Electronic Supplementary Material (ESI) for RSC Advances.

Delocalization Quantitatively Mapped For Prototypic Organic Nitroanions As Well As Azidoform Anion

Anatoly M. Belostotskii

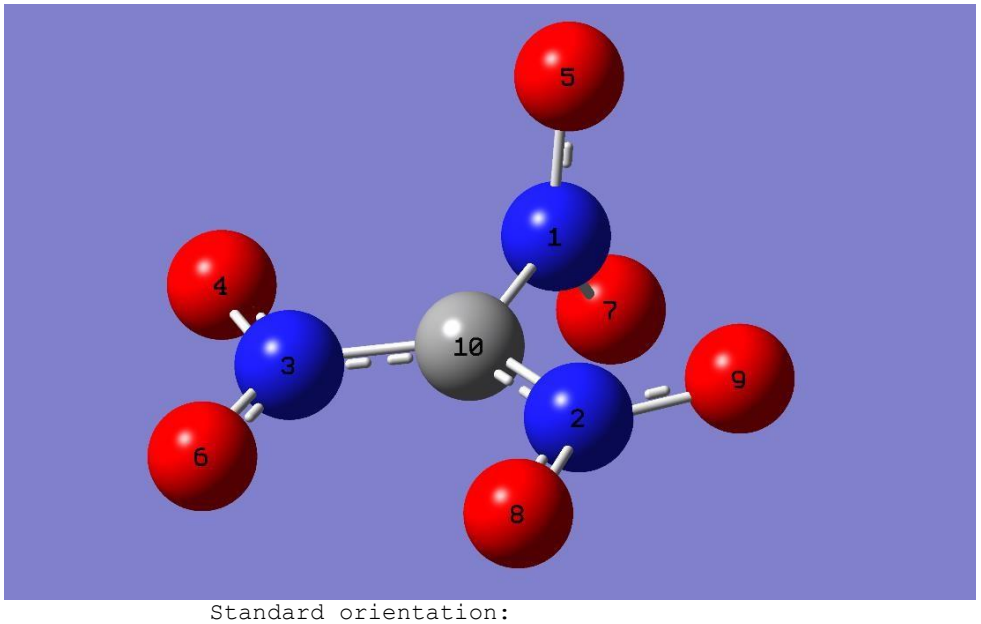
Chemistry Department, Bar-Ilan University, Ramat-Gan 5290002, Israel

ELECTRONIC SUPPLEMENTARY INFORMATION

Content

1. Anion **1,** conformer **1A**

Geometry optimized at the MP2/aug-cc-pVTZ level



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.347822	-0.000405	0.000084
2	7	0	-0.701597	1.240836	-0.000124
3	7	0	-0.702374	-1.240422	-0.000048
4	8	0	0.082883	-2.220090	-0.000326
5	8	0	1.919098	-0.000721	-1.092700
6	8	0	-1.940068	-1.353206	0.000230
7	8	0	1.918938	-0.000386	1.093035
8	8	0	-1.939223	1.354407	0.000081
9	8	0	0.084330	2.219971	-0.000363
10	6	0	-0.102436	0.000023	0.000162

ENERGY (a.u):

MP2=-652.5633233

ESP charges:

1	N	0.655174
2	N	0.655077
3	N	0.830848
4	O	-0.477818
5	O	-0.473187
6	O	-0.478040
7	O	-0.522604
8	O	-0.522623
9	O	-0.473199
10	C	-0.193627

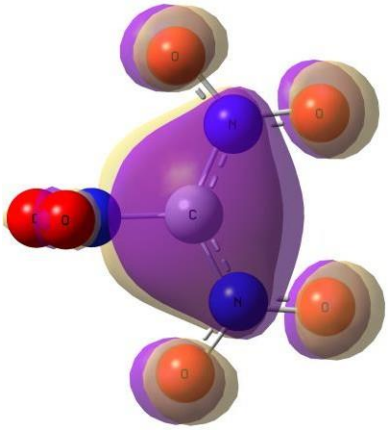
Wiberg bond index matrix in the NAO basis:

Atom		1	2	3	4	5	6	7	8	9
1.	N	0.0000	0.0078	0.0054	0.0061	1.4373	0.0061	1.3759	0.0182	0.0144
2.	N	0.0078	0.0000	0.0054	0.0061	0.0144	0.0061	0.0182	1.3758	1.4373

3.	N	0.0054	0.0054	0.0000	1.5298	0.0091	1.5299	0.0065	0.0065	0.0091
4.	O	0.0061	0.0061	1.5298	0.0000	0.0032	0.3369	0.0034	0.0034	0.0032
5.	O	1.4373	0.0144	0.0091	0.0032	0.0000	0.0032	0.2250	0.0150	0.0171
6.	O	0.0061	0.0061	1.5299	0.3369	0.0032	0.0000	0.0034	0.0034	0.0032
7.	O	1.3759	0.0182	0.0065	0.0034	0.2250	0.0034	0.0000	0.0147	0.0150
8.	O	0.0182	1.3758	0.0065	0.0034	0.0150	0.0034	0.0147	0.0000	0.2250
9.	O	0.0144	1.4373	0.0091	0.0032	0.0171	0.0032	0.0150	0.2250	0.0000
10.	C	1.1511	1.1512	0.9019	0.0497	0.1240	0.0497	0.1131	0.1131	0.1240

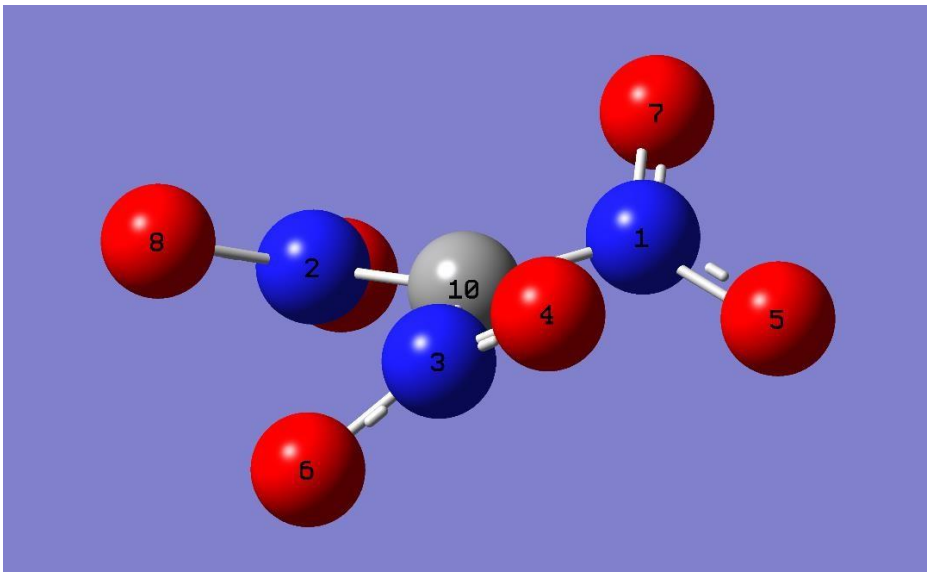
	Atom	10
1.	N	1.1511
2.	N	1.1512
3.	N	0.9019
4.	O	0.0497
5.	O	0.1240
6.	O	0.0497
7.	O	0.1131
8.	O	0.1131
9.	O	0.1240
10.	C	0.0000

Highest occupied NLMO



2. Anion **1,** conformer **1B**

Geometry optimized at the MP2/aug-cc-pVTZ level



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.098883	1.402566	0.000004
2	7	0	-1.263974	-0.615604	0.000168
3	7	0	1.165096	-0.786890	-0.000188
4	8	0	2.193083	-0.317341	0.516251
5	8	0	1.103199	1.922112	-0.515220
6	8	0	1.112897	-1.915745	-0.516867
7	8	0	-0.822605	2.057822	0.515310
8	8	0	-1.370770	-1.740528	0.517009
9	8	0	-2.215828	-0.006509	-0.516467
10	6	0	0.000029	0.000167	-0.000002

ENERGY (a.u):

MP2=-652.5624146

Zero-point correction= 0.042696 (Hartree/Particle)
Thermal correction to Energy= 0.051288
Thermal correction to Enthalpy= 0.052232
Thermal correction to Gibbs Free Energy= 0.006971
Sum of electronic and zero-point Energies= -652.519718
Sum of electronic and thermal Energies= -652.511127
Sum of electronic and thermal Enthalpies= -652.510183
Sum of electronic and thermal Free Energies= -652.555444

ESP charges:

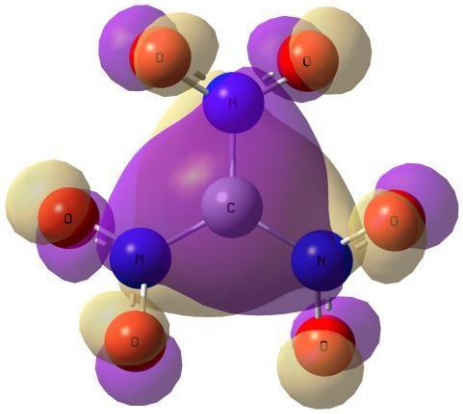
1	N	0.578040
2	N	0.578657
3	N	0.573669
4	O	-0.428754
5	O	-0.430473
6	O	-0.428948
7	O	-0.430886

```
     8  O   -0.430392
     9  O   -0.430694
    10  C   -0.150220
```

Wiberg bond index matrix in the NAO basis:

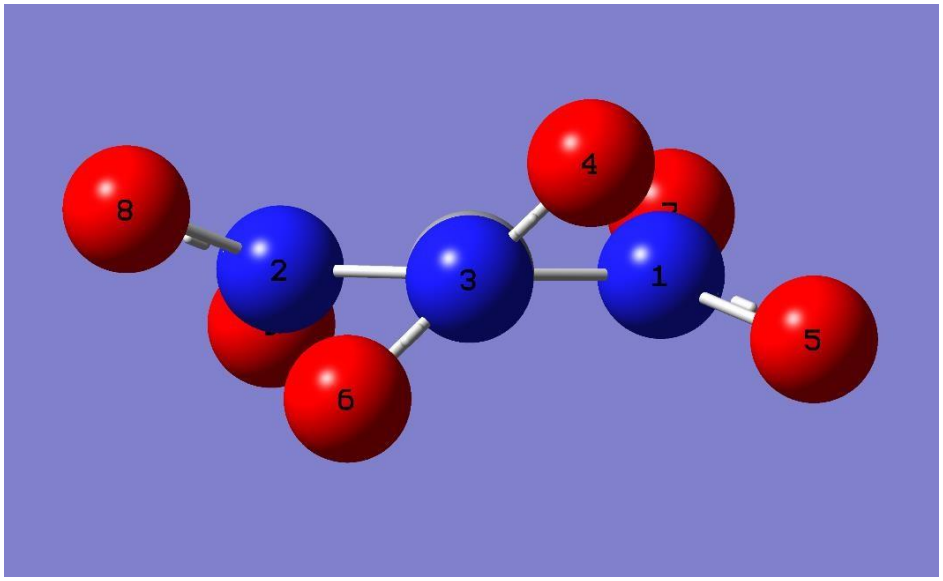
Atom		1	2	3	4	5	6	7
1.	N	0.0000	0.0109	1.4330	1.4620	0.0202	0.0071	1.1305
2.	N	0.0109	0.0000	0.0202	0.0071	1.4338	1.4628	1.1287
3.	O	1.4330	0.0202	0.0000	0.2375	0.0097	0.0070	0.1067
4.	O	1.4620	0.0071	0.2375	0.0000	0.0070	0.0066	0.1321
5.	O	0.0202	1.4338	0.0097	0.0070	0.0000	0.2381	0.1063
6.	O	0.0071	1.4628	0.0070	0.0066	0.2381	0.0000	0.1316
7.	N	1.1305	1.1287	0.1067	0.1321	0.1063	0.1316	0.0000

Highest occupied NLMO



3. Anion **1**, conformational transition state TS_{AB}

(Fig. 2 in the main text)



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.706721	1.236073	-0.036400
2	7	0	-0.706971	-1.235948	0.036365
3	7	0	1.392822	-0.000106	0.000007
4	8	0	1.979033	0.801798	0.754380
5	8	0	-0.057710	2.226274	-0.455048
6	8	0	1.979047	-0.802129	-0.754227
7	8	0	-1.896785	1.303145	0.343326
8	8	0	-0.058136	-2.226360	0.454815
9	8	0	-1.897121	-1.302728	-0.343193
10	6	0	-0.040089	-0.000023	-0.000040

ENERGY (a.u):

MP2=-652.0401204

Zero-point correction=	0.042606	(Hartree/Particle)
Thermal correction to Energy=	0.050409	
Thermal correction to Enthalpy=	0.051353	
Thermal correction to Gibbs Free Energy=	0.008527	
Sum of electronic and zero-point Energies=	-651.997515	
Sum of electronic and thermal Energies=	-651.989711	
Sum of electronic and thermal Enthalpies=	-651.988767	
Sum of electronic and thermal Free Energies=	-652.031593	

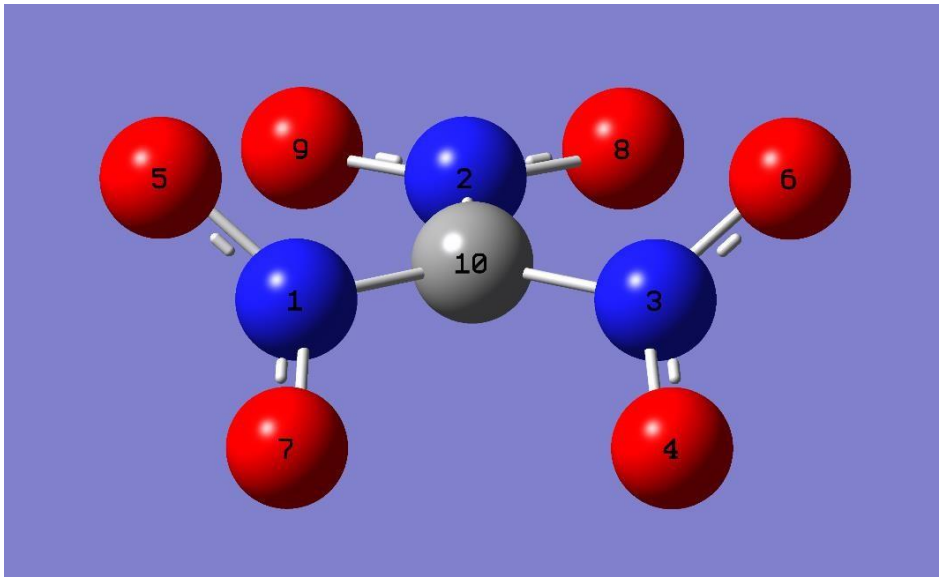
FREQUENCIES

Frequencies --	-33.3867	62.0796	72.7949
Frequencies --	132.3482	228.0215	235.0817
Frequencies --	423.7169	425.0005	464.2306
Frequencies --	482.6380	699.1030	721.7875
Frequencies --	723.2050	786.4117	787.0221
Frequencies --	871.1294	1190.3732	1201.5398

```
Frequencies --  1346.0654             1384.7792             1425.3653
Frequencies --  1643.3358             1674.9206             1720.7960
```

4. Anion **1**, conformational transition state TS_{AA}

(Fig. 2 in the main text)



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.228084	-0.704584	0.077023
2	7	0	0.000455	1.419674	-0.165665
3	7	0	1.227541	-0.705222	0.077095
4	8	0	1.318663	-1.832886	-0.456087
5	8	0	-2.147853	-0.185736	0.745993
6	8	0	2.147096	-0.187210	0.746978
7	8	0	-1.319242	-1.832820	-0.454996
8	8	0	1.101024	2.009193	-0.271212
9	8	0	-1.099524	2.010262	-0.271260
10	6	0	-0.000116	0.014084	-0.039081

ENERGY (a.u):

MP2=-652.0318078

Zero-point correction=	0.042379 (Hartree/Particle)
Thermal correction to Energy=	0.050190
Thermal correction to Enthalpy=	0.051134
Thermal correction to Gibbs Free Energy=	0.008204
Sum of electronic and zero-point Energies=	-651.989429
Sum of electronic and thermal Energies=	-651.981618
Sum of electronic and thermal Enthalpies=	-651.980674
Sum of electronic and thermal Free Energies=	-652.023604

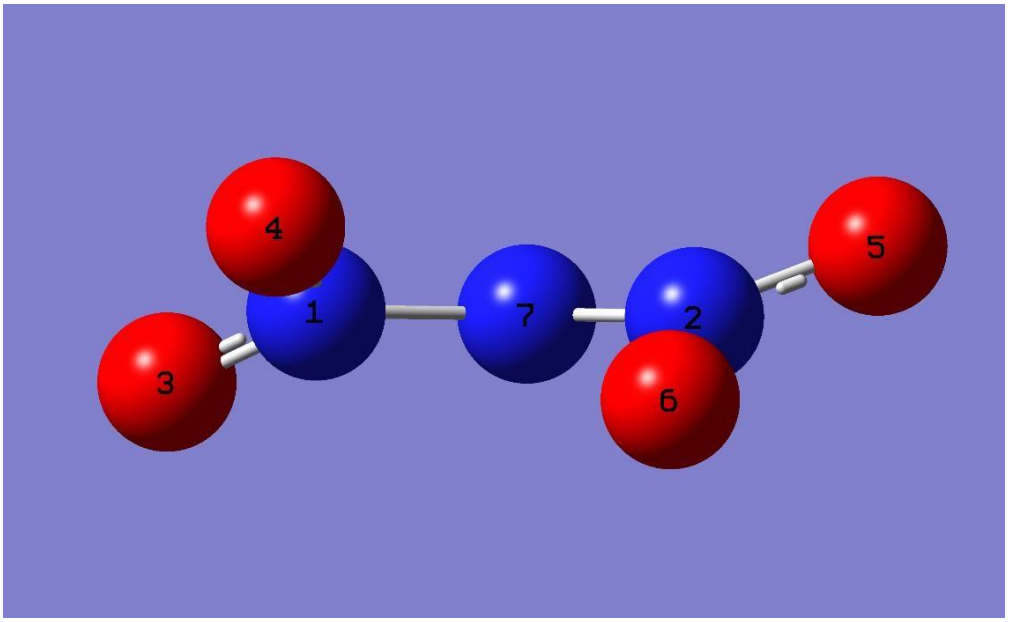
FREQUENCIES

Frequencies --	-81.9723	47.3008	94.3046
Frequencies --	112.8435	247.9997	256.9534

```
Frequencies --    371.0053              431.9304              447.9455
Frequencies --    499.8687              709.4900              720.4818
Frequencies --    736.7080              781.5909              786.9882
Frequencies --    869.7574             1183.0439             1186.7115
Frequencies --   1333.5173             1352.2965             1413.2038
Frequencies --   1635.0506             1684.0452             1699.2693
```

5. Anion **2**

Geometry optimized at the MP2/aug-cc-pVTZ level



Standard orientation (harmonic approximation)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.142414	-0.060506	-0.057356
2	7	0	1.142402	-0.060513	0.057403
3	8	0	-2.161356	-0.662053	0.328647
4	8	0	-1.173983	1.071922	-0.556355
5	8	0	2.161533	-0.661869	-0.328319
6	8	0	1.173781	1.071898	0.556409
7	7	0	0.000040	-0.816006	-0.000482

Vibration Averaged Geometry

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.148489	-0.059770	-0.057785
2	7	1.148485	-0.059785	0.057836
3	8	-2.167236	-0.665340	0.326971
4	8	-1.181966	1.075439	-0.555296
5	8	2.167421	-0.665160	-0.326642
6	8	1.181748	1.075409	0.555346
7	7	0.000043	-0.817986	-0.000484

ENERGY (a.u):

MP2=-464.3503795

```
Zero-point correction=                           0.028568 (Hartree/Particle)
 Thermal correction to Energy=                    0.034215
 Thermal correction to Enthalpy=                  0.035159
 Thermal correction to Gibbs Free Energy=        -0.001823
 Sum of electronic and zero-point Energies=           -464.321812
 Sum of electronic and thermal Energies=              -464.316164
 Sum of electronic and thermal Enthalpies=            -464.315220
 Sum of electronic and thermal Free Energies=         -464.352203
```

ESP charges:

```
     1  N    0.985177
     2  N    0.986353
     3  O   -0.593078
     4  O   -0.553319
     5  O   -0.593004
     6  O   -0.553253
     7  N   -0.678876
```

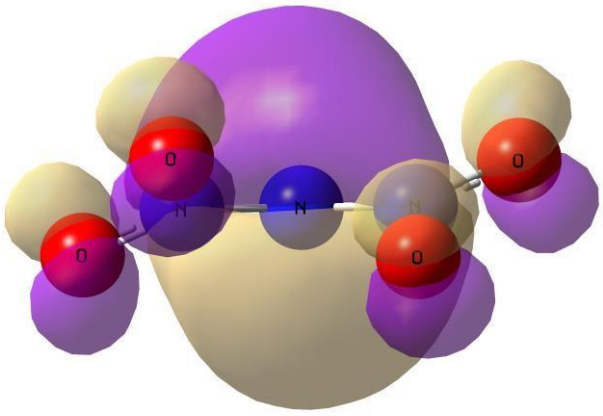
FREQUENCIES (harmonic approximation)

```
 Frequencies --     93.2264               105.0274               281.7234
 Frequencies --    483.6861               503.4058               738.0236
 Frequencies --    755.8613               767.0907               839.7728
 Frequencies --    980.1390              1078.3638              1248.8441
 Frequencies --   1391.3191              1613.5408              1659.7658
```

Wiberg bond index matrix in the NAO basis:

Atom		1	2	3	4	5	6	7
1.	N	0.0000	0.0109	1.4330	1.4620	0.0202	0.0071	1.1305
2.	N	0.0109	0.0000	0.0202	0.0071	1.4338	1.4628	1.1287
3.	O	1.4330	0.0202	0.0000	0.2375	0.0097	0.0070	0.1067
4.	O	1.4620	0.0071	0.2375	0.0000	0.0070	0.0066	0.1321
5.	O	0.0202	1.4338	0.0097	0.0070	0.0000	0.2381	0.1063
6.	O	0.0071	1.4628	0.0070	0.0066	0.2381	0.0000	0.1316
7.	N	1.1305	1.1287	0.1067	0.1321	0.1063	0.1316	0.0000

Highest occupied NLMO



Internal coordinates for the equilibrium structure

```
                      Interatomic distances:
                  1          2          3          4          5
     1  N    0.000000
     2  N    2.287696   0.000000
```

```
3  O    1.244628   3.369012   0.000000
4  O    1.237897   2.650424   2.182843   0.000000
5  O    3.369143   1.244604   4.372525   3.766125   0.000000
6  O    2.650246   1.237880   3.765847   2.598122   2.182738
7  N    1.370845   1.370807   2.191725   2.291636   2.191640
               6          7
6  O    0.000000
7  N    2.291719   0.000000
                     Interatomic angles:
  N2-N1-O3=143.3294       N2-N1-O4= 92.619        O3-N1-O4=123.1118
  N2-O4-O3= 87.8241       N1-N2-O5=143.3468       O4-N2-O5=148.2459
  N1-N2-O6= 92.6099       O3-N1-O6=148.2302       N1-O4-O6= 78.7144
  N2-O6-O4= 78.7232       O3-O4-O6=103.5971       N1-O6-O5= 87.8352
  O5-N2-O6=123.1052       O4-O6-O5=103.611        N1-N7-N2=113.1115
  O3-N1-N7=113.7687       N2-N7-O3=140.9652       O4-N1-N7=122.8295
  N2-N7-O4= 89.0336       O4-O3-N7= 63.1819       N1-N7-O5=140.9834
  O5-N2-N7=113.7661       O3-N7-O5=171.9391       O4-N7-O5=114.27
  N1-N7-O6= 89.0207       O6-N2-N7=122.8417       O3-N7-O6=114.2502
  O4-N7-O6= 69.0631       O6-O5-N7= 63.1875
                        Dihedral angles:
O5-N2-N1-O3=  71.94    O5-N2-N1-O4=-120.35    O5-N2-O4-O3= 105.9
O6-N2-N1-O3=-120.34    O6-N2-N1-O4=  47.37    O6-O4-N1-O3= 150.3
O3-O4-O6-N2=  56.31    O5-O6-N1-O3= 105.93    O5-O6-O4-N1=  56.3
O5-N2-O6-O4= 150.36    O5-O6-O4-O3=  70.38    O3-N1-N7-N2=-157.4
O4-N1-N7-N2=  28.58    N7-N1-O4-O3= 173.43    O4-O3-N7-N2=  37.2
O5-N2-N7-N1=-157.5     O5-N7-N1-O3=-175.86    O5-N2-N7-O3=-175.9
O5-N7-N1-O4=  10.16    O5-N2-N7-O4=-144.96    O5-N7-O3-O4=  22.1
O6-N2-N7-N1=  28.49    O6-N7-N1-O3=-144.94    O6-N2-N7-O3=  10.0
O6-N7-N1-O4=  41.08    O6-N2-N7-O4=  41.03    O6-N7-O3-O4=  42.2
O6-O5-N7-N1=  37.19    N7-N2-O6-O5= 173.46    O6-O5-N7-O3=  21.6
O6-O5-N7-O4=  42.23
```

Internal coordinates for the vibration-averaged structure (anharmonic potential energy well)

```
                     Interatomic distances:
               1          2          3          4          5
1  N    0.000000
2  N    2.299882   0.000000
3  O    1.246033   3.381292   0.000000
4  O    1.239894   2.663769   2.186199   0.000000
5  O    3.381426   1.246007   4.383658   3.781581   0.000000
6  O    2.663563   1.239875   3.781277   2.611641   2.186100
7  N    1.377425   1.377385   2.197185   2.300004   2.197103
               6          7
6  O    0.000000
7  N    2.300069   0.000000
                     Interatomic angles:
  N2-N1-O3=143.2288       N2-N1-O4= 92.7021       O3-N1-O4=123.1472
  N2-O4-O3= 87.8252       N1-N2-O5=143.2466       O4-N2-O5=148.3716
  N1-N2-O6= 92.6916       O3-N1-O6=148.3559       N1-O4-O6= 78.7503
  N2-O6-O4= 78.7604       O3-O4-O6=103.6661       N1-O6-O5= 87.8369
  O5-N2-O6=123.1416       O4-O6-O5=103.6809       N1-N7-N2=113.2026
  O3-N1-N7=113.6633       N2-N7-O3=141.0671       O4-N1-N7=122.9009
  N2-N7-O4= 89.1721       O4-O3-N7= 63.2968       N1-N7-O5=141.0851
  O5-N2-N7=113.6612       O3-N7-O5=172.0276       O4-N7-O5=114.4495
  N1-N7-O6= 89.1586       O6-N2-N7=122.9118       O3-N7-O6=114.4294
  O4-N7-O6= 69.1854       O6-O5-N7= 63.3017
                        Dihedral angles:
O5-N2-N1-O3=  71.43    O5-N2-N1-O4=-120.72    O5-N2-O4-O3= 105.3
O6-N2-N1-O3=-120.71    O6-N2-N1-O4=  47.14    O6-O4-N1-O3= 150.5
O3-O4-O6-N2=  55.99    O5-O6-N1-O3= 105.31    O5-O6-O4-N1=  55.9
O5-N2-O6-O4= 150.6     O5-O6-O4-O3=  69.94    O3-N1-N7-N2=-157.5
O4-N1-N7-N2=  28.45    N7-N1-O4-O3= 173.44    O4-O3-N7-N2=  37.1
O5-N2-N7-N1=-157.61    O5-N7-N1-O3=-175.91    O5-N2-N7-O3=-176.0
O5-N7-N1-O4=  10.09    O5-N2-N7-O4=-145.15    O5-N7-O3-O4=  22.0
O6-N2-N7-N1=  28.36    O6-N7-N1-O3=-145.13    O6-N2-N7-O3=   9.9
```

```
O6-N7-N1-O4=  40.87    O6-N2-N7-O4=  40.82    O6-N7-O3-O4=  42.0
O6-O5-N7-N1=  37.06    N7-N2-O6-O5= 173.47    O6-O5-N7-O3=  21.5
O6-O5-N7-O4=  42.05
```

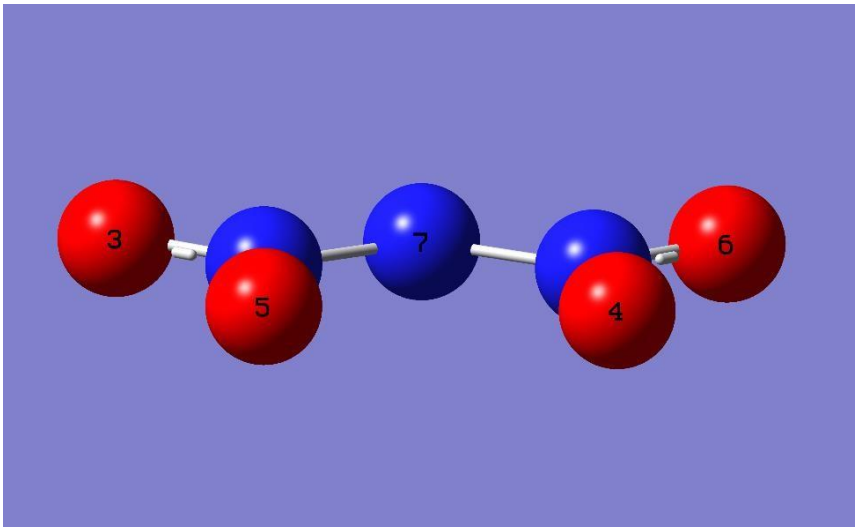
Vibration-averaged geometry (Cartesian coordinates; anharmonic potential energy well)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.148489	-0.059770	-0.057785
2	7	1.148485	-0.059785	0.057836
3	8	-2.167236	-0.665340	0.326971
4	8	-1.181966	1.075439	-0.555296
5	8	2.167421	-0.665160	-0.326642
6	8	1.181748	1.075409	0.555346
7	7	0.000043	-0.817986	-0.000484

6. Anion **2,** conformational transition state TS_c

(Fig. 4 in the main text**)**

Geometry optimized at the MP2/aug-cc-pVTZ level



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.171891	-0.052686	0.000198
2	7	0	-1.171920	-0.052646	-0.000278
3	8	0	-2.173018	-0.794895	0.001594
4	8	0	1.256543	1.181273	0.002437
5	8	0	-1.256362	1.181325	-0.002409
6	8	0	2.172936	-0.795002	-0.001432
7	7	0	-0.000085	-0.777754	-0.000137

ENERGY (a.u):

MP2=-464.3474563

Zero-point correction=	0.028247 (Hartree/Particle)
Thermal correction to Energy=	0.033095
Thermal correction to Enthalpy=	0.034039
Thermal correction to Gibbs Free Energy=	-0.000992
Sum of electronic and zero-point Energies=	-464.319210
Sum of electronic and thermal Energies=	-464.314361
Sum of electronic and thermal Enthalpies=	-464.313417
Sum of electronic and thermal Free Energies=	-464.348448

FREQUENCIES

Frequencies --	-82.1695	146.4261	299.3347
Frequencies --	436.9987	477.7910	760.7999
Frequencies --	769.1215	796.2711	821.7657
Frequencies --	966.7209	1066.2068	1246.6131
Frequencies --	1360.6564	1594.4298	1655.7002

Internal coordinates for the vibration-averaged structure (anharmonic potential energy well)

Interatomic distances:

		1	2	3	4	5
1	N	0.000000				
2	N	2.354551	0.000000			
3	O	3.438095	1.247987	0.000000		
4	O	1.238501	2.733875	3.969559	0.000000	
5	O	2.733740	1.238502	2.182002	2.522700	0.000000
6	O	1.247982	3.438073	4.358775	2.181940	3.969418
7	N	1.384682	1.384585	2.179396	2.334648	2.334510

		6	7
6	O	0.000000	
7	N	2.179481	0.000000

Interatomic angles:

N1-N2-O3=143.4169	N2-N1-O4= 93.896	O3-N2-O4=170.2863
N1-N2-O5= 93.8887	N1-O5-O3= 88.0115	O3-N2-O5=122.6944
N1-O4-O5= 86.1041	N2-O5-O4= 86.1109	O3-O5-O4=114.883
N2-N1-O6=143.415	O4-N1-O6=122.689	N2-O4-O6= 88.0085
O5-N1-O6=170.2863	O5-O4-O6=114.8789	N1-N7-N2=116.4764
N1-N7-O3=148.6318	O3-N2-N7=111.6539	O4-N1-N7=125.6565
N2-N7-O4= 90.9432	O3-N7-O4=123.0986	N1-N7-O5= 90.9399
O5-N2-N7=125.6517	O5-O3-N7= 64.7239	O4-N7-O5= 65.4068
O6-N1-N7=111.6545	N2-N7-O6=148.6301	O3-N7-O6=179.2143
O4-O6-N7= 64.7278	O5-N7-O6=123.0936	

Dihedral angles:

O4-N1-N2-O3=-179.74	O5-N2-N1-O4= 0.2	O3-O5-O4-N1= 0.2
O4-O5-N2-O3= 179.86	O6-N1-N2-O3= 0.3	O6-N1-O4-N2= 179.9
O6-O4-N2-O3= 0.95	O6-N1-N2-O5=-179.76	O6-N1-O5-O3= 0.8
O6-N1-O4-O5= 179.87	O6-O4-O5-N2= 0.26	O6-O4-O5-O3= 0.3
O3-N2-N7-N1=-179.89	O4-N1-N7-N2= 0.12	O4-N1-N7-O3= 0.0
O4-N7-N2-O3=-179.84	O5-N2-N7-N1= 0.13	O5-O3-N7-N1= 0.2
N7-N2-O5-O3= 179.98	O5-N7-N1-O4= 0.17	O5-N2-N7-O4= 0.1
O5-O3-N7-O4= 0.2	O6-N1-N7-N2=-179.91	O6-N1-N7-O3= 179.9
O6-N7-N2-O3=-179.98	N7-N1-O6-O4=-179.97	O4-O6-N7-N2= 0.1
O4-O6-N7-O3=-179.06	O6-N1-N7-O5=-179.86	O6-N7-N2-O5= 0.0
O6-N7-O3-O5= 179.25	O5-N7-O6-O4= 0.19	

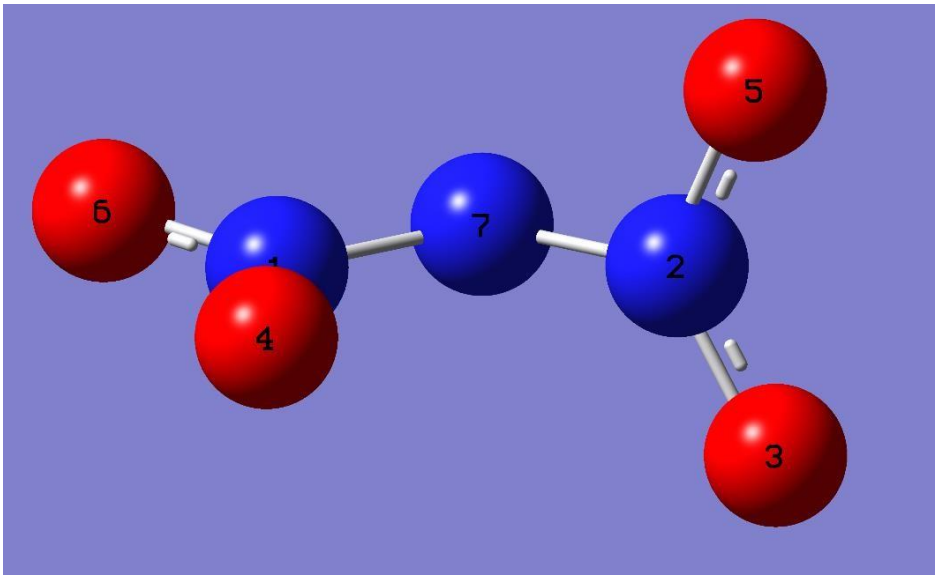
Vibration-averaged geometry (Cartesian coordinates; anharmonic potential energy well)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.177263	-0.052238	-0.000203
2	7	1.177289	-0.052196	0.000283
3	8	2.179427	-0.795962	-0.001602
4	8	-1.261436	1.183397	-0.002448
5	8	1.261260	1.183454	0.002420
6	8	-2.179347	-0.796069	0.001438
7	7	0.000083	-0.781073	0.000139

7. Anion **2,** conformational transition state TS_d

(Fig. 4 in the main text**)**

Geometry optimized at the MP2/aug-cc-pVTZ level



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.162034	0.055419	-0.024537
2	7	0	-1.149267	-0.123159	-0.104986
3	8	0	-1.761610	0.739170	-0.748317
4	8	0	1.058358	1.046616	0.709797
5	8	0	-1.628231	-0.696609	0.890357
6	8	0	2.253149	-0.478350	-0.295794
7	7	0	0.076711	-0.629973	-0.505614

ENERGY (a.u):

MP2=-464.3407641

Zero-point correction= 0.028012 (Hartree/Particle)
Thermal correction to Energy= 0.033008
Thermal correction to Enthalpy= 0.033953
Thermal correction to Gibbs Free Energy= -0.001526
Sum of electronic and zero-point Energies= -464.312752
Sum of electronic and thermal Energies= -464.307756
Sum of electronic and thermal Enthalpies= -464.306811
Sum of electronic and thermal Free Energies= -464.342290

FREQUENCIES

Frequencies -- -110.4307 123.8860 193.5452
Frequencies -- 470.1739 599.1815 637.1434

```
Frequencies --    741.5330               754.8300               845.3163
Frequencies --    957.1520              1070.1211              1241.7850
Frequencies --   1386.0283              1616.2160              1658.9313
```

Internal coordinates for the vibration-averaged structure (anharmonic potential energy well)

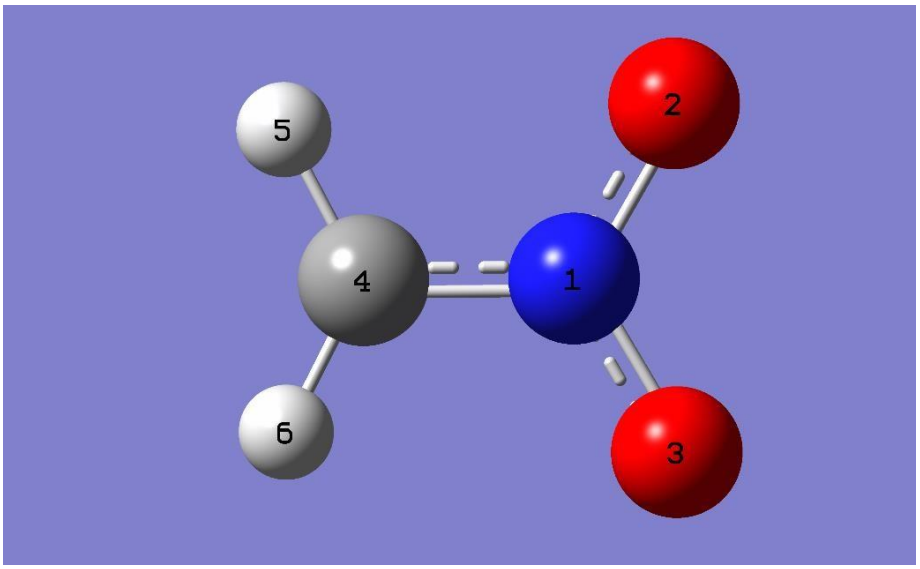
```
                          Interatomic distances:
                   1          2          3          4          5
     1  N    0.000000
     2  N    2.239133   0.000000
     3  O    2.963090   1.229214   0.000000
     4  O    1.257269   2.462302   3.005311   0.000000
     5  O    2.965313   1.229247   2.176225   3.009467   0.000000
     6  O    1.253801   3.402623   4.096085   2.203184   4.097690
     7  N    1.334076   1.426851   2.273583   2.264574   2.273253
                   6          7
     6  O    0.000000
     7  N    2.189547   0.000000
                          Interatomic angles:
       N1-N2-O3=114.1851        N2-N1-O4= 84.5832        O3-N1-O4= 79.7272
       O3-N2-O4=103.9371        N1-N2-O5=114.3339        N1-O3-O5= 68.5185
       O3-N2-O5=124.5518        O4-N1-O5= 79.8273        O4-N2-O5=104.1798
       O4-O3-O5= 68.8905        N2-N1-O6=152.7591        O3-N1-O6=149.8647
       O4-N1-O6=122.6577        N2-O4-O6= 93.4922        O3-O4-O6=102.6144
       O5-N1-O6=149.7904        O5-O4-O6=102.5442        N1-N7-N2=108.3423
       N1-N7-O3=107.5674        O3-N2-N7=117.5476        O4-N1-N7=121.8018
       N2-N7-O4= 80.1883        O3-N7-O4= 82.9403        N1-N7-O5=107.7155
       O5-N2-N7=117.5176        O3-O5-N7= 61.412         O4-N7-O5= 83.0879
       O6-N1-N7=115.5405        N2-N7-O6=139.4517        O3-N7-O6=133.193
       O4-O6-N7= 62.0645        O5-N7-O6=133.3166
                              Dihedral angles:
     O4-N1-N2-O3=  76.03     O5-N2-O3-N1= 149.06     O5-N2-N1-O4= -76.2
     O5-O3-N1-O4= -86.05     O5-N2-O4-O3=-131.71     O6-N1-N2-O3=-103.9
     O6-N1-O4-N2=-179.99     O6-N1-O4-O3= 158.1      O6-O4-N2-O3=-114.2
     O6-N1-N2-O5= 103.71     O6-N1-O3-O5= 132.68     O6-N1-O5-O4= 141.3
     O6-O4-N2-O5= 114.08     O6-O4-O3-O5=  94.88     O3-N2-N7-N1=  93.2
     O4-N1-N7-N2=   0.01     O4-N1-N7-O3=  30.14     O4-N7-N2-O3=  93.2
     O5-N2-N7-N1= -93.54     O3-O5-N7-N1=  99.85     N7-N2-O5-O3=-172.7
     O5-N7-N1-O4= -30.16     O5-N2-N7-O4= -93.54     O4-N7-O5-O3=  86.0
     O6-N1-N7-N2= 179.99     O6-N1-N7-O3=-149.87     O6-N7-N2-O3=  93.2
     N7-N1-O6-O4=-179.99     O4-O6-N7-N2=  0.        O4-O6-N7-O3=  41.0
     O6-N1-N7-O5= 149.83     O6-N7-N2-O5= -93.54     O6-N7-O5-O3= 120.7
     O5-N7-O6-O4= -41.14
```

Vibration-averaged geometry (Cartesian coordinates; anharmonic potential energy well)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.116557	0.021365	0.001386
2	7	-1.113943	-0.174737	-0.009939
3	8	-1.639120	0.110630	-1.084053
4	8	0.888526	1.255891	0.069756
5	8	-1.642039	-0.015020	1.088540
6	8	2.277347	-0.451834	-0.024416
7	7	0.129071	-0.874267	-0.048361

8. Anion **3**

Geometry optimized at the MP3/aug-cc-pVTZ level



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.044276	0.000245	0.000079
2	8	0	0.683595	1.098259	0.000000
3	8	0	0.684353	-1.097957	0.000001
4	6	0	-1.283023	-0.000444	-0.000349
5	1	0	-1.778271	0.952041	0.000771
6	1	0	-1.777104	-0.953512	0.000759

ENERGY (a.u):

MP2=-244.0627292

MP3=-244.0491347

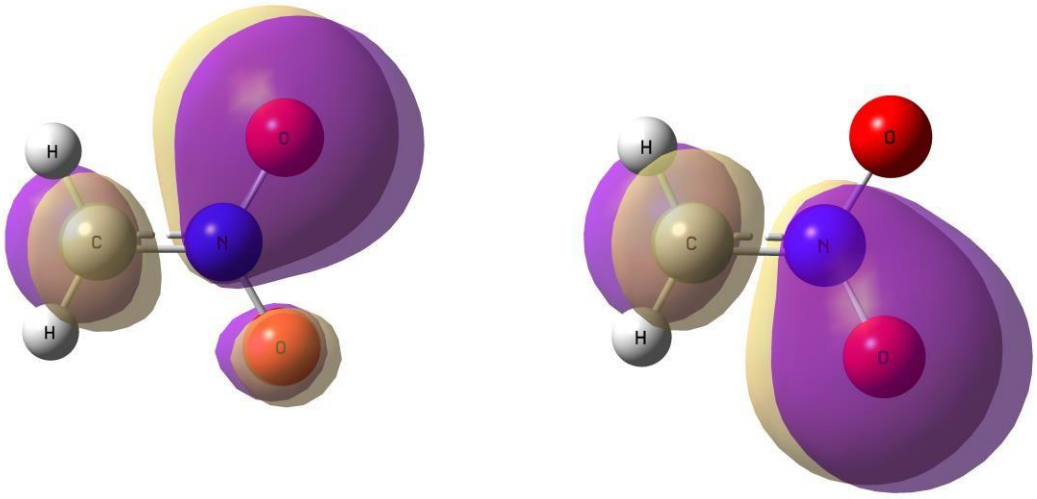
ESP charges:

1	N	0.892910
2	O	-0.732160
3	O	-0.731750
4	C	-0.736867
5	H	0.153798
6	H	0.154069

Wiberg bond index matrix in the NAO basis:

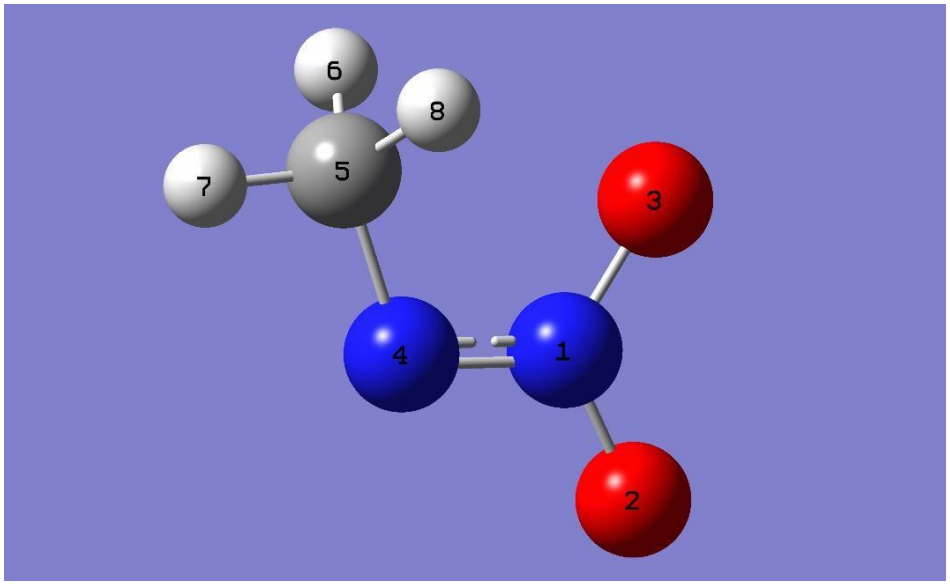
Atom		1	2	3	4	5	6
1.	N	0.0000	1.1757	1.1764	1.3037	0.0048	0.0048
2.	O	1.1757	0.0000	0.1486	0.1876	0.0158	0.0038
3.	O	1.1764	0.1486	0.0000	0.1879	0.0038	0.0157
4.	C	1.3037	0.1876	0.1879	0.0000	0.9115	0.9115
5.	H	0.0048	0.0158	0.0038	0.9115	0.0000	0.0008
6.	H	0.0048	0.0038	0.0157	0.9115	0.0008	0.0000

Two highest occupied NLMOs



9. Anion **4**

Geometry optimized at the MP3/aug-cc-pVTZ level



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.523783	-0.018490	-0.000752
2	8	0	1.670180	-0.525086	0.000555
3	8	0	0.390610	1.237348	0.000010
4	7	0	-0.497946	-0.803867	-0.000389
5	6	0	-1.739193	-0.056401	0.000312
6	1	0	-1.840513	0.594288	-0.875156
7	1	0	-2.549317	-0.787143	-0.002294
8	1	0	-1.842195	0.589662	0.879046

ENERGY (a.u):

MP2=-299.3322808

MP3=-299.318175

ESP charges:

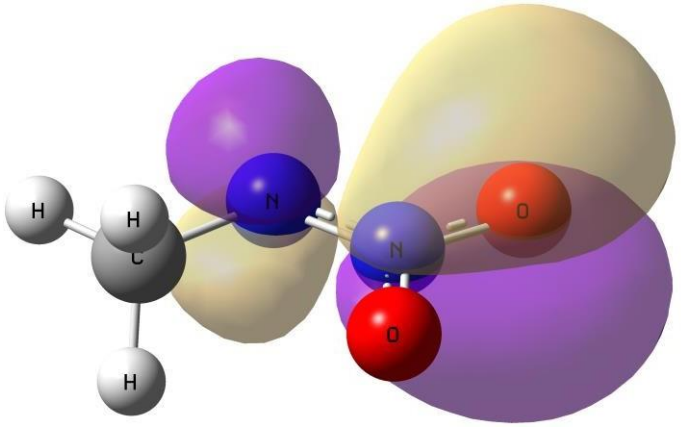
1	N	1.110367
2	O	-0.764995
3	O	-0.714478
4	N	-0.805446
5	C	0.497264
6	H	-0.106562
7	H	-0.110179
8	H	-0.105970

Wiberg bond index matrix in the NAO basis:

Atom		1	2	3	4	5	6	7	8
1.	N	0.0000	1.2234	1.1950	1.3051	0.0104	0.0075	0.0065	0.0075
2.	O	1.2234	0.0000	0.1567	0.1756	0.0217	0.0052	0.0010	0.0052
3.	O	1.1950	0.1567	0.0000	0.1927	0.0108	0.0086	0.0062	0.0086

4.	N	1.3051	0.1756	0.1927	0.0000	0.9622	0.0141	0.0084	0.0141
5.	C	0.0104	0.0217	0.0108	0.9622	0.0000	0.8865	0.9034	0.8865
6.	H	0.0075	0.0052	0.0086	0.0141	0.8865	0.0000	0.0003	0.0007
7.	H	0.0065	0.0010	0.0062	0.0084	0.9034	0.0003	0.0000	0.0003
8.	H	0.0075	0.0052	0.0086	0.0141	0.8865	0.0007	0.0003	0.0000

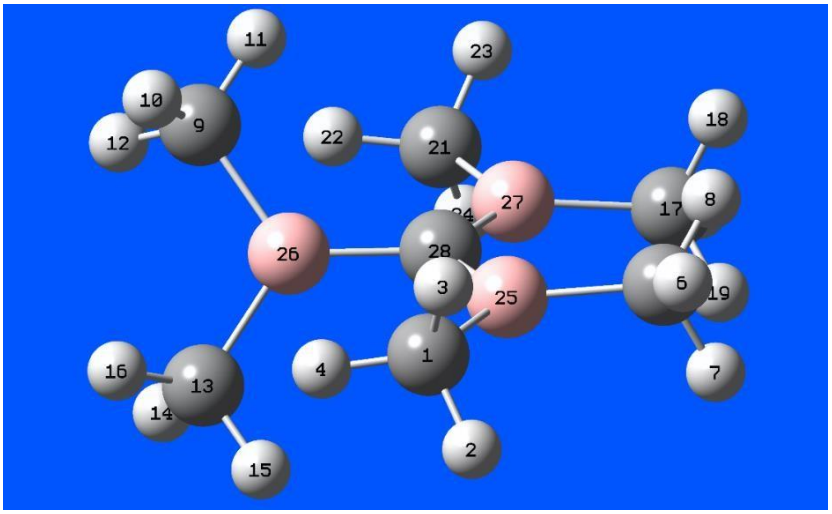
Highest occupied NLMO



10. Anion 5 (conformers 5*A* and 5*B*)

Geometry optimized at the MP2/aug-cc-pVTZ level

Conformer 5*A*



Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.009193	-2.762762	-0.134521
2	1	-0.422754	-3.445693	0.608072
3	1	-0.182898	-3.235119	-1.106190
4	1	1.088211	-2.738085	0.014499
5	6	-2.343376	-1.544665	-0.295141
6	1	-2.570564	-2.506953	-0.766652
7	1	-2.839091	-1.554497	0.683499
8	1	-2.822637	-0.757159	-0.875894
9	6	2.360601	0.787011	-1.080626
10	1	2.804966	0.020218	-1.729392
11	1	1.782457	1.458104	-1.714936
12	1	3.202832	1.335658	-0.643614
13	6	2.359348	-0.790660	1.080642
14	1	2.804890	-0.024572	1.729429
15	1	1.780149	-1.460861	1.714930
16	1	3.200733	-1.340612	0.643641
17	6	-2.340997	1.548242	0.295236
18	1	-2.836781	1.558739	-0.683366
19	1	-2.821391	0.761510	0.876103
20	1	-2.566692	2.510915	0.766684
21	6	0.013389	2.762776	0.134415
22	1	1.092355	2.736477	-0.014687
23	1	-0.417593	3.446333	-0.608163
24	1	-0.177919	3.235447	1.106085
25	5	-0.753751	-1.339421	-0.095422
26	5	1.477210	-0.001124	0.000007
27	5	-0.751702	1.340587	0.095411
28	6	-0.050999	0.000048	-0.000009

ENERGY (a.u):

MP2=-351.3684623

ESP atomic charges

1	C	-0.394853
2	H	0.024454
3	H	0.007295
4	H	0.034351
5	C	-0.363742
6	H	0.005461
7	H	0.021612
8	H	0.029495
9	C	-0.519737
10	H	0.026276
11	H	0.054614
12	H	0.060481
13	C	-0.520417
14	H	0.026384
15	H	0.054962
16	H	0.060538
17	C	-0.365706
18	H	0.022155
19	H	0.030078
20	H	0.005760
21	C	-0.403999
22	H	0.036663
23	H	0.026721
24	H	0.009530
25	B	0.702272
26	B	0.981649
27	B	0.705916
28	C	-1.358210

Wiberg bond index matrix in the NAO basis:

Atom		1	2	3	4	5	6	7	8	9
1.	C	0.0000	0.8874	0.8840	0.8923	0.0065	0.0032	0.0014	0.0070	0.0007
2.	H	0.8874	0.0000	0.0008	0.0008	0.0011	0.0001	0.0002	0.0003	0.0001
3.	H	0.8840	0.0008	0.0000	0.0008	0.0011	0.0002	0.0004	0.0001	0.0005
4.	H	0.8923	0.0008	0.0008	0.0000	0.0095	0.0004	0.0002	0.0005	0.0002
5.	C	0.0065	0.0011	0.0011	0.0095	0.0000	0.8954	0.8816	0.8887	0.0003
6.	H	0.0032	0.0001	0.0002	0.0004	0.8954	0.0000	0.0007	0.0006	0.0003
7.	H	0.0014	0.0002	0.0004	0.0002	0.8816	0.0007	0.0000	0.0010	0.0001
8.	H	0.0070	0.0003	0.0001	0.0005	0.8887	0.0006	0.0010	0.0000	0.0000
9.	C	0.0007	0.0001	0.0005	0.0002	0.0003	0.0003	0.0001	0.0000	0.0000
10.	H	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.8734
11.	H	0.0001	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.8877
12.	H	0.0001	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.8865
13.	C	0.0010	0.0003	0.0003	0.0019	0.0004	0.0001	0.0002	0.0001	0.0076
14.	H	0.0012	0.0000	0.0001	0.0006	0.0001	0.0000	0.0000	0.0000	0.0011
15.	H	0.0006	0.0000	0.0002	0.0001	0.0001	0.0000	0.0000	0.0000	0.0100
16.	H	0.0003	0.0000	0.0000	0.0002	0.0003	0.0000	0.0001	0.0000	0.0010
17.	C	0.0004	0.0000	0.0001	0.0001	0.0020	0.0006	0.0003	0.0017	0.0004
18.	H	0.0001	0.0001	0.0001	0.0000	0.0003	0.0000	0.0002	0.0006	0.0002
19.	H	0.0001	0.0000	0.0000	0.0000	0.0017	0.0003	0.0006	0.0002	0.0001
20.	H	0.0002	0.0000	0.0000	0.0000	0.0006	0.0001	0.0000	0.0003	0.0001
21.	C	0.0004	0.0002	0.0002	0.0001	0.0004	0.0002	0.0001	0.0001	0.0010
22.	H	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0019
23.	H	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0003
24.	H	0.0002	0.0000	0.0001	0.0000	0.0001	0.0000	0.0001	0.0000	0.0003
25.	B	0.8172	0.0076	0.0092	0.0046	0.8187	0.0047	0.0107	0.0061	0.0105
26.	B	0.0059	0.0010	0.0007	0.0022	0.0089	0.0003	0.0016	0.0006	0.8054
27.	B	0.0087	0.0025	0.0028	0.0003	0.0022	0.0009	0.0026	0.0006	0.0053
28.	C	0.0051	0.0104	0.0103	0.0016	0.0055	0.0098	0.0072	0.0025	0.0081

Atom	10	11	12	13	14	15	16	17	18

1.	C	0.0001	0.0001	0.0001	0.0010	0.0012	0.0006	0.0003	0.0004	0.0001
2.	H	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0001
3.	H	0.0000	0.0000	0.0000	0.0003	0.0001	0.0002	0.0000	0.0001	0.0001
4.	H	0.0000	0.0001	0.0000	0.0019	0.0006	0.0001	0.0002	0.0001	0.0000
5.	C	0.0002	0.0001	0.0001	0.0004	0.0001	0.0001	0.0003	0.0020	0.0003
6.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0006	0.0000
7.	H	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000	0.0001	0.0003	0.0002
8.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0017	0.0006
9.	C	0.8734	0.8877	0.8865	0.0076	0.0011	0.0100	0.0010	0.0004	0.0002
10.	H	0.0000	0.0008	0.0011	0.0011	0.0006	0.0001	0.0002	0.0001	0.0000
11.	H	0.0008	0.0000	0.0007	0.0100	0.0001	0.0006	0.0002	0.0001	0.0000
12.	H	0.0011	0.0007	0.0000	0.0010	0.0002	0.0002	0.0002	0.0003	0.0001
13.	C	0.0011	0.0100	0.0010	0.0000	0.8734	0.8877	0.8865	0.0003	0.0001
14.	H	0.0006	0.0001	0.0002	0.8734	0.0000	0.0008	0.0011	0.0002	0.0000
15.	H	0.0001	0.0006	0.0002	0.8877	0.0008	0.0000	0.0007	0.0001	0.0000
16.	H	0.0002	0.0002	0.0002	0.8865	0.0011	0.0007	0.0000	0.0001	0.0001
17.	C	0.0001	0.0001	0.0003	0.0003	0.0002	0.0001	0.0001	0.0000	0.8816
18.	H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0001	0.8816	0.0000
19.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8887	0.0010
20.	H	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.8954	0.0007
21.	C	0.0012	0.0006	0.0003	0.0007	0.0001	0.0001	0.0001	0.0065	0.0014
22.	H	0.0006	0.0001	0.0002	0.0002	0.0000	0.0001	0.0000	0.0095	0.0002
23.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0011	0.0002
24.	H	0.0001	0.0002	0.0000	0.0005	0.0000	0.0000	0.0000	0.0011	0.0004
25.	B	0.0006	0.0004	0.0020	0.0053	0.0013	0.0007	0.0013	0.0022	0.0026
26.	B	0.0179	0.0059	0.0096	0.8054	0.0178	0.0059	0.0096	0.0089	0.0016
27.	B	0.0013	0.0007	0.0013	0.0105	0.0006	0.0004	0.0020	0.8187	0.0107
28.	C	0.0054	0.0024	0.0099	0.0081	0.0054	0.0024	0.0099	0.0055	0.0072

Atom		19	20	21	22	23	24	25	26	27
1.	C	0.0001	0.0002	0.0004	0.0001	0.0002	0.0002	0.8172	0.0059	0.0087
2.	H	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.0076	0.0010	0.0025
3.	H	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001	0.0092	0.0007	0.0028
4.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0046	0.0022	0.0003
5.	C	0.0017	0.0006	0.0004	0.0001	0.0000	0.0001	0.8187	0.0089	0.0022
6.	H	0.0003	0.0001	0.0002	0.0000	0.0000	0.0000	0.0047	0.0003	0.0009
7.	H	0.0006	0.0000	0.0001	0.0000	0.0001	0.0001	0.0107	0.0016	0.0026
8.	H	0.0002	0.0003	0.0001	0.0000	0.0000	0.0000	0.0061	0.0006	0.0006
9.	C	0.0001	0.0001	0.0010	0.0019	0.0003	0.0003	0.0105	0.8054	0.0053
10.	H	0.0000	0.0000	0.0012	0.0006	0.0000	0.0001	0.0006	0.0179	0.0013
11.	H	0.0000	0.0000	0.0006	0.0001	0.0000	0.0002	0.0004	0.0059	0.0007
12.	H	0.0000	0.0000	0.0003	0.0002	0.0000	0.0000	0.0020	0.0096	0.0013
13.	C	0.0000	0.0003	0.0007	0.0002	0.0001	0.0005	0.0053	0.8054	0.0105
14.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0013	0.0178	0.0006
15.	H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0007	0.0059	0.0004
16.	H	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0013	0.0096	0.0020
17.	C	0.8887	0.8954	0.0065	0.0095	0.0011	0.0011	0.0022	0.0089	0.8187
18.	H	0.0010	0.0007	0.0014	0.0002	0.0002	0.0004	0.0026	0.0016	0.0107
19.	H	0.0000	0.0006	0.0070	0.0005	0.0003	0.0001	0.0006	0.0006	0.0061
20.	H	0.0006	0.0000	0.0032	0.0004	0.0001	0.0002	0.0009	0.0003	0.0047
21.	C	0.0070	0.0032	0.0000	0.8923	0.8874	0.8840	0.0087	0.0059	0.8173
22.	H	0.0005	0.0004	0.8923	0.0000	0.0008	0.0008	0.0003	0.0022	0.0046
23.	H	0.0003	0.0001	0.8874	0.0008	0.0000	0.0008	0.0025	0.0010	0.0077
24.	H	0.0001	0.0002	0.8840	0.0008	0.0008	0.0000	0.0028	0.0007	0.0092
25.	B	0.0006	0.0009	0.0087	0.0003	0.0025	0.0028	0.0000	0.0476	0.0851
26.	B	0.0006	0.0003	0.0059	0.0022	0.0010	0.0007	0.0476	0.0000	0.0476
27.	B	0.0061	0.0047	0.8173	0.0046	0.0077	0.0092	0.0851	0.0476	0.0000
28.	C	0.0025	0.0098	0.0051	0.0016	0.0104	0.0103	1.0634	0.9201	1.0634

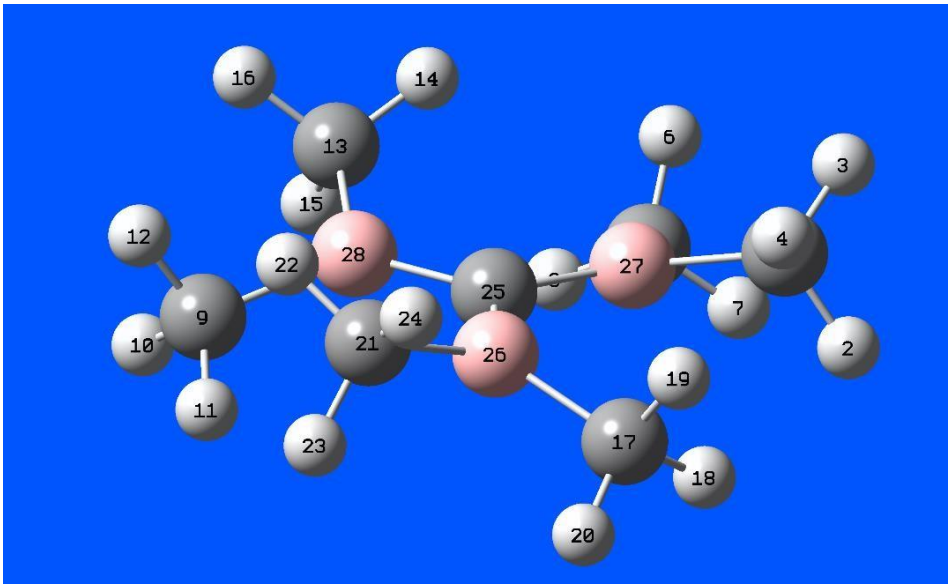
Atom		28
1.	C	0.0051
2.	H	0.0104
3.	H	0.0103
4.	H	0.0016
5.	C	0.0055

6.	H	0.0098
7.	H	0.0072
8.	H	0.0025
9.	C	0.0081
10.	H	0.0054
11.	H	0.0024
12.	H	0.0099
13.	C	0.0081
14.	H	0.0054
15.	H	0.0024
16.	H	0.0099
17.	C	0.0055
18.	H	0.0072
19.	H	0.0025
20.	H	0.0098
21.	C	0.0051
22.	H	0.0016
23.	H	0.0104
24.	H	0.0103
25.	B	1.0634
26.	B	0.9201
27.	B	1.0634
28.	C	0.0000

ESP atomic charges

1	C	-0.354016
2	H	0.013979
3	H	-0.003269
4	H	0.024118
5	C	-0.302438
6	H	-0.011186
7	H	0.007043
8	H	0.013302
9	C	-0.448461
10	H	0.007020
11	H	0.033677
12	H	0.042210
13	C	-0.448553
14	H	0.007102
15	H	0.033627
16	H	0.042261
17	C	-0.303723
18	H	0.007248
19	H	0.013494
20	H	-0.010598
21	C	-0.354803
22	H	0.024307
23	H	0.014190
24	H	-0.003254
25	B	0.663492
26	B	0.944876
27	B	0.664111
28	C	-1.315758

Conformer 5*B*



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.737615	0.366570	0.456289
2	1	0	-3.347736	0.651378	-0.425045
3	1	0	-3.403584	-0.259085	1.084605
4	1	0	-2.508297	1.288225	1.013125
5	6	0	-1.914015	-1.991273	-0.456409
6	1	0	-2.214478	-2.593962	0.424841
7	1	0	-2.824492	-1.916240	-1.085016
8	1	0	-1.160613	-2.569789	-1.013009
9	6	0	2.681528	-0.662005	-0.456254
10	1	0	3.072064	-1.488193	-1.084450
11	1	0	2.805839	0.279538	-1.013158
12	1	0	3.353482	-0.620413	0.425145
13	6	0	1.051268	-2.554110	0.456395
14	1	0	0.138187	-2.816431	1.012780
15	1	0	1.110336	-3.225020	-0.424800
16	1	0	1.925788	-2.817747	1.085250
17	6	0	-0.767549	2.653283	-0.456079
18	1	0	-1.645293	2.290151	-1.012671
19	1	0	-1.139216	3.214661	0.425303
20	1	0	-0.247410	3.404399	-1.084589
21	6	0	1.686372	2.187513	0.456084
22	1	0	2.369937	1.528101	1.012874
23	1	0	2.237969	2.573328	-0.425395
24	1	0	1.477710	3.077184	1.084321
25	6	0	-0.000004	0.000012	-0.000036
26	5	0	0.286429	1.509032	0.000020
27	5	0	-1.450059	-0.506459	-0.000023
28	5	0	1.163611	-1.002576	-0.000009

ESP atomic charges

1	C	-0.439335
2	H	0.059849
3	H	0.007692
4	H	0.028212

5	C	-0.400396
6	H	0.051404
7	H	-0.000399
8	H	0.015253
9	C	-0.431509
10	H	0.007973
11	H	0.022445
12	H	0.058422
13	C	-0.441988
14	H	0.028114
15	H	0.060552
16	H	0.008242
17	C	-0.419702
18	H	0.021620
19	H	0.054970
20	H	0.003114
21	C	-0.441708
22	H	0.027448
23	H	0.061216
24	H	0.009138
25	C	-1.347681
26	B	0.801074
27	B	0.791916
28	B	0.804063

Wiberg bond index matrix in the NAO basis:

Atom		1	2	3	4	5	6	7	8	9
1.	C	0.0000	0.9457	0.9428	0.9473	0.0070	0.0030	0.0012	0.0064	0.0007
2.	H	0.9457	0.0000	0.0008	0.0008	0.0011	0.0001	0.0001	0.0003	0.0001
3.	H	0.9428	0.0008	0.0000	0.0008	0.0010	0.0001	0.0004	0.0001	0.0004
4.	H	0.9473	0.0008	0.0008	0.0000	0.0086	0.0004	0.0002	0.0004	0.0002
5.	C	0.0070	0.0011	0.0010	0.0086	0.0000	0.9528	0.9409	0.9447	0.0002
6.	H	0.0030	0.0001	0.0001	0.0004	0.9528	0.0000	0.0006	0.0006	0.0002
7.	H	0.0012	0.0001	0.0004	0.0002	0.9409	0.0006	0.0000	0.0009	0.0001
8.	H	0.0064	0.0003	0.0001	0.0004	0.9447	0.0006	0.0009	0.0000	0.0000
9.	C	0.0007	0.0001	0.0004	0.0002	0.0002	0.0002	0.0001	0.0000	0.0000
10.	H	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.9333
11.	H	0.0001	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.9431
12.	H	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.9449
13.	C	0.0010	0.0002	0.0003	0.0020	0.0004	0.0000	0.0001	0.0000	0.0082
14.	H	0.0010	0.0000	0.0001	0.0007	0.0001	0.0000	0.0000	0.0000	0.0010
15.	H	0.0007	0.0000	0.0002	0.0001	0.0001	0.0000	0.0000	0.0000	0.0092
16.	H	0.0003	0.0000	0.0000	0.0001	0.0002	0.0000	0.0001	0.0000	0.0009
17.	C	0.0004	0.0000	0.0000	0.0000	0.0021	0.0006	0.0002	0.0016	0.0004
18.	H	0.0001	0.0001	0.0001	0.0000	0.0002	0.0000	0.0001	0.0004	0.0001
19.	H	0.0002	0.0000	0.0000	0.0000	0.0016	0.0003	0.0004	0.0003	0.0000
20.	H	0.0002	0.0000	0.0000	0.0000	0.0006	0.0001	0.0000	0.0003	0.0000
21.	C	0.0003	0.0001	0.0001	0.0001	0.0004	0.0002	0.0001	0.0002	0.0010
22.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0020
23.	H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002
24.	H	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0003
25.	B	0.8470	0.0079	0.0094	0.0047	0.8499	0.0048	0.0109	0.0063	0.0096
26.	B	0.0064	0.0008	0.0006	0.0023	0.0080	0.0002	0.0013	0.0004	0.8297
27.	B	0.0082	0.0019	0.0022	0.0003	0.0022	0.0007	0.0020	0.0005	0.0052
28.	C	0.0051	0.0097	0.0093	0.0014	0.0054	0.0090	0.0066	0.0022	0.0084

Atom		10	11	12	13	14	15	16	17	18
1.	C	0.0001	0.0001	0.0001	0.0010	0.0010	0.0007	0.0003	0.0004	0.0001
2.	H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
3.	H	0.0000	0.0000	0.0000	0.0003	0.0001	0.0002	0.0000	0.0000	0.0001
4.	H	0.0000	0.0001	0.0000	0.0020	0.0007	0.0001	0.0001	0.0000	0.0000
5.	C	0.0002	0.0001	0.0001	0.0004	0.0001	0.0001	0.0002	0.0021	0.0002
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000
7.	H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0001	0.0002	0.0001

8.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0016	0.0004
9.	C	0.9333	0.9431	0.9449	0.0082	0.0010	0.0092	0.0009	0.0004	0.0001
10.	H	0.0000	0.0007	0.0009	0.0010	0.0006	0.0001	0.0001	0.0001	0.0000
11.	H	0.0007	0.0000	0.0008	0.0092	0.0001	0.0005	0.0002	0.0001	0.0000
12.	H	0.0009	0.0008	0.0000	0.0009	0.0001	0.0002	0.0001	0.0002	0.0001
13.	C	0.0010	0.0092	0.0009	0.0000	0.9333	0.9431	0.9449	0.0002	0.0001
14.	H	0.0006	0.0001	0.0001	0.9333	0.0000	0.0007	0.0009	0.0002	0.0000
15.	H	0.0001	0.0005	0.0002	0.9431	0.0007	0.0000	0.0008	0.0001	0.0000
16.	H	0.0001	0.0002	0.0001	0.9449	0.0009	0.0008	0.0000	0.0001	0.0001
17.	C	0.0001	0.0001	0.0002	0.0002	0.0002	0.0001	0.0001	0.0000	0.9409
18.	H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0001	0.9409	0.0000
19.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9447	0.0009
20.	H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.9528	0.0006
21.	C	0.0010	0.0007	0.0003	0.0007	0.0001	0.0001	0.0001	0.0070	0.0012
22.	H	0.0007	0.0001	0.0001	0.0002	0.0000	0.0001	0.0000	0.0086	0.0002
23.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0011	0.0001
24.	H	0.0001	0.0002	0.0000	0.0004	0.0000	0.0000	0.0000	0.0010	0.0004
25.	B	0.0005	0.0003	0.0016	0.0052	0.0010	0.0006	0.0010	0.0022	0.0020
26.	B	0.0177	0.0061	0.0096	0.8297	0.0177	0.0061	0.0096	0.0080	0.0013
27.	B	0.0010	0.0006	0.0010	0.0096	0.0005	0.0003	0.0016	0.8499	0.0109
28.	C	0.0048	0.0019	0.0091	0.0084	0.0048	0.0019	0.0091	0.0054	0.0066

Atom		19	20	21	22	23	24	25	26	27
1.	C	0.0002	0.0002	0.0003	0.0001	0.0001	0.0001	0.8470	0.0064	0.0082
2.	H	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0079	0.0008	0.0019
3.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0094	0.0006	0.0022
4.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0047	0.0023	0.0003
5.	C	0.0016	0.0006	0.0004	0.0000	0.0000	0.0000	0.8499	0.0080	0.0022
6.	H	0.0003	0.0001	0.0002	0.0000	0.0000	0.0000	0.0048	0.0002	0.0007
7.	H	0.0004	0.0000	0.0001	0.0000	0.0001	0.0001	0.0109	0.0013	0.0020
8.	H	0.0003	0.0003	0.0002	0.0000	0.0000	0.0000	0.0063	0.0004	0.0005
9.	C	0.0000	0.0000	0.0010	0.0020	0.0002	0.0003	0.0096	0.8297	0.0052
10.	H	0.0000	0.0000	0.0010	0.0007	0.0000	0.0001	0.0005	0.0177	0.0010
11.	H	0.0000	0.0000	0.0007	0.0001	0.0000	0.0002	0.0003	0.0061	0.0006
12.	H	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000	0.0016	0.0096	0.0010
13.	C	0.0000	0.0002	0.0007	0.0002	0.0001	0.0004	0.0052	0.8297	0.0096
14.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0010	0.0177	0.0005
15.	H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0006	0.0061	0.0003
16.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0010	0.0096	0.0016
17.	C	0.9447	0.9528	0.0070	0.0086	0.0011	0.0010	0.0022	0.0080	0.8499
18.	H	0.0009	0.0006	0.0012	0.0002	0.0001	0.0004	0.0020	0.0013	0.0109
19.	H	0.0000	0.0006	0.0064	0.0004	0.0003	0.0001	0.0005	0.0004	0.0063
20.	H	0.0006	0.0000	0.0030	0.0004	0.0001	0.0001	0.0007	0.0002	0.0048
21.	C	0.0064	0.0030	0.0000	0.9473	0.9457	0.9428	0.0082	0.0064	0.8470
22.	H	0.0004	0.0004	0.9473	0.0000	0.0008	0.0008	0.0003	0.0023	0.0047
23.	H	0.0003	0.0001	0.9457	0.0008	0.0000	0.0008	0.0019	0.0008	0.0079
24.	H	0.0001	0.0001	0.9428	0.0008	0.0008	0.0000	0.0022	0.0006	0.0094
25.	B	0.0005	0.0007	0.0082	0.0003	0.0019	0.0022	0.0000	0.0442	0.0819
26.	B	0.0004	0.0002	0.0064	0.0023	0.0008	0.0006	0.0442	0.0000	0.0442
27.	B	0.0063	0.0048	0.8470	0.0047	0.0079	0.0094	0.0819	0.0442	0.0000
28.	C	0.0022	0.0090	0.0051	0.0014	0.0097	0.0093	1.1299	0.9577	1.1299

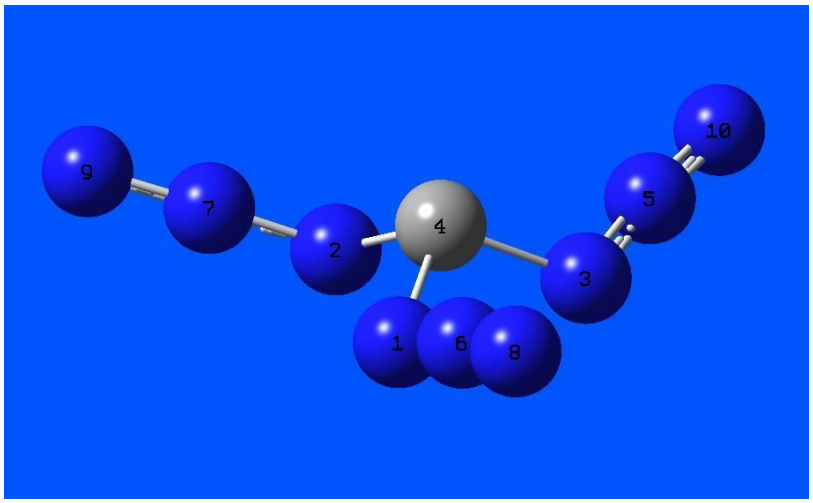
Atom		28
1.	C	0.0051
2.	H	0.0097
3.	H	0.0093
4.	H	0.0014
5.	C	0.0054
6.	H	0.0090
7.	H	0.0066
8.	H	0.0022
9.	C	0.0084
10.	H	0.0048
11.	H	0.0019
12.	H	0.0091
13.	C	0.0084

14.	H	0.0048
15.	H	0.0019
16.	H	0.0091
17.	C	0.0054
18.	H	0.0066
19.	H	0.0022
20.	H	0.0090
21.	C	0.0051
22.	H	0.0014
23.	H	0.0097
24.	H	0.0093
25.	B	1.1299
26.	B	0.9577
27.	B	1.1299
28.	C	0.0000

11. Anion 6 (conformers 6*A* and 6*B*)

Geometry optimized at the B2PLYP/QZVP level

Conformer 6*A*



Symmetry point group: C_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.203923	-1.344331	-0.386622
2	7	0	-1.266281	0.495383	-0.386714
3	7	0	1.062042	0.848781	-0.386629
4	6	0	-0.000082	-0.000061	0.238392
5	7	0	1.171416	1.992917	0.003346
6	7	0	1.140355	-2.010981	0.003076
7	7	0	-2.311799	0.017990	0.003195
8	7	0	1.993320	-2.717614	0.315394
9	7	0	-3.350373	-0.367023	0.315427
10	7	0	1.357467	3.084930	0.315192

ENERGY (a.u):

E = -530.5891487

ESP atomic charges

1	N	-0.267040
2	N	-0.273830
3	N	-0.269719
4	C	-0.416494
5	N	0.589630
6	N	0.583473
7	N	0.593259

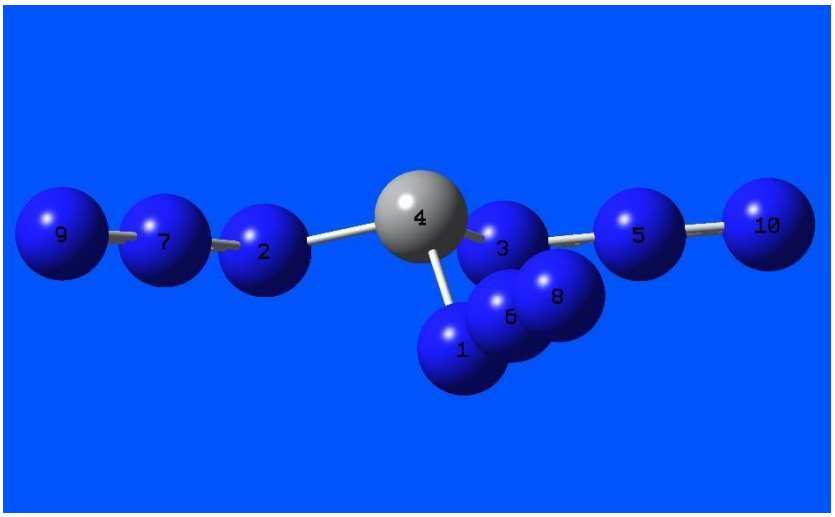
```
     8  N   -0.510669
     9  N   -0.514879
    10  N   -0.513731

Wiberg bond index matrix in the NAO basis:
```

Atom		1	2	3	4	5	6	7	8	9
1.	N	0.0000	0.0211	0.0211	0.8718	0.0088	1.5171	0.0061	0.5604	0.0114
2.	N	0.0211	0.0000	0.0211	0.8718	0.0061	0.0088	1.5172	0.0028	0.5604
3.	N	0.0211	0.0211	0.0000	0.8718	1.5171	0.0061	0.0088	0.0114	0.0028
4.	C	0.8718	0.8718	0.8718	0.0000	0.0368	0.0368	0.0368	0.0676	0.0675
5.	N	0.0088	0.0061	1.5171	0.0368	0.0000	0.0014	0.0014	0.0033	0.0020
6.	N	1.5171	0.0088	0.0061	0.0368	0.0014	0.0000	0.0014	2.1209	0.0033
7.	N	0.0061	1.5172	0.0088	0.0368	0.0014	0.0014	0.0000	0.0020	2.1209
8.	N	0.5604	0.0028	0.0114	0.0676	0.0033	2.1209	0.0020	0.0000	0.0040
9.	N	0.0114	0.5604	0.0028	0.0675	0.0020	0.0033	2.1209	0.0040	0.0000
10.	N	0.0028	0.0114	0.5605	0.0675	2.1209	0.0020	0.0033	0.0040	0.0040

Atom		10
1.	N	0.0028
2.	N	0.0114
3.	N	0.5605
4.	C	0.0675
5.	N	2.1209
6.	N	0.0020
7.	N	0.0033
8.	N	0.0040
9.	N	0.0040
10.	N	0.0000

Conformer 6*B*



Symmetry point group: C_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	0.000104	0.790985	0.634525
2	7	0	-1.137950	-1.258690	0.132072
3	7	0	1.137390	-1.259087	0.131980
4	6	0	-0.000154	-0.420343	-0.321055
5	7	0	2.262215	-0.845535	-0.051235
6	7	0	0.000507	1.893446	0.122339
7	7	0	-2.262652	-0.844807	-0.051156
8	7	0	0.000893	2.972678	-0.271122
9	7	0	-3.366119	-0.543913	-0.186157
10	7	0	3.365743	-0.544784	-0.186056

ENERGY (a.u):

E =-530.5895105

ESP atomic charges

1	N	-0.280684
2	N	-0.294287
3	N	-0.294413
4	C	-0.414870
5	N	0.617164
6	N	0.618799
7	N	0.617153
8	N	-0.523002
9	N	-0.522947
10	N	-0.522913

Wiberg bond index matrix in the NAO basis:

Atom		1	2	3	4	5	6	7	8	9
1.	N	0.0000	0.0203	0.0203	0.8181	0.0064	1.5236	0.0064	0.5626	0.0115
2.	N	0.0203	0.0000	0.0246	0.8890	0.0086	0.0090	1.5198	0.0097	0.5615
3.	N	0.0203	0.0246	0.0000	0.8890	1.5198	0.0090	0.0086	0.0097	0.0022
4.	C	0.8181	0.8890	0.8890	0.0000	0.0392	0.0226	0.0392	0.0575	0.0710
5.	N	0.0064	0.0086	1.5198	0.0392	0.0000	0.0010	0.0014	0.0029	0.0012
6.	N	1.5236	0.0090	0.0090	0.0226	0.0010	0.0000	0.0010	2.1284	0.0033
7.	N	0.0064	1.5198	0.0086	0.0392	0.0014	0.0010	0.0000	0.0029	2.1149
8.	N	0.5626	0.0097	0.0097	0.0575	0.0029	2.1284	0.0029	0.0000	0.0070
9.	N	0.0115	0.5615	0.0022	0.0710	0.0012	0.0033	2.1149	0.0070	0.0000
10.	N	0.0115	0.0022	0.5614	0.0710	2.1149	0.0033	0.0012	0.0070	0.0016

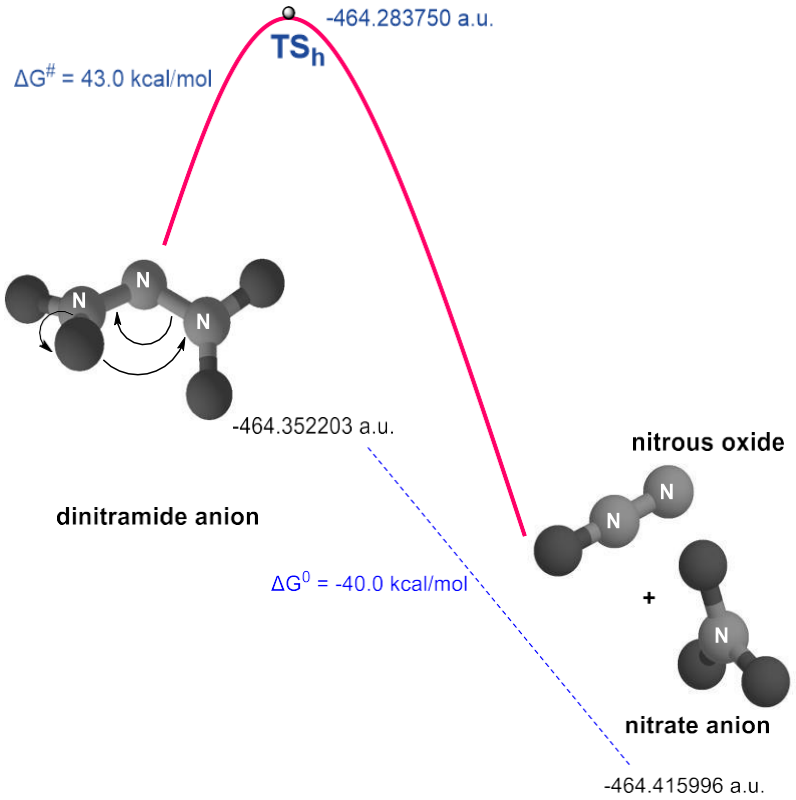
Atom		10
1.	N	0.0115
2.	N	0.0022
3.	N	0.5614
4.	C	0.0710
5.	N	2.1149
6.	N	0.0033
7.	N	0.0012
8.	N	0.0070
9.	N	0.0016
10.	N	0.0000

12. Decomposition of dinitramide anion 2 with extruding nitrate anion; gas phase

anion **2** → N_2O + NO_3^-

(Ref. 30a in the main text)

Reaction energy profile (this work)



A similar scheme is given in Ref. 30a.

Located transition state TS_h

Optimized at the MP2/aug-cc-pVTZ level without applying geometry constrains. The transition state of similar geometry for this reaction was also located in Ref. 30a with using other QM calculation methods.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.040415	-0.022152	0.000184
2	7	0	-1.183121	0.177295	-0.000540
3	8	0	1.557692	0.048252	1.094520
4	8	0	1.558991	0.044821	-1.093879
5	8	0	-2.349380	-0.179632	0.000486

6	8	0	-0.177546	-1.101014	0.001141
7	7	0	-0.531301	1.202083	-0.002236

ENERGY (a.u):

MP2=-464.2791025

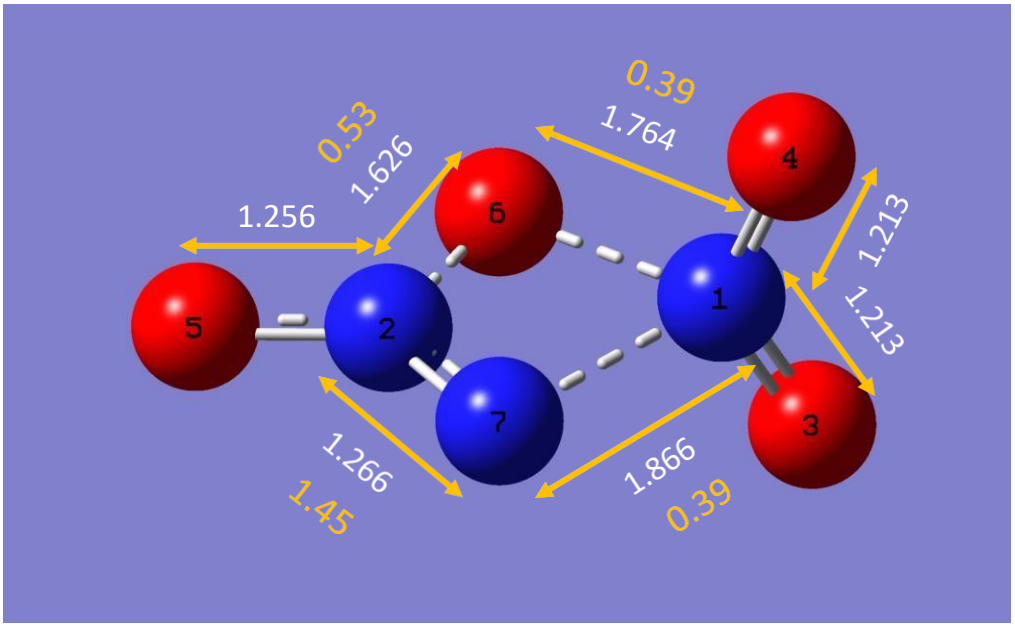
Zero-point correction=	0.025085 (Hartree/Particle)
Thermal correction to Energy=	0.030659
Thermal correction to Enthalpy=	0.031604
Thermal correction to Gibbs Free Energy=	-0.004648
Sum of electronic and zero-point Energies=	-464.254018
Sum of electronic and thermal Energies=	-464.248443
Sum of electronic and thermal Enthalpies=	-464.247499
Sum of electronic and thermal Free Energies=	-464.283750

FREQUENCIES

Frequencies --	-1110.9758	109.4785	291.2047
Frequencies --	313.9511	379.4667	501.9597
Frequencies --	536.7568	633.9017	708.2200
Frequencies --	779.6508	812.2218	1236.3553
Frequencies --	1307.5553	1681.1908	1718.9218

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7
1. N	0.0000	0.0179	1.4208	1.4206	0.0240	0.5598	0.2560
2. N	0.0179	0.0000	0.0202	0.0202	1.3613	0.5296	1.7051
3. O	1.4208	0.0202	0.0000	0.2733	0.0142	0.1348	0.0919
4. O	1.4206	0.0202	0.2733	0.0000	0.0142	0.1348	0.0919
5. O	0.0240	1.3613	0.0142	0.0142	0.0000	0.1130	0.3513
6. O	0.5598	0.5296	0.1348	0.1348	0.1130	0.0000	0.2303
7. N	0.2560	1.7051	0.0919	0.0919	0.3513	0.2303	0.0000



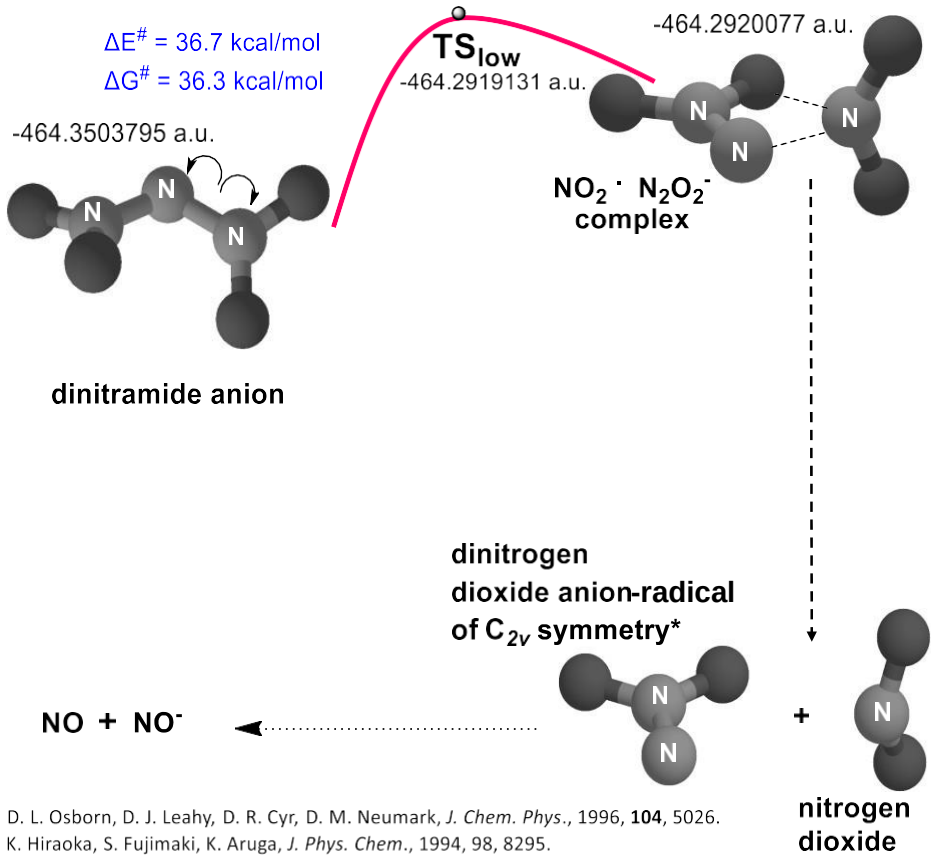
Modeled geometry of transition state TS_h of the above mentioned electrocyclic reaction. Numbers in white and yellow show interatomic distances and calculated bond orders (as Wiberg indexes), respectively.

13. Low barrier decomposition of dinitramide anion 2 yielding NO_2 and $N_2O_2^-$; gas phase

anion **2** → NO_2 + $N_2O_2^-$

(Ref. 30a in the main text)

Reaction energy profile (this work)



This scheme differs from that from Ref. 30a by supplying the transition state TS_{low} as well as the related supramolecular product $N_2O{\bullet}N_2O_4^-$. Dotted arrows show further transformations (not modeled in this study).

Located transition state TS_{low}

Optimized at the MP2/aug-cc-pVTZ level without applying geometry constrains

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.049795	0.000001	0.013746
2	7	0	-1.111478	-0.000002	0.092463
3	8	0	1.571896	-1.094440	-0.000359
4	8	0	1.571884	1.094447	-0.000377

5	8	0	-2.358823	0.000001	-0.056536
6	8	0	-0.358643	-0.000013	-1.047681
7	7	0	-0.425533	0.000006	1.156595

ENERGY (a.u):

MP2=-464.2919131

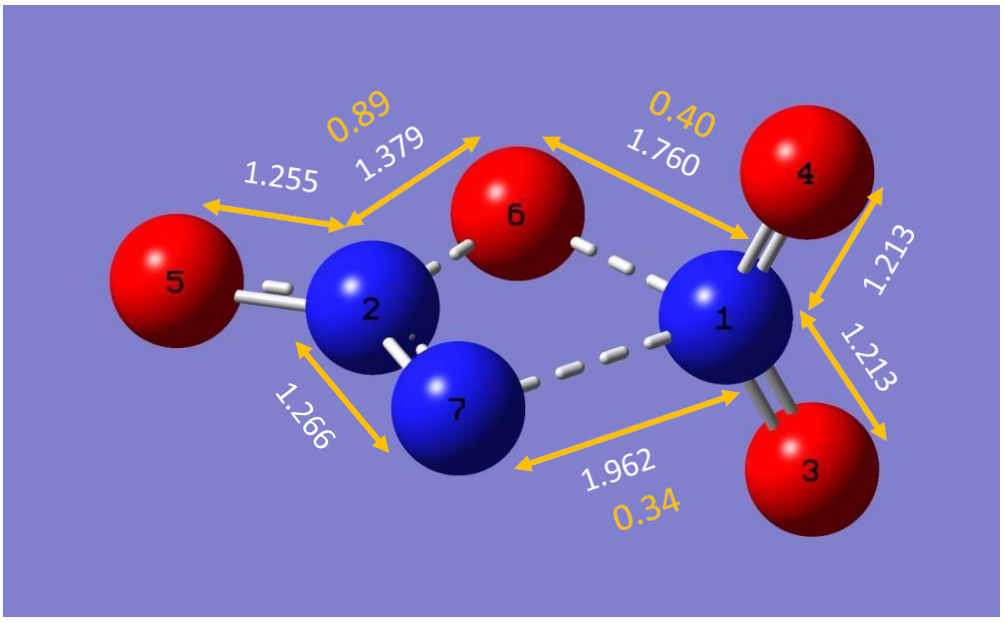
Zero-point correction=	0.026879	(Hartree/Particle)
Thermal correction to Energy=	0.031965	
Thermal correction to Enthalpy=	0.032909	
Thermal correction to Gibbs Free Energy=	-0.002393	
Sum of electronic and zero-point Energies=	-464.265035	
Sum of electronic and thermal Energies=	-464.259949	
Sum of electronic and thermal Enthalpies=	-464.259004	
Sum of electronic and thermal Free Energies=	-464.294306	

FREQUENCIES

Frequencies --	-319.4284	135.1018	299.4855
Frequencies --	421.2430	490.0892	578.1320
Frequencies --	634.9801	719.6690	774.5096
Frequencies --	814.6672	1036.1578	1202.6873
Frequencies --	1342.5246	1667.5673	1681.5214

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7
1. N	0.0000	0.0164	1.4112	1.4112	0.0347	0.3932	0.3888
2. N	0.0164	0.0000	0.0109	0.0109	1.2287	0.9134	1.4524
3. O	1.4112	0.0109	0.0000	0.2416	0.0125	0.1288	0.1340
4. O	1.4112	0.0109	0.2416	0.0000	0.0125	0.1288	0.1340
5. O	0.0347	1.2287	0.0125	0.0125	0.0000	0.1146	0.2748
6. O	0.3932	0.9134	0.1288	0.1288	0.1146	0.0000	0.2224
7. N	0.3888	1.4524	0.1340	0.1340	0.2748	0.2224	0.0000



Modeled geometry of transition state TS_{low}. Numbers in white and yellow show interatomic distances and calculated bond orders (as Wiberg indexes), respectively.

Located molecular complex $NO_2 \bullet N_2O_2^-$

Optimized at the MP2/aug-cc-pVTZ level without applying geometry constrains; gas phase

ENERGY (a.u):

MP2=-464.2920077

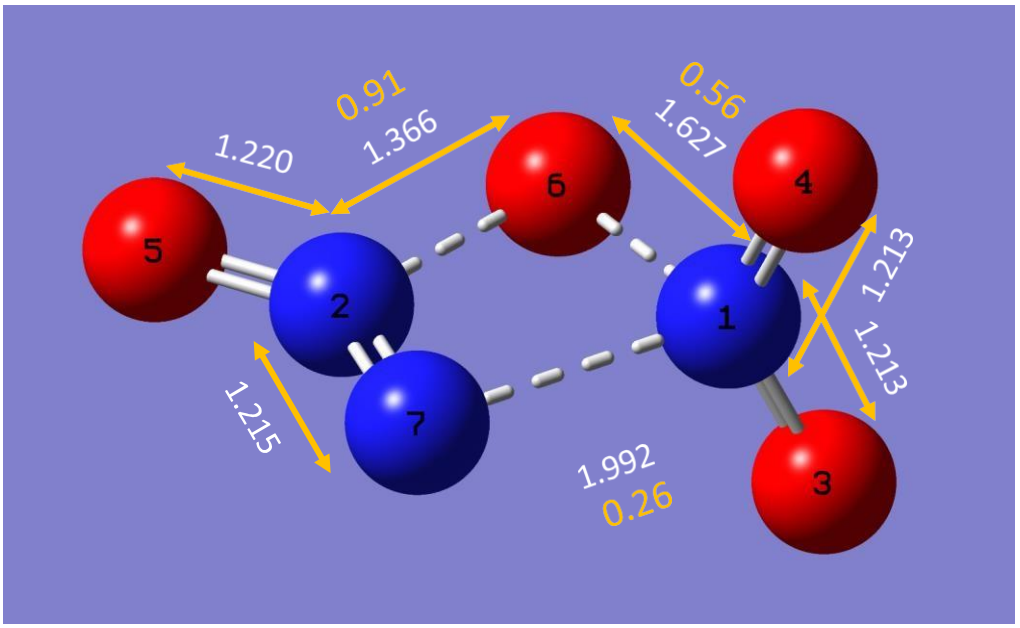
```
 Zero-point correction=                           0.027811 (Hartree/Particle)
 Thermal correction to Energy=                    0.033414
 Thermal correction to Enthalpy=                  0.034358
 Thermal correction to Gibbs Free Energy=        -0.001907
 Sum of electronic and zero-point Energies=           -464.264196
 Sum of electronic and thermal Energies=              -464.258594
 Sum of electronic and thermal Enthalpies=            -464.257650
 Sum of electronic and thermal Free Energies=         -464.293915
```

FREQUENCIES

```
Frequencies --    127.5237               229.4753               286.4937
Frequencies --    417.0530               472.6021               621.7733
Frequencies --    647.4614               710.5426               804.7340
Frequencies --    829.6252              1107.2098              1183.9340
Frequencies --   1365.7881              1697.4090              1706.1872
```

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7
1. N	0.0000	0.0162	1.4135	1.4135	0.0340	0.3988	0.3379
2. N	0.0162	0.0000	0.0105	0.0105	1.2320	0.8900	1.4583
3. O	1.4135	0.0105	0.0000	0.2463	0.0123	0.1265	0.1276
4. O	1.4135	0.0105	0.2463	0.0000	0.0123	0.1265	0.1276
5. O	0.0340	1.2320	0.0123	0.0123	0.0000	0.1118	0.2789
6. O	0.3988	0.8900	0.1265	0.1265	0.1118	0.0000	0.2186
7. N	0.3379	1.4583	0.1276	0.1276	0.2789	0.2186	0.0000



Numbers in white and yellow show interatomic distances and calculated bond orders (as Wiberg indexes), respectively.

σ Bonding in the N–N unit in NBO representation

(bold: occupancy; italics: atomic orbital coefficient; underlined: formal orbital number)

σ bonding orbital

```
   4. (1.80032) BD ( 1) N   1 - N   7
            ( 47.00%)   0.6855* N   1 s( 12.40%)p 7.05( 87.43%)d 0.01(  0.13%)
                                          f 0.00(  0.04%)
            ( 53.00%)   0.7280* N   7 s(  2.94%)p32.93( 96.83%)d 0.08(  0.23%)
                                          f 0.00(  0.00%)
```

σ* antibonding orbital

```
 318. (0.68566) BD*( 1) N   1 - N   7
            ( 53.00%)   0.7280* N   1 s( 12.40%)p 7.05( 87.43%)d 0.01(  0.13%)
                                          f 0.00(  0.04%)
            ( 47.00%)  -0.6855* N   7 s(  2.94%)p32.93( 96.83%)d 0.08(  0.23%)
                                          f 0.00(  0.00%)
```