Supporting Information for

Predicting the Electrochemical Behavior of Lithium Nitrite in Acetonitrile with Quantum Chemical Methods

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Supporting Information Available. Complete ref 26, RMP2 and RCCSD(T) reaction/activation energies as a function of basis set size (Table S1), the performance of several DFT methods in reproducing the redox potentials of oxygenated nitrogen compounds (Table S2), parameters employed in the CV simulation of NO_2^- oxidation under Ar (Table S3), additional computational (Figures S1, S2) and experimental details (Table S4, Figures S3−S6), Cartesian coordinates, electronic states, and absolute energies (in Hartrees) for tested molecular structures obtained with the B3LYP functional. This material is available free of charge via the Internet at http://pubs.acs.org.

Ref 26: Bylaska, E. J.; de Jong, W. A.; Govind, N.; Kowalski, K.; Straatsma, T. P.; Valiev, M.; Wang, D.; Apra, E.; Windus, T. L.; Hammond, J.; Nichols, P.; Hirata, S.; Hackler, M. T.; Zhao, Y.; Fan, P.-D.; Harrison, R. J.; Dupuis, M.; Smith, D. M. A.; Nieplocha, J.; Tipparaju, V.; Krishnan, M.; Wu, Q.; Van Voorhis, T.; Auer, A. A.; Nooijen, M.; Brown, E.; Cisneros, G.; Fann, G. I.; Fruchtl, H.; Garza, J.; Hirao, K.; Kendall, R.; Nichols, J. A.; Tsemekhman, K.; Wolinski, K.; Anchell, J.; Bernholdt, D.; Borowski, P.; Clark, T.; Clerc, D.; Dachsel, H.; Deegan, M.; Dyall, K.; Elwood, D.; Glendening, E.; Gutowski, M.; Hess, A.; Jaffe, J.; Johnson, B.; Ju, J.; Kobayashi, R.; Kutteh, R.; Lin, Z.; Littlefield, R.; Long, X.; Meng, B.; Nakajima, T.; Niu, S.; Pollack, L.; Rosing, M.; Sandrone, G.; Stave, M.; Taylor, H.; Thomas, G.; van Lenthe, J.; Wong A.; Zhang, Z. "NWChem, A Computational Chemistry Package for Parallel Computers, Version 5.1" (2007), Pacific Northwest National Laboratory, Richland, Washington 99352-0999, USA.

Table S1. RMP2 and RCCSD(T) reaction and activation energies as a function of basis set size (aug-cc-pVnZ, n = D, T, Q, 5) (kcal/mol)

Reaction[a]	RMP2/aug-cc-pVnZ					RCCSD(T)/aug-cc-pVnZ		
	D	T	Q	5	CBS	D	T	CBS[b]
$2NO_2 = N_2O_4$	-22.17	-24.92	-25.37	-25.35	-25.35	-13.28	-15.36	-15.79
$NO_2 + NO = N_2O_3$	-14.62	-16.66	-17.07	-17.12	-17.12	-9.03	-10.26	-10.71
$NO_2^- + NO_2 = NO_3^- + NO$	-13.08	-13.01	-13.14	-13.09	-13.09	-16.42	-16.50	-16.58
$NO_2^- + 1/2N_2O_4 = NO_3^- + NO$	-2.00	-0.55	-0.45	-0.42	-0.42	-9.78	-8.82	-8.68
$N_2O_4 = NO^+ + NO_3^-$	165.8	168.1	168.1	167.9	167.9	157.7	160.3	160.1
$N_2O_4 = NO_2^+ + NO_2^-$	182.8	183.6	184.1	183.9	183.9	182.0	183.1	183.4
$N_2O_3 = NO^+ + NO_2^-$	171.3	172.8	172.9	172.8	172.8	169.9	171.6	171.6
$2NO + O_2 = 2NO_2$	-34.04	-38.55	-40.28	-40.65	-40.71[c]	-21.74	-25.92	-28.08
$2NO_2 + 1/2O_2 = N_2O_5$	-16.77	-20.94	-21.75	-21.86	-21.86	-12.34	-15.48	-16.40
$2AN = (AN)_2$	-7.30	-7.13	-7.00	-6.94	-6.94	-6.76		-6.40
$NO^+ + (AN)_2 = NO^+(AN)_2$	-42.99	-43.45	-43.19	-43.16	-43.16	-43.31		-43.48
$NO_2^+ + (AN)_2 = NO_2^+(AN)_2$	-41.44	-42.21	-41.96	-42.06	-42.06	-42.16		-42.79
$NO_2^- + (AN)_2 = NO_2^-(AN)_2$	-22.28	-21.70	-21.48	-21.41	-21.41	-23.12		-22.25
$NO_3^- + (AN)_2 = NO_3^-(AN)_2$	-21.19	-20.56	-20.29	-20.32	-20.32	-22.11		-21.24
$2NO_2 =$ TS1	8.19	7.38	7.46	7.51	7.51	13.63	14.42	14.55
$2NO_2 =$ *trans*-ONO-NO_2	-5.25	-6.84	-6.85	-6.85	-6.85	-7.45	-8.08	-8.09
$2NO_2 = C_{2v}$-N_2O_4	-12.02	-12.34	-12.33	-12.31	-12.31	-0.51	0.80	0.83
C_{2v}-N_2O_4 = TS2	4.56	4.25	4.25	4.24	4.24	0.48	0.04	0.03
C_{2v}-N_2O_4 = *cis*-ONO-NO_2	7.90	6.82	6.81	6.78	6.78	-4.96	-6.72	-6.76
cis-ONO-NO_2 = TS3	1.71	1.90	1.81	1.80	1.80	2.05	2.22	2.11
cis-ONO-NO_2 = *trans*-ONO-NO_2	-1.13	-1.33	-1.33	-1.32	-1.32	-1.97	-2.16	-2.16
trans-ONO-$NO_2 = NO_3^- + NO^+$	148.8	149.5	149.5	149.4	149.4	151.9	153.0	152.4

[a]The notations for different NO_2 dimers and transition states for interconversion among them are defined in Figure 4. AN stands for acetonitrile (CH_3CN).

[b]Estimated by combining RMP2/CBS energies with RCCSD(T) corrections (Eq 2 and 3).

[c]When the difference in the reaction/activation energies changed by more than 0.25 kcal/mol upon extension of the basis set, we used an extrapolation scheme based on a polynomial function of inverse powers of 4 and 5 to estimate the MP2 CBS limit[S1,S2] reaction/activation energies $\Delta E = \Delta E_{CBS} + B/(l_{max}+1)^4 + C/(l_{max}+1)^5$, where l_{max} is the value of the highest angular momentum function in the basis set and ΔE_{CBS}, B, and C are the fitting parameters.

Table S2. The performance of several DFT methods in reproducing the experimental redox potentials of oxygenated nitrogen compounds in acetonitrile (vs Li^+/Li, V)[a]

method	$NO_2 + e \rightleftharpoons NO_2^-$	$NO^+ + e \rightleftharpoons NO$	$NO_2^+ + e \rightleftharpoons NO_2$	$NO_3 + e \rightleftharpoons NO_3^-$	MUE[b]
expt	*3.50*	*4.17*	*4.77*	*4.95*	
B3LYP/6-311+G*	3.45	4.81	5.23	4.95	0.29
B3LYP/aug-cc-pVTZ	3.38	4.73	5.09	4.87	0.27
M06-L/6-311+G*	3.06	4.52	4.75	4.50	0.32
M06-L/aug-cc-pVTZ	2.93	4.27	4.39	4.37	0.41
M06/6-311+G*	**3.44**	**4.56**	**4.86**	**5.09**	**0.17**
M06/aug-cc-pVTZ	**3.25**	**4.35**	**4.54**	**4.90**	**0.18**
M06-2X/6-311+G*	3.53	4.58	5.19	5.35	0.31
M06-2X/aug-cc-pvTZ	3.49	4.50	5.03	5.32	0.24

[a]Redox potentials are calculated using the thermodynamic cycle shown in Figure 3. Zero point energies and thermal corrections are obtained at the B3LYP/6-311+G* level. The results with the lowest MUE are shown in bold.

[b]Mean unsigned error.

Table S3. Parameters employed in the simulation of NO_2^- oxidation under Ar via the mechanism shown in reactions 9−12 (Model 1) and reactions 9, 11, 12, and 14−19 (Model 2)

Parameter	Model 1	Model 2
$C_{NO_2^-}$ (mM)	10	10
Disk area (cm^2)	0.196	0.196
E^o_9 (V); $k_{s,9}$ ($cm\ s^{-1}$)	3.551; 9.50×10^{-3}	3.565; 1.19×10^{-2}
E^o_{12} (V); $k_{s,12}$ ($cm\ s^{-1}$)	4.075; 1.86×10^{-1}	4.051; 2.19×10^{-1}
E^o_{18} (V); $k_{s,18}$ ($cm\ s^{-1}$)		*3.691*;[b] 5.44×10^{-2}
E^o_{19} (V); $k_{s,19}$ ($cm\ s^{-1}$)		*3.659*;[b] 1.84×10^{-4}
K_{10}; $k_{f,10}$ ($M^{-1}\ s^{-1}$)	7.05×10^{-4}; 2.00×10^{8}	
K_{11}; $k_{f,11}$ ($M^{-1}\ s^{-1}$)	*7.02*$\times10^{8}$;[b] 1.18×10^{7}	*1.59*$\times10^{8}$;[b] 2.77×10^{9}
K_{14} (M^{-1}); $k_{f,14}$ ($M^{-1}\ s^{-1}$)		1.42×10^{4}; 5.24×10^{3}
K_{15} (M^{-1}); $k_{f,15}$ ($M^{-1}\ s^{-1}$)		4.12×10^{3}; 1.00×10^{7}
K_{16}; $k_{f,16}$ ($M^{-1}\ s^{-1}$)		8.30×10^{-5}; 2.00×10^{8}
K_{17}; $k_{f,17}$ ($M^{-1}\ s^{-1}$)		1.11×10^{4}; 1.84×10^{4}
D_{NO_2}; $D_{NO_2^-}$ ($cm^2\ s^{-1}$)	2.51×10^{-4}; 6.50×10^{-6}	6.81×10^{-5}; 1.01×10^{-5}
D_{NO^+}; D_{NO} ($cm^2\ s^{-1}$)	2.09×10^{-5}; 6.77×10^{-5}	4.12×10^{-5}; 4.17×10^{-4}
$D_{NO_3^-}$; $D_{N_2O_3}$ ($cm^2\ s^{-1}$)	2.73×10^{-5}	2.12×10^{-5}; 7.40×10^{-4}
$D_{N_2O_4}$; $D_{trans\text{-}ONO\text{-}NO_2}$ ($cm^2\ s^{-1}$)		10^{-5}; 10^{-5}

[a]Subscripts for the redox potentials (E^o), equilibrium constants (K), heterogeneous rate constant (k_s) and homogeneous rate constants (k_f) correspond to the numbering of reactions in the text. Electron-transfer coefficients were set to 0.5. The fitting was performed after subtracting the background current in 0.5 M LiTFSI/AN electrolyte and full IR compensation. [b]Parameters that are not independent, but can be expressed through other parameters are shown in *italic*.

Further computational details

Free energy profile for the reaction between NO_2^- and NO_2. Figure S1 describes two possible reaction pathways through which the direct oxygen transfer from NO_2 to NO_2^- could take place. As expected, a transition state where a close contact between oxygen atoms of two reacting species is avoided has a lower energy. The calculated transition state energy of 35 kcal/mol is far too high to account for the observed reaction rate in acetonitrile at room temperature. Instead, the computed barrier is consistent with the reported[S3,S4] slow rate of reaction (4) during the anodic oxidation of nitrite ion in pure $NaNO_2$ and $NaNO_3$-KNO_3 eutectic melts at T = 520−603 K. From these results, we can conclude that an NO_2 radical is not directly involved in the reaction with NO_2^-.

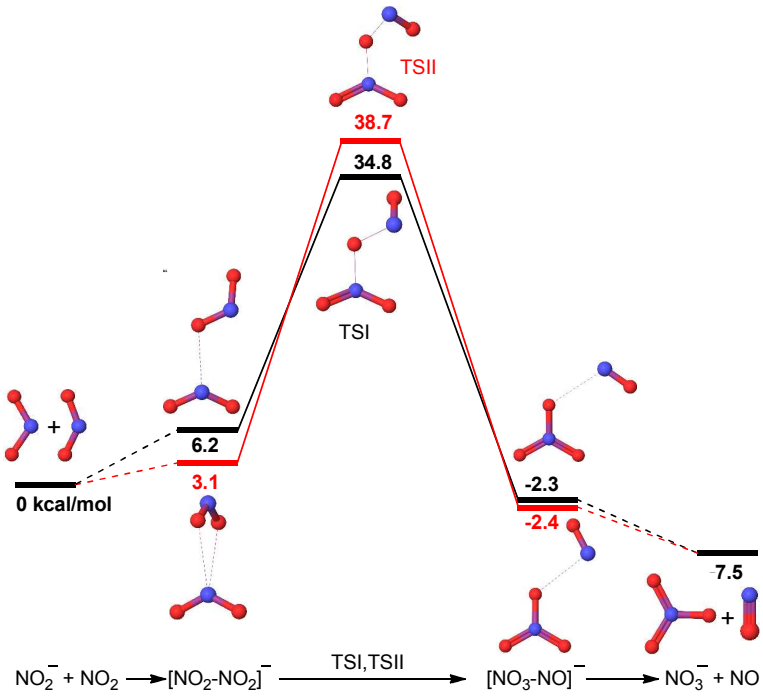

Figure S1. Free energy profile for the reaction of NO_2^- with NO_2 obtained at the B3LYP/6-311+G* level and solvation effects included through the polarizable continuum model

Free energy profile for the reaction between NO_2^- and NO_2. Figure S2 describes the free energy profile for the direct oxygen transfer from the most stable form of NO_2 dimer (a symmetric D_{2h} dimer) to NO_2^-. The activation energy for this reaction is significantly decreased (by 9 kcal/mol), as compared to the reaction that involves NO_2 (Figure S1). However, the calculated reaction barrier is still too high (26 kcal/mol) to support high reaction rates observed in our experiments.

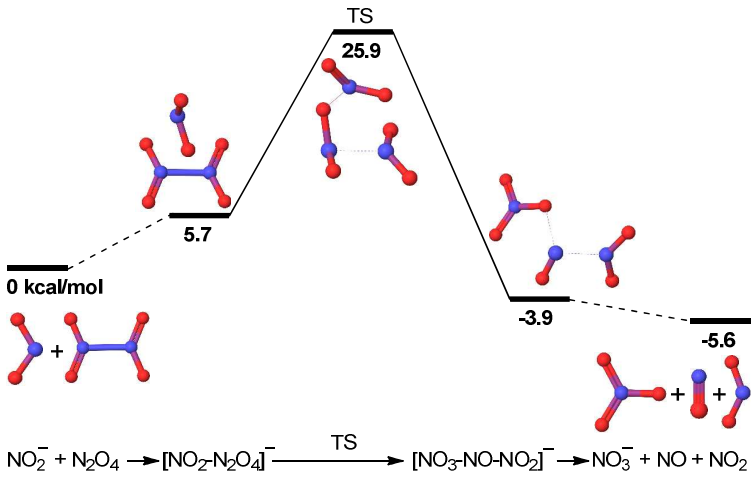

Figure S2. Free energy profile for the reaction of NO_2^- with N_2O_4 obtained at the B3LYP/6-311+G* level and solvation effects included through the polarizable continuum model

Further experimental details

UV-visible analysis of the $LiNO_2$ and N_2O_4/NO_2 reaction product in acetonitrile (AN). The NO_2 gas was first condensed in -78 °C (acetone/dry ice mixture) in a sealed tube, and then acetonitrile (AN) was added to make a solution. A 20 mL of N_2O_4/NO_2 solution (~30 mM based on NO_2) was taken in a sealed flask in a dry box, and then 21 mM of $LiNO_2$ was slowly added into the flask. After stirring of the reaction mixture for 10 min, a portion of solution was taken out and analyzed by UV/visible spectroscopy. The reference spectra for

N_2O_4/NO_2 and $LiNO_3$ in AN were generated by using pure AN as a reference. All UV/Visible data are presented in Figure S3.

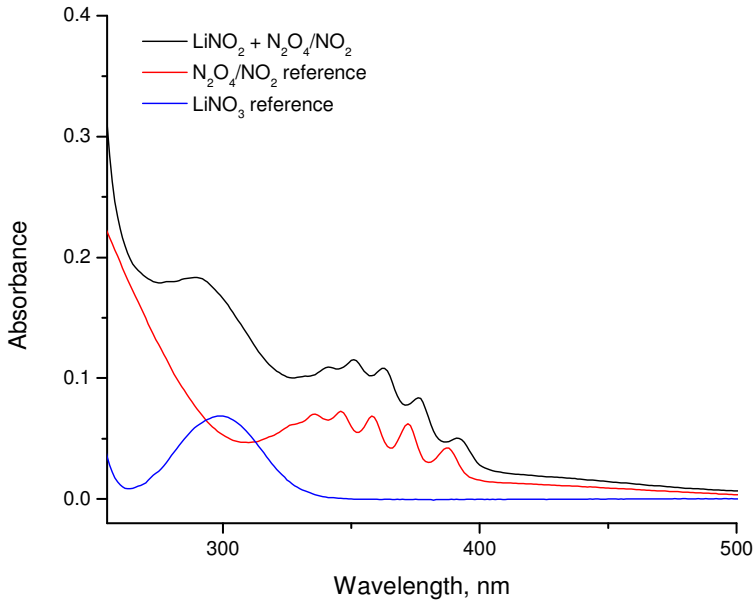

Figure S3. The UV-visible data of the reaction product of $LiNO_2$ + NO_2/N_2O_4 (black) in acetonitrile and reference data for condensed N_2O_4/NO_2 (red) and $LiNO_3$ (blue) in acetonitrile.

Redox Chemistry of $NOBF_4$ in acetonitrile. The cyclic voltammetry of $NOBF_4$ (10 mM) was performed in acetonitrile (AN) using 0.5M LiTFSI as a supporting salt under Ar in a dry glove box. A traditional three electrode electrochemical cell was used as described in the experimental section of the main text. All potentials were measured relative to Li^+/Li scale. The cyclic voltammogram of the $NOBF_4$ on a Pt electrode (surface area = 0.196 cm^2) clearly shows a well-defined quasi-reversible NO^+/NO redox couple at E_{mid} = ½(E_a+E_c) = 4.05 V vs Li^+/Li with different scan rates as shown in Figure S4 and Table S4.

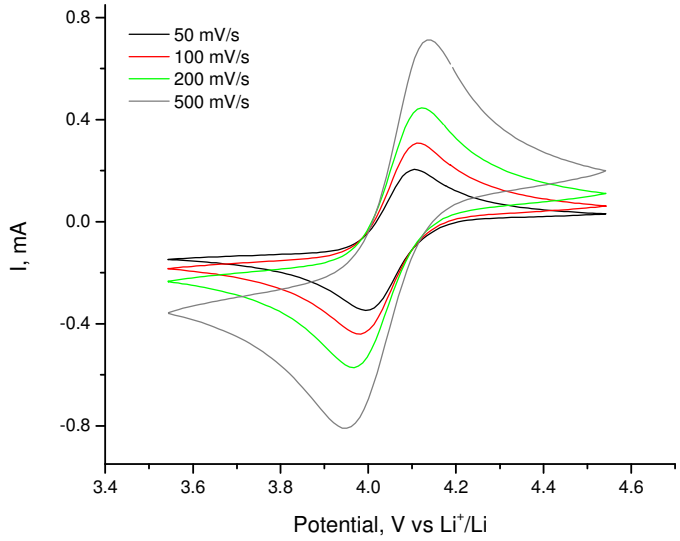

Figure S4. IR corrected cyclic voltammograms for 10 mM $NOBF_4$ in 0.5 LiTFSI/acetonitrile under Ar on Pt macroelectrode (surface area = 0.196 cm^2) at different scan rates.

Table S4. The electrochemical parameters for NO^+/NO redox couple in acetonitrile

Scan rate, mV/s	E_c, V	E_a, V	$E_{mid} = ½(E_a+E_c)$, V	ΔE (E_a-E_c), mV
50	3.992	4.106	4.049	114
100	3.981	4.113	4.047	132
200	3.965	4.126	4.046	161
500	3.945	4.147	4.046	202

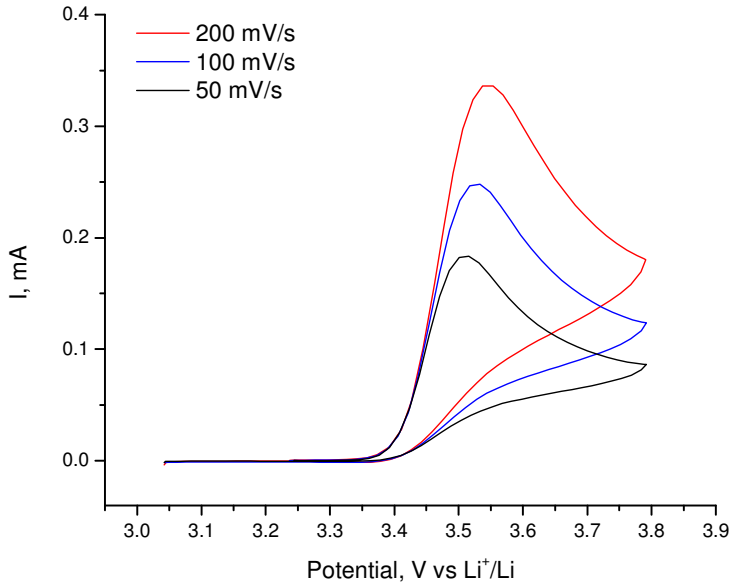

Figure S5. IR corrected cyclic voltammograms for the oxidation of 10 mM $LiNO_2$ under Ar in 0.5M LiTFSI/acetonitrile electrolyte on a Pt macroelectrode (surface area = 0.196 cm^2) at different scan rates when the potential scan is reversed after the first oxidation wave.

Electrochemistry of $NOBF_4$ in acetonitrile in presence of $LiNO_3$. To probe the mechanism of $LiNO_2$ electrochemistry in acetonitrile under Ar, and to confirm the NO^+/NO redox peak splitting in the presence of NO_3^-, a series of experiments with NO^+ (10 mM) on a Pt electrode was performed with incremental addition of $LiNO_3$ (1.0 to 6.0 mM) into the electrolyte. The electrolyte was stirred under Ar for 10 min after each addition of $LiNO_3$, and then CV data were recorded. The results are presented in Figure S6. The NO^+/NO reversible redox peak at 4.05V vs Li^+/Li was splitted to two peaks after adding 3.0 mM or higher of $LiNO_3$ into the electrolyte under Ar. The explanation for NO/NO^+ peak splitting in the presence of NO_3^- in acetonitrile under Ar was described in the main text.

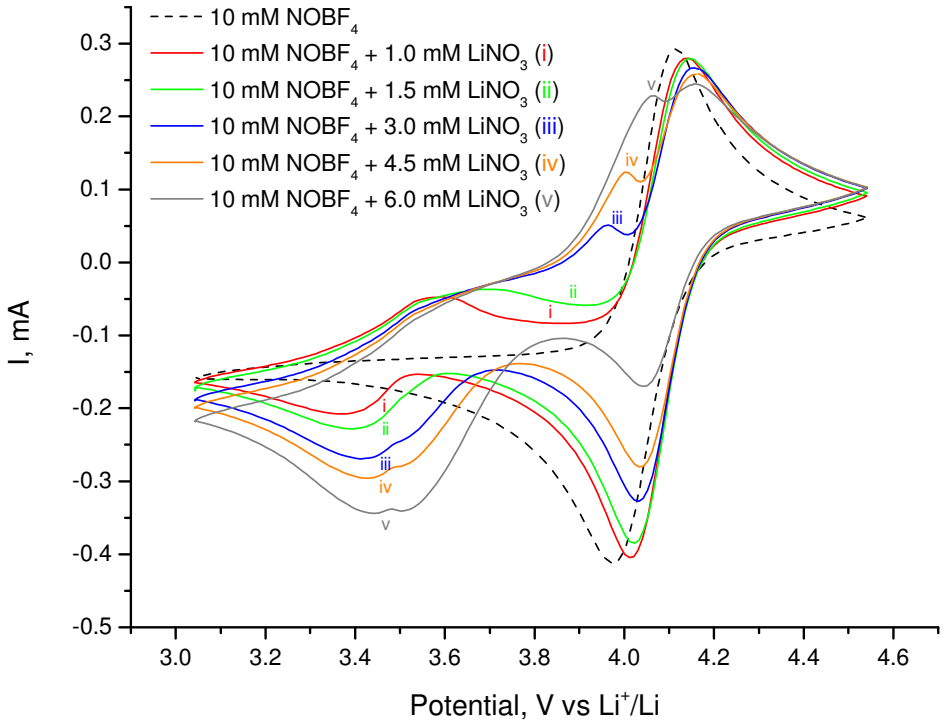

Figure S6. IR-corrected steady-state cyclic voltammograms for the oxidation of 10 mM $NOBF_4$ in 0.5 M LiTFSI/AN electrolyte under argon (dotted curve) and in the presence of 1.0 mM to 6.0 mM $LiNO_3$ (solid curves i–v) on a Pt macroelectrode (surface area = 0.196 cm^2) at a scan rate of 100 mV/s.

References:

S1. Klopper, W. J. Chem. Phys. 1995, 102, 6168-1-12.

S2. Xantheas, S. S. J. Chem. Phys. 1996, 104, 8821–8824.

S3. Martins, M. E.; Calandra, A. J. Arvía, A. J. *Electrochim. Acta* **1970**, *15*, 111–126.

S4. Calandra, A. J.; Arvía, A. J. *Electrochim. Acta* **1967**, *12*, 95–99.

NO_2 ($^2A_1$, C_{2v} symmetry) B3LYP/6-311+G* Total energy: -205.140695863041

N	0.3926398349	1.1964061547	0.0000000000
O	-0.3391172869	2.1390418223	0.0000000000
O	1.5781515207	1.0602075980	0.0000000000

NO ($^2\Pi$, $C_{\infty v}$ symmetry)B3LYP/6-311+G* Total energy: -129.931655243532

N	-4.1268277183	1.7365556252	0.0000000000
O	-2.9803387508	1.7960513018	0.0000000000

O_2 ($^3\Sigma_g^-$, $D_{\infty h}$ symmetry)B3LYP/6-311+G* Total energy: -150.370414977926

O	-4.3854195390	1.7231080916	0.0000000000
O	-3.1812804610	1.7856919084	0.0000000000

N_2O_3 ($^1A'$, C_s symmetry) B3LYP/6-311+G* Total energy: -335.086823283403

N	0.0000437915	-0.0121398905	0.8847795625
O	0.0000604571	1.0971109119	1.3463557497
O	-0.0002011656	-1.0904088208	1.4129039161
N	0.0002589458	0.0050499492	-0.9950911232
O	-0.0002891224	1.0957815152	-1.3015634855

N_2O_5 (^1A, C_2 symmetry) B3LYP/6-311+G* Total energy: -485.481439851617

N	2.3610821964	-3.5949026898	1.5101536857
O	1.9216704140	-2.5066601395	1.3243059600
O	2.8746976234	-3.8819541079	2.9049752161
N	3.4744385359	-2.6938715588	3.6247492704
O	4.0110345415	-1.8807364078	2.9442891612
O	3.3487565898	-2.8232006573	4.7977113383
O	2.4366674545	-4.5711083717	0.8397117591

NO^+ ($^1\Sigma^+$, $C_{\infty v}$ symmetry) B3LYP/6-311+G* Total energy: -129.572616830426

N	-4.0798719241	1.7389915468	0.0000000000
O	-3.0214471580	1.7939187245	0.0000000000

NO_2^- ($^1A_1$, C_{2v} symmetry) B3LYP/6-311+G* Total energy: -205.224985601710

N	0.3255136884	1.0770731624	0.0000000000
O	-0.2845728792	2.1770384780	0.0000000000
O	1.5823740661	1.1266834425	0.0000000000

NO_2^+ ($^1A_1$, C_{2v} symmetry) B3LYP/6-311+G* Total energy: -204.775736828781

N	0.5503632957	1.4767899319	0.0000109824
O	-0.4234526987	2.0252620132	-0.0000047963
O	1.5244047141	0.9285197147	-0.0000048185

NO_3^- ($^1A_1'$, D_{3h}) B3LYP/6-311+G* Total energy: -280.457548415786

N	-1.6674448934	0.1609058579	0.6672114847
O	-1.7259601756	0.8895343268	-0.3589935274
O	-0.7405138173	-0.6841071241	0.7877993179
O	-2.5358382929	0.2773441635	1.5726856951

N_2O_4 (^1A_g, D_{2h} symmetry) B3LYP/6-311+G* Total energy: -410.302858567872

N	0.0000000005	-0.0000000035	0.9043701806

O	-0.0000000074	1.0961720989	1.3610433707
O	0.0000000067	-1.0961720967	1.3610433903
N	0.0000000031	-0.0000000028	-0.9043701871
O	0.0000000058	1.0961721042	-1.3610433688
O	-0.0000000082	-1.0961721009	-1.3610433864

C_{2v}-N_2O_4 ($^1A_1$, open shell singlet, C_{2v} symmetry) B3LYP/6-311+G*
Total energy: -410.283277466757

N	0.3489864056	1.3240465766	-0.0350406281
O	-0.1969951452	2.3835603683	-0.0275018466
O	1.4872411870	0.9719841826	-0.0009820494
N	-1.6105807019	-1.0097793300	-0.1275538079
O	-1.2746067191	-0.6308048670	-1.2085623705
O	-1.3336641905	-0.6599497339	0.9797285662

trans-ONO-NO_2 (^1A, C_1 symmetry)B3LY/6-311+G* Total energy: -410.284041838678

N	1.9638294359	-2.8025609436	2.6330872256
O	3.2223139402	-1.7561949163	2.7205361945
O	1.9656415447	-3.2510817916	1.5958361071
N	3.3602465311	-1.2045874052	4.0231907671
O	4.0125446413	-0.1976925258	4.0334530274
O	2.8407478713	-1.8000017182	4.9325329612

cis-ONO-NO_2 (^1A, C_2 symmetry) B3LYP/6-311+G* Total energy: -410.280370352480

N	2.2654344315	-3.6269573317	1.3437717393
O	2.0865396392	-2.5628363000	1.0436289489
O	2.9955818126	-3.8654163747	2.8773565442
N	3.4207133657	-2.7372008366	3.5828811996
O	3.7817474413	-1.7857079957	2.9213599324
O	3.3865136813	-2.8562016094	4.7785450737

TS1 ($^1A'$, open shell singlet, C_s symmetry) B3LYP/6-311+G*
Total energy: -410.259350977313

N	2.4053755965	-4.4912652304	2.9674660181
O	3.3067497065	-3.7947486905	2.4419508326
N	3.4831474387	-2.2582936267	3.7150254934
O	4.3123291379	-1.5223417651	3.3302488348
O	2.7269751580	-2.3834327085	4.6015733196
O	2.0147802187	-5.5189682972	2.4814885874

TS2 ($^1A'$, open shell singlet, C_s symmetry) B3LYP/6-311+G*
Total energy: -410.277685167077

N	-0.0407898786	0.8697365986	0.5116009662
O	-0.6011476024	1.9070775369	0.5067656213
O	1.0776167195	0.4973678898	0.5339653050
N	-1.6747729043	-1.0844991916	-0.1479800374
O	-1.2780969295	-0.6325550764	-1.1861051030
O	-1.3247824356	-0.6496092066	0.9475950329

TS3 (^1A, open shell singlet, C_1 symmetry) B3LYP/6-311+G*
Total energy: -410.276555761936

N	-0.7058314081	-1.2794047265	-0.8904218604
O	0.4315870620	0.0969367467	-0.8282492433
O	-1.7480904907	-0.9520382569	-0.6720020983
N	0.6174413615	0.5599614332	0.4518693610
O	1.3622771853	1.5021625383	0.5375869892
O	0.0300050770	-0.0191358276	1.3503441437

AN ($^1A_1$, C_{3v} symmetry) B3LYP/6-311++G** Total energy: -132.796196988129

H	-1.1540041695	-1.4075780042	-2.7782810885
H	-0.2014266488	0.0593576537	-2.4760903720
C	-1.0880632750	-0.5011750920	-2.1731550492
H	-0.9818267230	-0.7861752387	-1.1245460557
N	-3.2282924062	0.9554596682	-2.4976699292
C	-2.2828030042	0.3119662661	-2.3543109413

$(AN)_2$ (^1A_g, C_{2h} symmetry) B3LYP/6-311++G** Total energy: -265.599007067309

C	-1.7332114584	-3.7336579045	0.9748179751
H	-2.3546922968	-4.4684331599	1.4903520681
H	-2.3480145683	-3.1990473976	0.2478235942
H	-0.9243621667	-4.2497483459	0.4526900057
N	-0.6934157223	-2.0628995014	2.6874915912
C	-1.1633585128	-2.7983136342	1.9335734706
C	2.7342572346	-2.5694348285	2.2063046315
H	3.3506786965	-3.1033794026	2.9321462798
H	3.3541424816	-1.8339662596	1.6895393434
H	1.9255785059	-2.0545252261	2.7298308365
N	1.6914523224	-4.2402143311	0.4955891736
C	2.1631478128	-3.5050404372	1.2484758700

$NO^+(AN)_2$ (^1A, C_1 symmetry) B3LYP/6-311++G** Total energy: -395.255096306382

N	0.9652076409	-0.2105910780	-0.2582446810
O	0.7300977712	-1.1515084405	-0.7310079924
C	0.7430801338	-0.4478682578	4.6105307635
H	1.7548013917	-0.2478651710	4.9696566274
H	0.0726406396	0.3335373636	4.9741705221
H	0.4105294130	-1.4135604716	4.9968888879
N	0.7205357898	-0.5008473598	2.0085066563
C	0.7326765364	-0.4696980109	3.1596859748
C	-2.2243480112	3.3127007164	-1.3538616402
H	-2.2342355934	4.0044971577	-0.5090520945
H	-1.8545672770	3.8340344999	-2.2393043088
H	-3.2413560054	2.9630785502	-1.5432435642
N	-0.6902403657	1.2775896133	-0.8260657131
C	-1.3642982022	2.1828968739	-1.0549574251

$NO_2^+(AN)_2$ (^1A, C_1 symmetry) B3LYP/6-311++G** Total energy: -470.445010919090

N	0.3800548969	0.4689334022	0.0628978730
O	-0.6822135718	0.2066768944	0.2750473832
O	1.4425690504	0.7312197968	-0.1492368096
C	1.5469148381	-0.1962349633	5.0681648965
H	1.9636224113	-1.1936725949	5.2223625551

H	2.2812427499	0.5491711816	5.3804518134
H	0.6473562972	-0.0877730575	5.6776240952
N	0.9594107283	0.1381230922	2.5530390875
C	1.2191991028	-0.0097363231	3.6654229538
C	-0.7756772358	1.1266738347	-4.9447176909
H	-1.5239118954	1.9146668771	-5.0512651216
H	0.1221937217	1.4100815587	-5.4976633099
H	-1.1724121911	0.1982090374	-5.3604174478
N	-0.1969967410	0.7957438282	-2.4276234317
C	-0.4532695630	0.9421573278	-3.5411007915

$NO_2^-(AN)_2$ ($^1A'$, C_s symmetry) B3LYP/6-311++G**
Total energy: -470.859983699822

N	-0.6750042682	0.9258434890	-0.4680212378
O	-0.3210311000	1.9849303789	0.1238215564
O	-0.7840765560	0.9942774621	-1.7129190350
C	-0.5014551519	0.4481131259	2.8067603408
H	0.1408787957	-0.4052856104	2.5787644757
H	-1.5413436158	0.1163594693	2.7677239118
H	-0.3562297156	1.2017343739	2.0145039713
N	0.0497261850	1.3664312087	5.1859309738
C	-0.1933032451	0.9636542515	4.1305957928
C	0.1553434216	3.9554206898	-2.5083873576
H	-0.2042903256	2.9164736262	-2.4647901889
H	1.1350523960	3.9820565644	-2.0272290988
H	-0.5317931273	4.5643162223	-1.9175221169
N	0.3181788873	4.8798609175	-4.9438538804
C	0.2454577852	4.4690545267	-3.8661496352

$NO_3^-(AN)_2$ ($^1A'$, C_s symmetry) B3LYP/6-311++G** Total energy: -546.089277771172

N	-0.2019422509	-0.6355057081	0.4369935034
O	-0.9652364270	-0.1399549962	1.3039931032
O	-0.3033042637	-0.2638161129	-0.7705822285
C	2.0183938677	-2.0723877155	-2.0532965597
H	1.6760005497	-3.0508267386	-1.7115973213
H	2.8464937213	-1.7605970356	-1.4142405206
H	1.1970150504	-1.3626517922	-1.9000972981
N	2.7941245544	-2.2021918396	-4.5421643452
C	2.4476790548	-2.1416960206	-3.4417632695
C	-2.6817704173	1.8681946267	-0.5225313055
H	-3.0555935620	1.1566773481	-1.2610460797
H	-1.8623149615	2.4290455513	-0.9757099746
H	-2.2670190848	1.2922986097	0.3129044441
N	-4.5883734603	3.4905933617	0.2162574920
C	-3.7442137942	2.7711750880	-0.1067521064
O	0.6550322351	-1.4910225448	0.7574622355

$(AN)_8$ (^1A, D_2 symmetry) B3LYP/6-31G** Total energy: -1062.13403697206

C	-3.2314020172	-0.1260702745	0.4304202486
H	-2.9582905781	-0.9738402229	-0.2042701252
H	-3.1398508887	-0.4194842029	1.4793736915

H	-4.2561151812	0.1755324658	0.2000297413
N	-1.5893434616	1.8537261221	-0.0694210859
C	-2.3215098939	0.9797096951	0.1548299670
C	0.8467757667	-2.2175674097	5.5546309813
H	-0.1010301885	-2.0031519854	5.0527324150
H	1.2516728565	-3.1560034797	5.1650812424
H	0.6790777631	-2.3090501568	6.6310820184
N	2.5371460288	-0.2829956663	5.0387438054
C	1.7887431167	-1.1383246430	5.2781320352
C	-3.1281084811	3.2713532710	-2.8676250643
H	-2.5658712925	2.9418264280	-3.7460374255
H	-3.6194588494	4.2240166774	-3.0827515801
H	-2.4376380226	3.3954876179	-2.0286197285
N	-4.8909704265	1.4335271516	-2.2503419901
C	-4.1178932332	2.2556860310	-2.5250763463
C	4.5754881845	-1.8962073125	2.6791600574
H	4.3275707765	-1.5124776860	1.6854974951
H	4.4463510410	-1.0951313985	3.4125360476
H	5.6127468220	-2.2414650167	2.6911422180
N	2.9347988094	-3.8532949946	3.2658450672
C	3.6710205847	-2.9931758147	3.0065094804
C	0.9358439807	1.2185881672	2.2927274013
H	0.4311827495	2.0894500394	1.8670566259
H	1.5156805124	1.5001537103	3.1753214380
H	1.6100801680	0.7948147732	1.5431405831
N	-0.8375562507	-0.5957050422	2.9481352002
C	-0.0534195009	0.2121932562	2.6604527501
C	0.4890380051	0.1508316661	-2.4338410549
H	0.2029311660	1.0103237486	-1.8210846715
H	1.5111776330	-0.1423671486	-2.1816833468
H	0.4141576185	0.4245713166	-3.4892805991
N	-1.1484974916	-1.8289997760	-1.9192207006
C	-0.4197688188	-0.9540938306	-2.1511167895
C	-3.7116310709	-1.2096336281	-4.2249794480
H	-3.2133014211	-1.9344744162	-3.5751099542
H	-4.5353703999	-0.7457796592	-3.6749679890
H	-4.1017461175	-1.7181848343	-5.1106674991
N	-1.9913337862	0.6481731494	-4.8999178229
C	-2.7551175642	-0.1780077762	-4.6116475539
C	0.4024116018	-3.2602014171	0.8926916980
H	-0.2986522044	-2.8206326377	1.6077716830
H	-0.1496201614	-3.5924094440	0.0099313378
H	0.9156557437	-4.1003789580	1.3672339314
N	2.1525174426	-1.4367717392	0.2012623585
C	1.3785925788	-2.2486184452	0.5048736016

$NO^{+}(AN)_8$ (^1A, C_1 symmetry) B3LYP/6-31G** Total energy: -1191.78460647794

N	0.0379058935	0.2776493755	0.5422309829
O	0.5274059472	-0.4507369274	-0.1022299816
C	1.1664374002	-1.1955128834	4.4672691414
H	1.5278115681	-0.7993525419	5.4199238230

H	0.0959974277	-1.4047620214	4.5405130110
H	1.6922980292	-2.1217580515	4.2231997883
N	1.5598697136	0.5362693002	2.5456139696
C	1.3844301232	-0.2302266477	3.4010799421
C	-0.1457227338	-4.6064475020	0.8791151585
H	0.2315519342	-5.5764105714	0.5440691353
H	-0.8565138566	-4.7656474065	1.6943384152
H	-0.6504350051	-4.1019849431	0.0500839225
N	1.8334400493	-3.0999661959	1.6979875833
C	0.9577173807	-3.7720214262	1.3383660613
C	-1.9339833647	3.0704582110	-2.1361750337
H	-1.1902909721	3.7480464882	-1.7086210161
H	-1.6024075932	2.7604463026	-3.1304278460
H	-2.8991318439	3.5795463037	-2.2032232002
N	-2.1194976330	0.9563402887	-0.6054882432
C	-2.0388461095	1.8966791860	-1.2837064150
C	2.6896505768	1.2780973837	-3.8002571406
H	3.0780535255	0.9404263599	-2.8344651149
H	3.1535028076	0.6961137621	-4.6014295630
H	2.9398921875	2.3328051344	-3.9440533774
N	0.0907457596	0.9578391788	-3.8468644134
C	1.2423628919	1.1018384766	-3.8302534273
C	-3.9939632002	-0.8504713491	1.6195931671
H	-4.4893905552	-0.3769841754	2.4713427462
H	-4.0972176385	-0.2122520917	0.7378154041
H	-4.4640976237	-1.8180857591	1.4252105096
N	-1.4393999229	-1.1555979548	2.1013244575
C	-2.5749717477	-1.0239892231	1.8935539981
C	-1.9602293955	-1.7605151878	-3.8923872590
H	-3.0505368948	-1.6906007635	-3.8514674444
H	-1.5445730936	-0.8074667398	-4.2326905155
H	-1.6831238594	-2.5496614349	-4.5966858996
N	-0.9955740799	-2.2874894972	-1.5157761266
C	-1.4268533533	-2.0599906267	-2.5693425531
C	4.8057080025	-1.8598106163	0.6320828132
H	5.5271919208	-1.3687881976	1.2906895968
H	4.1334028950	-2.4862970567	1.2256346274
H	5.3486564718	-2.4835949189	-0.0831865543
N	3.3676297861	-0.0736885821	-0.6331426470
C	4.0120135692	-0.8626014895	-0.0753825163
C	3.1177141092	3.1548335204	1.0034079946
H	3.0814553792	2.7189615155	2.0051944952
H	3.9687665519	2.7331793323	0.4629653937
H	3.2298475413	4.2397006479	1.0773621770
N	0.9027693014	2.5382185364	-0.2460344792
C	1.8853812583	2.8170310087	0.3082041040

$NO_2^+(AN)_8$ (^1A, C_2 symmetry) B3LYP/6-31G** Total energy: -1266.94858342307

N	-0.1718681118	0.2995255555	-0.4425043586
O	-1.2950996687	0.2454842084	-0.4611366954
O	0.9522730436	0.3200299672	-0.4348512394

C	-5.6740795217	1.2434814757	-0.6988701810
H	-6.7163906415	0.9267072552	-0.7919725190
H	-5.4153490864	1.3226457855	0.3609575146
H	-5.5589478372	2.2209625801	-1.1748862507
N	-4.0845172860	-0.5112258307	-1.8196222469
C	-4.7942696674	0.2683844490	-1.3335263176
C	-1.8384902901	2.0603440709	3.9579819677
H	-2.8352630803	1.6387408474	3.7999444527
H	-1.4204233129	1.6680621626	4.8888664259
H	-1.9088574569	3.1488041920	4.0321004433
N	-0.3433836091	1.3778670360	1.9223977739
C	-0.9956546964	1.6859971854	2.8300158748
C	-2.1952025442	-1.8730901057	-4.3331578815
H	-3.1384976210	-1.6651363856	-3.8192456182
H	-2.1889876223	-1.3698275406	-5.3037493133
H	-2.0915810654	-2.9500568973	-4.4903240700
N	-0.2539406648	-0.9759243362	-2.8249504667
C	-1.1048468991	-1.3782896437	-3.5038149299
C	-3.4881960392	-2.4802499573	1.2364148640
H	-2.4199047091	-2.7073583938	1.1753382826
H	-3.9724227870	-3.1790661829	1.9236201975
H	-3.9275937397	-2.5877834999	0.2409668694
N	-3.8082568157	-0.0100093729	2.0482190093
C	-3.6688921224	-1.1083950526	1.6982937441
C	5.2609547170	1.2729043794	0.4522875123
H	6.3243412326	1.0367871265	0.3582358875
H	4.9722180257	1.9582093735	-0.3497702931
H	5.0909103930	1.7534348457	1.4194596215
N	3.8219453909	-0.9068168480	0.2498185894
C	4.4651154067	0.0546692494	0.3493956073
C	1.2695134251	4.4685646265	-2.8506291205
H	1.2617669659	5.3829695480	-2.2515081593
H	2.2968272444	4.1084339526	-2.9562588594
H	0.8574380661	4.6890487148	-3.8389580805
N	-0.1247736043	2.5936533876	-1.6741148596
C	0.4823447716	3.4316878536	-2.1967054507
C	2.0894396173	-3.6369871107	1.3891221662
H	2.0629483702	-4.5945081628	0.8621256425
H	3.0016224553	-3.0950859456	1.1225121741
H	2.0763318088	-3.8231491047	2.4663935188
N	0.0519858217	-2.1497976988	0.6918748913
C	0.9458480344	-2.8197976758	1.0062894337
C	3.2893272053	-0.6632750548	-3.3821807419
H	3.8051108152	-0.7731608079	-4.3397584620
H	3.7554240029	-1.3192288117	-2.6419355821
H	2.2401860468	-0.9513556118	-3.4959288602
N	3.4267209115	1.8121367270	-2.5347520190
C	3.3681976276	0.7183249867	-2.9202312018

$NO_2^-(AN)_8$ (^1A, C_1 symmetry) B3LYP/6-31G** Total energy: -1267.34384306372

N	-0.3646982524	0.2383980620	0.2291877844

O	-0.3660081352	1.0479348930	-0.7409518827
O	-1.3561860497	-0.5411402935	0.2861188629
C	-3.1871632383	2.3994376006	-1.4626931659
H	-2.2892505236	1.8281326608	-1.1843241557
H	-2.8798365727	3.3767142930	-1.8460407603
H	-3.8068658356	2.5518411815	-0.5742273938
N	-4.5302893557	1.0778776347	-3.2838504981
C	-3.9416386864	1.6749298428	-2.4790102093
C	-2.1793120782	-0.2600052838	3.4381396318
H	-1.8731881960	-0.5470522687	2.4238183477
H	-2.0315650238	-1.1062394364	4.1154127904
H	-3.2428399648	-0.0050437645	3.4231469628
N	-0.7232088278	1.7734944551	4.2211190369
C	-1.3782010791	0.8759233191	3.8810254109
C	2.7918047240	0.7462437292	-1.6062359340
H	1.7404961795	0.9831219109	-1.3982980989
H	3.1041062160	1.2461431577	-2.5279870486
H	2.8772459623	-0.3369463745	-1.7386344440
N	4.2617982929	1.5545727444	0.4071247477
C	3.6207052364	1.1938360717	-0.4927886569
C	0.3224725607	-3.4082614773	0.1389080027
H	0.9196580523	-3.7006972478	1.0074225304
H	-0.3179901284	-2.5617860864	0.4123900548
H	-0.3127685224	-4.2386834284	-0.1807504348
N	1.8842347700	-2.6728879543	-1.8333667254
C	1.1961772664	-3.0059642524	-0.9581887879
C	-1.4601145858	-1.3269168155	-3.0438806100
H	-1.3019601491	-0.6755974607	-2.1765775209
H	-0.4965591433	-1.5027873394	-3.5298830566
H	-2.1419472124	-0.8291278019	-3.7394215203
N	-2.4886682807	-3.6026751058	-2.2489084426
C	-2.0323670327	-2.5962998085	-2.6084584179
C	0.8616561434	3.5041666760	1.2837328280
H	0.4282148513	3.2509304879	2.2566772283
H	0.4463757849	2.8253022299	0.5299243946
H	1.9441731087	3.3488259946	1.3272170905
N	0.3299450023	5.9947139079	0.6625342720
C	0.5670704394	4.8920444342	0.9409491062
C	2.0698073573	-0.2145876246	2.7033914627
H	1.7305548867	0.3330914471	3.5872079756
H	3.0438641069	0.1709442551	2.3889371095
H	1.3475197836	-0.0420358195	1.8945629148
N	2.2063289993	-2.7827483253	3.2077117586
C	2.1539287266	-1.6418225941	2.9929888682
C	-4.4888891777	-1.2992706028	-0.2187088600
H	-3.4658410903	-0.9039937755	-0.2193119333
H	-4.4376996058	-2.3722960565	-0.4225135782
H	-5.0599540540	-0.8157427044	-1.0164972966
N	-5.5802171617	-0.8376114813	2.1189730402
C	-5.1083463006	-1.0487720964	1.0781652944

$NO_3^-(AN)_8$ (^1A, C_1 symmetry) B3LYP/6-31G** Total energy: -1342.54429897864

N	-0.5057339025	0.5985002812	-0.2263358908
O	-0.3443519523	1.5461279369	-1.0462012701
O	0.3726347106	0.3328706627	0.6236021151
O	-1.5693613667	-0.0932691271	-0.2755936371
C	-3.3073871682	2.4792832413	-1.9529598634
H	-2.3280363396	2.0802803763	-1.6577937100
H	-3.1625368856	3.3744480542	-2.5647659050
H	-3.8610968331	2.7582080427	-1.0517507350
N	-4.6388359024	0.6697425936	-3.3017874559
C	-4.0540022643	1.4766951683	-2.7041845386
C	-1.8033316602	-0.4727340807	3.1312962184
H	-1.7132807227	-0.3971026020	2.0426159389
H	-1.3245631845	-1.4019219242	3.4535900219
H	-2.8610902359	-0.4947690210	3.4084182856
N	-0.5775604069	1.5607284649	4.2404378861
C	-1.1273961518	0.6608479856	3.7524875231
C	2.8766639833	0.8141337556	-1.5427256390
H	1.8582724241	1.2022783334	-1.4309360887
H	3.3322156270	1.2301583402	-2.4463537839
H	2.8207033795	-0.2746052271	-1.6396346677
N	4.2937833099	1.4807250683	0.5584700176
C	3.6696010371	1.1806151217	-0.3747611214
C	0.1221940712	-3.0240982590	0.1220672373
H	0.6472512435	-3.2332742124	1.0584558115
H	-0.4756438048	-2.1162181345	0.2512097338
H	-0.5399461105	-3.8570750002	-0.1297150542
N	1.8206200068	-2.6211317665	-1.8329000933
C	1.0757483557	-2.8078989149	-0.9605620953
C	-1.7385501058	-1.5973254181	-3.2021355677
H	-1.6208190129	-0.8822905010	-2.3803948255
H	-0.7591108934	-1.7915549662	-3.6477767433
H	-2.4117823095	-1.1668553797	-3.9480915620
N	-2.7505183346	-3.8154482886	-2.2404455562
C	-2.3014934293	-2.8372751888	-2.6782859222
C	1.0033228555	3.5510464267	1.4123146330
H	0.5174975034	3.1755458274	2.3183765236
H	0.5405468646	3.0721296852	0.5434428030
H	2.0583008187	3.2615135331	1.4355831740
N	0.7836560434	6.1589533537	1.2619899616
C	0.8816821013	5.0033988996	1.3316051440
C	2.4347449084	-0.1056064762	3.1257733860
H	2.0415036481	0.5715748103	3.8886024592
H	3.5264684575	-0.1226660086	3.1708453285
H	2.1292499901	0.2669548240	2.1456141087
N	1.4495250476	-2.5086175761	3.4770685942
C	1.8908947502	-1.4441790155	3.3267068972
C	-4.6305022778	-1.3788872812	-0.1251035054
H	-3.7359356581	-0.7556813826	-0.2129370585
H	-4.3762288034	-2.3895538133	-0.4570589035
H	-5.4047179231	-0.9770290358	-0.7843398821

N	-5.4398230756	-1.3948279868	2.3678840544
C	-5.0895242541	-1.3933696642	1.2601719661

$[NO_2\text{-}NO_2]^-$ (^2A, C_1 symmetry) Reactant_I B3LYP/6-311+G*
Total energy: -410.387282931640

N	0.2473650863	1.3346053633	-0.0913180290
O	0.0318078456	2.4278926986	0.3945109510
O	1.3172257335	0.7640996017	-0.1437841853
N	-1.4207134652	-1.2805721651	-0.0356579135
O	-1.6355753995	-0.1287210254	0.4052524178
O	-2.2737969906	-2.1546583911	0.1999461685

$[NO_3\text{-}NO]^-$ ($^2A''$, C_s symmetry) Product_I B3LYP/6-311+G*
Total energy: -410.395910623203

N	0.3411280192	1.4060387700	0.0041875125
O	-0.4503649113	2.3789251757	0.0246303402
O	1.5792592906	1.5840744250	-0.0379164777
O	-0.1299576523	0.2261774670	0.0265989232
N	1.0988128091	-1.8771937874	0.1096642748
O	0.2132008862	-2.6241484350	0.1609894987

$[NO_2\text{-}NO_2]^-$ (^2A, C_1 symmetry) TSI B3LYP/6-311+G*
Total energy: -410.344287365517

N	0.5888767795	1.2867625079	0.0222764040
O	-0.1328595354	2.1525309781	-0.4615470839
O	1.5592556542	1.4499953713	0.7631609151
N	-1.4032255811	-0.2473213185	-0.3040940354
O	-0.0221193678	-0.1278728484	0.1823697952
O	-1.5372383554	-1.3246803709	-0.8609083132

$[NO_2\text{-}NO_2]^-$ ($^2A_1$, C_{2v} symmetry) Reactant_II B3LYP/6-311+G*
Total energy: -410.393901730093

N	0.3091586501	1.2752334842	-0.0340079899
O	-0.1558910001	2.4036713061	-0.0294278126
O	1.5017677319	1.0177474139	-0.0017476018
N	-1.6662331471	-1.0697985671	-0.1292730003
O	-1.2436512202	-0.5951157856	-1.1877048387
O	-1.3025807893	-0.6258231221	0.9636118863

$[NO_3\text{-}NO]^-$ ($^2A''$, C_s symmetry) Product_II B3LYP/6-311+G*
Total energy: -410.395750579048

N	0.1847691639	1.5086896127	0.0365697885
O	-0.5917373318	2.4927547433	0.0068948780
O	1.4288015648	1.6716278963	0.0130030709
O	-0.2954000994	0.3366176540	0.0910063749
N	1.1120180972	-1.7458382805	0.0174667559
O	2.2385963221	-1.4987222599	-0.0692254162

$[NO_2\text{-}NO_2]^-$ (^2A, C_1 symmetry) TSII B3LYP/6-311+G*
Total energy: -410.337492762418

N	0.5413455499	1.3526656879	0.0352515085

O	-0.1005786178	2.3810973855	-0.2204751962
O	1.6775951455	1.2797389759	0.5356955778
N	-1.0896928864	-0.4554272772	-0.7345779104
O	-1.1450237252	0.2134072943	-1.7333090575
O	-0.2942807226	0.1334836085	0.3651919567

$[NO_2\text{-}N_2O_4]^-$ (^{1}A, C_1 symmetry) Reactant B3LYP/6-311+G*
Total energy: -615.554816719723

N	0.8337287543	1.5543842929	0.1233642699
O	-0.0443211950	1.4339995281	-0.7718712586
O	1.8567447940	2.1958919012	-0.1613793995
N	-1.5295368717	-0.3321698217	0.0193681057
O	-1.0707285620	-0.5674703663	1.0959000648
O	-1.6116869633	-0.9658137864	-0.9938442957
N	-2.4681692615	1.1228081314	-0.0115978632
O	-2.9854874780	1.3427682921	-1.0671530628
O	-2.5109220731	1.6930623645	1.0394965374

$[NO_3\text{-}NO\text{-}NO_2]^-$ (^{1}A, C_1 symmetry) Product B3LYP/6-311+G*
Total energy: -615.573109841403

N	0.6448132154	1.1456805128	0.1656877047
O	0.3856207866	1.7314584113	-0.9058988944
O	1.6392232101	1.4341404733	0.8500102271
N	-2.0495966710	-0.0487549029	-0.5914849261
O	-1.8884285428	0.2331609623	-1.6752414874
O	-0.1367093212	0.2176230779	0.5782824942
N	-1.7950451044	-1.9895892543	-0.5108587897
O	-2.0408499590	-2.6043493897	0.5065524345
O	-1.4723926435	-2.4611584436	-1.5848868608

$[NO_2\text{-}N_2O_4]^-$ (^{1}A, C_1 symmetry) TS B3LYP/6-311++G**
Total energy: -615.527159814307

N	0.6712705488	1.2300927622	-0.1173237716
O	0.1041650831	2.0230661017	-0.8037442857
O	1.8453345395	1.0336756655	0.0470611382
N	-1.3584141824	-0.4229808643	0.1275593522
O	-0.3260841527	0.1850092392	0.7865009269
O	-1.1760460872	-0.7618116410	-1.0137156186
N	-2.8050083052	1.1459970845	0.0835715760
O	-3.4280219331	1.2567443128	-0.9636339833
O	-3.0986142379	1.7351128781	1.1185265104