

The HNO^- radical anion: a proposed intermediate in diazeniumdiolate synthesis using NO and alkoxides

Zhe-Chen Wang,¹ Ya-Ke Li,^{2,3} Sheng-Gui He,² and Veronica M. Bierbaum¹

¹ Department of Chemistry and Biochemistry, University of Colorado, Boulder, Colorado 80309, USA

² Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100190, China

³ University of Chinese Academy of Sciences, Beijing, 100049, China

Supporting Information

1. DFT calculated and fully optimized structures used in this paper.
2. List of relative energies used in Figure 2 – Table S1.

1. DFT calculated and fully optimized structures used in this paper.

CH₃O⁻

Charge -1, Multiplicity 1

Z-Matrix:

C	-0.53880500	-0.00015600	0.00000100
H	-1.03913300	0.51262800	-0.88915700
H	-1.03913900	0.51473100	0.88794100
H	-1.03885600	-1.02683500	0.00121200
O	0.79374500	0.00005200	0.00000000

Energy:

Zero-point correction=	0.034498 (Hartree/Particle)
Thermal correction to Energy=	0.037410
Thermal correction to Enthalpy=	0.038355
Thermal correction to Gibbs Free Energy=	0.012256
Sum of electronic and zero-point Energies=	-115.112315
Sum of electronic and thermal Energies=	-115.109403
Sum of electronic and thermal Enthalpies=	-115.108459
Sum of electronic and thermal Free Energies=	-115.134558

CH₂O

Charge 0, Multiplicity 1

Z-Matrix:

C	-0.00000600	0.52749200	0.00000000
H	0.94009100	1.11448600	0.00000000
H	-0.94001300	1.11464500	0.00000000
O	-0.00000600	-0.67426000	0.00000000

Energy:

Zero-point correction=	0.026502 (Hartree/Particle)
Thermal correction to Energy=	0.029370
Thermal correction to Enthalpy=	0.030314
Thermal correction to Gibbs Free Energy=	0.004844
Sum of electronic and zero-point Energies=	-114.515347
Sum of electronic and thermal Energies=	-114.512479
Sum of electronic and thermal Enthalpies=	-114.511535
Sum of electronic and thermal Free Energies=	-114.537005

HNO⁻

Charge -1, Multiplicity 2

Z-Matrix:

N	0.06352400	0.64526200	0.00000000
H	-0.95285500	0.94816100	0.00000000
O	0.06352400	-0.68312400	0.00000000

Energy:

Zero-point correction=	0.012102 (Hartree/Particle)
Thermal correction to Energy=	0.014963
Thermal correction to Enthalpy=	0.015907
Thermal correction to Gibbs Free Energy=	-0.010008
Sum of electronic and zero-point Energies=	-130.527535
Sum of electronic and thermal Energies=	-130.524674
Sum of electronic and thermal Enthalpies=	-130.523730
Sum of electronic and thermal Free Energies=	-130.549645

N₂O

Charge 0, Multiplicity 1

Z-Matrix:

N	0.00000000	0.00000000	-0.07294200
N	0.00000000	0.00000000	-1.19838200
O	0.00000000	0.00000000	1.11240800

Energy:

Zero-point correction=	0.011007 (Hartree/Particle)
Thermal correction to Energy=	0.013719
Thermal correction to Enthalpy=	0.014663
Thermal correction to Gibbs Free Energy=	-0.010313
Sum of electronic and zero-point Energies=	-184.707219
Sum of electronic and thermal Energies=	-184.704507
Sum of electronic and thermal Enthalpies=	-184.703563
Sum of electronic and thermal Free Energies=	-184.728539

NO

Charge 0, Multiplicity 2

Z-Matrix:

N	0.00000000	0.00000000	-0.61228400
O	0.00000000	0.00000000	0.53574900

Energy:

Zero-point correction=	0.004510 (Hartree/Particle)
Thermal correction to Energy=	0.006871
Thermal correction to Enthalpy=	0.007815
Thermal correction to Gibbs Free Energy=	-0.015478
Sum of electronic and zero-point Energies=	-129.927147
Sum of electronic and thermal Energies=	-129.924785
Sum of electronic and thermal Enthalpies=	-129.923841
Sum of electronic and thermal Free Energies=	-129.947135

OH⁻

Charge -1, Multiplicity 1

Z-Matrix:

O	0.00000000	0.00000000	0.10737700
H	0.00000000	0.00000000	-0.85901300

Energy:

Zero-point correction=	0.008540 (Hartree/Particle)
Thermal correction to Energy=	0.010900
Thermal correction to Enthalpy=	0.011845
Thermal correction to Gibbs Free Energy=	-0.007716
Sum of electronic and zero-point Energies=	-75.818908
Sum of electronic and thermal Energies=	-75.816548
Sum of electronic and thermal Enthalpies=	-75.815604
Sum of electronic and thermal Free Energies=	-75.835164

Table S1: Figure 2 is using Total Energy (Hartree) from the H-N distance of 320 pm (step 1) to 120 pm (step 100). Note that the following relative energies are extracted from a Gaussian fixed-coordinate scanning file with the key word "modredundant" and may be close but not equal to the fully optimized energies of the corresponding structures.

1.0000000000	-245.0959304710
2.0000000000	-245.0959704060
3.0000000000	-245.0960123280
4.0000000000	-245.0960562910
5.0000000000	-245.0961023530
6.0000000000	-245.0961505710
7.0000000000	-245.0962010040
8.0000000000	-245.0962537040
9.0000000000	-245.0963087210
10.0000000000	-245.0963661020
11.0000000000	-245.0964258960
12.0000000000	-245.0964881480
13.0000000000	-245.0965529010
14.0000000000	-245.0966201980
15.0000000000	-245.0966900730
16.0000000000	-245.0967625600
17.0000000000	-245.0968376950
18.0000000000	-245.0969155120
19.0000000000	-245.0969960570
20.0000000000	-245.0970793880
21.0000000000	-245.0971655680
22.0000000000	-245.0972546550
23.0000000000	-245.0973466850
24.0000000000	-245.0974416530
25.0000000000	-245.0975395110

26.0000000000	-245.0976401760
27.0000000000	-245.0977435560
28.0000000000	-245.0978495720
29.0000000000	-245.0979581730
30.0000000000	-245.0980693380
31.0000000000	-245.0981830680
32.0000000000	-245.0982993750
33.0000000000	-245.0984182490
34.0000000000	-245.0985396240
35.0000000000	-245.0986633670
36.0000000000	-245.0987893100
37.0000000000	-245.0989172780
38.0000000000	-245.0990471140
39.0000000000	-245.0991784570
40.0000000000	-245.0993116080
41.0000000000	-245.0994464870
42.0000000000	-245.0995824570
43.0000000000	-245.0997196060
44.0000000000	-245.0998577690
45.0000000000	-245.0999967610
46.0000000000	-245.1001363840
47.0000000000	-245.1002765580
48.0000000000	-245.1004170630
49.0000000000	-245.1005572130
50.0000000000	-245.1006970310
51.0000000000	-245.1008364270
52.0000000000	-245.1009751400
53.0000000000	-245.1011129430

54.0000000000	-245.1012497520
55.0000000000	-245.1013852180
56.0000000000	-245.1015192130
57.0000000000	-245.1016514490
58.0000000000	-245.1017816900
59.0000000000	-245.1019097190
60.0000000000	-245.1020353240
61.0000000000	-245.1021583210
62.0000000000	-245.1022785530
63.0000000000	-245.1023958740
64.0000000000	-245.1025101570
65.0000000000	-245.1026212930
66.0000000000	-245.1027291880
67.0000000000	-245.1028337670
68.0000000000	-245.1029349830
69.0000000000	-245.1030328130
70.0000000000	-245.1031272750
71.0000000000	-245.1032184360
72.0000000000	-245.1033064030
73.0000000000	-245.1033913420
74.0000000000	-245.1034734680
75.0000000000	-245.1035530440
76.0000000000	-245.1036303680
77.0000000000	-245.1037057760
78.0000000000	-245.1037796440
79.0000000000	-245.1038523990
80.0000000000	-245.1039245380
81.0000000000	-245.1039966350

82.0000000000	-245.1040693410
83.0000000000	-245.1041433830
84.0000000000	-245.1042195510
85.0000000000	-245.1042987080
86.0000000000	-245.1043817450
87.0000000000	-245.1044697180
88.0000000000	-245.1045638640
89.0000000000	-245.1046656180
90.0000000000	-245.1047766280
91.0000000000	-245.1048988430
92.0000000000	-245.1050341320
93.0000000000	-245.1051847280
94.0000000000	-245.1053529940
95.0000000000	-245.1055415830
96.0000000000	-245.1057534990
97.0000000000	-245.1059921550
98.0000000000	-245.1062614090
99.0000000000	-245.1065659100
100.0000000000	-245.1069115870