

## Supplementary Materials:

# Evaluating the atmospheric loss of H<sub>2</sub> by NO<sub>3</sub> radicals: a theoretical study

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### Optimized geometries of various species in the H<sub>2</sub> + NO<sub>3</sub> reaction using G3B3 theory

TS: NO<sub>3</sub> + H<sub>2</sub> → HNO<sub>3</sub> + H

O

O, 1, B1

O, 1, B2, 2, A1

N, 2, B3, 1, A2, 3, D1, 0

H, 1, B4, 4, A3, 2, D2, 0

H, 1, B5, 4, A4, 2, D3, 0

B1 = 2.24138616

B2 = 2.14289043

B3 = 1.20911441

B4 = 1.2046473

B5 = 2.13971303

A1 = 60.1033463

A2 = 32.75957236

A3 = 108.17363282

A4 = 110.58324343

D1 = 0

D2 = -0.00016525

D3 = -0.00071326

**Frequencies:** 1742.7293(i), 168.4829, 360.8313, 602.7442, 649.7943, 761.9105, 827.1083, 894.0376, 1196.9248

**H<sub>2</sub>:** Optimized at G3B3

H

H, 1, B1

B1 = 0.74278797

**Frequencies:** 4453.12

**NO<sub>3</sub>:** Optimized at G3B3

N

O, 1, B1

O, 1, B2, 2, A1

O, 1, B3, 2, A2, 3, D1, 0

B1 = 1.239184

B2 = 1.239184

B3 = 1.238824

A1 = 119.93293126

A2 = 120.03353437

D1 = 180

**Frequencies:** 203.0754, 209.9418, 790.2457, 1138.9543, 1147.3374, 1150.5727

**HNO<sub>3</sub>:** Optimized at G3B3

O

O, 1, B1,

O, 1, B2, 2, A1

N, 3, B3, 1, A2, 2,

H, 1, B4, 4, A3, 3, D1, 0

B1 = 2.22629094

B2 = 2.19331432

B3 = 1.20262393

B4 = 0.97854839

A1 = 59.60125846

A2 = 35.98981463

A2 = 102.61480736

D1 = 180

**Frequencies:** 504.6885, 581.1024, 651.4258, 769.3275, 916.3726, 1346.4982, 1373.1928, 1802.7541, 3668.3679.

TS: NO<sub>3</sub> + CH<sub>4</sub> → HNO<sub>3</sub> + CH<sub>3</sub>

O

O, 1, B1

O, 1, B2, 2, A1

N, 3, B3, 1, A2, 2, D1, 0

C, 1, B4, 4, A3, 3, D2, 0

H, 1, B5, 4, A4, 3, D3, 0

H, 5, B6, 1, A5, 4, D4, 0

H, 5, B7, 1, A6, 4, D5, 0

H, 5, B8, 1, A7, 4, D6, 0

B1 = 2.23198091

B2 = 2.15307876

B3 = 1.21441493

B4 = 2.54296766

B5 = 1.22804328

B6 = 1.08890072

B7 = 1.08957367

B8 = 1.08890210

A1 = 60.02157598

A2 = 36.26198079

A3 = 109.54611657

A4 = 107.75703177

A5 = 103.47394069

A6 = 101.68448035

A7 = 103.45332871

D1 = -0.00099786

D2 = 180

D3 = -179.98879979

D4 = 60.07285416

D5 = -179.94868995

D6 = -59.97967869

**Frequencies:** 1610.3351(i), 48.0386, 76.7290, 126.9953, 413.9952, 431.3833, 522.7556, 678.2558, 724.2253, 771.5175, 924.3643, 1087.6799, 1211.9060, 1346.5319, 1360.3373, 1443.8627, 1448.4073, 1713.5619, 3096.8581, 3241.3526, 3246.0072.

CH<sub>4</sub>

C

H, 1, B1

H, 1, B2, 2, A1  
 H, 1, B3, 2, A2, 3, D1, 0  
 H, 1, B4, 2, A3, 3, D2, 0  
 B1 = 1.09351122  
 B2 = 1.09351122  
 B3 = 1.09351122  
 B4 = 1.09351122  
 A1 = 109.47122063  
 A2 = 109.47122063  
 A3 = 109.47122063  
 D1 = 120.00000000  
 D2 = -120.00000000

**Frequencies:** 1373.5436, 1373.5436, 1373.5436, 1593.3084, 1593.3084, 3051.3248, 3160.9657, 3160.9657m 3160.9657.

CH<sub>3</sub>  
 C  
 H, 1, B1  
 H, 1, B2, 2, A1  
 H, 1, B3, 3, A2, 2, D1, 0  
 B1 = 1.08279310  
 B2 = 1.08279264  
 B3 = 1.08279264  
 A1 = 119.99996550  
 A2 = 120.00001479  
 D1 = -179.91531434

**Frequencies:** 453.4895, 1431.1441, 1431.1441, 3142.8528, 3317.4233, 3317.4238

TS: NO<sub>3</sub> + HCl → Cl + HNO<sub>3</sub>

O  
 O, 1, B1  
 O, 2, B2, 1, A1  
 N, 1, B3, 3, A2, 2, D1, 0  
 H, 1, B4, 4, A3, 2, D2, 0  
 Cl, 1, B5, 4, A4, 2, D3, 0  
 B1 = 2.20986032  
 B2 = 2.14150617  
 B3 = 1.21072617  
 B4 = 1.38883793  
 B5 = 2.51237320  
 A1 = 60.42076234  
 A2 = 32.92963813  
 A3 = 101.75053282  
 A4 = 71.59311434  
 D1 = 0.00038751  
 D2 = -179.98467289  
 D3 = -179.99176470

**Frequencies:** 1057.2906 (i), 101.4819, 190.5316, 432.9443, 642.7350, 741.4154, 760.1939, 793.1172, 990.7807, 1229.3885, 1451.4274, 1635.2128

HCl  
 Cl  
 H, 1, B1  
 B1 = 1.29000000  
**Frequencies:** 2934.5027