
H	-3.1071245736	-0.5071389489	-3.0882572564
C	0.2138478571	-2.2801164168	2.4740228671
C	0.8139782179	-3.0187449059	1.4568067323
C	-0.5949447915	-2.9168487257	3.4118923344
C	0.5860629335	-4.3832102504	1.3672124746
H	1.4635571748	-2.5235861231	0.7459273216
C	-0.8222217066	-4.2818188930	3.3160576877
H	-1.0487969797	-2.3387700522	4.2061249792
C	-0.2339819763	-5.0143583899	2.2939022897
H	1.0547747920	-4.9545003743	0.5781418707
H	-1.4593285102	-4.7725689090	4.0386162245
H	-0.4101587790	-6.0787735140	2.2220071374
N	1.0037487409	-0.3667657478	3.7587268773
H	1.5155849926	-1.0013727119	4.3463123437
H	1.2528150403	0.6120594267	3.7480946840
H	-2.4236058804	-0.9453448197	1.4297988528

TSa01

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N	-1.6539294810	2.3451026936	-0.2139056381
O	-1.7104641630	1.5016959539	-1.2091692457
C	-0.5662436008	2.8749507654	0.1902856532
H	-2.5255203347	2.4617276976	0.3067030903
N	0.9866436730	-0.2320773152	-0.2684483418
N	2.0057901500	-0.2585628420	0.5047630850
C	-0.2103834071	-0.1083527687	0.3337107462
C	3.1948351237	-0.3807697642	-0.2319245079

C	-1.2822402271	-0.1466675729	-0.5756229480
C	-0.3391605487	-0.0122502240	1.8271419189
O	4.2141790936	-0.4664377490	0.6346868056
O	3.3479095396	-0.4043224434	-1.4303788118
H	-1.0487008860	-0.5276120600	-1.5596039154
C	-2.6539486014	-0.4865742939	-0.0697154501
H	-1.3520669567	0.2479796211	2.1218767145
H	0.3511096034	0.7339193009	2.2197294708
H	-0.0679858582	-0.9612731278	2.2958637048
C	5.5054633356	-0.5990807122	0.0460648359
O	-3.0494442883	-1.6671238047	-0.5179439723
O	-3.3067496321	0.2183630552	0.6608766616
H	6.2053251785	-0.6700034291	0.8719690401
H	5.7351201164	0.2682918212	-0.5701946986
H	5.5532333470	-1.4961099558	-0.5683649199
C	-4.3379087312	-2.1086611312	-0.0647791038
H	-4.4903029421	-3.0819392144	-0.5162374857
H	-5.1032549852	-1.4081622167	-0.3901588250
H	-4.3446548377	-2.1814864829	1.0200642852
H	0.3351582200	2.6878996603	-0.3734867935
H	-0.6027218992	3.5159265389	1.0575656454

TSb01

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N	0.3950335041	2.2965568468	-0.0696411267
O	0.3469807875	1.0349598334	-0.6803459811
C	1.4213533009	2.9350718799	-0.4379656284
H	-0.6219687806	0.6555743887	-0.4362033874
N	-0.9977731548	-1.5394401065	0.0505974495
N	-1.5795297949	-0.3773265068	0.0954895279
C	0.3302704674	-1.4942410824	0.1366534598
C	-2.9737649290	-0.4419011924	0.0524318944
C	0.9029475272	-0.2867479877	0.5876670665
C	1.1067013095	-2.7169987034	-0.2569396149
O	-3.4438912596	0.8038548540	-0.0546694466
O	-3.6666746315	-1.4265527375	0.1074500952
H	0.3755202494	0.2456469877	1.3713581927
C	2.3793502662	-0.0266049389	0.6052031681
H	0.4312173399	-3.5691553993	-0.2278675076
H	1.5039678523	-2.6262021792	-1.2677642452
H	1.9420977926	-2.9061568988	0.4141832628
C	-4.8669756318	0.9172048565	-0.0976597399
O	2.9890117003	-0.4732855600	-0.4777857585
O	2.9138044176	0.5566258855	1.5118454247
H	-5.0780252723	1.9782775351	-0.1721945409
H	-5.2624396521	0.3895262752	-0.9630525626
H	-5.3051020788	0.5046393197	0.8088149827
C	4.4066215057	-0.2484254662	-0.5336375657

H	4.7351910121	-0.6775769535	-1.4726266994
H	4.6130130587	0.8190906693	-0.5033336208
H	4.8908455021	-0.7390673212	0.3071794411
H	2.1372615624	2.5293474845	-1.1473980056
H	1.5536090297	3.9238672173	-0.0203425342

TSA-MeF

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C	-0.8666075770	0.1501268607	-0.3806687762
C	-2.1363039906	0.7358338368	-0.1775042405
H	-0.8571461630	-0.8069881029	-0.8798491126
N	-0.2078924936	-0.3676393519	1.2159509199
O	-1.1142584429	-0.0881466708	2.1975190953
H	-1.8836918587	0.2305730914	1.6501496797
C	1.0175849838	-0.4831282583	1.6106020514
C	-2.3183561593	2.2222074968	0.0261738496
H	-1.9697975048	2.8097358624	-0.8283178655
H	-3.3763977017	2.4335494380	0.1605375787
H	-1.7851689080	2.5897483593	0.9052159696
C	0.1993826839	1.0516066729	-0.9472020139
O	0.5358955395	0.9916223825	-2.1027797287
O	0.6738238231	1.9437130646	-0.0841522409
C	1.6391742924	2.8608856861	-0.6118542557
H	1.9274846084	3.4964643073	0.2177762498
H	2.4990334704	2.3125022381	-0.9928745740
H	1.1963891974	3.4493125823	-1.4125184519
C	-3.3094950065	-0.0774053655	-0.3433319813
O	-4.4672897299	0.3152375317	-0.3441737559
O	-3.0342903507	-1.4063782705	-0.4835218804
C	-4.1631068923	-2.2555324946	-0.6440047185
H	-3.7675967794	-3.2602930725	-0.7581704887
H	-4.8110505947	-2.2064187999	0.2297497356
H	-4.7376820585	-1.9770453848	-1.5257230851
C	2.0501571634	-0.7776668726	0.5956906510
C	1.8285202031	-1.7525480246	-0.3728649623
C	3.2367637269	-0.0477985189	0.5967572872
C	2.7900448842	-1.9891329501	-1.3436144208
H	0.9142494335	-2.3303158590	-0.3526649020
C	4.1914600315	-0.2851074575	-0.3795545423
H	3.3973251213	0.7193996001	1.3431468364
C	3.9674524337	-1.2533952813	-1.3504515028
H	2.6204105173	-2.7496669499	-2.0927369633
H	5.1066212343	0.2902186918	-0.3862704656
H	4.7137589589	-1.4360679086	-2.1112622372
N	1.3793302996	-0.3157450707	2.8868609253
H	2.2965663357	-0.5925993258	3.1903286846
H	0.6782032692	-0.1110557121	3.5792406521

TSA-cN

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C	0.9609811975	-0.1689119444	0.4894420604
C	0.3987086079	-1.1975928762	-0.2627071393
H	0.3553759464	0.2433931990	1.2862902983
N	0.8079072247	1.6524534122	-0.4160264346
O	-0.4387313122	2.1297793975	-0.2015485794
H	-0.9884535020	1.3006214404	-0.0305107299
C	1.6089917210	2.3805908952	-1.0626718090
C	1.1860725722	-2.2463200914	-0.9958812281
H	1.5782137833	-1.8585198184	-1.9370455786
H	2.0289730181	-2.6151722740	-0.4139771005
H	0.5236376105	-3.0791555378	-1.2204918835
C	2.4250070409	-0.1545578321	0.8002090920
O	2.8475081862	-0.1272791357	1.9257180347
O	3.1815859246	-0.1852883645	-0.2889448761
C	4.5997417504	-0.2050861571	-0.0619424283
H	5.0541145909	-0.2263650163	-1.0456126005
H	4.8996650892	0.6865305684	0.4836951101
H	4.8693107157	-1.0913363955	0.5073756844
C	-3.0051926522	-0.4941184084	0.0346566913
O	-3.5894966850	-1.5315358420	-0.1381830040
O	-3.5983513531	0.6710180737	0.2999615275
C	-5.0244665636	0.6293198365	0.3773590098
H	-5.3379244440	-0.0394793996	1.1763424214
H	-5.3404046316	1.6452133507	0.5868781313
H	-5.4426010656	0.2862007536	-0.5665086670
N	-0.9441384655	-1.3107416924	-0.3024921215
N	-1.6152664190	-0.2629201467	-0.0086864088
H	2.6152927267	2.0143693210	-1.2007067455
H	1.2864303876	3.3364266842	-1.4623387266

TSA-cO1

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C	-1.3391717550	0.0370069168	-0.5470891574
C	-0.1933541154	-0.4569291645	0.0656850592
H	-1.2201190305	0.3972950695	-1.5641847539
N	-1.6194844536	1.8974306720	0.0653166276
O	-2.6661545781	2.6213514724	-0.3997200644
H	-3.3433291581	1.9296737300	-0.5550899912
C	-0.6557604071	2.5128374316	0.5897291638
C	-0.1895522619	-1.2544394879	1.3407168127
H	-0.4391967921	-2.3015806220	1.1720280048
H	0.8001596567	-1.2028453330	1.7888411143
H	-0.9111201191	-0.8584896748	2.0565592139
C	-2.7231903176	-0.4790555155	-0.2742606491

O	-3.7255103997	0.1883403564	-0.4160634272
O	-2.7374132792	-1.7475584721	0.0673270868
C	-4.0340569350	-2.3329071588	0.2786849232
H	-3.8460270194	-3.3665686414	0.5426767484
H	-4.5447957272	-1.8119289911	1.0844058140
H	-4.6205447642	-2.2653708212	-0.6340409934
C	2.3771156002	0.8303085367	-1.9071250872
O	3.3971006349	0.3356248554	-1.4930471625
O	2.3389780291	1.6883220038	-2.9327117709
C	3.6019017054	1.9921027925	-3.5220662294
H	4.0692907864	1.0876909492	-3.9068218993
H	3.3946726414	2.6843661804	-4.3310330083
H	4.2619010421	2.4527052486	-2.7894352078
N	1.0197325658	-0.1634285599	-0.4633020964
N	1.0596722854	0.6495808194	-1.4442280800
H	0.1904032494	1.9137870304	0.8998437212
H	-0.6833161037	3.5868370169	0.7282033986

TSA-cO2

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C	-1.3576062330	-0.2451519632	-0.6068101514
C	-0.2432835884	-0.4260068771	0.2060183785
H	-1.2282999602	-0.3352832770	-1.6775679468
N	-1.6218729511	1.6908440031	-0.6969922793
O	-1.7807932355	2.2602459945	0.5345117349
H	-2.4207794495	1.6629845877	0.9659664769
C	-0.9645049839	2.3645380912	-1.5446891170
C	-0.3306017341	-0.7492363606	1.6701158216
H	0.6517692497	-1.0589023055	2.0194052738
H	-0.6380232686	0.1204736936	2.2554392556
H	-1.0389419748	-1.5523282059	1.8734201444
C	-2.6989185953	-0.6285289568	-0.0650205615
O	-3.2699079662	-0.0226134443	0.8134221669
O	-3.1621023574	-1.7182416870	-0.6396404735
C	-4.4225165331	-2.2064245026	-0.1469804055
H	-4.6335983122	-3.0999936727	-0.7217905449
H	-4.3373247672	-2.4380995341	0.9117186459
H	-5.1925232345	-1.4545696557	-0.2997844237
C	2.3919061305	0.4810298141	-1.8839347179
O	3.4086673064	0.2225913839	-1.2903664728
O	2.3650541999	1.0319782562	-3.1017494301
C	3.6421000302	1.3080928401	-3.6757274999
H	4.2155491516	0.3893496373	-3.7825838166
H	3.4434416387	1.7451713780	-4.6482748220
H	4.1952035309	2.0063280746	-3.0506759750
N	0.9945272106	-0.1886317048	-0.2900042589
N	1.0564203526	0.2766762153	-1.4752741470
H	-0.7803800635	1.9068220864	-2.5037405492

H	-0.6142830627	3.3640233012	-1.3107921754
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TSA-EcN

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C	-0.8100956033	1.4194961027	-0.3119894250
C	-1.4972110948	1.2663902481	0.8880582727
H	-1.3786828146	1.2795835233	-1.2186581693
N	0.2100266777	-0.3025492853	-0.6013433535
O	-0.0724016370	-1.1241362297	0.4778354619
H	-1.0113621601	-1.3194529246	0.3437973506
C	1.4623324016	-0.2916117308	-0.9562053544
C	-1.0556210402	1.8141479590	2.2147326681
H	-0.2369161632	1.2241634827	2.6317248645
H	-0.7157529937	2.8458750990	2.1491839756
H	-1.8960013676	1.7630132998	2.9037160454
C	0.3061766914	2.4016698012	-0.4601173110
O	0.3644705509	3.1808127183	-1.3788700412
O	1.2225040581	2.3081695772	0.4947020674
C	2.3433009884	3.1936833468	0.3765113405
H	2.9985601279	2.9501700089	1.2050183244
H	2.8462512178	3.0266296722	-0.5738793473
H	2.0114342453	4.2275581658	0.4377431254
C	-4.1459213334	-0.7997214286	-0.0285001871
O	-5.0059511590	-0.6339900955	0.8011659855
O	-4.2626985295	-1.6509586218	-1.0536437664
C	-5.4956426178	-2.3663101340	-1.1146045234
H	-6.3298692611	-1.6732339272	-1.2045113284
H	-5.4314527758	-2.9979623635	-1.9940334916
H	-5.6276856567	-2.9722863675	-0.2203260800
N	-2.6458543451	0.5499018742	0.9012056216
N	-2.8923389677	-0.1666659636	-0.1299835694
C	2.5511540414	-1.0130053403	-0.2629422261
C	2.6936246680	-0.9043941001	1.1188850512
C	3.4643080004	-1.7558581448	-1.0060123211
C	3.7527827819	-1.5369097824	1.7491295260
H	1.9838564268	-0.3182244883	1.6851955885
C	4.5119057280	-2.4017260449	-0.3662400667
H	3.3441916474	-1.8407559499	-2.0781033584
C	4.6574985733	-2.2898536254	1.0095603843
H	3.8725339109	-1.4445631095	2.8196465967
H	5.2127347494	-2.9890778122	-0.9428201458
H	5.4771521266	-2.7895972063	1.5075357500
N	1.8051116214	0.4319088566	-2.0345904399
H	1.1071469788	0.8947770713	-2.5945438262
H	2.7735593070	0.6107528689	-2.2345646682

TSA-EcO

0 1

C	2.0905810243	0.5027516292	-0.1610580840
C	1.6332406669	1.2203203375	0.9374471282
H	1.7459070297	0.7986356384	-1.1422952375
N	0.9972245321	-1.1779606874	-0.1911871533
O	0.9488008866	-1.6269454324	1.1211725696
H	1.8882995431	-1.7562775432	1.3257235858
C	-0.1678641293	-1.0444814716	-0.7662038310
C	2.3190241479	1.2747428102	2.2720071977
H	2.1286757818	0.3703910034	2.8535674752
H	3.3973612857	1.3861420145	2.1760704805
H	1.9277346480	2.1232741388	2.8293638693
C	3.4078528145	-0.1921675338	-0.0998646748
O	3.7155106578	-0.9667590227	0.7768786054
O	4.1855385666	0.1226353022	-1.1209520387
C	5.4755635201	-0.5075983351	-1.1457432636
H	5.9734268359	-0.1225572314	-2.0277773960
H	6.0305606666	-0.2520389766	-0.2463685954
H	5.3567240202	-1.5865160838	-1.2087551765
C	-1.5782848772	2.0257676547	-0.1127143701
O	-2.1342114412	2.5809552237	0.8012142724
O	-2.1938642961	1.6637968675	-1.2469753928
C	-3.6020423351	1.8971499037	-1.2770273872
H	-3.8143663806	2.9574963212	-1.1574679932
H	-3.9428554098	1.5484889568	-2.2461444887
H	-4.0887838020	1.3370959518	-0.4792624874
N	0.4009572129	1.7829345700	0.8797554109
N	-0.2453589451	1.5885502407	-0.2036551019
N	-0.1684564594	-0.7919592679	-2.1015586727
H	0.7309018574	-0.6367297277	-2.5317926389
H	-0.9030181712	-0.1745712630	-2.4198248212
C	-1.4890534327	-1.2793423063	-0.1352994896
C	-2.4970914531	-1.8672242654	-0.8977204145
C	-1.7637152663	-0.8712520994	1.1705156917
C	-3.7640021306	-2.0491687968	-0.3609313199
H	-2.2844847411	-2.1890623284	-1.9077450319
C	-3.0341957546	-1.0394163407	1.6947847491
H	-0.9920095662	-0.3976069578	1.7592607490
C	-4.0356040543	-1.6323595591	0.9335863565
H	-4.5373504042	-2.5139173843	-0.9567338366
H	-3.2441103846	-0.7032350271	2.7008243145
H	-5.0241832634	-1.7677759229	1.3507714418

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C	-2.1269787961	0.6265675278	0.8001083951
C	-1.3770694038	1.4753064722	-0.0349361199

H	-1.9267100510	0.6915083562	1.8598742939
N	-1.1525965283	-1.0811270274	0.8723541525
O	-0.3403627343	-0.9085870515	1.9958458959
H	0.1842367452	-0.0996469028	1.8187573764
C	-0.4893541317	-1.4203028332	-0.2129174892
C	-1.7310230505	1.9471726191	-1.4107605774
H	-2.7722556895	1.7484039886	-1.6499871320
H	-1.5547303637	3.0211024900	-1.4846261500
H	-1.0958648452	1.4712635590	-2.1610867984
C	-3.5585584714	0.2815661274	0.5342472058
O	-4.4378283623	0.5609512985	1.3037801494
O	-3.7567283513	-0.3455555777	-0.6237214817
C	-5.1201603855	-0.6866511745	-0.9277717130
H	-5.0914121270	-1.1731817103	-1.8957394516
H	-5.5083107191	-1.3597752047	-0.1677784736
H	-5.7241933651	0.2159889141	-0.9659623894
C	2.0254178746	1.8690452632	0.3287204110
O	2.2643208911	1.2833090139	1.3618151387
O	2.9779522583	2.3829890973	-0.4567051678
C	4.3151366044	2.1701781462	-0.0073208172
H	4.5150771183	1.1028661628	0.0792547680
H	4.9581810414	2.6181022074	-0.7574012984
H	4.4719757472	2.6439412817	0.9597684452
N	-0.1436961401	1.5924964820	0.4689400266
N	0.7768814871	2.0769223832	-0.2794203233
C	0.9695659440	-1.6837587782	-0.2519114699
C	1.7319995435	-1.0208544381	-1.2127960850
C	1.5829277798	-2.5489576968	0.6498941663
C	3.1047564457	-1.2116590766	-1.2595237936
H	1.2566071431	-0.3246127512	-1.8917575657
C	2.9519570506	-2.7515233800	0.5839224371
H	0.9888208018	-3.0568479927	1.3950668422
C	3.7143701640	-2.0788411716	-0.3635149173
H	3.6948500818	-0.6788022250	-1.9924493971
H	3.4257444963	-3.4307399136	1.2787989388
H	4.7845987581	-2.2298439711	-0.4008324587
N	-1.1375988589	-1.4299967296	-1.3725453069
H	-0.6868673814	-1.7872915205	-2.1970253850
H	-2.1189092202	-1.1902262632	-1.4103878809

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C	-1.8420661730	0.5433599988	0.3133636010
C	-0.9588492329	1.3431700786	-0.4185969046
H	-1.6632330523	0.5058447451	1.3794261007
N	-1.4185356318	-1.3123496190	-0.0350492303
O	-1.2492660794	-1.4391630284	-1.4088145793
H	-2.1191399186	-1.1675547166	-1.7427208392

C	-0.4477669553	-1.8084394070	0.6810986818
C	-1.1295191780	1.7672615924	-1.8429354607
H	-0.3549721123	1.3117290678	-2.4646657568
H	-2.1015162499	1.4807764316	-2.2327754127
H	-1.0072827291	2.8474102415	-1.9316649107
C	-3.2799209543	0.4211595155	-0.0891797454
O	-3.6657731308	-0.0150630028	-1.1490422713
O	-4.0796155060	0.8534913511	0.8692791308
C	-5.4871247641	0.7970519862	0.5893672559
H	-5.9769016266	1.1809680000	1.4763991033
H	-5.7181311929	1.4126333966	-0.2764247979
H	-5.7835152999	-0.2314237019	0.3980308613
C	2.1747030052	2.5176009075	0.4728488423
O	2.3903794985	2.1097554319	1.5897594173
O	3.0418673071	3.2807566390	-0.2061658168
C	4.2494256303	3.5937302043	0.4837656348
H	4.7961111261	2.6844762270	0.7266080278
H	4.8291411048	4.2132193782	-0.1922819559
H	4.0324571370	4.1359220972	1.4022518927
N	0.1610900081	1.6224347817	0.2751786339
N	1.0511915475	2.3016395741	-0.3431021019
C	0.8255351353	-2.3240457518	0.1425403718
C	1.5156052222	-1.5944042691	-0.8244576623
C	1.3698041829	-3.4979338560	0.6569853392
C	2.7503675634	-2.0407145898	-1.2657876270
H	1.0900144240	-0.6788741280	-1.2117544941
C	2.5964678533	-3.9501333531	0.1948907703
H	0.8267284812	-4.0605977015	1.4048669574
C	3.2869746608	-3.2206248120	-0.7632115070
H	3.2938140136	-1.4704287793	-2.0061307804
H	3.0123477240	-4.8689179582	0.5839834833
H	4.2455571773	-3.5714376280	-1.1204170884
N	-0.6036401955	-1.8285493303	2.0136490459
H	-1.4794508363	-1.5649023271	2.4343309741
H	0.1970250167	-1.9438306866	2.6103678177

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C	-1.2318230661	-0.0426002911	-0.6931969917
C	-0.2146395714	-0.7634444955	-0.0466137531
H	-0.9582964844	0.4220378705	-1.6312952618
N	-1.3305454932	1.7057738046	0.1402263838
O	-0.0893773690	2.2325507697	0.1336348365
H	0.5081370495	1.5186529873	-0.2020040262
C	-2.2640962826	2.4194079439	0.5961924681
C	-0.4054011984	-1.8099559948	1.0026395568
H	-1.4478596554	-2.0968551288	1.1053890886
H	0.1831511932	-2.6924327921	0.7516554542

H	-0.0399757153	-1.4512092491	1.9674934601
C	-2.6483178612	-0.5372581880	-0.6874257935
O	-3.1556206493	-0.9995375347	-1.6737073556
O	-3.2378774809	-0.4345954888	0.4933186540
C	-4.5813067999	-0.9426449685	0.5661217403
H	-4.8990960773	-0.7811443906	1.5893426199
H	-5.2186889015	-0.3995760945	-0.1274726803
H	-4.5872077870	-2.0016687337	0.3206331435
C	3.1745587272	-0.0863317401	-0.0985249660
O	3.2646019818	0.9849419746	-0.6544140354
O	4.2325381528	-0.7792915733	0.3358855770
C	5.5006497470	-0.1696938003	0.1013788374
H	5.5555609136	0.7955425923	0.6012722670
H	6.2392092937	-0.8507699827	0.5103242254
H	5.6636602336	-0.0300684787	-0.9654957404
N	0.9953710430	-0.2835632170	-0.3612058991
N	2.0083863709	-0.7838118009	0.2439038983
H	-3.2570614203	1.9973405924	0.6026826775
H	-2.0637258930	3.4174664078	0.9698006146

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C	-1.2154165387	0.1283759811	-0.4629980773
C	-0.1336870318	-0.3109596440	0.3042297887
H	-0.9723177942	0.4512485424	-1.4695097253
N	-1.7018789651	1.9089572193	0.1208898558
O	-2.8713014249	2.5116197169	-0.1951499124
H	-3.4366391560	1.7512458169	-0.4569237345
C	-0.8186453139	2.5973808851	0.6949037971
C	-0.2583612582	-0.9221481991	1.6652011597
H	0.3192980724	-0.3454831801	2.3896405553
H	-1.2953930525	-0.9573344196	1.9908642746
H	0.1463667825	-1.9352838838	1.6733132611
C	-2.5730805396	-0.5261157084	-0.3863062184
O	-3.6265010730	0.0475873104	-0.5608774000
O	-2.4756402428	-1.8198831983	-0.1872210138
C	-3.7126600946	-2.5557926850	-0.1819220766
H	-3.4351627270	-3.5867658568	0.0006124684
H	-4.3586652968	-2.1811489892	0.6077896956
H	-4.2046208555	-2.4498230863	-1.1453228603
C	3.2649667388	-0.0982700024	-0.2937694208
O	3.3947135033	0.4266067340	-1.3751574642
O	4.3062410682	-0.4952540548	0.4524158102
C	5.5904904340	-0.2553632223	-0.1168934999
H	5.7431543413	0.8105182523	-0.2765367580
H	6.3114085874	-0.6365271806	0.5986195449
H	5.6890993729	-0.7755134839	-1.0679017000
N	1.0531541741	-0.0450445731	-0.2623951930

N	2.0872017312	-0.4026492136	0.4042432636
H	0.1252593081	2.1110132050	0.9004883050
H	-1.0044847494	3.6314229181	0.9556952742

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C	-1.2113272443	0.0016188155	-0.4407968314
C	-0.1384288079	-0.2971777544	0.4093180313
H	-0.9752034979	0.0367248499	-1.4966566663
N	-1.6266437750	1.8605836944	-0.2902767742
O	-2.1486390378	2.2798682145	0.8885055328
H	-2.6987813062	1.5186025090	1.1703680986
C	-1.1044683034	2.7301679376	-1.0390863327
C	-0.2591426766	-0.6029227288	1.8694019712
H	0.2280747689	0.1777202715	2.4575668200
H	-1.2974777791	-0.6761078401	2.1830376118
H	0.2507818742	-1.5372368239	2.1058317440
C	-2.5734067412	-0.5450703388	-0.1231212131
O	-3.3067896798	-0.1105165338	0.7382949718
O	-2.8560273691	-1.5779952268	-0.8834232864
C	-4.1214777037	-2.2187189014	-0.6379196373
H	-4.1819799898	-3.0269548699	-1.3564613474
H	-4.1479604338	-2.6000871211	0.3794964038
H	-4.9266889624	-1.5042934518	-0.7874078860
C	3.2605783487	-0.2458429654	-0.2220057409
O	3.3891222594	-0.0375627936	-1.4055413321
O	4.3019736836	-0.4009833072	0.6078777634
C	5.5864527156	-0.2949315976	-0.0007252125
H	5.7134836539	0.6865431715	-0.4538845527
H	6.3088182175	-0.4382972076	0.7958373200
H	5.7102702066	-1.0592394114	-0.7656748472
N	1.0495205564	-0.1738592868	-0.2031010021
N	2.0810750241	-0.3746893890	0.5277583950
H	-0.6368087200	2.3837548648	-1.9499697483
H	-1.1170622811	3.7788392208	-0.7668222529

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C	1.1777517629	-0.0401848871	0.6195150778
C	0.0426196993	-0.5902973129	0.0168032145
H	1.0376755104	0.3815530394	1.6038295327
N	1.5210889741	1.7954048465	-0.1413346196
O	0.2631513251	2.2333779501	-0.5340412339
H	-0.3196119659	1.9711700110	0.2130252713
C	2.4506929526	2.2553352463	-0.9269017492
C	0.0725194471	-1.5777889848	-1.1151757020

H	0.3755710706	-1.0927917882	-2.0446221099
H	0.7618174959	-2.4015258422	-0.9373697791
H	-0.9295744611	-1.9783240402	-1.2491128286
C	2.5107808229	-0.7021057243	0.4688512504
O	3.1617825617	-1.0430533845	1.4236755509
O	2.8750702008	-0.8893450766	-0.7901903235
C	4.1625442622	-1.4927072040	-0.9758854084
H	4.3270165105	-1.5129779890	-2.0473415661
H	4.9235388416	-0.8918742584	-0.4803824523
H	4.1625475161	-2.5001043963	-0.5655225786
C	-2.5602097072	0.9330341706	1.7644217900
O	-3.4703966927	0.1422334428	1.7647381208
O	-2.6229925102	2.1391498099	2.3370187295
C	-3.8634513853	2.4477606172	2.9723731022
H	-4.0768844023	1.7231969438	3.7555991286
H	-3.7434246381	3.4392588036	3.3950824743
H	-4.6730061488	2.4404698414	2.2452810603
N	-1.1779355887	-0.2844891123	0.5039797160
N	-1.2799152975	0.7831217371	1.2052131868
N	2.1679617299	3.0312758000	-1.9840772195
H	2.8956701836	3.5900269532	-2.3950164296
H	1.2120780604	3.3128030568	-2.1276549304
C	3.8659978007	1.9425572824	-0.6439221387
C	4.3030770332	1.8123166819	0.6715103857
C	4.7753669567	1.8180186921	-1.6935295748
C	5.6409561702	1.5558668350	0.9338634831
H	3.5966189028	1.9300759204	1.4818531277
C	6.1114354997	1.5673752536	-1.4259397570
H	4.4348414040	1.8975124512	-2.7174958554
C	6.5460508225	1.4376005866	-0.1122960785
H	5.9766410964	1.4581625507	1.9567248189
H	6.8130825992	1.4668701710	-2.2421723205
H	7.5895587447	1.2434998064	0.0942360742

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C	1.4160661468	0.6168826719	-0.4512334033
C	1.0546592566	1.9569346642	-0.3888696053
H	0.7419454460	-0.0703468901	-0.9437166125
N	1.1336350238	-0.1919981060	1.3507420378
O	1.5525855195	0.7535222745	2.2795777195
H	2.4751127117	0.9095254780	2.0230155244
C	-0.0500516192	-0.6631819584	1.6365792721
C	2.0073274044	3.0919199537	-0.1338242697
H	2.2998802221	3.1453422758	0.9165968743
H	2.9190361283	3.0113332216	-0.7231255919
H	1.5067638064	4.0231524436	-0.3904936502
C	2.8582400440	0.2354158556	-0.4546268876

O	3.6702418919	0.6565107055	0.3373951180
O	3.1359915739	-0.6388858065	-1.4076871369
C	4.4988560175	-1.0841891943	-1.4739776504
H	4.5394142810	-1.7835780266	-2.3007263689
H	5.1577923191	-0.2379444170	-1.6528451587
H	4.7731758519	-1.5719039277	-0.5415388998
C	-2.4146418954	1.8575255223	-0.6509688901
O	-2.7818147232	3.0066359725	-0.6913080835
O	-3.2553432855	0.8177972556	-0.7074229109
C	-4.6368686280	1.1527859979	-0.8168582083
H	-4.8219709771	1.7070822311	-1.7351648723
H	-5.1719792542	0.2088663089	-0.8316751737
H	-4.9507828923	1.7540126121	0.0341533676
N	-0.2513948269	2.3008228924	-0.4971585558
N	-1.1044351524	1.3531752611	-0.5308834589
C	-0.6069607129	-1.6996599250	0.7472998592
C	0.2491599863	-2.5669560708	0.0716613679
C	-1.9844060812	-1.8170215118	0.5834087085
C	-0.2721749791	-3.5451204618	-0.7609104283
H	1.3178836252	-2.4811251988	0.2150172659
C	-2.5008411077	-2.7987039856	-0.2468576076
H	-2.6494608141	-1.1143200738	1.0658153194
C	-1.6467792566	-3.6640044185	-0.9185065261
H	0.3947689816	-4.2191130794	-1.2803307848
H	-3.5709608559	-2.8799297377	-0.3794143062
H	-2.0523034540	-4.4285368395	-1.5669830254
N	-0.7364207954	-0.2716175454	2.7146361062
H	-0.3257906641	0.4003067377	3.3411470455
H	-1.5358572626	-0.7957141613	3.0238634807

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C	-0.2223282588	0.5512317124	-0.9384187560
C	-1.2823856876	1.1764200924	-0.2469248576
H	-0.5346329990	-0.0519449423	-1.7799744384
N	0.1997951258	-1.0742330890	0.0038595305
O	-0.8842046207	-1.8867909326	-0.3019411186
H	-1.6536525113	-1.2759842200	-0.3587567436
C	1.3257207162	-1.7382151509	-0.0579190455
C	-1.2122879316	2.3058492043	0.7290785346
H	-0.2682260692	2.8325956326	0.6811995756
H	-2.0301622715	2.9992967929	0.5342322690
H	-1.3628496787	1.9288940422	1.7444167810
C	1.1303875153	1.1369438098	-1.2187704311
O	1.7398350175	0.8389499257	-2.2150931650
O	1.5765630147	1.9737295272	-0.2981681239
C	2.8957880017	2.4899996102	-0.5258073908
H	3.1385783724	3.0762957709	0.3530931391

H	3.5954797625	1.6647924127	-0.6443153970
H	2.9002578649	3.1101003956	-1.4191874015
C	-4.4822713925	-0.0793550828	0.0840489628
O	-4.4435553319	-1.1658719696	-0.4519003544
O	-5.5953014301	0.4173998966	0.6426000227
C	-6.7425994418	-0.4250479720	0.5709700313
H	-6.5524574631	-1.3704672747	1.0758769216
H	-7.5418987685	0.1138649637	1.0686789329
H	-7.0077418218	-0.6217995975	-0.4661452289
N	-2.4077060597	0.4738785508	-0.4075008550
N	-3.4397263066	0.8280333923	0.2766213822
C	2.5751941504	-1.0721866740	0.3604095826
C	3.7657176380	-1.3210637781	-0.3204528862
C	2.5713636944	-0.2507140337	1.4854662247
C	4.9479332738	-0.7546282512	0.1296925099
H	3.7619903625	-1.9425864447	-1.2063372263
C	3.7582478598	0.3070641301	1.9348633067
H	1.6421065651	-0.0722863481	2.0087874387
C	4.9456990772	0.0523995378	1.2611126938
H	5.8701187722	-0.9432023986	-0.4016217483
H	3.7566100634	0.9344482215	2.8152565345
H	5.8711328441	0.4847230661	1.6162939119
N	1.3754204767	-3.0169653538	-0.4250358406
H	2.2125467448	-3.5549537146	-0.2812996740
H	0.5261661312	-3.4900514596	-0.6878666032

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C	-1.1350693449	-0.8550166198	-0.3209409228
C	0.0003585539	-1.6689690776	-0.2547562320
H	-1.0184571382	0.0721370221	-0.8643411164
N	-1.4354364586	-0.0440411724	1.4234940690
O	-1.3804782260	-1.0609813489	2.3713899642
H	-2.0560433463	-1.6831942459	2.0533778463
C	-0.6304027527	0.9377641638	1.7312572127
C	0.0360697491	-3.0892221182	0.2151504514
H	0.6028472414	-3.1627746282	1.1457147535
H	-0.9624121481	-3.4819446384	0.3834039643
H	0.5513318043	-3.7133591917	-0.5157732195
C	-2.5040466911	-1.4579120327	-0.4085310403
O	-3.0106811064	-2.1557955737	0.4407571272
O	-3.0931846032	-1.1334954293	-1.5443685484
C	-4.4043384720	-1.6823354306	-1.7535409169
H	-4.7198644826	-1.3237131479	-2.7260640464
H	-4.3567444869	-2.7683921200	-1.7391733706
H	-5.0773669659	-1.3331531910	-0.9745540697
C	3.3110991315	-0.8476781751	-0.8388118141
O	3.3227632194	0.3081561672	-1.1936591922

O	4.4256340515	-1.5829729256	-0.7164198097
C	5.6401022400	-0.9060828701	-1.0297006030
H	5.7740606081	-0.0443912770	-0.3784042622
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H	5.6342589774	-0.5722495743	-2.0657638853
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C	-0.5497530712	2.0818655845	0.8066851507
C	-1.6818861714	2.4938783808	0.1058016095
C	0.6641258846	2.7396453930	0.6184667980
C	-1.5974203343	3.5592875205	-0.7759782492
H	-2.6232601308	1.9865517780	0.2684128168
C	0.7422049791	3.8041467889	-0.2657736920
H	1.5517560375	2.4008579808	1.1358448875
C	-0.3867874509	4.2150653769	-0.9619074887
H	-2.4781640499	3.8821532514	-1.3131788116
H	1.6878185511	4.3049932731	-0.4185765081
H	-0.3225257797	5.0457295246	-1.6512226667
N	0.1388830550	0.9114035447	2.8199184734
H	0.0688481603	0.1287810634	3.4498780065
H	0.5925713273	1.7495984281	3.1400662675