frontiers

Supplementary Material

Rotational rest frequencies and first astronomical search of protonated methylamine

by

Philipp C. Schmid, Sven Thorwirth, Christian P. Endres, Matthias Töpfer, Álvaro Sánchez-Monge, Andreas Schwörer, Peter Schilke, Stephan Schlemmer, Oskar Asvany

1 OPTIMIZED STRUCTURES - INTERNAL COORDINATES

1.1 $CH_3NH_3^+$

```
H3CNH3+ staggered, fc-CCSD(T)/cc-pVTZ
H
N 1 r1*
C 2 r2* 1 a1*
H 3 r3* 2 a2* 1 d180
H 2 r1* 3 a1* 1 d120
H 2 r1* 3 a1* 1 m120
H 3 r3* 2 a2* 4 d120
H 3 r3* 2 a2* 4 m120

r1   =        1.021888670486178
r2   =        1.509832038338843
a1   =      111.322729722338764
r3   =        1.086221357830763
a2   =      108.094967345682846
d180 =      180.000000000000000
d120 =      119.999999999999886
m120 =     -119.999999999999886

H3CNH3+ eclipsed, fc-CCSD(T)/cc-pVTZ
H
N 1 r1*
C 2 r2* 1 a1*
H 3 r3* 2 a2* 1 d0
H 2 r1* 3 a1* 1 d120
H 2 r1* 3 a1* 1 m120
H 3 r3* 2 a2* 4 d120
H 3 r3* 2 a2* 4 m120

r1   =        1.020980858044073
r2   =        1.522931178746826
a1   =      111.622873263568593
r3   =        1.085212195189002
a2   =      108.398509681501920
d0   =        0.000000000000000
d120 =      120.000000000000014
```

```
m120 =     -120.000000000000014

H3CNH3+ staggered, ae-CCSD(T)/cc-pwCVQZ
H
N 1 r1*
C 2 r2* 1 a1*
H 3 r3* 2 a2* 1 d180
H 2 r1* 3 a1* 1 d120
H 2 r1* 3 a1* 1 m120
H 3 r3* 2 a2* 4 d120
H 3 r3* 2 a2* 4 m120

r1   =        1.019717090636783
r2   =        1.502545184585313
a1   =      111.322827518148856
r3   =        1.083735104990842
a2   =      108.209722042561509
d180 =      180.000000000000000
d120 =      120.000000000000213
m120 =     -120.000000000000213

H3CNH3+ eclipsed, ae-CCSD(T)/cc-pwCVQZ
H
N 1 r1*
C 2 r2* 1 a1*
H 3 r3* 2 a2* 1 d0
H 2 r1* 3 a1* 1 d120
H 2 r1* 3 a1* 1 m120
H 3 r3* 2 a2* 4 d120
H 3 r3* 2 a2* 4 m120

r1   =        1.018821061587891
r2   =        1.515603898808069
a1   =      111.642903272376515
r3   =        1.082786158743740
a2   =      108.535443965366582
d0   =        0.000000000000000
d120 =      120.000000000000199
m120 =     -120.000000000000199
```

1.2 C_2H_6

```
H3CCH3 eclipsed, fc-CCSD(T)/cc-pVTZ
H
C 1 r1*
C 2 r2* 1 a1*
H 3 r1* 2 a1* 1 d180
H 2 r1* 3 a1* 1 d120
H 2 r1* 3 a1* 1 m120
H 3 r1* 2 a1* 4 d120
H 3 r1* 2 a1* 4 m120
```

```
r1   =        1.091820232420359
r2   =        1.528947845669051
a1   =      111.198814812642979
d180 =      180.000000000000000
d120 =      119.999999999999886
m120 =     -119.999999999999886

H3CCH3 staggered, fc-CCSD(T)/cc-pVTZ
H
C 1 r1*
C 2 r2* 1 a1*
H 3 r1* 2 a1* 1 d0
H 2 r1* 3 a1* 1 d120
H 2 r1* 3 a1* 1 m120
H 3 r1* 2 a1* 4 d120
H 3 r1* 2 a1* 4 m120

r1   =        1.090756660712056
r2   =        1.542576023555226
a1   =      111.639722122523679
d0   =        0.000000000000000
d120 =      119.999999999999986
m120 =     -119.999999999999986

H3CCH3 staggered, ae-CCSD(T)/cc-pwCVQZ
H
C 1 r1*
C 2 r2* 1 a1*
H 3 r1* 2 a1* 1 d180
H 2 r1* 3 a1* 1 d120
H 2 r1* 3 a1* 1 m120
H 3 r1* 2 a1* 4 d120
H 3 r1* 2 a1* 4 m120

r1   =        1.089182409753815
r2   =        1.522900851019744
a1   =      111.229246806209161
d180 =      180.000000000000000
d120 =      119.999999999999986
m120 =     -119.999999999999986

H3CCH3 eclipsed, ae-CCSDT(T)/cc-pwCVQZ
H
C 1 r1*
C 2 r2* 1 a1*
H 3 r1* 2 a1* 1 d0
H 2 r1* 3 a1* 1 d120
H 2 r1* 3 a1* 1 m120
H 3 r1* 2 a1* 4 d120
```

```
H 3 r1* 2 a1* 4 m120

r1   =         1.088162642081549
r2   =         1.536482403275187
a1   =       111.672526685471595
d0   =         0.000000000000000
d120 =       120.000000000000043
m120 =      -120.000000000000043
```

2 ENERGIES

Table S1. Total energies (hartree) and harmonic zero-point vibrational energies (kcal/mol) of $CH_3NH_3^+$ and C_2H_6 calculated at the fc-CCSD(T)/cc-pVTZ and ae-CCSD(T)/cc-pwCVQZ levels.

Molecule	Basis set	Energy / hartree	ZPVE / kcal/mol
$CH_3NH_3^+$ staggered	cc-pVTZ	−96.0563235	49.96
$CH_3NH_3^+$ eclipsed	cc-pVTZ	−96.0525711	49.63
$CH_3NH_3^+$ staggered	cc-pwCVQZ	−96.1975778	···
$CH_3NH_3^+$ eclipsed	cc-pwCVQZ	−96.1938923	···
C_2H_6 staggered	cc-pVTZ	−79.6744450	46.90
C_2H_6 eclipsed	cc-pVTZ	−79.6699792	46.61
C_2H_6 staggered	cc-pwCVQZ	−79.8082653	···
C_2H_6 eclipsed	cc-pwCVQZ	−79.8038965	···