

Supplementary Material

Oxidative Repair of Pyrimidine Cyclobutane Dimers by Nitrate Radicals ($\text{NO}_3^\bullet$): A Kinetic Study and Computational Study

Tomas Haddad,¹ Joses G. Nathanael,¹ Jonathan M. White¹ and Uta Wille^{1,*}

¹School of Chemistry, Bio21 Institute, The University of Melbourne, 30 Flemington Road, Parkville, Victoria 3010, Australia.

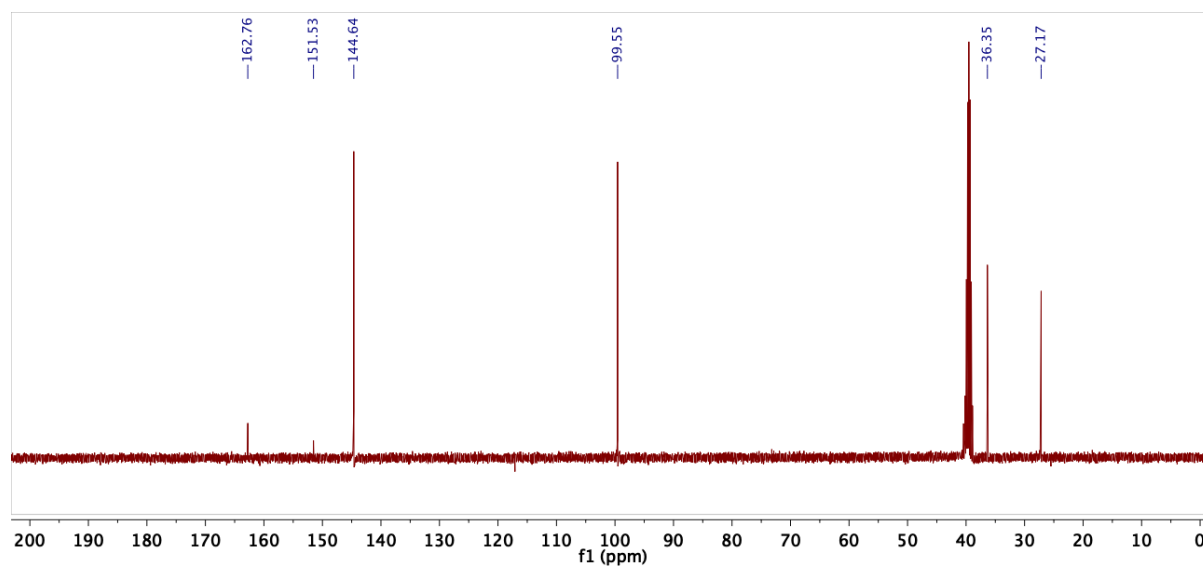
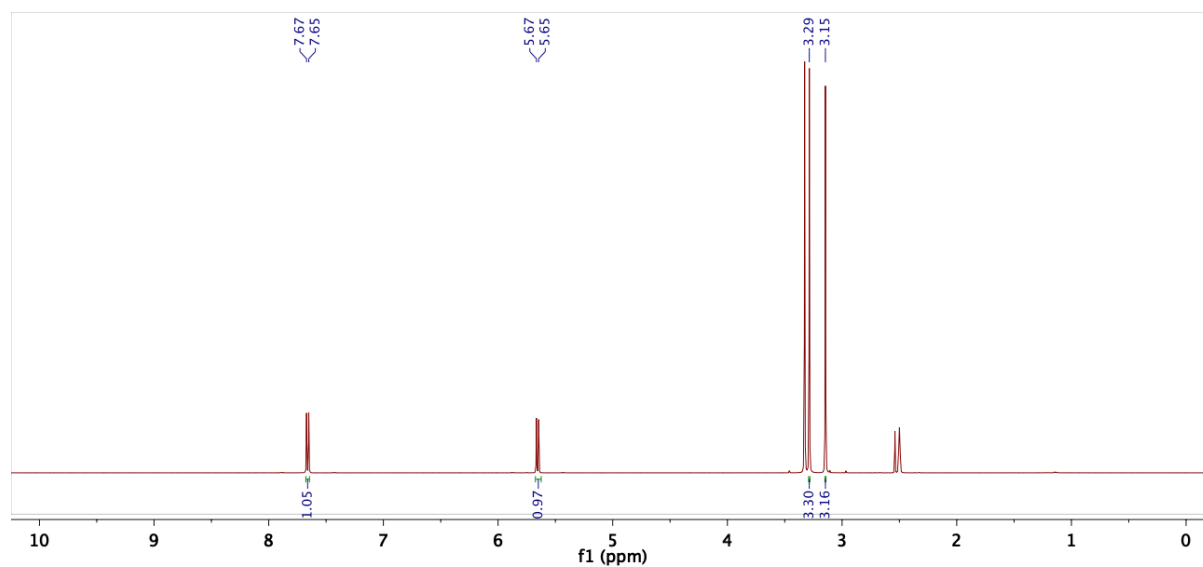
* Correspondence: uwille@unimelb.edu.au

Contents

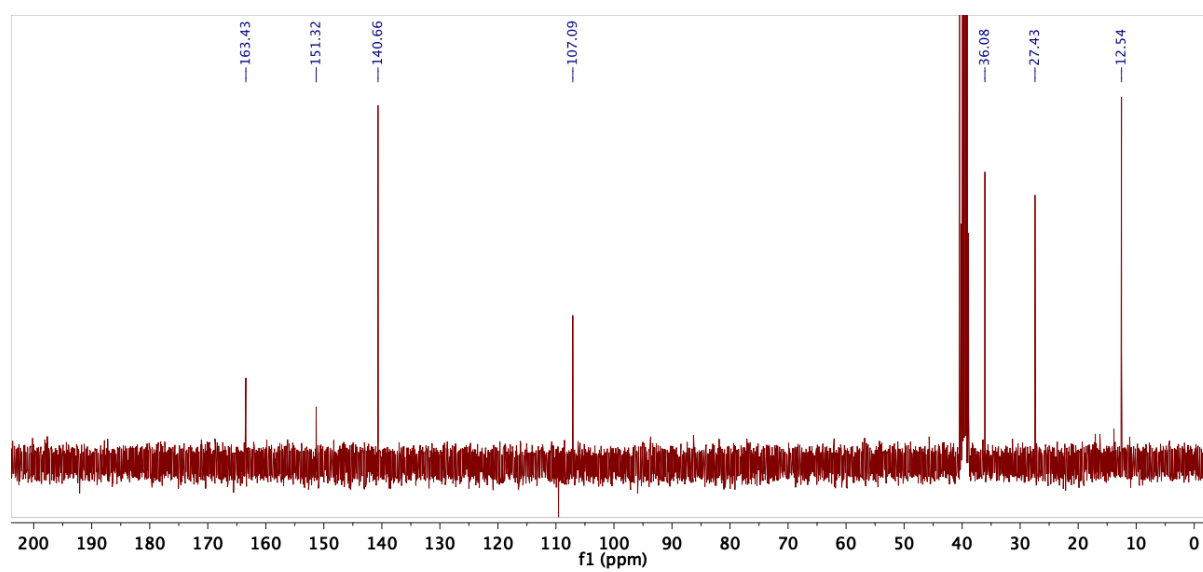
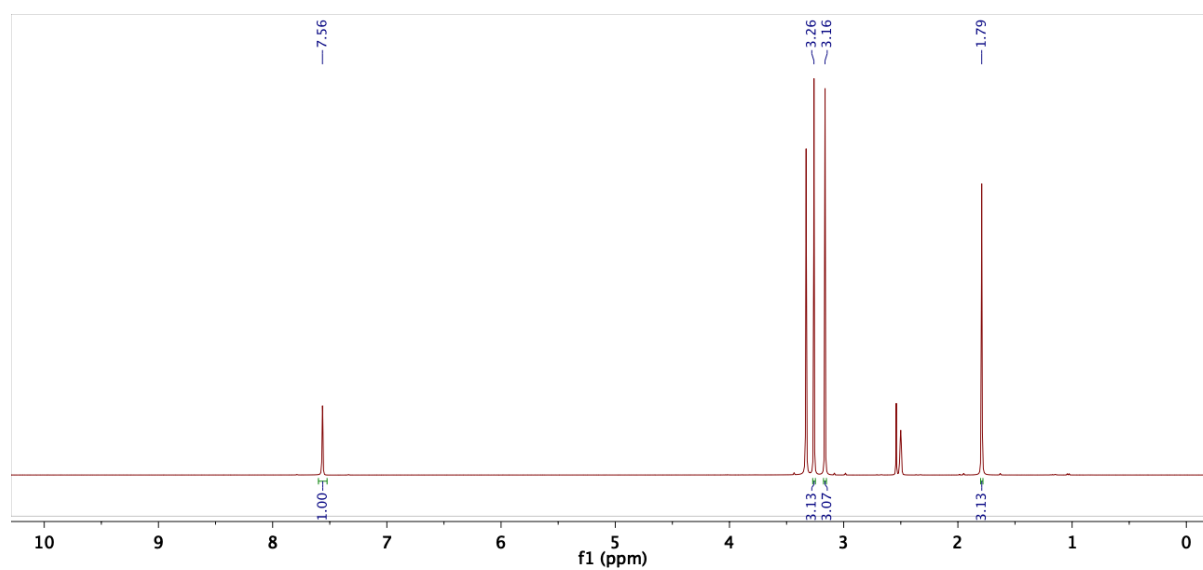
1. NMR spectra of substrates used in the laser flash photolysis study	2
2. Crystallographic Data	14
3. Laser flash photolysis studies	18
4. Gaussian Archive Entries for the DFT calculations.....	21

1. NMR spectra of substrates used in the laser flash photolysis study

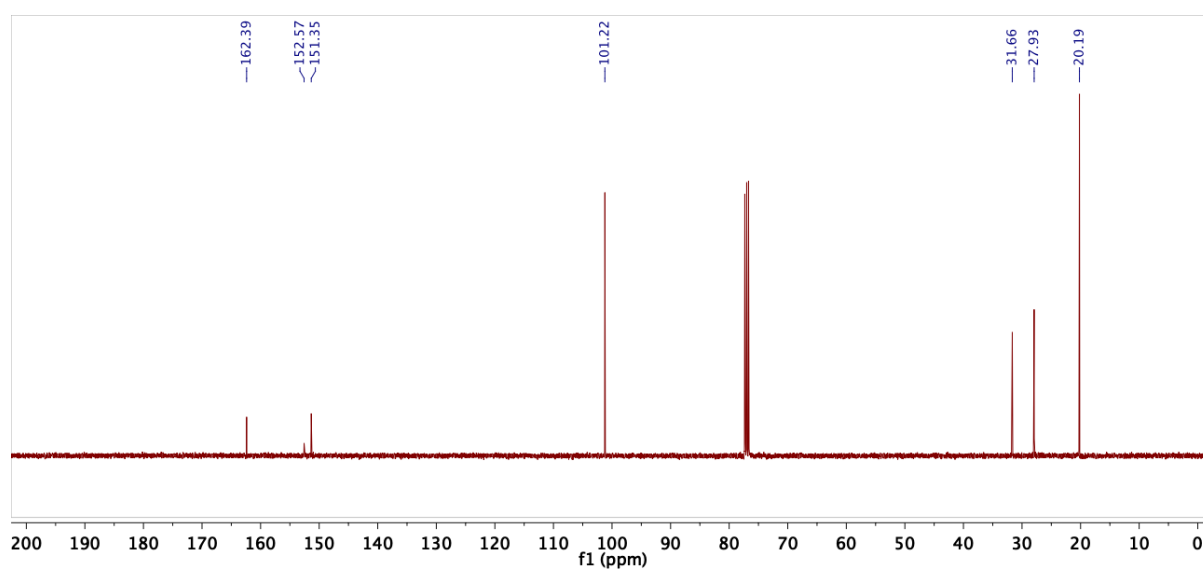
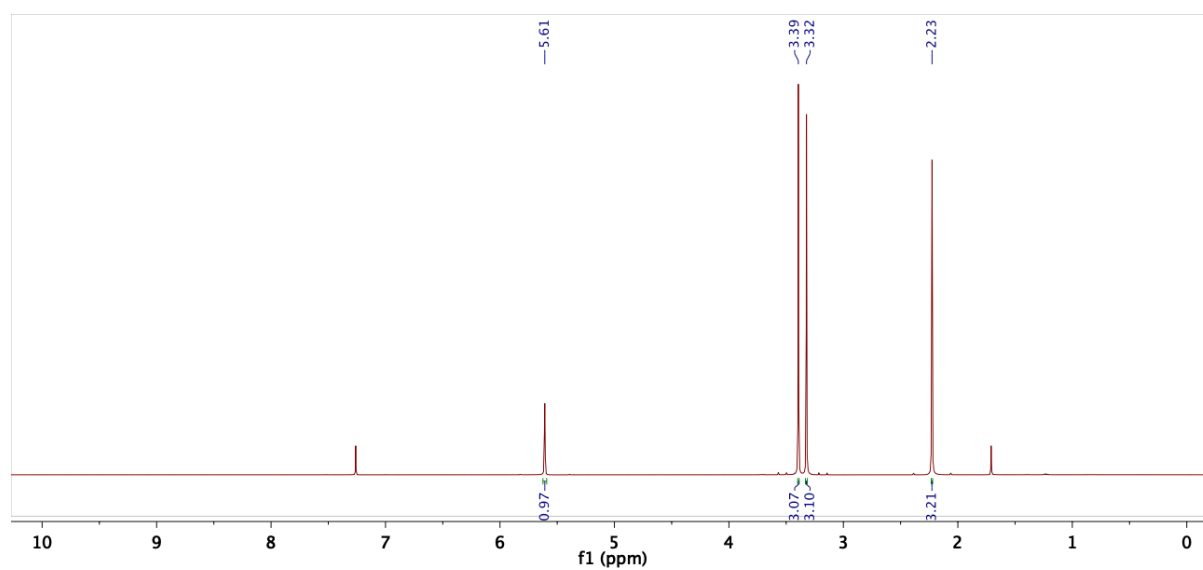
1.1. 1,3-Dimethyluracil (DMU)



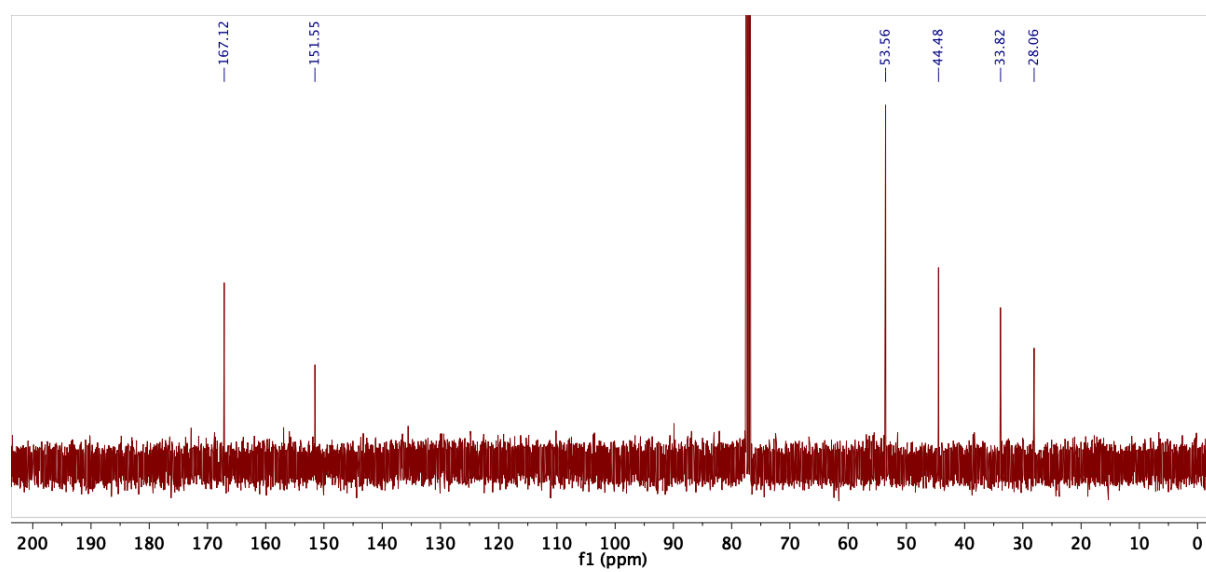
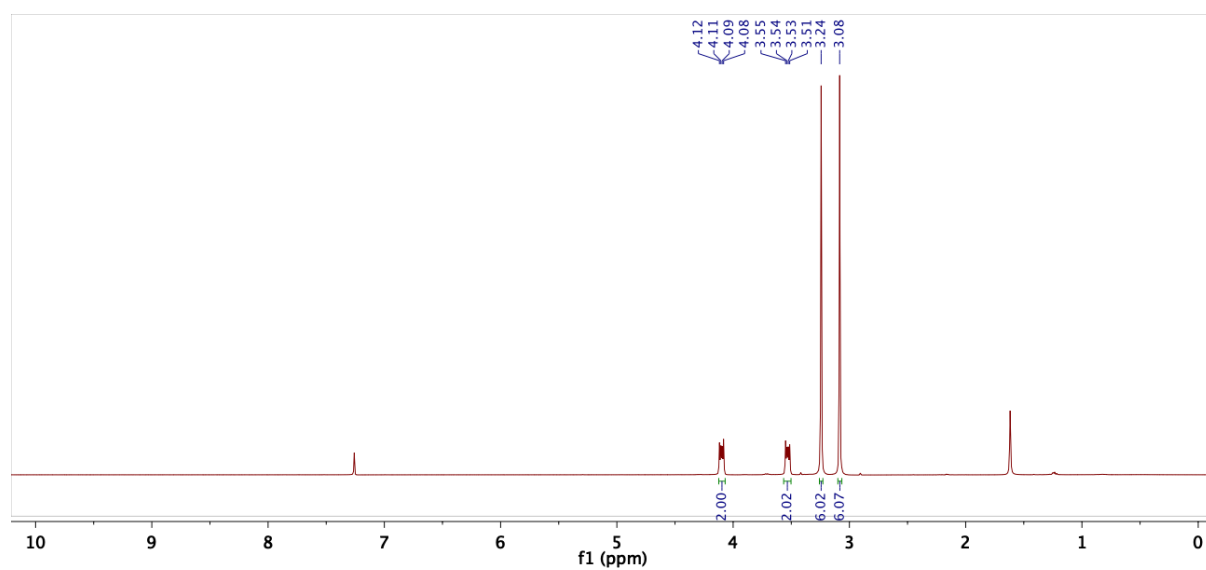
1.2. 1,3-Dimethylthymine (DMT)



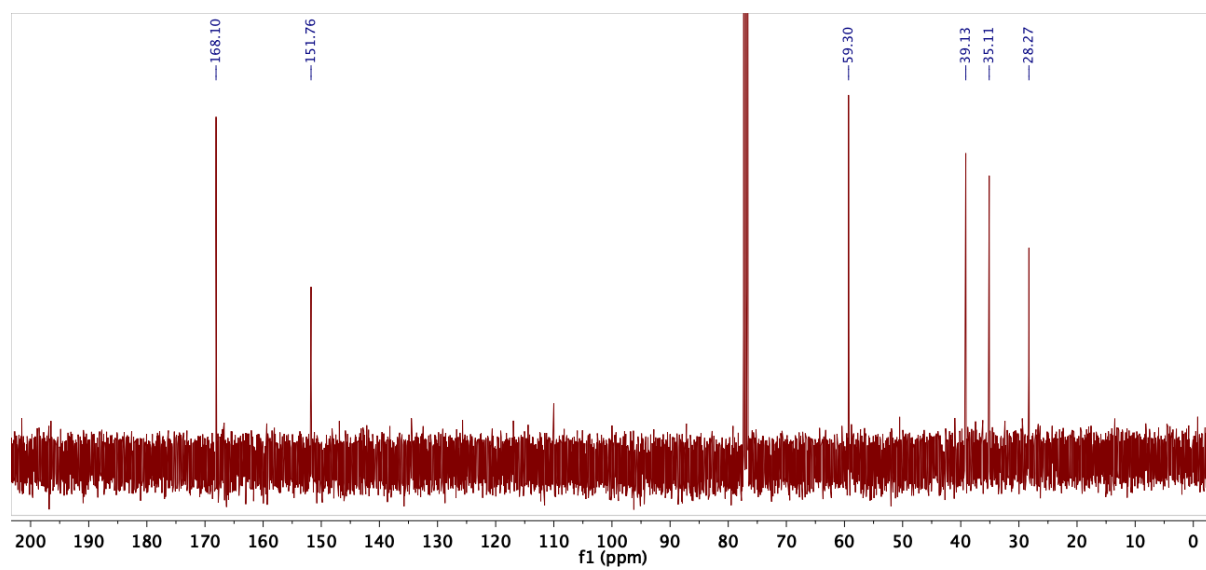
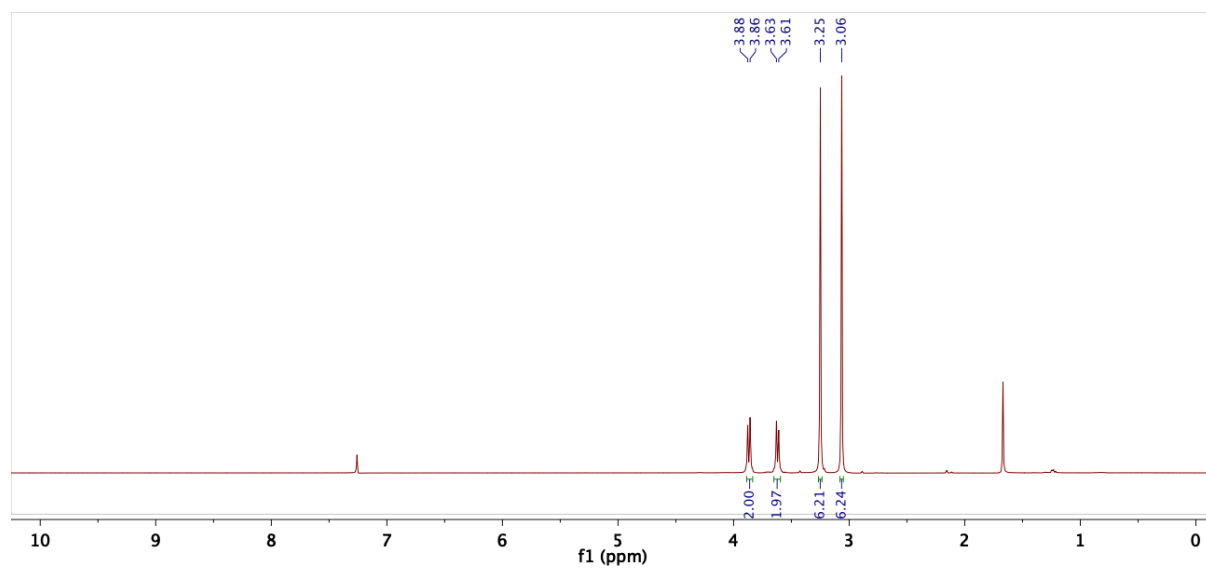
1.3. 1,3,6-Trimethyluracil (DMU^{6-Me})



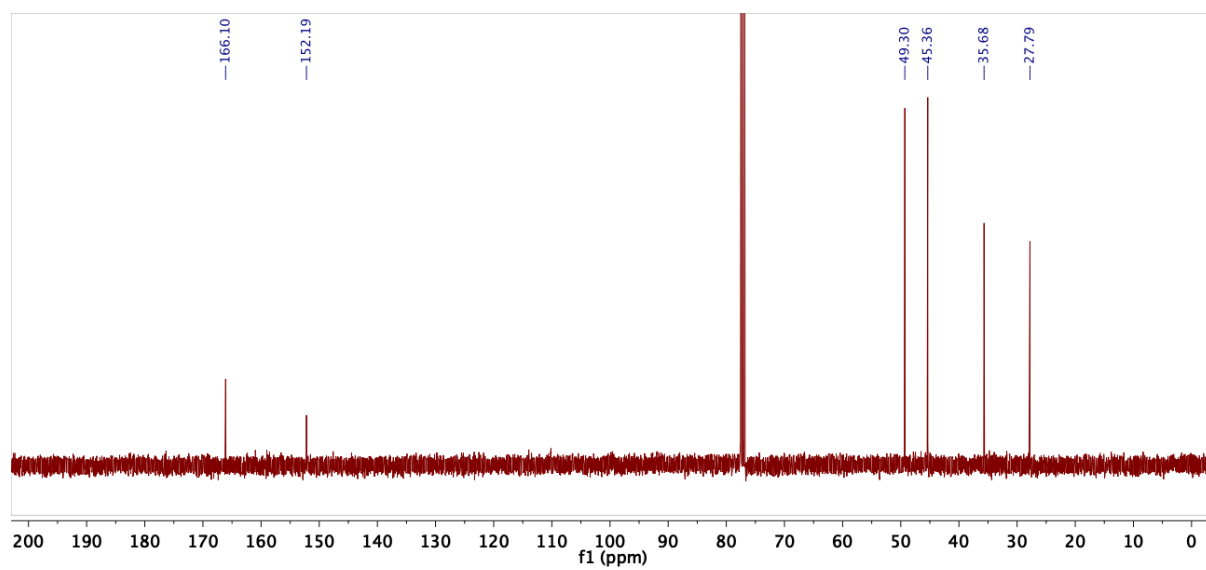
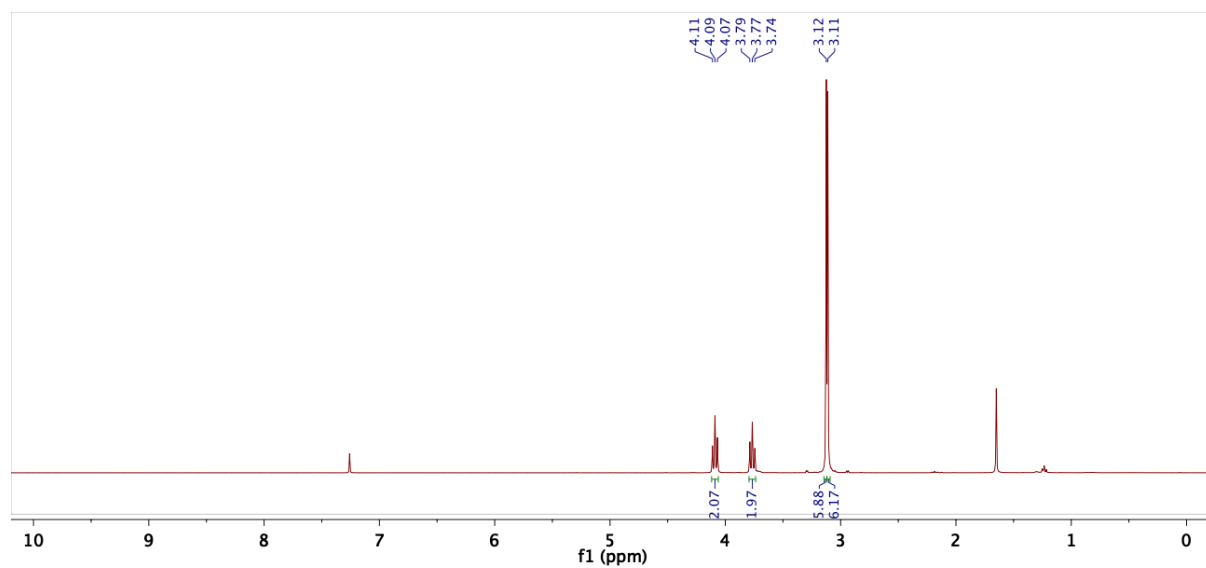
1.4. *trans,anti*-DMU cyclobutane dimer (*t,a*-DMU<>DMU)



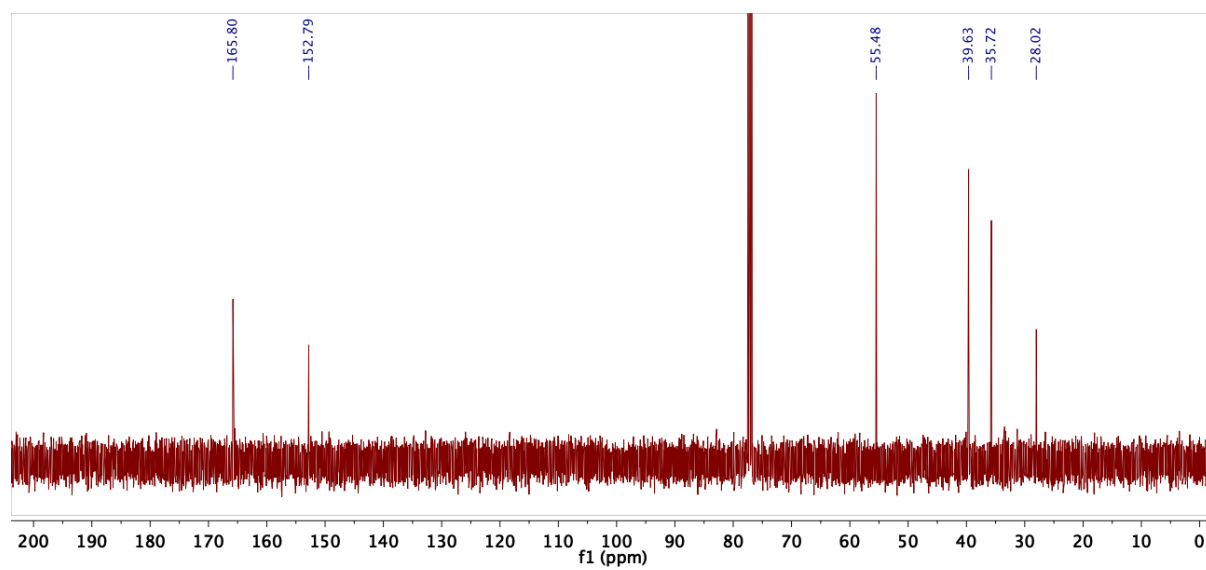
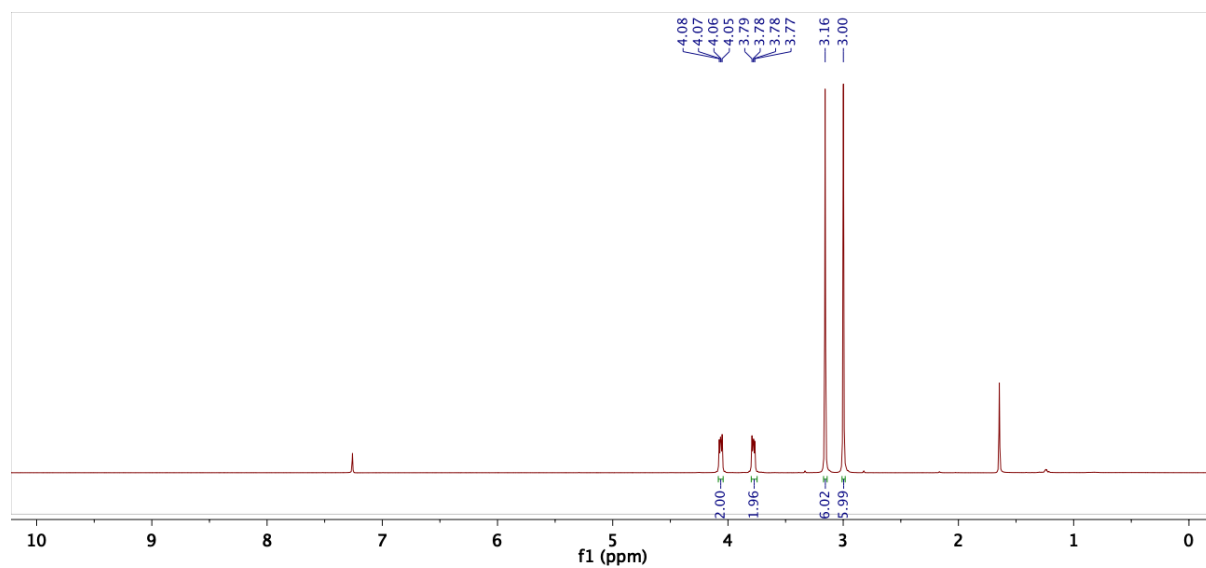
1.5. *trans,syn*-DMU cyclobutane dimer (*t,s*-DMU<>DMU)



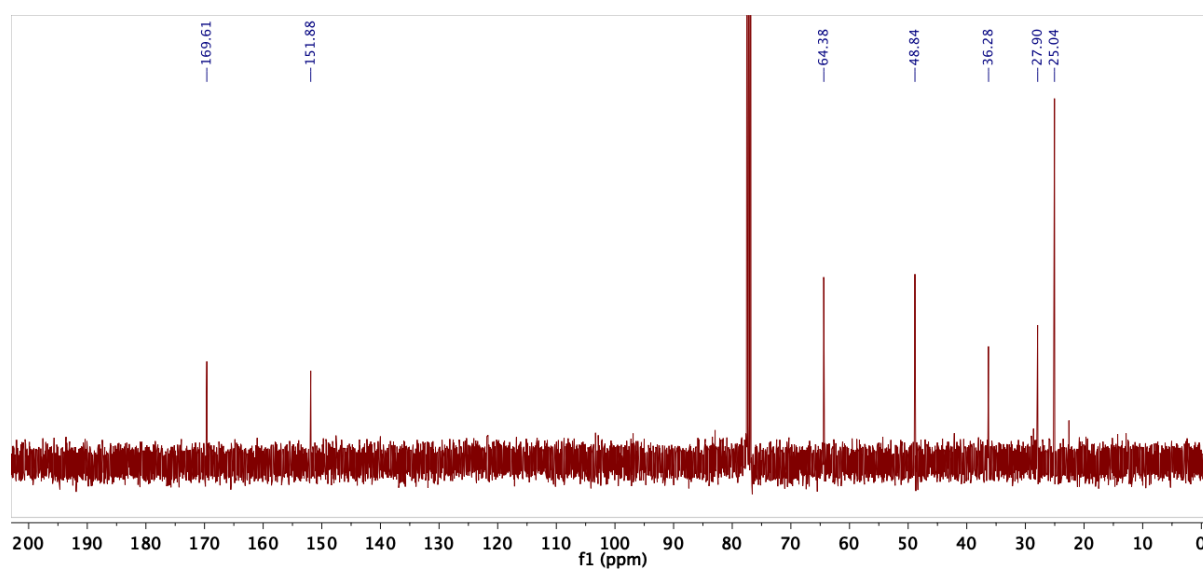
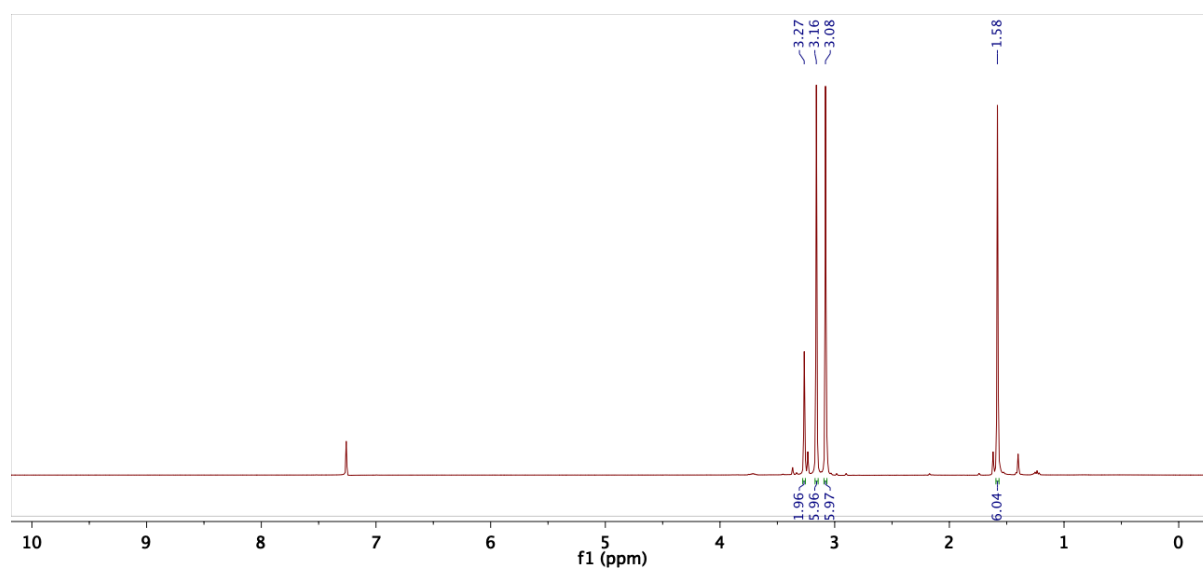
1.6. *cis,anti*-DMU cyclobutane dimer (*c,a*-DMU $\leftrightarrow$ DMU)



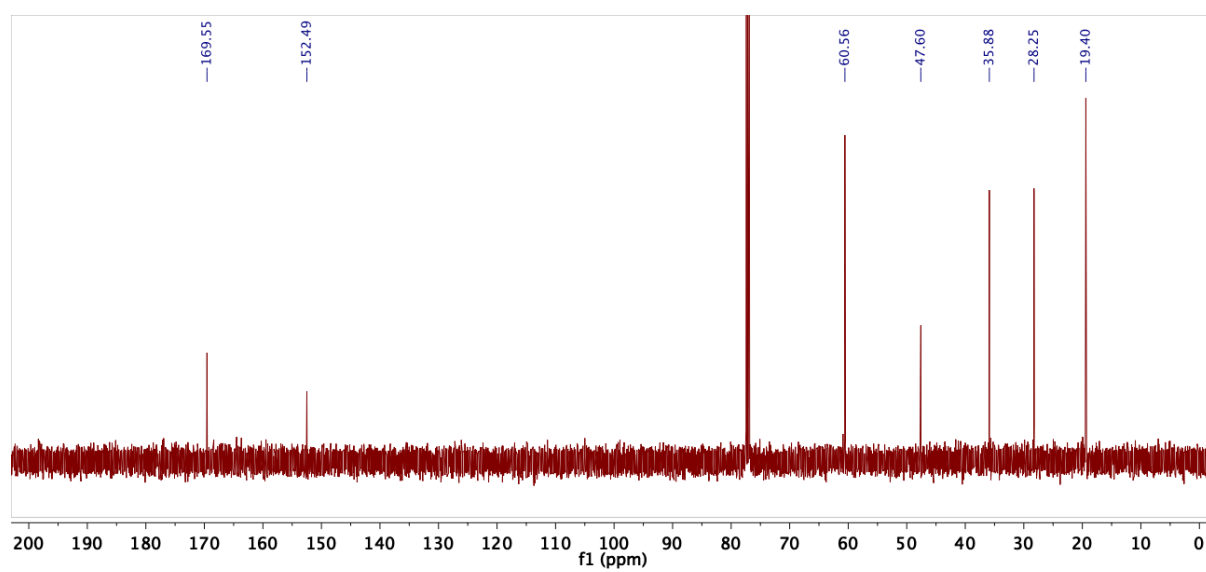
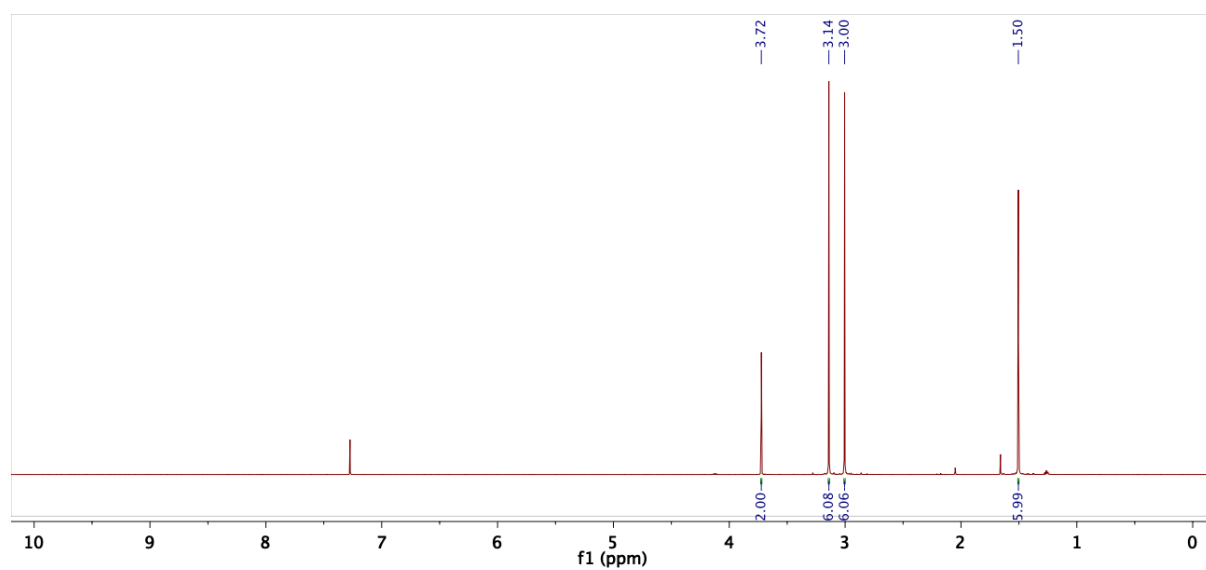
1.7. *cis,syn*-DMU cyclobutane dimer (*c,s*-DMU<>DMU)



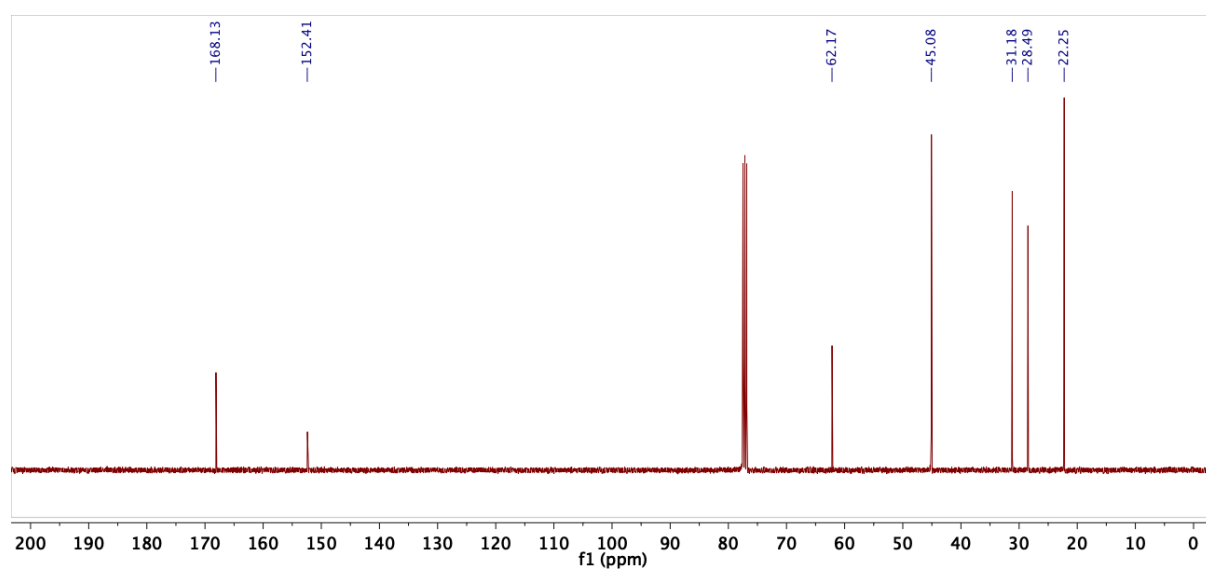
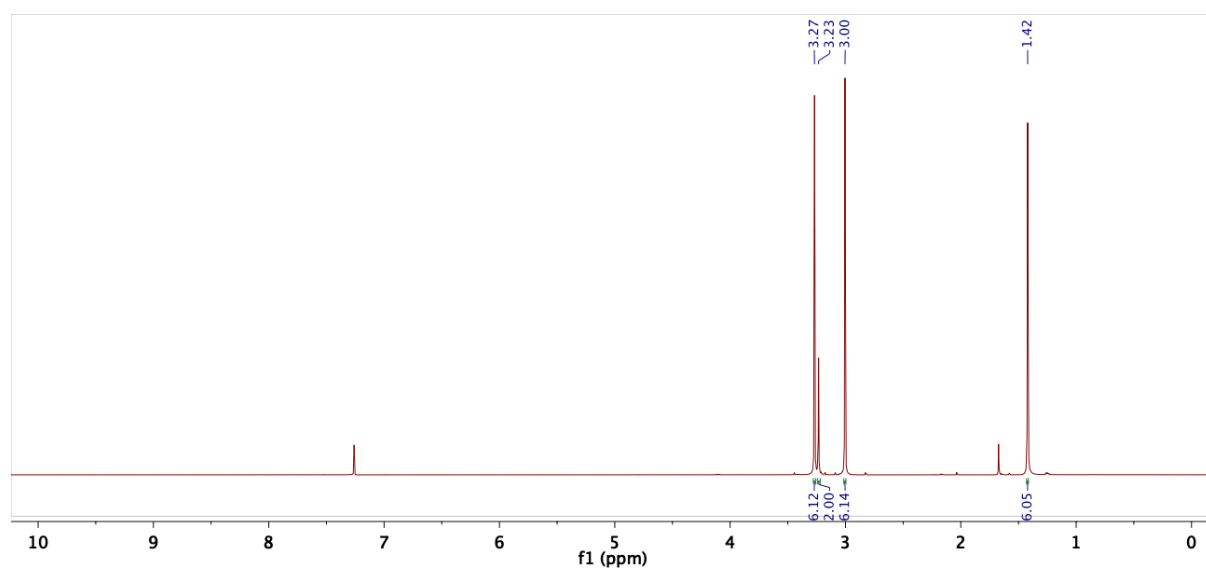
1.8. *cis,anti*-DMT cyclobutane dimer (*c,a*-DMT<>DMT)



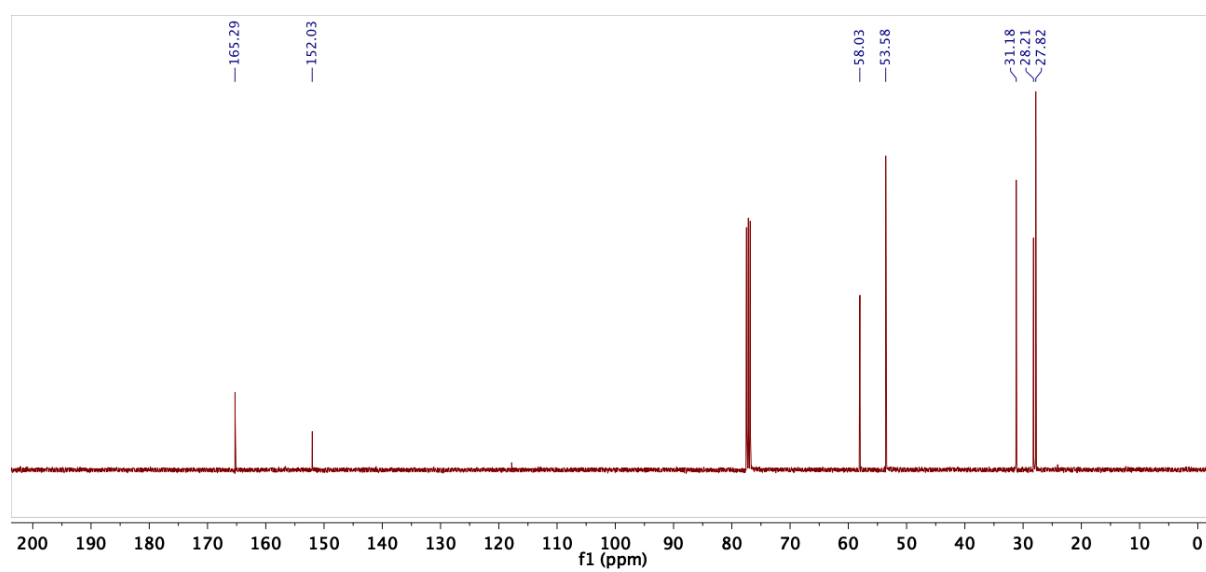
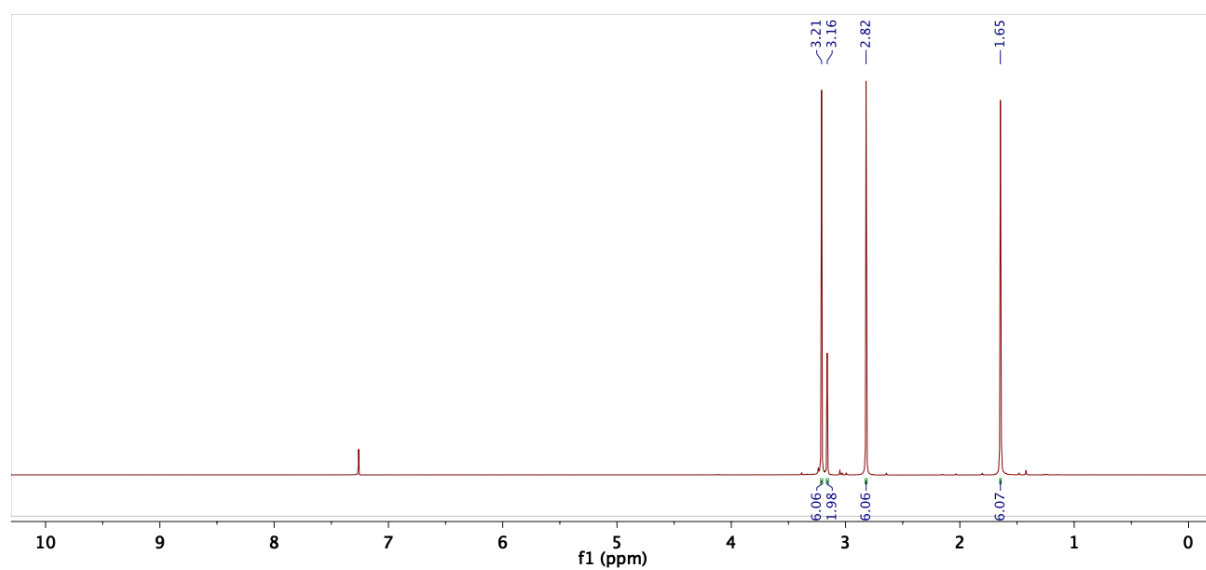
1.9. *cis,syn*-DMT cyclobutane dimer (*c,s*-DMT<>DMT)



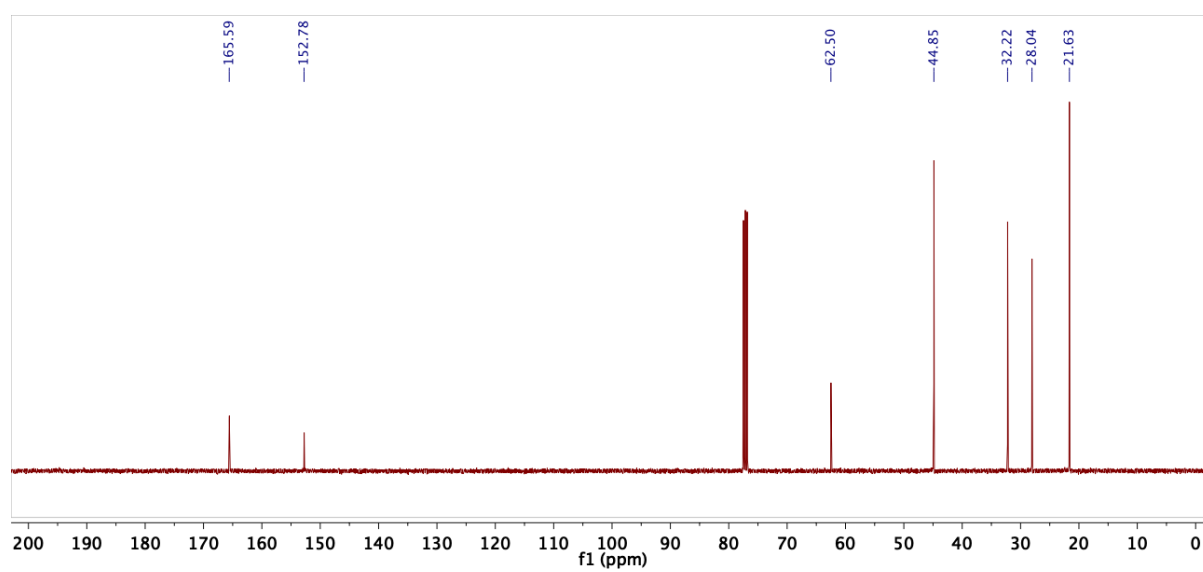
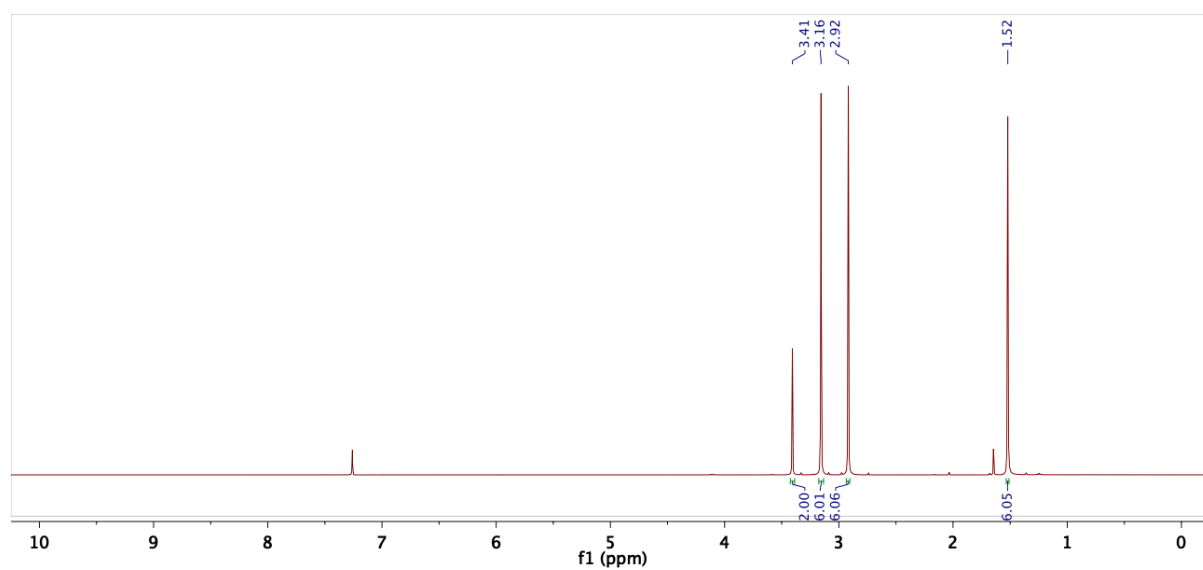
1.10. *trans,syn*-DMU^{6-Me} cyclobutane dimer (*t,s*-DMU^{6-Me}<>DMU^{6-Me})



1.11. *cis,anti*-DMU^{6-Me} cyclobutane dimer (*c,α*-DMU^{6-Me}<>DMU^{6-Me})

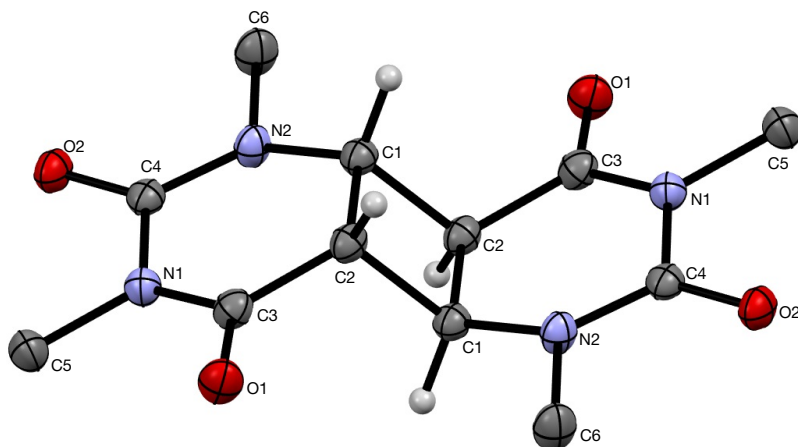


1.12. *cis,syn*-DMU^{6-Me} cyclobutane dimer (*c,s*-DMU^{6-Me}<>DMU^{6-Me})



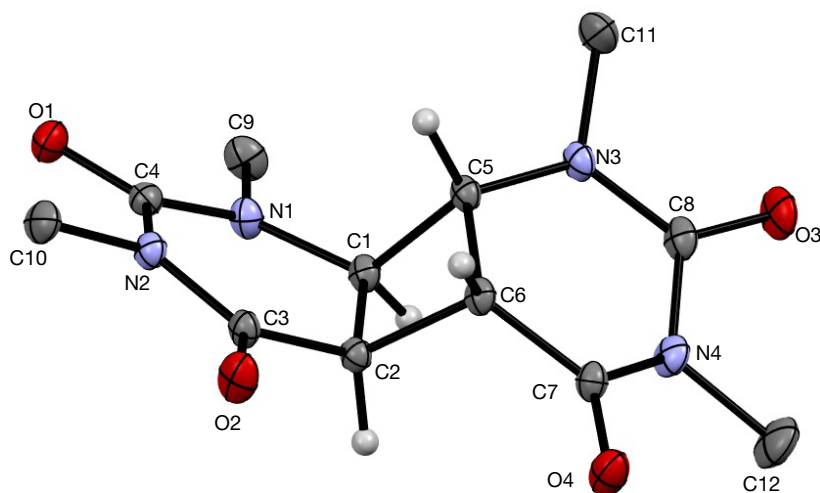
2. Crystallographic Data

t,a-DMU<>DMU



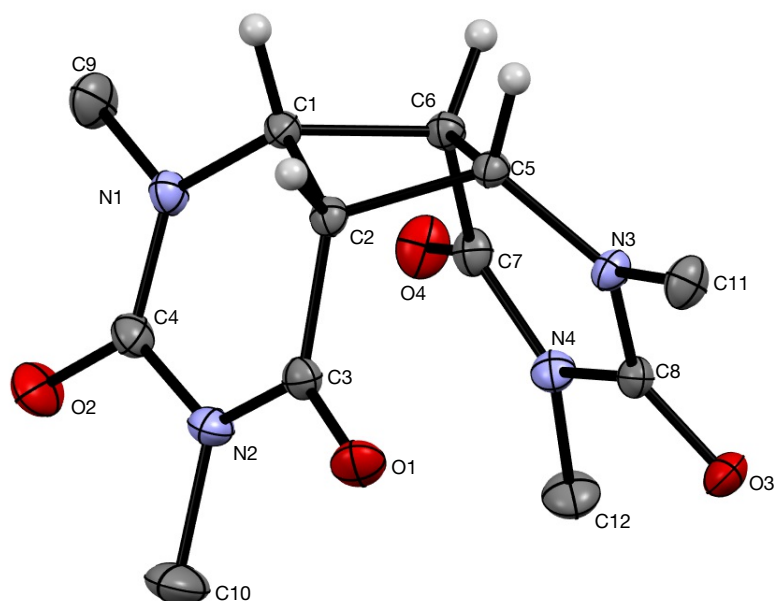
Crystal data. $C_{12}H_{16}N_4O_4$, $M = 280.29$, $T = 100.0$ K, $\lambda = 1.54184$ Å, Monoclinic, space group $P2_1/c$, $a = 8.3382(3)$, $b = 12.2526(3)$, $c = 6.5401(2)$ Å, $\beta = 110.724(3)^\circ$, $V = 624.93(4)$ Å³, $Z = 4$, $D_c = 1.490$ mg M⁻³, $\mu(\text{Cu-K}\alpha) 0.959$ mm⁻¹, $F(000) = 296$ crystal size $0.41 \times 0.30 \times 0.03$ mm³, 7094 reflections measured $\theta_{\text{max}} = 77.86^\circ$, 1307 independent reflections [$R(\text{int}) = 0.0457$], the final R was 0.0416 [$I > 2\sigma(I)$, 1203 data] and $wR(F^2)$ was 0.1132 (all data), GOF 1.120

t,s-DMU<>DMU



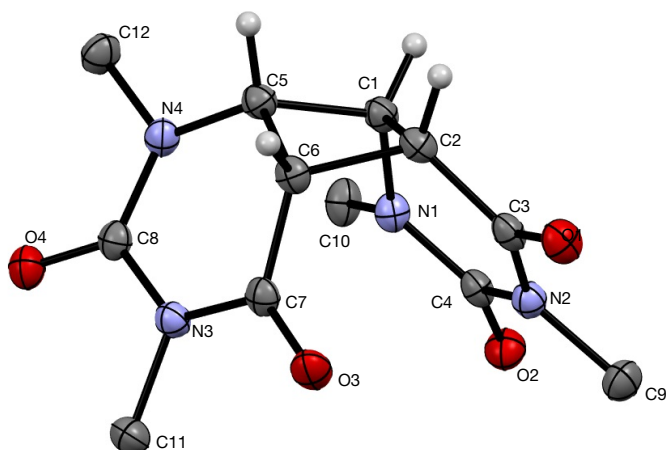
Crystal data. $C_{12}H_{16}N_4O_4$, $M = 280.29$, $T = 100.0$ K, $\lambda = 0.71073$ Å, Monoclinic, space group $I2/a$, $a = 18.4981(6)$, $b = 7.1521(2)$, $c = 20.1708(6)$ Å, $\beta = 109.501(4)^\circ$, $V = 2515.52(14)$ Å³, $Z = 8$, $D_c = 1.480$ mg M⁻³, $\mu(\text{Mo-K}\alpha) 0.113$ mm⁻¹, $F(000) = 1184$ crystal size $0.75 \times 0.57 \times 0.35$ mm³, 23109 reflections measured $\theta_{\text{max}} = 44.93^\circ$, 7955 independent reflections [$R(\text{int}) = 0.0242$], the final R was 0.0492 [$I > 2\sigma(I)$, 6242 data] and $wR(F^2)$ was 0.1542 (all data), GOF 1.045.

c,α-DMU<>DMU



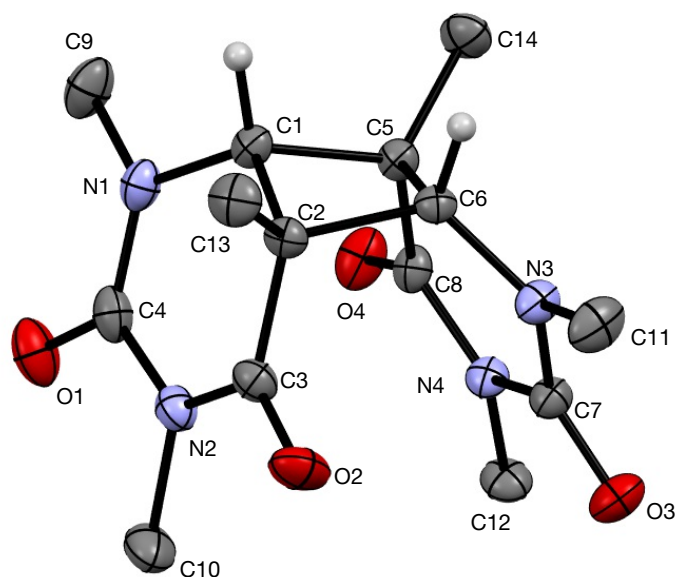
Crystal data. $C_{12}H_{16}N_4O_4$, $M = 308.34$, $T = 100.0$ K, $\lambda = 0.71073$ Å, Orthorhombic, space group $Pbca$, $a = 12.3523(4)$, $b = 13.8595(5)$, $c = 15.3599(55)$ Å, $V = 2629.56(15)$ Å³, $Z = 8$, $D_c = 1.416$ mg M⁻³ $\mu(Mo-K\alpha)$ 0.108 mm⁻¹, $F(000) = 1184$ crystal size $0.6 \times 0.4 \times 0.30$ mm³, 23200 reflections measured $\theta_{max} = 40.97^\circ$, 8238 independent reflections [$R(int) = 0.0359$], the final R was 0.0521 [$I > 2\sigma(I)$, 5785 data] and $wR(F^2)$ was 0.1500 (all data), GOF 1.036.

c,s-DMU<>DMU



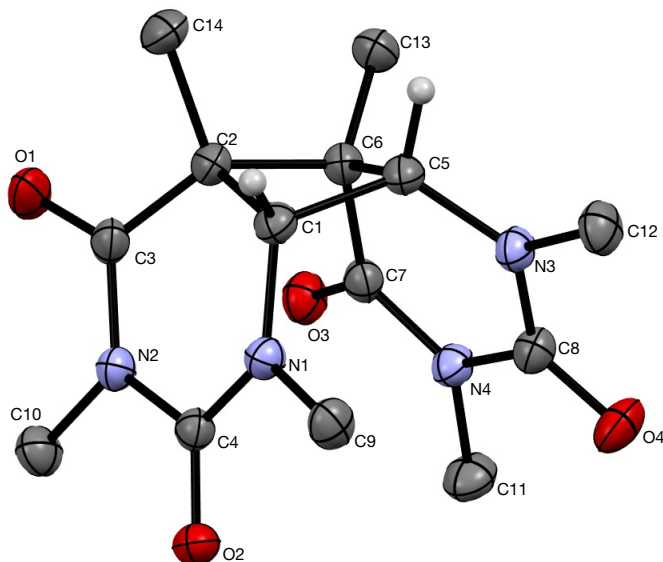
Crystal data. $C_{12}H_{16}N_4O_4$, $M = 280.29$, $T = 100.0$ K, $\lambda = 1.54184$ Å, Triclinic, space group $P-1$, $a = 10.2610(4)$ $b = 10.7301(3)$, $c = 11.3273(4)$ Å, $\alpha = 94.454(3)^\circ$, $\beta = 91.337(3)^\circ$, $\gamma = 92.297(3)^\circ$, $V = 1241.95(7)$ Å³, $Z = 4$ $Z' = 2$, $D_c = 1.499$ mg M⁻³ $\mu(Cu-K\alpha)$ 0.965 mm⁻¹, $F(000) = 592$ crystal size $0.36 \times 0.25 \times 0.03$ mm³, 14239 reflections measured $\theta_{max} = 78.10^\circ$, 5143 independent reflections [$R(int) = 0.0413$], the final R was 0.0409 [$I > 2\sigma(I)$, 4571 data] and $wR(F^2)$ was 0.1142 (all data), GOF 1.069.

***c,α*-DMT<>DMT**



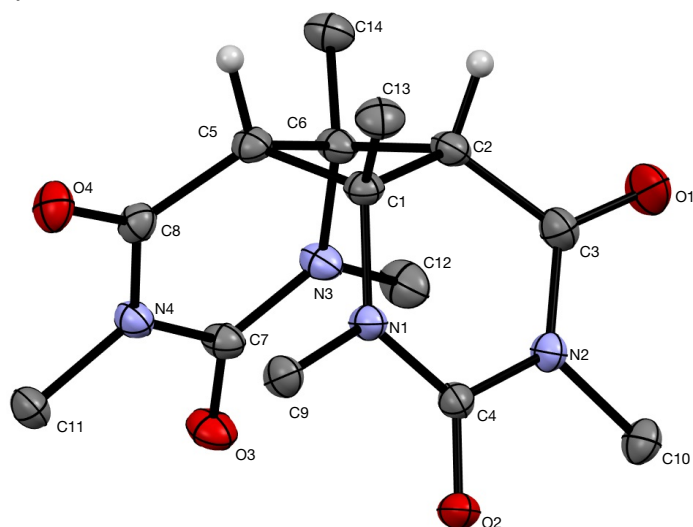
Crystal data. $C_{14}H_{20}N_4O_4$, $M = 308.34$, $T = 100.0$ K, $\lambda = 0.71073$ Å, Monoclinic, space group Cc , $a = 7.7634(2)$, $b = 15.0640(4)$, $c = 13.0966(5)$ Å, $\beta = 102.529(3)^\circ$, $V = 1495.15(8)$ Å³, $Z = 4$, $D_c = 1.370$ mg M^{-1} , $\mu(\text{Mo-K}\alpha) 0.102$ mm⁻¹, $F(000) = 656$ crystal size $0.62 \times 0.57 \times 0.30$ mm³, 12434 reflections measured $\theta_{\max} = 40.97^\circ$, 6416 independent reflections [$R(\text{int}) = 0.0264$], the final R was 0.0423 [$I > 2\sigma(I)$, 5486 data] and $wR(F^2)$ was 0.1104 (all data), GOF 0.974.

***c,s*-DMT<>DMT**



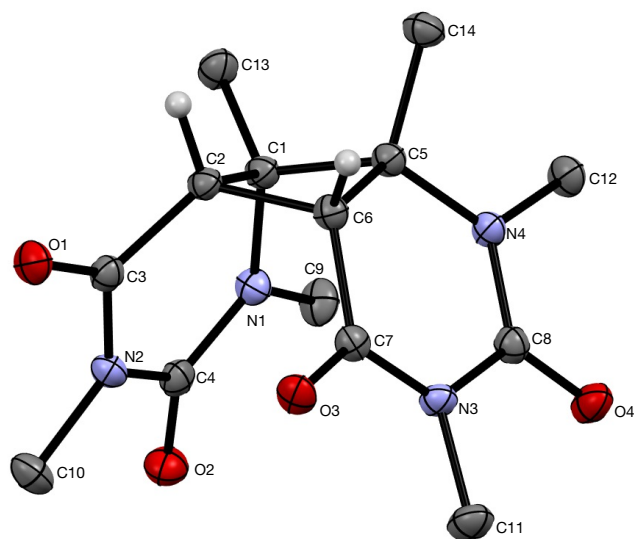
Crystal data. $C_{14}H_{20}N_4O_4$, $M = 308.34$, $T = 100.0$ K, $\lambda = 1.54184$ Å, Monoclinic, space group $P2_1/n$, $a = 8.1766(2)$, $b = 13.9470(3)$, $c = 12.9664(2)$ Å, $\beta = 99.158(2)^\circ$, $V = 1459.83(5)$ Å³, $Z = 4$, $D_c = 1.403$ mg M^{-1} , $\mu(\text{Cu-K}\alpha) 0.871$ mm⁻¹, $F(000) = 656$ crystal size $0.40 \times 0.27 \times 0.25$ mm³, 18485 reflections measured $\theta_{\max} = 77.51^\circ$, 3068 independent reflections [$R(\text{int}) = 0.0583$], the final R was 0.0460 [$I > 2\sigma(I)$, 2879 data] and $wR(F^2)$ was 0.1282 (all data), GOF 1.045.

***c*,*α*-DMU^{6-Me} <> DMU^{6-Me}**



Crystal data. $C_{14}H_{20}N_4O_4$, $M = 308.34$, $T = 100.0$ K, $\lambda = 1.54184$ Å, Monoclinic, space group $P2_1/n$, $a = 8.45200(10)$, $b = 13.9402(2)$, $c = 12.7899(2)$ Å, $\beta = 104.7110(10)^\circ$, $V = 1457.54(4)$ Å³, $Z = 4$, $D_c = 1.405$ mg M⁻³, $\mu(\text{Cu-K}\alpha) = 0.873$ mm⁻¹, $F(000) = 656$ crystal size $0.20 \times 0.19 \times 0.02$ mm³, 18548 reflections measured $\theta_{\text{max}} = 78.01^\circ$, 3069 independent reflections [$R(\text{int}) = 0.0544$], the final R was 0.0413 [$I > 2\sigma(I)$, 2811 data] and $wR(F^2)$ was 0.1183 (all data), GOF 1.085.

***c*,*s*-DMU^{6-Me} <> DMU^{6-Me}**



Crystal data. $C_{14}H_{20}N_4O_4$, $M = 308.34$, $T = 100.0$ K, $\lambda = 1.54184$ Å, Triclinic, space group $P-1$, $a = 7.0055(3)$, $b = 8.0358(3)$, $c = 13.0069(6)$ Å, $\alpha = 81.767(3)^\circ$, $\beta = 75.877(4)^\circ$, $\gamma = 83.973(3)^\circ$, $V = 700.90(5)$ Å³, $Z = 2$, $D_c = 1.461$ mg M⁻³, $\mu(\text{Cu-K}\alpha) = 0.907$ mm⁻¹, $F(000) = 328$ crystal size $0.39 \times 0.10 \times 0.06$ mm³, 7962 reflections measured $\theta_{\text{max}} = 77.63^\circ$, 2901 independent reflections [$R(\text{int}) = 0.0459$], the final R was 0.0521 [$I > 2\sigma(I)$, 2598 data] and $wR(F^2)$ was 0.1446 (all data), GOF 0.992.

3. Laser flash photolysis studies

Time-dependent decay plots of $\text{NO}_3^\bullet$ signals at 630 nm for its reaction with each compound are fitted according to the exponential decay fitting available on Igor Pro 6.03 (WaveMetrics, Inc.; Lake Oswego, OR, USA). The fitting used for the calculations follows the equation: $y = y_0 + Ae^{-invTau*x}$; where y is the optical density, OD (proportional to $[\text{NO}_3^\bullet]$) and x is the time (unit in ns). The value of k_{obs} corresponds to the value of $invTau$.

Second-order rate coefficients, k , for the reactions of $\text{NO}_3^\bullet$ with various substrates were obtained from the slopes of k_{obs} vs [substrate] plots. These plots are shown in Figure S1–8 below. The intercept is due to the reaction of $\text{NO}_3^\bullet$ with the solvent (see ref [26] in the manuscript).

Error determination: each result is reported as the average of three different runs. For example, if three different runs produced this set of data: $(x_1 \pm \sigma_1)$, $(x_2 \pm \sigma_2)$ and $(x_3 \pm \sigma_3)$, then the result would be taken as $\frac{x_1 + x_2 + x_3}{3}$ and σ is the overall standard deviation obtained following the statistical equation below:

$$\sigma = \sqrt{\frac{\sigma_1^2 + \sigma_2^2 + \sigma_3^2}{3} + \frac{2}{9}(x_1^2 + x_2^2 + x_3^2 - x_1 \cdot x_2 - x_2 \cdot x_3 - x_3 \cdot x_1)}, \text{ where}$$

x_1, x_2, x_3 are the result from each respective run and $\sigma_1, \sigma_2, \sigma_3$ are the standard deviation of each result. Overall errors are given as 2σ statistical uncertainties. Typical errors measured in these experiments are around 5–15%.

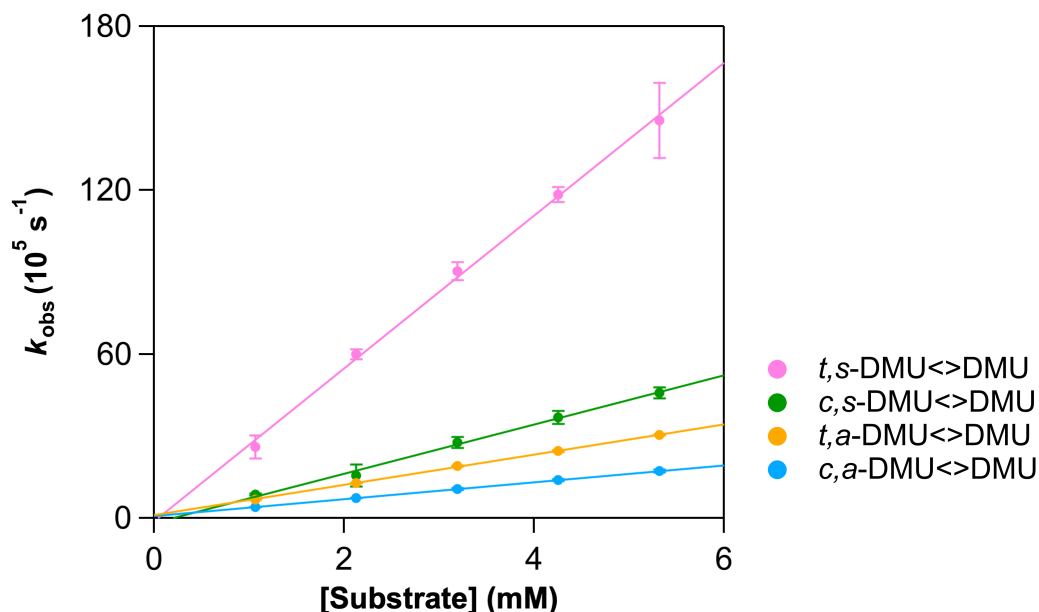


Figure S1. Plot of pseudo-first-order rate coefficient (k_{obs}) versus [DMU<->DMU] (see Table 2). Error bars shown are 2σ statistical uncertainties. From the linear regression analysis: t,s -DMU<->DMU: intercept = $-1.2 \times 10^5 \text{ s}^{-1}$, $k = 2.8 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$, $R^2 = 0.9979$; c,s -DMU<->DMU: intercept = $-1.8 \times 10^5 \text{ s}^{-1}$, $k = 9.0 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$, $R^2 = 0.9951$; t,a -DMU<->DMU: intercept = $1.1 \times 10^5 \text{ s}^{-1}$, $k = 5.5 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$, $R^2 = 0.9997$; c,a -DMU<->DMU: intercept = $6.8 \times 10^4 \text{ s}^{-1}$, $k = 3.1 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$, $R^2 = 0.9999$.

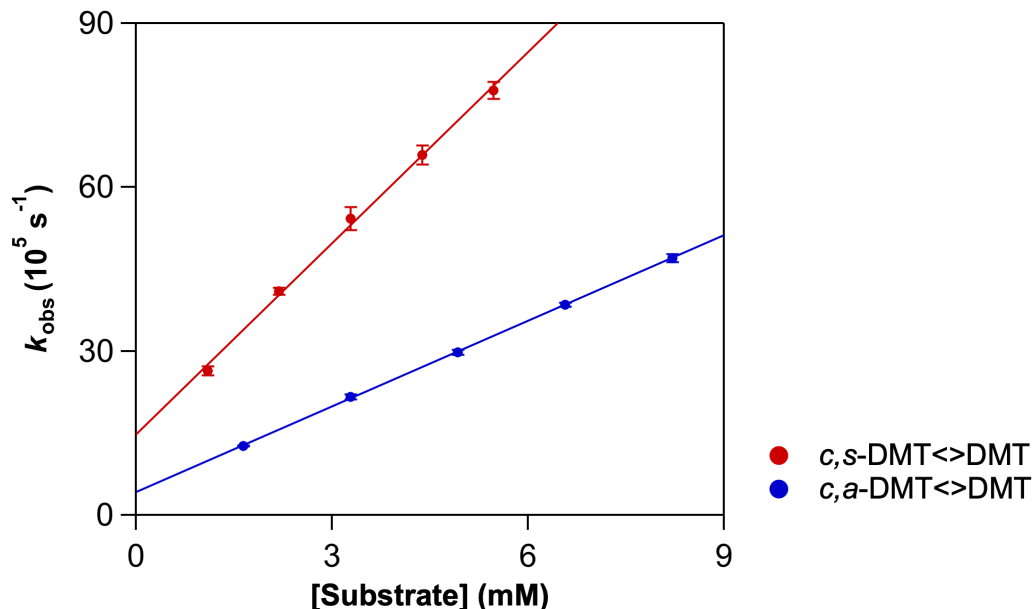


Figure S2. Plot of pseudo-first-order rate coefficient (k_{obs}) versus [DMT<->DMT] (see Table 2). Error bars shown are 2σ statistical uncertainties. From the linear regression analysis: c,s -DMT<->DMT: intercept = $1.5 \times 10^6 \text{ s}^{-1}$, $k = 1.2 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$, $R^2 = 0.9975$; c,a -DMT<->DMT: intercept = $4.2 \times 10^5 \text{ s}^{-1}$, $k = 5.2 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$, $R^2 = 0.9998$.

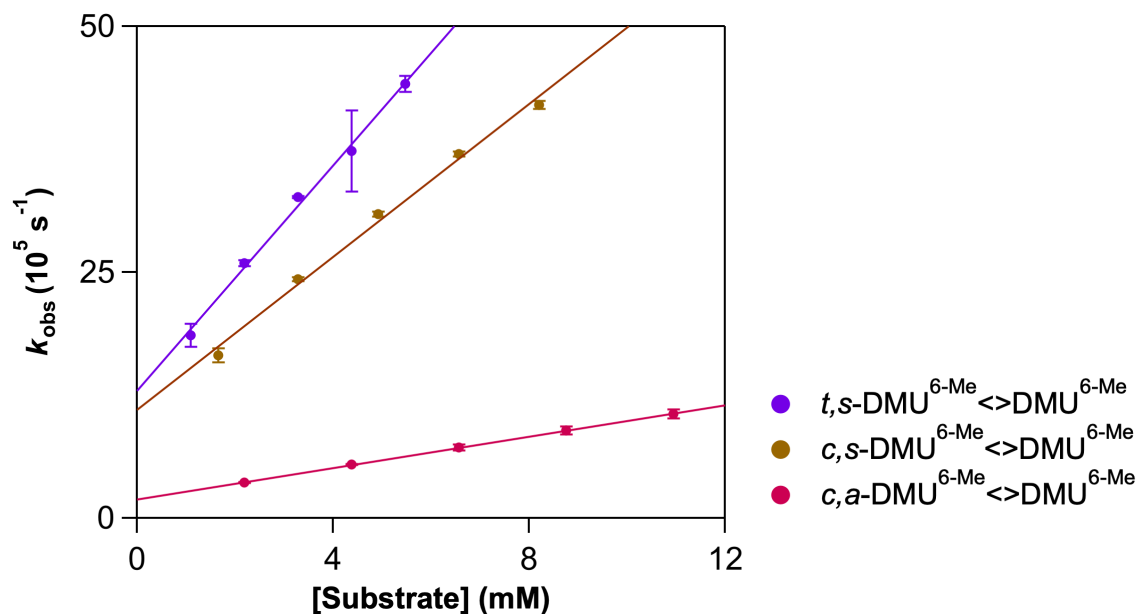


Figure S3. Plot of pseudo-first-order rate coefficient (k_{obs}) versus $[\text{DMU}^{6\text{-Me}} \leftrightarrow \text{DMU}^{6\text{-Me}}]$ (see Table 2). Error bars shown are 2σ statistical uncertainties. From the linear regression analysis: $t,s\text{-DMU}^{6\text{-Me}} \leftrightarrow \text{DMU}^{6\text{-Me}}$: intercept = $1.3 \times 10^6 \text{ s}^{-1}$, $k = 5.7 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$, $R^2 = 0.9951$; $c,s\text{-DMU}^{6\text{-Me}} \leftrightarrow \text{DMU}^{6\text{-Me}}$: intercept = $1.1 \times 10^6 \text{ s}^{-1}$, $k = 3.9 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$, $R^2 = 0.9934$; $c,a\text{-DMU}^{6\text{-Me}} \leftrightarrow \text{DMU}^{6\text{-Me}}$: intercept = $1.9 \times 10^5 \text{ s}^{-1}$, $k = 8.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$, $R^2 = 0.9996$.

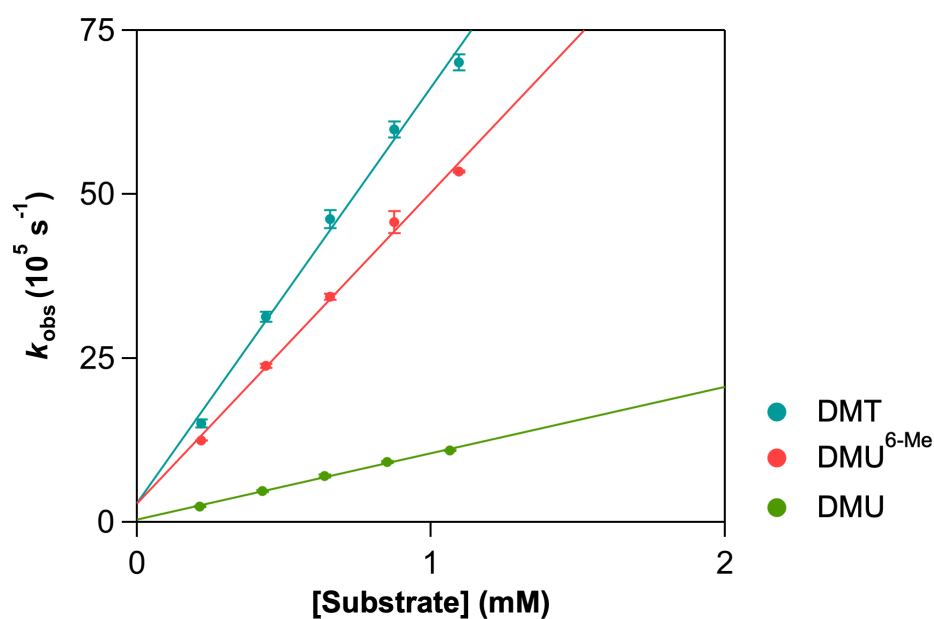


Figure S4. Plot of pseudo-first-order rate coefficient (k_{obs}) versus [pyrimidine] (see Table 2). Error bars shown are 2σ statistical uncertainties. From the linear regression analysis: DMT: intercept = $2.9 \times 10^5 \text{ s}^{-1}$, $k = 6.3 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$, $R^2 = 0.9932$; $\text{DMU}^{6\text{-Me}}$: intercept = $2.8 \times 10^5 \text{ s}^{-1}$, $k = 4.8 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$, $R^2 = 0.9960$; DMU: intercept = $4.5 \times 10^4 \text{ s}^{-1}$, $k = 1.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$, $R^2 = 0.9969$.

4. Gaussian Archive Entries for the DFT calculations

Performed using the Gaussian software package (see ref. [30] in the manuscript).

Scheme 3

c, α -DMU $\leftrightarrow$ DMU

```
1\1\GINC-SPARTAN-RC021\FOpt\RM062X\6-31+G(d)\C12H16N4O4\UWILLE\10-Oct-2018\0\#p M062X/6-31+G* scf=(qc,direct) nosymm scrf=(cpcm,solvent=acetonitrile) opt=(calcfc,maxcycle=500) freq=noraman\geom&freq\0,1\N,0.5924551445,-0.531099967,0.613546273\C,0.8238438367,-0.0108077247,1.8486850816\N,2.1627926582,0.3270236441,2.1667753272\C,3.2691948095,0.0182479522,1.4020896844\C,3.0409565644,-0.5553319923,0.0299151326\C,1.5803104727,-0.4643371363,-0.4252449771\C,3.3775235135,0.4672407211,-1.1156444729\C,1.905219482,0.8886797597,-1.1564236226\C,-0.8017070508,-0.7212766706,0.2244072796\O,-0.0611168104,0.1542215064,2.6769451692\C,2.4191414437,0.9526995985,3.4660545909\O,4.3993006605,0.2339377671,1.8123411669\H,3.53305229,-1.5284253158,-0.0279833035\H,3.6543421931,-0.0860566195,-2.0141402426\H,1.4426043586,1.0359667302,-2.1344808205\H,1.3528515791,-1.2256910378,-1.1727443745\H,-1.2754721127,0.2402073207,-0.001048279\H,-0.8238867663,-1.3559868859,-0.6624627563\H,-1.3426916602,-1.2112214117,1.0333347842\H,2.8224797363,0.2198956113,4.1697932089\H,1.482530781,1.3519967558,3.8452061138\H,3.1489158789,1.7520009166,3.3288186188\C,1.6114638295,2.0892792569,-0.2975976608\C,4.0393192653,2.6019529941,-0.1409948844\N,2.681082064,2.7951402594,0.2145088087\N,4.3289602553,1.5227008757,-0.9168422278\O,0.4617491759,2.4050962105,-0.032332528\O,4.8877312792,3.3978630963,0.2371995921\C,5.7391589428,1.2246134905,-1.1467033276\H,6.1815152325,0.7442493164,-0.2671373556\H,5.8115541851,0.5546236771,-2.0048910185\H,6.2742561282,2.1484917898,-1.3625812509\C,2.3637269905,3.9025813675,1.1187933135\H,3.2731931792,4.1935621442,1.6375427666\H,1.9678210021,4.7535834275,0.558161614\H,1.609091198,3.5631426024,1.8298366863\Version=AM64L-G09RevB.01\HF=-986.5313252\RMSD=0.000e+00\RMSF=5.094e-06\Dipole=0.0776866,-2.0615351,-2.5908068\Quadrupole=-7.3705267,0.1734364,7.1970902,-11.7785984,-10.7258104,1.4251307\PG=C01 [X(C12H16N4O4)]\@Sum of electronic and thermal Free Energies= -986.281771 Hartrees
```

NO₃[•]

```
1\1\GINC-R125\FOpt\UM062X\6-31+G(d)\N1O3(2)\ROOT\03-May-2016\0\# M062X/6-31+G* freq=noraman scf=(qc,direct) geom=checkpoint guess=check scrf=(cpcm,solvent=acetonitrile) nosymm opt=(z-matrix,readfc,maxcycle=500)\freq&geom\0,2\N,0.8689333182,3.3208672997,-0.5219369421\O,-0.4478434627,3.3964213064,-0.4486150722\O,1.3026841701,2.2112633696,-0.677978757\O,1.4389129813,4.3740110238,-0.4206602213\Version=ES64L-G09RevD.01\HF=-280.1036456\S2=0.75616\S2-1=0.\S2A=0.750029\RMSD=0.000e+00\RMSF=3.042e-05\Dipole=-0.3658701,0.0196907,0.0197095\Quadrupole=-0.9798125,-0.5823941,1.5622066,-2.3377363,0.4524744,-0.1929561\PG=C01 [X(N1O3)]\@Sum of electronic and thermal Free Energies= -280.116807 Hartrees
```

Reactant complex between NO₃[•] and c, α -DMU $\leftrightarrow$ DMU (no CT interactions)

```
1\1\GINC-SPARTAN-RC210\FOpt\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\23-O
```

ct-2018\0\#p M062X/6-31+G* scf=(qc,direct) nosymm scrf=(cpcm,solvent=acetonitrile) opt=(calcf, maxcycle=500) freq=noraman\geom&freq\0,2\N,0.7041407994,0.2860562581,1.3870956175\C,0.9894048069,1.0047062067,2.5058747002\N,2.3323536396,1.4219689104,2.6820122625\C,3.4023636787,1.0203504699,1.908576045\C,3.1149761293,0.2161353056,0.6692279497\C,1.6300099769,0.1976604074,0.2948591888\C,3.3561212822,1.0365319149,-0.6490865876\C,1.8709728814,1.4132832542,-0.6723364163\C,-0.7033407281,0.0012827302,1.1241328525\O,0.1470885979,1.2804608444,3.349219636\C,2.6411826418,2.2598031428,3.8428672644\O,4.5459820122,1.3329761814,2.2022922011\H,3.6325198879,-0.7422343399,0.7481454088\H,3.6011564921,0.3464600858,-1.4578090611\H,1.3500420518,1.3810123991,-1.6316300521\H,1.3832061762,-0.6840533929,-0.2985756874\H,-1.2259446924,0.9049732715,0.792992722\H,-0.7572006939,-0.7584250161,0.3429050638\H,-1.1743998394,-0.3781691911,2.0305349819\H,3.1263362364,1.666666361,4.6224544064\H,1.7120770621,2.6777106918,4.220476825\H,3.3191522917,3.0548907878,3.5288434298\C,1.5874737888,2.7355335841,-0.012876756\C,4.0029031649,3.3202691812,-0.0877987053\N,2.6598963931,3.5431409236,0.3066690931\N,4.2839194009,2.1304785555,-0.6840842218\O,0.4443542878,3.0668113618,0.2614912297\O,4.8461195527,4.1866128121,0.0988612093\C,2.354705453,4.7888837217,1.0139122555\H,3.2814980473,5.1930857087,1.4115839801\H,1.8961024774,5.5115783295,0.3338240251\H,1.6557582884,4.5681615721,1.8219973656\O,3.5070659787,-2.2310210074,-1.3717549044\O,1.6110151662,-2.5963434292,-2.3813309697\O,3.1424646512,-3.8661979056,-2.7634153478\N,2.8026554341,-2.8457480924,-2.1132399881\C,5.6903181562,1.821507219,-0.9238733457\H,5.7419397136,1.0012048901,-1.6416546266\H,6.1894735883,2.6970291674,-1.3373342461\H,6.1837861669,1.5248916447,0.008340842\Version=AM64L-G09RevB.01\HF=-1266.6374156\S2=0.760929\S2-1=0.\S2A=0.750071\RMSD=0.000e+00\RM SF=5.205e-06\Dipole=-0.0042955,-2.5823465,-2.2693671\Quadrupole=-4.6462711,-1.3123376,5.9586087,-14.4753153,-8.9385068,-3.15848\PG=C01 [X(C12H16N5O7)]\@

Sum of electronic and thermal Free Energies= -1266.388891 Hartrees

CT complex between NO₃^{*} and c,α-DMU<>DMU

1\1\GINC-SPARTAN-RC183\FOpt\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\28-O
ct-2018\0\#p M062X/6-31+G* scf=(qc,direct) nosymm scrf=(cpcm,solvent=acetonitrile) opt=(calcf, maxcycle=500) freq=noraman\geom&freq\0,2\N,0.84483777,0.3570499846,0.6765805848\C,1.141312553,0.8826946495,1.9644096508\N,2.4614370418,1.2294567449,2.1972156821\C,3.5392856142,0.958580913,1.3478023155\C,3.2492776225,0.4644405837,-0.0410592972\C,1.7677331143,0.5131191879,-0.4146151931\C,3.472253959,1.5772326772,-1.1334627016\C,1.9828699148,1.9279605231,-1.0577662684\C,-0.558140588,0.1094103741,0.3814007122\O,0.265312367,0.9942634043,2.7881000997\C,2.7820092514,1.8067487184,3.5094422072\O,4.67525251,1.170899196,1.7178434694\H,3.7718919803,-0.481455905,-0.1962175977\H,3.7152680936,1.0930087215,-2.0801923051\H,1.4487610411,2.1099445795,-1.9922860819\H,1.5086107811,-0.2187936472,-1.1784391926\H,-1.0498387738,1.0752548527,0.2144251991\H,-0.6100850726,-0.505989191,-0.5148070579\H,-1.0183708668,-0.3941368526,1.2301039668\H,3.1722214936,1.0322859044,4.1736939172\H,1.8737347104,2.2327791067,3.9277076671\H,3.5381002785,2.5784950548,3.3688297749\C,1.6862512907,3.054998579,-0.0996176414\C,4.0847072112,3.711417143,-0.1117753088\N,2.7371980141,3.8290290351,0.3274387522\N,4.3848820144,2.6592

060273,-0.9192932928\O,0.547108901,3.2429769363,0.3004298791\O,4.91025
36151,4.5413282523,0.2349741683\C,2.414289765,4.9123249764,1.262323716
7\H,3.3436438488,5.3006695724,1.6686394624\H,1.87250434,5.7063603112,0
.7429848386\H,1.7842572567,4.5137845286,2.0584977095\O,1.6232042018,-1
.5733229028,1.5199935583\O,1.0801671668,-2.4242840406,-0.4042945043\O,
1.7792948947,-3.6883045692,1.207652567\N,1.4855250892,-2.597767512,0.7
403039016\C,5.7911286831,2.4441000859,-1.2527834353\H,5.8388399773,1.8
268805415,-2.1510890332\H,6.2659390342,3.4047139206,-1.4466964487\H,6.
3103193806,1.9387890744,-0.4317117406\\Version=AM64L-G09RevB.01\HF=-12
66.6566234\S2=0.758654\S2-1=0.\S2A=0.750055\RMSD=0.000e+00\RMSF=4.476e
-06\Dipole=-0.080398,1.9417678,-2.4383985\Quadrupole=2.3795697,-15.426
3199,13.0467502,1.3078399,-12.2127895,1.6073906\PG=C01 [X(C12H16N5O7)]\\@
Sum of electronic and thermal Free Energies= -1266.399329 Hartrees

TS1

1\1\GINC-SPARTAN-RC122\FTS\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\27-Mar-2019\0\#p M062X/6-31+G* scf=verytight freq=noraman nosymm geom=chec
kpoint guess=check scrf=(cpcm,solvent=acetonitrile) opt=(ts,noeigentes
t,readfc,maxcycle=500)\geom&freq\0,2\N,0.9024991452,0.9626914433,0.8
715820506\C,1.1120327003,0.994257509,2.2773742326\N,2.4104384153,1.199
9299461,2.7046799828\C,3.5340981146,1.2446355171,1.8711404994\C,3.3455
302214,0.620934381,0.5189864698\C,1.9289921743,0.6959482757,-0.0195048
037\C,3.8134845729,1.4176435781,-0.7498671979\C,2.35545433,1.761676140
4,-1.1022750306\C,-0.4757051902,1.0026772971,0.4074836588\O,0.16590070
54,0.9409694403,3.0264885066\C,2.5665250707,1.4852445663,4.1364133164\O,
4.5968723948,1.6763570649,2.2592505797\H,3.7473972052,-0.396193139,0
.5855687129\H,4.2421255174,0.7269129888,-1.475532992\H,2.0181940508,1.
5828401243,-2.1227363692\H,1.6445862623,-0.3212846165,-0.5337999277\H,
-0.9935494293,1.8451065973,0.8677937728\H,-0.4696313757,1.0974907583,-
0.6767008359\H,-0.9635240931,0.0689659255,0.7127944251\H,3.6303991073,
1.4940723155,4.3588609865\H,2.0612236787,0.7061891927,4.7064265949\H,2
.1258502528,2.4566443109,4.3710884627\C,1.9242150308,3.1341174982,-0.6
374241801\C,4.2604336579,3.7031071656,-0.0454661358\N,2.8546832887,3.8
790501632,0.0558349981\N,4.6912272931,2.5424537369,-0.6090890553\O,0.7
777486709,3.5148215731,-0.7918773484\O,5.0115440809,4.5824431673,0.342
7136983\C,2.389412078,5.1361263706,0.6507759468\H,3.0993064134,5.43402
77603,1.4181914222\H,2.3181405148,5.9187893062,-0.109350484\H,1.406785
4988,4.9625516898,1.0864026677\O,1.3762593309,-1.7300089207,1.40345123
04\O,1.3234968737,-1.8419890972,-0.7660360013\O,0.9685176428,-3.607573
4085,0.4130007142\N,1.2197026353,-2.4104209666,0.3793410718\C,6.129455
0229,2.2851219863,-0.5997113103\H,6.4551403292,1.9482114315,0.38986086
78\H,6.3433011919,1.5142409221,-1.3414477532\H,6.6577026153,3.19957000
48,-0.8659204433\\Version=AM64L-G09RevB.01\HF=-1266.6447554\S2=0.75679
\S2-1=0.\S2A=0.750036\RMSD=2.254e-09\RMSF=6.011e-06\Dipole=0.7645193,2
.2425924,-0.894789\Quadrupole=9.7724469,-20.3283394,10.5558926,-5.4021
865,-7.4114326,2.5848514\PG=C01 [X(C12H16N5O7)]\\@
Vimag = -147.6194 cm⁻¹
Sum of electronic and thermal Free Energies= -1266.392612 Hartrees

Product complex between HNO₃ and c,α-DMU<>DMU radical 1

1\1\GINC-SPARTAN-RC176\FOpt\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\22-N

```

ov-2018\0\#p M062X/6-31+G* scf=(qc,direct) nosymm scrf=(cpcm,solvent=
acetonitrile) opt=(calcf, maxcycle=500) freq=noraman\geom&freq\0,2\N
,0.8908211456,0.8114236794,0.8495188383\C,1.0820129775,0.8532733732,2.
2201108556\N,2.3661405113,1.1862712832,2.6832718175\C,3.4721467563,1.4
084178092,1.8747925606\C,3.3614740092,0.8174755337,0.4918699844\C,1.95
36623658,0.7934571152,-0.0220103371\C,3.7288505286,1.6899579214,-0.759
8954462\C,2.2327940802,1.8193066692,-1.1304533948\C,-0.4870998574,0.68
84255601,0.3659979019\O,0.1584312837,0.684993381,2.9957944647\C,2.4765
077513,1.4647754811,4.1182856593\O,4.4768431344,1.9587103722,2.2828031
027\H,3.8843653029,-0.1470313319,0.5319388962\H,4.272354707,1.08960471
71,-1.4893150693\H,1.945396719,1.5727400212,-2.1539664402\H,1.73187114
05,-1.1771049336,-0.5510120567\H,-1.1010215287,1.4858170847,0.78577365
11\H,-0.466453487,0.7734973486,-0.7200703577\H,-0.89588041,-0.28234260
39,0.6591479923\H,3.5330174304,1.4770354436,4.3761418678\H,1.959776350
3,0.6805618608,4.6689341238\H,2.0278220967,2.4330431607,4.3539094123\C
,1.6133106663,3.1364471059,-0.7262691369\C,3.8155122412,4.0112720426,-
0.0205131473\N,2.3989541652,3.9912032487,0.0244322659\N,4.4260352031,2
.9327979186,-0.581523124\O,0.4402602839,3.3763926168,-0.9527866128\O,4
.4229037915,4.9819527623,0.4064428768\C,1.7424383061,5.1666479259,0.60
31203367\H,2.3568647335,5.533565604,1.4216927779\H,1.6219477761,5.9533
178265,-0.1468332095\H,0.7633418051,4.8614913014,0.9687528378\O,2.1087
757318,-1.9140675497,1.4802565865\O,1.5575273992,-2.1530502226,-0.6333
74301\O,1.5867052567,-3.860662031,0.6777751142\N,1.7675336125,-2.67649
96556,0.6016732926\C,5.8845072224,2.8853831095,-0.5295453877\H,6.22553
63969,2.5629956575,0.4600155112\H,6.2309425697,2.1800060879,-1.2866049
375\H,6.2829504809,3.8751822654,-0.7482093295\Version=AM64L-G09RevB.0
1\HF=-1266.6624059\S2=0.754428\S2-1=0\S2A=0.750015\RMSD=0.000e+00\RMS
F=2.906e-06\Dipole=0.5726994,-0.4095804,-1.8224853\Quadrupole=9.406627
5,-17.3473593,7.9407318,-10.1319667,-11.6760453,-0.075247\PG=C01 [X(C1
2H16N5O7)]\@

```

Sum of electronic and thermal Free Energies= -1266.408965 Hartrees

TS2

```

1\1\GINC-SPARTAN-RC144\FTS\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\09-Apr-2019\0\#p M062X/6-31+G* scf=(qc,direct) nosymm freq=noraman scrf=(c
pcm,solvent=acetonitrile) opt=(ts,noeigentest,calcf, maxcycle=500)\geom&freq\0,2\N,0.3126256486,0.9512551237,0.8248114805\C,0.7980037597,1
.204579832,2.0730079827\N,2.2055626742,1.2569703847,2.220182178\C,3.12
38952724,0.8542687843,1.2752232267\C,2.6043590759,0.5741498626,-0.1059
620681\C,1.1491024767,0.9379157985,-0.3218138512\C,3.0348678992,1.6104
549327,-1.2071324115\C,1.6802545306,2.2885279916,-0.9769431962\C,-1.13
63070161,1.0052119187,0.6484105129\O,0.0730096082,1.3806184253,3.03876
58686\C,2.7312321355,1.598470842,3.5441017581\O,4.3137812916,0.7630671
62,1.5242299235\H,2.88576178,-0.5237924546,-0.3507169095\H,3.085925389
7,1.1227572563,-2.1803155713\H,1.1219744704,2.6061948685,-1.859957889\
H,0.6842340959,0.3430940847,-1.1103875653\H,-1.3787938193,0.5660998513
,-0.3195621464\H,-1.6211167198,0.4346144515,1.4401675422\H,-1.48615678
84,2.0418334653,0.6799212495\H,2.9603243558,0.6874665498,4.1043335763\
H,1.9809683247,2.1794549299,4.0735681319\H,3.6460544185,2.1764966985,3
.4121898005\C,1.7368660569,3.4091193248,0.0265422008\C,4.2190557317,3.
4251983804,-0.0911236326\N,2.9788627584,3.8243130102,0.4614703736\N,4.

```

1920437644,2.4178001617,-1.012693\O,0.7118216914,3.9009484837,0.466648
 1982\O,5.2516590327,3.9817351113,0.2447754782\C,2.9954728241,4.8633782
 16,1.495339638\H,2.2875759408,4.5860533895,2.277533355\H,4.0025072515,
 4.9295742237,1.8975595827\H,2.6989934825,5.8253848184,1.0698697089\O,3
 .0971157502,-2.0344767026,-0.2629814186\O,1.8790083199,-1.7528764864,1
 .5306992822\O,2.4488637256,-3.7309910788,0.840176311\N,2.4284387986,-2
 .5209173303,0.7706582321\C,5.4776446061,1.9077830313,-1.4818482299\H,5
 .3017718335,1.321139704,-2.3842935453\H,6.1361365386,2.7439820043,-1.7
 133149544\H,5.9432210293,1.2767219793,-0.7171522027\\Version=AM64L-G09
 RevB.01\HF=-1266.6299813\S2=0.759387\S2-1=0.\S2A=0.750056\RMSE=0.000e+
 00\RMSF=3.734e-06\Dipole=-0.7218235,0.8326277,-3.1650497\Quadrupole=-5
 .36091,-7.0749506,12.4358606,3.1712063,-9.0030658,-2.6116134\PG=C01 [X
 (C12H16N5O7)]\\@

Vimag = - 434.7993 cm⁻¹

Sum of electronic and thermal Free Energies= -1266.380428 Hartrees

Product complex between HNO₃ and *c*,*α*-DMU<>DMU radical 2

1\1\GINC-SPARTAN-RC035\FOpt\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\20-A
 pr-2019\0\p M062X/6-31+G* scf=(qc,direct) nosymm freq=noraman scrf=(
 cpcm,solvent=acetonitrile) opt=(calcf, maxcycle=500)\geom&freq\0,2\N
 ,-0.1136613921,2.0106330295,1.1350890396\C,0.3261077248,1.8696863604,2
 .4125960319\N,1.6110125885,1.2955027765,2.6274844204\C,2.5005983098,0.
 9930093824,1.6270567343\C,1.9632870888,1.0143131073,0.2956003806\C,0.5
 970901181,1.5098416005,-0.0049498283\C,2.5616681615,1.6023006943,-0.96
 19870761\C,1.3047415677,2.511771773,-1.0128088137\C,-1.4596895224,2.54
 61752545,0.9410741364\O,-0.3389779481,2.2209563597,3.3753347603\C,2.06
 69301445,1.210787583,4.0169819969\O,3.6920174595,0.7378234483,1.884962
 5355\H,4.5632638517,-0.364525315,1.2184305926\H,2.5852768323,0.8943610
 796,-1.7935323444\H,0.8120696107,2.6447235028,-1.976790488\H,-0.020719
 3045,0.8044722984,-0.5753327424\H,-1.6142489659,2.6870509138,-0.129048
 8436\H,-2.2095291386,1.8544590636,1.3351251851\H,-1.5529853642,3.50956
 49996,1.4437792963\H,2.8296746567,0.4372886938,4.0765140635\H,1.215436
 4092,0.9583140533,4.644406001\H,2.488427288,2.1670386632,4.3390567654\
 C,1.5118423682,3.8419029388,-0.3385121096\C,3.939988727,3.4179409241,-
 0.1268474966\N,2.739249876,4.0600605744,0.2632599252\N,3.8194176886,2.
 2905059436,-0.8790462819\O,0.6051213029,4.6508297684,-0.2558658498\O,5
 .0195892304,3.8915530491,0.1936397398\C,2.8847383747,5.2694695886,1.07
 78114613\H,1.9413600422,5.4439275638,1.5918297636\H,3.6842537733,5.106
 6346726,1.7970185141\H,3.1253856457,6.1332544415,0.4521101909\O,5.2044
 293221,-1.1040877733,0.9255387965\O,3.5902827872,-1.2489879139,-0.5400
 906402\O,5.2862393517,-2.5966250188,-0.6249813964\N,4.6560651748,-1.68
 70648529,-0.1475113068\C,5.0519519408,1.6064504905,-1.2550620929\H,4.8
 044599423,0.8315196568,-1.9814823423\H,5.7402173492,2.3207229857,-1.70
 82094698\H,5.538794927,1.1572736387,-0.3827572084\\Version=AM64L-G09Re
 vB.01\HF=-1266.6708816\S2=0.756927\S2-1=0.\S2A=0.750036\RMSE=0.000e+00
 \RMSF=7.756e-06\Dipole=-1.9228294,-0.0586715,-1.2138969\Quadrupole=-14
 .4776559,-3.4760471,17.953703,4.8141481,-0.2002481,-7.3782712\PG=C01 [
 X(C12H16N5O7)]\\@

Sum of electronic and thermal Free Energies= -1266.416357 Hartrees

TS3

1\1\GINC-SPARTAN-RC025\FTS\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\02-Ma
y-2019\0\#p M062X/6-31+G* scf=(qc,direct) nosymm scrf=(cpcm,solvent=a
cetonitrile) opt=(ts,noeigentest,calcfc,maxcycle=500) freq=noraman\geom
&freq\0,2\N,0.1899008492,0.42713851,0.2057875182\C,-0.5210092073,1.
3069913938,1.0726284739\N,0.1133199969,2.4870179824,1.4106657936\C,1.4
866220628,2.7347272445,1.2924233924\C,2.3062380853,1.7877054029,0.4639
793085\C,1.4656291274,0.795839554,-0.3481719179\C,2.7396140599,2.41338
27138,-0.9147093803\C,1.5080349609,1.7785349068,-1.5680039502\C,-0.281
443493,-0.8769113354,0.0758960762\O,-1.6321055433,1.0201180434,1.44855
22291\C,-0.6890173296,3.4470405824,2.1797636622\O,1.9836576274,3.71414
93789,1.8063827919\H,3.0990085879,1.3724494115,1.0877919667\H,3.657434
6121,1.9264012524,-1.2471253182\H,1.6249032897,1.3119237086,-2.5477477
139\H,2.0143506204,-0.1171399039,-0.5803047388\H,-1.3565992785,-0.9487
843817,0.2347048532\H,0.0931259941,-1.3570272941,-0.8283155383\H,0.216
3050854,-1.4571877518,0.9914846158\H,-0.6897237791,3.1748125211,3.2381
484696\H,-1.7071525559,3.432229709,1.7955705965\H,-0.2453033329,4.432
1077676,2.0533912301\C,0.3084585555,2.6983335431,-1.6045073694\C,1.793
969926,4.6450307781,-1.1768328413\N,0.5248742375,4.0327737391,-1.35105
4991\N,2.8766046164,3.8273943116,-1.0840029846\O,-0.8055194881,2.24795
91558,-1.8190067907\O,1.8702522661,5.8625324805,-1.1234051351\C,-0.635
4275312,4.9299961424,-1.3588404265\H,-1.5118532222,4.3520667018,-1.072
1809322\H,-0.4579890724,5.7339635988,-0.647824209\H,-0.7848442166,5.35
20136939,-2.3558774145\O,1.2945940214,0.0229334923,2.6515801686\O,0.95
93145035,-2.0815579184,2.2313912072\O,2.1680872865,-1.4969899906,3.912
7504635\N,1.488457611,-1.1661218283,2.9508018241\C,4.1556067767,4.4470
735628,-0.7460135437\H,4.2951468727,5.3432844875,-1.349715675\H,4.1884
640196,4.7137948665,0.315419288\H,4.9495913978,3.7328105049,-0.9674670
586\Version=AM64L-G09RevB.01\HF=-1266.6502794\S2=0.756651\S2-1=0.S2A
=0.750033\RMSD=0.000e+00\RMSF=5.008e-06\Dipole=0.8227895,0.4443105,-3.
911542\Quadrupole=18.2609782,-8.7152459,-9.5457323,0.941861,-19.009263
3,8.5654934\PG=C01 [X(C12H16N5O7)]\@

$V_{\text{imag}} = -249.0161 \text{ cm}^{-1}$

Sum of electronic and thermal Free Energies= -1266.396360 Hartrees

Product complex between HNO₃ and α , α -DMU $\leftrightarrow$ DMU radical 3

1\1\GINC-SPARTAN-RC017\FOpt\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\04-M
ay-2019\0\#p M062X/6-31+G* scf=(qc,direct) nosymm scrf=(cpcm,solvent=
acetonitrile) opt=(calcfc,maxcycle=500) freq=noraman\geom&freq\0,2\N
,0.0613813717,0.5684563109,-0.0380625524\C,-0.6227390751,1.4010101059,
0.8277917971\N,-0.0041863134,2.6170788294,1.1593741845\C,1.347991582,2.
.890588133,1.022696384\C,2.1745442671,1.9443912464,0.1967499967\C,1.32
83407954,0.9563104611,-0.6124904497\C,2.6033150781,2.5691153027,-1.182
2034246\C,1.3739461037,1.9288693781,-1.8367917813\C,-0.4361226249,-0.6
968193815,-0.2784852894\O,-1.7145039815,1.1038519431,1.2799840725\C,-0
.8032330222,3.5793399877,1.9237174962\O,1.8399864463,3.8872578225,1.52
23002076\H,2.9743773449,1.5404956335,0.8199948396\H,3.5240849258,2.088
6050506,-1.5164991678\H,1.4989891308,1.4637022666,-2.816469004\H,1.889
810706,0.0501784348,-0.8422057254\H,-1.4614613874,-0.8840579101,0.0086
980401\H,0.0371664067,-1.2515842404,-1.0779316344\H,0.4193672908,-1.53
75640483,1.3816123253\H,-0.6375764807,3.4487921601,2.9964178443\H,-1.8

527038918,3.4157462764,1.6917176192\H,-0.4990571748,4.5840984017,1.6314849504\C,0.1848244421,2.8547416035,-1.8923416092\C,1.65010583,4.8020014299,-1.3959802447\N,0.3881894385,4.1830811301,-1.5788977603\N,2.738382171,3.9861652249,-1.3477593441\O,-0.9244210857,2.4330527079,-2.1765882989\O,1.7237114099,6.0190336999,-1.3061369894\C,-0.7967858434,5.044365589,-1.5630992265\H,-1.6041190552,4.5109747729,-1.0605583847\H,-0.5507116661,5.956903293,-1.0268257868\H,-1.1081599626,5.2862853412,-2.5828171066\O,1.4082266599,0.0771558719,2.5208312115\O,0.7869815512,-2.003510852,2.1853004642\O,1.9006160165,-1.4774003228,3.9491421228\N,1.4083699052,-1.0629770153,2.9349160251\C,4.0173888085,4.5934013162,-0.9924068783\H,4.1188349928,5.5490293699,-1.5047132263\H,4.0840305145,4.7508912183,0.0897468835\H,4.8153772551,3.9223576478,-1.3140576199\\Version=AM64L-G09RevB.01\HF=-1266.6664788\S2=0.754331\S2-1=0.\S2A=0.750014\RMSD=0.000e+00\RMSF=8.061e-06\Dipole=1.6761848,-1.5082899,-2.1959921\Quadrupole=16.5402775,-14.6591623,-1.8811152,-2.7244036,-13.191387,3.4668492\PG=C01 [X(C12H16N5O7)]\\@
Sum of electronic and thermal Free Energies= -1266.412229 Hartrees

TS4

1\1\GINC-SPARTAN-RC139\FTS\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\03-Jul-2019\O\#p M062X/6-31+G* scrf=(cpcm,solvent=acetonitrile) nosymm opt=(ts,noeigentest,calcf, maxcycle=500) freq=noraman\geom&freq\0,2\N,0.405930614,1.8435587371,5.3826780387\C,1.6887042457,1.5452990122,5.0712997333\N,1.9421874358,1.1465074308,3.717555669\C,0.9599420365,0.8223961772,2.7768476331\C,-0.4656309275,1.1335652431,3.1241705225\C,-0.6063549223,2.0051895921,4.3761066461\C,-1.0299288964,2.3572782181,2.3090790833\C,-0.6522887505,3.2857437803,3.4682033979\O,2.6151031635,1.5896659251,5.8625077492\C,3.2961479241,0.8986276396,3.3474668946\O,1.2720650214,0.3310843548,1.7086445551\H,-1.0456670777,0.2097527448,3.0774884799\H,-2.1120025389,2.2509619327,2.2223154145\H,-1.3661406877,4.0597774416,3.7568436606\H,-1.5816730086,1.8632032795,4.842786778\H,3.4798858753,-0.2349679519,3.3839868306\H,3.9819680458,1.3639997468,4.0510914066\H,3.4712875881,1.159345732,2.30227491\C,0.704920828,3.916059001,3.3007110593\C,0.7233151506,3.2884412447,0.8931301518\N,1.3242190138,3.7960142353,2.0734883344\N,-0.4961801869,2.6995233163,1.0239801551\O,1.2543974886,4.4787093547,4.2346320904\O,1.2980456813,3.4003063481,-0.1797356215\C,2.6718633602,4.3599625702,1.9591923128\H,3.1300014651,3.9717561591,1.0536033961\H,2.6258907615,5.4512616938,1.9137117127\H,3.2476883367,4.0654377683,2.8374908031\O,3.7446248997,-1.3769178027,1.1462536499\O,2.8881807999,-1.7262773057,3.119870592\O,2.2855415229,-2.9477937695,1.4955664335\N,2.9889215535,-2.0172996724,1.8339247838\C,-1.0481967999,2.0272827142,-0.1488595538\H,-2.1235344623,1.9131189753,-0.0040298494\H,-0.8629884561,2.6352665584,-1.033226677\H,-0.589266053,1.0415702659,-0.281925847\C,0.1547195209,2.4089191273,6.7061401009\H,-0.9032070909,2.2798562758,6.937817422\H,0.7563969849,1.8803172138,7.4441401979\H,0.4087767311,3.4740590719,6.7199519702\\Version=AM64L-G09RevB.01\HF=-1266.6339406\S2=0.759251\S2-1=0.\S2A=0.750059\RMSD=6.354e-09\RMSF=1.518e-06\Dipole=-3.7516294,1.4255184,1.5708088\Quadrupole=1.9709044,-7.8166877,5.8457832,-6.8032374,-19.7811033,6.4824809\PG=C01 [X(C12H16N5O7)]\\@
Vimag = - 698.6018 cm⁻¹
Sum of electronic and thermal Free Energies= - 1266.382868 Hartrees

Product complex between HNO₃ and *c*,*α*-DMU<>DMU radical 4

1\1\GINC-SPARTAN-RC040\FOpt\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\15-M
ay-2019\0\#p M062X/6-31+G* scf=(qc,direct) nosymm scrf=(cpcm,solvent=
acetonitrile) opt=(calcf, maxcycle=500) freq=noraman\geom&freq\0,2\N
,4.1131558329,-1.0955670807,2.1922391812\C,4.5614513794,-1.2338325814,
3.4630778475\N,5.9800110817,-1.3597834951,3.643053977\C,6.9060943254,-
1.5084475835,2.6074796872\C,6.414130483,-1.3541622951,1.1976835655\C,5
.001278222,-0.768997787,1.1130273639\C,6.915810043,-0.0150031776,0.537
6821811\C,5.6173587378,0.6701573613,0.9747576547\C,2.6917302861,-0.804
4679886,2.0185955733\O,3.832528249,-1.2701353258,4.4406863898\C,6.4532
969223,-1.3411058653,4.9488535418\O,8.0842660525,-1.7107318855,2.85070
67318\H,6.6215763861,-2.2737565371,0.6461310157\H,6.9485788645,-0.1470
079495,-0.5448779157\H,5.1296069235,1.3438516123,0.2672508111\H,4.5186
662562,-1.0412159082,0.173599305\H,2.4299970013,-0.9902959235,0.975775
8921\H,2.1028248096,-1.4581761439,2.6605814101\H,2.4766275271,0.240021
8637,2.2662356746\H,0.4519590191,2.1067132993,-0.1401437272\H,5.728754
9488,-1.2531356172,5.7389870592\H,7.5138830159,-1.4612898968,5.0875577
866\C,5.7380206782,1.3692533396,2.3043845292\C,8.2157018643,1.25725746
23,2.1573926409\N,7.0022530844,1.521608368,2.838284967\N,8.1313413934,
0.6172210488,0.9596520388\O,4.7419342223,1.7499389729,2.8998768734\O,9
.2753252329,1.6172280236,2.6508868468\C,7.1166602971,2.1262758383,4.16
80972236\H,8.0011751503,1.7221665028,4.6564703299\H,7.2047838339,3.213
6772642,4.0918547956\H,6.2224775447,1.8709941979,4.7345372795\O,-1.382
8441378,0.9478555067,0.0334652097\O,0.7015211429,1.4310106395,0.523712
4247\O,-0.2791811317,-0.2254944942,1.4895492779\N,-0.4109577049,0.6613
32463,0.6908957536\C,9.3797135705,0.1798308095,0.3431411551\H,9.191602
9501,-0.0071321681,-0.7152624179\H,10.1284261329,0.9641173143,0.445296
4174\H,9.7454206093,-0.7372101841,0.8185624484\Version=AM64L-G09RevB.
01\HF=-1266.6557497\S2=0.756651\S2-1=0.\S2A=0.750032\RMSD=0.000e+00\RM
SF=1.827e-05\Dipole=-0.4616772,0.4350508,-4.1412135\Quadrupole=-16.265
6626,19.846649,-3.5809864,-6.0400537,-40.8634909,1.4788986\PG=C01 [X(C
12H16N5O7)]\@
Sum of electronic and thermal Free Energies= -1266.405151 Hartrees

c,*α*-DMU<>DMU radical 1

1\1\GINC-SPARTAN-RC103\FOpt\UM062X\6-31+G(d)\C12H15N4O4(2)\UWILLE\28-M
ar-2019\0\#p M062X/6-31+G* scf=(qc,direct) nosymm scrf=(cpcm,solvent=
acetonitrile) freq=noraman opt=(calcf, maxcycle=500)\geom&freq\0,2\N
,0.8864153537,0.7265418852,0.8136124541\C,1.048410152,0.9045594253,2.1
677133882\N,2.3239060204,1.2960410811,2.6261040908\C,3.4526496502,1.44
07806304,1.8342399799\C,3.3572068713,0.8073574344,0.4668937704\C,1.957
8540515,0.7791078988,-0.0525179268\C,3.7191252876,1.6888996678,-0.7826
517039\C,2.2193013523,1.8426160977,-1.1233855116\C,-0.4748672304,0.528
8966619,0.31234396\O,0.1184915915,0.7843437139,2.949784652\C,2.4045411
491,1.6802819149,4.0380731974\O,4.4650592334,1.9830602284,2.2396587044
\H,3.8880037846,-0.1518768633,0.5187081592\H,4.2399312718,1.0878864254
, -1.527758291\H,1.9069499319,1.6455200882,-2.1508665482\H,-1.128183557
8,1.3224734975,0.6771501461\H,-0.4325513376,0.5589192061,-0.7762411865
\H,-0.8563906323,-0.4410405566,0.6401213332\H,3.4549722992,1.706105912
4,4.3186746393\H,1.8690481422,0.9439399241,4.6349568515\H,1.9581224256

,2.6662887362,4.1909137342\C,1.6209723864,3.1390904728,-0.6361888481\C
 ,3.8519465115,3.9827271753,0.0138858784\N,2.4397475954,3.9534929044,0.
 1282310005\N,4.4355836448,2.922147062,-0.6076638949\O,0.4390379445,3.3
 899294866,-0.7982582101\O,4.4755654773,4.9430793241,0.4416339741\C,1.8
 149184306,5.0934221491,0.8031684486\H,2.4463867567,5.3863832123,1.6389
 820718\H,1.6991991308,5.9380960796,0.1181035492\H,0.8354280459,4.77896
 97162,1.1595897386\C,5.8935528566,2.8573794207,-0.5968271176\H,6.25549
 43736,2.4787389194,0.3653695928\H,6.2133257663,2.1907068597,-1.3994550
 88\H,6.2983122696,3.8532032083,-0.7713429879\\Version=AM64L-G09RevB.01
 \HF=-985.8680127\S2=0.755741\S2-1=0.\S2A=0.750022\RMSD=0.000e+00\RMSF=
 4.593e-06\Dipole=0.5554728,-1.9713031,-1.4744285\Quadrupole=4.3076627,
 -11.3032781,6.9956154,-14.4277047,-9.446187,-2.7997301\PG=C01 [X(C12H1
 5N4O4)]\\@
 Sum of electronic and thermal Free Energies= - 985.633734 Hartrees

TS5

1\1\GINC-SPARTAN-RC068\FTS\UM062X\6-31+G(d)\C12H15N4O4(2)\UWILLE\03-Apr-2019\0\#p M062X/6-31+G* nosymm scf=(qc,direct) freq=noraman geom=checkpoint guess=check scrf=(cpcm,solvent=acetonitrile) opt=(ts,noeigent est,readfc,maxcycle=500)\geom&freq\0,2\N,1.2110060703,1.3610781922,1.1596912569\C,1.5369929278,1.1868247357,2.4868642209\N,2.8121754711,0.6875975077,2.767625768\C,3.7190576142,0.1988554093,1.8270668737\C,3.3240824829,0.3948769388,0.4232334846\C,2.0857441371,1.0020999567,0.1651520457\C,3.7950081452,1.8991218004,-0.8913861622\C,2.3020459727,1.6852383856,-1.1691507951\C,-0.1286720629,1.877546644,0.8664087207\O,0.7553683723,1.4690385888,3.3877509046\C,3.1351687798,0.564873682,4.1911689474\O,4.7784357993,-0.3152684019,2.1620506017\H,3.7649048604,-0.3171179796,-0.2718458001\H,4.5426927599,1.5854812727,-1.6217096298\H,2.1447427418,1.0250427835,-2.0263057988\H,-0.1771367272,2.9542139706,1.0520815616\H,-0.36418987,1.6631902918,-0.1750696556\H,-0.8469309083,1.372055467,1.5122174689\H,4.1807587171,0.2795179182,4.271217496\H,2.5017668974,-0.1943293263,4.6555065157\H,2.962458042,1.5230291748,4.6812926316\C,1.5270197568,2.9650367407,-1.4099402702\C,3.1613107581,4.0625962242,0.0658787166\N,1.9329195506,4.0234115789,-0.6309292645\N,4.0840424917,3.0947092675,-0.2253997531\O,0.5881832837,3.0314078931,-2.1835504515\O,3.3973766564,4.9870759689,0.8321156071\C,1.1176792512,5.2385905332,-0.5731860151\H,0.9816660549,5.5272015192,0.4689302662\H,1.6077036075,6.0523938405,-1.1125485803\H,0.1574899578,5.01638146,-1.0340881171\C,5.3834949824,3.1895550285,0.4363716192\H,5.311095866,2.8325749349,1.4692643986\H,6.0859196513,2.5610202587,-0.1130869296\H,5.7260919088,4.2231487394,0.4310611174\\Version=AM64L-G09RevB.01\HF=-985.8256283\S2=0.783526\S2-1=0.\S2A=0.750356\RMSD=0.000e+00\RMSF=6.313e-06\Dipole=0.3400916,-0.3557083,-1.5632574\Quadrupole=6.9318482,-2.8110505,-4.1207977,2.6517441,-11.9725677,-4.6144658\PG=C01 [X(C12H15N4O4)]\\@
 V_{imag} = - 946.4302 cm⁻¹
 Sum of electronic and thermal Free Energies= - 985.596437 Hartrees

DMU-DMU radical 5

1\1\GINC-SPARTAN-RC098\FOpt\UM062X\6-31+G(d)\C12H15N4O4(2)\UWILLE\04-Apr-2019\0\#p M062X/6-31+G* nosymm scf=(qc,direct) geom=checkpoint guess=check scrf=(cpcm,solvent=acetonitrile) opt=(readfc,maxcycle=500) fr

```

eq=noraman\geom&freq\0,2\N,1.1551685327,0.7726875185,1.3185058698\C,
1.1720956764,0.2008215241,2.5880620424\N,2.2792213372,0.4577056678,3.3
780078602\C,3.3932257611,1.2012292816,2.9746905788\C,3.3178885052,1.71
68493835,1.6272592381\C,2.2298933439,1.499005952,0.8528626042\C,3.4691
275436,2.1137721993,-1.2592156493\C,2.1573103221,2.0869433814,-0.56261
96811\C,-0.0163061888,0.4793900178,0.4788977919\O,0.2540328396,-0.4938
127056,3.0014523128\C,2.2553610446,-0.1339179404,4.7163357898\O,4.3436
163199,1.3799016698,3.7304929582\H,4.1685263292,2.279705273,1.26451909
1\H,3.9555287951,1.1949644174,-1.5545040763\H,1.4629392618,1.490272080
1,-1.1587482813\H,-0.7850784557,0.0649527177,1.1249325105\H,-0.3788103
871,1.400123723,0.0247592836\H,0.2417522765,-0.2566672264,-0.287501928
8\H,3.1688921237,0.1634656205,5.224179553\H,2.2008520221,-1.2212211107
,4.6372898233\H,1.3816292035,0.2278952049,5.260726592\C,1.5357236194,3
.4779206523,-0.4417772843\C,3.7694716782,4.4667298229,-0.8255117777\N,
2.3911478635,4.5506915479,-0.5544130455\N,4.2639468559,3.2365594813,-1
.1604224137\O,0.3473788136,3.6110633953,-0.2075657055\O,4.4728013404,5
.4679900718,-0.7812278003\C,1.8745481853,5.904999458,-0.3300188013\H,2
.3031897612,6.3168427856,0.5854634741\H,2.1474646859,6.5390465647,-1.1
734798054\H,0.7935285365,5.8383184645,-0.2408875385\C,5.6808709537,3.1
820255322,-1.52707704\H,6.2951110592,3.4702365937,-0.6719380123\H,5.91
61936848,2.1599507187,-1.8193266853\H,5.8792277758,3.8616282919,-2.357
4458472\Version=AM64L-G09RevB.01\HF=-985.8886355\S2=0.757217\S2-1=0.\
S2A=0.750033\RMSD=0.000e+00\RMSF=2.563e-06\Dipole=0.160622,-0.7966496,
-2.5464936\Quadrupole=2.1254929,-3.6819931,1.5565003,-10.4272144,-17.2
934009,-4.7855847\PG=C01 [X(C12H15N4O4)]\@\
Sum of electronic and thermal Free Energies= - 985.660622 Hartrees

```

TS6

```

1\1\GINC-SPARTAN-RC045\FTS\UM062X\6-31+G(d)\C12H15N4O4(2)\UWILLE\22-Ap
r-2019\0\#p M062X/6-31+G* scrf=(cpcm,solvent=acetonitrile) opt=(ts,no
eigentest,calcfc,maxcycle=500) freq=noraman scf=(qc,direct) nosymm\geom
&freq\0,2\N,0.9242520621,0.7452452003,1.2511131613\C,0.8666617623,0
.290065887,2.5666865465\N,2.027656221,0.4065233864,3.3091890296\C,3.24
83341769,0.9148113528,2.8283134467\C,3.2236957943,1.3525623833,1.44589
60114\C,2.0780971216,1.2410395491,0.7511596118\C,3.6030765008,2.227560
5936,-1.5786740228\C,2.2490748811,2.1671817409,-1.3837601352\C,-0.2975
557684,0.5955998448,0.4535962635\O,-0.1604675788,-0.1845369825,3.03093
96093\C,1.9418771883,-0.0667828707,4.6909633329\O,4.2352990781,0.96476
91217,3.5565036783\H,4.1404832168,1.7480988488,1.025076627\H,4.1593236
641,1.4068490631,-2.0170885186\H,1.6746638466,1.373470311,-1.842920427
6\H,-1.1306797026,1.0655511779,0.97750653\H,-0.1440141529,1.0936979917
,-0.5002231761\H,-0.5137001822,-0.4645520426,0.3056754166\H,2.90661037
3,0.1057790289,5.1603194384\H,1.7005160633,-1.1314441946,4.7019520674\
H,1.1588558227,0.4812179824,5.2176572078\C,1.5353350352,3.3742651873,-
0.9698097472\C,3.7386531485,4.4347373402,-0.6409406789\N,2.355380456,4
.4301110138,-0.5609217601\N,4.3365184981,3.2984264011,-1.175504329\O,0
.3159369236,3.4691755723,-0.9481832276\O,4.4067310057,5.3892740071,-0
.2776092954\C,5.7951944201,3.3294061281,-1.3090653136\H,6.2521151259,3
.4390390234,-0.3241851699\H,6.115040563,2.3932384702,-1.7636545343\H,6
.0891679369,4.1706769962,-1.9379775746\C,1.745824541,5.6565939315,-0.04
21813231\H,2.1434321864,5.8640140155,0.9522538409\H,1.9770460718,6.493

```

5993525,-0.7036907902\H,0.6715964896,5.4985595472,0.0035006648\\Version=AM64L-G09RevB.01\HF=-985.843034\S2=0.774585\S2-1=0.\S2A=0.750319\RMSD=0.000e+00\RMSF=3.932e-06\Dipole=0.9800826,-0.392881,-2.9250545\Quadrupole=5.4948371,-4.204679,-1.2901581,-2.4340099,-23.2560818,-5.4368622\PG=C01 [X(C12H15N4O4)]\\@

V_{imag} = - 276.5855 cm⁻¹

Sum of electronic and thermal Free Energies= - 985.615810 Hartrees

Product complex 6

1\1\GINC-SPARTAN-RC027\FOpt\UM062X\6-31+G(d)\C12H15N4O4(2)\UWILLE\11-Apr-2019\0\#p M062X/6-31+G* scf=(qc,direct) nosymm geom=checkpoint guess=check scrf=(cpcm,solvent=acetonitrile) opt=(readfc,maxcycle=500) freq=noraman\geom&freq\0,2\N,0.9824096517,0.7703476284,1.321422705\C,1.449126233,1.4257926023,2.462400129\N,2.8264028462,1.5538691475,2.5506040258\C,3.7591204135,0.9842830624,1.6640795672\C,3.1947365779,0.270210569,0.528998902\C,1.8611160296,0.2363812102,0.4615536087\C,3.4978172231,2.5029907674,-1.9928877527\C,2.1531719365,2.4303346228,-2.0836727771\C,-0.4672608588,0.6130173498,1.1574601765\O,0.6695896729,1.8606063329,3.2945624937\C,3.3812678924,2.2944195356,3.6866550624\O,4.9588115471,1.1204997411,1.8727706198\H,3.8573635828,-0.1702844429,-0.204455316\H,4.1527740159,2.1061066047,-2.7608209337\H,1.6648250338,1.9741086484,-2.9338939985\H,-0.9374908156,1.5968328932,1.139721767\H,-0.6382652728,0.1084382469,0.2071077676\H,-0.8669331947,0.0190120148,1.9811297111\H,4.0546289857,3.0621181273,3.3022641822\H,3.934732259,1.6120628348,4.3355039219\H,2.5572684899,2.7458066395,4.2336777987\C,1.3321831101,2.97016092,-1.022777734\C,3.4229275343,3.6485046703,0.1149595704\N,2.0403995264,3.5645221305,0.0339057946\N,4.1315305484,3.0686236674,-0.9221185038\O,0.1047289127,2.9352143293,-0.9976024033\O,3.9926271714,4.1952864193,1.0501397285\C,1.2713286583,4.2194602191,1.0931858935\H,1.8492156064,4.1981698295,2.0154583094\H,1.0651598865,5.2581112298,0.8187383487\H,0.3299522736,3.6870634735,1.2166891423\C,5.5922115092,3.1087563009,-0.8211550666\H,5.9075448163,2.5628945802,0.0706917351\H,6.0067678235,2.6398439302,-1.7125521716\H,5.9304073739,4.144243992,-0.7565533039\\Version=AM64L-G09RevB.01\HF=-985.8566938\S2=0.762337\S2-1=0.\S2A=0.750062\RMSD=0.000e+00\RMSF=1.365e-05\Dipole=0.5256627,-1.003988,-2.0748904\Quadrupole=1.6597545,-3.6363019,1.9765473,2.7858552,-19.6834985,-8.2027226\PG=C01 [X(C12H15N4O4)]\\@

Sum of electronic and thermal Free Energies= - 985.627383 Hartrees

[c,α-DMU<>DMU]**

1\1\GINC-SPARTAN-RC161\FOpt\UM062X\6-31+G(d)\C12H16N4O4(1+,2)\UWILLE\01-May-2019\0\#p M062X/6-31+G* scf=(qc,direct) geom=checkpoint guess=check nosymm scrf=(cpcm,solvent=acetonitrile) opt=(readfc,maxcycle=500) freq=noraman\geom&freq\1,2\N,0.5809621878,-0.4308021578,0.5675167236\C,0.852602314,-0.0136781354,1.9275098167\N,2.1532403993,0.3127361666,2.2209910168\C,3.2823214717,0.051235069,1.4185026107\C,3.0532826902,-0.5431284321,0.0583105517\C,1.5978683621,-0.4919682549,-0.41636914\C,3.3982289522,0.4543935197,-1.1133605095\C,1.9306456607,0.8761574509,-1.1641646908\C,-0.7959013236,-0.7084279596,0.2328157213\O,-0.0654483222,0.053923442,2.7015295491\C,2.3616805537,0.8738254546,3.5655876153\O,4.393416814,0.3163949351,1.810132537\H,3.5352092845,-1.5217917823,0.0141

236455\H,3.674804881,-0.1237816677,-1.995260392\H,1.4435339058,0.99935
63457,-2.132767365\H,1.340637516,-1.2533128921,-1.1547177968\H,-1.4245
393025,0.0850614491,0.6432358895\H,-0.8897418942,-0.7902907986,-0.8477
895129\H,-1.078011768,-1.6538934162,0.7178120305\H,2.2708541762,0.0815
064206,4.3116814947\H,1.6048338628,1.6369644493,3.7442562949\H,3.35816
6815,1.306331365,3.5926228102\C,1.6102782935,2.0512544133,-0.262494301
1\C,4.0234554972,2.6409657698,-0.2342541044\N,2.6624556125,2.821128219
7,0.1509293188\N,4.3340194859,1.5185750666,-0.9356520105\O,0.458579751
7,2.2418997005,0.0977947251\O,4.8437690197,3.4841953079,0.0803524825\C
,5.7512009368,1.2591055866,-1.1872300224\H,6.2461406404,0.9104111419,-
0.2754803738\H,5.8274324868,0.4950302648,-1.9613269392\H,6.2282611714,
2.1753177267,-1.5334721853\C,2.391612808,3.9767051516,1.0157256791\H,3
.1602681772,4.0248138928,1.7853599225\H,2.4060392009,4.8965653464,0.42
76857598\H,1.4111034116,3.8359858703,1.4645652586\\Version=AM64L-G09Re
vB.01\HF=-986.2682661\S2=0.757026\S2-1=0.\S2A=0.750039\RMSD=0.000e+00\
RMSF=1.559e-05\Dipole=-2.0339145,-3.8121874,-2.0550153\Quadrupole=-0.2
894152,-5.3776347,5.6670499,-8.4819206,-6.6888319,2.0213963\PG=C01 [X(
C12H16N4O4)]\\@

Sum of electronic and thermal Free Energies= -986.022675 Hartrees

TS7

1\1\GINC-SPARTAN-RC110\FTS\UM062X\6-31+G(d)\C12H16N4O4(1+,2)\UWILLE\04
-May-2019\0\#p M062X/6-31+G* scrf=(cpcm,solvent=acetonitrile) scf=(qc
,direct) nosymm opt=(ts,noeigentest,calcfc,maxcycle=500) freq=noraman\
\geom&freq\1,2\N,0.6135988043,-0.4996714719,0.5936742645\C,0.88468608
21,0.0410125324,1.8973685974\N,2.1989564018,0.3382734961,2.1895124287\
C,3.2990935586,0.0396551005,1.3825321047\C,3.0273960907,-0.5362279601,
0.0167112014\C,1.5667340862,-0.6664510199,-0.3185736311\C,3.3672783123
,0.4803966729,-1.1550482844\C,1.9672471283,1.0055282682,-1.3015484954\
C,-0.8053605229,-0.7092577538,0.2784017241\O,-0.0284341159,0.217140224
1,2.6607289568\C,2.4352138613,0.917638952,3.5217641389\O,4.4310545769,
0.2634954316,1.7435391834\H,3.5657626795,-1.4837843629,-0.0815355088\H
,3.6698450152,-0.095043442,-2.0299527635\H,1.3991335652,0.9173157369,-
2.2246449164\H,1.2870265304,-1.2587812774,-1.1865469263\H,-1.311545895
3,0.2572762924,0.3184225526\H,-0.8744501952,-1.1399741093,-0.718075116
2\H,-1.2310497931,-1.3828681004,1.0222324761\H,2.3331043937,0.14141602
29,4.2827260368\H,1.7004188743,1.7024517671,3.6955018049\H,3.442664066
4,1.3254014735,3.5322020459\C,1.5874246768,2.1230115659,-0.391782694\C
,4.0105259498,2.6137464327,-0.160575603\N,2.6404166348,2.8018527221,0.
1757402274\N,4.3236789766,1.515470347,-0.907179798\O,0.4172562017,2.35
79160513,-0.1384962329\O,4.8388348361,3.4151305351,0.2281513622\C,5.74
44221328,1.2226081115,-1.1015928317\H,6.1887739345,0.8462822121,-0.175
5007151\H,5.8348869763,0.4725639405,-1.8875570901\H,6.2557926378,2.133
7736071,-1.4104665601\C,2.3426780355,3.9171691651,1.0810427851\H,3.093
5381231,3.9359805802,1.869339077\H,2.3652061446,4.8629185545,0.5346767
951\H,1.3514572346,3.755393702,1.499511404\\Version=AM64L-G09RevB.01\H
F=-986.2607268\S2=0.763636\S2-1=0.\S2A=0.750083\RMSD=0.000e+00\RMSF=8.
734e-06\Dipole=-1.3557169,-3.7196215,-2.5846822\Quadrupole=1.4783438,-
6.2291921,4.7508483,-7.5725233,-9.0291707,1.8781646\PG=C01 [X(C12H16N4
O4)]\\@

Vimag = - 414.2506 cm⁻¹

Sum of electronic and thermal Free Energies= -986.015923 Hartrees

DMU-DMU radical cation 7

```
1\1\GINC-SPARTAN-RC101\FOpt\UM062X\6-31+G(d)\C12H16N4O4(1+,2)\UWILLE\O
8-May-2019\0\#p M062X/6-31+G* scrf=(cpcm,solvent=acetonitrile) scf=(q
c,direct) nosymm opt=(calcf, maxcycle=500) freq=noraman\geom&freq\1,
2\N,0.6821778494,-1.0702319236,0.526863714\C,0.6500466653,-0.173741898
4,1.6856713995\N,1.8369742503,0.4153117732,2.036892347\C,3.0504134754,
0.1865112848,1.3819371874\C,2.9431225366,-0.410382217,0.0070195126\C,1
.7304679661,-1.2025296218,-0.2124420372\C,2.9877055182,0.8136742918,-1
.08723511\C,1.7912756903,1.6808397086,-0.9716302023\C,-0.5770653769,-1
.7998701879,0.2741421689\O,-0.3884450174,-0.0259923135,2.2658370022\C,
1.8095930519,1.2310728165,3.2619269851\O,4.1084773507,0.5451565853,1.8
404168722\H,3.8271864447,-1.0189402966,-0.20343357\H,3.006168644,0.314
2869028,-2.0595742331\H,0.8591622295,1.4224126874,-1.4591069884\H,1.67
40714189,-1.8920881818,-1.0520137407\H,-1.3570515603,-1.0691128383,0.0
635600018\H,-0.4203646826,-2.4585194207,-0.5769206972\H,-0.828962519,-
2.3692529538,1.1673421122\H,1.5784897076,0.5987118246,4.1202759097\H,1
.0454410897,2.0009706105,3.1506586566\H,2.793202046,1.6795844564,3.378
4421018\C,1.8278677514,2.8785341776,-0.1526686738\C,4.2801912664,2.653
9275335,-0.0930381312\N,3.0735199244,3.2014682281,0.3738518135\N,4.196
7542738,1.5622637704,-0.9237136672\O,0.8241585509,3.5372559493,0.09411
02027\O,5.3477299367,3.1516693583,0.2198844925\C,5.4570867719,0.920451
9996,-1.2900767724\H,5.8937522622,0.3982305304,-0.4313581739\H,5.26239
11492,0.2116710025,-2.0962824902\H,6.1575300538,1.6780471148,-1.639202
2404\C,3.1840624098,4.3551707609,1.2682060587\H,3.946861036,4.14582206
33,2.0168582027\H,3.462473387,5.2508431721,0.706860278\H,2.2168014479,
4.5055352509,1.7426387089\Version=AM64L-G09RevB.01\HF=-986.2826871\S2
=0.759225\S2-1=0.\S2A=0.750061\RMSD=0.000e+00\RMSF=1.268e-05\Dipole=-1
.9380375,-5.5854938,-2.1884891\Quadrupole=-4.5929402,-2.5812556,7.1741
959,-10.1537985,-8.623473,3.2094169\PG=C01 [X(C12H16N4O4)]\@\@
Sum of electronic and thermal Free Energies= -986.037421 Hartrees
```

TS8

```
1\1\GINC-SPARTAN-RC124\FTS\UM062X\6-31+G(d)\C12H16N4O4(1+,2)\UWILLE\15
-May-2019\0\#p M062X/6-31+G* scf=(qc,direct) scrf=(cpcm,solvent=aceto
nitrile) nosymm opt=(ts,noeigentest,calcf, maxcycle=500) freq=noraman\
geom&freq\1,2\N,0.6918470688,-1.0657189074,0.5653824139\C,0.69125554
19,-0.1321841601,1.6631740487\N,1.9043170047,0.4284623993,1.9917274753
\C,3.1121323951,0.1275190798,1.3516821456\C,2.9776114164,-0.590281471,
0.0704927455\C,1.7688119945,-1.3081757097,-0.1381567927\C,3.011511234,
0.8856352149,-1.1958000393\C,1.783274417,1.6080920444,-0.9627020352\C,
-0.5997176314,-1.7233685602,0.2983885941\O,-0.3390382209,0.1048282369,
2.2398720133\C,1.8938144613,1.3504682033,3.1354335616\O,4.1779415309,0
.5414797807,1.7597199751\H,3.8815933244,-1.0954633277,-0.2615905078\H,
3.0518961126,0.2778393203,-2.0957928454\H,0.8456267598,1.2759895784,-1
.3906645483\H,1.685301084,-2.044341338,-0.9332623195\H,-1.3224274587,-
0.9628474834,0.0024474297\H,-0.4524247093,-2.4460646319,-0.5008772644\
H,-0.9338551308,-2.2184216412,1.2091270665\H,1.599397028,0.8156776547,
4.0396147976\H,1.1794067782,2.1514478123,2.9327202437\H,2.899376612,1.
7494534998,3.2451342745\C,1.7649597664,2.7437110283,-0.0514478099\C,4.
```

2276621363,2.6674786759,-0.0754227717\N,3.0106608339,3.1509604555,0.41
 22243316\N,4.1778228104,1.575551021,-0.9380307463\O,0.7237539489,3.272
 3404278,0.3125543735\O,5.2818203515,3.1841269955,0.2302385464\C,5.4656
 705029,1.0066379668,-1.3396640607\H,5.9473673743,0.5324752449,-0.47952
 64127\H,5.2885331286,0.2715989539,-2.1244710877\H,6.1053537431,1.80170
 98845,-1.7204566253\C,3.093875921,4.2748955115,1.3498040769\H,3.837327
 169,4.0439285655,2.1125131966\H,3.3877865462,5.1841708515,0.820502464\
 H,2.1130201554,4.4091548232,1.7998110928\\Version=AM64L-G09RevB.01\HF=
 -986.2789482\S2=0.764412\S2-1=0.\S2A=0.750154\RMSD=0.000e+00\RMSF=4.32
 7e-06\Dipole=-1.0854515,-4.5359627,-2.916895\Quadrupole=-0.5594884,-1.
 6295327,2.1890212,-4.7234966,-11.4441688,1.8089792\PG=C01 [X(C12H16N4O4)]\\@
 Vimag = - 393.0411 cm⁻¹
 Sum of electronic and thermal Free Energies= -986.034539 Hartrees

Product complex 8

1\1\GINC-SPARTAN-RC145\FOpt\UM062X\6-31+G(d)\C12H16N4O4(1+,2)\UWILLE\1
 7-Apr-2019\0\#p M062X/6-31+G* scf=(qc,direct) nosymm scrf=(cpcm,solve
 nt=acetonitrile) opt=(calcf, maxcycle=500) freq=noraman\geom&freq\1,
 2\N,0.6403645677,0.3267668402,1.2826714756\C,1.1565357203,1.1738082352
 ,2.3001207563\N,2.5074899632,1.4558342078,2.2252783568\C,3.3625117537,
 0.9955639044,1.2220159478\C,2.7440709587,0.1626066009,0.2005488424\C,3
 .8299192995,2.4052636677,-1.5933395887\C,2.4861325124,2.1210563282,-1.
 4218461981\C,-0.8022154242,0.0642368462,1.344840542\O,0.4204311366,1.5
 976027377,3.1614973047\C,3.1130802275,2.2768029436,3.2809208784\O,4.53
 60574641,1.3382954274,1.2004764827\H,3.3816373754,-0.3362314883,-0.517
 4865517\H,4.4348445609,1.8727878508,-2.3198593523\H,1.9669244072,1.465
 3179201,-2.1085675531\H,-1.3319625088,1.0134998263,1.2538880903\H,-1.0
 626016744,-0.595411816,0.519998391\H,-1.0415176614,-0.4028245065,2.300
 1634148\H,3.6946601678,3.0778416353,2.8206484527\H,3.7798419091,1.6557
 94543,3.8822304987\H,2.3171981165,2.6830057608,3.8996149381\C,1.695086
 3884,2.8993681698,-0.4767760232\C,3.7626627857,4.0949417724,0.11588439
 27\N,2.4056791335,3.8718556995,0.2345963195\N,4.4524326992,3.315389414
 2,-0.8470487456\O,0.5092888858,2.6914468741,-0.2675047725\O,4.35825584
 94,4.910355291,0.7841492538\C,1.692343382,4.7390164128,1.1811688829\H,
 2.0993566108,4.6084254263,2.1847242086\H,1.8181614299,5.7794342166,0.8
 781983891\H,0.6421344076,4.4599127792,1.1606274206\C,5.9000179044,3.53
 88855518,-0.9342634073\H,6.3531304172,3.2572073837,0.0176907025\H,6.29
 09928058,2.9191967148,-1.7385113566\H,6.0887948403,4.5927700922,-1.136
 6461263\C,1.405458544,-0.1720103007,0.3147643869\H,0.9218269642,-0.830
 0332925,-0.3997597332\\Version=AM64L-G09RevB.01\HF=-986.3022859\S2=0.7
 61366\S2-1=0.\S2A=0.750098\RMSD=0.000e+00\RMSF=3.651e-05\Dipole=0.2265
 199,-2.4714928,-2.9979315\Quadrupole=16.0443154,-5.8744351,-10.1698803
 ,18.9516973,-16.4589548,-8.6456865\PG=C01 [X(C12H16N4O4)]\\@
 Sum of electronic and thermal Free Energies= -986.060299 Hartrees

Scheme 4

c,s-DMU<>DMU

1\1\GINC-SPARTAN-RC177\FOpt\RM062X\6-31+G(d)\C12H16N4O4\UWILLE\09-Nov-
 2018\0\#p M062X/6-31+G* freq=noraman nosymm scrf=(cpcm,solvent=aceton

itrile) scf=(qc,direct) opt=(calcf, maxcycle=500)\\geom&freq\\0,1\\N,0.
 5562084402,-0.3914194966,0.6161038585\\C,0.837464784,0.0583844246,1.864
 7903936\\N,2.1933970512,0.3176233997,2.1841233034\\C,3.2690063167,-0.058
 3684986,1.4132997941\\C,2.992828783,-0.5928319565,0.0286485332\\C,1.5387
 425502,-0.4377475411,-0.4313263189\\C,3.3939944203,0.4054786454,-1.1079
 096175\\C,1.9314979787,0.8732298212,-1.1956887557\\C,-0.8463377666,-0.67
 17059984,0.3179274138\\O,-0.0335136579,0.2311910774,2.7081749677\\C,2.48
 87371022,0.8780197119,3.5051506016\\O,4.4134031767,0.0493487254,1.82589
 51903\\H,3.4380289665,-1.5869164124,-0.0430796534\\H,3.6983354323,-0.142
 0025298,-1.9995706352\\H,1.5125715043,0.9909479571,-2.1987262898\\H,1.26
 9524549,-1.2194007349,-1.1439646404\\H,-1.4614313119,0.2226766606,0.452
 2061351\\H,-0.9141287403,-1.0038912075,-0.7182675035\\H,-1.2231083565,-1
 .4566435732,0.977648258\\H,2.8281908021,0.0929505329,4.1860641118\\H,1.5
 82818938,1.3362882655,3.891934662\\H,3.2766523759,1.6237444368,3.396614
 2198\\O,2.3864436505,3.8668626424,0.7697398603\\O,5.6242685904,1.2430678
 228,-1.0685923453\\N,4.0159466527,2.5328584752,-0.0941474135\\N,1.699972
 2504,2.0683325449,-0.4144146978\\C,2.6612830914,2.8644151422,0.11924210
 53\\C,4.4523767414,1.4220662666,-0.784721521\\C,0.3204334681,2.529131249
 6,-0.2724188516\\H,-0.313918062,1.8948795566,-0.8933947277\\H,-0.0144724
 441,2.4681523466,0.7682530632\\H,0.2329896848,3.564414344,-0.6096464448
 \\C,4.9972430516,3.4706622219,0.4543100962\\H,4.9056652537,4.4429463692,
 -0.0334729335\\H,4.8257836725,3.5886481919,1.5250123487\\H,5.9859260606,
 3.0552061168,0.2754574333\\Version=AM64L-G09RevB.01\\HF=-986.5286182\\RM
 SD=0.000e+00\\RMSF=4.065e-06\\Dipole=-2.1755177,-1.5144918,-2.3487472\\Qu
 adrupole=-18.6124473,7.9678234,10.6446239,-5.1748287,-0.4803499,-2.556
 1842\\PG=C01 [X(C12H16N4O4)]\\@
 Sum of electronic and thermal Free Energies= - 986.279902 Hartrees

[NO₃⁻] [c,s-DMU<->DMU]**

1\\1\\GINC-SPARTAN-RC202\\FOpt\\UM062X\\6-31+G(d)\\C12H16N5O7(2)\\UWILLE\\19-N
 ov-2018\\0\\#p M062X\\6-31+G* freq=noraman nosymm scrf=(cpcm,solvent=ace
 tonitrile) scf=(qc,direct) opt=(calcf, maxcycle=500)\\geom&freq\\0,2\\N
 ,0.7516155944,-0.2105386631,0.7406917513\\C,1.1136661226,0.4669779132,1
 .9197150855\\N,2.438402585,0.8792803562,2.0271656482\\C,3.4757939167,0.2
 883947511,1.3130862921\\C,3.117607225,-0.3382342264,-0.0130790105\\C,1.6
 311745606,-0.4403466211,-0.2521436482\\C,3.4164080548,0.6212417185,-1.2
 193028816\\C,1.9976466461,1.1144830606,-1.3790526612\\C,-0.6358418318,-0
 .6787208726,0.6587273125\\O,0.2842792522,0.7054864435,2.7674310297\\C,2.
 7877283212,1.6330171958,3.236276122\\O,4.6281473778,0.3767297975,1.6774
 347822\\H,3.6144195499,-1.3083393984,-0.0874693568\\H,3.7454357306,0.052
 6047716,-2.0883524125\\H,1.4104263724,0.8650403555,-2.2604410208\\H,1.29
 75204777,-1.1463842512,-1.005857536\\H,-1.3203826405,0.1579871025,0.800
 5804303\\H,-0.7843040252,-1.1283474654,-0.3212217594\\H,-0.8030924306,-1
 .4227326316,1.4408772189\\H,2.9240999049,0.9545933543,4.0826614411\\H,1.
 9826160113,2.3339175978,3.4474660712\\H,3.7163124675,2.1676509663,3.041
 4192938\\O,2.1809389816,4.0235453855,0.5968887878\\O,5.600840422,1.59785
 12679,-1.1794680531\\N,3.9344216525,2.7810111199,-0.1892006359\\N,1.6709
 074914,2.2841073476,-0.7709330661\\C,2.5848995767,3.0867941517,-0.05465
 37441\\C,4.4259947502,1.6989799279,-0.9100115595\\C,0.2742361255,2.73268
 17318,-0.7569609656\\H,-0.2828181063,2.1300235398,-1.4734219704\\H,-0.14
 64893766,2.6065073476,0.2448249596\\H,0.2274843057,3.7859723416,-1.0319
 738823\\C,4.9223542455,3.7005314909,0.3890228068\\H,5.4113965455,4.26546

71638,-0.4067466625\H,4.4049830034,4.3749684798,1.0662679423\H,5.66482
8797,3.1118867638,0.929565433\N,1.9204637168,-3.033261659,1.8119670174
\O,2.3873735282,-1.9916173742,2.3359063708\O,1.7487257141,-3.071127420
9,0.5734160026\O,1.6292333843,-4.0109458602,2.5190070273\\Version=AM64
L-G09RevB.01\HF=-1266.6670469\S2=0.754281\S2-1=0.\S2A=0.750013\RMSD=0.
000e+00\RMSF=8.601e-06\Dipole=-2.110686,5.3321211,-5.0503131\Quadrupol
e=-1.7661727,-6.9164712,8.6826438,20.3164547,-12.0998043,15.2251075\PG
=C01 [X(C12H16N5O7)]\\@
Sum of electronic and thermal Free Energies= -1266.413007 Hartrees

TS9

1\1\GINC-SPARTAN-RC071\FTS\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\02-Ma
y-2019\0\#p M062X/6-31+G* nosymm scf=(qc,direct) scrf=(cpcm,solvent=a
cetonitrile) opt=(ts,noeigentest,calcfc,maxcycle=500) freq=noraman\\ge
om&freq\\0,2\N,2.3083333226,2.0345106919,2.3885163472\C,3.0604655495,2
.6232943695,3.4225610373\N,4.4460511904,2.5498647709,3.3358928006\C,5.
1497421898,1.8569395414,2.3555023309\C,4.3451711261,1.4222827315,1.165
9890919\C,2.8400514535,1.3467147336,1.3238147343\C,4.1248587091,2.4650
499093,0.0145258242\C,2.6678710544,2.0035806429,-0.1581807955\C,0.8534
084042,2.1750162926,2.4891865809\O,2.4930275959,3.1838729796,4.3351194
625\C,5.2184470691,3.1532655702,4.4282460424\O,6.3419976328,1.66309828
63,2.4516466434\H,4.7673147614,0.5013208275,0.7611683878\H,4.776232265
1,2.3337772876,-0.8521829108\H,2.5560233993,1.1995654484,-0.8834546578
\H,2.3378352303,0.1998614468,1.2413739141\H,0.5216607589,1.7818625037,
3.452074168\H,0.5705061516,3.229543672,2.4212772752\H,0.406031861,1.60
18571851,1.677065262\H,5.4149178072,2.4117353788,5.2062670181\H,4.6447
587086,3.9800244262,4.8399160557\H,6.1598760255,3.5116278249,4.0156698
679\O,0.9336586682,5.0781932723,0.1486392165\O,5.3369158068,4.34868204
64,0.8090616108\N,3.0765330679,4.5773954841,0.762898809\N,1.7059357607
,3.0086843261,-0.3761242491\C,1.8354472911,4.2601208822,0.1711953501\C
,4.2482452275,3.8795439669,0.5356946349\C,0.4512572944,2.7150232827,-1
.072122294\H,0.1973472605,3.5589376306,-1.7134065012\H,0.5966665815,1.
8175172376,-1.6710521566\H,-0.3626213319,2.5460009476,-0.3610947889\C,
3.1845024686,5.8964707684,1.3956788034\H,2.2362232214,6.1229140257,1.8
781011745\H,3.9858181116,5.8510173807,2.1315901112\H,3.4127647595,6.66
30843808,0.6507837139\N,0.8002990407,-1.1384559099,0.5098697934\O,0.41
20069098,-0.0995521037,-0.0278886084\O,1.8836455694,-1.0980139667,1.22
39544993\O,0.2260910259,-2.2099431726,0.4130314007\\Version=AM64L-G09R
evB.01\HF=-1266.6530746\S2=0.754896\S2-1=0.\S2A=0.750021\RMSD=0.000e+0
0\RMSF=5.422e-06\Dipole=0.6821861,1.8181857,-0.4244235\Quadrupole=-7.2
879726,-4.5064538,11.7944264,2.7625593,-3.3915176,1.8015062\PG=C01 [X(
C12H16N5O7)]\\@

Vimag = -686.3235 cm⁻¹

Sum of electronic and thermal Free Energies= -1266.402488 Hartrees

Product complex between HNO₃ and c,s-DMU<>DMU radical 9

1\1\GINC-SPARTAN-RC053\FOpt\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\17-A
pr-2019\0\#p M062X/6-31+G* freq=noraman nosymm scrf=(cpcm,solvent=ace
tonitrile) scf=(qc,direct) opt=(calcfc,maxcycle=500)\\geom&freq\\0,2\N
,2.242345803,2.0848127804,2.3391331192\C,2.9382735164,2.5477963828,3.4
439669337\N,4.3330989255,2.4114967752,3.4575665527\C,5.0932165365,1.81

65710966,2.4613835417\C,4.3396511442,1.414388741,1.2250623717\C,2.8315
969762,1.4217150515,1.2815982622\C,4.2188394385,2.4402148013,0.0405884
381\C,2.7530635645,1.9956209687,-0.1601453259\C,0.7926625836,2.3062040
159,2.3461100984\O,2.3580562135,3.0768723681,4.3754922688\C,4.99987746
65,2.9152894137,4.6628084758\O,6.2903368859,1.6410104725,2.5732316547\
H,4.7543234308,0.4733055437,0.8556147474\H,4.913473826,2.2872979285,-0
.7880554484\H,2.6735970284,1.1983873134,-0.9007064325\H,2.0769015829,-
0.3399396648,1.3016144661\H,0.5668466598,3.3754486392,2.3069283574\H,0
.3726069224,1.7991723929,1.4775967672\H,0.3659575884,1.8840736227,3.25
76955788\H,4.632719425,2.3801271928,5.5398909294\H,4.791148514,3.98008
51783,4.7750902083\H,6.0673702725,2.7508473264,4.5427864651\O,1.084856
308,5.1391775918,-0.0578840612\O,5.4230167514,4.3098316077,0.883498836
8\N,3.1809611445,4.5963947527,0.6783973049\N,1.8265981379,3.0374864587
,-0.4813799489\C,1.9590487602,4.2898920056,0.0327313452\C,4.3404866196
,3.860366369,0.547663801\C,0.6022775275,2.7388687296,-1.2202057898\H,0
.7643790517,1.8272013565,-1.7950209036\H,-0.2486108296,2.5926703213,-0
.54645025\H,0.3793051624,3.5657363536,-1.8949542863\C,3.2908123487,5.9
245976651,1.2883656385\H,3.6225084805,6.6622044248,0.552606276\H,2.314
1115826,6.2063252737,1.674801414\H,4.0181076023,5.8655043019,2.0967722
482\N,0.6513817775,-1.234386283,0.4347864857\O,0.4366269184,-0.1850094
665,-0.137586697\O,1.6749450952,-1.2636518125,1.3165126146\O,0.0557882
566,-2.2712859907,0.3162959421\\Version=AM64L-G09RevB.01\HF=-1266.6629
821\S2=0.753672\S2-1=0.\S2A=0.75001\RMSD=0.000e+00\RMSF=2.410e-06\Dipo
le=-0.3242033,-0.45147,-0.923747\Quadrupole=-9.1894708,-5.0041679,14.1
936387,-8.1551222,-8.2516515,-3.6483042\PG=C01 [X(C12H16N5O7)]\\@
Sum of electronic and thermal Free Energies= -1266.410971 Hartrees

[c,s-DMU<>DMU]**

1\1\GINC-SPARTAN-RC098\FOpt\UM062X\6-31+G(d)\C12H16N4O4(1+,2)\UWILLE\2
7-Apr-2019\0\\#p M062X/6-31+G* scf=(qc,direct) nosymm scrf=(cpcm,solve
nt=acetonitrile) opt=(calcf, maxcycle=500) freq=noraman\\geom&freq\\1,
2\N,1.8642688205,1.0918408269,2.6316492151\C,2.2427811546,2.2090706238
,3.40315375\N,3.4599496756,2.8109060401,3.0895507192\C,4.4344448843,2.
2380782187,2.2801483811\C,3.9843731635,1.1494392241,1.3309829472\C,2.5
52391538,0.713460664,1.5346984676\C,3.790223698,1.682144072,-0.1321899
558\C,2.2913819128,1.8519894032,-0.0438948023\C,0.5857330048,0.4614477
005,2.9936088324\O,1.5251857927,2.6154589374,4.2856143128\C,3.82941410
12,3.9811918399,3.8988503811\O,5.5753842239,2.6430005861,2.2688601877\
H,4.6979354336,0.3231905054,1.3893968762\H,4.0651342862,0.9149719177,-
0.8556017926\H,1.6155448356,1.2259686722,-0.6231594955\H,2.2594172465,
-0.2471333981,1.1187390006\H,-0.2244476866,1.1859128958,2.9001716723\H
,0.4214403445,-0.3784871719,2.3215191363\H,0.6445800355,0.1141996519,4
.0254654147\H,4.1876613767,3.6635417039,4.8806439999\H,2.9498571552,4.
6126042949,4.0105972329\H,4.6188519299,4.5136502217,3.3721848574\O,2.1
552945189,5.2431914699,0.8872507893\O,5.6307358336,2.9625031574,-0.967
9783349\N,3.9702143877,4.1145188186,0.0716731016\N,1.8220911774,3.0789
306754,0.2812195585\C,2.6417826653,4.2230964987,0.4587213874\C,4.55072
26012,2.9528852061,-0.4269438582\C,0.3842073972,3.2884471352,0.4962635
744\H,-0.1352358507,2.3620232205,0.2541132852\H,0.2059034149,3.5619400
696,1.5390396453\H,0.0342386038,4.0958251086,-0.1475678028\C,4.7999960
691,5.3267868151,0.081626238\H,4.9034737085,5.7151596526,-0.9333535402

\H,4.3188253738,6.064473039,0.7186844199\H,5.7812281725,5.0633267028,0.4773311983\\Version=AM64L-G09RevB.01\HF=-986.2857249\S2=0.754512\S2-1=0.\S2A=0.750014\RMSD=0.000e+00\RMSF=2.092e-06\Dipole=-2.9235485,-3.3971965,-1.0240276\Quadrupole=-4.9790671,5.1147692,-0.1357022,6.3880344,10.7043191,-0.5148233\PG=C01 [X(C12H16N4O4)]\\@
Sum of electronic and thermal Free Energies= -986.039591 Hartrees

Product complex 10

1\1\GINC-SPARTAN-RC018\FOpt\UM062X\6-31+G(d)\C12H16N4O4(1+,2)\UWILLE\01-Jul-2019\0\\#p M062X/6-31+G* scf=verytight nosymm scrf=(cpcm,solvent=acetonitrile) freq=noraman opt=(calcf, maxcycle=500)\\geom&freq\\1,2\N,2.0870107693,0.6370890541,2.5380463667\C,2.1892761744,1.9416113744,3.0830989138\N,3.4037377981,2.581461157,2.9154950127\C,4.5339753157,1.9988640188,2.3245739843\C,4.2862139818,0.731393593,1.6476455918\C,3.0941626086,0.0676345527,1.8719856389\C,3.6016243423,1.7747650545,-0.6227137804\C,2.2734615971,2.0790638002,-0.3731095454\O,1.2387357558,2.43820023,3.6466482596\C,3.5802070018,3.884713246,3.571061427\O,5.6124996585,2.5652186262,2.3448078664\H,5.1192727694,0.2304342522,1.170871734\H,3.8726409669,0.8554354147,-1.1255550738\H,1.4794427882,1.3617946483,-0.5588448687\H,2.9203307411,-0.9316893971,1.4861073832\H,4.0255120598,3.7435620398,4.5586408479\H,2.6077884764,4.3627745014,3.6615462952\H,4.2470432983,4.4892450355,2.9573088825\O,2.4696032061,5.3358272712,0.8754921023\O,5.7721669062,2.6901653578,-0.8464419219\N,4.1614919594,4.0279665383,0.049444598\N,1.9105471062,3.2549878675,0.1393934426\C,2.8533475354,4.2969725502,0.3879065498\C,4.611257282,2.8268106059,-0.5116257015\C,0.5088064168,3.5783365736,0.4413525532\H,-0.105653539,2.7297078034,0.1470921164\H,0.4083494961,3.7657977297,1.5127353777\H,0.2220630042,4.4702471719,-0.1153892362\C,5.1692599029,5.078815261,0.2425469725\H,5.559930321,5.3849479723,-0.7292197992\H,4.6951523868,5.9206435931,0.7401902356\H,5.9776293229,4.67316549,0.852880684\C,0.812174208,-0.0604303648,2.7674168665\H,0.6268164145,-0.1183528519,3.8398997207\H,0.0048679464,0.4918461275,2.2853869619\H,0.8932658707,-1.0585042283,2.3420497917\\Version=AM64L-G09RevB.01\HF=-986.2967905\S2=0.758958\S2-1=0.\S2A=0.75007\RMSD=6.463e-09\RMSF=9.335e-06\Dipole=-3.2584973,-3.5923172,-1.0373355\Quadrupole=-8.6291034,6.5967842,2.0323192,2.0292549,8.8432341,-4.3642958\PG=C01 [X(C12H16N4O4)]\\@
Sum of electronic and thermal Free Energies= -986.050761 Hartrees

Selected geometries of other NO₃[•] – pyrimidine cyclobutane dimer complexes

[NO₃[•]] [t,s-DMU<>DMU]^{••}

1\1\GINC-SPARTAN-RC202\FOpt\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\22-Nov-2018\0\\#p M062X/6-31+G* scf=(qc,direct) scrf=(cpcm,solvent=acetonitrile) nosymm freq=noraman opt=(calcf, maxcycle=500)\\geom&freq\\0,2\N,0.0295877366,0.093442265,2.0139133447\C,-0.3463439909,-0.3758195756,3.2860575568\N,0.6449967839,-0.490794351,4.2550779181\C,1.9845866368,-0.1837693966,4.070512169\C,2.4118757614,0.2205027641,2.6768472356\C,1.282208239,0.491619789,1.7174005494\C,3.0193149935,1.6375009137,2.6563564334\C,4.2067892751,1.7408155498,1.7227298167\N,4.2026096253,2.7970312432,0.8300692278\C,3.0406422998,3.4219279768,0.3940316306\N,1.87299798

56,3.2495527169,1.1674817387\C,1.7879410072,2.3649745566,2.1798952837\
C,-1.0499906656,0.2353099454,1.0276056428\O,-1.4990018097,-0.666552460
4,3.5137847186\C,0.1863372305,-0.9550120968,5.5711635593\O,2.794136509
4,-0.2431680908,4.9707948998\H,3.1061619421,-0.546750288,2.3123243062\
O,5.1394536514,0.9722706588,1.8139720527\C,5.3766923279,2.9641431793,-
0.0324755352\O,3.0155352769,4.1315325035,-0.5860317416\C,0.6848804569,
3.9805551401,0.712022208\H,1.5191305119,0.5703862813,0.656105734\H,-0.
6047486099,0.6010307479,0.1025343628\H,-1.522771157,-0.7347092717,0.87
12764355\H,-1.7898377456,0.9454324032,1.4011767408\H,1.0544442247,-1.0
108407983,6.2220483776\H,-0.2747204969,-1.93742945,5.4657379837\H,-0.5
426637496,-0.2498810668,5.9723356065\H,6.2544900208,2.6673061618,0.536
6576628\H,5.4471702161,4.0100169133,-0.3234629509\H,5.2718668786,2.333
3160752,-0.9197144197\H,0.925367272,5.0401703211,0.6284153316\H,0.3802
167378,3.5840671704,-0.2589197849\H,-0.1037615066,3.8286661529,1.44792
28172\H,0.9937210783,2.5634905355,2.8977195855\H,3.3638052625,1.977260
3346,3.6412663889\N,2.2244708029,1.2398678433,-1.6735873468\O,3.047174
0123,0.8201973862,-0.8214912331\O,1.0767978806,1.5721757088,-1.2940574
623\O,2.5473960941,1.3291776084,-2.8652488444\\Version=AM64L-G09RevB.0
1\HF=-1266.6714479\S2=0.755344\S2-1=0.\S2A=0.750019\RMSD=0.000e+00\RMS
F=3.588e-06\Dipole=-2.5953719,1.0397628,5.2754114\Quadrupole=-17.97758
1,17.3788484,0.5987326,1.5004122,11.1907349,20.8125799\PG=C01 [X(C12H1
6N5O7)]\\@

CT complex between NO₃⁻ and t, α -DMU<->DMU

1\1\GINC-SPARTAN-RC023\FOpt\UM062X\6-31+G(d)\C12H16N5O7(2)\UWILLE\18-M
ay-2019\0\#p M062X/6-31+G* scf=(qc,direct) nosymm freq=noraman scrf=(
cpcm,solvent=acetonitrile) opt=(calcf, maxcycle=500)\geom&freq\0,2\C
,2.6271242557,2.8250451434,2.8523724378\C,1.3528823108,3.423228929,2.2
548563972\C,3.0828227015,4.2566257898,3.275603421\C,4.5306184403,4.570
8894023,3.0237476544\N,4.8064563535,5.3077026492,1.8985517359\C,3.8628
116899,5.6346640212,0.8958676909\N,2.5666550144,5.2567421267,1.0730999
959\C,2.0136568363,4.8390886807,2.3395494649\H,3.2801498096,2.37977815
13,2.0994843397\O,5.3944467936,4.1655896231,3.7834497024\C,6.197585292
3,5.6740689951,1.6180079353\O,4.2429551424,6.2122047676,-0.11234797\C,
1.6040889176,5.7081555177,0.0712480577\H,1.0961725122,3.0832816363,1.2
497438627\H,6.7600399468,5.5743530189,2.543234342\H,6.2291708242,6.702
5243342,1.2631742948\H,6.6177628316,5.0134361737,0.8559921722\H,1.4096
510332,6.781249207,0.1732059263\H,1.9878181271,5.5035671802,-0.9275788
541\H,0.6718195371,5.1601113003,0.2203898658\H,1.3794485962,5.62575158
61,2.7621028558\H,2.8655953933,4.4625367493,4.3269601336\C,3.575334231
2,1.0991669794,4.3679657126\H,3.225861745,0.2336172347,4.9283507436\H,
4.1493279013,0.7926007575,3.4941960085\H,4.190964403,1.7367078347,5.01
35944124\C,-0.9048368645,2.7031718535,5.2777305653\H,-1.7292752957,3.2
082775751,4.7826161918\H,-1.1711648054,1.6693005068,5.504228783\H,-0.6
370688638,3.2229700387,6.198495867\N,0.241619375,2.7098042189,4.360307
2561\N,2.4248380627,1.8587047702,3.8993032598\C,0.1207433919,3.3252611
347,3.114030768\C,1.3587142332,2.039566869,4.8233546948\O,1.4437658533
,1.5989419121,5.944387427\O,-0.9264252846,3.8165108498,2.7488802518\O,
1.5627778223,0.4794027056,2.4085202331\O,0.3915594271,-1.2779508831,2.
0396025063\O,0.3363293873,-0.3507300483,3.9964580673\N,0.7304289212,-0
.4181812924,2.8389347895\\Version=AM64L-G09RevB.01\HF=-1266.6507637\S2

=0.759114\S2-1=0.\S2A=0.750065\RMSE=0.000e+00\RMSF=5.321e-06\Dipole=1.1015326,2.6879314,0.6262698\Quadrupole=-1.59404,6.9679679,-5.3739279,1.720577,7.4319134,23.0953158\PG=C01 [X(C12H16N5O7)]\@

[NO₃⁻] [c,s-DMT<>DMT]**

1\1\GINC-SPARTAN-RC018\FOpt\UM062X\6-31+G(d)\C14H20N5O7(2)\UWILLE\17-A
pr-2019\0\#p M062X/6-31+G* nosymm scrf=(cpcm,solvent=acetonitrile) sc
f=(qc,direct) opt=(calcf, maxcycle=500) freq=noraman\geom&freq\0,2\N
,1.0951375696,-0.0086088672,0.5071495148\C,1.4490808955,0.7084884097,1
.6609151436\N,2.7872495546,1.0627555519,1.7890019565\C,3.818748225,0.4
314819932,1.1010499393\C,3.4852548032,-0.2197932929,-0.2336366302\C,1.
9856784227,-0.2705567714,-0.46971756\C,3.7815377761,0.7844616808,-1.44
45986121\C,2.3613998606,1.2931883479,-1.557391731\C,-0.3048930867,-0.4
326901081,0.410218823\O,0.6071669117,1.0281890237,2.4696183925\C,3.138
4711684,1.8370478989,2.9845117539\O,4.9613193785,0.4822467534,1.503043
1938\H,1.7699926894,1.0557499405,-2.4412891674\H,1.6314251027,-0.97516
48251,-1.2178717872\H,-0.9616301385,0.4379292456,0.4348821018\H,-0.430
2499826,-0.9794571832,-0.5220854882\H,-0.5336827197,-1.0845662424,1.25
58397911\H,3.2007181272,1.1819206927,3.8575262184\H,2.3712192891,2.592
8916572,3.1408126826\H,4.1054041263,2.306176543,2.80964999\O,2.5365235
687,4.1804986798,0.4477125302\O,5.9679224929,1.7453547595,-1.279575317
3\N,4.2882390914,2.9221199256,-0.3150592987\N,2.0342263763,2.462376871
7,-0.9486109268\C,2.9420008835,3.2466954117,-0.2078177867\C,4.78427549
12,1.8530511965,-1.0508278948\C,0.6414478178,2.9240525148,-0.949464683
4\H,0.0864433,2.3286599651,-1.6735906403\H,0.2085706911,2.8028496397,0
.0479939848\H,0.6082417139,3.977988496,-1.2243878277\C,5.2760813562,3.
805560981,0.3177814107\H,5.8195534208,4.3600041998,-0.4492746823\H,4.7
480399602,4.4909840008,0.9754932373\H,5.9735471188,3.1889828207,0.8870
565933\N,1.7553922243,-2.7513152044,1.9064547939\O,2.4153582235,-1.763
3906483,2.317530642\O,1.5471579724,-2.8826654648,0.6808796607\O,1.3129
343838,-3.5843879042,2.7153100708\C,4.2198700186,-1.5559488784,-0.3361
892718\H,3.9997068158,-2.1568575858,0.5455263703\H,3.9075776126,-2.107
1416995,-1.2248234305\H,5.2950494273,-1.3645365884,-0.387155514\C,4.22
09449821,0.088642381,-2.7278265251\H,4.2880995689,0.828611204,-3.52999
95876\H,5.2002796096,-0.3726679142,-2.5972724446\H,3.5015979051,-0.677
9646081,-3.0273319879\Version=AM64L-G09RevB.01\HF=-1345.2627675\S2=0.
754358\S2-1=0.\S2A=0.750013\RMSE=0.000e+00\RMSF=2.881e-06\Dipole=-0.92
18698,4.9403628,-5.7803168\Quadrupole=0.3320542,-5.837301,5.5052468,15
.9181713,-15.6506357,13.5994319\PG=C01 [X(C14H20N5O7)]\@

CT complex between NO₃⁻ and c,a-DMT<>DMT

1\1\GINC-SPARTAN-RC155\FOpt\UM062X\6-31+G(d)\C14H20N5O7(2)\UWILLE\02-M
ay-2019\0\#p M062X/6-31+G* scf=(qc,direct) nosymm scrf=(cpcm,solvent=
acetonitrile) freq=noraman opt=(calcf, maxcycle=500)\geom&freq\0,2\N
,0.4788730084,-0.4895035935,0.5060504557\C,0.6975566406,-0.027817843,1
.7646875152\N,2.0448015978,0.2825100614,2.1130414212\C,3.1514085351,-0
.0140409074,1.3616431844\C,2.9190814719,-0.6571290628,0.0059241177\C,1
.4954831725,-0.4517773884,-0.5018091079\C,3.3550426992,0.4331186227,-1
.1865914643\C,1.9000255764,0.9006924681,-1.2026903895\C,-0.9129786127,
-0.6495045995,0.0867306907\O,-0.1901554605,0.1264587002,2.5853844838\C
,2.2865885453,0.8747255995,3.4339208919\O,4.2834565949,0.2327221548,1.

7459474285\H,-1.4673629985,-1.169075259,0.8676245533\H,-1.374129095,0.325544406,-0.1006504262\H,-0.9275009194,-1.2445183639,-0.8268365245\H,2.6595240249,0.1138655677,4.1237073612\H,1.3490616749,1.2822657302,3.8009576197\H,3.0350687837,1.6606162431,3.329796334\C,1.6635466709,2.089650233,-0.3048493709\C,4.0979087324,2.530127543,-0.1216952837\N,2.7799743801,2.7780259916,0.1983725525\N,4.3568740646,1.3244570303,-0.8548560182\O,0.5447646016,2.4523598959,-0.0185046524\O,5.0242602826,3.234638832,0.1914524684\C,5.7506841305,0.9948015869,-1.1058192251\H,6.2350485958,1.8517878509,-1.5797221635\H,6.2364840106,0.8065329921,-0.1418645657\H,5.7816426727,0.1133315435,-1.7441768558\C,2.5195026464,3.9429116955,1.0577264622\H,3.4015415405,4.1257383718,1.6670024627\H,2.3032364329,4.8178539325,0.4404686077\H,1.6582279531,3.7143467384,1.6829063397\C,3.5900800496,-2.0041373451,-0.096294395\H,4.6538612537,-1.9229949529,0.1428585946\H,3.123938018,-2.6833696749,0.6293464701\H,3.4588845815,-2.4133285645,-1.0994223703\C,1.2955866184,1.1533690706,-2.5821184809\H,0.2204650044,1.3237677725,-2.4774864559\H,1.7517855308,2.0306265911,-3.0509080772\H,1.4670630993,0.2791742366,-3.2146610229\H,1.2635024765,-1.1796528667,-1.2838073587\H,3.6532896758,-0.2025736103,-2.0305838067\O,2.5782403235,-1.845324584,-3.2443730271\O,3.840840215,-2.8065619938,-4.7175860849\O,4.6963303918,-1.4105435958,-3.3018033151\N,3.7048048073,-2.0274602565,-3.7646405728\\Version=AM64L-G09RevB.01\HF=-1345.2488681\S2=0.757536\S2-1=0.\S2A=0.75004\RMSD=0.000e+00\RMSF=1.046e-05\Dipole=-0.329065,3.3981514,3.1625311\Quadrupole=6.6814652,13.5984427,-20.2799079,25.8003999,29.8604146,-26.2172622\PG=C01 [X(C14H20N5O7)]\\@

[NO₃⁻] [c,s-DMU^{6Me}<>DMU^{6Me}]⁺⁺

1\1\GINC-SPARTAN-RC071\FOpt\UM062X\6-31+G(d)\C14H20N5O7(2)\UWILLE\03-May-2020\0\#p M062X/6-31+G* scrf=(cpcm,solvent=acetonitrile) nosymm fr eq=noraman opt=(calcf, maxcycle=500)\geom&freq\0,2\N,0.6924511807,-0.7689400225,0.1675165408\C,0.5815303918,0.2456333307,1.1971339331\N,1.7542476169,0.7134121664,1.7382127383\C,3.0060452444,0.4406408553,1.2092690145\C,2.996126773,-0.1976535002,-0.1498687795\C,1.8305469867,-1.0632907447,-0.3967904987\C,3.0234871563,0.9699853444,-1.2844868969\C,1.9149973326,1.93768079,-1.1996517629\C,-0.5267839108,-1.5604370043,-0.0858263197\O,-0.5074656221,0.6147488798,1.5572600952\C,1.6256639847,1.508252522,2.9649210844\O,4.0353281915,0.8005498354,1.741599828\H,3.9177950356,-0.77019469,-0.2768308948\H,3.0174060184,0.447741489,-2.2450946787\H,-1.2594260357,-1.2987583768,0.670697773\H,-0.911733943,-1.3234142833,-1.0794680568\H,-0.2749171165,-2.6179132323,-0.0117292033\H,1.1664290188,0.8944821994,3.7421184238\H,1.0019657187,2.3821435889,2.7717823354\H,2.6251141407,1.8154793794,3.2630154594\O,3.4771775196,4.3929791694,0.8340343195\O,5.3961096338,1.0440342091,-1.5479361759\N,4.4363296664,2.8378754897,-0.5318612449\N,2.083385059,3.0056125662,-0.3353777004\C,3.325976196,3.4674588693,0.0519215375\C,4.3959399293,1.6132281787,-1.1519605201\C,0.9045776732,3.7417852879,0.1339118495\H,0.4359792031,4.2721138979,-0.6985747783\H,0.1867661807,3.0413799728,0.5685162665\H,1.2257307744,4.4561180261,0.88762771\C,5.7523147077,3.4193456742,-0.2524985373\H,6.417789676,3.1547256584,-1.0713177761\H,5.6478844865,4.4990062839,-0.1783995757\H,6.1453783097,3.0203774885,0.686718134\N,1.8758565247,-2.5537299796,2.6689223777\O,0.7779182261,-1.954712033,2.6917862665\O,2.7172870128,-2.2652928415,1.7785634883\O,2.1376304049,-3.422510

3325,3.5118417342\C,1.9386191661,-2.1910458817,-1.3557423512\H,1.94655
38778,-3.1227093089,-0.774038127\H,1.0908684176,-2.2235827642,-2.04414
34602\H,2.8710598841,-2.1289477685,-1.9171324957\C,0.6529228496,1.8163
823254,-1.987200343\H,0.6934885928,0.9344634212,-2.6304997209\H,-0.243
3026627,1.7337698828,-1.35757703\H,0.5075965282,2.692706982,-2.6332459
816\\Version=AM64L-G09RevB.01\HF=-1345.2796765\S2=0.757328\S2-1=0.\S2A
=0.750041\RMSD=3.166e-09\RMSF=4.617e-06\Dipole=-2.741581,2.3905389,-6.
0854827\Quadrupole=-9.4412311,7.8992504,1.5419807,9.2230536,-18.202939
9,20.2552912\PG=C01 [X(C14H20N5O7)]\\@

CT complex between NO₃⁻ and c,α-DMU^{6Me}<>DMU^{6Me}

1\1\GINC-SPARTAN-RC053\FOpt\UM062X\6-31+G(d)\C14H20N5O7(2)\UWILLE\14-M
ay-2019\0\#p M062X/6-31+G* scf=(qc,direct) nosymm scrf=(cpcm,solvent=
acetonitrile) freq=noraman opt=(calcf, maxcycle=500)\geom&freq\0,2\N
,-2.2534536989,-2.8356247884,-1.7537537928\C,-2.2346972561,-2.83884741
,-0.3940111536\N,-0.9877439499,-2.9818702296,0.2622855788\C,0.21454458
17,-3.0723141756,-0.3795785825\C,0.1791380547,-3.4438499591,-1.8410957
002\C,-1.1360836948,-3.2084154241,-2.6068437514\C,0.926944349,-2.44636
06752,-2.8165263627\C,-0.4471151746,-2.0007503407,-3.3680209326\C,-3.5
58497625,-2.6301834229,-2.3869381896\O,-3.2418246612,-2.675812944,0.27
89204228\C,-0.991132714,-2.8095591635,1.7185541511\O,1.2845953305,-2.9
150253477,0.1883239688\H,0.5742212471,-4.4628204344,-1.912623468\H,-0.
5248459978,-2.0172649837,-4.4570781887\H,-4.1058926495,-1.8708220325,-
1.8299481652\H,-3.3997696276,-2.2725024075,-3.4044418323\H,-4.14002584
59,-3.5571919585,-2.4056679117\H,-1.8532309901,-3.3311092162,2.1282326
125\H,-1.0489956152,-1.7484311331,1.9749243116\H,-0.0673706457,-3.2311
070798,2.108368818\C,-0.9652287561,-0.6936834487,-2.8544658207\C,0.984
0964471,-0.3466571653,-1.4141716626\N,-0.3507884196,-0.1881790648,-1.6
949516974\N,1.6618019319,-1.4019990844,-2.1270660676\O,-1.9421796732,-
0.1525028866,-3.3160476401\O,1.5865551615,0.3222912143,-0.6125252\C,3.
0906614664,-1.5196417281,-1.9336412946\H,3.4218123073,-0.7314581977,-1
.2641504801\H,3.3016432908,-2.5053180944,-1.5073016896\H,3.5670123108,
-1.4223482188,-2.9165118111\C,-1.036038578,0.8907347737,-0.9715257199\
H,-0.7325869197,0.8483708279,0.0730354028\H,-0.7708841031,1.8619205745
,-1.3969747102\H,-2.1073446748,0.7244417167,-1.0652235727\C,-1.5166878
341,-4.3725237637,-3.5149810706\H,-1.8422261701,-5.2167868975,-2.89918
00172\H,-2.3230678853,-4.0964543327,-4.1979915535\H,-0.6654059574,-4.6
943971671,-4.1174987697\C,1.8048243286,-3.1361067151,-3.8493542901\H,2
.2080972575,-2.3910787172,-4.5412028559\H,2.6231764615,-3.6876633237,-
3.3813919833\H,1.2054100608,-3.8481664354,-4.417543182\O,1.4067932775,
0.1810806543,-3.9429288454\O,3.3407450827,-0.2646932606,-4.8103447128\
O,2.1613325334,1.3828218115,-5.5633487266\N,2.321618637,0.4394130552,-
4.7891058615\\Version=AM64L-G09RevB.01\HF=-1345.2476392\S2=0.757801\S2
-1=0.\S2A=0.750048\RMSD=0.000e+00\RMSF=6.378e-06\Dipole=-1.3567207,-4.
7339884,1.6696964\Quadrupole=-7.0329786,32.6221334,-25.5891549,-7.2750
296,20.4903323,36.9774362\PG=C01 [X(C14H20N5O7)]\\@

[NO₃⁻] [t,s-DMU^{6Me}<>DMU^{6Me}]^{•+}

1\1\GINC-SPARTAN-RC126\FOpt\UM062X\6-31+G(d)\C14H20N5O7(2)\UWILLE\25-J
un-2019\0\#p M062X/6-31+G* scf=(qc,direct) nosymm scrf=(cpcm,solvent=
acetonitrile) freq=noraman opt=(calcf, maxcycle=500)\geom&freq\0,2\N

, -0.023956772, -0.1436526953, -0.0210330368\C, -0.3714068523, -0.935520932
2, 1.1047889662\N, 0.6115027886, -1.2014058086, 2.0441572646\C, 1.894112926
6, -0.685662852, 1.9986791226\C, 2.3353448655, -0.090223751, 0.6819452038\C
, 1.2400959979, 0.1973609406, -0.3136469883\C, 2.9902913527, 1.2920205108, 0
.8754348834\C, 4.2244735148, 1.4328256735, 0.0120315836\N, 4.2908128487, 2.
5348685244, -0.8163538666\C, 3.2413269665, 3.4189469203, -1.0522566214\N, 2
.0466094335, 3.2344732924, -0.3304534345\C, 1.856445846, 2.239662149, 0.573
8245271\C, -1.0986287745, 0.043218576, -1.0066142257\O, -1.4995707252, -1.3
522490609, 1.2317067987\C, 0.1962728649, -1.9951989015, 3.2076006504\O, 2.6
47355528, -0.7299454743, 2.9472689292\H, 3.0354240991, -0.8321455076, 0.270
9033039\O, 5.1160017381, 0.6124590792, 0.077335963\C, 5.5067520408, 2.76297
88283, -1.6086582399\O, 3.361114371, 4.32153723, -1.8521278098\C, 0.9747973
302, 4.2141519804, -0.5720695588\H, -0.9387152013, 0.9827209298, -1.5318346
212\H, -1.0987729099, -0.7930264882, -1.7114160521\H, -2.0466391022, 0.0765
77464, -0.4770058133\H, 1.0949139292, -2.2650111111, 3.7568137148\H, -0.312
7428447, -2.8897409303, 2.8508895047\H, -0.4714138606, -1.4095426937, 3.842
962117\H, 6.2763110818, 2.0961796666, -1.2294843696\H, 5.8123201275, 3.8024
461232, -1.4972207971\H, 5.3092947989, 2.5497409285, -2.6608865905\H, 0.870
5302451, 4.8683153216, 0.296263975\H, 1.2417977135, 4.8017403908, -1.444874
0365\H, 0.0375937442, 3.6878579306, -0.7560391193\H, 3.3450594461, 1.410542
8355, 1.9101732952\C, 0.7734410682, 2.4076352431, 1.5937034349\H, -0.221159
1221, 2.4877924435, 1.1456249652\H, 0.7665511847, 1.5755994631, 2.299753847
3\H, 0.9596485345, 3.3222750501, 2.172174164\C, 1.6168901567, 0.4285328355,
-1.7434685191\H, 1.1221841887, 1.2958331794, -2.1898294395\H, 2.6963756257
, 0.5488224919, -1.8474789672\H, 1.3278067948, -0.4613208757, -2.3167135127
\O, 2.6812633044, -3.2243789381, 0.8560945765\O, 0.7322423884, -4.155813789
2, 0.7184481698\O, 1.2862911898, -2.590365407, -0.6708605098\N, 1.568261129
2, -3.3357827856, 0.2995621689\\Version=AM64L-G09RevB.01\HF=-1345.269674
3\S2=0.752848\S2-1=0.\S2A=0.750007\RMSD=0.000e+00\RMSF=5.337e-06\Dipol
e=-1.6043225, 8.4683633, -1.200346\Quadrupole=-2.7294447, -11.3475516, 14.
0769963, 21.9605296, -7.6642813, 10.6091799\PG=C01 [X(C14H20N5O7)]\\@