Electronic Supplementary Information:

Impacts of acid-group on the hydrolysis of 2-dinitromethylene-5,5-dinitropyrimidine-4,6-dione

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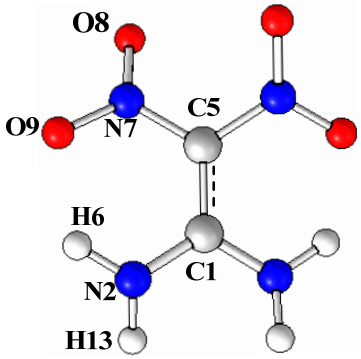
Calculated bond lengths (in angstrom) of FOX-7 by multiple methods are shown in Table S1; The calculated single point energy and active free energy ($\Delta G^{\neq}$) by multiple methods for the first step in the direct hydrolysis of NMP in the formamide phase are shown in Table S2; Optimized geometries of reactant NMP are shown in Fig. S1; Potential energy diagrams for the internal rotation of the dihedral angles in NMP are shown in Fig. S2 and Fig. S3; Optimized geometries of species in the direct hydrolysis of NMP calculated at the B3LYP/6-311G(d,p) with CPCM model in the gas, formamide, and DMSO phase are shown in Fig. S4, Fig. S10, and Fig. S11; Optimized geometries of species in the H_2O catalyzed hydrolysis of NMP calculated at the B3LYP/6-311G(d,p) with CPCM model in the gas, formamide, and DMSO phase are shown in Fig. S5, Fig. S12, and Fig. S13; Optimized geometries of species in the HSO_4^--catalyzed hydrolysis of NMP via calculated at the B3LYP/6-311G(d,p) with CPCM model in the gas, formamide, and DMSO phases are shown in Fig. S6, Fig. S14, and Fig. S15; Optimized geometries of species in the HSO_4^--catalyzed decomposition of DMA calculated at the B3LYP/6-311G(d,p) level in the gas, formamide, and DMSO phases are shown in Fig. S7, Fig. S16 and Fig. S17; Schematic energy diagram of the corresponding direct decomposition process of DMA obtained in the gas phase are shown in Fig. S8 and Fig. S9; Relative energies (in kcal mol^{-1}) of species in the decomposition of DMA in the gas, formamide, and DMSO phases are shown in Table S3; Activation (free) energies (in kcal mol^{-1}) for the hydrolysis paths A to

C in the gas, formamide, and DMSO phases are shown in Table S4; Calculated the dipole moments (μ, in debye) of the rate-determining step for the direct hydrolysis path A by multiple methods are shown in Table S5; Calculated TST/Eckart rate constants (s^{-1}) of each elementary reaction for the hydrolysis of NMP at temperature ranges of 233-400 K are shown in Table S6; Structural and energetic informations. See DOI: 10.1039/x0xx00000x.

Content

Method details

Table S1 Calculated bond lengths (in angstrom) of FOX-7 by multiple methods[a].



Bond	B3LYP	B3LYP-D3	M06-2X	B3PW91	B3LYP[b]	Ref.[c]
C1-N2	1.345	1.346	1.342	1.341	1.343	1.325
C1-C5	1.421	1.420	1.411	1.419	1.432	1.456
N2-H6	1.015	1.015	1.011	1.017	1.019	0.841
N2-H13	1.007	1.007	1.006	1.006	1.008	0.837
C5-N7	1.438	1.439	1.345	1.432	1.431	1.427
N7-O8	1.216	1.216	1.204	1.211	1.222	1.242
N7-O9	1.249	1.248	1.233	1.243	1.256	1.242

[a]The calculated methods (B3LYP, B3LYP-D3, M06-2X, and B3PW91) in the second, third, fourth and fifth column combine the basis set 6-311G(d,p); [b]B3LYP/6-311G(d,p); [c]Reference 7(a) (R. Gilardi, CCCD 127539. Cambridge Structural Database, Cambridge Crystallographic Data Center, Cambridge, U.K., 1999).

The bond lengths of FOX-7 are calculated by multiple methods in the revised manuscript (Table S1). The calculated bond lengths were compared with the experimental ones in crystal structure (CCCD 127539, Cambridge Crystallographic Data Center, 1999). It is found that the calculated bond lengths by B3LYP/6-311G(d,p), B3LYP-D3/6-311G(d,p), M06-2X/6-311G(d,p), B3PW91/6-311G(d,p), and B3LYP/agu-cc-pvdz are very close, and are in good agreement with the experimental observations. It is indicated that the geometry optimization is hardly affected by the calculation method. Therefore, the time-saving method of B3LYP/6-311G(d,p) was selected to optimize the geometries in the present work.

Table S2 Calculated single point energy and the active free energy ($\Delta G^{\neq}$) by multiple methods for the first step in the direct hydrolysis of NMP in the formamide phase[a].

Methods[b]	A-IM1	A-TS1	A-IM2	$\Delta G^{\neq}$
B3LYP-D3/6-311++G(3df,3pd)	-1348.954028	-1348.871855	-1348.944123	51.56
M06-2X-D3/6-311++G(3df,3pd)	-1348.418659	-1348.335550	-1348.411515	52.15
M06-HF-D3/6-311++G(3df,3pd)	-1348.616819	-1348.536816	-1348.607674	49.75
BP86/6-311++G(3df,3pd)	-1349.035945	-1347.582792	-1347.654653	45.70
B2PLYP/aug-cc-pvdz	-1347.570221	-1347.487673	-1347.558281	51.80
CCSD(T)/6-311G(d,p)[c]	-1345.059067	-1344.976275	-1345.054105	51.95

[a]The second, third, fourth column are shown in Hartree, the fifth column is shown in kcal/mol; [b]The single-point energies were calculated based on the optimized geometries obtained via B3LYP/6-311G(d,p) method; [c]Since the species of the first step in the direct hydrolysis of NMP contain as much as 26 atoms, CCSD(T) calculation in this process may expend enormous resource to result in the lager basis set is not used in the present work.

Based on the optimized geometries, the single-point energies of the first step in the direct hydrolysis of NMP in formamide phase were estimated at DFT functions (B3LYP-D3, M06-2X-D3, M06-HF-D3, and BP86 with 6-311++G(3df,3pd)), double hybrid functions B2PLYP/aug-cc-pvdz, and CCSD(T)/6-311G(d,p) so as to grasp a suited method (shown in Table S2). The accuracy of B3LYP-D3/6-311++G(3df,3pd)//B3LYP/6-311G(d,p) and M06-2X-D3/6-311++G(3df,3pd)//B3LYP/6-311G(d,p) energies is gauged by comparison to CCSD(T)/6-311G(d,p)//B3LYP/6-311G(d,p) and B2PLYP/aug-cc-pvdz//B3LYP/6-311G(d,p) energies of the first step in the direct hydrolysis of NMP in the formamide phase. It is found that the difference in the energy barrier is less than 0.5 kcal mol^{-1}, indicating that the accuracy as well as the reliability of the former two methods is comparable to that of the latter two methods. Therefore, B3LYP-D3/6-311++G(3df,3pd)//B3LYP/6-311G(d,p) was intentionally used to calculate the single-point energies due to its relatively high efficiency.

The theoretical rate coefficients of conventional transition state theory with an asymmetric Eckart tunneling correction (TST/Eckart) (*Phys. Rev.*, 1930, **35**, 1303; *J. Phys. Chem.*, 1979, **83**, 29216; *J. Phys. Chem.*, 1962, **66**, 532) for the elementary reactions incorporated in the titled reaction system are calculated. The temperature increases from 233 to 400 K. The relationship is shown in eqn. (1).

$$k(T) = \kappa(T)\sigma\frac{k_{\mathrm{B}}T}{h}\frac{Q^{\neq}(T)}{Q_{\mathrm{A}}(T)Q_{\mathrm{B}}(T)}\exp(-E_a/RT) \qquad (1)$$

where $\kappa(T)$ is the asymmetric Eckart tunneling correction factor, σ is the reaction symmetry number, k_B is the Boltzmann constant, h is the Planck constant, $Q^{\neq}(T)$ is the partition function for the transition state, $Q_A(T)$ and $Q_B(T)$ are the partition functions for the reactants and *Ea* is the activation energy barrier. The total molar partition function includes translation (Q_{trans}), vibration (Q_{vib}), rotation (Q_{rot}), electronic (Q_{ele}) and torsional (Q_{tor}) partition functions ($Q=Q_{trans}Q_{vib}Q_{rot}Q_{ele}Q_{tor}$) (*J. Phys. Chem. A*, 2014, **118**, 12089). The overall rate coefficients of the formation of final products are deduced by using the steady-state approximation (SSA), and fitted to the modified three parameters Arrhenius expressions as shown in Eq. (2).

$$k = A \times T^{n} \times \exp(-E_a/RT) \qquad (2)$$

All the kinetic calculations are performed by implementing VKLab program (*J. Comput. Chem*., 1998, **19**, 1039).

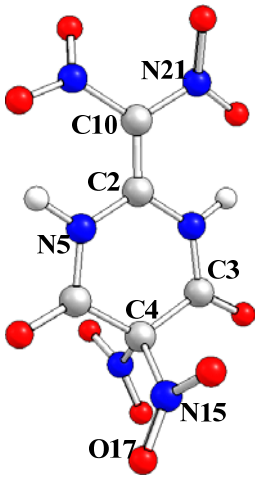


Fig. S1 Optimized geometries of reactant NMP.

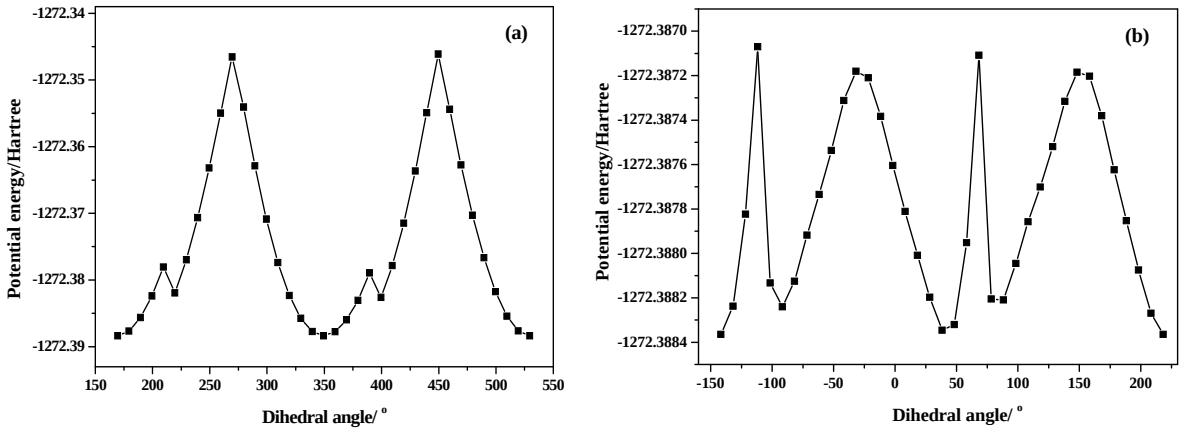


Fig. S2 Potential energy diagram for the internal rotation of the dihedral angles in NMP. (a) N5-C2-C10-N21 dihedral angle; (b) C3-C4-N15-O17 dihedral angle.

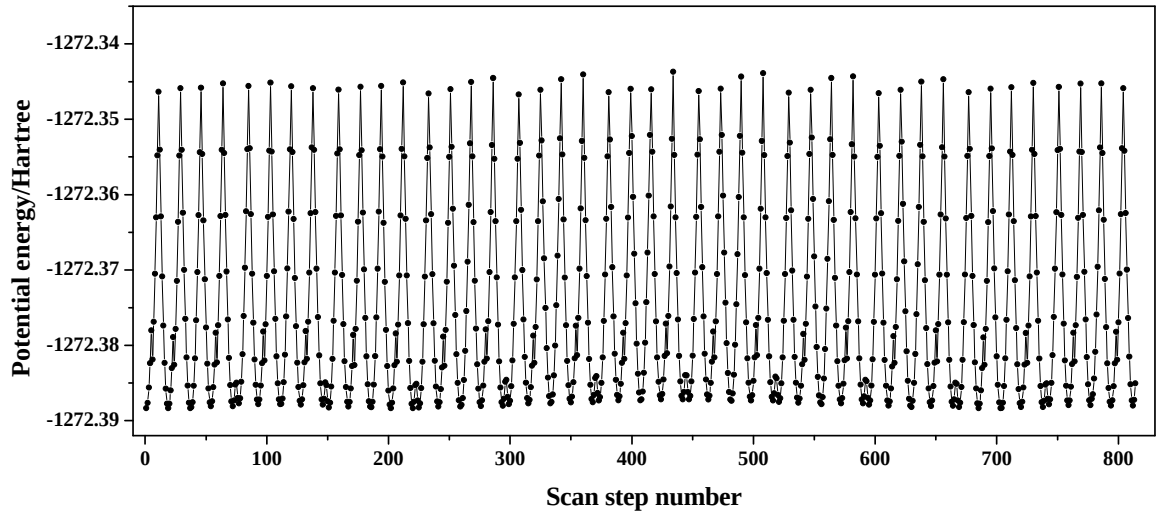


Fig. S3 Potential energy diagram for the simultaneous rotation of the dihedral angle N5-C2-C10-N21 and C3-C4-N15-O17 in NMP (10 ^{o}/step).

The internal rotation of -NO_2 in C10 and C4 in NMP is discussed as follows.

The configuration of NMP was optimized by the B3LYP/6-311G(d,p) method (shown in Fig. S1). The potential energy diagrams for the internal rotation of lateral -NO_2 in C10 and C4 in NMP were calculated when the optimized geometry of NMP was taken as the initial structure, and are shown in Fig. S2(a) and Fig. S2(b), respectively. The potential energy diagram for the simultaneous rotation of lateral -NO_2 in C10 and C4 in NMP was also considered (shown in Fig. S3).

As shown in Fig. S2 and Fig. S3, the initial structure of NMP was found to not only have the lowest energy, but also have a very good symmetry, resulting in that the rotation of the lateral groups may have good periodicity, and thus the number of the spatial configurations may distinctly decrease. Based on these calculations, we believe that the torsional dependencies of lateral groups may be fairly weak during the reaction process.

The calculation strategy for geometry searching was discussed as follows.

First, the possible structure of transition states is searched via B3LYP/6-311G(d,p) method in the hydrolysis of NMP based on the optimized structure of NMP. Next, the intrinsic reaction coordinate (IRC) analysis is performed to ensure that the structure of every transition state obtained does connect the corresponding reactant and product. Finally, the obtained structures are conformed via the vibrational frequency calculations, via which whether the obtained structures are the ones of the transition states or local minima points.

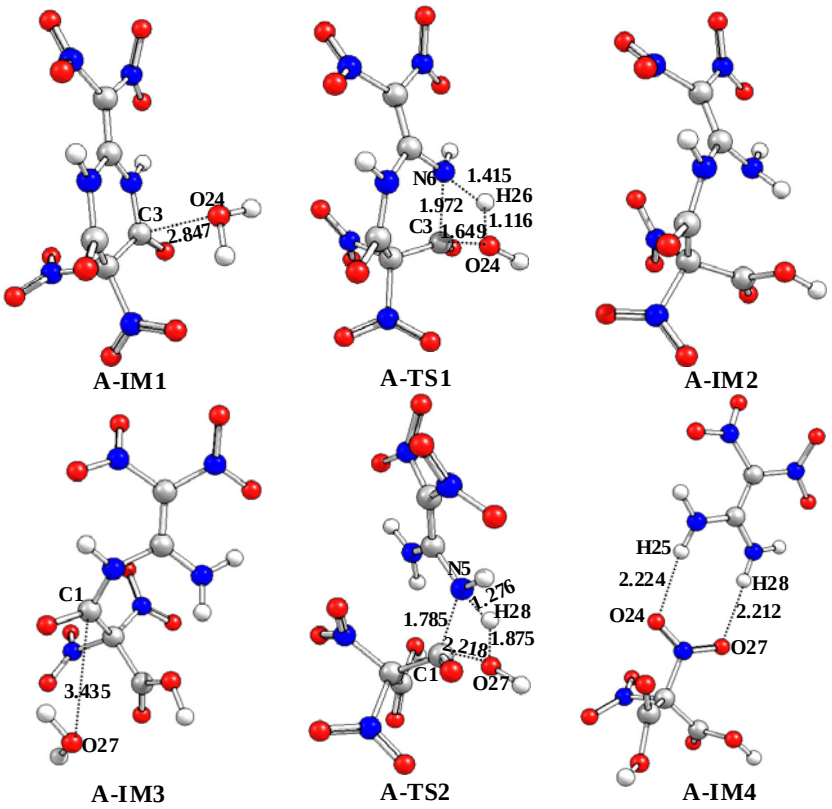


Fig. S4 Optimized geometries of species in the direct hydrolysis of NMP calculated at the B3LYP/6-311G(d,p) level in the gas phase (bond lengths are in angstrom).

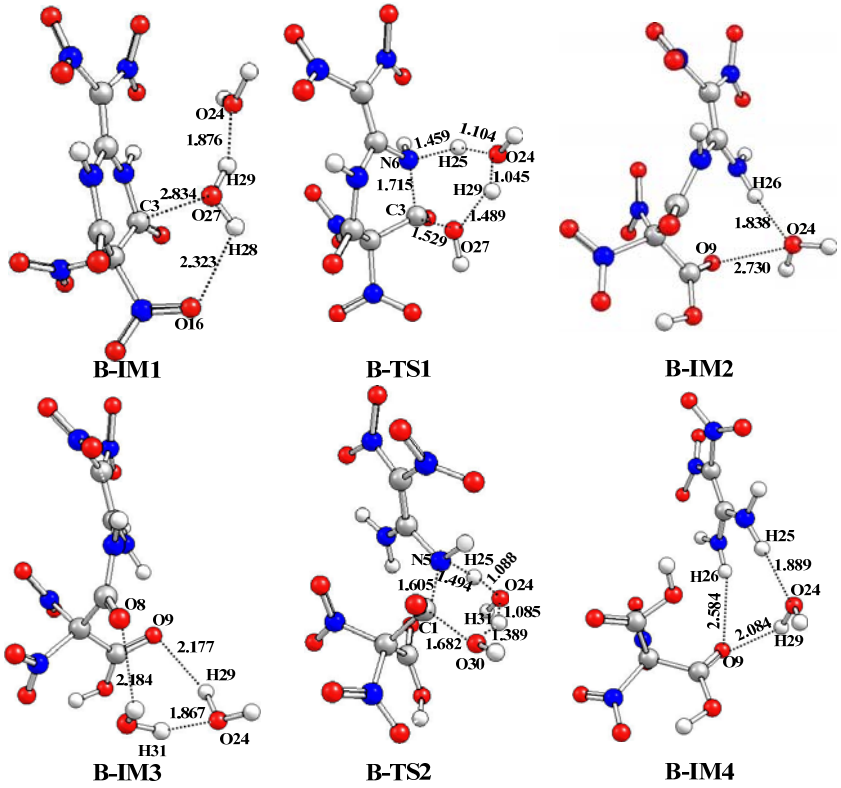


Fig. S5 Optimized geometries of species in the H_2O catalyzed hydrolysis of NMP calculated at the B3LYP/6-311G(d,p) level in the gas phase (bond lengths are in angstrom).

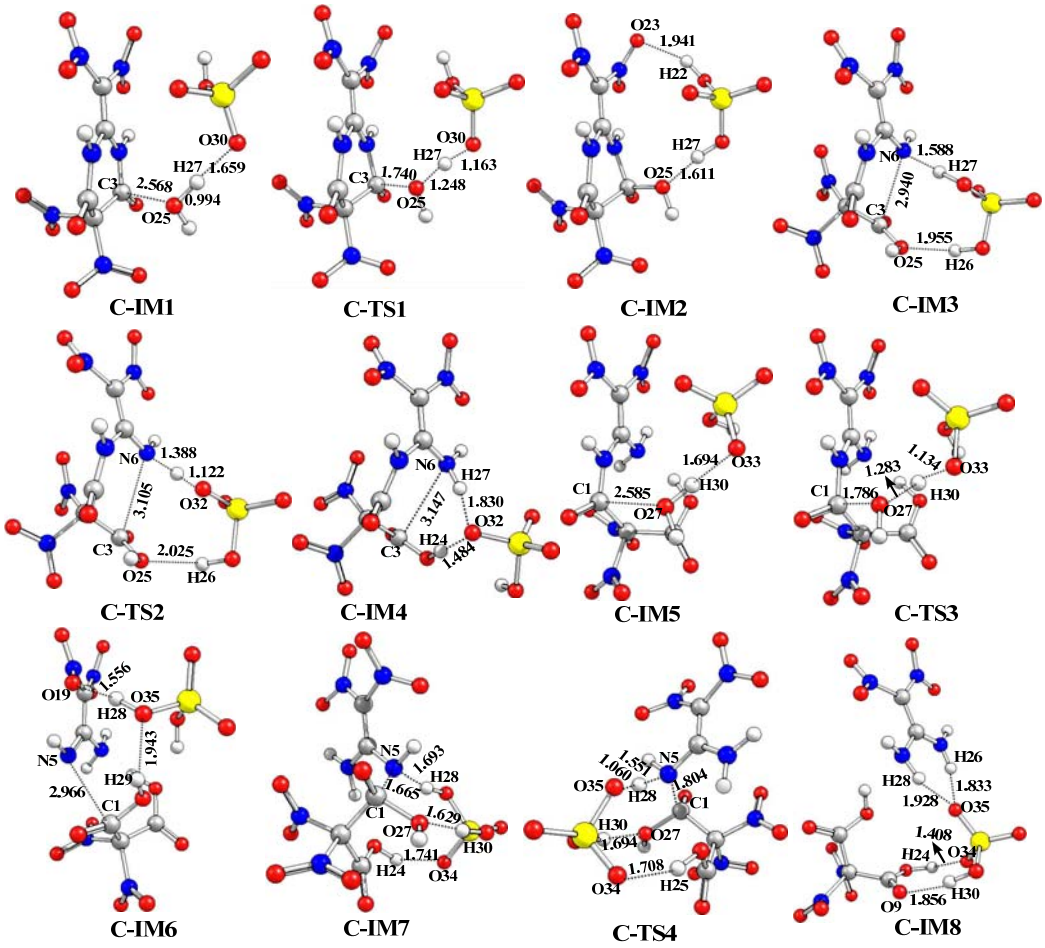


Fig. S6 Optimized geometries of species in the HSO_4^--catalyzed hydrolysis of NMP calculated at the B3LYP/6-311G(d,p) level in the gas phase (bond lengths are in angstrom).

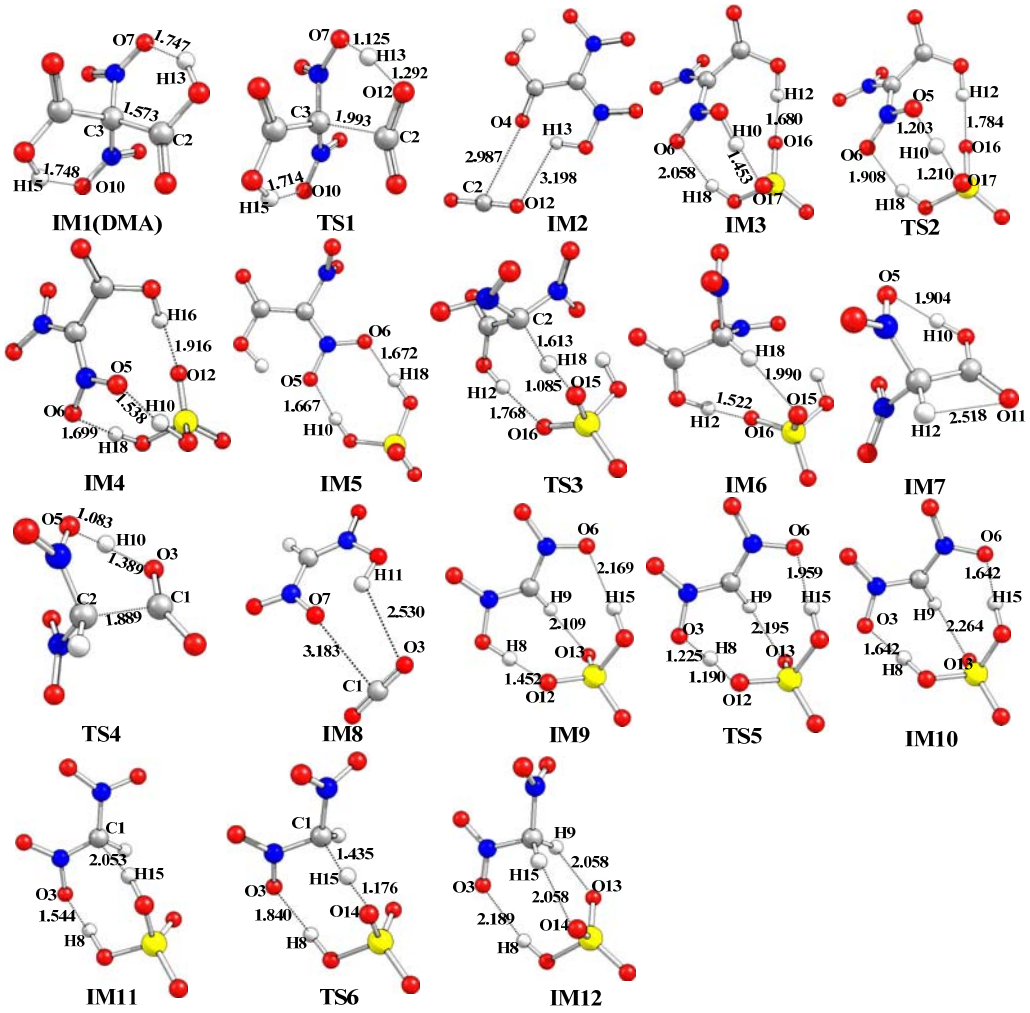


Fig. S7 Optimized geometries of species in the HSO_4^--catalyzed decomposition of DMA calculated at the B3LYP/6-311G(d,p) level in the gas phase (bond lengths are in angstrom).

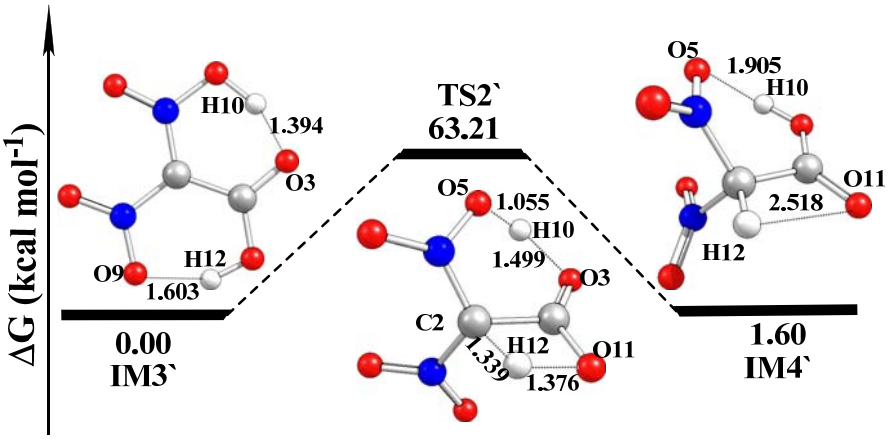


Fig. S8 Schematic energy diagram of the corresponding direct decomposition process of DMA obtained via B3LYP-D3/6-311++G(3df,3pd)//B3LYP/6-311G(d,p) in the gas phase.

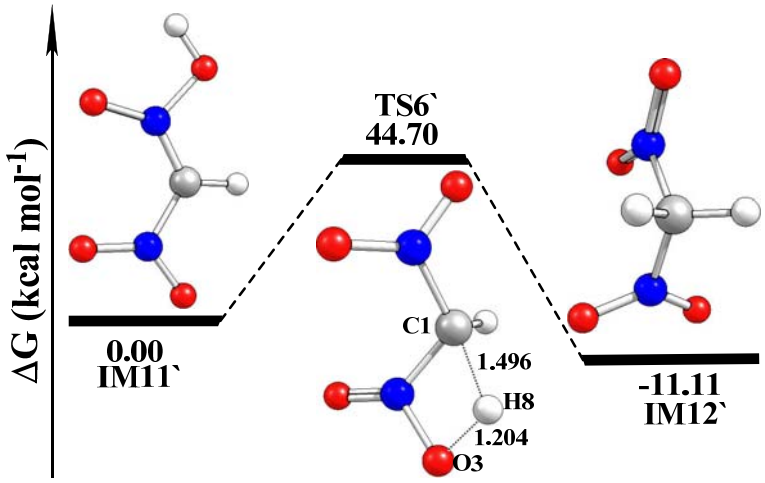


Fig. S9 Schematic energy diagram of the corresponding direct decomposition process of DMA obtained via B3LYP-D3/6-311++G(3df,3pd)//B3LYP/6-311G(d,p) in the gas phase.

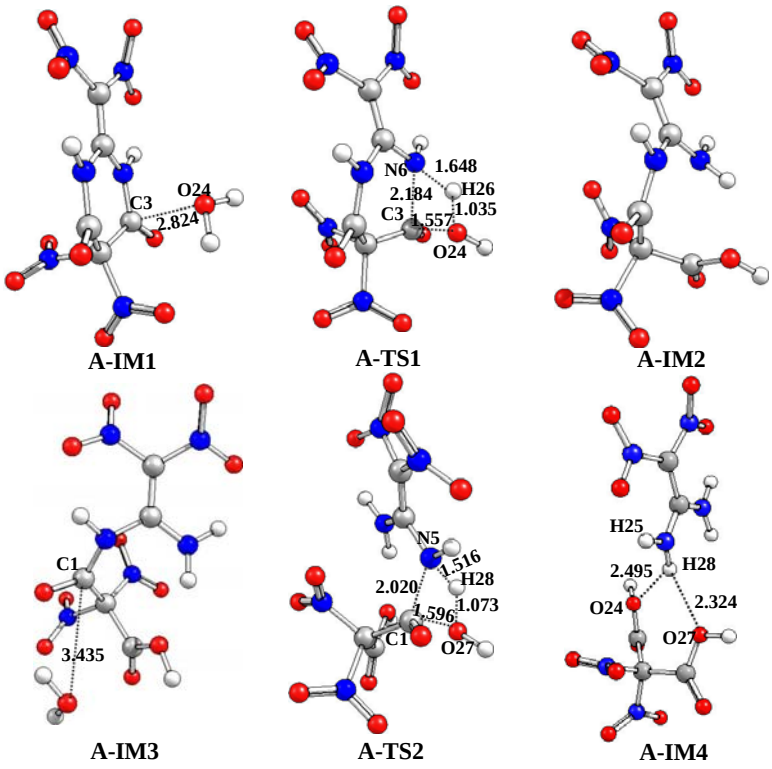


Fig. S10 Optimized geometries of species in the direct hydrolysis of NMP calculated at the B3LYP/6-311G(d,p) with CPCM model in the formamide phase (bond lengths are in angstrom).

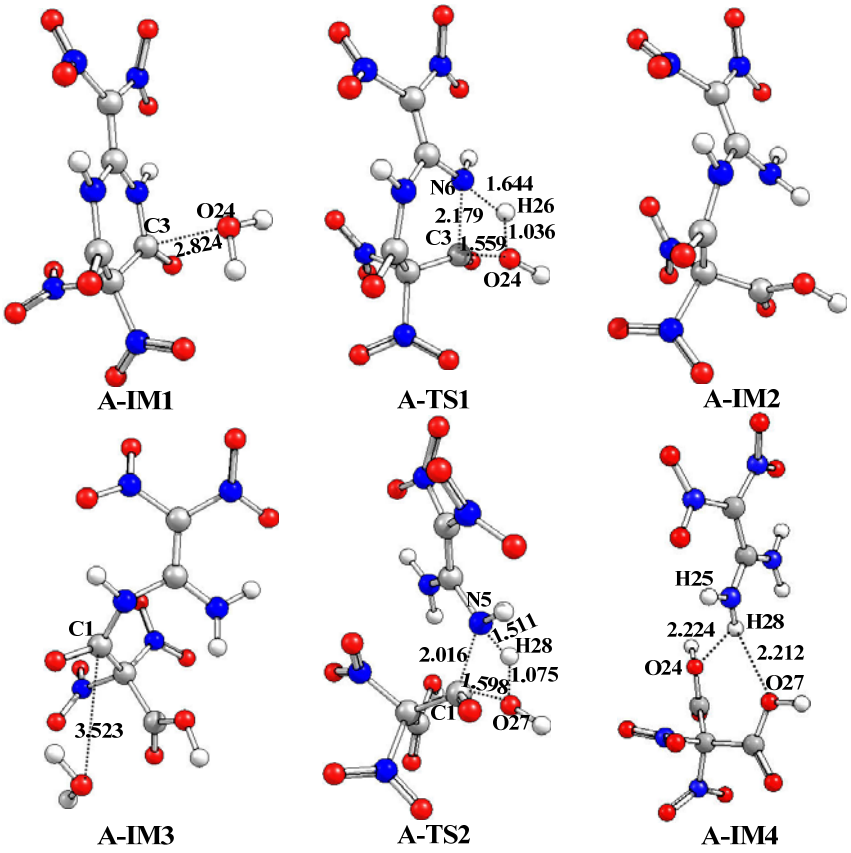


Fig. S11 Optimized geometries of species in the direct hydrolysis of NMP calculated at the B3LYP/6-311G(d,p) with CPCM model in the DMSO phase (bond lengths are in angstrom).

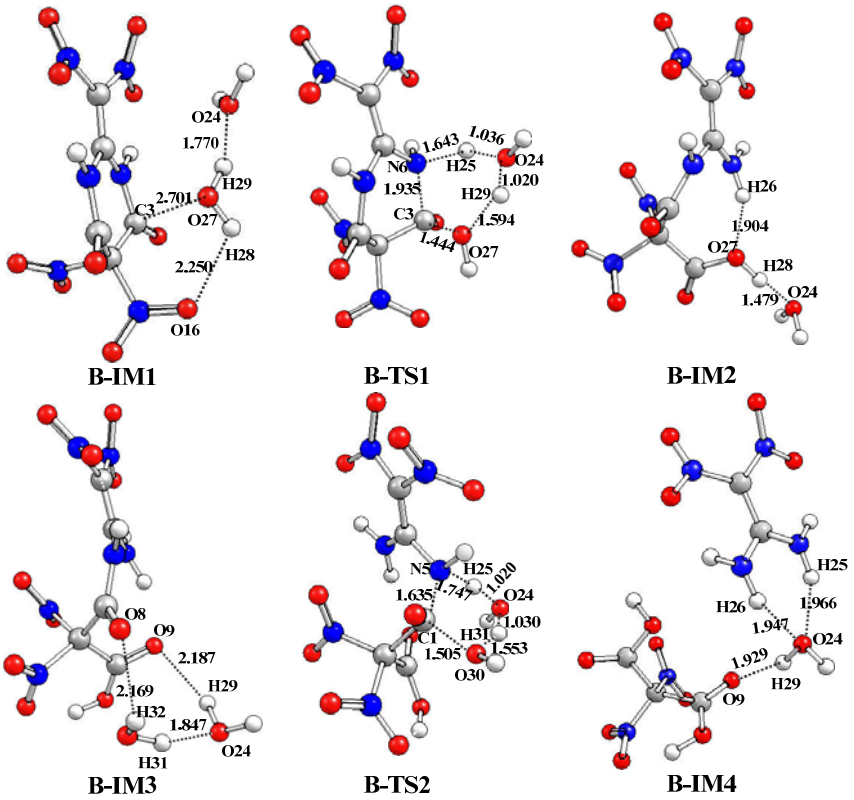


Fig. S12 Optimized geometries of species in the H_2O catalyzed hydrolysis of NMP calculated at the B3LYP/6-311G(d,p) with CPCM model in the formamide phase (bond lengths are in angstrom).

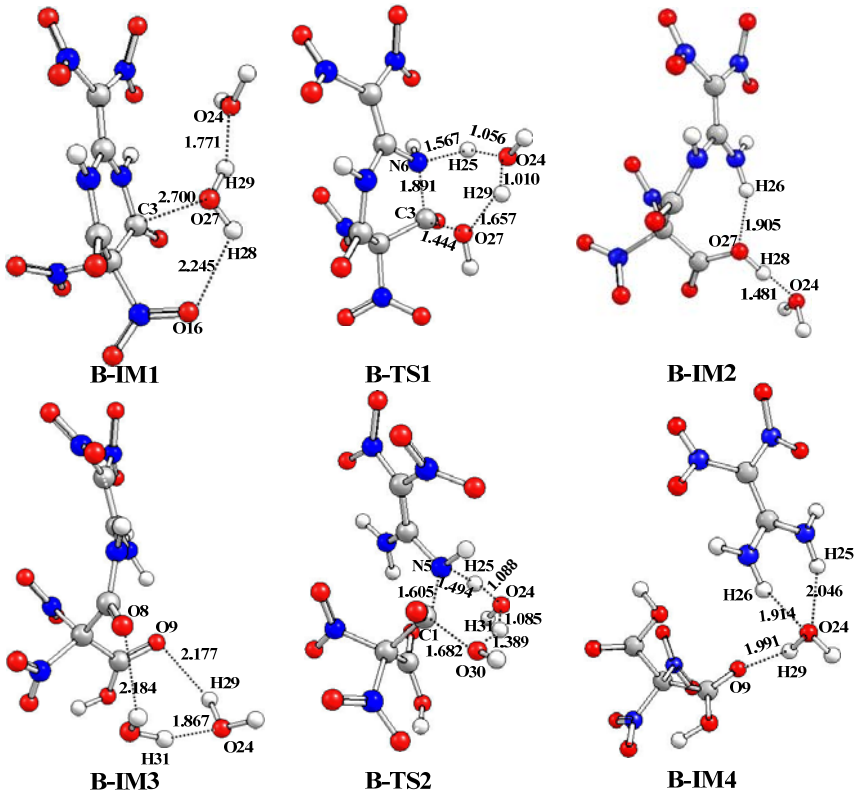


Fig. S13 Optimized geometries of species in the H_2O catalyzed hydrolysis of NMP calculated at the B3LYP/6-311G(d,p) with CPCM model in the DMSO phase (bond lengths are in angstrom).

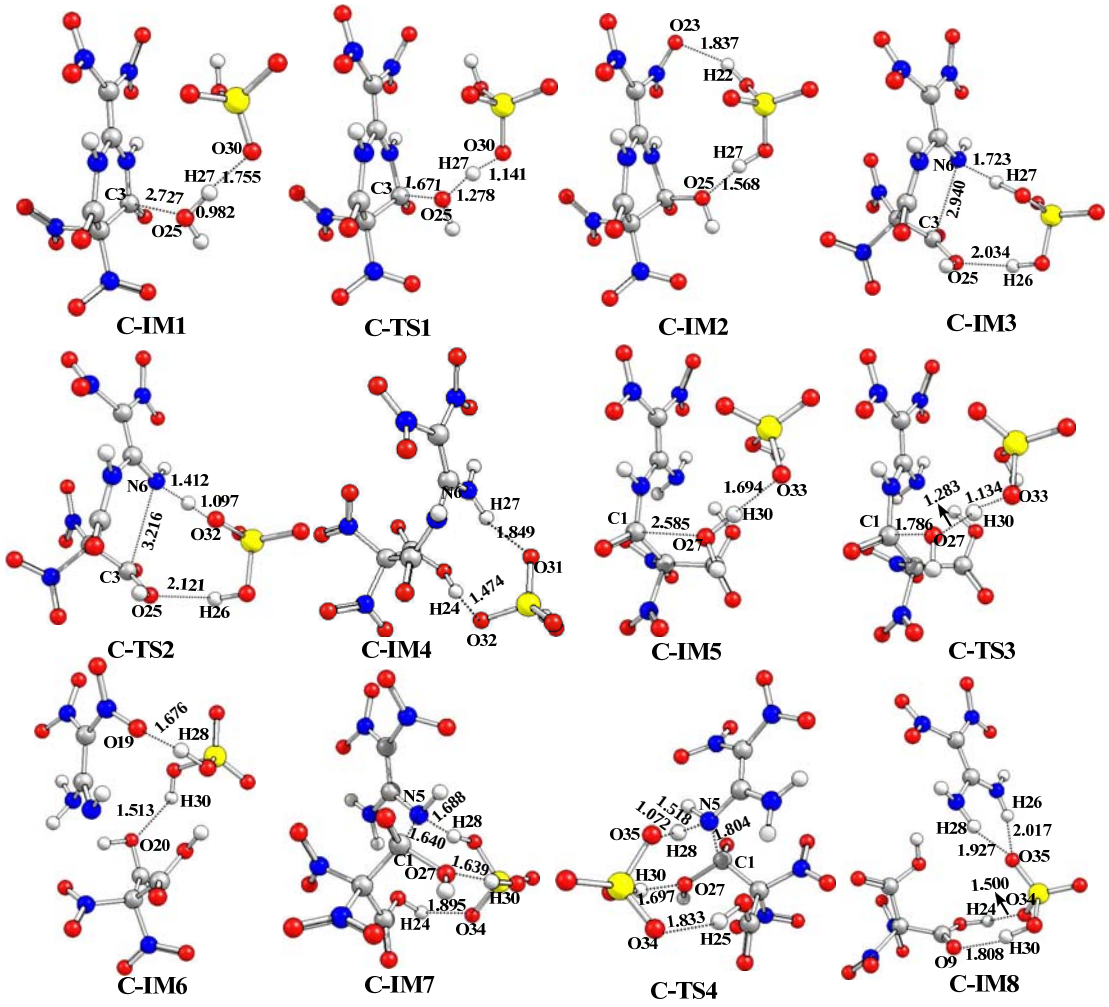


Fig. S14 Optimized geometries of species in the HSO_4^--catalyzed hydrolysis of NMP via calculated at the B3LYP/6-311G(d,p) with CPCM model in the formamide phase (bond lengths are in angstrom).

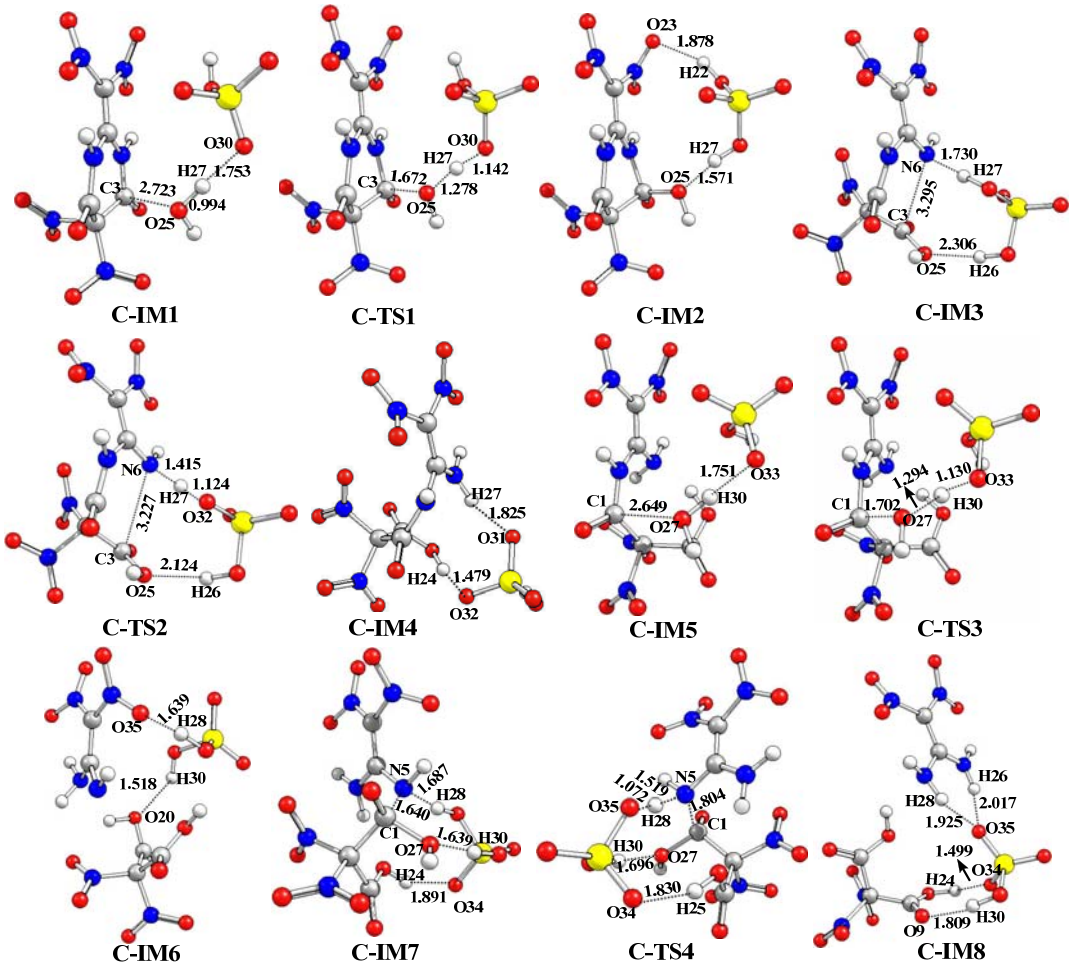


Fig. S15 Optimized geometries of species in the HSO_4^--catalyzed hydrolysis of NMP via calculated at the B3LYP/6-311G(d,p) with CPCM model in the DMSO phase (bond lengths are in angstrom).

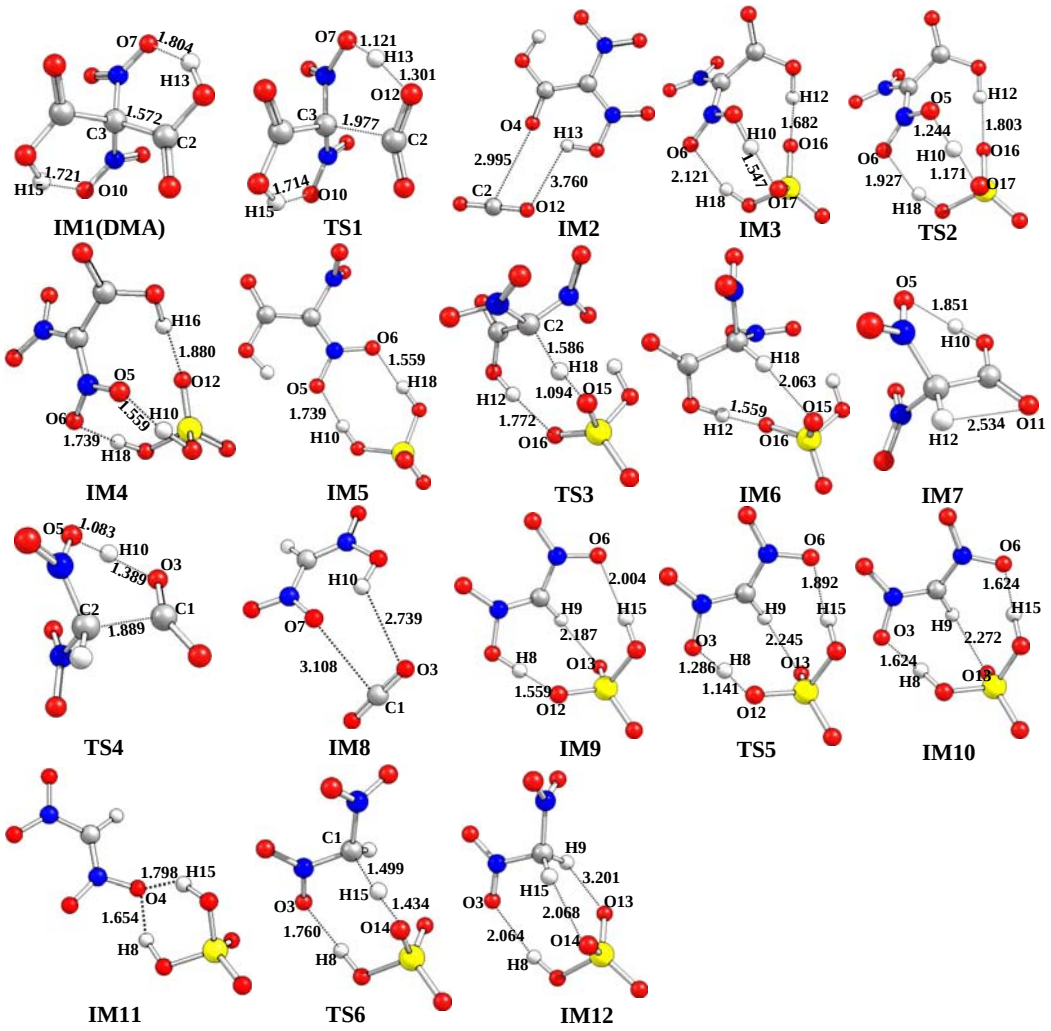


Fig. S16 Optimized geometries of species in the HSO_4^--catalyzed decomposition of DMA calculated at the B3LYP/6-311G(d,p) level in the formamide phase (bond lengths are in angstrom).

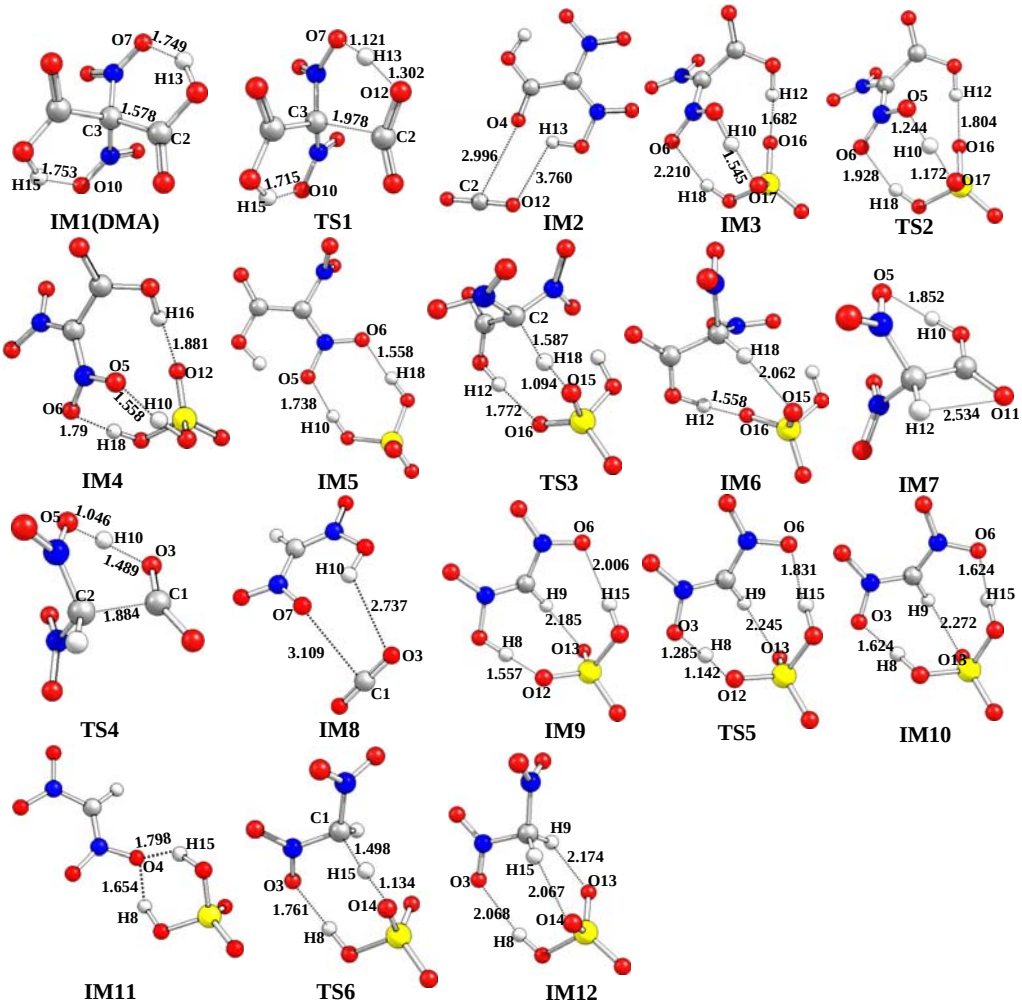


Fig. 17 Optimized geometries of species in the HSO_4^--catalyzed decomposition of DMA calculated at the B3LYP/6-311G(d,p) level in the DMSO phase (bond lengths are in angstrom).

Table S3 Relative energies (in kcal mol^{-1}) of species in the decomposition of DMA in the gas, formamide, and DMSO phases[a].

System	ΔE	ΔG(g)	ΔG(f)	ΔG(g)	$\Delta G(g)^{\neq}$	$\Delta G(f)^{\neq}$	$\Delta G(g)^{\neq}$
IM1(DMA)+HSO_4^-	0.00	0.00	0.00	0.00			
TS1+HSO_4^-	14.30	15.04	14.06	13.26			
IM2+HSO_4^-	-22.98	-26.48	-28.58	-29.40			
IM3+CO_2	-55.30	-51.79	-31.13	-32.20			
TS2+CO_2	-56.44	-52.48	-31.30	-32.38			
IM4+CO_2	-55.73	-52.33	-30.93	-32.01			
IM5+CO_2	-59.82	-58.57	-38.11	-39.16			
TS3+CO_2	-46.00	-42.59	-20.52	-21.61			
IM6+CO_2	-60.44	-57.43	-30.93	-32.01			
IM7+HSO_4^-+CO_2	-18.49	-29.18	-32.35	-33.11			
TS4+HSO_4^-+CO_2	-0.38	-10.15	-12.66	-13.44			
IM8+HSO_4^-+CO_2	-36.33	-50.28	-52.29	-53.06			
IM9+2CO_2	-62.82	-69.80	-53.16	-54.16			
TS5+2CO_2	-62.72	-69.48	-52.55	-53.59			
IM10+2CO_2	-61.34	-68.81	-52.62	-53.66			
IM11+2CO_2	-61.76	-71.60	-52.71	-53.74			
TS6+2CO_2	-56.92	-64.57	-48.03	-49.06			
IM12+2CO_2	-59.44	-67.86	-60.64	-61.49			
$CH_2(NO_2)_2$+HSO_4^-+2CO_2	-38.08	-59.67	-63.47	-64.21			
IM1 → IM2					15.04	14.06	13.26
IM3 → IM4					-0.96	-0.17	-0.18
IM5 → IM6					15.98	17.59	17.55
IM7 → IM8					19.03	19.69	19.67
IM9 → IM10					0.32	0.61	0.57
IM11 → IM12					7.03	4.68	4.68

[a]The gas, formamide, and DMSO phase are denoted as (g), (f), and (d).

Table S4 Activation (free) energies (in kcal mol^{-1}) for the hydrolysis paths A to C in the gas, formamide, and DMSO phase[a].

System	$\Delta E(g)^{\neq}$	$\Delta G(g)^{\neq}$	$\Delta G(f)^{\neq}$	$\Delta G(d)^{\neq}$
A-IM1→A-IM2	53.40	54.93	51.56	52.73
A-IM3→A-IM4	47.16	49.68	45.02	45.14
B-IM1→B-IM2	45.02	47.92	36.59	38.81
B-IM3→B-IM4	36.12	38.58	34.28	33.45
C-IM1→C-IM2	9.05	10.75	17.81	16.67
C-IM3→C-IM4	-1.25	-0.62	-1.23	-1.25
C-IM5→C-IM6	12.16	12.85	19.94	19.84
C-IM7→C-IM8	-0.74	-0.56	-0.81	-0.78

[a]The gas, formamide, and DMSO phase are denoted as (g), (f), and (d).

Table S5 Calculated the dipole moments (μ, in debye) of the rate-determining step for the direct hydrolysis path A by multiple methods.

Path A	B3LYP/ 6-311G(d,p)	B3LYP-D3/ 6-311G(d,p)	M062X /6-311G(d,p)	B3PW91 /6-311G(d,p)	B3LYP /aug-cc-pvdz
A-IM1	2.4	2.4	2.9	2.4	2.2
A-TS1	5.8	6.0	5.3	4.6	5.4

Table S6 Calculated TST/Eckart rate constants[a] (s^{-1}) of each elementary reaction for the hydrolysis of NMP at temperature ranges of 233-400 K.

T/K	$k_{A1}^{TST/Eckart}$	$k_{A2}^{TST/Eckart}$	$k_{B1}^{TST/Eckart}$	$k_{B2}^{TST/Eckart}$	$k_{C1}^{TST/Eckart}$	$k_{C2}^{TST/Eckart}$	$k_{C3}^{TST/Eckart}$	$k_{C4}^{TST/Eckart}$
233	2.38×10^{-35}	5.16×10^{-26}	8.13×10^{-31}	1.52×10^{-21}	5.21×10^{5}	7.24×10^{10}	9.19×10^{2}	3.91×10^{12}
243	1.06×10^{-33}	3.58×10^{-25}	3.49×10^{-29}	2.81×10^{-20}	1.00×10^{5}	7.79×10^{10}	2.16×10^{3}	4.02×10^{12}
253	3.98×10^{-32}	2.55×10^{-24}	1.11×10^{-27}	4.12×10^{-19}	1.83×10^{5}	8.32×10^{10}	4.75×10^{3}	4.13×10^{12}
263	1.25×10^{-30}	1.86×10^{-23}	2.72×10^{-26}	4.94×10^{-18}	3.18×10^{5}	8.82×10^{10}	9.82×10^{3}	4.24×10^{12}
268	6.53×10^{-30}	5.04×10^{-23}	1.23×10^{-25}	1.59×10^{-17}	4.12×10^{5}	9.07×10^{10}	1.38×10^{4}	4.29×10^{12}
273	3.25×10^{-29}	1.37×10^{-22}	5.26×10^{-25}	4.92×10^{-17}	5.30×10^{5}	9.31×10^{10}	1.93×10^{4}	4.34×10^{12}
278	1.55×10^{-28}	3.74×10^{-22}	2.13×10^{-24}	1.46×10^{-16}	6.74×10^{5}	9.54×10^{10}	2.65×10^{4}	4.39×10^{12}
283	7.03×10^{-28}	1.02×10^{-21}	8.22×10^{-24}	4.17×10^{-16}	8.51×10^{5}	9.77×10^{10}	3.60×10^{4}	4.44×10^{12}
288	3.05×10^{-27}	2.76×10^{-21}	3.02×10^{-23}	1.15×10^{-15}	1.06×10^{6}	9.99×10^{10}	4.84×10^{4}	4.49×10^{12}
298	5.05×10^{-26}	2.00×10^{-20}	3.58×10^{-22}	7.86×10^{-15}	1.63×10^{6}	1.04×10^{11}	8.49×10^{4}	4.58×10^{12}
303	1.93×10^{-25}	5.30×10^{-20}	1.16×10^{-21}	1.96×10^{-14}	1.99×10^{6}	1.06×10^{11}	1.11×10^{5}	4.63×10^{12}
308	7.10×10^{-25}	1.39×10^{-19}	3.61×10^{-21}	4.74×10^{-14}	2.42×10^{6}	1.08×10^{11}	1.44×10^{5}	4.67×10^{12}
323	2.82×10^{-23}	2.31×10^{-18}	8.80×10^{-20}	5.68×10^{-13}	4.18×10^{6}	1.14×10^{11}	2.97×10^{5}	4.80×10^{12}
343	2.38×10^{-21}	7.78×10^{-17}	4.01×10^{-18}	1.11×10^{-11}	8.02×10^{6}	1.20×10^{11}	7.06×10^{5}	4.96×10^{12}
363	1.26×10^{-19}	1.97×10^{-15}	1.19×10^{-16}	1.55×10^{-10}	1.43×10^{7}	1.26×10^{11}	1.53×10^{6}	5.11×10^{12}
400	7.05×10^{-17}	3.78×10^{-13}	2.56×10^{-14}	1.01×10^{-8}	3.56×10^{7}	1.34×10^{11}	5.15×10^{6}	5.36×10^{12}

[a] k_{A1}, k_{A2}, k_{B1}, k_{B2}, k_{C1}, k_{C2}, k_{C3}, and k_{C4} denote the rate constant of the relevant elementary reaction of A-TS1, A-TS2, B-TS1, B-TS2, C-TS1, C-TS2, C-TS3, and C-TS4, respectively.

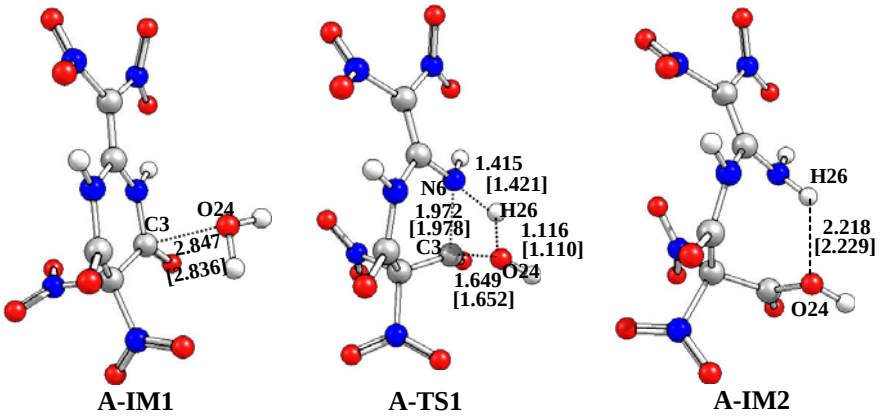
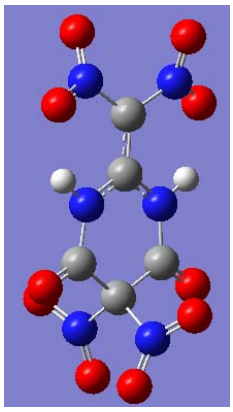


Fig. S18 Optimized geometries in the gas phase for the first-step hydrolysis in path A (bond lengths are in angstrom). For the bond lengths of species, the values in no-bracket and square brackets respect the calculated results at the B3LYP/6-311G(d,p) and B3LYP-D3/6-311G(d,p) method, respectively.

Structural and Energetic Informations

NMP

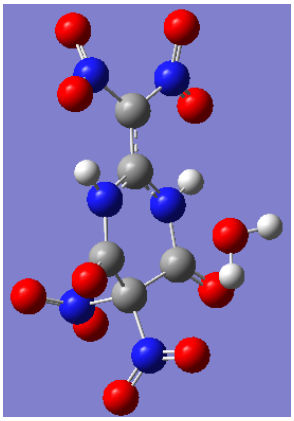


Sum of electronic and zero-point Energies = -1272.265886 Hartree
Sum of electronic and thermal Energies = -1272.248083 Hartree
Sum of electronic and thermal Enthalpies = -1272.247139 Hartree
Sum of electronic and thermal Free Energies = -1272.314648 Hartree

Coordinates

C	1.06493800	-1.30584000	0.13410600
C	-1.01817300	-0.00003100	-0.00009000
C	1.06498400	1.30580800	-0.13385600
C	1.86622600	-0.00004300	-0.00010900
N	-0.31086000	-1.16073400	0.12515800
N	-0.31081600	1.16063700	-0.12541200
H	-0.87703300	2.00031900	-0.28069200
O	1.60653900	-2.36403000	0.28098400
O	1.60657200	2.36408300	-0.28015900
C	-2.40987400	0.00002800	0.00004300
H	-0.87708800	-2.00037900	0.28055200
N	-3.18651100	-1.22740300	-0.09340800
O	-4.28534000	-1.17052800	-0.59682900
O	-2.65542100	-2.27330400	0.31096300
N	2.71442200	0.09197400	1.28997500
O	2.09075600	0.56626500	2.22522400
O	3.82568700	-0.36064100	1.28780600
N	2.71392900	-0.09207500	-1.29017700
O	2.09042100	-0.56718000	-2.22513400
O	3.82490400	0.36138900	-1.28850400
N	-3.18639800	1.22751200	0.09345700
O	-2.65536400	2.27333600	-0.31120800
O	-4.28510900	1.17075500	0.59716000

A-IM1



Sum of electronic and zero-point Energies= -1348.704896 Hartree

Sum of electronic and thermal Energies= -1348.683628 Hartree

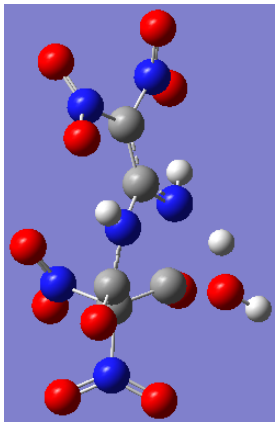
Sum of electronic and thermal Enthalpies= -1348.682684 Hartree

Sum of electronic and thermal Free Energies= -1348.757206 Hartree

C	-1.05535100	1.29137000	0.10440200
C	1.02915700	-0.00123100	0.00110000
C	-1.04035000	-1.19900200	-0.53213500
C	-1.79801400	-0.04932600	0.14384200
N	0.31592400	1.12852400	0.27697400
N	0.33300200	-1.11707000	-0.36216000
H	0.90102600	-1.88900200	-0.71999400
O	-1.59577400	2.35652800	0.06835400
O	-1.58532400	-2.09831700	-1.10217600
C	2.42177400	-0.01614300	0.07904000
H	0.88000500	1.95089900	0.51022500
N	3.20768100	1.19401600	0.21768000
O	4.35639000	1.18427600	-0.16670200
O	2.64084700	2.19746200	0.68427600
N	-1.99606700	-0.41600300	1.66192500
O	-1.80011900	-1.57418200	1.95782900
O	-2.32498800	0.49456600	2.38353800
N	-3.19815400	0.06806900	-0.47034100
O	-4.13762700	-0.21923900	0.22962900
O	-3.22498800	0.42424100	-1.63191200
N	3.18267700	-1.25476100	-0.00461400

O	2.69216900	-2.18648600	-0.65952300
O	4.22856800	-1.32358900	0.60151100
O	-0.53202800	0.77510100	-2.61879400
H	-1.46908500	0.66973700	-2.82531000
H	-0.30770100	1.65203900	-2.94690700

A-TS1



Sum of electronic and zero-point Energies = -1348.623440 Hartree

Sum of electronic and thermal Energies = -1348.603991 Hartree

Sum of electronic and thermal Enthalpies = -1348.603047 Hartree

Sum of electronic and thermal Free Energies = -1348.672636 Hartree

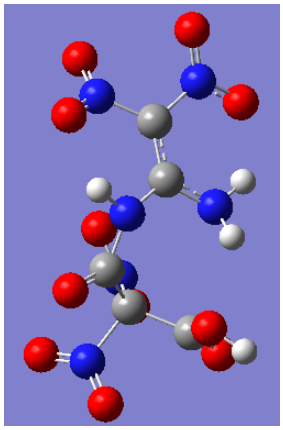
Imaginary frequency = -1131.2997 cm^{-1}

Coordinates：

C	-1.53752500	1.38610200	-0.20635200
C	1.10148900	0.15874000	-0.44456000
C	-0.99342800	-1.11760100	-0.76984300
C	-1.79146900	-0.08547200	0.08111900
N	0.42240300	1.33209100	-0.41631800
N	0.36601900	-0.92099400	-0.89776800
H	0.90862000	-1.73629500	-1.18964600
O	-1.92156000	2.34528100	0.35634900
O	-1.55834300	-2.06548700	-1.24220000
C	2.44359800	0.00387500	-0.11673000
H	0.91450500	2.05487400	0.10903700
N	3.29950400	1.14482800	0.15040000
O	4.48537100	1.04316500	-0.09003100
O	2.75878400	2.17694600	0.57061100
N	-1.52078400	-0.30458500	1.60123200
O	-0.57895400	-1.01882800	1.87947500
O	-2.26953400	0.26781500	2.35281500
N	-3.29978400	-0.39729600	-0.13992600
O	-3.76336400	-1.28501300	0.52818600

O	-3.84720500	0.26653600	-0.99551400
N	3.09301200	-1.29336200	-0.04808800
O	2.65175100	-2.19423000	-0.77836500
O	4.00507600	-1.43720800	0.73702600
O	-1.39700400	1.49682100	-1.84519200
H	-1.88173200	2.28859700	-2.12881200
H	-0.32012000	1.62780700	-1.58439200

A-IM2



Sum of electronic and zero-point Energies= -1348.691743 Hartree

Sum of electronic and thermal Energies= -1348.671669 Hartree

Sum of electronic and thermal Enthalpies= -1348.670725 Hartree

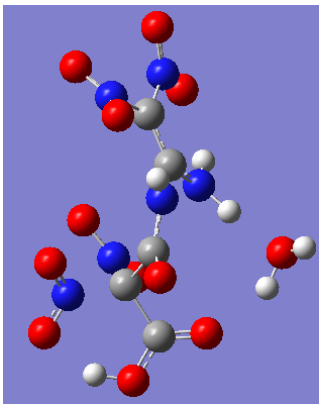
Sum of electronic and thermal Free Energies= -1348.742817 Hartree

Coordinates：

C	-2.24737000	1.35800500	-0.48095900
C	1.20651700	0.34348300	-0.58851100
C	-0.95999300	-0.91540700	-0.88246800
C	-1.82575100	-0.02700300	0.06658600
N	0.67880300	1.58592700	-0.52758600
N	0.38326900	-0.63807800	-1.11274600
H	0.88651300	-1.45845400	-1.45511100
O	-2.71281600	2.24252800	0.16221300
O	-1.47658800	-1.87004900	-1.39771700
C	2.49302600	0.03357400	-0.17609900
H	1.29127500	2.29436300	-0.13122700
N	3.48345100	1.04845600	0.10790100
O	4.65717800	0.75030400	0.01768800
O	3.07368400	2.18677800	0.38685200
N	-1.25977600	0.07480100	1.49967300
O	-0.19850500	-0.48524800	1.70353900
O	-1.94710600	0.65979300	2.29972400
N	-3.16643700	-0.83496900	0.23851200
O	-3.15755300	-1.70829800	1.06740000
O	-4.06409500	-0.50502500	-0.50284400

N	2.94457600	-1.34231100	-0.01412000
O	2.50188600	-2.18302300	-0.80852000
O	3.70514200	-1.58904500	0.89558800
O	-2.03481900	1.39082700	-1.81518700
H	-2.46660500	2.18728000	-2.16449800
H	0.07177500	1.84776700	-1.29177700

A-IM3



Sum of electronic and zero-point Energies = -1425.136756 Hartree

Sum of electronic and thermal Energies = -1425.113928 Hartree

Sum of electronic and thermal Enthalpies = -1425.112984 Hartree

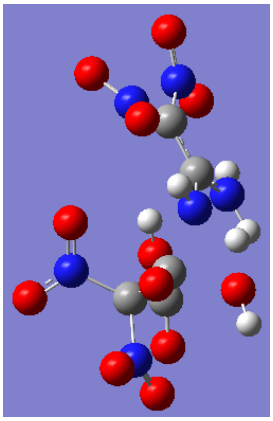
Sum of electronic and thermal Free Energies = -1425.190716 Hartree

Coordinates：

C	-3.05426900	-0.64255700	0.06439200
C	1.26709700	-0.58402600	0.32277000
C	-0.94727300	0.20123200	1.22957200
C	-1.80068600	0.28928400	-0.07932900
N	0.79415900	-1.69854500	-0.23966000
N	0.41693300	0.03413500	1.23741500
H	0.89377700	0.54382000	1.98254300
O	-2.91246000	-1.70089700	0.61092700
O	-1.56986700	0.46404400	2.22626100
C	2.52120800	-0.02896200	0.07827000
H	1.40168400	-2.12380200	-0.93342500
N	3.54313000	-0.73305600	-0.65565600
O	4.70606700	-0.42307300	-0.47985400
O	3.17432500	-1.65458500	-1.40104200
N	-1.13889200	-0.00736500	-1.46152900
O	-0.23374800	0.73300500	-1.77972300
O	-1.60407300	-0.92965900	-2.09226800
N	-2.11902400	1.81764500	-0.22409300
O	-1.35437700	2.59857800	0.27026900
O	-3.10797600	2.09750900	-0.89702200
N	2.89524600	1.27930800	0.58592400
O	2.44332200	1.61269100	1.69304600

O	3.60887500	1.98135600	-0.09797000
O	-4.19183500	-0.23687600	-0.44789500
H	-4.09691400	0.66412500	-0.82436300
H	0.17381100	-2.30535500	0.32193200
O	-0.79398300	-3.35495200	1.33700900

A-TS2



Sum of electronic and zero-point Energies = -1425.055989 Hartree

Sum of electronic and thermal Energies = -1425.034522 Hartree

Sum of electronic and thermal Enthalpies = -1425.033578 Hartree

Sum of electronic and thermal Free Energies = -1425.107673 Hartree

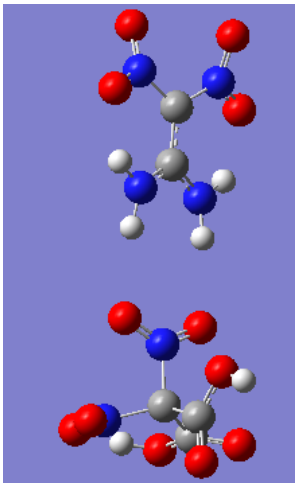
Imaginary frequency = -1523.8901 cm^{-1}

Coordinates：

C	-3.36650800	0.00506500	0.02650800
C	1.33433200	-0.70736400	0.68238900
C	-1.15724400	0.30055100	1.24111300
C	-1.79425800	0.13038900	-0.17378000
N	1.00952200	-1.97841500	0.44287000
N	0.43513500	-0.01072900	1.52427500
H	0.84810100	0.86937700	1.85102800
O	-3.79147600	-0.50929700	1.01443900
O	-1.55030700	1.23696700	1.88049800
C	2.48029300	-0.08531800	0.19572300
H	1.58059000	-2.49717700	-0.21509700
N	3.51494500	-0.82354000	-0.49365100
O	4.63849200	-0.36420400	-0.52868300
O	3.19944300	-1.92494000	-0.97259200
N	-1.36500700	-1.08543300	-1.04270700
O	-0.57906900	-0.86931600	-1.94234500
O	-1.85331600	-2.14931000	-0.73368800
N	-1.32358500	1.35750500	-0.99944700
O	-0.23958900	1.81200100	-0.73769700
O	-2.06781700	1.75370500	-1.88909400
N	2.72224900	1.34076400	0.35586400

O	2.28843500	1.88757100	1.38138200
O	3.31248600	1.92121000	-0.52809700
O	-4.11490500	0.42100400	-0.97778900
H	-3.57641200	0.93722200	-1.61474000
H	0.19158500	-2.38062300	0.88222000
O	-1.32378600	-1.25956000	2.02190800
H	-2.12639300	-1.24060100	2.56314400
H	-0.19872500	-0.79584700	2.28534500

A-IM4



Sum of electronic and zero-point Energies = -1425.136756 Hartree

Sum of electronic and thermal Energies = -1425.113928 Hartree

Sum of electronic and thermal Enthalpies = -1425.112984 Hartree

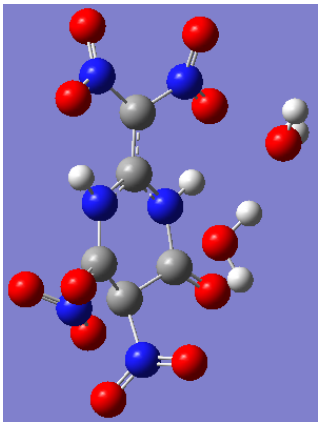
Sum of electronic and thermal Free Energies = -1425.190716 Hartree

Coordinates：

C	3.81414200	1.40761300	-0.46327100
C	-2.74284000	0.01958000	-0.09725400
C	3.66073300	-0.19295100	1.49686700
C	3.25284400	0.01195400	0.01602300
N	-2.06678600	1.16183000	-0.28964100
N	-2.02672700	-1.10880300	0.01990300
H	-2.54642700	-1.96845400	0.16153200
O	3.96176100	2.25281400	0.36304900
O	4.80692000	-0.30387000	1.79879100
C	-4.16811200	0.00451900	-0.01902400
H	-2.61484000	2.01088700	-0.37664200
N	-4.92784500	1.21187200	0.13910700
O	-6.03185500	1.16174000	0.64942900
O	-4.39888900	2.28593900	-0.21958300
N	1.71318000	0.02527100	-0.15844900
O	1.17818300	-1.03452400	-0.41801700
O	1.16832200	1.09425000	0.01376500
N	3.72007200	-1.22416900	-0.78545900
O	3.89621800	-2.24665300	-0.17908200
O	3.83209600	-1.06660000	-1.99779700
N	-4.91564900	-1.21788300	-0.09402700

O	-4.32766900	-2.28154900	0.19935400
O	-6.07123200	-1.19071400	-0.47553300
O	4.02189100	1.55575100	-1.75744300
H	3.93534900	0.69697100	-2.22060500
H	-1.06889100	1.18622700	-0.14502800
O	2.59800900	-0.21818300	2.29565800
H	2.90071700	-0.32023900	3.21250100
H	-1.05026300	-1.11371400	-0.23257500

B-IM1



Sum of electronic and zero-point Energies = -1425.146919 Hartree

Sum of electronic and thermal Energies = -1425.122742 Hartree

Sum of electronic and thermal Enthalpies = -1425.121798 Hartree

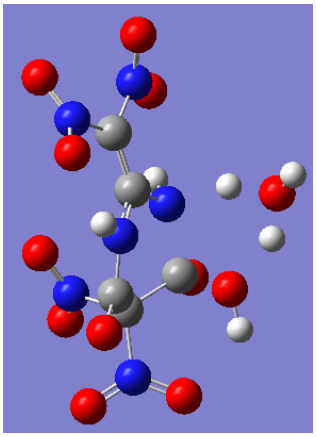
Sum of electronic and thermal Free Energies = -1425.202288 Hartree

Coordinates：

C	-1.10500400	0.98722900	0.74560500
C	0.87447200	-0.33994000	0.16016100
C	-1.21487100	-0.94168100	-0.95799400
C	-1.95740800	-0.10435300	0.09188600
N	0.22063100	0.58350800	0.91564000
N	0.13610600	-1.11442600	-0.67701600
H	0.67409400	-1.70756600	-1.31290100
O	-1.54130000	1.99804200	1.20914500
O	-1.75898700	-1.44330700	-1.89617500
C	2.26694100	-0.47508900	0.23719200
H	0.82530400	1.16800400	1.49778300
N	3.10028800	0.55212400	0.80263100
O	4.23386400	0.67984800	0.38760200
O	2.59565300	1.31621600	1.65028100
N	-2.40188500	-1.06126900	1.25814100
O	-2.14176200	-2.23684900	1.11383500
O	-2.94557700	-0.52720300	2.19392500
N	-3.24309600	0.45219100	-0.53871000
O	-4.26284600	-0.15422400	-0.30957900
O	-3.10483400	1.42502000	-1.24860300
N	2.97154300	-1.59551700	-0.36136500
O	2.42968800	-2.17683200	-1.31377200

O	4.02759600	-1.93255500	0.12887200
O	-0.28513300	1.60653200	-1.76742900
H	-1.03311900	2.17230500	-1.98147100
H	0.47065000	2.18693800	-1.57395500
H	2.38639000	3.13516900	-0.09588300
H	2.92527500	2.86314300	-1.50726600
O	2.13882800	2.78390300	-0.95843200

B-TS1



Sum of electronic and zero-point Energies = -1425.080099 Hartree

Sum of electronic and thermal Energies = -1425.059177 Hartree

Sum of electronic and thermal Enthalpies = -1425.058233 Hartree

Sum of electronic and thermal Free Energies = -1425.130844 Hartree

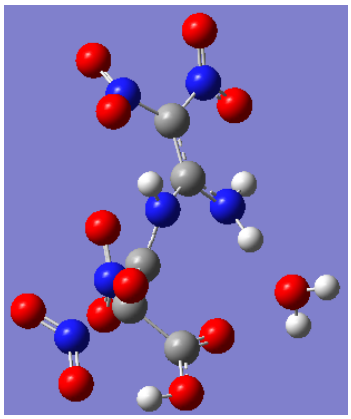
Imaginary frequency = -621.9617 cm^{-1}

Coordinates：

C	-1.35338100	1.22661600	0.17155300
C	1.04628400	-0.00055300	-0.25431400
C	-1.04819900	-1.08878400	-0.96109500
C	-1.80339200	-0.28621500	0.11472300
N	0.35653400	1.10627000	0.21570200
N	0.32243300	-0.85421200	-1.03910900
H	0.86228800	-1.53943200	-1.56956000
O	-1.75744800	1.97088000	1.03602100
O	-1.59507300	-1.86377700	-1.69517500
C	2.39551600	-0.20989000	-0.02332200
H	0.66536700	1.37835300	1.14965500
N	3.23042900	0.79534400	0.61043800
O	4.40358200	0.84381200	0.29668300
O	2.67945600	1.57838500	1.39248700
N	-1.58453900	-0.86245200	1.51968300
O	-0.52904800	-1.45774100	1.68709400
O	-2.42637900	-0.62177400	2.34624700
N	-3.30672900	-0.42580600	-0.20002900
O	-3.83693100	-1.44444400	0.16218100
O	-3.82880300	0.48109300	-0.83177400
N	3.07892900	-1.43747400	-0.40061800

O	2.63593900	-2.05846300	-1.37760500
O	4.01777200	-1.79904300	0.27423500
O	-1.47597300	1.67696800	-1.28466600
H	-2.43553600	1.76858600	-1.41195900
H	-0.51535300	2.80300500	-1.44570000
H	0.64401300	2.32276900	-0.53756400
H	1.00815700	3.22449600	-1.95587300
O	0.42174300	3.18704100	-1.18782300

B-IM2



Sum of electronic and zero-point Energies = -1425.133492 Hartree

Sum of electronic and thermal Energies = -1425.110296 Hartree

Sum of electronic and thermal Enthalpies = -1425.109352 Hartree

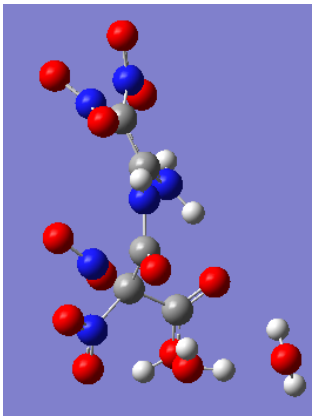
Sum of electronic and thermal Free Energies = -1425.188158 Hartree

Coordinates：

C	-2.55008800	1.10032200	0.22357200
C	1.30141900	0.53251700	-0.34351200
C	-0.93119000	-0.40429100	-1.11323500
C	-1.78834500	-0.26845300	0.20129100
N	0.86574300	1.67157900	0.18427500
N	0.41500000	-0.14322000	-1.18214400
H	0.87703600	-0.68382300	-1.91606000
O	-2.07785000	2.02051200	0.82690500
O	-1.53368300	-0.83003200	-2.06885700
C	2.57837300	0.00296500	-0.14957500
H	1.50135900	2.13207200	0.82749000
N	3.63142000	0.74999000	0.48644500
O	4.78631200	0.43054800	0.27496600
O	3.29925400	1.72026400	1.18858800
N	-1.12208400	-0.47939100	1.57873900
O	0.02805600	-0.85499700	1.60654500
O	-1.86706000	-0.30718900	2.51897300
N	-2.72501100	-1.53557800	0.12014600
O	-2.25747800	-2.55930400	0.54340600
O	-3.83022400	-1.39490600	-0.37748200
N	2.93112100	-1.33349700	-0.59198700
O	2.42447900	-1.73797300	-1.65169600

O	3.68315600	-1.99078500	0.09512700
O	-3.62950400	1.18537800	-0.52490200
H	-3.92515300	0.28978200	-0.80002900
H	-1.68116200	3.50917600	-0.85988400
H	0.15226900	2.21353800	-0.31033500
H	-0.82375900	3.76025700	-2.12515500
O	-0.99232200	3.12991800	-1.41852200

B-IM3



Sum of electronic and zero-point Energies= -1501.576568 Hartree

Sum of electronic and thermal Energies= -1501.551114 Hartree

Sum of electronic and thermal Enthalpies= -1501.550170 Hartree

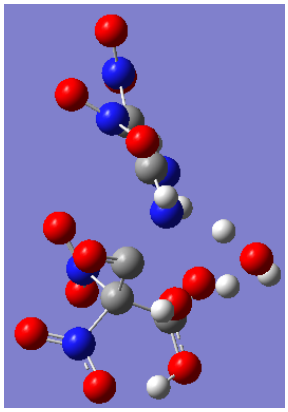
Sum of electronic and thermal Free Energies= -1501.632619 Hartree

Coordinates：

C	2.22362400	0.94793800	-0.32205800
C	-1.58938300	0.53818300	0.31769800
C	0.60165100	-0.58385900	0.94956400
C	1.39943700	-0.37417000	-0.38417700
N	-1.04544500	1.58879200	-0.30063600
N	-0.74018400	-0.26676000	1.05883200
H	-1.21559100	-0.78916200	1.79891100
O	1.74913400	1.85704200	0.32817800
O	1.17625300	-1.08692300	1.87861600
C	-2.95231200	0.23031500	0.27092000
H	-1.67176200	2.15199400	-0.86815000
N	-3.92684900	1.14830600	-0.26393600
O	-5.08460700	1.04525500	0.09036800
O	-3.51522400	2.03199400	-1.03581800
N	0.51678500	-0.36005400	-1.67940900
O	-0.34111600	-1.21434400	-1.73102000
O	0.80159700	0.46101300	-2.52316700
N	2.25012000	-1.65715200	-0.66883900
O	1.88362200	-2.69436600	-0.19590300
O	3.17968000	-1.50192700	-1.45418900
N	-3.47982500	-1.01902500	0.78824100
O	-2.91398000	-1.51520700	1.77654800

O	-4.42602000	-1.52369900	0.22364600
O	3.29997700	1.07392500	-1.04459500
H	3.56491400	0.19193500	-1.39186600
H	3.37727600	-0.81356200	2.01998000
H	-0.15448900	1.95179400	0.02571100
H	4.11039500	0.48599700	1.62207100
O	3.82282500	-0.38346800	1.28217800
O	4.19438200	2.31104400	1.94187500
H	3.36885700	2.59373900	1.52480000
H	4.88789700	2.75535500	1.44336000

B-TS2



Sum of electronic and zero-point Energies = -1501.519857 Hartree

Sum of electronic and thermal Energies = -1501.497073 Hartree

Sum of electronic and thermal Enthalpies = -1501.496128 Hartree

Sum of electronic and thermal Free Energies = -1501.572318 Hartree

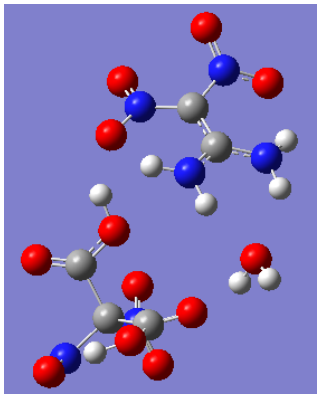
Imaginary frequency = -696.2591 cm^{-1}

Coordinates：

C	2.41884400	-0.18762000	-1.18553300
C	-1.39970300	-0.00637800	-0.72890900
C	0.73881300	0.80513000	0.58885600
C	1.79147000	-0.36344500	0.21662700
N	-1.06849900	-0.91865200	-1.63832400
N	-0.42956100	1.00395900	-0.49309200
H	-0.94148300	1.76824900	-0.02626400
O	1.70422500	-0.34809900	-2.15331600
O	0.42039400	0.92716600	1.74821800
C	-2.63820100	0.03617800	-0.08664600
H	-1.70377200	-1.69804900	-1.77108600
N	-3.71830200	-0.85530300	-0.42690400
O	-4.85266400	-0.56135500	-0.10079600
O	-3.43238800	-1.86705500	-1.09050600
N	1.19531000	-1.78593800	0.29617300
O	0.12267300	-1.93016400	0.83011200
O	1.91273500	-2.65231600	-0.17253300
N	2.79102900	-0.36145200	1.39586500
O	2.48345400	-0.98497700	2.37287900
O	3.81461300	0.31428100	1.26677000
N	-2.93911900	1.01317500	0.95013700

O	-2.47092900	2.15682900	0.81344300
O	-3.62027600	0.66708500	1.88828800
O	3.66094800	0.20338600	-1.29195400
H	4.01854700	0.39161900	-0.38894800
H	1.72205600	2.67887800	0.79022900
H	-0.14540800	-0.88138600	-2.05751800
H	1.37141700	2.48548200	-1.25024400
O	1.69489600	2.07440300	0.03699900
O	0.80534000	2.40858000	-2.17311300
H	0.12719100	1.71249600	-1.68421300
H	1.32392000	1.90688100	-2.82124000

B-IM4



Sum of electronic and zero-point Energies = -1501.613080 Hartree

Sum of electronic and thermal Energies = -1501.587930 Hartree

Sum of electronic and thermal Enthalpies = -1501.586986 Hartree

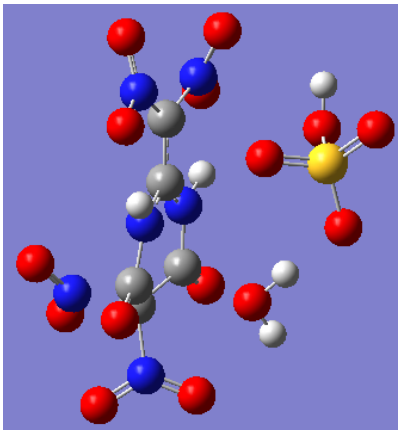
Sum of electronic and thermal Free Energies = -1501.671876 Hartree

Coordinates：

C	2.25668700	1.28101400	0.21471100
C	-2.72914200	1.03284700	0.35993200
C	1.64207300	-1.21456100	0.52162200
C	2.62225500	-0.18734000	-0.15744300
N	-1.91278800	1.28117500	1.38567000
N	-2.99848600	2.04431600	-0.46960500
H	-3.55146700	1.84619100	-1.29331300
O	1.51349900	1.89650100	-0.50063700
O	2.02359400	-2.27102600	0.92497100
C	-3.33138900	-0.26679200	0.17611200
H	-1.66010900	0.49676000	1.97028300
N	-2.77449800	-1.44267700	0.70161800
O	-3.10595900	-2.53829500	0.29540600
O	-1.85310100	-1.32058500	1.58552700
N	2.54685700	-0.30450600	-1.69296200
O	1.73542300	-1.08143400	-2.14206600
O	3.32119500	0.40503600	-2.29684300
N	4.03723700	-0.63234300	0.23948400
O	4.61706500	-1.38360300	-0.49289100
O	4.43601400	-0.22614000	1.33111600
N	-4.49688800	-0.43048900	-0.66651000
O	-4.64017300	0.36373100	-1.61255900

O	-5.29945200	-1.30227000	-0.39751300
O	2.71984300	1.73593200	1.36092100
H	3.39604000	1.11338400	1.71470900
H	-0.26616200	-1.24924900	0.96893900
H	-1.36730900	2.13966700	1.36355300
H	-0.32770600	4.46507400	0.68872300
O	0.44508600	-0.67931900	0.55924800
O	-0.60339700	3.60344700	0.36203000
H	-2.46101200	2.89773500	-0.36819300
H	0.18769200	3.19530400	-0.03185800

C-IM1



Sum of electronic and zero-point Energies = -2048.548370 Hartree

Sum of electronic and thermal Energies = -2048.521870 Hartree

Sum of electronic and thermal Enthalpies = -2048.520925 Hartree

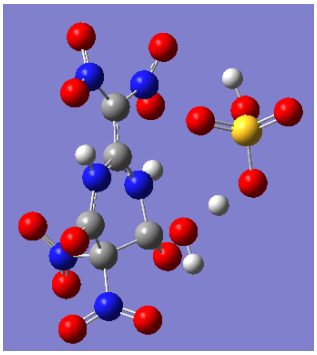
Sum of electronic and thermal Free Energies = -2048.607674 Hartree

Coordinates：

C	1.59860400	-0.29838900	1.26185600
C	-0.18875100	0.86298000	0.03559300
C	1.69069200	0.03896500	-1.30069200
C	2.48191400	-0.07042300	0.02125500
N	0.39771400	0.39778200	1.17409200
N	0.43647400	0.59909700	-1.14005400
H	-0.12008500	0.79251400	-1.97583400
O	1.98322900	-0.80732900	2.27538000
O	2.15594400	-0.24446800	-2.36659000
C	-1.38025300	1.59530100	0.07779400
H	-0.13260000	0.53796200	2.03531700
N	-2.17604800	1.65846700	1.27874800
O	-3.38529100	1.74446500	1.18556100
O	-1.57946200	1.59365900	2.36819500
N	3.20342600	1.29386500	0.28848200
O	2.88483500	2.22982200	-0.41756200
O	3.98813300	1.30547000	1.21008600
N	3.62335700	-1.08150800	-0.14941100
O	4.58578800	-0.65543200	-0.75688100
O	3.48019400	-2.19950500	0.28903300
N	-1.92361200	2.26491200	-1.08032500

O	-1.48913600	1.95635100	-2.19801900
O	-2.72605400	3.16511700	-0.90057300
O	0.79992300	-2.19276100	-0.27565200
H	1.28819400	-2.88668600	0.17541700
H	-0.15518300	-2.46590100	-0.24972200
S	-2.78308600	-1.94100800	-0.26406300
O	-1.72680400	-2.96351800	-0.06589200
O	-2.82999800	-1.23364100	1.26683300
O	-4.13192600	-2.46139200	-0.48405200
O	-2.36338900	-0.84665700	-1.16109700
H	-3.66123600	-0.74211600	1.31408100

C-TS1



Sum of electronic and zero-point Energies = -2048.536160 Hartree

Sum of electronic and thermal Energies = -2048.511275 Hartree

Sum of electronic and thermal Enthalpies = -2048.510331 Hartree

Sum of electronic and thermal Free Energies = -2048.592735 Hartree

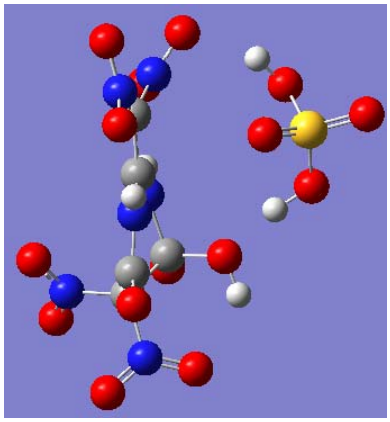
Imaginary frequency = -541.4682 cm^{-1}

Coordinates：

C	1.39422400	-0.74706300	0.97295900
C	-0.18386100	0.95562900	0.03369300
C	1.79768300	0.40885800	-1.30237800
C	2.46111500	-0.08387700	-0.00290100
N	0.28993000	0.23024100	1.05052300
N	0.53529300	0.94178900	-1.12713500
H	0.07486300	1.37237500	-1.93089700
O	1.73483300	-1.29666900	2.00045800
O	2.33502500	0.34719800	-2.37638900
C	-1.37392700	1.71465400	0.12135200
H	-0.20220100	0.26686100	1.93729000
N	-2.25855100	1.52824600	1.23597500
O	-3.46978300	1.53724300	1.04808800
O	-1.74815800	1.31095900	2.34375900
N	3.09122200	1.09088300	0.75676000
O	2.75995500	2.21220700	0.40234400
O	3.82594700	0.81094200	1.67647600
N	3.62190100	-1.00737700	-0.38187100
O	4.67230500	-0.46228800	-0.64424300
O	3.40562800	-2.20430500	-0.43823200
N	-1.84542200	2.57780600	-0.91806500

O	-1.32257400	2.49378300	-2.04563800
O	-2.69993300	3.40693700	-0.64781100
O	0.72851100	-1.82764200	-0.21792200
H	1.38799000	-2.53452900	-0.24098100
H	-0.40932800	-2.31368300	-0.05226900
S	-2.67704200	-2.05110400	-0.36700600
O	-1.43518100	-2.85504300	0.03303800
O	-3.05742000	-1.41545800	1.10612600
O	-3.75689100	-2.93066800	-0.77102500
O	-2.34186500	-0.91672800	-1.22680500
H	-3.67387000	-0.67743700	0.97148100

C-IM2



Sum of electronic and zero-point Energies = -2048.536192 Hartree

Sum of electronic and thermal Energies = -2048.510931 Hartree

Sum of electronic and thermal Enthalpies = -2048.509987 Hartree

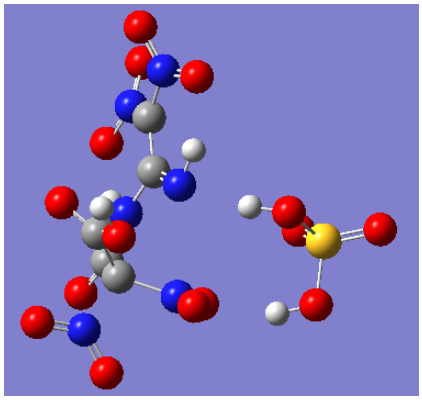
Sum of electronic and thermal Free Energies = -2048.593776 Hartree

Coordinates：

C	1.39217500	-0.86012400	0.93107000
C	-0.08302900	1.02919900	0.07791800
C	1.87991300	0.45609300	-1.28293800
C	2.52783400	-0.13950300	-0.02534000
N	0.36437700	0.26607700	1.06409400
N	0.63780800	1.03388200	-1.08326400
H	0.20508600	1.51979400	-1.86920600
O	1.76015900	-1.35291600	1.99318700
O	2.39446300	0.41217300	-2.37136300
C	-1.27668800	1.80127200	0.17023400
H	-0.09341100	0.31635800	1.96616500
N	-2.20983600	1.49581700	1.20461600
O	-3.41608800	1.45523100	0.94126200
O	-1.76473800	1.20035200	2.32103500
N	3.20228000	0.92940900	0.80554700
O	2.86352200	2.08780500	0.58976900
O	3.97436500	0.55532900	1.65991000
N	3.61924900	-1.10464100	-0.48387300
O	4.71560500	-0.63755800	-0.69916700
O	3.30185800	-2.27291400	-0.65064100
N	-1.73003800	2.70838000	-0.83668900
O	-1.16028100	2.70370800	-1.94506400

O	-2.61721900	3.49906500	-0.55438600
O	0.70033400	-1.76183900	-0.06645700
H	1.34431600	-2.46909800	-0.22301500
H	-0.78966500	-2.35213100	0.09559900
S	-2.87769700	-1.95825600	-0.40455700
O	-1.66908300	-2.85295100	0.07389400
O	-3.40535400	-1.41043600	1.02979200
O	-3.87748100	-2.84133900	-0.95348000
O	-2.39864000	-0.81334800	-1.16338600
H	-3.66266900	-0.46982000	0.94545400

C-IM3



Sum of electronic and zero-point Energies = -2048.534931 Hartree

Sum of electronic and thermal Energies = -2048.508947 Hartree

Sum of electronic and thermal Enthalpies = -2048.508003 Hartree

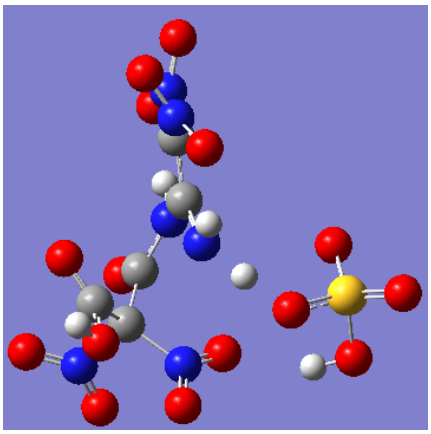
Sum of electronic and thermal Free Energies = -2048.594901 Hartree

Coordinates：

C	1.22632600	-1.93892500	1.30737000
C	-1.18014300	-0.61250800	-0.04127900
C	0.84127500	-1.48875300	-1.20953500
C	1.76594500	-1.26078700	0.03196100
N	-0.48451800	-0.01596500	0.88490900
N	-0.47226500	-1.13713900	-1.12779100
H	-1.06549300	-1.48070000	-1.89131700
O	1.77280100	-1.48465400	2.43779400
O	1.32320800	-2.00935700	-2.18945000
C	-2.61369600	-0.83760200	-0.04045400
H	-1.10148600	0.21309800	1.66486800
N	-3.36217300	-0.66595000	1.17142000
O	-4.37499100	-1.32708300	1.35621800
O	-2.91464600	0.11869800	2.03219000
N	2.16526400	0.21499500	0.13233600
O	1.85955200	0.89875100	-0.84115300
O	2.79854300	0.58403500	1.08689500
N	3.12382100	-1.97487300	-0.32320900
O	3.97250400	-1.29926400	-0.85949300
O	3.19375800	-3.14828500	-0.03391500
N	-3.36575400	-1.22862300	-1.18553400

O	-2.75365100	-1.69328800	-2.18062600
O	-4.57615200	-1.05784000	-1.20919500
O	0.49049300	-2.88240600	1.22734800
H	1.38168000	-2.01059600	3.15187700
H	1.95086900	2.74920800	-0.71097800
S	0.11109300	3.70293600	-0.19068800
O	1.69442600	3.67181900	-0.50406800
O	-0.00019400	2.71419900	1.06303500
O	-0.61015600	3.13062200	-1.31014300
O	-0.15779900	5.03400400	0.28617300
H	-0.15349000	1.76676500	0.79038300

C-TS2



Sum of electronic and zero-point Energies = -2048.532938

Sum of electronic and thermal Energies = -2048.507259

Sum of electronic and thermal Enthalpies = -2048.506315

Sum of electronic and thermal Free Energies = -2048.592572 Hartree

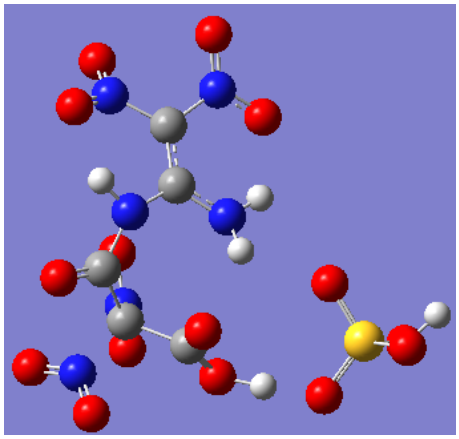
Imaginary frequency = -579.7861 cm^{-1}

Coordinates：

C	-0.66994400	1.99780200	1.29531000
C	1.29290300	0.10727300	-0.06831900
C	-0.55177800	1.35556400	-1.21990800
C	-1.44610500	1.51458900	0.05271100
N	0.57627800	-0.38868100	0.92204400
N	0.61167000	0.62858000	-1.16245700
H	1.22219600	0.81409800	-1.96582300
O	-1.27516400	1.73479700	2.45211100
O	-0.89955300	1.91682800	-2.23006600
C	2.72247400	0.21057500	-0.06909400
H	1.18170000	-0.68340500	1.68672900
N	3.47215500	0.00815600	1.14685200
O	4.51762500	0.61761300	1.30653600
O	2.98950700	-0.73474700	2.02040300
N	-2.35589500	0.27918800	0.19158500
O	-2.34847300	-0.45924700	-0.78105700
O	-3.03863300	0.17582100	1.17802800
N	-2.46443200	2.66822400	-0.30338900
O	-3.52796800	2.33126200	-0.76645600
O	-2.07764300	3.79448000	-0.08747300

N	3.50370400	0.51403900	-1.23075000
O	2.92871900	0.99636700	-2.23334500
O	4.69258400	0.24012300	-1.24212500
O	0.33087700	2.64523200	1.16545100
H	-0.70625000	2.10192000	3.14647700
H	-2.70292600	-2.45446200	-0.81586600
S	-0.91994100	-3.40021700	-0.12388100
O	-2.46842900	-3.38563700	-0.67317900
O	-0.96474900	-2.30813400	0.95890400
O	-0.04682200	-2.98324200	-1.22037500
O	-0.75384100	-4.72875100	0.43285000
H	-0.22962200	-1.27814900	0.79753900

C-IM4



Sum of electronic and zero-point Energies = -2048.562182 Hartree

Sum of electronic and thermal Energies = -2048.535795 Hartree

Sum of electronic and thermal Enthalpies = -2048.534851 Hartree

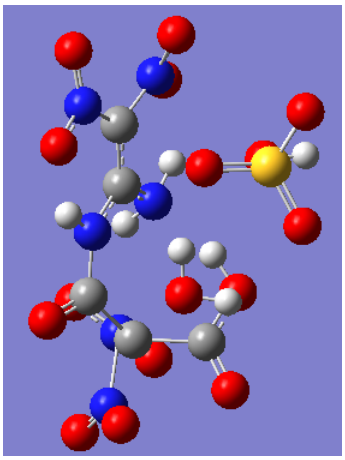
Sum of electronic and thermal Free Energies = -2048.623284 Hartree

Coordinates：

C	1.30236600	1.36346600	-0.33192100
C	-1.49155700	-0.79408700	-0.47944900
C	-1.16335300	1.69125900	-0.97510600
C	-0.06284800	2.01578700	0.07773100
N	-0.25128100	-1.18346900	-0.23370400
N	-1.69100200	0.41454700	-1.13197300
H	-2.58792400	0.45953900	-1.61588500
O	2.14174300	1.27348000	0.63437300
O	-1.58215600	2.58839100	-1.66206800
C	-2.62383800	-1.56778100	-0.14560800
H	-0.11269500	-2.04030600	0.28848100
N	-2.52480400	-2.93391200	0.28596500
O	-3.48618800	-3.67193900	0.12707800
O	-1.44399700	-3.31614600	0.76201800
N	-0.47631200	1.72654700	1.52810500
O	-1.42853400	0.98169600	1.69469500
O	0.18001700	2.26089700	2.39105400
N	0.09770000	3.56533600	0.02568800
O	-0.75127400	4.20906900	0.60176900
O	1.04204000	3.98765800	-0.60246400
N	-3.96823600	-1.04439400	-0.21237100
O	-4.23648800	-0.22884300	-1.11270900

O	-4.77814700	-1.40788600	0.62045800
O	1.39412200	1.00980400	-1.48726100
H	3.00612600	0.68049100	0.37264600
H	4.17482800	-3.23873000	1.08682100
S	3.81878900	-1.57647500	-0.21868700
O	4.26556700	-2.28562000	1.21676000
O	2.38235400	-1.87218600	-0.36783800
O	4.69764700	-2.12580900	-1.24273600
O	4.07881200	-0.13485400	0.10471400
H	0.54782300	-0.84353700	-0.76167900

C-IM5



Sum of electronic and zero-point Energies = -2124.955995 Hartree

Sum of electronic and thermal Energies = -2124.927008 Hartree

Sum of electronic and thermal Enthalpies = -2124.926064 Hartree

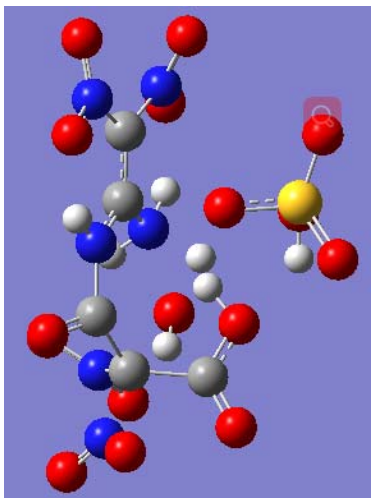
Sum of electronic and thermal Free Energies = -2125.017302 Hartree

Coordinates：

C	2.18393300	1.35015100	-0.62698200
C	-0.60924200	-1.27975200	-0.23747000
C	1.62896500	-0.89868300	0.97214700
C	2.52251200	-0.09571500	-0.04293900
N	-0.11782000	-1.03503600	-1.50450500
N	0.28029600	-1.24408600	0.78644200
H	-0.15986600	-1.48391400	1.68456200
O	2.97189500	2.23100300	-0.46500800
O	2.14580800	-1.25646300	1.99594500
C	-1.95727100	-1.55729300	-0.00336700
H	-0.85604000	-1.11519700	-2.20243800
N	-2.93644000	-1.47420400	-1.07985100
O	-4.05519700	-1.09819600	-0.82607800
O	-2.55838200	-1.79270400	-2.22374300
N	2.87663700	-0.99320400	-1.24154500
O	2.54446500	-2.17348400	-1.16698600
O	3.44247300	-0.47525100	-2.17484200
N	3.88985900	0.05373700	0.72611500
O	4.80186500	-0.65070300	0.33321300
O	3.90234400	0.83129900	1.63761900
N	-2.48614700	-1.91530000	1.28935000

O	-1.74019600	-1.80493700	2.27900200
O	-3.59993600	-2.40064300	1.35680500
O	1.12449100	1.45611800	-1.39861700
H	0.51732600	0.68213000	-1.38865100
H	0.65704300	-1.65491200	-1.72597800
S	-2.29674400	2.22460100	0.13140700
O	-3.68321600	2.65856100	-0.02010000
O	-1.94517900	1.37425900	-1.31131100
O	-2.05588600	1.14050300	1.11511500
O	-1.28946300	3.29715400	0.18080300
H	-2.12168500	1.98650000	-2.03644200
O	0.65387000	1.58102300	1.61644400
H	0.56074400	2.47675200	1.26269800
H	-0.28573500	1.31911700	1.67726900

C-TS3



Sum of electronic and zero-point Energies =-2124.941308 Hartree

Sum of electronic and thermal Energies = -2124.914084 Hartree

Sum of electronic and thermal Enthalpies = -2124.913140 Hartree

Sum of electronic and thermal Free Energies = -2125.001534 Hartree

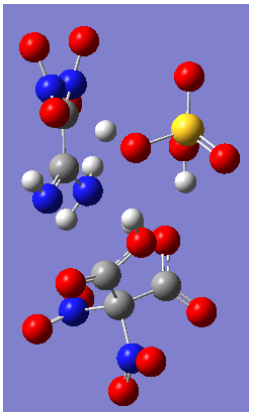
Imaginary frequency = -444.0354 cm^{-1}

Coordinates：

C	2.19738900	0.97779800	-1.04072200
C	-0.73568300	-1.39051500	-0.08942000
C	1.40558900	-0.50147200	1.15387300
C	2.43635600	-0.20220500	-0.02641100
N	-0.14594700	-1.48206000	-1.35510300
N	0.05866200	-1.08214200	0.92922300
H	-0.43612000	-1.06061800	1.82500700
O	2.97996300	1.87260900	-1.13594700
O	1.88408900	-0.79520800	2.22913300
C	-2.11821700	-1.63812500	0.08254300
H	-0.84446200	-1.76907600	-2.04451700
N	-3.00383500	-1.82191800	-1.04818400
O	-4.15640700	-1.45826900	-0.95792400
O	-2.53376800	-2.33118700	-2.08864200
N	2.79570100	-1.46037400	-0.83207100
O	2.44390800	-2.54143300	-0.38000700
O	3.37221600	-1.28678100	-1.88618900
N	3.75441900	0.14204800	0.74257000
O	4.68029400	-0.63227600	0.60822200

O	3.73821200	1.14568100	1.40969600
N	-2.74244000	-1.71875100	1.37831600
O	-2.09715600	-1.31547300	2.36180500
O	-3.83417300	-2.25207700	1.47960900
O	1.11931400	0.87184600	-1.81539300
H	0.61459200	0.02429800	-1.67895800
H	0.59913500	-2.17513600	-1.32913500
S	-1.94633200	2.74786300	-0.06016700
O	-3.38648600	2.84501800	-0.11410200
O	-1.52561500	1.87662300	-1.39613900
O	-1.53805700	1.80259900	1.10084400
O	-1.12198800	3.94853100	-0.07593400
H	-0.58544600	2.03948100	-1.58294500
O	0.81467600	1.26779100	1.12057600
H	1.38124500	1.72839000	1.75069300
H	-0.42832600	1.59238100	1.16321600

C-IM6



Sum of electronic and zero-point Energies = -2124.981573 Hartree

Sum of electronic and thermal Energies = -2124.953568 Hartree

Sum of electronic and thermal Enthalpies = -2124.952624 Hartree

Sum of electronic and thermal Free Energies = -2125.043622 Hartree

Coordinates：

C	2.34609500	0.15523200	-1.44908700
C	-1.10755500	-1.60260200	0.24483900
C	1.97535000	0.55437700	1.13195300
C	2.77238500	-0.20303900	0.02233400
N	-0.47516900	-2.03161900	-0.96209900
N	-0.29386900	-1.35391500	1.20193700
H	-0.78018400	-1.00908300	2.02480400
O	3.14255400	0.72557000	-2.14110100
O	2.12651500	0.37198400	2.29983000
C	-2.56970900	-1.44621500	0.22665700
H	-1.13866200	-2.43484800	-1.61929100
N	-3.40119800	-2.05564700	-0.77001700
O	-4.52857800	-1.63227300	-0.97587400
O	-2.91541800	-3.00164800	-1.43198700
N	2.78269300	-1.71252500	0.29109300
O	3.18816900	-2.07662500	1.36567900
O	2.42206200	-2.42631900	-0.63425400
N	4.25600100	0.23012600	0.14704200
O	5.09200400	-0.57889200	-0.19105900
O	4.44217500	1.36385100	0.53165700
N	-3.23616700	-0.76574700	1.25137500
O	-2.55260800	0.05498300	1.96431300

O	-4.40978800	-0.96917600	1.51520100
O	1.10304500	-0.08877200	-1.81723100
H	0.55319600	-0.85909800	-1.40350700
H	0.23348700	-2.72201800	-0.73100800
S	-1.73845700	2.71907900	-0.37343300
O	-3.16652600	2.85494200	-0.49655300
O	-1.34859000	1.48761600	-1.34463500
O	-1.35846900	2.14825500	1.07891600
O	-0.83252500	3.82202100	-0.59636600
H	-0.38180400	1.35829200	-1.40313400
O	1.18954600	1.45172000	0.54789700
H	0.55964100	1.85088200	1.18159100
H	-1.90432800	1.33143600	1.35450800

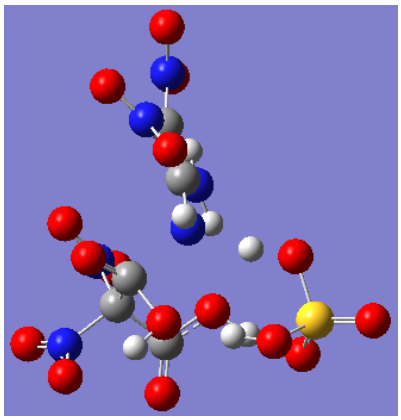
C-IM7

Sum of electronic and zero-point Energies = -2124.962660 Hartree
Sum of electronic and thermal Energies = -2124.935410 Hartree
Sum of electronic and thermal Enthalpies = -2124.934466 Hartree
Sum of electronic and thermal Free Energies = -2125.021529 Hartree

Coordinates：

C	2.04593700	-1.28399600	-0.80650200
C	-1.54228100	0.43657700	-0.45364000
C	0.21591100	-0.81225800	1.08876400
C	0.85331600	-1.84324000	-0.01477100
N	-1.25501400	0.10575000	-1.71336300
N	-0.45175700	0.54593900	0.39724100
H	-0.77312000	0.98825900	1.26151000
O	3.16510700	-1.69427800	-0.69768500
O	-0.50640400	-1.33620200	1.92283200
C	-2.86440600	0.69264000	-0.02933000
H	-2.02280200	-0.05176000	-2.35378600
N	-3.96734300	0.78440700	-0.93109700
O	-4.99336200	1.34628600	-0.57284400
O	-3.82176400	0.32487400	-2.08332700
N	-0.18224200	-2.46578300	-0.95452700
O	-1.24197800	-2.80156500	-0.47855900
O	0.15748400	-2.58860900	-2.12363800
N	1.39613900	-3.04646900	0.80110700
O	1.16008300	-4.15568700	0.37164600
O	2.05656600	-2.79183700	1.78834800
N	-3.18831300	0.91350800	1.36784400
O	-2.37751100	1.55070500	2.05549600
O	-4.23062700	0.45874500	1.80113800
O	1.66844000	-0.23870100	-1.55343000
H	2.42739400	0.38803600	-1.65771200
H	-0.28286500	0.05552000	-1.98921800
S	2.50702700	2.76488400	-0.18169400
O	3.20568400	1.83787800	-1.08136200
O	2.62046900	2.23360200	1.31234000
O	0.94748500	2.68773800	-0.47471900
O	2.89930100	4.14779800	-0.18916400
H	2.20976500	1.32194900	1.41514000
O	1.45225000	-0.10874600	1.59039500
H	1.81401700	-0.72478400	2.24271300
H	0.51423700	1.80882400	-0.18883000

C-TS4



Sum of electronic and zero-point Energies = -2124.963894 Hartree

Sum of electronic and thermal Energies = -2124.937028 Hartree

Sum of electronic and thermal Enthalpies = -2124.936084 Hartree

Sum of electronic and thermal Free Energies = -2125.022463 Hartree

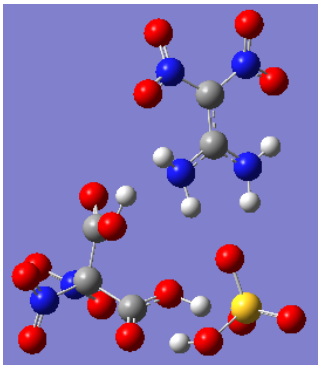
Imaginary frequency = -163.8158 cm^{-1}

Coordinates：

C	-2.03598900	1.31155500	-0.79632600
C	1.51308300	-0.54480300	-0.46068100
C	-0.25665100	0.86394600	1.12485600
C	-0.82344000	1.85502000	-0.01710600
N	1.22335400	-0.27153900	-1.73498100
N	0.42503700	-0.63450700	0.38673500
H	0.75002600	-1.01973900	1.27539600
O	-3.13970400	1.76180100	-0.68510300
O	0.51603000	1.34140800	1.92922500
C	2.84610100	-0.74515100	-0.02704100
H	1.98888300	-0.11754800	-2.37882000
N	3.95370200	-0.82034900	-0.92320100
O	5.00098100	-1.33058200	-0.54828900
O	3.79434000	-0.40295400	-2.09043300
N	0.24930700	2.38985300	-0.97164600
O	1.32856200	2.66798300	-0.50229500
O	-0.08909100	2.51668000	-2.13900200
N	-1.32312900	3.11608400	0.74096500
O	-1.06134700	4.19425100	0.25238500
O	-1.97364900	2.92482200	1.74825100
N	3.17101400	-0.91761600	1.37532700

O	2.37061600	-1.54830700	2.08204000
O	4.20272400	-0.42911200	1.79896800
O	-1.69155000	0.24736800	-1.52373500
H	-2.46086400	-0.37675900	-1.60141100
H	0.25029000	-0.20286200	-2.00115500
S	-2.54320600	-2.72391500	-0.16943600
O	-3.25816300	-1.78023000	-1.04414900
O	-2.66035100	-2.21133800	1.34144200
O	-1.00170500	-2.63679700	-0.46320900
O	-2.95596100	-4.10177400	-0.18607800
H	-2.25420400	-1.30894600	1.44297500
O	-1.46127400	0.17726100	1.62243500
H	-1.79149200	0.76546400	2.31592200
H	-0.50862600	-1.75770500	-0.13616400

C-IM8



Sum of electronic and zero-point Energies = -2125.040926 Hartree

Sum of electronic and thermal Energies = -2125.012777 Hartree

Sum of electronic and thermal Enthalpies = -2125.011832 Hartree

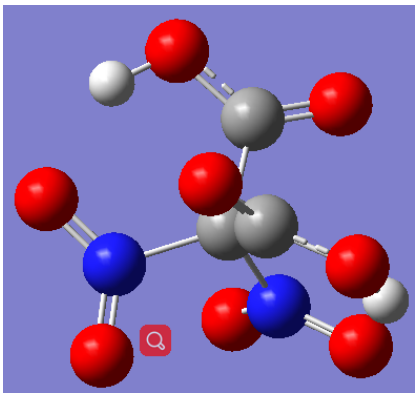
Sum of electronic and thermal Free Energies = -2125.105336 Hartree

Coordinates：

C	-2.71630000	-0.28069800	-0.20983500
C	2.85090600	-0.23847400	0.09076000
C	-1.26741300	1.75344800	-0.13184100
C	-2.74686200	1.27624200	-0.16046100
N	2.55761700	-1.13839600	-0.83838100
N	1.94872500	-0.10271800	1.10720000
H	2.33355600	0.30353900	1.95277300
O	-3.13931300	-0.92613200	0.72650800
O	-0.79953500	2.54230700	-0.89753800
C	4.01588600	0.58767800	0.02424200
H	3.15672900	-1.19079500	-1.65124000
N	5.02957100	0.38630000	-0.96388000
O	6.16249700	0.79658400	-0.76089000
O	4.72414900	-0.25472400	-1.99108000
N	-3.47817600	1.95214800	-1.33259300
O	-3.62647000	3.15248400	-1.21069500
O	-3.85136000	1.25906100	-2.25212700
N	-3.54153400	1.73367400	1.07487200
O	-4.73604700	1.52596200	1.02135900
O	-2.92844600	2.25791800	1.97987200
N	4.24311400	1.64877500	0.96325700
O	3.71700500	1.55662800	2.09154200
O	4.90517600	2.61619600	0.62579100

O	-2.09652200	-0.68629400	-1.26685200
H	-1.86131100	-1.72506800	-1.21706500
H	1.75300500	-1.75139400	-0.67890300
S	-0.65971000	-3.41436300	0.15286800
O	-1.47448500	-3.07090200	-1.06767200
O	-1.70166100	-3.28922100	1.39497700
O	0.37275000	-2.35977000	0.38145300
O	-0.17535700	-4.77828800	0.18583800
H	-2.27776000	-2.51069000	1.24168600
O	-0.64027700	1.06925600	0.81611900
H	0.33451500	1.14647000	0.75190200
H	1.28724700	-0.87843900	1.19159300

IM1(DMA)



Sum of electronic and zero-point Energies = -826.753318 Hartree

Sum of electronic and thermal Energies = -826.741627 Hartree

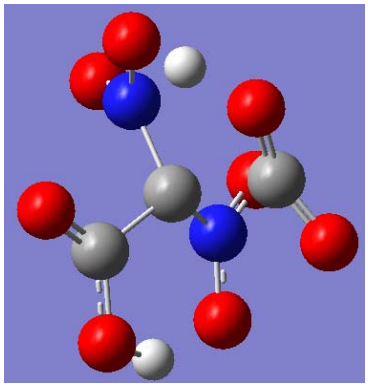
Sum of electronic and thermal Enthalpies = -826.740683 Hartree

Sum of electronic and thermal Free Energies = -826.793162 Hartree

Coordinates：

C	0.32435700	-0.94043100	-1.22199200
C	-0.32420600	-0.94280100	1.22027900
C	0.00003000	-0.00390400	0.00009700
O	-0.61410500	-1.41692800	-1.78772200
O	0.61422300	-1.42139800	1.78430500
N	1.09876100	0.94633600	0.52043800
O	0.72052100	1.81747900	1.26339200
O	2.25305500	0.73189300	0.18198800
N	-1.09887200	0.94717200	-0.51838800
O	-0.72073900	1.81987900	-1.25957600
O	-2.25314200	0.73194800	-0.18040500
O	1.58733700	-1.17309500	-1.49249200
H	2.16400500	-0.61820800	-0.92310900
O	-1.58719700	-1.17649600	1.49000600
H	-2.16393300	-0.61977700	0.92250000

TS1



Sum of electronic and zero-point Energies = -826.731390 Hartree

Sum of electronic and thermal Energies = -826.720120 Hartree

Sum of electronic and thermal Enthalpies = -826.719175 Hartree

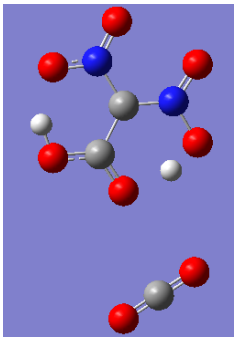
Sum of electronic and thermal Free Energies = -826.770039 Hartree

Imaginary frequency = -724.0300 cm^{-1}

Coordinates：

C	-0.09946600	1.15544900	-1.37885400
C	0.08121000	0.81365600	1.33825700
C	0.04790000	-0.14547700	0.12325600
O	0.97412300	1.44850600	-1.75000600
O	-0.95082800	1.19054500	1.81457200
N	-1.16162900	-0.97401800	0.19594300
O	-1.16858400	-2.10124400	0.57801400
O	-2.25394300	-0.38858200	-0.14910400
N	1.21395700	-0.98093500	-0.22854300
O	1.04050100	-1.92509100	-0.96814800
O	2.31612500	-0.58436800	0.16098700
O	-1.30686300	1.34291000	-1.50430500
H	-1.94744600	0.51062900	-0.75233600
O	1.27887500	1.20723400	1.72539100
H	1.96804700	0.71298000	1.22536900

IM2



Sum of electronic and zero-point Energies = -826.793450 Hartree

Sum of electronic and thermal Energies = -826.780532 Hartree

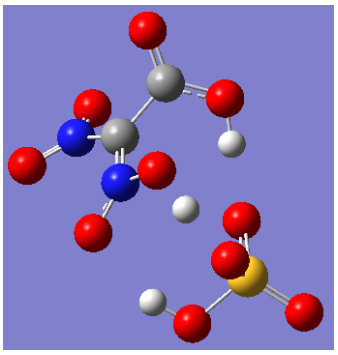
Sum of electronic and thermal Enthalpies = -826.779588 Hartree

Sum of electronic and thermal Free Energies = -826.842258 Hartree

Coordinates：

C	4.09305100	0.04260900	0.02279200
C	-0.04381900	-0.88199200	-0.03390000
C	-1.23021300	0.00504200	-0.00444800
O	4.52790300	-1.03181900	0.02282200
O	1.09114200	-0.39851900	-0.07941400
N	-1.06160100	1.37908600	0.00822500
O	-1.93442000	2.19977600	0.06327900
O	0.19596400	1.84612000	-0.03790900
N	-2.57800700	-0.51007500	0.00721600
O	-3.53575600	0.22566200	-0.05148200
O	-2.68488500	-1.75820700	0.07353100
O	3.67317100	1.12576900	0.02371300
H	0.80783800	0.99890500	-0.07009100
O	-0.21438200	-2.17469800	-0.01208800
H	-1.19459900	-2.34860400	0.03571800

IM3



Sum of electronic and zero-point Energies = -1338.002024 Hartree

Sum of electronic and thermal Energies = -1337.987677 Hartree

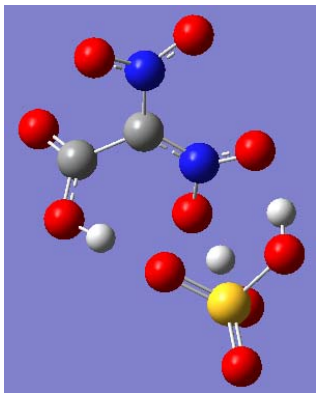
Sum of electronic and thermal Enthalpies = -1337.986733 Hartree

Sum of electronic and thermal Free Energies = -1338.044861 Hartree

Coordinates：

C	-1.87247000	1.42897100	0.07943200
C	-1.61590600	-0.05971600	0.22002800
O	-2.93963000	1.89894100	0.37398500
N	-2.44134500	-0.96011600	-0.54808900
O	-2.96046500	-0.46783700	-1.54879000
O	-2.59960000	-2.11250000	-0.16781900
N	-0.64040300	-0.54132500	0.97265400
O	-0.18993100	-1.69048300	1.00474500
O	-0.08825900	0.40059200	1.79293200
H	0.94992700	0.33077300	1.63497000
O	-0.86746900	2.14133100	-0.40610800
H	-0.06086500	1.59526000	-0.60568100
S	2.46307000	0.10381200	-0.30110200
O	1.26101300	0.63554300	-0.99885100
O	2.38322000	-1.52383000	-0.49918600
O	2.33106300	0.30814500	1.18525500
O	3.75025400	0.47651500	-0.85028700
H	1.56273900	-1.82381800	-0.06738900

TS2



Sum of electronic and zero-point Energies = -1338.003976 Hartree

Sum of electronic and thermal Energies = -1337.990127 Hartree

Sum of electronic and thermal Enthalpies = -1337.989183 Hartree

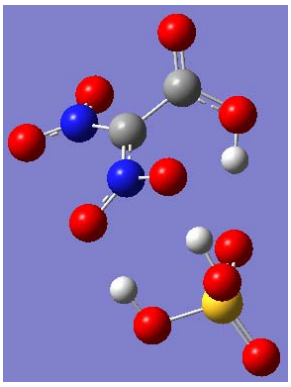
Sum of electronic and thermal Free Energies = -1338.046109 Hartree

Imaginary frequency = -554.4435 cm^{-1}

Coordinates：

C	1.92012500	-1.41735900	0.08162000
C	1.63666000	0.06161600	0.22059200
O	2.98574300	-1.88578700	0.38111100
N	2.48148100	0.97831100	-0.49522000
O	3.06513000	0.50292900	-1.47146500
O	2.59992500	2.13392900	-0.10606000
N	0.60704700	0.50873800	0.93704600
O	0.14361200	1.66479500	0.92662800
O	0.02684300	-0.41566700	1.69660000
H	-1.15999300	-0.34641700	1.51234000
O	0.92901300	-2.15197800	-0.42179800
H	0.12148800	-1.62289200	-0.61445800
S	-2.48817100	-0.09551500	-0.31586800
O	-1.34319200	-0.69295800	-1.03186100
O	-2.33831800	1.51609200	-0.47118900
O	-2.32662500	-0.33578600	1.19208600
O	-3.82003200	-0.40458400	-0.78077900
H	-1.48797100	1.77478600	-0.05622500

IM4



Sum of electronic and zero-point Energies = -1338.002532 Hartree

Sum of electronic and thermal Energies = -1337.988256 Hartree

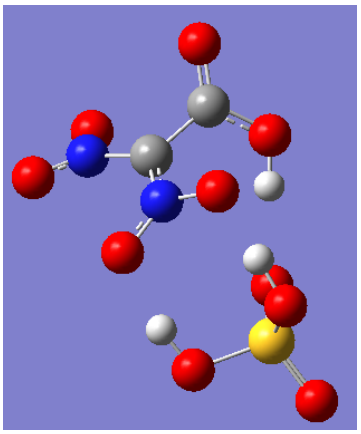
Sum of electronic and thermal Enthalpies = -1337.987312 Hartree

Sum of electronic and thermal Free Energies = -1338.045566 Hartree

Coordinates：

C	-2.00281200	1.39679300	0.06456500
C	-1.67348500	-0.06562100	0.22494900
O	-3.07956900	1.85250800	0.34058200
N	-2.49363500	-1.01743800	-0.46039200
O	-3.12316200	-0.57385100	-1.42723800
O	-2.55881200	-2.17764600	-0.06730200
N	-0.60446800	-0.44686700	0.94229600
O	-0.11940500	-1.61123700	0.92585100
O	-0.03392700	0.47650900	1.64044100
H	1.49586200	0.46369700	1.48187100
O	-1.02396400	2.16108500	-0.44206800
H	-0.20682000	1.65076200	-0.60384800
S	2.52862400	0.07354500	-0.35239400
O	1.41473600	0.72806300	-1.04244700
O	2.25089300	-1.50256100	-0.33057700
O	2.47834800	0.47246800	1.17853100
O	3.87387400	0.25464400	-0.83223300
H	1.36538400	-1.66793300	0.10154900

IM5



Sum of electronic and zero-point Energies = -1338.002529 Hartree

Sum of electronic and thermal Energies = -1337.988252 Hartree

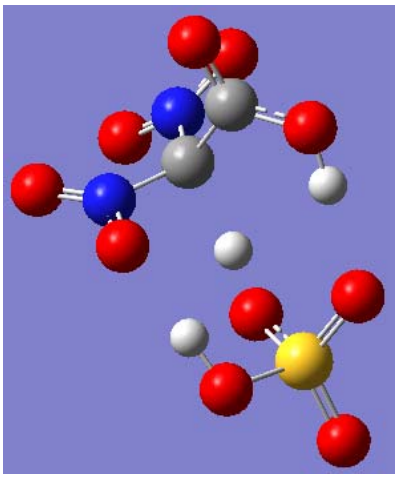
Sum of electronic and thermal Enthalpies = -1337.987308 Hartree

Sum of electronic and thermal Free Energies = -1338.045566 Hartree

Coordinates：

C	-2.00315600	1.39667800	0.06440200
C	-1.67340700	-0.06566700	0.22470200
O	-3.08020800	1.85185500	0.34038200
N	-2.49345900	-1.01768700	-0.46031800
O	-3.12289500	-0.57444200	-1.42736800
O	-2.55857900	-2.17780800	-0.06690600
N	-0.60443600	-0.44645300	0.94233100
O	-0.03386700	0.47736300	1.63987000
O	-0.11922200	-1.61086100	0.92653200
H	1.49647100	0.46361200	1.48203800
O	-1.02466700	2.16129400	-0.44203700
H	-0.20714900	1.65140100	-0.60332700
S	2.52874200	0.07351700	-0.35242100
O	1.41532000	0.72922400	-1.04201500
O	2.25006000	-1.50240600	-0.33135600
O	2.47880200	0.47161500	1.17879300
O	3.87409300	0.25407700	-0.83213100
H	1.36474300	-1.66765600	0.10121300

TS3



Sum of electronic and zero-point Energies = -1337.986268

Sum of electronic and thermal Energies = -1337.972343

Sum of electronic and thermal Enthalpies = -1337.971399

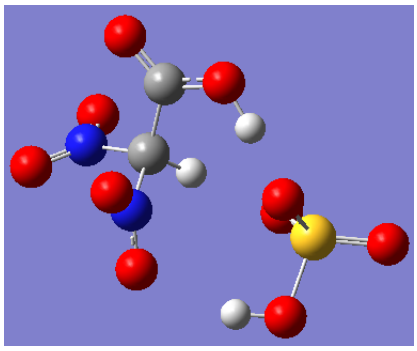
Sum of electronic and thermal Free Energies = -1338.029280 Hartree

Imaginary frequency = -206.9405 cm^{-1}

Coordinates：

C	-1.44104200	-1.38133300	-0.46210300
C	-1.13743600	0.04329500	0.06593100
O	-2.47969100	-1.62207400	-1.01678800
N	-2.03874000	0.39460300	1.15967100
O	-2.46798200	-0.55840200	1.81571500
O	-2.21729800	1.56929600	1.45329700
N	-1.11115400	0.96195600	-1.05653400
O	-0.25108100	0.65870300	-1.92793800
O	-1.82814300	1.93265600	-1.16029200
H	1.45044700	0.58021100	-1.55141800
O	-0.51190300	-2.31463300	-0.27557300
H	0.34355400	-1.94822600	0.03242100
S	2.41039700	-0.00966200	0.27899100
O	2.02520200	-1.42291100	0.18444800
O	1.27037400	0.75817700	1.03606900
O	2.37542900	0.62274700	-1.19685300
O	3.69301000	0.33174000	0.83842000
H	0.29644700	0.41254600	0.70617600

IM6



Sum of electronic and zero-point Energies = -1338.002532 Hartree

Sum of electronic and thermal Energies = -1337.988256 Hartree

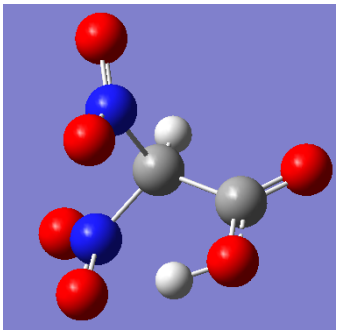
Sum of electronic and thermal Enthalpies = -1337.987312 Hartree

Sum of electronic and thermal Free Energies = -1338.045566 Hartree

Coordinates：

C	1.47917500	1.46507500	-0.28040100
C	1.14439200	0.01715100	0.18620000
O	2.59842200	1.89457300	-0.18576500
N	2.33509900	-0.55715100	0.92355700
O	2.47739800	-0.14337100	2.05664400
O	3.05114100	-1.35296300	0.34429100
N	0.85899200	-0.90050300	-0.99268700
O	0.23760000	-1.92341900	-0.73592500
O	1.28721100	-0.58198900	-2.08067500
H	-1.85009600	-1.82860400	-0.38137900
O	0.44855900	2.13148300	-0.73623400
H	-0.41999100	1.59620500	-0.74152600
S	-2.44062400	0.11420200	0.29328200
O	-1.64220600	0.69448300	-0.84653000
O	-1.60065800	0.01240800	1.50655500
O	-2.71922500	-1.43631500	-0.20089800
O	-3.77067300	0.67367800	0.45608200
H	0.27948700	-0.03315000	0.85916100

IM7



Sum of electronic and zero-point Energies = -638.158384 Hartree

Sum of electronic and thermal Energies = -638.149366 Hartree

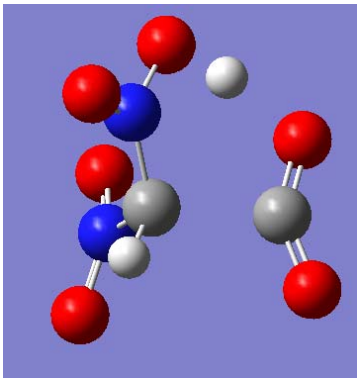
Sum of electronic and thermal Enthalpies = -638.148422 Hartree

Sum of electronic and thermal Free Energies = -638.194555 Hartree

Coordinates：

C	1.44099700	-0.35744300	-0.27505300
C	-0.02127000	0.07337800	-0.57534900
O	1.66918300	-0.93339100	0.89455200
N	-0.34822400	1.35896400	0.20282000
O	-0.64235900	2.31931900	-0.47455500
O	-0.26667600	1.29427400	1.41364500
N	-1.08367000	-0.94504400	-0.18608100
O	-0.97483600	-1.47779800	0.91182500
O	-1.95999600	-1.13952100	-0.99815300
O	2.27763000	-0.11325400	-1.09234800
H	0.83054600	-1.08124300	1.37291400
H	-0.14921000	0.29115800	-1.62741100

TS4



Sum of electronic and zero-point Energies = -638.130051 Hartree

Sum of electronic and thermal Energies = -638.121566 Hartree

Sum of electronic and thermal Enthalpies = -638.120622 Hartree

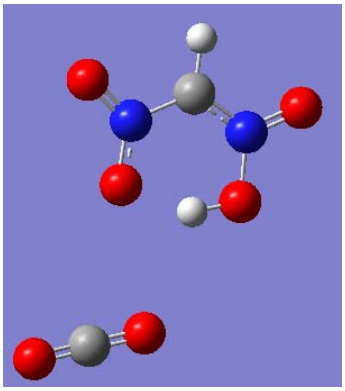
Sum of electronic and thermal Free Energies = -638.164750 Hartree

Imaginary frequency = -606.9505 cm^{-1}

Coordinates：

C	-0.89611500	1.35192700	-0.07080900
C	0.02375000	-0.19191300	-0.65214100
O	-0.39624800	1.65670800	1.01271100
N	-0.66491200	-1.27103600	0.13527200
O	-1.49728100	-1.88579600	-0.50427300
O	-0.38003600	-1.41732000	1.30847400
N	1.39764800	-0.02955200	-0.31251700
O	1.65757500	0.37431300	0.90316500
O	2.28565000	-0.15928700	-1.10970100
O	-1.74086700	1.63352900	-0.84807200
H	0.76007800	0.90796600	1.19060800
H	-0.08538200	-0.38110400	-1.71062800

IM8



Sum of electronic and zero-point Energies = -638.187918 Hartree

Sum of electronic and thermal Energies = -638.178437 Hartree

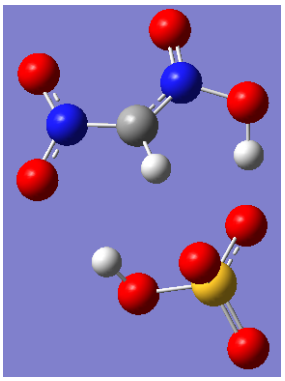
Sum of electronic and thermal Enthalpies = -638.177492 Hartree

Sum of electronic and thermal Free Energies = -638.227340 Hartree

Coordinates：

C	3.21632200	-0.43096000	0.00131700
C	-2.00568000	0.51887700	0.00218600
O	2.39971100	-1.25796000	-0.00117500
N	-0.86030500	1.33030300	-0.00111200
O	-1.03389600	2.53729900	0.00062600
O	0.27855700	0.79384000	-0.00569700
N	-1.96431500	-0.82549300	0.00084600
O	-0.77731100	-1.48205600	-0.00387900
O	-2.96228900	-1.51315400	0.00371200
O	4.03963500	0.38399100	0.00395400
H	-0.07897400	-0.75272500	-0.00558800
H	-2.96779900	0.99587500	0.00610700

IM9



Sum of electronic and zero-point Energies = -1149.387006 Hartree

Sum of electronic and thermal Energies = -1149.375225 Hartree

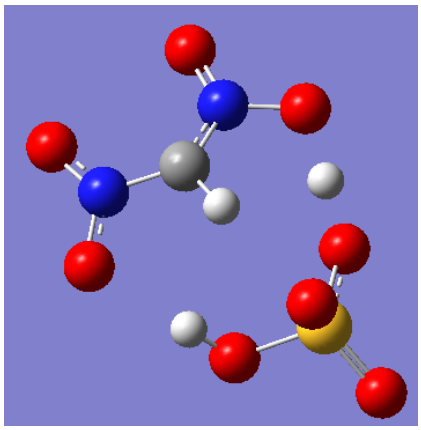
Sum of electronic and thermal Enthalpies = -1149.374280 Hartree

Sum of electronic and thermal Free Energies = -1149.426654 Hartree

Coordinates：

C	-1.33772500	-0.00055500	0.49945600
N	-1.72831900	1.20420000	0.07916800
O	-2.78642100	1.53377900	-0.42532700
O	-0.78928800	2.18129200	0.26370200
N	-1.99440100	-1.18498900	0.09926500
O	-3.15913200	-1.18679600	-0.28110200
O	-1.28058800	-2.20768000	0.16582700
H	0.12934200	1.76098100	-0.02768600
H	-0.39338800	-0.10796900	1.01052800
S	2.08393000	0.00339400	-0.00047800
O	1.31386200	1.15289500	-0.60597300
O	3.50556800	0.05945100	-0.29528700
O	1.55521800	-1.33102100	-0.82383600
O	1.67412800	-0.22477300	1.39970700
H	0.73977200	-1.65564200	-0.40264900

TS5



Sum of electronic and zero-point Energies = -1149.388662 Hartree

Sum of electronic and thermal Energies = -1149.377498 Hartree

Sum of electronic and thermal Enthalpies = -1149.376554 Hartree

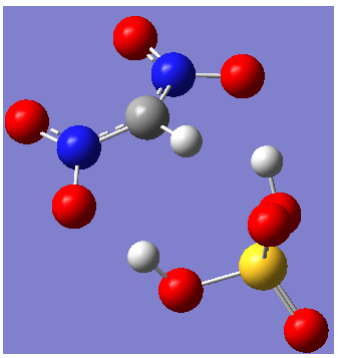
Sum of electronic and thermal Free Energies = -1149.427181 Hartree

Imaginary frequency = -620.1423 cm^{-1}

Coordinates：

C	-1.35312400	0.00525500	0.56396200
N	-1.68628300	1.23027800	0.10418900
O	-2.73461100	1.55061100	-0.43648400
O	-0.73583800	2.14047900	0.27770800
N	-1.95868400	-1.16886200	0.10455000
O	-3.09206800	-1.19518900	-0.36199200
O	-1.22811700	-2.19110700	0.20299000
H	0.32180500	1.63893600	-0.08426200
H	-0.43667500	-0.10218200	1.11573700
S	2.04391900	-0.02382400	-0.00422600
O	1.30002800	1.19091100	-0.59305600
O	3.42697000	-0.01263200	-0.43391400
O	1.38685300	-1.31019000	-0.76487700
O	1.73573400	-0.17263700	1.42215900
H	0.57408000	-1.61896700	-0.30908900

IM10



Sum of electronic and zero-point Energies = -1149.387657 Hartree

Sum of electronic and thermal Energies = -1149.376176 Hartree

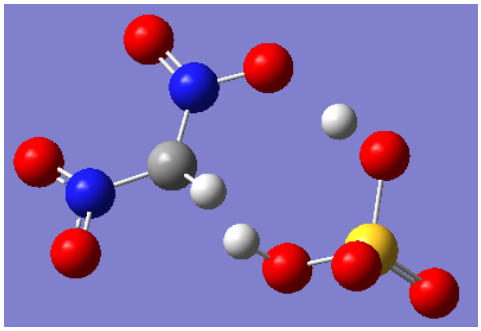
Sum of electronic and thermal Enthalpies = -1149.375232 Hartree

Sum of electronic and thermal Free Energies = -1149.426526 Hartree

Coordinates：

C	-1.38743300	0.00008200	0.60309100
N	-1.81919600	1.21221700	0.11281600
O	-2.90348500	1.39098900	-0.43290600
O	-0.97189400	2.16418200	0.26177800
N	-1.81928000	-1.21216500	0.11270600
O	-2.90313100	-1.39115300	-0.43362400
O	-0.97212300	-2.16400700	0.26229600
H	0.49325300	1.58446300	-0.19952400
H	-0.47847300	-0.00027300	1.17360200
S	2.04215100	-0.00006000	-0.00139100
O	1.32866900	1.25911400	-0.66982500
O	3.39990100	-0.00036100	-0.49223200
O	1.32789400	-1.25813800	-0.67077800
O	1.77062000	-0.00061700	1.43163800
H	0.49312300	-1.58414400	-0.19979600

IM11



Sum of electronic and zero-point Energies = -1149.382915 Hartree

Sum of electronic and thermal Energies = -1149.370868 Hartree

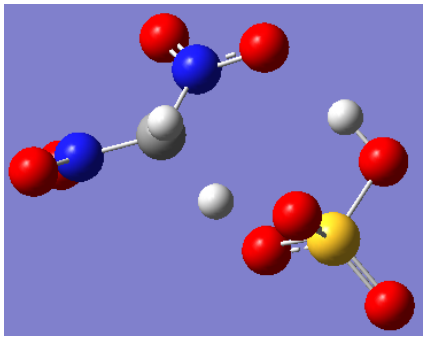
Sum of electronic and thermal Enthalpies = -1149.369924 Hartree

Sum of electronic and thermal Free Energies = -1149.424094 Hartree

Coordinates：

C	-1.39353300	-0.10644000	0.34966800
N	-1.42241600	1.26573800	0.15669200
O	-2.29847900	1.86267100	-0.45361700
O	-0.43021700	1.90437100	0.66978800
N	-2.49248700	-0.94430000	0.02595000
O	-3.34556900	-0.60615000	-0.79305200
O	-2.48590000	-2.05147400	0.59321800
H	1.01534600	1.51903700	0.28665700
H	-0.80485800	-0.44455100	1.18580000
S	2.22435300	-0.26439100	-0.02684400
O	3.52294400	-0.48583800	-0.61412200
O	1.15198100	-0.83302800	-1.09505300
O	1.95328700	1.29601500	-0.05276600
O	1.89768600	-0.80208800	1.28375600
H	0.23950800	-0.73147200	-0.72466000

TS6



Sum of electronic and zero-point Energies= -1149.381625 Hartree

Sum of electronic and thermal Energies= -1149.370086 Hartree

Sum of electronic and thermal Enthalpies= -1149.369142 Hartree

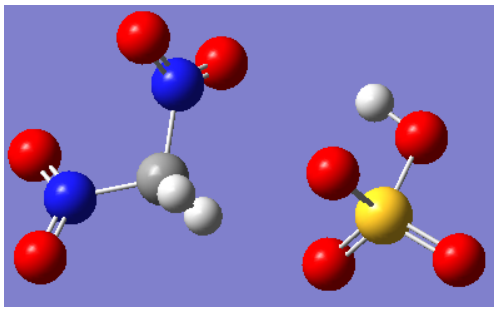
Sum of electronic and thermal Free Energies= -1149.421565 Hartree

Imaginary frequency = -866.2294 cm^{-1}

Coordinates：

C	-1.25437600	-0.11995600	0.33957900
N	-1.44129400	1.30164400	0.14551900
O	-2.42791800	1.77516700	-0.38767700
O	-0.49250200	2.00444900	0.56014200
N	-2.38621500	-0.97259200	0.00933400
O	-2.98238700	-0.80979500	-1.04770500
O	-2.61591800	-1.88893100	0.80400100
H	1.28565000	1.61745800	0.28660200
H	-0.92302600	-0.30791200	1.35357700
S	2.16754500	-0.30802000	-0.04777700
O	3.39877400	-0.67516900	-0.71599600
O	0.94666800	-0.63790400	-0.95557800
O	2.17031100	1.32005800	-0.01824900
O	1.92294400	-0.77619500	1.31371100
H	-0.08429700	-0.45828800	-0.41837600

IM12



Sum of electronic and zero-point Energies = -1144.810203 Hartree

Sum of electronic and thermal Energies = -1144.798347 Hartree

Sum of electronic and thermal Enthalpies = -1144.797403 Hartree

Sum of electronic and thermal Free Energies = -1144.851526 Hartree

Coordinates：

C	-1.26430500	-0.33315100	0.20091000
N	-1.28491600	1.15133000	0.16599300
O	-1.91225900	1.68259300	1.01666100
O	-0.68747800	1.69320400	-0.69920500
N	-2.63047900	-0.81974800	-0.12312900
O	-3.29799600	-0.17560800	-0.85821700
O	-2.92422600	-1.86415200	0.34939600
H	1.74427900	1.50585600	-0.91016700
H	-1.00534400	-0.64164500	1.19345700
S	2.18962900	-0.31131800	0.04778500
O	3.45784500	-0.84074000	0.41923300
O	1.45945400	-1.07753300	-0.93956000
O	2.55078800	1.06728000	-0.68563400
O	1.32773100	0.07830000	1.14488900
H	-0.57027200	-0.71206000	-0.53385800