

**Nitrosation mechanisms, kinetics, and dynamics of the guanine and 9-methylguanine radical cations by nitric oxide — Radical-radical combination at different electron configurations**

Jonathan Benny,<sup>a,b</sup> Toru Saito<sup>\*c</sup>, and Jianbo Liu<sup>\*a,b</sup>

<sup>a</sup> Department of Chemistry and Biochemistry, Queens College of the City University of New York, 65-30 Kissena Blvd., Queens, NY 11367, USA;

<sup>b</sup> The Ph.D. Program in Chemistry, the Graduate Center of the City University of New York, 365 5th Ave., New York, NY 10016, USA;

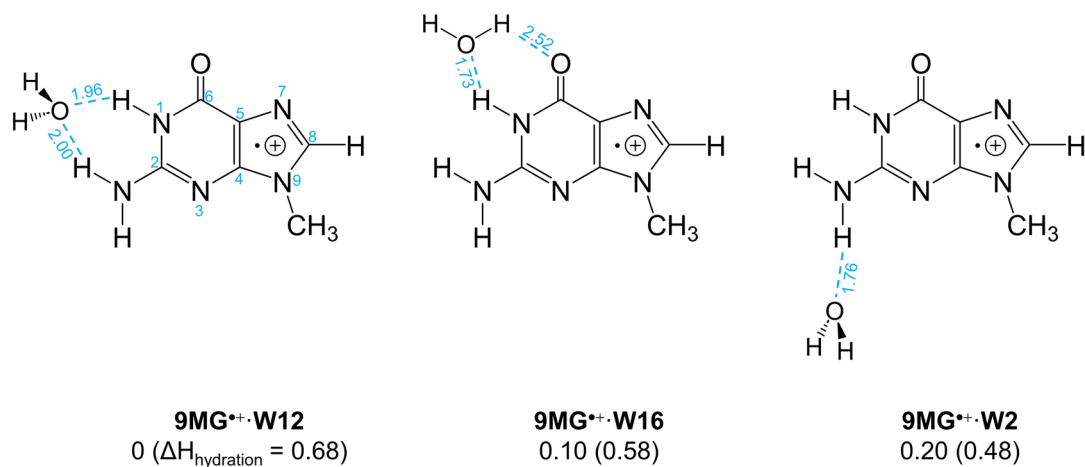
<sup>c</sup> Department of Biomedical Information Science, Graduate School of Information Science, Hiroshima City University, 731-3194 Hiroshima, Japan

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\* Corresponding author email: jianbo.liu@qc.cuny.edu. Tel: 1-718-997-3271.  
Co-corresponding author email: tsaito@hiroshima-cu.ac.jp.



**Fig. S1** Low-energy conformers of 9MG<sup>•+</sup>·H<sub>2</sub>O, with atomic numbering scheme. Hydration sites are indicated by the last two numbers in the notation, and hydrogen bonds are depicted by blue dashed lines with lengths shown in Å. Relative enthalpies (eV, with respect to the global minima) and hydration energies (in parentheses) were evaluated at the DLPNO-CCSD(T)/aug-cc-pVTZ//ωB97XD/6-31+G(d,p) level of theory, including 298 K thermal corrections.

**Table S1.** Experimental and calculated ionization energies (0 K, eV) for •NO and 9MG

|     | Experiment <sup>68</sup> | ωB97XD/<br>6-31+G(d,p)   | DLPNO-CCSD(T)/<br>aug-cc-pVTZ | CASSCF/<br>6-31+G(d,p) | CASMP2/<br>6-31+G(d,p) |
|-----|--------------------------|--------------------------|-------------------------------|------------------------|------------------------|
| •NO | 9.2643                   | 9.75                     | 9.20                          | 7.56                   | 9.06                   |
| 9MG | –                        | 7.53                     | 7.63                          | 6.88                   | 7.69                   |
|     | CASMP2/<br>6-311+G(d,p)  | CASMP2/<br>6-311++G(d,p) | CASMP2/<br>ANO-RCC-VTZP       | CASPT2/<br>6-31G(d,p)  | CASPT2/<br>ANO-L-VTZP  |
| •NO | 8.42                     | 8.42                     | 8.16                          | 8.99                   | 9.12                   |
| 9MG | 7.74                     | 7.72                     | 4.89                          | 7.14                   | 7.81                   |

**Table S2.** Reaction  $\Delta H$  (298 K, eV) calculated at different levels of theory

| Species  | $\omega$ B97XD/<br>6-31+G(d,p) <sup>a</sup>                                      | DLPNO-CCSD(T)/<br>aug-cc-pVTZ  | CASPT2/<br>ANO-L-VTZP  |
|--|--|--|--|
| <sup>1,CS</sup> [2-NHNO-3H-9MG] <sup>+</sup>         | -0.66 (1.49) <sup>b</sup>  | -0.14 (1.80)   | -0.64 (1.25)   |
| <sup>1,CS</sup> [3-NO-9MG] <sup>+</sup>              | -0.53 (-0.13)  | -0.09 (0.15)   | -0.58 (-0.50)  |
| <sup>1,CS</sup> [5-NO-9MG] <sup>+</sup>              | -0.64 (-0.50)  | -0.36 (-0.20)  | -0.74 (-0.57)  |
| <sup>1,CS</sup> [7-NO-9MG] <sup>+</sup>              | -1.21 (barrierless)  | -0.78 (barrierless)  | -1.20 (barrierless)  |
| <sup>1,CS</sup> [8-NO-9MG] <sup>+</sup>              | -0.61 (barrierless)  | -0.19 (barrierless)  | -0.44 (barrierless)  |
| <sup>1,CS</sup> [7H-8-NO-9MG] <sup>+</sup>           | -1.60 (0.96)   | -1.03 (1.44)   | -1.39 (1.15)   |
| <sup>1,CS</sup> [7H-8-ON-9MG] <sup>+</sup>           | 0.92 (3.63)  | 1.52 (4.06)  | 1.26 (3.90)  |
| <sup>1,CS</sup> [4,5-NO-9MG] <sup>+</sup>            | 1.54 (1.57)  | 1.98 (2.01)  | 1.95 (1.77)  |
| <sup>1,CS</sup> [7,8-NO-9MG] <sup>+</sup>            | 1.00 (1.01)  | 1.55 (1.57)  | 1.13 (1.15)  |
| <sup>1,OS</sup> precursor                            | -1.00  | —  | —  |
| <sup>1,OS</sup> [8- $\dot{O}N$ -9MG] <sup>+</sup>    | 1.13 (1.46)  | —  | —  |
| <sup>1,OS</sup> [7H-8- $\dot{O}N$ -9MG] <sup>+</sup> | 0.64 (3.41)  | —  | —  |
| <sup>1,OS</sup> [2,4- $\dot{N}O$ -9MG] <sup>+</sup>  | 2.82 (2.92)  | —  | —  |
| <sup>1,OS</sup> [5,8- $\dot{N}O$ -9MG] <sup>+</sup>  | 1.45 (1.79)  | —  | —  |
| <sup>1,OS</sup> [5,8- $\dot{O}N$ -9MG] <sup>+</sup>  | 1.19 (1.59)  | —  | —  |
| <sup>1,OS</sup> [7,8- $\dot{O}N$ -9MG] <sup>+</sup>  | 2.19 (2.29)  | —  | —  |
| <sup>3</sup> precursor                               | -0.58  | -0.13  | -0.43  |
| <sup>3</sup> [2NHNO-3H-9MG] <sup>+</sup>             | 1.10 (3.18)  | 1.89 (3.86)  | 1.47 (3.33)  |
| <sup>3</sup> [3-NO-9MG] <sup>+</sup>                 | 1.11 (1.15)  | 1.88 (1.91)  | 1.39 (1.35)  |
| <sup>3</sup> [4-NO-9MG] <sup>+</sup>                 | 1.04 (1.08)  | 1.70 (1.72)  | 1.40 (1.37)  |
| <sup>3</sup> [5-NO-9MG] <sup>+</sup>                 | 0.37 (0.49)  | 1.00 (1.05)  | 0.56 (0.73)  |
| <sup>3</sup> [7-NO-9MG] <sup>+</sup>                 | 0.42 (0.84)  | 1.26 (1.60)  | 0.72 (1.05)  |
| <sup>3</sup> [8-NO-9MG] <sup>+</sup>                 | 0.16 (0.41)  | 0.81 (1.01)  | 0.45 (0.62)  |
| <sup>3</sup> [7H-8NO-9MG] <sup>+</sup>               | -1.19 (1.48)   | -0.31 (2.28)   | -0.89 (1.75)   |
| <sup>3</sup> [3-ON-9MG] <sup>+</sup>                 | 2.31 (2.35)  | 2.91 (2.94)  | 2.50 (2.52)  |
| <sup>3</sup> [4-ON-9MG] <sup>+</sup>                 | 1.70 (1.74)  | 2.19 (2.30)  | 1.92 (2.08)  |
| <sup>3</sup> [5-ON-9MG] <sup>+</sup>                 | 1.05 (1.17)  | 1.57 (1.74)  | 1.30 (1.45)  |
| <sup>3</sup> [7-ON-9MG] <sup>+</sup>                 | 1.66 (1.96)  | 2.34 (2.60)  | 1.87 (2.14)  |
| <sup>3</sup> [8-ON-9MG] <sup>+</sup>                 | 0.77 (1.03)  | 1.30 (1.63)  | 1.06 (1.31)  |
| <sup>3</sup> [7H-8-ON-9MG] <sup>+</sup>              | -0.21 (2.37)   | 0.51 (2.99)  | 0.12 (2.53)  |
| <sup>3</sup> [2,4-NO-9MG] <sup>+</sup>               | 2.97 (3.13)  | 3.49 (3.69)  | 3.37 (3.38)  |
| <sup>3</sup> [5,8-NO-9MG] <sup>+</sup>               | 1.36 (1.93 from [5-NO-9MG] <sup>+</sup> ,<br>1.75 from <sup>3</sup> precursor)   | 1.94 (2.54 from [5-NO-9MG] <sup>+</sup> ,<br>2.27 from <sup>3</sup> precursor)   | 1.70 (2.11 from [5-NO-9MG] <sup>+</sup> ,<br>1.86 from <sup>3</sup> precursor)   |
| <sup>3</sup> [7,8-NO-9MG] <sup>+</sup>               | 1.21 (1.73)  | 1.96 (2.43)  | 1.52 (1.89)  |
| <sup>3</sup> [4,5-ON-9MG] <sup>+</sup>               | 1.92 (1.93)  | 2.61 (2.65)  | 2.45 (2.29)  |
| <sup>3</sup> [5,8-ON-9MG] <sup>+</sup>               | 1.59 (2.25 from [5-ON-9MG] <sup>+</sup> ,<br>1.81 from [8-NO-9MG] <sup>+</sup> ) | 2.18 (2.74 from [5-ON-9MG] <sup>+</sup> ,<br>2.43 from [8-NO-9MG] <sup>+</sup> ) | 1.93 (2.36 from [5-ON-9MG] <sup>+</sup> ,<br>2.13 from [8-NO-9MG] <sup>+</sup> ) |
| <sup>3</sup> [7,8-ON-9MG] <sup>+</sup>               | 2.05 (2.08)  | 2.75 (2.83)  | 2.57 (2.45)  |

<sup>a</sup> The DFT energy of reactant <sup>\*</sup>NO was calculated by subtracting experimental IE(<sup>\*</sup>NO) from the energy of NO<sup>+</sup>, and spin projection was applied to singlet biradicals; <sup>b</sup> Numbers in parentheses indicate corresponding activation barriers.

**Table S3.**  $\langle \widehat{S}^2 \rangle$  and T1 diagnostic for reaction structures along with energy difference at different levels of theory <sup>a,b</sup>

| Species  | $\langle \widehat{S}^2 \rangle$   | T1  | $\Delta_{\omega B97XD-CASPT2}$   | $\Delta_{CCSD(T)-CASPT2}$   |
|--|---|---|--|---|
| <sup>1,CS</sup> [2-NHNO-3H-9MG] <sup>+</sup>               | 0.0000 (0.0000)   | 0.0147 (0.0152)   | -0.02 (0.24)   | 0.50 (0.55)   |
| <sup>1,CS</sup> [3-NO-9MG] <sup>+</sup>                    | 0.0000 (0.0000)   | 0.0148 (0.0161)   | 0.05 (0.37)  | 0.49 (0.65)   |
| <sup>1,CS</sup> [5-NO-9MG] <sup>+</sup>                    | 0.0000 (0.0000)   | 0.0160 (0.0159)   | 0.10 (0.07)  | 0.38 (0.37)   |
| <sup>1,CS</sup> [7-NO-9MG] <sup>+</sup>                    | 0.0000 (barrierless)  | 0.0158 (barrierless)  | -0.01  | 0.42  |
| <sup>1,CS</sup> [8-NO-9MG] <sup>+</sup>                    | 0.0000 (barrierless)  | 0.0162 (barrierless)  | -0.17  | 0.25  |
| <sup>1,CS</sup> [7H-8-NO-9MG] <sup>+</sup>                 | 0.0000 (0.0000)   | 0.0145 (0.0157)   | -0.21 (-0.19)  | 0.36 (0.29)   |
| <sup>1,CS</sup> [7H-8-ON-9MG] <sup>+</sup>                 | 0.0000 (0.0000)   | 0.0171 (0.0181)   | -0.34 (0.63)   | 0.26 (0.16)   |
| <sup>1,CS</sup> [4,5-NO-9MG] <sup>+</sup>                  | 0.0000 (0.0000)   | 0.0190 (0.0182) <sup>a</sup>  | -0.41 (-0.20)  | 0.03 (0.24)   |
| <sup>1,CS</sup> [7,8-NO-9MG] <sup>+</sup>                  | 0.0000 (0.0000)   | 0.0167 (0.0180)   | -0.13 (-0.14)  | 0.42 (0.42)   |
| <sup>1,OS</sup> precursor                                  | 0.7168 (0.0648)   | —   | —  | —   |
| <sup>1,OS</sup> [8- $\dot{O}\dot{N}$ -9MG] <sup>+</sup>    | 0.8292 (0.0000)   | —   | —  | —   |
| <sup>1,OS</sup> [7H-8- $\dot{O}\dot{N}$ -9MG] <sup>+</sup> | 0.9129 (0.9028)   | —   | —  | —   |
| <sup>1,OS</sup> [2,4- $\dot{N}O$ -9MG] <sup>+</sup>        | 0.9328 (0.0000)   | —   | —  | —   |
| <sup>1,OS</sup> [5,8- $\dot{N}O$ -9MG] <sup>+</sup>        | 1.0074 (0.0000)   | —   | —  | —   |
| <sup>1,OS</sup> [5,8- $\dot{O}\dot{N}$ -9MG] <sup>+</sup>  | 0.9336 (0.6254)   | —   | —  | —   |
| <sup>1,OS</sup> [7,8- $\dot{O}\dot{N}$ -9MG] <sup>+</sup>  | 1.0134 (0.9733)   | —   | —  | —   |
| <sup>3</sup> precursor                                     | 2.0204  | 0.0200  | -0.15  | 0.30  |
| <sup>3</sup> [2NHNO-3H-9MG] <sup>+</sup>                   | 2.0098 (2.0095)   | 0.0211 (0.0217)   | -0.37 (-0.15)  | 0.42 (0.53)   |
| <sup>3</sup> [3-NO-9MG] <sup>+</sup>                       | 2.0113 (2.0248)   | 0.0203 (0.0207)   | -0.28 (-0.20)  | 0.49 (0.56)   |
| <sup>3</sup> [4-NO-9MG] <sup>+</sup>                       | 2.0125 (2.0161)   | 0.0200 (0.0199)   | -0.36 (-0.29)  | 0.30 (0.35)   |
| <sup>3</sup> [5-NO-9MG] <sup>+</sup>                       | 2.0093 (2.0245)   | 0.0202 (0.0184)   | -0.19 (-0.24)  | 0.44 (0.32)   |
| <sup>3</sup> [7-NO-9MG] <sup>+</sup>                       | 2.0174 (2.0265)   | 0.0227 (0.0217)   | -0.30 (-0.21)  | 0.54 (0.55)   |
| <sup>3</sup> [8-NO-9MG] <sup>+</sup>                       | 2.0085 (2.0303)   | 0.0191 (0.0197)   | -0.29 (-0.21)  | 0.36 (0.39)   |
| <sup>3</sup> [7H-8NO-9MG] <sup>+</sup>                     | 2.0354 (2.0212)   | 0.0209 (0.0208)   | -0.30 (-0.27)  | 0.58 (0.53)   |
| <sup>3</sup> [3-ON-9MG] <sup>+</sup>                       | 2.0088 (2.0217)   | 0.0161 (0.0172)   | -0.19 (-0.17)  | 0.41 (0.42)   |
| <sup>3</sup> [4-ON-9MG] <sup>+</sup>                       | 2.0085 (2.0198)   | 0.0172 (0.0183)   | -0.22 (-0.34)  | 0.27 (0.22)   |
| <sup>3</sup> [5-ON-9MG] <sup>+</sup>                       | 2.0086 (2.0298)   | 0.0175 (0.0191)   | -0.25 (-0.28)  | 0.27 (0.29)   |
| <sup>3</sup> [7-ON-9MG] <sup>+</sup>                       | 2.0088 (2.0308)   | 0.0169 (0.0201)   | -0.21 (-0.18)  | 0.47 (0.46)   |
| <sup>3</sup> [8-ON-9MG] <sup>+</sup>                       | 2.0083 (2.0330)   | 0.0166 (0.0198)   | -0.29 (-0.28)  | 0.24 (0.32)   |
| <sup>3</sup> [7H-8-ON-9MG] <sup>+</sup>                    | 2.0088 (2.0086)   | 0.0170 (0.0176)   | -0.33 (-0.16)  | 0.39 (0.46)   |
| <sup>3</sup> [2,4-NO-9MG] <sup>+</sup>                     | 2.0133 (2.0479)   | 0.0181 (0.0226)   | -0.40 (-0.25)  | 0.12 (0.31)   |
| <sup>3</sup> [5,8-NO-9MG] <sup>+</sup>                     | 2.0112 (2.0497 from [5-NO-9MG] <sup>+</sup> , 2.0707 from <sup>3</sup> precursor)   | 0.0187 (0.0238 from [5-NO-9MG] <sup>+</sup> , 0.023 from <sup>3</sup> precursor)    | -0.34 (-0.18 from [5-NO-9MG] <sup>+</sup> , -0.11 from <sup>3</sup> precursor)   | 0.24 (0.43 from [5-NO-9MG] <sup>+</sup> , 0.41 from <sup>3</sup> precursor)   |
| <sup>3</sup> [7,8-NO-9MG] <sup>+</sup>                     | 2.0163 (2.0298)   | 0.0198 (0.0217)   | -0.31 (-0.16)  | 0.44 (0.54)   |
| <sup>3</sup> [4,5-ON-9MG] <sup>+</sup>                     | 2.0319 (2.0258)   | 0.0227 (0.0266)   | -0.53 (-0.36)  | 0.16 (0.36)   |
| <sup>3</sup> [5,8-ON-9MG] <sup>+</sup>                     | 2.0108 (2.0511 from [5-ON-9MG] <sup>+</sup> , 2.0449 from [8-NO-9MG] <sup>+</sup> ) | 0.0186 (0.0221 from [5-ON-9MG] <sup>+</sup> , 0.0243 from [8-NO-9MG] <sup>+</sup> ) | -0.34 (-0.11 from [5-ON-9MG] <sup>+</sup> , -0.32 from [8-NO-9MG] <sup>+</sup> ) | 0.25 (0.38 from [5-ON-9MG] <sup>+</sup> , 0.30 from [8-NO-9MG] <sup>+</sup> ) |
| <sup>3</sup> [7,8-ON-9MG] <sup>+</sup>                     | 2.0204 (2.0307)   | 0.0216 (0.0228)   | -0.52 (-0.37)  | 0.18 (0.38)   |

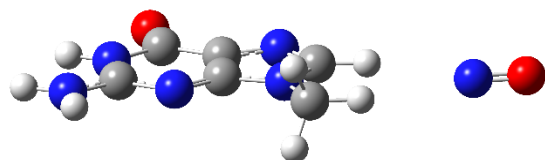
<sup>a</sup>  $\langle \widehat{S}^2 \rangle$  was evaluated at  $\omega B97XD/6-31+G(d,p)$  and T1 diagnostic was conducted at DLPNO-CCSD(T)/aug-cc-pVTZ;<sup>b</sup> numbers in parentheses are for corresponding activation barriers.

### Cartesian coordinates for the ion-molecule encounter and TS-like structures in Fig. 3

#### $1.0^{\text{S}}$ [ion-molecule encounter]<sup>+</sup>

N1 0.933181 -0.611436 -0.000023  
 C2 1.459247 0.641953 -0.000030  
 H3 2.529631 0.809287 -0.000039  
 N4 0.542372 1.621584 -0.000023  
 C5 -0.618852 0.978828 -0.000011  
 C6 -1.988124 1.488001 0.000003  
 O7 -2.373661 2.624889 0.000006  
 N8 -2.921395 0.402833 0.000014  
 H9 -3.891517 0.701158 0.000025  
 C10 -2.610203 -0.918151 0.000013  
 N11 -3.578588 -1.823501 0.000024  
 H12 -4.560045 -1.588262 0.000034  
 H13 -3.314933 -2.799417 0.000022  
 N14 -1.338619 -1.386575 0.000000  
 C15 -0.426543 -0.444722 -0.000011  
 C16 1.646244 -1.887457 -0.000029  
 H17 2.716219 -1.683421 -0.000023  
 H18 1.378004 -2.453453 0.892605  
 H19 1.378012 -2.453442 -0.892671  
 O20 6.020385 0.260607 0.000048  
 N21 4.908794 -0.026780 0.000007

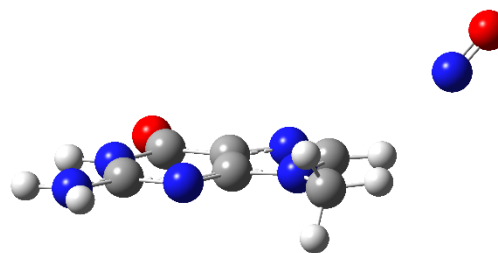
Zero-point correction= 0.151792 (Hartree/Particle)  
 Thermal correction to Energy= 0.165873  
 Thermal correction to Enthalpy= 0.166817  
 Thermal correction to Gibbs Free Energy= 0.107289  
 Sum of electronic and zero-point Energies= -711.140605  
 Sum of electronic and thermal Energies= -711.126524  
 Sum of electronic and thermal Enthalpies= -711.125579  
 Sum of electronic and thermal Free Energies= -711.185108



#### $1.0^{\text{S}}$ [TS-like]<sup>+</sup>

N1 0.957308 -0.618629 -0.585715  
 C2 1.456500 0.633104 -0.763787  
 H3 2.492020 0.800426 -1.029900  
 N4 0.562281 1.613755 -0.568318  
 C5 -0.557446 0.973399 -0.255280  
 C6 -1.886859 1.484798 0.069005  
 O7 -2.267942 2.621791 0.125810  
 N8 -2.782855 0.402122 0.339593  
 H9 -3.724604 0.701917 0.570597  
 C10 -2.472106 -0.918681 0.307940  
 N11 -3.403640 -1.821613 0.580670  
 H12 -4.355922 -1.584696 0.816532  
 H13 -3.141725 -2.797450 0.547980  
 N14 -1.237366 -1.389100 0.007444  
 C15 -0.360769 -0.449477 -0.253011  
 C16 1.653451 -1.895925 -0.727304  
 H17 2.707188 -1.694819 -0.913316  
 H18 1.549095 -2.467509 0.195211  
 H19 1.226911 -2.454624 -1.561151  
 O20 5.474560 0.352729 1.033017  
 N21 4.561052 -0.081209 0.488906

Zero-point correction= 0.151504 (Hartree/Particle)  
 Thermal correction to Energy= 0.164875  
 Thermal correction to Enthalpy= 0.165819  
 Thermal correction to Gibbs Free Energy= 0.108054  
 Sum of electronic and zero-point Energies= -711.140469  
 Sum of electronic and thermal Energies= -711.127098  
 Sum of electronic and thermal Enthalpies= -711.126154  
 Sum of electronic and thermal Free Energies= -711.183920



**Cartesian coordinates for closed-shell  
singlet structures optimized at  
 $\omega$ B97XD/6-31+G(d,p) (Scheme 2)**

**9MG<sup>+</sup>**

N1 1.951120 -0.354584 -0.005039  
 C2 2.319075 0.954049 -0.004604  
 H3 3.359068 1.254438 -0.006930  
 N4 1.291153 1.814596 -0.002631  
 C5 0.216436 1.034973 -0.000529  
 C6 -1.205059 1.373616 0.001955  
 O7 -1.725524 2.455144 0.004320  
 N8 -1.999348 0.182762 0.001632  
 H9 -2.998658 0.360699 0.003190  
 C10 -1.529628 -1.090373 -0.000748  
 N11 -2.379559 -2.107285 -0.002613  
 H12 -3.382588 -1.994398 -0.003318  
 H13 -1.998202 -3.043651 -0.004190  
 N14 -0.209714 -1.400163 -0.001254  
 C15 0.580653 -0.354432 -0.001405  
 C16 2.813072 -1.534839 0.008346  
 H17 2.706734 -2.055164 0.960914  
 H18 2.530148 -2.196868 -0.810227  
 H19 3.844839 -1.211461 -0.122750

Zero-point correction= 0.146470 (Hartree/Particle)  
 Thermal correction to Energy= 0.156361  
 Thermal correction to Enthalpy= 0.157305  
 Thermal correction to Gibbs Free Energy= 0.110574  
 Sum of electronic and zero-point Energies= -581.292006  
 Sum of electronic and thermal Energies= -581.282115  
 Sum of electronic and thermal Enthalpies= -581.281170  
 Sum of electronic and thermal Free Energies= -581.327901

**\*NO**

O1 0.000000 0.000000 0.537659  
 N2 0.000000 0.000000 -0.614468

Zero-point correction= 0.004646 (Hartree/Particle)  
 Thermal correction to Energy= 0.007007  
 Thermal correction to Enthalpy= 0.007951  
 Thermal correction to Gibbs Free Energy= -0.015348  
 Sum of electronic and zero-point Energies= -129.845210  
 Sum of electronic and thermal Energies= -129.842849  
 Sum of electronic and thermal Enthalpies= -129.841905  
 Sum of electronic and thermal Free Energies= -129.865205

**1,OS precursor**

C1 1.037219 0.721493 -0.103862  
 C2 0.303095 -0.540323 -0.124599  
 H3 0.592376 2.720136 0.092946  
 C4 -1.218635 1.728395 0.208943  
 C5 -0.379846 -2.519309 -0.304196  
 N6 0.135708 1.814043 0.088676  
 N7 0.729494 -1.793280 -0.333229  
 N8 -1.522513 -1.795015 -0.090209  
 N9 -1.892866 0.562646 0.187252  
 C10 -1.123290 -0.492520 0.009775  
 N11 -1.928928 2.842469 0.353880  
 H12 -2.933005 2.757430 0.425485

H13 -1.519677 3.764051 0.370157  
 O14 2.218398 0.914830 -0.211164  
 H15 -0.409800 -3.593654 -0.433163  
 C16 -2.899404 -2.280276 -0.056544  
 H17 -3.432823 -1.943509 -0.946592  
 H18 -2.882286 -3.369066 -0.027477  
 H19 -3.396791 -1.899642 0.835795  
 O20 -0.550968 0.321057 2.980616  
 N21 -0.005626 -0.576429 2.548807

Zero-point correction= 0.152163 (Hartree/Particle)  
 Thermal correction to Energy= 0.165751  
 Thermal correction to Enthalpy= 0.166695  
 Thermal correction to Gibbs Free Energy= 0.110828  
 Sum of electronic and zero-point Energies= -711.145183  
 Sum of electronic and thermal Energies= -711.131595  
 Sum of electronic and thermal Enthalpies= -711.130651  
 Sum of electronic and thermal Free Energies= -711.186518

**TS-<sup>1,CS</sup>[2-NHNO-3H-9MG]<sup>+</sup>**

C1 1.204490 0.912467 0.074738  
 C2 0.199825 1.953474 -0.046126  
 O3 0.268379 3.141110 0.086407  
 N4 -1.099099 1.359028 -0.394450  
 C5 -1.275718 0.055580 -0.582731  
 N6 -2.435318 -0.699189 -0.875946  
 H7 -2.986614 -0.479586 -1.707320  
 N8 -0.356516 -0.873840 -0.463534  
 C9 0.897845 -0.427344 -0.135970  
 N10 2.525715 1.043944 0.374163  
 C11 2.995316 -0.178489 0.343477  
 N12 2.046050 -1.126816 0.035642  
 C13 2.236047 -2.566565 -0.090380  
 H14 3.281594 -2.792298 0.115745  
 H15 1.609466 -3.094006 0.630849  
 H16 1.996471 -2.889482 -1.105041  
 H17 4.022711 -0.457130 0.534301  
 H18 -1.855253 2.025866 -0.511956  
 N19 -3.538818 -0.919797 0.401597  
 O20 -3.040574 -0.729882 1.407203  
 H21 -1.431735 -1.581232 -0.825803

Zero-point correction= 0.149477 (Hartree/Particle)  
 Thermal correction to Energy= 0.161596  
 Thermal correction to Enthalpy= 0.162540  
 Thermal correction to Gibbs Free Energy= 0.110222  
 Sum of electronic and zero-point Energies= -711.063691  
 Sum of electronic and thermal Energies= -711.051572  
 Sum of electronic and thermal Enthalpies= -711.050628  
 Sum of electronic and thermal Free Energies= -711.102946

**1,CS[2-NHNO-3H-9MG]<sup>+</sup>**

C1 1.458635 0.715738 0.000011  
 C2 0.775146 1.986893 0.000004  
 O3 1.163574 3.115700 -0.000001  
 N4 -0.685891 1.759530 -0.000002  
 C5 -1.330900 0.593372 0.000006  
 N6 -2.705783 0.583947 0.000014  
 H7 -3.212799 1.461406 0.000032

N8 -0.639285 -0.546891 0.000015  
 C9 0.741543 -0.462728 0.000008  
 N10 2.795266 0.446397 -0.000008  
 C11 2.870149 -0.857345 -0.000022  
 N12 1.635432 -1.478824 -0.000022  
 C13 1.362971 -2.911976 0.000034  
 H14 2.315775 -3.439687 -0.000596  
 H15 0.810019 -3.194218 0.898832  
 H16 0.808974 -3.194072 -0.898165  
 H17 3.783928 -1.435737 -0.000041  
 H18 -1.210414 2.629663 -0.000010  
 N19 -3.578750 -0.496208 -0.000008  
 O20 -3.056878 -1.573926 -0.000030  
 H21 -1.161228 -1.420913 0.000024

Zero-point correction= 0.155891 (Hartree/Particle)  
 Thermal correction to Energy= 0.167762  
 Thermal correction to Enthalpy= 0.168706  
 Thermal correction to Gibbs Free Energy= 0.117414  
 Sum of electronic and zero-point Energies= -711.142273  
 Sum of electronic and thermal Energies= -711.130402  
 Sum of electronic and thermal Enthalpies= -711.129458  
 Sum of electronic and thermal Free Energies= -711.180750

### TS-<sup>1,CS</sup>[3-NO-9MG]<sup>+</sup>

C1 -0.968070 1.578035 -0.243948  
 C2 0.406239 1.118914 -0.113417  
 H3 -2.797343 0.742358 -0.717894  
 C4 -1.466228 -0.837944 -0.672875  
 C5 2.501755 0.914353 -0.033732  
 N6 -1.835414 0.464361 -0.551897  
 N7 1.551926 1.823329 0.047517  
 N8 2.035143 -0.356524 -0.243258  
 N9 -0.204200 -1.257981 -0.484635  
 C10 0.676877 -0.240890 -0.314993  
 N11 -2.400011 -1.763433 -0.906667  
 H12 -2.092538 -2.710104 -1.078527  
 H13 -3.368119 -1.536276 -1.074670  
 O14 -1.437187 2.677104 -0.131556  
 H15 3.560602 1.117805 0.054705  
 C16 2.813186 -1.577944 -0.418324  
 H17 2.659020 -1.974509 -1.422710  
 H18 3.866657 -1.338520 -0.278633  
 H19 2.510246 -2.322005 0.319347  
 O20 -1.146853 -0.617847 2.305861  
 N21 -0.211551 -0.935458 1.794322

Zero-point correction= 0.153012 (Hartree/Particle)  
 Thermal correction to Energy= 0.165364  
 Thermal correction to Enthalpy= 0.166308  
 Thermal correction to Gibbs Free Energy= 0.113979  
 Sum of electronic and zero-point Energies= -711.123419  
 Sum of electronic and thermal Energies= -711.111067  
 Sum of electronic and thermal Enthalpies= -711.110123  
 Sum of electronic and thermal Free Energies= -711.1624518

### <sup>1,CS</sup>[3-NO-9MG]<sup>+</sup>

C1 1.592887 -1.426919 0.157027  
 C2 0.146247 -1.378207 0.158100  
 H3 3.154200 -0.117430 -0.288799

C4 1.489706 1.049048 -0.283104  
 C5 -1.892838 -1.868194 -0.057179  
 N6 2.145923 -0.103016 -0.164914  
 N7 -0.727932 -2.419937 0.159010  
 N8 -1.835320 -0.501236 -0.217582  
 N9 0.115097 1.053877 -0.165749  
 C10 -0.520648 -0.189842 -0.053697  
 N11 2.120005 2.195857 -0.489157  
 H12 1.602202 3.058326 -0.584763  
 H13 3.126344 2.257033 -0.428191  
 O14 2.360823 -2.326788 0.317525  
 H15 -2.835526 -2.393868 -0.122423  
 C16 -2.968015 0.342542 -0.595436  
 H17 -3.416172 0.807038 0.282339  
 H18 -2.637662 1.106744 -1.299940  
 H19 -3.702751 -0.289230 -1.093767  
 O20 -1.428937 2.175832 0.967267  
 N21 -0.364882 2.289950 0.493097

Zero-point correction= 0.155418 (Hartree/Particle)  
 Thermal correction to Energy= 0.167374  
 Thermal correction to Enthalpy= 0.168318  
 Thermal correction to Gibbs Free Energy= 0.117590  
 Sum of electronic and zero-point Energies= -711.137549  
 Sum of electronic and thermal Energies= -711.125593  
 Sum of electronic and thermal Enthalpies= -711.124649  
 Sum of electronic and thermal Free Energies= -711.175378

### TS-<sup>1,CS</sup>[5-NO-9MG]<sup>+</sup>

C1 0.604707 -1.465333 -0.588315  
 C2 -0.383995 -0.418989 -0.425493  
 H3 2.612998 -1.695065 -0.248177  
 C4 2.179155 0.271355 0.244457  
 C5 -2.052970 0.893807 -0.670377  
 N6 1.878177 -1.002248 -0.158812  
 N7 -1.702713 -0.354048 -0.852866  
 N8 -1.026438 1.680915 -0.200610  
 N9 1.280723 1.249539 0.305654  
 C10 0.056985 0.865068 -0.049856  
 N11 3.441834 0.543389 0.589874  
 H12 3.663474 1.490183 0.858418  
 H13 4.184405 -0.135867 0.555177  
 O14 0.453290 -2.600997 -0.975247  
 H15 -3.042163 1.295221 -0.845053  
 C16 -1.035525 3.125195 0.002909  
 H17 -0.439742 3.611414 -0.771440  
 H18 -2.064570 3.479495 -0.045858  
 H19 -0.613559 3.352945 0.982056  
 O20 -2.372421 -1.521989 1.630389  
 N21 -1.751290 -1.837698 0.773015

Zero-point correction= 0.153449 (Hartree/Particle)  
 Thermal correction to Energy= 0.165695  
 Thermal correction to Enthalpy= 0.166639  
 Thermal correction to Gibbs Free Energy= 0.114719  
 Sum of electronic and zero-point Energies= -711.136822  
 Sum of electronic and thermal Energies= -711.124576  
 Sum of electronic and thermal Enthalpies= -711.123632  
 Sum of electronic and thermal Free Energies= -711.175552



**<sup>1,CS</sup>[5-NO-9MG]<sup>+</sup>**

C1 1.079841 -1.211842 -0.652765  
 C2 -0.277124 -0.908062 -0.153325  
 H3 2.873163 -0.222758 -0.820859  
 C4 1.484008 1.198762 -0.230674  
 C5 -2.384636 -0.805021 -0.363137  
 N6 1.909105 -0.062689 -0.548002  
 N7 -1.425511 -1.664206 -0.400297  
 N8 -1.974788 0.529232 -0.184323  
 N9 0.195983 1.521422 -0.036548  
 C10 -0.632676 0.501499 -0.135935  
 N11 2.384083 2.170357 -0.145623  
 H12 2.054203 3.105809 0.046305  
 H13 3.374788 2.021237 -0.260794  
 O14 1.516988 -2.263662 -1.027931  
 H15 -3.437446 -1.039308 -0.465013  
 C16 -2.831438 1.711352 -0.177966  
 H17 -3.267534 1.859997 -1.167386  
 H18 -3.621049 1.584652 0.563459  
 H19 -2.219797 2.573805 0.084487  
 O20 0.756052 -0.494273 2.201841  
 N21 -0.027229 -1.171271 1.730698

Zero-point correction= 0.153807 (Hartree/Particle)  
 Thermal correction to Energy= 0.166692  
 Thermal correction to Enthalpy= 0.167636  
 Thermal correction to Gibbs Free Energy= 0.114011  
 Sum of electronic and zero-point Energies= -711.142692  
 Sum of electronic and thermal Energies= -711.129806  
 Sum of electronic and thermal Enthalpies= -711.128862  
 Sum of electronic and thermal Free Energies= -711.182488

**<sup>1,CS</sup>[7-NO-9MG]<sup>+</sup> (barrierless)**

N1 0.316494 1.949882 0.004345  
 C2 1.597724 1.575398 0.005219  
 H3 2.448507 2.242579 0.007147  
 N4 1.683862 0.246740 0.003202  
 C5 0.398075 -0.277911 0.000048  
 C6 -0.136046 -1.620432 0.000291  
 O7 0.439825 -2.682431 0.001325  
 N8 -1.552896 -1.553411 -0.000736  
 H9 -1.994365 -2.466242 -0.000700  
 C10 -2.320343 -0.416528 -0.000267  
 N11 -3.651917 -0.555051 0.000117  
 H12 -4.114836 -1.448980 0.000562  
 H13 -4.214802 0.281509 0.000459  
 N14 -1.799708 0.801075 -0.000221  
 C15 -0.464945 0.799896 0.000611  
 C16 -0.212246 3.313944 -0.005639  
 H17 -0.740384 3.485249 -0.943903  
 H18 -0.902300 3.430339 0.829790  
 H19 0.615865 4.014460 0.092002  
 O20 3.153678 -1.505186 -0.006575  
 N21 3.144305 -0.358406 0.001159

Zero-point correction= 0.154464 (Hartree/Particle)  
 Thermal correction to Energy= 0.167305  
 Thermal correction to Enthalpy= 0.168249  
 Thermal correction to Gibbs Free Energy= 0.114605

Sum of electronic and zero-point Energies= -711.163586  
 Sum of electronic and thermal Energies= -711.150745  
 Sum of electronic and thermal Enthalpies= -711.149801  
 Sum of electronic and thermal Free Energies= -711.203446

**<sup>1,CS</sup>[8-NO-9MG]<sup>+</sup> (barrierless)**

C1 -1.324582 1.573763 -0.137616  
 C2 -0.061767 0.821818 -0.322728  
 H3 -3.283882 1.140677 0.277227  
 C4 -2.298822 -0.684147 0.221366  
 C5 1.958840 0.127433 -0.556814  
 N6 -2.390419 0.681400 0.135248  
 N7 1.118071 1.262748 -0.586328  
 N8 1.138600 -1.042976 -0.436427  
 N9 -1.164389 -1.376728 0.057355  
 C10 -0.105826 -0.636825 -0.208449  
 N11 -3.403216 -1.369218 0.486594  
 H12 -3.330692 -2.374888 0.552090  
 H13 -4.305576 -0.940654 0.625373  
 O14 -1.490610 2.758252 -0.196891  
 H15 2.739153 0.088094 -1.315937  
 O16 3.753196 0.793924 0.850725  
 C17 1.634472 -2.412304 -0.384565  
 H18 2.143617 -2.591860 0.565768  
 H19 0.783582 -3.087157 -0.471747  
 H20 2.321880 -2.578237 -1.215022  
 N21 2.703828 0.300228 0.927046

Zero-point correction= 0.154245 (Hartree/Particle)  
 Thermal correction to Energy= 0.166798  
 Thermal correction to Enthalpy= 0.167742  
 Thermal correction to Gibbs Free Energy= 0.114563  
 Sum of electronic and zero-point Energies= -711.141102  
 Sum of electronic and thermal Energies= -711.128549  
 Sum of electronic and thermal Enthalpies= -711.127605  
 Sum of electronic and thermal Free Energies= -711.180784

**TS-<sup>1,CS</sup>[7H-8-NO-9MG]<sup>+</sup>**

C1 1.330569 -1.602652 0.032649  
 C2 0.099687 -0.815277 0.026852  
 H3 3.340650 -1.208438 -0.049840  
 C4 2.405773 0.642363 -0.065859  
 C5 -1.913182 -0.051903 0.144584  
 N6 2.447606 -0.727060 -0.040369  
 N7 -1.177172 -1.227307 0.030898  
 N8 -1.099125 1.050323 0.088610  
 N9 1.272242 1.347780 -0.026079  
 C10 0.185121 0.594562 0.017678  
 N11 3.556266 1.307605 -0.127970  
 H12 3.519539 2.316431 -0.145735  
 H13 4.456901 0.857200 -0.171238  
 O14 1.464351 -2.794493 0.087521  
 H15 -1.809418 -0.907839 1.128418  
 O16 -3.957525 -0.920861 -0.200599  
 C17 -1.503106 2.457330 0.152977  
 H18 -2.530719 2.543939 -0.196756  
 H19 -0.832825 3.027311 -0.489377  
 H20 -1.420362 2.814099 1.180763  
 N21 -3.343751 0.096314 -0.240076

Zero-point correction= 0.150138 (Hartree/Particle)  
 Thermal correction to Energy= 0.162253  
 Thermal correction to Enthalpy= 0.163197  
 Thermal correction to Gibbs Free Energy= 0.111589  
 Sum of electronic and zero-point Energies= -711.083021  
 Sum of electronic and thermal Energies= -711.070906  
 Sum of electronic and thermal Enthalpies= -711.069962  
 Sum of electronic and thermal Free Energies= -711.121570

**1,CS[7H-8-NO-9MG]<sup>+</sup>**

C1 -1.297569 1.598137 -0.000001  
 C2 -0.100688 0.786243 0.000001  
 H3 -3.311139 1.252268 -0.000004  
 C4 -2.413207 -0.624559 0.000001  
 C5 1.929902 -0.014154 0.000004  
 N6 -2.427861 0.753732 -0.000001  
 N7 1.221348 1.116025 0.000001  
 N8 1.099666 -1.076268 0.000007  
 N9 -1.299080 -1.341668 0.000002  
 C10 -0.191140 -0.597914 0.000003  
 N11 -3.589977 -1.257606 0.000001  
 H12 -3.584067 -2.266478 0.000002  
 H13 -4.477163 -0.781105 0.000000  
 O14 -1.377252 2.802952 -0.000004  
 H15 1.627590 2.048041 0.000001  
 O16 3.901886 0.937342 -0.000007  
 C17 1.472846 -2.494872 -0.000010  
 H18 2.558174 -2.571544 0.000537  
 H19 1.055926 -2.963192 0.891582  
 H20 1.056838 -2.962956 -0.892154  
 N21 3.349605 -0.136313 0.000008

Zero-point correction= 0.156290 (Hartree/Particle)  
 Thermal correction to Energy= 0.168421  
 Thermal correction to Enthalpy= 0.169366  
 Thermal correction to Gibbs Free Energy= 0.118087  
 Sum of electronic and zero-point Energies= -711.176891  
 Sum of electronic and thermal Energies= -711.164759  
 Sum of electronic and thermal Enthalpies= -711.163814  
 Sum of electronic and thermal Free Energies= -711.215093

**TS-1,CS[7H-8-ON-9MG]<sup>+</sup>**

C1 -1.419254 1.549573 -0.047577  
 C2 -0.132863 0.862536 -0.067195  
 H3 -3.387314 1.000167 0.128907  
 C4 -2.309737 -0.770489 0.125274  
 C5 1.919292 0.258506 -0.327541  
 N6 -2.460185 0.589940 0.090366  
 N7 1.107885 1.374581 -0.161752  
 N8 1.203462 -0.906560 -0.203493  
 N9 -1.125979 -1.384878 0.036570  
 C10 -0.106455 -0.546914 -0.054209  
 N11 -3.398964 -1.524791 0.247181  
 H12 -3.280617 -2.527158 0.271163  
 H13 -4.329325 -1.146818 0.333363  
 O14 -1.652213 2.725118 -0.124152  
 H15 1.638991 1.067081 -1.325061  
 C16 1.716776 -2.275467 -0.270042

H17 2.804759 -2.239207 -0.258550  
 H18 1.348981 -2.822760 0.597839  
 H19 1.361967 -2.751093 -1.185117  
 O20 3.267118 0.282361 -0.177370  
 N21 3.661891 0.550778 1.090751

Zero-point correction= 0.149645 (Hartree/Particle)  
 Thermal correction to Energy= 0.161429  
 Thermal correction to Enthalpy= 0.162373  
 Thermal correction to Gibbs Free Energy= 0.111628  
 Sum of electronic and zero-point Energies= -710.984610  
 Sum of electronic and thermal Energies= -710.972826  
 Sum of electronic and thermal Enthalpies= -710.971882  
 Sum of electronic and thermal Free Energies= -711.022627

**1,CS[7H-8-ON-9MG]<sup>+</sup>**

C1 1.562784 1.489967 -0.000003  
 C2 0.254683 0.888462 0.000010  
 H3 3.491472 0.810014 -0.000033  
 C4 2.290840 -0.887415 -0.000022  
 C5 -1.876379 0.440538 0.000047  
 N6 2.537344 0.466378 -0.000022  
 N7 -1.008541 1.438911 0.000040  
 N8 -1.262046 -0.748043 0.000033  
 N9 1.070231 -1.402647 -0.000005  
 C10 0.107394 -0.479198 0.000009  
 N11 3.343072 -1.713339 -0.000041  
 H12 3.166219 -2.706285 -0.000045  
 H13 4.298008 -1.394169 -0.000059  
 O14 1.847227 2.664753 0.000000  
 H15 -1.242576 2.426727 0.000040  
 C16 -1.825591 -2.110310 0.000097  
 H17 -2.432918 -2.258656 -0.890583  
 H18 -0.970797 -2.785152 0.000132  
 H19 -2.432900 -2.258572 0.890807  
 O20 -3.245276 0.742743 0.000076  
 N21 -4.076418 -0.204995 -0.000247

Zero-point correction= 0.155024 (Hartree/Particle)  
 Thermal correction to Energy= 0.167300  
 Thermal correction to Enthalpy= 0.168244  
 Thermal correction to Gibbs Free Energy= 0.116263  
 Sum of electronic and zero-point Energies= -711.084533  
 Sum of electronic and thermal Energies= -711.072257  
 Sum of electronic and thermal Enthalpies= -711.071313  
 Sum of electronic and thermal Free Energies= -711.123293

**TS-1,CS[4,5-NO-9MG]<sup>+</sup>**

C1 1.371983 -1.254586 -0.234323  
 C2 -0.109762 -1.021473 -0.042938  
 H3 3.079071 -0.165039 -0.341358  
 C4 1.547426 1.233108 -0.084830  
 C5 -2.041209 -0.764501 -0.899315  
 N6 2.079157 -0.052020 -0.215991  
 N7 -1.059312 -1.639202 -0.819430  
 N8 -1.860468 0.434911 -0.299635  
 N9 0.282815 1.511647 0.124132  
 C10 -0.535990 0.425304 0.296660  
 N11 2.425629 2.232549 -0.183668

H12 2.081619 3.174684 -0.068517  
 H13 3.398150 2.100713 -0.411422  
 O14 1.888555 -2.324983 -0.381180  
 H15 -2.965866 -0.975241 -1.427203  
 O16 -0.482408 -1.218543 1.533900  
 C17 -2.732481 1.607592 -0.349186  
 H18 -2.140641 2.469773 -0.658741  
 H19 -3.520697 1.420920 -1.078534  
 H20 -3.177856 1.790193 0.629597  
 N21 -0.868215 -0.033664 1.682877

Zero-point correction= 0.153866 (Hartree/Particle)  
 Thermal correction to Energy= 0.165170  
 Thermal correction to Enthalpy= 0.166114  
 Thermal correction to Gibbs Free Energy= 0.116802  
 Sum of electronic and zero-point Energies= -711.060974  
 Sum of electronic and thermal Energies= -711.049671  
 Sum of electronic and thermal Enthalpies= -711.048726  
 Sum of electronic and thermal Free Energies= -711.098038

**1,CS[4,5-NO-9MG]<sup>+</sup>**

C1 1.360722 -1.266223 -0.223480  
 C2 -0.118571 -1.019834 -0.015895  
 H3 3.076321 -0.195315 -0.358153  
 C4 1.565921 1.221038 -0.079351  
 C5 -2.045331 -0.750539 -0.896516  
 N6 2.079591 -0.070809 -0.218955  
 N7 -1.081215 -1.632607 -0.807524  
 N8 -1.845368 0.456999 -0.301958  
 N9 0.305923 1.515433 0.134095  
 C10 -0.525536 0.438586 0.292684  
 N11 2.457557 2.208692 -0.176755  
 H12 2.126705 3.155120 -0.058395  
 H13 3.429709 2.063785 -0.397872  
 O14 1.865504 -2.342053 -0.371580  
 H15 -2.976883 -0.951151 -1.415819  
 O16 -0.518894 -1.225116 1.487235  
 C17 -2.708659 1.636000 -0.352152  
 H18 -2.107131 2.495564 -0.650065  
 H19 -3.490778 1.459252 -1.090532  
 H20 -3.163090 1.816065 0.623042  
 N21 -0.893490 -0.029156 1.666929

Zero-point correction= 0.154574 (Hartree/Particle)  
 Thermal correction to Energy= 0.166289  
 Thermal correction to Enthalpy= 0.167233  
 Thermal correction to Gibbs Free Energy= 0.117222  
 Sum of electronic and zero-point Energies= -711.060341  
 Sum of electronic and thermal Energies= -711.048626  
 Sum of electronic and thermal Enthalpies= -711.047682  
 Sum of electronic and thermal Free Energies= -711.097693

**TS-1,CS[7,8-NO-9MG]<sup>+</sup>**

C1 -1.085616 -1.583847 0.189129  
 C2 0.060055 -0.734076 0.194948  
 H3 -3.114678 -1.304928 -0.015794  
 C4 -2.269372 0.578900 -0.142965  
 C5 2.149302 0.302872 0.404835  
 N6 -2.251550 -0.772262 0.002027  
 N7 1.447295 -0.973612 0.298830

N8 1.225729 1.251832 0.117186  
 N9 -1.155790 1.327424 -0.135475  
 C10 -0.047124 0.636221 0.022929  
 N11 -3.436721 1.201564 -0.302939  
 H12 -3.428125 2.203921 -0.419423  
 H13 -4.321711 0.720186 -0.324781  
 O14 -1.171800 -2.781019 0.312519  
 H15 2.880644 0.476197 1.196320  
 O16 3.089466 -0.501581 -0.669518  
 C17 1.430250 2.695563 0.242907  
 H18 2.303335 2.876004 0.872354  
 H19 1.589423 3.138616 -0.740646  
 H20 0.546423 3.135466 0.703916  
 N21 2.282237 -1.514727 -0.534865

Zero-point correction= 0.154623 (Hartree/Particle)  
 Thermal correction to Energy= 0.165997  
 Thermal correction to Enthalpy= 0.166942  
 Thermal correction to Gibbs Free Energy= 0.116849  
 Sum of electronic and zero-point Energies= -711.080406  
 Sum of electronic and thermal Energies= -711.069032  
 Sum of electronic and thermal Enthalpies= -711.068087  
 Sum of electronic and thermal Free Energies= -711.118180

**1,CS[7,8-NO-9MG]<sup>+</sup>**

C1 1.098955 -1.588254 -0.138839  
 C2 -0.049707 -0.740316 -0.200937  
 H3 3.130424 -1.299336 0.025765  
 C4 2.274807 0.584383 0.102356  
 C5 -2.142182 0.264839 -0.383698  
 N6 2.264600 -0.771653 -0.002973  
 N7 -1.412165 -0.976567 -0.240897  
 N8 -1.223345 1.242099 0.028892  
 N9 1.159024 1.330873 0.112424  
 C10 0.040904 0.651411 -0.017334  
 N11 3.440711 1.216135 0.212150  
 H12 3.428716 2.221425 0.303084  
 H13 4.329767 0.741197 0.217293  
 O14 1.177536 -2.790175 -0.199580  
 H15 -2.651443 0.441866 -1.336710  
 O16 -3.136083 -0.435828 0.481173  
 C17 -1.449998 2.674081 -0.175829  
 H18 -2.330062 2.980639 0.388935  
 H19 -0.579557 3.203583 0.208282  
 H20 -1.578122 2.904372 -1.237746  
 N21 -2.331401 -1.535543 0.470982

Zero-point correction= 0.155853 (Hartree/Particle)  
 Thermal correction to Energy= 0.167370  
 Thermal correction to Enthalpy= 0.168315  
 Thermal correction to Gibbs Free Energy= 0.118309  
 Sum of electronic and zero-point Energies= -711.080999  
 Sum of electronic and thermal Energies= -711.069482  
 Sum of electronic and thermal Enthalpies= -711.068537  
 Sum of electronic and thermal Free Energies= -711.118543

**Cartesian coordinates for singlet biradical structures optimized at  $\omega$ B97XD/6-31+G(d,p) (Scheme 3)**

**<sup>1,0S</sup>precursor**

C1 1.037219 0.721493 -0.103862  
 C2 0.303095 -0.540323 -0.124599  
 H3 0.592376 2.720136 0.092946  
 C4 -1.218635 1.728395 0.208943  
 C5 -0.379846 -2.519309 -0.304196  
 N6 0.135708 1.814043 0.088676  
 N7 0.729494 -1.793280 -0.333229  
 N8 -1.522513 -1.795015 -0.090209  
 N9 -1.892866 0.562646 0.187252  
 C10 -1.123290 -0.492520 0.009775  
 N11 -1.928928 2.842469 0.353880  
 H12 -2.933005 2.757430 0.425485  
 H13 -1.519677 3.764051 0.370157  
 O14 2.218398 0.914830 -0.211164  
 H15 -0.409800 -3.593654 -0.433163  
 C16 -2.899404 -2.280276 -0.056544  
 H17 -3.432823 -1.943509 -0.946592  
 H18 -2.882286 -3.369066 -0.027477  
 H19 -3.396791 -1.899642 0.835795  
 O20 -0.550968 0.321057 2.980616  
 N21 -0.005626 -0.576429 2.548807

Zero-point correction= 0.152163 (Hartree/Particle)  
 Thermal correction to Energy= 0.165751  
 Thermal correction to Enthalpy= 0.166695  
 Thermal correction to Gibbs Free Energy= 0.110828  
 Sum of electronic and zero-point Energies= -711.145183  
 Sum of electronic and thermal Energies= -711.131595  
 Sum of electronic and thermal Enthalpies= -711.130651  
 Sum of electronic and thermal Free Energies= -711.186518

**TS-<sup>1,0S</sup>[8- $\dot{O}N$ -9MG]<sup>+</sup>**

C1 1.522574 1.514634 0.049512  
 C2 0.175280 0.908359 0.205243  
 H3 3.445409 0.859827 -0.224368  
 C4 2.266763 -0.845758 -0.156762  
 C5 -1.913578 0.433433 0.465856  
 N6 2.499974 0.504322 -0.125139  
 N7 -0.953193 1.478863 0.393538  
 N8 -1.225039 -0.820794 0.283477  
 N9 1.053872 -1.409307 -0.027237  
 C10 0.067885 -0.556894 0.140420  
 N11 3.298569 -1.658406 -0.322999  
 H12 3.117897 -2.652853 -0.346113  
 H13 4.249638 -1.338848 -0.430989  
 O14 1.806903 2.676344 0.073030  
 H15 -2.525029 0.482444 1.364966  
 C16 -1.821285 -2.148742 0.398571  
 H17 -2.886442 -2.092512 0.174227  
 H18 -1.320180 -2.811646 -0.307073  
 H19 -1.688014 -2.528179 1.415262  
 O20 -2.903444 0.612274 -0.744893

N21 -4.018009 0.182840 -0.614219

Zero-point correction= 0.152525 (Hartree/Particle)  
 Thermal correction to Energy= 0.164835  
 Thermal correction to Enthalpy= 0.165779  
 Thermal correction to Gibbs Free Energy= 0.112448  
 Sum of electronic and zero-point Energies= -711.067706  
 Sum of electronic and thermal Energies= -711.055395  
 Sum of electronic and thermal Enthalpies= -711.054451  
 Sum of electronic and thermal Free Energies= -711.107783

**<sup>1,0S</sup>[8- $\dot{O}N$ -9MG]<sup>+</sup>**

C1 1.540132 1.505101 0.039787  
 C2 0.179584 0.913508 0.176360  
 H3 3.460494 0.832544 -0.201472  
 C4 2.265043 -0.862027 -0.126263  
 C5 -1.930426 0.461724 0.411853  
 N6 2.510849 0.486584 -0.108008  
 N7 -0.935810 1.507069 0.317087  
 N8 -1.228970 -0.815432 0.277709  
 N9 1.046413 -1.416144 -0.008346  
 C10 0.058341 -0.562720 0.135409  
 N11 3.291446 -1.683845 -0.269755  
 H12 3.103330 -2.677296 -0.283613  
 H13 4.246486 -1.373048 -0.369900  
 O14 1.829817 2.664743 0.050553  
 H15 -2.483964 0.524726 1.353069  
 C16 -1.879971 -2.119985 0.307651  
 H17 -2.601973 -2.187245 -0.508592  
 H18 -1.112475 -2.883749 0.187789  
 H19 -2.391751 -2.251812 1.262543  
 O20 -2.851848 0.629263 -0.690345  
 N21 -4.032516 0.157515 -0.493012

Zero-point correction= 0.154030 (Hartree/Particle)  
 Thermal correction to Energy= 0.166271  
 Thermal correction to Enthalpy= 0.167215  
 Thermal correction to Gibbs Free Energy= 0.114932  
 Sum of electronic and zero-point Energies= -711.072916  
 Sum of electronic and thermal Energies= -711.060675  
 Sum of electronic and thermal Enthalpies= -711.059731  
 Sum of electronic and thermal Free Energies= -711.112013

**TS-<sup>1,0S</sup>[7H-8- $\dot{O}N$ -9MG]<sup>+</sup>**

C1 1.342910 1.592426 0.014832  
 C2 0.106029 0.823619 -0.044414  
 H3 3.350213 1.169675 -0.008218  
 C4 2.389983 -0.666750 -0.034349  
 C5 -1.909457 0.096551 0.092376  
 N6 2.450862 0.700469 -0.025213  
 N7 -1.169972 1.258844 -0.061739  
 N8 -1.125888 -1.023434 0.063810  
 N9 1.243907 -1.354028 -0.012197  
 C10 0.169001 -0.584495 -0.014916  
 N11 3.530502 -1.351621 -0.059569  
 H12 3.478356 -2.359812 -0.065355  
 H13 4.438843 -0.915870 -0.089579  
 O14 1.494349 2.781930 0.080971  
 H15 -1.770004 0.960008 1.084868

C16 -1.582352 -2.414685 0.119571  
 H17 -2.219844 -2.621650 -0.740582  
 H18 -0.694563 -3.044586 0.090880  
 H19 -2.130371 -2.583964 1.046609  
 O20 -3.229437 -0.044825 -0.248778  
 N21 -4.024927 0.972538 -0.015773

Zero-point correction= 0.149123 (Hartree/Particle)  
 Thermal correction to Energy= 0.161309  
 Thermal correction to Enthalpy= 0.162254  
 Thermal correction to Gibbs Free Energy= 0.109861  
 Sum of electronic and zero-point Energies= -711.013643  
 Sum of electronic and thermal Energies= -711.001456  
 Sum of electronic and thermal Enthalpies= -711.000512  
 Sum of electronic and thermal Free Energies= -711.052905

### <sup>1,0s</sup>[7H-8-ÖN-9MG]<sup>+</sup>

C1 1.564830 1.484534 0.007653  
 C2 0.256382 0.890378 -0.015253  
 H3 3.490386 0.794813 0.045585  
 C4 2.282957 -0.896593 0.022695  
 C5 -1.883826 0.455576 -0.055248  
 N6 2.535142 0.455074 0.027820  
 N7 -1.008281 1.450323 -0.040819  
 N8 -1.267238 -0.735298 -0.046643  
 N9 1.059722 -1.405046 0.001211  
 C10 0.104068 -0.473479 -0.015293  
 N11 3.331404 -1.728598 0.040684  
 H12 3.149533 -2.720449 0.040784  
 H13 4.287520 -1.413918 0.058680  
 O14 1.858740 2.657724 0.010698  
 H15 -1.235357 2.438649 -0.035524  
 C16 -1.852121 -2.082911 -0.096530  
 H17 -2.580687 -2.139131 -0.905000  
 H18 -1.026678 -2.766695 -0.290360  
 H19 -2.321419 -2.321608 0.856975  
 O20 -3.206351 0.717050 -0.119060  
 N21 -4.053056 -0.198582 0.304549

Zero-point correction= 0.155134 (Hartree/Particle)  
 Thermal correction to Energy= 0.167356  
 Thermal correction to Enthalpy= 0.168300  
 Thermal correction to Gibbs Free Energy= 0.116760  
 Sum of electronic and zero-point Energies= -711.104427  
 Sum of electronic and thermal Energies= -711.092205  
 Sum of electronic and thermal Enthalpies= -711.091261  
 Sum of electronic and thermal Free Energies= -711.142801

### TS-<sup>1,0s</sup>[2,4-ÑO-9MG]<sup>+</sup>

C1 0.706108 -0.282949 0.146780  
 C2 0.162132 1.051077 -0.144507  
 C3 -1.243931 1.446651 0.197379  
 C4 -1.409470 -0.858311 -0.363921  
 C5 2.261596 1.136236 -0.421886  
 O6 -1.603802 2.543699 0.505619  
 N7 1.172316 1.859507 -0.546943  
 N8 2.080751 -0.143909 0.012737  
 N9 -0.122168 -0.581176 -0.926626  
 N10 -2.222384 -1.731349 -1.043783  
 H11 -1.747387 -2.356307 -1.681232

H12 -3.091666 -1.363003 -1.404141  
 C13 3.055311 -1.232107 0.060905  
 H14 3.026150 -1.711465 1.040247  
 H15 4.047407 -0.810303 -0.096029  
 H16 2.838118 -1.958414 -0.725839  
 N17 -2.038600 0.301541 0.156266  
 H18 -3.005944 0.326800 0.459278  
 N19 -0.991393 -1.485433 1.095773  
 O20 0.145842 -1.135404 1.364859  
 H21 3.256863 1.508484 -0.636572

Zero-point correction= 0.151934 (Hartree/Particle)  
 Thermal correction to Energy= 0.163318  
 Thermal correction to Enthalpy= 0.164262  
 Thermal correction to Gibbs Free Energy= 0.115202  
 Sum of electronic and zero-point Energies= -711.011200  
 Sum of electronic and thermal Energies= -710.999817  
 Sum of electronic and thermal Enthalpies= -710.998872  
 Sum of electronic and thermal Free Energies= -711.047932

### <sup>1,0s</sup>[2,4-ÑO-9MG]<sup>+</sup>

C1 0.612211 -0.295781 0.033266  
 C2 0.291000 1.192181 -0.009652  
 C3 -1.166275 1.572298 0.037470  
 C4 -1.463537 -0.924940 -0.172130  
 C5 2.390326 1.002274 -0.230780  
 O6 -1.558020 2.699739 0.169627  
 N7 1.344095 1.912657 -0.158422  
 N8 2.049986 -0.253695 -0.141015  
 N9 -0.197292 -0.867739 -0.957428  
 N10 -2.477893 -1.769181 -0.625935  
 H11 -2.323282 -2.745325 -0.405898  
 H12 -2.721841 -1.631462 -1.599414  
 C13 2.894106 -1.448997 -0.169919  
 H14 2.779483 -1.976008 0.778994  
 H15 3.930797 -1.146922 -0.311054  
 H16 2.569864 -2.083304 -0.996547  
 N17 -1.951884 0.443782 -0.098221  
 H18 -2.958566 0.564733 -0.035884  
 N19 -0.997508 -1.380239 1.166869  
 O20 0.254471 -0.885255 1.293764  
 H21 3.418424 1.321115 -0.367793

Zero-point correction= 0.153104 (Hartree/Particle)  
 Thermal correction to Energy= 0.164395  
 Thermal correction to Enthalpy= 0.165339  
 Thermal correction to Gibbs Free Energy= 0.116591  
 Sum of electronic and zero-point Energies= -711.010966  
 Sum of electronic and thermal Energies= -710.999674  
 Sum of electronic and thermal Enthalpies= -710.998730  
 Sum of electronic and thermal Free Energies= -711.047479

### TS-<sup>1,0s</sup>[5,8-ÑO-9MG]<sup>+</sup>

C1 1.237033 -1.402879 -0.015659  
 C2 -0.188336 -0.904692 -0.032372  
 H3 3.158040 -0.713543 0.045260  
 C4 1.936512 0.958720 0.015730  
 C5 -2.099759 -0.330438 -0.682472  
 N6 2.200663 -0.377783 0.008533

N7 -0.957639 -0.930400 -1.237354  
 N8 -1.623048 0.976479 -0.328536  
 N9 0.704685 1.468442 -0.128628  
 C10 -0.309401 0.661651 -0.186221  
 N11 2.939709 1.812039 0.132094  
 H12 2.730402 2.800743 0.097258  
 H13 3.902425 1.527038 0.236861  
 O14 1.543980 -2.556910 -0.001943  
 H15 -3.075843 -0.429324 -1.145343  
 O16 -2.168303 -1.033751 0.730080  
 C17 -2.308299 2.080041 0.339927  
 H18 -1.746819 2.995524 0.153839  
 H19 -3.299773 2.178085 -0.102220  
 H20 -2.395188 1.906379 1.416188  
 N21 -0.962249 -1.222209 1.102386

Zero-point correction= 0.153449 (Hartree/Particle)  
 Thermal correction to Energy= 0.164543  
 Thermal correction to Enthalpy= 0.165488  
 Thermal correction to Gibbs Free Energy= 0.116372  
 Sum of electronic and zero-point Energies= -711.037116  
 Sum of electronic and thermal Energies= -711.026022  
 Sum of electronic and thermal Enthalpies= -711.025078  
 Sum of electronic and thermal Free Energies= -711.074194

### <sup>1,0S</sup>[5,8-~~N~~O-9MG]<sup>+</sup>

C1 1.194051 -1.406164 -0.222838  
 C2 -0.199945 -0.855537 -0.059697  
 H3 3.132820 -0.765751 -0.058811  
 C4 1.950606 0.929317 0.081506  
 C5 -2.210637 -0.374787 -0.299717  
 N6 2.181735 -0.411199 -0.043947  
 N7 -1.235572 -1.165577 -1.027888  
 N8 -1.554707 0.932159 -0.309609  
 N9 0.731558 1.495865 -0.003725  
 C10 -0.263680 0.663313 -0.135463  
 N11 2.979054 1.736396 0.272933  
 H12 2.796267 2.728307 0.346099  
 H13 3.931562 1.413817 0.360627  
 O14 1.477500 -2.545622 -0.438141  
 H15 -3.242165 -0.386623 -0.637120  
 O16 -2.113502 -0.899343 1.049607  
 C17 -2.215395 2.229788 -0.245937  
 H18 -1.460528 3.003772 -0.379435  
 H19 -2.953006 2.294410 -1.046679  
 H20 -2.702309 2.349787 0.724723  
 N21 -0.808444 -1.186728 1.268199

Zero-point correction= 0.155260 (Hartree/Particle)  
 Thermal correction to Energy= 0.166346  
 Thermal correction to Enthalpy= 0.167290  
 Thermal correction to Gibbs Free Energy= 0.118575  
 Sum of electronic and zero-point Energies= -711.064689  
 Sum of electronic and thermal Energies= -711.053603  
 Sum of electronic and thermal Enthalpies= -711.052659  
 Sum of electronic and thermal Free Energies= -711.101374

### TS-<sup>1,0S</sup>[5,8-O~~N~~-9MG]<sup>+</sup>

C1 1.197829 -1.402160 -0.213095  
 C2 -0.189217 -0.833945 -0.186830

H3 3.124125 -0.748054 0.003432  
 C4 1.933190 0.947991 0.061816  
 C5 -2.206118 -0.405838 -0.372823  
 N6 2.171824 -0.397621 -0.024727  
 N7 -1.224031 -1.217140 -1.019744  
 N8 -1.575223 0.924806 -0.312553  
 N9 0.715771 1.506716 -0.036442  
 C10 -0.278808 0.668459 -0.184121  
 N11 2.962107 1.759945 0.239807  
 H12 2.778498 2.752926 0.290904  
 H13 3.915490 1.441104 0.329184  
 O14 1.486410 -2.553829 -0.345251  
 H15 -3.221430 -0.416496 -0.755659  
 C16 -2.250121 2.205591 -0.153152  
 H17 -1.505275 2.996604 -0.234590  
 H18 -2.994816 2.314364 -0.942876  
 H19 -2.732862 2.254432 0.825524  
 O20 -0.880928 -1.135717 1.274214  
 N21 -2.114463 -0.885149 1.059604

Zero-point correction= 0.152955 (Hartree/Particle)  
 Thermal correction to Energy= 0.164063  
 Thermal correction to Enthalpy= 0.165007  
 Thermal correction to Gibbs Free Energy= 0.116211  
 Sum of electronic and zero-point Energies= -711.056104  
 Sum of electronic and thermal Energies= -711.044996  
 Sum of electronic and thermal Enthalpies= -711.044052  
 Sum of electronic and thermal Free Energies= -711.092848

### <sup>1,0S</sup>[5,8-O~~N~~-9MG]<sup>+</sup>

C1 1.181001 -1.405152 -0.198766  
 C2 -0.214451 -0.836828 -0.094302  
 H3 3.118231 -0.767521 -0.063852  
 C4 1.943821 0.936483 0.066375  
 C5 -2.228062 -0.371927 -0.329882  
 N6 2.168308 -0.409661 -0.052489  
 N7 -1.217221 -1.117168 -1.078056  
 N8 -1.565645 0.950554 -0.256870  
 N9 0.730036 1.509287 0.007709  
 C10 -0.275184 0.683543 -0.123842  
 N11 2.984558 1.734726 0.230407  
 H12 2.812352 2.728548 0.303472  
 H13 3.936427 1.404955 0.293964  
 O14 1.453654 -2.556608 -0.357007  
 H15 -3.231289 -0.346075 -0.744391  
 C16 -2.229388 2.242571 -0.153095  
 H17 -1.474290 3.023810 -0.233043  
 H18 -2.949530 2.338577 -0.967061  
 H19 -2.740882 2.317832 0.809101  
 O20 -0.839152 -1.201988 1.176608  
 N21 -2.164815 -0.971093 1.013025

Zero-point correction= 0.155085 (Hartree/Particle)  
 Thermal correction to Energy= 0.166239  
 Thermal correction to Enthalpy= 0.167183  
 Thermal correction to Gibbs Free Energy= 0.118267  
 Sum of electronic and zero-point Energies= -711.060448  
 Sum of electronic and thermal Energies= -711.049295  
 Sum of electronic and thermal Enthalpies= -711.048351  
 Sum of electronic and thermal Free Energies= -711.097266

**TS-<sup>1,0s</sup>[7,8-O<sup>-</sup>N-9MG]<sup>+</sup>**

C1 1.093783 -1.539692 -0.189970  
 C2 -0.107176 -0.722390 -0.317795  
 H3 3.097971 -1.226435 0.133514  
 C4 2.209691 0.647377 0.136471  
 C5 -2.193917 0.130179 -0.424943  
 N6 2.226852 -0.714805 0.039685  
 N7 -1.367097 -1.107318 -0.582200  
 N8 -1.249003 1.212202 -0.257806  
 N9 1.094480 1.389097 0.047196  
 C10 -0.011943 0.705694 -0.154315  
 N11 3.354270 1.285789 0.336938  
 H12 3.327117 2.292878 0.414404  
 H13 4.245164 0.819864 0.418504  
 O14 1.184893 -2.735745 -0.260755  
 H15 -2.921628 0.320713 -1.217888  
 C16 -1.631442 2.611862 -0.135900  
 H17 -2.163801 2.767803 0.805438  
 H18 -0.724432 3.214960 -0.150701  
 H19 -2.274160 2.884621 -0.975497  
 O20 -2.165108 -1.527861 0.778646  
 N21 -2.759285 -0.345497 0.837302

Zero-point correction= 0.152315 (Hartree/Particle)  
 Thermal correction to Energy= 0.163922  
 Thermal correction to Enthalpy= 0.164866  
 Thermal correction to Gibbs Free Energy= 0.114537  
 Sum of electronic and zero-point Energies= -711.037958  
 Sum of electronic and thermal Energies= -711.026351  
 Sum of electronic and thermal Enthalpies= -711.025407  
 Sum of electronic and thermal Free Energies= -711.075736

**<sup>1,0s</sup>[7,8-O<sup>-</sup>N-9MG]<sup>+</sup>**

C1 1.046413 -1.554248 -0.157807  
 C2 -0.117096 -0.702357 -0.288181  
 H3 3.064387 -1.304571 0.138966  
 C4 2.237625 0.597488 0.118550  
 C5 -2.194415 0.221124 -0.370512  
 N6 2.209779 -0.765325 0.049384  
 N7 -1.417823 -1.023410 -0.550935  
 N8 -1.216231 1.262544 -0.188864  
 N9 1.142238 1.368810 0.044442  
 C10 0.012415 0.717023 -0.135764  
 N11 3.405733 1.205065 0.282131  
 H12 3.410342 2.213400 0.344566  
 H13 4.283922 0.713751 0.349946  
 O14 1.096075 -2.756216 -0.217038  
 H15 -2.916967 0.460352 -1.156546  
 C16 -1.543082 2.679306 -0.098469  
 H17 -2.078905 2.876066 0.832746  
 H18 -0.611960 3.244134 -0.113350  
 H19 -2.162423 2.965670 -0.951409  
 N20 -2.827361 -0.382948 0.817590  
 O21 -2.185312 -1.565279 0.588532

Zero-point correction= 0.154335 (Hartree/Particle)  
 Thermal correction to Energy= 0.166013  
 Thermal correction to Enthalpy= 0.166957

Thermal correction to Gibbs Free Energy= 0.116416  
 Sum of electronic and zero-point Energies= -711.038663  
 Sum of electronic and thermal Energies= -711.026985  
 Sum of electronic and thermal Enthalpies= -711.026041  
 Sum of electronic and thermal Free Energies= -711.076581

**Cartesian coordinates for triplet structures optimized at  $\omega$ B97XD/6-31+G(d,p) (Scheme 4)**

**<sup>3</sup>precursor**

N1 -1.914874 0.419985 -0.510058  
 C2 -2.291514 -0.882506 -0.603539  
 H3 -3.333085 -1.173807 -0.646164  
 N4 -1.269694 -1.749619 -0.637054  
 C5 -0.190338 -0.980025 -0.563470  
 C6 1.227448 -1.330694 -0.533292  
 O7 1.738487 -2.416479 -0.576587  
 N8 2.029443 -0.151042 -0.439093  
 H9 3.026357 -0.338334 -0.406778  
 C10 1.568196 1.121055 -0.348105  
 N11 2.424566 2.126141 -0.232482  
 H12 3.425766 2.002529 -0.202050  
 H13 2.050627 3.063512 -0.175038  
 N14 0.251459 1.443774 -0.372538  
 C15 -0.545188 0.408543 -0.477438  
 C16 -2.768298 1.603527 -0.437300  
 H17 -2.602221 2.114740 0.511568  
 H18 -2.534257 2.272531 -1.265864  
 H19 -3.807542 1.284885 -0.505646  
 O20 -0.718064 -0.335173 2.736559  
 N21 0.423262 -0.210987 2.646804

Zero-point correction= 0.151687 (Hartree/Particle)  
 Thermal correction to Energy= 0.165824  
 Thermal correction to Enthalpy= 0.166768  
 Thermal correction to Gibbs Free Energy= 0.106420  
 Sum of electronic and zero-point Energies= -711.141788  
 Sum of electronic and thermal Energies= -711.127651  
 Sum of electronic and thermal Enthalpies= -711.126707  
 Sum of electronic and thermal Free Energies= -711.187055

**TS-<sup>3</sup>[2-NHNO-3H-9MG]<sup>+</sup>**

C1 1.266799 0.892458 0.064992  
 C2 0.289299 1.965524 -0.007356  
 O3 0.394650 3.147856 0.126379  
 N4 -1.044816 1.405350 -0.309842  
 C5 -1.246014 0.107999 -0.469377  
 N6 -2.452693 -0.642744 -0.786771  
 H7 -2.859008 -0.460099 -1.709535  
 N8 -0.371405 -0.853686 -0.378700  
 C9 0.912324 -0.439754 -0.121517  
 N10 2.598186 0.984441 0.323044  
 C11 3.028549 -0.253544 0.290576  
 N12 2.041968 -1.174066 0.024371  
 C13 2.181170 -2.622401 -0.078662  
 H14 3.219107 -2.880349 0.127745  
 H15 1.539955 -3.113292 0.655240  
 H16 1.925775 -2.954125 -1.086523  
 H17 4.052300 -0.562202 0.452906  
 H18 -1.797805 2.084101 -0.378200  
 N19 -3.535692 -0.560610 0.157239  
 O20 -3.371031 -0.969925 1.291301  
 H21 -1.510853 -1.549966 -0.680398

Zero-point correction= 0.149661 (Hartree/Particle)  
 Thermal correction to Energy= 0.161469  
 Thermal correction to Enthalpy= 0.162413  
 Thermal correction to Gibbs Free Energy= 0.109718  
 Sum of electronic and zero-point Energies= -711.001297  
 Sum of electronic and thermal Energies= -710.989489  
 Sum of electronic and thermal Enthalpies= -710.988544  
 Sum of electronic and thermal Free Energies= -711.041240

**<sup>3</sup>[2-NHNO-3H-9MG]<sup>+</sup>**

C1 1.532436 0.671829 -0.023795  
 C2 0.868324 1.952741 -0.022943  
 O3 1.274862 3.074895 -0.052855  
 N4 -0.596217 1.752676 0.028084  
 C5 -1.256285 0.597259 0.051749  
 N6 -2.618097 0.578872 0.034723  
 H7 -3.133819 1.418071 0.289699  
 N8 -0.582451 -0.556614 0.051341  
 C9 0.802712 -0.496146 0.013254  
 N10 2.867314 0.384217 -0.054499  
 C11 2.926447 -0.918242 -0.035978  
 N12 1.681883 -1.523861 0.006428  
 C13 1.392591 -2.952661 0.035273  
 H14 2.338681 -3.492087 0.015654  
 H15 0.863247 -3.216493 0.953882  
 H16 0.811113 -3.242347 -0.843198  
 H17 3.831559 -1.509801 -0.050928  
 H18 -1.109967 2.628897 0.008400  
 N19 -3.247184 -0.618371 0.338435  
 O20 -4.104622 -1.125387 -0.373338  
 H21 -1.096821 -1.429401 0.099092

Zero-point correction= 0.154243 (Hartree/Particle)  
 Thermal correction to Energy= 0.166666  
 Thermal correction to Enthalpy= 0.167610  
 Thermal correction to Gibbs Free Energy= 0.113660  
 Sum of electronic and zero-point Energies= -711.078004  
 Sum of electronic and thermal Energies= -711.065582  
 Sum of electronic and thermal Enthalpies= -711.064638  
 Sum of electronic and thermal Free Energies= -711.118588

**TS-<sup>3</sup>[3-NO-9MG]<sup>+</sup>**

N1 0.976744 1.658979 -0.101873  
 C2 0.098097 2.704258 0.009120  
 H3 0.443155 3.729338 0.006304  
 N4 -1.160084 2.329229 0.110966  
 C5 -1.111193 0.980212 0.107496  
 C6 -2.204980 0.027523 0.053745  
 O7 -3.387683 0.183490 0.118999  
 N8 -1.690069 -1.325307 -0.132471  
 H9 -2.424718 -2.022429 -0.212971  
 C10 -0.411386 -1.712273 -0.148817  
 N11 -0.074157 -2.989232 -0.180329  
 H12 -0.766147 -3.721467 -0.108122  
 H13 0.900140 -3.261449 -0.190208  
 N14 0.594276 -0.763216 -0.169975  
 C15 0.201987 0.542180 -0.025152  
 C16 2.429966 1.754169 -0.238003



H17 2.919405 1.428995 0.680574  
 H18 2.762702 1.143372 -1.078027  
 H19 2.679596 2.796181 -0.433029  
 O20 2.896172 -1.384228 0.079766  
 N21 1.839433 -1.233747 0.644399

Zero-point correction= 0.152518 (Hartree/Particle)  
 Thermal correction to Energy= 0.164486  
 Thermal correction to Enthalpy= 0.165431  
 Thermal correction to Gibbs Free Energy= 0.113172  
 Sum of electronic and zero-point Energies= -711.075760  
 Sum of electronic and thermal Energies= -711.063792  
 Sum of electronic and thermal Enthalpies= -711.062848  
 Sum of electronic and thermal Free Energies= -711.115106

### **<sup>3</sup>[3-NO-9MG]<sup>+</sup>**

N1 -1.247857 -1.479530 0.017250  
 C2 -0.538947 -2.665186 0.009309  
 H3 -1.052666 -3.616602 0.011612  
 N4 0.755920 -2.499465 0.001491  
 C5 0.930579 -1.149106 0.019985  
 C6 2.159741 -0.391672 -0.031855  
 O7 3.304965 -0.728470 -0.062237  
 N8 1.866538 1.048422 -0.059299  
 H9 2.707501 1.616173 -0.106038  
 C10 0.681003 1.652201 0.012348  
 N11 0.557096 2.969631 0.081916  
 H12 1.368725 3.568535 0.127831  
 H13 -0.352628 3.407174 0.137935  
 N14 -0.450906 0.872795 -0.009981  
 C15 -0.294236 -0.516110 0.033783  
 C16 -2.705288 -1.354899 0.021498  
 H17 -3.044565 -0.860420 0.932423  
 H18 -3.042468 -0.805351 -0.858336  
 H19 -3.122802 -2.360342 -0.011013  
 O20 -2.520221 1.838282 -0.384510  
 N21 -1.643100 1.476856 0.389930

Zero-point correction= 0.154469 (Hartree/Particle)  
 Thermal correction to Energy= 0.166709  
 Thermal correction to Enthalpy= 0.167653  
 Thermal correction to Gibbs Free Energy= 0.114707  
 Sum of electronic and zero-point Energies= -711.077458  
 Sum of electronic and thermal Energies= -711.065218  
 Sum of electronic and thermal Enthalpies= -711.064274  
 Sum of electronic and thermal Free Energies= -711.117220

### **TS-<sup>3</sup>[3-ON-9MG]<sup>+</sup>**

N1 1.958069 -0.166974 0.235131  
 C2 2.479913 1.075413 -0.032225  
 H3 3.548335 1.238571 -0.065226  
 N4 1.565234 1.993129 -0.233812  
 C5 0.385634 1.327624 -0.141071  
 C6 -0.961959 1.861072 -0.112625  
 O7 -1.386626 2.961791 -0.289551  
 N8 -1.923749 0.800479 0.231245  
 H9 -2.876992 1.142711 0.316374  
 C10 -1.678386 -0.500624 0.370228  
 N11 -2.640134 -1.400113 0.480036

H12 -3.610708 -1.156809 0.342355  
 H13 -2.410921 -2.372588 0.636937  
 N14 -0.366011 -0.932376 0.444760  
 C15 0.613414 -0.003892 0.142174  
 C16 2.698414 -1.396035 0.507625  
 H17 2.267894 -1.896215 1.376094  
 H18 2.671598 -2.058052 -0.359247  
 H19 3.731233 -1.128620 0.726925  
 O20 -0.213635 -2.305151 -0.281393  
 N21 -0.270627 -2.180353 -1.558974

Zero-point correction= 0.151466 (Hartree/Particle)  
 Thermal correction to Energy= 0.163541  
 Thermal correction to Enthalpy= 0.164485  
 Thermal correction to Gibbs Free Energy= 0.112153  
 Sum of electronic and zero-point Energies= -711.031802  
 Sum of electronic and thermal Energies= -711.019727  
 Sum of electronic and thermal Enthalpies= -711.018783  
 Sum of electronic and thermal Free Energies= -711.071116

### **<sup>3</sup>[3-ON-9MG]<sup>+</sup>**

N1 1.833155 0.644574 0.038515  
 C2 1.806659 2.029071 0.030821  
 H3 2.726766 2.596723 0.050473  
 N4 0.603140 2.527487 0.005198  
 C5 -0.222318 1.441288 0.007516  
 C6 -1.664958 1.394812 -0.056843  
 O7 -2.489411 2.257542 -0.109043  
 N8 -2.128953 -0.000398 -0.061414  
 H9 -3.141011 -0.075801 -0.097629  
 C10 -1.400583 -1.114297 0.034813  
 N11 -1.944222 -2.317044 0.166696  
 H12 -2.944411 -2.427837 0.245760  
 H13 -1.371702 -3.144426 0.253090  
 N14 -0.046155 -0.985348 -0.028970  
 C15 0.527742 0.285543 0.038903  
 C16 3.038074 -0.183802 0.061519  
 H17 3.080109 -0.773157 0.977923  
 H18 3.069630 -0.834046 -0.814386  
 H19 3.896764 0.485520 0.031076  
 O20 0.690399 -2.094261 0.404720  
 N21 1.192786 -2.761973 -0.650324

Zero-point correction= 0.152904 (Hartree/Particle)  
 Thermal correction to Energy= 0.165413  
 Thermal correction to Enthalpy= 0.166357  
 Thermal correction to Gibbs Free Energy= 0.112516  
 Sum of electronic and zero-point Energies= -711.033871  
 Sum of electronic and thermal Energies= -711.021362  
 Sum of electronic and thermal Enthalpies= -711.020418  
 Sum of electronic and thermal Free Energies= -711.074259

### **TS-<sup>3</sup>[4-NO-9MG]<sup>+</sup>**

C1 -1.361807 1.344232 -0.070483  
 C2 0.110315 1.110831 -0.175059  
 H3 -3.052671 0.196105 -0.116169  
 C4 -1.442786 -1.085689 -0.502662  
 C5 2.160584 1.104385 -0.686809  
 N6 -2.044259 0.130164 -0.199952

N7 1.028468 1.904348 -0.616534  
 N8 1.975476 -0.139594 -0.352893  
 N9 -0.141839 -1.297234 -0.473872  
 C10 0.588998 -0.275289 0.083189  
 N11 -2.255476 -2.086942 -0.837501  
 H12 -1.845405 -2.994126 -1.005599  
 H13 -3.245215 -1.970142 -0.988011  
 O14 -1.901888 2.400913 0.094276  
 H15 3.118775 1.492477 -1.013531  
 O16 -0.269769 -0.505383 2.339417  
 C17 2.930827 -1.237960 -0.289051  
 H18 3.876918 -0.915520 -0.721245  
 H19 3.065970 -1.518448 0.758408  
 H20 2.518922 -2.080206 -0.846671  
 N21 0.726084 -0.387518 1.667685

Zero-point correction= 0.152123 (Hartree/Particle)  
 Thermal correction to Energy= 0.164173  
 Thermal correction to Enthalpy= 0.165117  
 Thermal correction to Gibbs Free Energy= 0.113293  
 Sum of electronic and zero-point Energies= -711.080035  
 Sum of electronic and thermal Energies= -711.067985  
 Sum of electronic and thermal Enthalpies= -711.067041  
 Sum of electronic and thermal Free Energies= -711.118865

### <sup>3</sup>[4-NO-9MG]<sup>+</sup>

C1 -1.398089 1.318206 -0.039987  
 C2 0.079530 1.112429 -0.162406  
 H3 -3.063629 0.130923 -0.083274  
 C4 -1.418202 -1.097358 -0.514881  
 C5 2.113860 1.130752 -0.744044  
 N6 -2.055318 0.096094 -0.184036  
 N7 0.956457 1.901618 -0.678626  
 N8 1.978215 -0.095519 -0.343268  
 N9 -0.116927 -1.280615 -0.473146  
 C10 0.599797 -0.260938 0.140019  
 N11 -2.208166 -2.104624 -0.888623  
 H12 -1.779381 -2.998867 -1.077243  
 H13 -3.193220 -1.994879 -1.070975  
 O14 -1.949262 2.364223 0.154318  
 H15 3.046843 1.530203 -1.125876  
 O16 -0.227915 -0.520504 2.358490  
 C17 2.964951 -1.166185 -0.274620  
 H18 3.889353 -0.832268 -0.743502  
 H19 3.137108 -1.412111 0.775735  
 H20 2.557920 -2.034084 -0.795773  
 N21 0.755929 -0.425541 1.652551

Zero-point correction= 0.153251 (Hartree/Particle)  
 Thermal correction to Energy= 0.165649  
 Thermal correction to Enthalpy= 0.166594  
 Thermal correction to Gibbs Free Energy= 0.113983  
 Sum of electronic and zero-point Energies= -711.079065  
 Sum of electronic and thermal Energies= -711.066667  
 Sum of electronic and thermal Enthalpies= -711.065723  
 Sum of electronic and thermal Free Energies= -711.118333

### TS-<sup>3</sup>[4-ON-9MG]<sup>+</sup>

C1 1.465726 -1.329523 -0.051888  
 C2 0.018519 -1.040225 -0.279332

H3 3.178565 -0.245578 0.207960  
 C4 1.644866 1.130502 -0.155445  
 C5 -1.987910 -0.927845 -0.947254  
 N6 2.185061 -0.133065 0.039424  
 N7 -0.879875 -1.773476 -0.836404  
 N8 -1.782072 0.295287 -0.559376  
 N9 0.352391 1.382018 -0.254628  
 C10 -0.455911 0.331581 0.046799  
 N11 2.505786 2.140608 -0.248214  
 H12 2.131761 3.074157 -0.340078  
 H13 3.505987 2.017702 -0.271137  
 O14 1.963660 -2.415625 0.037432  
 H15 -2.929022 -1.270733 -1.361978  
 C16 -2.705121 1.424484 -0.520592  
 H17 -3.606597 1.165903 -1.074003  
 H18 -2.948236 1.639339 0.522268  
 H19 -2.207838 2.283848 -0.971708  
 O20 -0.730608 0.339506 1.615042  
 N21 -1.648442 -0.424162 2.075650

Zero-point correction= 0.151425 (Hartree/Particle)  
 Thermal correction to Energy= 0.163529  
 Thermal correction to Enthalpy= 0.164473  
 Thermal correction to Gibbs Free Energy= 0.112446  
 Sum of electronic and zero-point Energies= -711.054433  
 Sum of electronic and thermal Energies= -711.042330  
 Sum of electronic and thermal Enthalpies= -711.041386  
 Sum of electronic and thermal Free Energies= -711.093412

### <sup>3</sup>[4-ON-9MG]<sup>+</sup>

C1 -1.503019 1.274772 -0.029245  
 C2 -0.045430 1.031327 -0.271482  
 H3 -3.166506 0.114557 0.261067  
 C4 -1.564605 -1.170447 -0.180133  
 C5 1.900679 0.911898 -1.111055  
 N6 -2.173682 0.056870 0.064313  
 N7 0.737808 1.685608 -1.049790  
 N8 1.832540 -0.222630 -0.494415  
 N9 -0.264734 -1.355649 -0.246678  
 C10 0.515584 -0.293030 0.192274  
 N11 -2.380172 -2.209687 -0.353674  
 H12 -1.966498 -3.122590 -0.474768  
 H13 -3.379102 -2.116995 -0.448991  
 O14 -2.024176 2.347940 0.082036  
 H15 2.772213 1.236742 -1.668588  
 C16 2.830165 -1.279689 -0.381092  
 H17 3.688324 -1.029666 -1.003277  
 H18 3.132143 -1.368077 0.664161  
 H19 2.369240 -2.211390 -0.713764  
 O20 0.743392 -0.396376 1.612222  
 N21 1.390555 0.622047 2.153743

Zero-point correction= 0.152759 (Hartree/Particle)  
 Thermal correction to Energy= 0.165156  
 Thermal correction to Enthalpy= 0.166100  
 Thermal correction to Gibbs Free Energy= 0.113170  
 Sum of electronic and zero-point Energies= -711.056126  
 Sum of electronic and thermal Energies= -711.043730  
 Sum of electronic and thermal Enthalpies= -711.042785  
 Sum of electronic and thermal Free Energies= -711.095715

**TS-<sup>3</sup>[5-NO-9MG]<sup>+</sup>**

C1 1.180586 -1.255280 -0.558624  
 C2 -0.212968 -0.874284 -0.162148  
 H3 3.058921 -0.429752 -0.434537  
 C4 1.724512 1.085645 0.019984  
 C5 -2.240123 -0.554309 -0.696170  
 N6 2.082467 -0.192082 -0.292581  
 N7 -1.361685 -1.500001 -0.637990  
 N8 -1.760273 0.733919 -0.399899  
 N9 0.447553 1.528240 0.009537  
 C10 -0.447845 0.596000 -0.166581  
 N11 2.666172 1.969838 0.299846  
 H12 2.382020 2.921141 0.492078  
 H13 3.647441 1.738698 0.352624  
 O14 1.552543 -2.303850 -0.990056  
 H15 -3.279485 -0.693738 -0.969958  
 O16 -1.071008 -0.910887 2.240404  
 C17 -2.527681 1.977131 -0.427756  
 H18 -2.992885 2.099629 -1.406849  
 H19 -3.289046 1.954600 0.352843  
 H20 -1.839787 2.801623 -0.244693  
 N21 -0.131140 -1.186160 1.564441

Zero-point correction= 0.152490 (Hartree/Particle)  
 Thermal correction to Energy= 0.164705  
 Thermal correction to Enthalpy= 0.165649  
 Thermal correction to Gibbs Free Energy= 0.112982  
 Sum of electronic and zero-point Energies= -711.100533  
 Sum of electronic and thermal Energies= -711.088319  
 Sum of electronic and thermal Enthalpies= -711.087375  
 Sum of electronic and thermal Free Energies= -711.140042

**<sup>3</sup>[5-NO-9MG]<sup>+</sup>**

C1 1.066770 -1.242227 -0.647930  
 C2 -0.259872 -0.887795 0.025475  
 H3 2.976454 -0.476507 -0.685479  
 C4 1.741151 1.029428 0.027368  
 C5 -2.275887 -0.481259 -0.629561  
 N6 2.031313 -0.234383 -0.406578  
 N7 -1.475837 -1.463750 -0.493287  
 N8 -1.732297 0.806503 -0.351738  
 N9 0.485866 1.513937 0.099355  
 C10 -0.451568 0.620189 -0.057441  
 N11 2.733980 1.851189 0.316067  
 H12 2.504459 2.798719 0.585066  
 H13 3.703734 1.570774 0.314113  
 O14 1.324494 -2.244296 -1.237715  
 H15 -3.307098 -0.559293 -0.955939  
 O16 -0.861959 -0.969767 2.318722  
 C17 -2.431271 2.081208 -0.490413  
 H18 -2.862064 2.155940 -1.490130  
 H19 -3.217006 2.149341 0.263495  
 H20 -1.708572 2.882604 -0.341992  
 N21 -0.061043 -1.262974 1.450156

Zero-point correction= 0.154415 (Hartree/Particle)  
 Thermal correction to Energy= 0.166593  
 Thermal correction to Enthalpy= 0.167537

Thermal correction to Gibbs Free Energy= 0.115030  
 Sum of electronic and zero-point Energies= -711.104764  
 Sum of electronic and thermal Energies= -711.092587  
 Sum of electronic and thermal Enthalpies= -711.091643  
 Sum of electronic and thermal Free Energies= -711.144150

**TS-<sup>3</sup>[5-ON-9MG]<sup>+</sup>**

C1 1.163277 -1.244246 -0.561192  
 C2 -0.223743 -0.862540 -0.130725  
 H3 3.044177 -0.421067 -0.469632  
 C4 1.717152 1.091594 0.020707  
 C5 -2.255679 -0.550575 -0.641717  
 N6 2.070165 -0.184280 -0.310512  
 N7 -1.381808 -1.493199 -0.592549  
 N8 -1.769440 0.748885 -0.364683  
 N9 0.441558 1.539221 0.028799  
 C10 -0.458808 0.613297 -0.146744  
 N11 2.664371 1.969541 0.297424  
 H12 2.385287 2.919753 0.502861  
 H13 3.645228 1.734172 0.340371  
 O14 1.519669 -2.293045 -1.004786  
 H15 -3.299873 -0.687383 -0.899100  
 C16 -2.541946 1.988219 -0.393213  
 H17 -3.002872 2.112398 -1.374302  
 H18 -3.307286 1.958040 0.383364  
 H19 -1.859416 2.815362 -0.202116  
 O20 -0.073169 -1.161393 1.507964  
 N21 -1.107525 -1.010207 2.200153

Zero-point correction= 0.151728 (Hartree/Particle)  
 Thermal correction to Energy= 0.163916  
 Thermal correction to Enthalpy= 0.164860  
 Thermal correction to Gibbs Free Energy= 0.112225  
 Sum of electronic and zero-point Energies= -711.075314  
 Sum of electronic and thermal Energies= -711.063126  
 Sum of electronic and thermal Enthalpies= -711.062182  
 Sum of electronic and thermal Free Energies= -711.114817

**<sup>3</sup>[5-ON-9MG]<sup>+</sup>**

C1 1.057387 -1.235464 -0.638486  
 C2 -0.254175 -0.888817 0.073466  
 H3 2.959518 -0.450343 -0.718859  
 C4 1.718310 1.045685 0.006738  
 C5 -2.283786 -0.531632 -0.556190  
 N6 2.015944 -0.215639 -0.428703  
 N7 -1.470244 -1.496910 -0.387526  
 N8 -1.754492 0.776206 -0.338998  
 N9 0.457948 1.520205 0.084176  
 C10 -0.472124 0.615843 -0.040235  
 N11 2.704463 1.878642 0.282662  
 H12 2.467570 2.825164 0.549356  
 H13 3.676948 1.607465 0.275589  
 O14 1.308054 -2.239885 -1.227136  
 H15 -3.318754 -0.635363 -0.863181  
 C16 -2.473856 2.034042 -0.516442  
 H17 -2.918507 2.064492 -1.512362  
 H18 -3.250754 2.119679 0.244987  
 H19 -1.761172 2.850720 -0.408090  
 O20 0.041334 -1.241473 1.442585

N21 -0.867974 -0.858062 2.322084

Zero-point correction= 0.153641 (Hartree/Particle)  
 Thermal correction to Energy= 0.165818  
 Thermal correction to Enthalpy= 0.166762  
 Thermal correction to Gibbs Free Energy= 0.114261  
 Sum of electronic and zero-point Energies= -711.079852  
 Sum of electronic and thermal Energies= -711.067675  
 Sum of electronic and thermal Enthalpies= -711.066730  
 Sum of electronic and thermal Free Energies= -711.119232

### TS-<sup>3</sup>[7-NO-9MG]<sup>+</sup>

N1 0.281695 1.950636 -0.051193  
 C2 1.550548 1.558769 -0.155313  
 H3 2.412209 2.211703 -0.140913  
 N4 1.630329 0.214881 -0.235404  
 C5 0.379727 -0.282931 -0.047195  
 C6 -0.146745 -1.627162 -0.120359  
 O7 0.440730 -2.671349 -0.237723  
 N8 -1.567130 -1.582495 0.001011  
 H9 -2.002989 -2.498480 -0.019337  
 C10 -2.335384 -0.457310 0.069457  
 N11 -3.659412 -0.582779 0.145157  
 H12 -4.130879 -1.473383 0.165495  
 H13 -4.214553 0.259268 0.187089  
 N14 -1.819779 0.779126 0.052673  
 C15 -0.499879 0.796528 0.029338  
 C16 -0.238591 3.318069 -0.034871  
 H17 -0.931010 3.445173 -0.867311  
 H18 -0.759114 3.487543 0.907830  
 H19 0.595083 4.011914 -0.131655  
 O20 3.512337 -1.352256 0.065350  
 N21 3.012677 -0.363752 0.492248

Zero-point correction= 0.152228 (Hartree/Particle)  
 Thermal correction to Energy= 0.164545  
 Thermal correction to Enthalpy= 0.165489  
 Thermal correction to Gibbs Free Energy= 0.112314  
 Sum of electronic and zero-point Energies= -711.087526  
 Sum of electronic and thermal Energies= -711.075209  
 Sum of electronic and thermal Enthalpies= -711.074264  
 Sum of electronic and thermal Free Energies= -711.127439

### <sup>3</sup>[7-NO-9MG]<sup>+</sup>

N1 -0.348183 1.960771 -0.005445  
 C2 -1.638302 1.595179 -0.003855  
 H3 -2.493314 2.254082 -0.005374  
 N4 -1.711844 0.257880 -0.001269  
 C5 -0.423517 -0.265288 -0.000209  
 C6 0.103235 -1.607368 0.001887  
 O7 -0.491094 -2.660312 0.004091  
 N8 1.515533 -1.548280 0.001200  
 H9 1.956783 -2.461409 0.002721  
 C10 2.283494 -0.408905 -0.001023  
 N11 3.613572 -0.549536 -0.002250  
 H12 4.076051 -1.443923 -0.002270  
 H13 4.177774 0.286447 -0.003517  
 N14 1.765430 0.810054 -0.001704  
 C15 0.430790 0.818869 -0.002015  
 C16 0.173933 3.328268 0.008321

H17 0.671601 3.512057 0.960850  
 H18 0.888043 3.439060 -0.807301  
 H19 -0.653888 4.023405 -0.123139  
 N20 -2.918967 -0.385633 -0.002735  
 O21 -2.960109 -1.613569 0.001511

Zero-point correction= 0.154355 (Hartree/Particle)  
 Thermal correction to Energy= 0.166803  
 Thermal correction to Enthalpy= 0.167747  
 Thermal correction to Gibbs Free Energy= 0.114607  
 Sum of electronic and zero-point Energies= -711.103329  
 Sum of electronic and thermal Energies= -711.090882  
 Sum of electronic and thermal Enthalpies= -711.089937  
 Sum of electronic and thermal Free Energies= -711.143077

### TS-<sup>3</sup>[7-ON-9MG]<sup>+</sup>

N1 0.344143 1.931094 0.010275  
 C2 1.621474 1.524123 0.029354  
 H3 2.494453 2.159011 -0.008247  
 N4 1.638580 0.197755 0.073261  
 C5 0.367388 -0.300885 -0.048178  
 C6 -0.183980 -1.632623 0.019532  
 O7 0.396383 -2.688985 0.083301  
 N8 -1.596991 -1.546286 -0.015288  
 H9 -2.058167 -2.448997 0.014466  
 C10 -2.341184 -0.391864 -0.019454  
 N11 -3.674105 -0.504653 -0.024622  
 H12 -4.154474 -1.389425 -0.039550  
 H13 -4.221215 0.342572 -0.026001  
 N14 -1.799361 0.818176 -0.011246  
 C15 -0.466092 0.801966 -0.037138  
 C16 -0.146889 3.308579 0.081145  
 H17 -0.865856 3.463171 -0.722941  
 H18 -0.631815 3.468759 1.044555  
 H19 0.695043 3.989651 -0.034220  
 O20 2.985665 -0.553794 -0.449912  
 N21 3.456498 -1.395841 0.332371

Zero-point correction= 0.150811 (Hartree/Particle)  
 Thermal correction to Energy= 0.163461  
 Thermal correction to Enthalpy= 0.164405  
 Thermal correction to Gibbs Free Energy= 0.110219  
 Sum of electronic and zero-point Energies= -711.046868  
 Sum of electronic and thermal Energies= -711.034218  
 Sum of electronic and thermal Enthalpies= -711.033274  
 Sum of electronic and thermal Free Energies= -711.087459

### <sup>3</sup>[7-ON-9MG]<sup>+</sup>

N1 -0.572673 1.849417 -0.035030  
 C2 -1.800735 1.323593 -0.129579  
 H3 -2.735896 1.861547 -0.173444  
 N4 -1.682867 0.000137 -0.176078  
 C5 -0.354502 -0.366227 -0.115308  
 C6 0.329520 -1.637477 -0.119499  
 O7 -0.133576 -2.749573 -0.184297  
 N8 1.721982 -1.399778 -0.029145  
 H9 2.275931 -2.249226 -0.026348  
 C10 2.338311 -0.174005 0.059356  
 N11 3.673624 -0.150278 0.140655  
 H12 4.243756 -0.980037 0.138140

H13 4.127661 0.747865 0.205830  
 N14 1.674005 0.972116 0.067772  
 C15 0.350744 0.814224 -0.020828  
 C16 -0.230687 3.271725 0.047660  
 H17 0.262829 3.462446 1.000609  
 H18 0.442001 3.521373 -0.772626  
 H19 -1.145896 3.857139 -0.025541  
 O20 -2.759917 -0.841489 -0.347900  
 N21 -3.116692 -1.397844 0.828990

Zero-point correction= 0.153726 (Hartree/Particle)  
 Thermal correction to Energy= 0.166188  
 Thermal correction to Enthalpy= 0.167133  
 Thermal correction to Gibbs Free Energy= 0.113705  
 Sum of electronic and zero-point Energies= -711.057577  
 Sum of electronic and thermal Energies= -711.045115  
 Sum of electronic and thermal Enthalpies= -711.044170  
 Sum of electronic and thermal Free Energies= -711.097598

### TS-<sup>3</sup>[8-NO-9MG]<sup>+</sup>

C1 -1.379547 1.478040 -0.181641  
 C2 -0.049267 0.880318 -0.415229  
 H3 -3.266403 0.816782 0.288669  
 C4 -2.080000 -0.876415 0.183226  
 C5 2.014696 0.412210 -0.718442  
 N6 -2.331493 0.463023 0.112725  
 N7 1.071132 1.454415 -0.702975  
 N8 1.360713 -0.833203 -0.613043  
 N9 -0.869770 -1.432761 -0.034314  
 C10 0.078125 -0.574918 -0.322785  
 N11 -3.072086 -1.699391 0.482953  
 H12 -2.867881 -2.688491 0.530890  
 H13 -4.014915 -1.391743 0.670363  
 O14 -1.688161 2.633886 -0.217575  
 H15 2.869719 0.492369 -1.379223  
 O16 2.214491 0.447598 1.834759  
 C17 2.028858 -2.127541 -0.548526  
 H18 2.515488 -2.243918 0.423120  
 H19 1.278572 -2.906042 -0.681170  
 H20 2.768352 -2.188321 -1.346953  
 N21 2.817108 0.663249 0.837113

Zero-point correction= 0.152753 (Hartree/Particle)  
 Thermal correction to Energy= 0.164866  
 Thermal correction to Enthalpy= 0.165810  
 Thermal correction to Gibbs Free Energy= 0.113240  
 Sum of electronic and zero-point Energies= -711.103306  
 Sum of electronic and thermal Energies= -711.091194  
 Sum of electronic and thermal Enthalpies= -711.090250  
 Sum of electronic and thermal Free Energies= -711.142819

### <sup>3</sup>[8-NO-9MG]<sup>+</sup>

C1 -1.414030 1.513401 -0.112996  
 C2 -0.080575 0.878198 -0.306021  
 H3 -3.333743 0.906715 0.264539  
 C4 -2.191207 -0.824015 0.183217  
 C5 2.014859 0.360498 -0.637700  
 N6 -2.401676 0.529893 0.125950  
 N7 1.037733 1.439142 -0.532657  
 N8 1.266869 -0.896137 -0.439367

N9 -1.000176 -1.417182 0.008999  
 C10 0.001872 -0.597141 -0.225206  
 N11 -3.230475 -1.606962 0.425994  
 H12 -3.071601 -2.604485 0.467839  
 H13 -4.166357 -1.261255 0.577287  
 O14 -1.672717 2.680262 -0.146941  
 H15 2.486679 0.386832 -1.623347  
 O16 2.857789 0.522867 1.546178  
 C17 1.883757 -2.215462 -0.427708  
 H18 2.620737 -2.264229 0.376709  
 H19 1.102514 -2.956058 -0.260988  
 H20 2.370269 -2.400031 -1.387208  
 N21 3.073849 0.504761 0.346761

Zero-point correction= 0.155384 (Hartree/Particle)  
 Thermal correction to Energy= 0.167436  
 Thermal correction to Enthalpy= 0.168380  
 Thermal correction to Gibbs Free Energy= 0.115903  
 Sum of electronic and zero-point Energies= -711.112216  
 Sum of electronic and thermal Energies= -711.100164  
 Sum of electronic and thermal Enthalpies= -711.099220  
 Sum of electronic and thermal Free Energies= -711.151697

### TS-<sup>3</sup>[7H-8-NO-9MG]<sup>+</sup>

C1 1.345776 1.595007 0.034626  
 C2 0.108687 0.822340 -0.010249  
 H3 3.354845 1.186941 -0.039047  
 C4 2.403580 -0.654587 -0.069562  
 C5 -1.914348 0.079867 0.152021  
 N6 2.458119 0.712615 -0.042680  
 N7 -1.160199 1.258674 0.014270  
 N8 -1.100462 -1.039463 0.106940  
 N9 1.263042 -1.349826 -0.029501  
 C10 0.179573 -0.592211 0.000649  
 N11 3.546754 -1.332248 -0.130692  
 H12 3.499574 -2.340588 -0.148727  
 H13 4.451902 -0.891040 -0.174962  
 O14 1.490430 2.784806 0.113403  
 H15 -1.757673 0.871139 1.168891  
 O16 -4.039525 0.865569 -0.253276  
 C17 -1.545480 -2.431707 0.154013  
 H18 -2.182495 -2.639768 -0.707199  
 H19 -0.655377 -3.058284 0.121021  
 H20 -2.093384 -2.610912 1.079746  
 N21 -3.248877 -0.054430 -0.168300

Zero-point correction= 0.150246 (Hartree/Particle)  
 Thermal correction to Energy= 0.162235  
 Thermal correction to Enthalpy= 0.163180  
 Thermal correction to Gibbs Free Energy= 0.110834  
 Sum of electronic and zero-point Energies= -711.064047  
 Sum of electronic and thermal Energies= -711.052058  
 Sum of electronic and thermal Enthalpies= -711.051114  
 Sum of electronic and thermal Free Energies= -711.103459

### <sup>3</sup>[7H-8-NO-9MG]<sup>+</sup>

C1 -1.588982 1.478436 -0.000008  
 C2 -0.274018 0.894669 -0.000007  
 H3 -3.513774 0.783502 0.000003  
 C4 -2.296692 -0.901435 0.000008

C5 1.886316 0.475242 0.000001  
 N6 -2.556943 0.447891 0.000001  
 N7 0.969407 1.466401 -0.000006  
 N8 1.244305 -0.731623 -0.000008  
 N9 -1.070051 -1.406654 0.000001  
 C10 -0.111310 -0.480734 -0.000006  
 N11 -3.338306 -1.739583 0.000025  
 H12 -3.148886 -2.730300 0.000037  
 H13 -4.297143 -1.432022 0.000042  
 O14 -1.884882 2.651361 -0.000015  
 H15 1.175472 2.458698 0.000000  
 O16 4.107285 -0.102456 0.000028  
 C17 1.864773 -2.057888 -0.000041  
 H18 2.473137 -2.184460 0.896155  
 H19 1.053783 -2.784880 -0.000124  
 H20 2.473234 -2.184361 -0.896185  
 N21 3.197933 0.711115 0.000028

Zero-point correction= 0.155352 (Hartree/Particle)  
 Thermal correction to Energy= 0.167689  
 Thermal correction to Enthalpy= 0.168633  
 Thermal correction to Gibbs Free Energy= 0.115647  
 Sum of electronic and zero-point Energies= -711.162198  
 Sum of electronic and thermal Energies= -711.149861  
 Sum of electronic and thermal Enthalpies= -711.148917  
 Sum of electronic and thermal Free Energies= -711.201902

### TS-<sup>3</sup>[8-ON-9MG]<sup>+</sup>

C1 -1.390540 1.473817 -0.172162  
 C2 -0.044547 0.892523 -0.388878  
 H3 -3.273018 0.789058 0.275652  
 C4 -2.067903 -0.891492 0.161280  
 C5 2.030108 0.443534 -0.639793  
 N6 -2.332495 0.447600 0.104962  
 N7 1.065523 1.480993 -0.650282  
 N8 1.378974 -0.812242 -0.595435  
 N9 -0.851957 -1.436326 -0.053169  
 C10 0.094955 -0.571292 -0.313334  
 N11 -3.055131 -1.725102 0.442323  
 H12 -2.842352 -2.712916 0.482485  
 H13 -4.002148 -1.427850 0.625947  
 O14 -1.707578 2.626279 -0.209184  
 H15 2.898356 0.544709 -1.280650  
 C16 2.059617 -2.101242 -0.532047  
 H17 2.519288 -2.229796 0.450891  
 H18 1.321203 -2.884162 -0.700312  
 H19 2.821012 -2.140321 -1.310948  
 O20 2.773842 0.637081 0.848237  
 N21 2.071859 0.399265 1.845046

Zero-point correction= 0.152340 (Hartree/Particle)  
 Thermal correction to Energy= 0.164355  
 Thermal correction to Enthalpy= 0.165300  
 Thermal correction to Gibbs Free Energy= 0.113005  
 Sum of electronic and zero-point Energies= -711.080410  
 Sum of electronic and thermal Energies= -711.068394  
 Sum of electronic and thermal Enthalpies= -711.067450  
 Sum of electronic and thermal Free Energies= -711.119745

### <sup>3</sup>[8-ON-9MG]<sup>+</sup>

C1 -1.413568 1.512152 -0.104831  
 C2 -0.074633 0.881476 -0.278166  
 H3 -3.338692 0.898624 0.232890  
 C4 -2.191303 -0.828946 0.156589  
 C5 2.021310 0.367365 -0.591681  
 N6 -2.403249 0.524895 0.108977  
 N7 1.048506 1.444836 -0.464341  
 N8 1.281503 -0.888686 -0.385774  
 N9 -0.995377 -1.419243 -0.001153  
 C10 0.009514 -0.597163 -0.206196  
 N11 -3.232317 -1.616545 0.371983  
 H12 -3.071319 -2.614098 0.407528  
 H13 -4.171796 -1.274802 0.510199  
 O14 -1.673544 2.678581 -0.135780  
 H15 2.473671 0.399118 -1.586735  
 C16 1.905600 -2.205215 -0.375688  
 H17 2.653066 -2.243443 0.418863  
 H18 1.130507 -2.948551 -0.193691  
 H19 2.380476 -2.393414 -1.340433  
 O20 3.091314 0.495991 0.312281  
 N21 2.738136 0.526453 1.590195

Zero-point correction= 0.154662 (Hartree/Particle)  
 Thermal correction to Energy= 0.166704  
 Thermal correction to Enthalpy= 0.167648  
 Thermal correction to Gibbs Free Energy= 0.115286  
 Sum of electronic and zero-point Energies= -711.089794  
 Sum of electronic and thermal Energies= -711.077752  
 Sum of electronic and thermal Enthalpies= -711.076807  
 Sum of electronic and thermal Free Energies= -711.129169

### TS-<sup>3</sup>[7H-8-ON-9MG]<sup>+</sup>

C1 -1.419254 1.549573 -0.047577  
 C2 -0.132863 0.862536 -0.067195  
 H3 -3.387314 1.000167 0.128907  
 C4 -2.309737 -0.770489 0.125274  
 C5 1.919292 0.258506 -0.327541  
 N6 -2.460185 0.589940 0.090366  
 N7 1.107885 1.374581 -0.161752  
 N8 1.203462 -0.906560 -0.203493  
 N9 -1.125979 -1.384878 0.036570  
 C10 -0.106455 -0.546914 -0.054209  
 N11 -3.398964 -1.524791 0.247181  
 H12 -3.280617 -2.527158 0.271163  
 H13 -4.329325 -1.146818 0.333363  
 O14 -1.652213 2.725118 -0.124152  
 H15 1.638991 1.067081 -1.325061  
 C16 1.716776 -2.275467 -0.270042  
 H17 2.804759 -2.239207 -0.258550  
 H18 1.348981 -2.822760 0.597839  
 H19 1.361967 -2.751093 -1.185117  
 O20 3.267118 0.282361 -0.177370  
 N21 3.661891 0.550778 1.090751

Zero-point correction= 0.149369 (Hartree/Particle)  
 Thermal correction to Energy= 0.161548  
 Thermal correction to Enthalpy= 0.162492  
 Thermal correction to Gibbs Free Energy= 0.108764  
 Sum of electronic and zero-point Energies= -711.031215

Sum of electronic and thermal Energies= -711.019035  
 Sum of electronic and thermal Enthalpies= -711.018091  
 Sum of electronic and thermal Free Energies= -711.071819

**<sup>3</sup>[7H-8-ON-9MG]<sup>+</sup>**

C1 -1.313933 1.586931 0.000000  
 C2 -0.118362 0.793583 0.000000  
 H3 -3.325516 1.211551 0.000000  
 C4 -2.402097 -0.649860 0.000000  
 C5 1.927201 0.027640 -0.000001  
 N6 -2.436430 0.724105 0.000000  
 N7 1.224090 1.153220 0.000000  
 N8 1.128786 -1.046372 0.000000  
 N9 -1.274864 -1.346092 0.000000  
 C10 -0.184166 -0.576627 0.000000  
 N11 -3.569786 -1.305409 0.000001  
 H12 -3.547265 -2.313436 0.000001  
 H13 -4.463925 -0.842999 0.000002  
 O14 -1.420052 2.792435 -0.000001  
 H15 1.590952 2.098337 0.000000  
 C16 1.552009 -2.449685 0.000000  
 H17 2.137057 -2.657878 0.896040  
 H18 0.643999 -3.050711 -0.000052  
 H19 2.137142 -2.657852 -0.895991  
 O20 3.255219 -0.110060 -0.000001  
 N21 3.982820 1.015133 0.000003

Zero-point correction= 0.154766 (Hartree/Particle)  
 Thermal correction to Energy= 0.167314  
 Thermal correction to Enthalpy= 0.168258  
 Thermal correction to Gibbs Free Energy= 0.114443  
 Sum of electronic and zero-point Energies= -711.126486  
 Sum of electronic and thermal Energies= -711.113938  
 Sum of electronic and thermal Enthalpies= -711.112993  
 Sum of electronic and thermal Free Energies= -711.166809

**TS-<sup>3</sup>[2,4-NO-9MG]<sup>+</sup>**

C1 0.632755 -0.285970 -0.156530  
 C2 0.352661 1.166273 -0.032042  
 C3 -1.082192 1.600486 -0.076336  
 C4 -1.522295 -0.879724 -0.130218  
 C5 2.452794 0.918657 -0.038271  
 O6 -1.450634 2.740567 -0.008641  
 N7 1.445137 1.852629 0.057448  
 N8 2.047585 -0.321222 -0.215694  
 N9 -0.216606 -0.995581 -0.915536  
 N10 -2.569675 -1.714988 -0.491750  
 H11 -2.451041 -2.674426 -0.191397  
 H12 -2.846682 -1.644104 -1.463107  
 C13 2.842437 -1.544875 -0.337252  
 H14 2.635215 -2.183164 0.523346  
 H15 3.897688 -1.277032 -0.361372  
 H16 2.563277 -2.052160 -1.261489  
 N17 -1.912397 0.498488 -0.243652  
 H18 -2.911968 0.680763 -0.223499  
 N19 -1.059212 -1.237915 1.261143  
 O20 0.126988 -0.797460 1.435603  
 H21 3.501900 1.186298 0.021998

Zero-point correction= 0.151064 (Hartree/Particle)  
 Thermal correction to Energy= 0.162469  
 Thermal correction to Enthalpy= 0.163414  
 Thermal correction to Gibbs Free Energy= 0.113062  
 Sum of electronic and zero-point Energies= -711.002484  
 Sum of electronic and thermal Energies= -710.991078  
 Sum of electronic and thermal Enthalpies= -710.990134  
 Sum of electronic and thermal Free Energies= -711.040486

**<sup>3</sup>[2,4-NO-9MG]<sup>+</sup>**

C1 0.608970 -0.293653 0.027702  
 C2 0.301314 1.194553 0.012324  
 C3 -1.155022 1.584380 0.030309  
 C4 -1.473535 -0.920474 -0.158928  
 C5 2.400118 0.992139 -0.206002  
 O6 -1.544331 2.714026 0.153104  
 N7 1.358894 1.911441 -0.118600  
 N8 2.048618 -0.261529 -0.150479  
 N9 -0.204518 -0.867734 -0.963166  
 N10 -2.490030 -1.765322 -0.604357  
 H11 -2.376555 -2.729148 -0.316403  
 H12 -2.701713 -1.677949 -1.590899  
 C13 2.884440 -1.462298 -0.199507  
 H14 2.758844 -2.008820 0.736822  
 H15 3.924205 -1.164402 -0.326226  
 H16 2.562684 -2.075968 -1.042427  
 N17 -1.942535 0.462837 -0.138595  
 H18 -2.950026 0.588605 -0.110088  
 N19 -1.021780 -1.359421 1.187133  
 O20 0.258457 -0.920116 1.279329  
 H21 3.431303 1.306621 -0.329174

Zero-point correction= 0.152884 (Hartree/Particle)  
 Thermal correction to Energy= 0.164269  
 Thermal correction to Enthalpy= 0.165213  
 Thermal correction to Gibbs Free Energy= 0.115180  
 Sum of electronic and zero-point Energies= -711.008630  
 Sum of electronic and thermal Energies= -710.997244  
 Sum of electronic and thermal Enthalpies= -710.996300  
 Sum of electronic and thermal Free Energies= -711.046334

**TS-<sup>3</sup>[4,5-ON-9MG]<sup>+</sup>**

C1 1.332119 -1.277026 -0.250304  
 C2 -0.132160 -1.038690 0.086321  
 H3 3.061445 -0.217108 -0.375508  
 C4 1.552160 1.196375 -0.130528  
 C5 -2.079901 -0.829072 -0.830210  
 N6 2.068318 -0.086264 -0.217437  
 N7 -1.119836 -1.715905 -0.639856  
 N8 -1.839693 0.421270 -0.382342  
 N9 0.269718 1.484653 -0.004967  
 C10 -0.541220 0.429035 0.198276  
 N11 2.425412 2.196441 -0.210272  
 H12 2.073452 3.138989 -0.123891  
 H13 3.415880 2.063052 -0.340848  
 O14 1.824376 -2.340952 -0.477621  
 H15 -3.013239 -1.068818 -1.328277  
 C16 -2.722910 1.576581 -0.413443  
 H17 -2.140597 2.443263 -0.731152

H18 -3.536743 1.383246 -1.111236  
 H19 -3.124026 1.750224 0.588873  
 O20 -0.788454 0.087733 1.759606  
 N21 -0.299930 -1.130239 1.627086

Zero-point correction= 0.151671 (Hartree/Particle)  
 Thermal correction to Energy= 0.163204  
 Thermal correction to Enthalpy= 0.164148  
 Thermal correction to Gibbs Free Energy= 0.113470  
 Sum of electronic and zero-point Energies= -711.046804  
 Sum of electronic and thermal Energies= -711.035272  
 Sum of electronic and thermal Enthalpies= -711.034328  
 Sum of electronic and thermal Free Energies= -711.085005

### <sup>3</sup>[4,5-ON-9MG]<sup>+</sup>

C1 1.368600 -1.250151 -0.216312  
 C2 -0.109593 -1.051460 0.096250  
 H3 3.063694 -0.143208 -0.350866  
 C4 1.508768 1.231130 -0.127856  
 C5 -2.024602 -0.817859 -0.926139  
 N6 2.065297 -0.041425 -0.206615  
 N7 -1.032202 -1.692345 -0.757997  
 N8 -1.849290 0.382338 -0.368167  
 N9 0.231641 1.480982 0.037571  
 C10 -0.553229 0.391925 0.302781  
 N11 2.360377 2.250186 -0.252061  
 H12 1.995590 3.186272 -0.156160  
 H13 3.346210 2.134190 -0.423736  
 O14 1.889077 -2.307684 -0.415281  
 H15 -2.919003 -1.052108 -1.493804  
 C16 -2.752167 1.518181 -0.363648  
 H17 -2.179146 2.404549 -0.646117  
 H18 -3.568076 1.337712 -1.062022  
 H19 -3.144463 1.650797 0.649429  
 O20 -0.781445 0.078492 1.730531  
 N21 -0.359041 -1.210487 1.600245

Zero-point correction= 0.152381 (Hartree/Particle)  
 Thermal correction to Energy= 0.164107  
 Thermal correction to Enthalpy= 0.165051  
 Thermal correction to Gibbs Free Energy= 0.114124  
 Sum of electronic and zero-point Energies= -711.047397  
 Sum of electronic and thermal Energies= -711.035671  
 Sum of electronic and thermal Enthalpies= -711.034727  
 Sum of electronic and thermal Free Energies= -711.085654

### TS-<sup>3</sup>[5,8-NO-9MG]<sup>+</sup> (from 5-NO)

C1 1.167033 -1.395340 -0.308743  
 C2 -0.207434 -0.833206 -0.075840  
 H3 3.108576 -0.762547 -0.119991  
 C4 1.926771 0.927355 0.083062  
 C5 -2.229946 -0.306593 -0.490391  
 N6 2.157393 -0.409766 -0.086121  
 N7 -1.373780 -1.307931 -0.818751  
 N8 -1.568415 0.918861 -0.395951  
 N9 0.707865 1.495131 -0.001226  
 C10 -0.267135 0.646816 -0.195965  
 N11 2.954645 1.725707 0.316485  
 H12 2.772831 2.714689 0.421712  
 H13 3.902773 1.395830 0.420752

O14 1.442846 -2.520259 -0.597408  
 H15 -3.294128 -0.347652 -0.684116  
 O16 -1.944810 -0.959696 1.334272  
 C17 -2.207024 2.230128 -0.304943  
 H18 -1.446501 2.989484 -0.480937  
 H19 -2.984430 2.302458 -1.065263  
 H20 -2.635986 2.357329 0.691405  
 N21 -0.663566 -1.054131 1.368199

Zero-point correction= 0.152575 (Hartree/Particle)  
 Thermal correction to Energy= 0.163821  
 Thermal correction to Enthalpy= 0.164766  
 Thermal correction to Gibbs Free Energy= 0.114745  
 Sum of electronic and zero-point Energies= -711.046597  
 Sum of electronic and thermal Energies= -711.035351  
 Sum of electronic and thermal Enthalpies= -711.034407  
 Sum of electronic and thermal Free Energies= -711.084428

### TS-<sup>3</sup>[5,8-NO-9MG]<sup>+</sup> (from <sup>3</sup>precursor)

C1 1.240515 -1.410770 -0.258760  
 C2 -0.131966 -0.845833 -0.264684  
 H3 3.151324 -0.740652 0.078116  
 C4 1.943414 0.940597 0.089665  
 C5 -2.181382 -0.396716 -0.371967  
 N6 2.199236 -0.396950 0.002436  
 N7 -1.216567 -1.356070 -0.871131  
 N8 -1.546829 0.880978 -0.458698  
 N9 0.719747 1.487517 -0.061738  
 C10 -0.246711 0.629512 -0.249158  
 N11 2.946790 1.768853 0.326627  
 H12 2.742254 2.757488 0.380679  
 H13 3.899856 1.465259 0.461433  
 O14 1.558872 -2.552563 -0.412118  
 H15 -3.208578 -0.464255 -0.712688  
 O16 -2.171004 -0.757479 1.117142  
 C17 -2.218665 2.165735 -0.289329  
 H18 -1.485192 2.953990 -0.454430  
 H19 -3.016854 2.249186 -1.026968  
 H20 -2.626283 2.247579 0.721484  
 N21 -0.958192 -1.024816 1.487873

Zero-point correction= 0.152784 (Hartree/Particle)  
 Thermal correction to Energy= 0.164141  
 Thermal correction to Enthalpy= 0.165085  
 Thermal correction to Gibbs Free Energy= 0.114713  
 Sum of electronic and zero-point Energies= -711.053305  
 Sum of electronic and thermal Energies= -711.041948  
 Sum of electronic and thermal Enthalpies= -711.041004  
 Sum of electronic and thermal Free Energies= -711.091375

### <sup>3</sup>[5,8-NO-9MG]<sup>+</sup>

C1 1.191455 -1.406527 -0.226439  
 C2 -0.201368 -0.852780 -0.062628  
 H3 3.131351 -0.770255 -0.061477  
 C4 1.952652 0.927123 0.082658  
 C5 -2.211973 -0.367731 -0.295005  
 N6 2.181013 -0.413733 -0.046342  
 N7 -1.245145 -1.180799 -1.012677  
 N8 -1.550937 0.935359 -0.313673



N9 0.734977 1.496393 0.000181  
 C10 -0.261476 0.665187 -0.136060  
 N11 2.983342 1.731129 0.275962  
 H12 2.803041 2.723217 0.352432  
 H13 3.935054 1.405913 0.362193  
 O14 1.472410 -2.546341 -0.443036  
 H15 -3.244011 -0.375815 -0.631103  
 O16 -2.115178 -0.887695 1.054741  
 C17 -2.208906 2.234875 -0.254706  
 H18 -1.452464 3.006642 -0.392065  
 H19 -2.947190 2.297577 -1.054934  
 H20 -2.694492 2.360112 0.715910  
 N21 -0.810600 -1.193491 1.263476

Zero-point correction= 0.155365 (Hartree/Particle)  
 Thermal correction to Energy= 0.166414  
 Thermal correction to Enthalpy= 0.167358  
 Thermal correction to Gibbs Free Energy= 0.117695  
 Sum of electronic and zero-point Energies= -711.067345  
 Sum of electronic and thermal Energies= -711.056297  
 Sum of electronic and thermal Enthalpies= -711.055352  
 Sum of electronic and thermal Free Energies= -711.105015

### TS-<sup>3</sup>[5,8-ON-9MG]<sup>+</sup> (from 5-NO)

C1 1.168382 -1.390428 -0.278728  
 C2 -0.220970 -0.828197 -0.100955  
 H3 3.103728 -0.744662 -0.119948  
 C4 1.916526 0.946070 0.064459  
 C5 -2.222684 -0.364850 -0.478614  
 N6 2.150972 -0.396003 -0.087383  
 N7 -1.354335 -1.317346 -0.850203  
 N8 -1.575089 0.925561 -0.358180  
 N9 0.700401 1.515300 -0.001093  
 C10 -0.287835 0.676420 -0.190161  
 N11 2.950109 1.744643 0.269917  
 H12 2.770647 2.735336 0.364525  
 H13 3.900885 1.416630 0.354380  
 O14 1.446036 -2.526995 -0.515327  
 H15 -3.274749 -0.386784 -0.737129  
 C16 -2.260020 2.207057 -0.249174  
 H17 -1.516009 2.998145 -0.334844  
 H18 -2.988182 2.295786 -1.056211  
 H19 -2.761305 2.274846 0.719064  
 O20 -0.676397 -1.065458 1.292987  
 N21 -2.008131 -0.947313 1.310933

Zero-point correction= 0.152838 (Hartree/Particle)  
 Thermal correction to Energy= 0.164008  
 Thermal correction to Enthalpy= 0.164953  
 Thermal correction to Gibbs Free Energy= 0.115007  
 Sum of electronic and zero-point Energies= -711.034692  
 Sum of electronic and thermal Energies= -711.023522  
 Sum of electronic and thermal Enthalpies= -711.022577  
 Sum of electronic and thermal Free Energies= -711.072523

### TS-<sup>3</sup>[5,8-ON-9MG]<sup>+</sup> (from 8-NO)

C1 1.214763 -1.408650 -0.245566  
 C2 -0.154474 -0.827130 -0.261144  
 H3 3.131371 -0.758990 0.066802  
 C4 1.940471 0.938356 0.079671

C5 -2.229557 -0.382603 -0.321387  
 N6 2.181592 -0.407047 0.000800  
 N7 -1.224787 -1.260785 -0.973442  
 N8 -1.557745 0.905447 -0.391065  
 N9 0.724421 1.495003 -0.050071  
 C10 -0.258646 0.649242 -0.229404  
 N11 2.962426 1.751287 0.292170  
 H12 2.775530 2.743401 0.346132  
 H13 3.912694 1.432937 0.411085  
 O14 1.508035 -2.558473 -0.391302  
 H15 -3.232532 -0.401432 -0.734676  
 O16 -0.951248 -1.065182 1.366014  
 C17 -2.218310 2.193222 -0.222589  
 H18 -1.473531 2.978640 -0.344592  
 H19 -2.994665 2.296784 -0.981445  
 H20 -2.659977 2.251382 0.776044  
 N21 -2.182857 -0.845062 1.102390

Zero-point correction= 0.153238 (Hartree/Particle)  
 Thermal correction to Energy= 0.164382  
 Thermal correction to Enthalpy= 0.165326  
 Thermal correction to Gibbs Free Energy= 0.115465  
 Sum of electronic and zero-point Energies= -711.050727  
 Sum of electronic and thermal Energies= -711.039583  
 Sum of electronic and thermal Enthalpies= -711.038638  
 Sum of electronic and thermal Free Energies= -711.088500

### <sup>3</sup>[5,8-ON-9MG]<sup>+</sup>

C1 1.176646 -1.404126 -0.216676  
 C2 -0.216101 -0.831027 -0.099789  
 H3 3.115611 -0.774006 -0.074160  
 C4 1.946884 0.932867 0.074851  
 C5 -2.237841 -0.368373 -0.295699  
 N6 2.166808 -0.413390 -0.058992  
 N7 -1.235371 -1.125241 -1.065351  
 N8 -1.556346 0.950466 -0.268919  
 N9 0.735399 1.510964 0.023390  
 C10 -0.268752 0.684187 -0.119247  
 N11 2.991239 1.724429 0.248691  
 H12 2.823169 2.717938 0.334394  
 H13 3.941469 1.389670 0.310189  
 O14 1.444967 -2.554339 -0.391045  
 H15 -3.245580 -0.335894 -0.698820  
 C16 -2.221735 2.243557 -0.199410  
 H17 -1.465709 3.022667 -0.290775  
 H18 -2.935700 2.321997 -1.020647  
 H19 -2.740494 2.338024 0.757435  
 O20 -0.837728 -1.219526 1.171752  
 N21 -2.162485 -0.937511 1.060118

Zero-point correction= 0.155075 (Hartree/Particle)  
 Thermal correction to Energy= 0.166222  
 Thermal correction to Enthalpy= 0.167166  
 Thermal correction to Gibbs Free Energy= 0.117244  
 Sum of electronic and zero-point Energies= -711.058779  
 Sum of electronic and thermal Energies= -711.047632  
 Sum of electronic and thermal Enthalpies= -711.046688  
 Sum of electronic and thermal Free Energies= -711.096610

### TS-<sup>3</sup>[7,8-NO-9MG]<sup>+</sup>

C1 0.938464 -1.585046 -0.199654  
 C2 -0.159567 -0.647553 -0.304787  
 H3 2.964760 -1.468740 0.121129  
 C4 2.274873 0.481723 0.150164  
 C5 -2.104216 0.432456 -0.378305  
 N6 2.149548 -0.869489 0.041415  
 N7 -1.484630 -0.832718 -0.550220  
 N8 -1.153590 1.364258 -0.212322  
 N9 1.228011 1.325025 0.073266  
 C10 0.078566 0.723313 -0.121081  
 N11 3.477318 1.010556 0.347039  
 H12 3.546194 2.014511 0.434088  
 H13 4.320410 0.461601 0.417443  
 O14 0.924255 -2.783574 -0.297187  
 H15 -3.074592 0.674266 -0.792798  
 O16 -2.813998 -0.591054 0.998276  
 C17 -1.339812 2.814713 -0.148969  
 H18 -1.081557 3.165940 0.850618  
 H19 -0.693222 3.288879 -0.887616  
 H20 -2.383611 3.040488 -0.362157  
 N21 -2.303840 -1.640139 0.390302

Zero-point correction= 0.153193 (Hartree/Particle)  
 Thermal correction to Energy= 0.164657  
 Thermal correction to Enthalpy= 0.165602  
 Thermal correction to Gibbs Free Energy= 0.114694  
 Sum of electronic and zero-point Energies= -711.053972  
 Sum of electronic and thermal Energies= -711.042508  
 Sum of electronic and thermal Enthalpies= -711.041563  
 Sum of electronic and thermal Free Energies= -711.092471

### <sup>3</sup>[7,8-NO-9MG]<sup>+</sup>

C1 1.095628 -1.542785 -0.165000  
 C2 -0.089224 -0.726119 -0.303926  
 H3 3.106558 -1.237818 0.136403  
 C4 2.226472 0.638841 0.122832  
 C5 -2.186461 0.140480 -0.399871  
 N6 2.237981 -0.721807 0.043650  
 N7 -1.397795 -1.086966 -0.508740  
 N8 -1.246187 1.204703 -0.212499  
 N9 1.107240 1.378944 0.047844  
 C10 0.000245 0.695454 -0.144204  
 N11 3.373648 1.281991 0.295961  
 H12 3.345743 2.289558 0.365498  
 H13 4.266510 0.818192 0.367076  
 O14 1.180019 -2.743782 -0.221679  
 H15 -2.924878 0.352587 -1.175730  
 O16 -2.808385 -0.406133 0.772111  
 C17 -1.611435 2.613480 -0.121078  
 H18 -2.100550 2.809634 0.835295  
 H19 -0.700552 3.206059 -0.195765  
 H20 -2.284770 2.867306 -0.942297  
 N21 -2.116670 -1.602907 0.658576

Zero-point correction= 0.155151 (Hartree/Particle)  
 Thermal correction to Energy= 0.166695  
 Thermal correction to Enthalpy= 0.167640  
 Thermal correction to Gibbs Free Energy= 0.116417  
 Sum of electronic and zero-point Energies= -711.073066

Sum of electronic and thermal Energies= -711.061522  
 Sum of electronic and thermal Enthalpies= -711.060577  
 Sum of electronic and thermal Free Energies= -711.111800

### TS-<sup>3</sup>[7,8-ON-9MG]<sup>+</sup>

C1 1.077794 -1.550641 -0.175514  
 C2 -0.108139 -0.715492 -0.303203  
 H3 3.088744 -1.265571 0.132765  
 C4 2.228542 0.621324 0.129965  
 C5 -2.183500 0.174037 -0.412193  
 N6 2.224854 -0.741399 0.041697  
 N7 -1.376112 -1.067644 -0.564292  
 N8 -1.226720 1.236349 -0.226745  
 N9 1.123200 1.378435 0.047797  
 C10 0.005167 0.710722 -0.140896  
 N11 3.384124 1.244311 0.316587  
 H12 3.372194 2.252026 0.389194  
 H13 4.268857 0.765929 0.392671  
 O14 1.150273 -2.748734 -0.238196  
 H15 -2.889200 0.381564 -1.221919  
 C16 -1.585363 2.643461 -0.114127  
 H17 -2.130718 2.810338 0.817720  
 H18 -0.667034 3.229200 -0.114172  
 H19 -2.207176 2.929257 -0.965118  
 N20 -2.827461 -0.352762 0.795562  
 O21 -2.219756 -1.536797 0.711999

Zero-point correction= 0.152927 (Hartree/Particle)  
 Thermal correction to Energy= 0.164386  
 Thermal correction to Enthalpy= 0.165330  
 Thermal correction to Gibbs Free Energy= 0.114231  
 Sum of electronic and zero-point Energies= -711.042168  
 Sum of electronic and thermal Energies= -711.030709  
 Sum of electronic and thermal Enthalpies= -711.029764  
 Sum of electronic and thermal Free Energies= -711.080864

### <sup>3</sup>[7,8-ON-9MG]<sup>+</sup>

C1 1.054057 -1.552210 -0.164120  
 C2 -0.115264 -0.705332 -0.294487  
 H3 3.069629 -1.290651 0.135935  
 C4 2.232186 0.606766 0.121455  
 C5 -2.194686 0.207817 -0.381322  
 N6 2.212007 -0.756280 0.045791  
 N7 -1.410528 -1.036688 -0.552554  
 N8 -1.222818 1.253332 -0.204153  
 N9 1.133707 1.372477 0.043932  
 C10 0.008466 0.713103 -0.140164  
 N11 3.396827 1.219040 0.293287  
 H12 3.396512 2.227116 0.359365  
 H13 4.276834 0.731506 0.364078  
 O14 1.111182 -2.753219 -0.223965  
 H15 -2.921483 0.435790 -1.166467  
 C16 -1.557561 2.667454 -0.102945  
 H17 -2.081041 2.856155 0.837085  
 H18 -0.630492 3.238527 -0.129006  
 H19 -2.191941 2.952067 -0.945144  
 N20 -2.812004 -0.376143 0.824360  
 O21 -2.181375 -1.560062 0.618842

|  |                             |
|--|-----------------------------|
| Zero-point correction=                       | 0.154265 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.165910                    |
| Thermal correction to Enthalpy=              | 0.166854                    |
| Thermal correction to Gibbs Free Energy=     | 0.115495                    |
| Sum of electronic and zero-point Energies=   | -711.041531                 |
| Sum of electronic and thermal Energies=      | -711.029886                 |
| Sum of electronic and thermal Enthalpies=    | -711.028942                 |
| Sum of electronic and thermal Free Energies= | -711.080302                 |