Supporting Information for:

Theoretical Prediction of Stable Noble-Gas Anions $XeNO_2^-$ and $XeNO_3^-$ with very Short Xenon-Nitrogen Bond Lengths

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SI1: Calculated structure of $XeNO_2^-$ at B3LYP/aug-cc-pVTZ level (in Å).

Xe	-0.18081100	0.05098600	0.00000000
N	0.42451200	1.77300900	0.00000000
O	0.42451200	-0.94777000	1.45820700
O	0.42451200	-0.94777000	-1.45820700

SI2: Calculated structure of $XeNO_2^-$ at MPW1PW91/aug-cc-pVTZ level (in Å).

Xe	-0.18166500	0.05001000	0.00000000
N	0.42651700	1.74877200	0.00000000
O	0.42651700	-0.93387200	1.43128500
O	0.42651700	-0.93387200	-1.43128500

SI3: Calculated structure of $XeNO_2^-$ at MP2/aug-cc-pVDZ level (in Å).

Xe	-0.18240100	0.05925700	0.00000000
N	0.42824600	1.75057200	0.00000000
O	0.42824600	-0.96586700	1.43461600
O	0.42824600	-0.96586700	-1.43461600

SI4: Calculated structure of $XeNO_2^-$ at MP2/aug-cc-pVTZ level (in Å).

Xe	-0.18726900	0.05182100	0.00000000
N	0.43967500	1.71768300	0.00000000
O	0.43967500	-0.92638200	1.40749200
O	0.43967500	-0.92638200	-1.40749200

SI5: Calculated structure of $XeNO_2^-$ at CCSD(T)/aug-cc-pVTZ level (in Å).

Xe	-0.18338000	0.05118700	0.00000000
N	0.43054400	1.76963100	0.00000000
O	0.43054400	-0.94696900	1.44507800
O	0.43054400	-0.94696900	-1.44507800

SI6: Calculated structure of $XeNO_2^-$ at CASPT2/aug-cc-pVTZ level (in Å).

Xe	-0.19536073	0.05267936	-0.00000117
N	0.47512930	1.77548600	0.03327729
O	0.48518036	-0.91846977	1.46459675
O	0.42899065	-0.95440732	-1.46535584

SI7: Calculated structure of transition state of $XeNO_2^-$ at B3LYP/aug-cc-pVTZ level (in Å).

(a) Transition state to $XeO + NO^-$.

Xe	0.06463300	-0.22507100	-0.07873100
N	-1.88320200	-0.37948300	0.33841500
O	1.88875500	0.28317000	0.29281300
O	-0.67722400	1.56810600	-0.05749400

(b) Transition state to $XeN^- + O_2$ (or $Xe + N + O_2^-$).

Xe	-0.17364401	-0.16966927	-0.04804687
N	-2.01692901	0.33407673	0.20084813
O	1.90956099	-0.55039327	0.16493413
O	1.02734899	1.40334373	-0.01635987

SI8: Calculated structure of transition state of $XeNO_2^-$ at MPW1PW91/aug-cc-pVTZ level (in Å).

(a) Transition state to $XeO + NO^-$.

Xe	-0.06379500	-0.22416100	-0.08233200
N	1.84637800	-0.36143900	0.35800300
O	0.66619300	1.53884400	-0.06552500
O	-1.85115800	0.29050000	0.30801500

(b) Transition state to $XeN^- + O_2$ (or $Xe + N + O_2^-$).

Xe	-0.17364400	-0.16966900	-0.04804700
N	-2.01692900	0.33407700	0.20084800
O	1.90956100	-0.55039300	0.16493400
O	1.02734900	1.40334400	-0.01636000

SI9: Calculated structure of transition state of $XeNO_2^-$ at MP2/aug-cc-pVDZ level (in Å).

(a) Transition state to $XeO + NO^-$.

Xe	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.78944886
O	1.69039562	0.00000000	-0.78567262
O	-0.09345430	1.87102713	0.62937839

(b) Transition state to $XeN^- + O_2$ (or $Xe + N + O_2^-$).

Xe	-0.23794700	0.14522500	0.00000000
N	0.55865900	1.78072900	0.00000000
O	0.55865900	-1.26920400	0.92127300
O	0.55865900	-1.26920400	-0.92127300

SI10: Calculated structure of transition state of $XeNO_2^-$ at MP2/aug-cc-pVTZ level (in Å).

(a) Transition state to XeO + NO^-.

Xe	0.11639900	-0.19419000	-0.19735200
N	-1.18247300	-0.66744500	0.92181900
O	1.48469000	0.66292500	0.64631500
O	-1.23572000	1.23186900	-0.12078200

(b) Transition state to XeN^- + O_2 (or Xe + N + O_2^-).

Xe	-0.25204300	0.13667100	0.00000000
N	0.59175400	1.72490400	0.00000000
O	0.59175400	-1.21591000	0.91603300
O	0.59175400	-1.21591000	-0.91603300

SI11: Calculated structure of transition state of $XeNO_2^-$ at MP4SDQ/aug-cc-pVTZ level (in Å).

(a) Transition state to XeO + NO^-.

Xe	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.82456903
O	1.63244189	0.00000000	-0.84758175
O	0.07726385	1.83201659	0.67944848

(b) Transition state to XeN^- + O_2 (or Xe + N + O_2^-).

Xe	-0.24605100	0.14694900	0.00000000
N	0.57768400	1.78604100	0.00000000
O	0.57768400	-1.27734500	0.92460900
O	0.57768400	-1.27734500	-0.92460900

SI12: Calculated structure of $XeNO_3^-$ at B3LYP/aug-cc-pVTZ level (in Å).

Xe	0.00000000	0.00000000	0.07431300
N	0.00000000	0.00000000	1.87901700
O	0.00000000	1.64377300	-0.71525100
O	-1.42354900	-0.82188700	-0.71525100
O	1.42354900	-0.82188700	-0.71525100

SI13: Calculated structure of $XeNO_3^-$ at MPW1PW91/aug-cc-pVTZ level (in Å).

Xe	0.00000000	0.00000000	0.07298000
N	0.00000000	0.00000000	1.85798100
O	0.00000000	1.62253800	-0.70611600
O	-1.40516000	-0.81126900	-0.70611600
O	1.40516000	-0.81126900	-0.70611600

SI14: Calculated structure of $XeNO_3^-$ at MP2/aug-cc-pVDZ level (in Å).

Xe	0.00000000	0.00000000	0.08051200
N	0.00000000	0.00000000	1.87233800
O	0.00000000	1.64695200	-0.72725100
O	-1.42630200	-0.82347600	-0.72725100
O	1.42630200	-0.82347600	-0.72725100

SI15: Calculated structure of $XeNO_3^-$ at MP2/aug-cc-pVTZ level (in Å).

Xe	0.00000000	0.00000000	0.07512500
N	0.00000000	0.00000000	1.84784400
O	0.00000000	1.61119200	-0.70798500
O	-1.39533300	-0.80559600	-0.70798500
O	1.39533300	-0.80559600	-0.70798500

SI16: Calculated structure of $XeNO_3^-$ at CCSD(T)/aug-cc-pVTZ level (in Å).

Xe	0.00000000	0.00000000	0.07496400
N	0.00000000	0.00000000	1.87499000
O	0.00000000	1.62850800	-0.71554000
O	-1.41032900	-0.81425400	-0.71554000
O	1.41032900	-0.81425400	-0.71554000

SI17: Calculated structure of transition state of $XeNO_3^-$ at B3LYP/aug-cc-pVTZ level (in Å).

Xe	-0.04929700	0.00000000	-0.17824600
N	1.80737200	-0.00000200	-0.63925500
O	-1.05011800	1.52868700	0.14440300
O	0.85154200	-0.00000100	1.47370200
O	-1.05012300	-1.52868500	0.14440300

SI18: Calculated structure of transition state of $XeNO_3^-$ at MPW1PW91/aug-cc-pVTZ level (in Å).

Xe	-0.04840800	0.00000000	-0.17798800
N	1.78995900	-0.00000100	-0.62016200
O	-1.03850200	1.50490200	0.14594200
O	0.83754900	-0.00000200	1.45217600
O	-1.03850500	-1.50490000	0.14594100

SI19: Calculated structure of transition state of $XeNO_3^-$ at MP2/aug-cc-pVDZ level (in Å).

Xe	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.82887710
O	1.57883480	0.00000000	-0.99712984
O	0.07337068	1.83231119	0.50109534
O	-1.57377870	0.12623992	-0.99713061

SI20: Calculated structure of $XeNO_2Li$ at B3LYP/aug-cc-pVTZ level (in Å), isomer (a).

Xe	-0.25606800	0.17589300	0.00000000
N	0.44882000	1.83865900	0.00000000
O	0.44882000	-1.00584400	1.32772100
O	0.44882000	-1.00584400	-1.32772100
Li	1.16827400	-2.09177600	0.00000000

SI21: Calculated structure of $XeNO_2Li$ at MPW1PW91/aug-cc-pVTZ level (in Å), isomer (a).

Xe	-0.25660400	0.17028600	0.00000000
N	0.44640000	1.81209400	0.00000000
O	0.44640000	-0.98027700	1.31238200
O	0.44640000	-0.98027700	-1.31238200
Li	1.19647300	-2.06521700	0.00000000

SI22: Calculated structure of $XeNO_2Li$ at MP2/aug-cc-pVDZ level (in Å).

Isomer (a)

Xe	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.79868243
O	1.74551142	0.00000000	-0.81990638
O	-0.29720055	1.71997090	-0.82004966
Li	1.43557547	1.70458697	-1.58454866

Isomer (b)

Xe	0.15590300	-0.09209400	-0.21806700
N	-0.85827700	-1.44037600	0.41517800
O	1.57990900	0.40553700	0.79774800
O	-1.02587000	1.38807800	-0.00786400
Li	-2.28103800	0.23559100	0.85009400

SI23: Calculated structure of $XeNO_2Li$ at MP2/aug-cc-pVTZ level (in Å), isomer (a).

Xe	0.23193600	0.00000300	-0.21149900
N	1.60064700	-0.00005700	0.92288000
O	-1.04719700	1.31529400	0.18790500
O	-1.04726900	-1.31524900	0.18786800
Li	-2.32444600	-0.00003200	0.65152900

SI24: Calculated structure of $XeNO_2Li$ at CCSD(T)/aug-cc-pVTZ level (in Å), isomer (a).

Xe	-0.26057400	0.17127200	0.00000000
N	0.45319700	1.83672100	0.00000000
Li	1.21582800	-2.08635400	0.00000000
O	0.45319700	-0.99041800	1.33189000
O	0.45319700	-0.99041800	-1.33189000

SI25: Calculated structure of transition state of $XeNO_2Li$ at B3LYP/aug-cc-pVTZ level (in Å), isomer (a).

Xe	0.25219900	-0.31159700	-0.12583600
N	1.25974600	0.94536300	0.83048200
O	-0.49290300	1.59953600	-0.44449600
O	-1.53079000	-0.71918200	0.47294600
Li	-2.08247000	1.05529400	0.25139100

SI26: Calculated structure of transition state of $XeNO_2Li$ at MPW1PW91/aug-cc-pVTZ level (in Å), isomer (a).

Xe	0.24981000	-0.30720200	-0.12400200
N	1.21690500	0.94452400	0.83530900
O	-0.47359400	1.56514900	-0.45514700
O	-1.50183400	-0.71356100	0.46773900
Li	-2.06821000	1.05484600	0.24939600

SI27: Calculated structure of transition state of $XeNO_2Li$ at MP2/aug-cc-pVDZ level (in Å), isomer (a).

Xe	-0.38258700	-0.11643900	-0.16592300
N	-0.53974900	1.15810500	1.10670800
O	0.86966800	-1.36783300	0.50580200
O	1.29973400	1.18424500	-0.46224500
Li	2.36091600	-0.11678100	0.28813800

SI28: Calculated structure of transition state of $XeNO_2Li$ at MP2/aug-cc-pVTZ level (in Å), isomer (a).

Xe	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.82506687
O	1.98227068	0.00000000	0.82641876
O	0.38005450	1.68087872	-0.70633979
Li	1.93737736	1.88066750	0.36599790

SI29: Calculated structure of $XeNO_3Li$ at B3LYP/aug-cc-pVTZ level (in Å), isomer (a).

N	-1.28657300	1.47450800	0.00000000
Xe	-0.03949200	0.18808300	0.00000000
O	-0.13220100	-1.13291800	1.31553300
O	1.70629700	0.63828300	0.00000000
O	-0.13220100	-1.13291800	-1.31553300
Li	-0.13220100	-2.48587400	0.00000000

SI30: Calculated structure of $XeNO_3Li$ at MPW1PW91/aug-cc-pVTZ level (in Å), isomer (a).

N	-1.27846600	1.45155500	0.00000000
Xe	-0.03896400	0.18433600	0.00000000
O	-0.12752100	-1.10956600	1.30360000
O	1.68452600	0.63312200	0.00000000
O	-0.12752100	-1.10956600	-1.30360000
Li	-0.12752100	-2.47564600	0.00000000

SI31: Calculated structure of $XeNO_3Li$ at MP2/aug-cc-pVDZ level (in Å).

Isomer (a)

N	0.00000000	0.00000000	0.00000000
Xe	0.00000000	0.00000000	1.78335398
O	1.66294661	0.00000000	2.67284417
O	-0.92743399	-1.24467395	2.71152965
O	-0.47560701	1.59348342	2.67284417
Li	1.16403172	1.56220279	3.68496650

Isomer (b)

N	0.00000000	0.00000000	1.97150300
Xe	0.00000000	0.00000000	0.20818700
O	0.00000000	1.53571900	-0.75544600
O	-1.32997100	-0.76785900	-0.75544600
O	1.32997100	-0.76785900	-0.75544600
Li	0.00000000	0.00000000	-2.30396500

Isomer (c)

N	1.11894000	-0.01448400	-1.39186900
Xe	-0.08532100	-0.00080300	-0.07499000
O	0.94897500	0.01224000	1.42427200
O	-1.14880400	-1.39252700	0.12023900
O	-1.14446900	1.39762500	0.09429100
Li	2.50970900	0.00201900	0.22738300

SI32: Calculated structure of $XeNO_3Li$ at MP2/aug-cc-pVTZ level (in Å), isomer (a).

N	-1.25647500	1.46145000	0.00000000
Xe	-0.03757100	0.18659300	0.00000000
O	-0.14095200	-1.09528100	1.30930800
O	1.68778000	0.58994700	0.00000000
O	-0.14095200	-1.09528100	-1.30930800
Li	-0.14095200	-2.50042800	0.00000000

SI33: Calculated structure of $XeNO_3Li$ at CCSD(T)/aug-cc-pVTZ level (in Å), isomer (a).

Xe	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.79117496
Li	1.93836069	0.00000000	-1.86588528
O	0.97208108	-1.31482100	-0.86698424
O	0.97208108	1.31482100	-0.86698424
O	-1.54517583	-0.00000000	-0.91156794

SI34: Calculated structure of transition state of $XeNO_3Li$ at B3LYP/aug-cc-pVTZ level (in Å), isomer (a).

N	1.00978100	1.61787200	-0.37158200
Xe	0.19134100	-0.08562100	-0.19202700
O	-0.63950500	0.92431700	1.20335000
O	0.92308600	-1.35839200	0.87706800
O	-1.58257500	-0.55306500	-0.71158400
Li	-2.33631200	0.39851900	0.67327700

SI35: Calculated structure of transition state of $XeNO_3Li$ at MPW1PW91/aug-cc-pVTZ level (in Å), isomer (a).

N	1.02598100	1.58276900	-0.36698700
Xe	0.18717200	-0.08930600	-0.19076000
O	-0.60589900	0.93555800	1.17702800
O	0.87814500	-1.35303700	0.87956700
O	-1.56508600	-0.52952700	-0.70063800
Li	-2.31547700	0.43972500	0.67409700

SI36: Calculated structure of transition state of $XeNO_3Li$ at MP2/aug-cc-pVDZ level (in Å), isomer (a).

N	0.22779400	1.80938700	-0.48307500
Xe	0.20807900	-0.03580300	-0.19356100
O	-0.77907100	0.67419900	1.31713200
O	1.45041000	-0.94635600	0.79450900
O	-1.39354500	-0.96781300	-0.68631800
Li	-2.35105200	-0.27086100	0.81040800

SI37: Calculated structure of transition state of $XeNO_3Li$ at MP2/aug-cc-pVTZ level (in Å), isomer (a).

N	0.40387300	1.76149800	-0.43874800
Xe	0.20198300	-0.04458900	-0.19147000
O	-0.72786300	0.72615500	1.25620500
O	1.29437500	-1.05101000	0.81391700
O	-1.40324700	-0.87034000	-0.68596800
Li	-2.34676800	-0.12037900	0.77912000

SI38: Calculated structure of XeF_2NO^- at MP2/aug-cc-pVDZ level (in Å).

F	0.03295100	0.57239500	2.09573200
Xe	0.03295100	0.05079700	0.00000000
N	1.48930800	-1.00212800	0.00000000
O	-1.59970500	-0.75390600	0.00000000
F	0.03295100	0.57239500	-2.09573200

SI39: Calculated structure of $XeFNO_2$ at MP2/aug-cc-pVDZ level (in Å).

Xe	-0.09520600	-0.11418300	0.00000000
N	-1.89017900	-0.03349500	0.00000000
O	0.88476100	-0.60481900	-1.40735100
O	0.88476100	-0.60481900	1.40735100
F	0.46846500	1.78638200	0.00000000

SI40: Calculated structure of $XeNO_2H$ at MP2/aug-cc-pVDZ level (in Å).

Xe	0.15580500	0.06045100	-0.18564500
N	1.58235200	-0.67388600	0.65052500
O	-1.44593900	-1.24999100	0.15196500
O	-0.72973000	1.51037600	0.45992800
H	-2.08458800	-0.63021000	0.57600900

SI41: Calculated structure of $XeNO_2CH_3$ at MP2/aug-cc-pVDZ level (in Å).

Xe	0.47847500	0.02842000	-0.17681200
N	1.35564800	-1.13614700	0.90625200
O	-0.08808500	1.66554300	0.38112200
O	-1.48263500	-0.79793900	-0.46574400
C	-2.44568900	-0.11472900	0.36900600
H	-2.52365500	-0.60862200	1.34947300
H	-2.16596500	0.94862800	0.49713000
H	-3.39769500	-0.17413300	-0.17955200

SI42: Calculated structure of $NXeO_2BeO_2XeN$ at MP2/aug-cc-pVDZ level (in Å).

N	0.00000000	3.90261000	-0.88192300
O	1.14411500	0.89171300	-0.84452700
O	-0.58362700	1.30649400	0.93263000
O	-1.14411500	-0.89171300	-0.84452700
O	0.58362700	-1.30649400	0.93263000
N	0.00000000	-3.90261000	-0.88192300
Xe	0.68894300	2.54796000	0.10046200
Xe	-0.68894300	-2.54796000	0.10046200
Be	0.00000000	0.00000000	0.02184000

SI43: Calculated structure of $XeNHO_2$ at MP2/aug-cc-pVDZ level (in Å).

H	-1.83369900	0.00004500	1.35214200
N	-1.78793700	-0.00090200	0.31335700
Xe	-0.00190900	0.00000100	-0.19648100
O	0.90401200	-1.42132100	0.44155600
O	0.90253200	1.42209900	0.44148400

SI44: Calculated structure of $XeNH_2O_2^+$ at MP2/aug-cc-pVDZ level (in Å).

H	-1.98254000	-0.17719200	1.12422800
H	-1.80608900	-1.59409400	0.22761300
N	-1.77923900	-0.55819600	0.17921400
Xe	0.11469400	0.01963300	-0.21601300
O	1.24626600	-1.04648100	0.61873800
O	0.00996500	1.62379000	0.51355900

SI45: The calculated S–T crossing point structure along the $XeNO_2^- \rightarrow XeO + NO^-$ reaction path (in Å).

Xe	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.39380023
O	1.47711131	0.00000000	-1.33270908
O	0.75108052	0.94012499	2.50596045

SI46: Dissociation energies (in kcal/mol) of $XeNO_2^-$ by various channels.

	B3LYP/aptz	MPW1PW91/aptz	MP2/apdz	MP2/aptz	CCSD(T)/aptz	CCSD(T)/apqz[a]
Xe + N(Q) + O(T) + O^-(D)	32.5	30.9	19.2	63.5	40.9	50.1
XeO + NO^- (S)	–51.1	–46.6	–45.4	–23.2	–36.8	–33.2
XeO + NO^- (T)	–79.5	–77.8	–71.0	–46.8	–61.4	–57.3
Xe + NO_2^-	–211.7	–211.9	–219.8	–190.7	–194.5	–191.2
Xe + N^-(S) + O_2 (S)	24.0	31.6	20.0	51.9	30.0	35.2
Xe + N^-(T) + O_2 (T)	–56.9	–56.4	–54.4	–16.5	–36.4	–30.4
Xe + N(D) + O_2^-(D)	–1.2	4.6	3.6	37.7	10.9	17.1
Xe + N(Q) + O_2^-(D)	–64.3	–64.9	–74.9	–37.6	–51.5	–44.5
XeN(D) + O_2^-(D)	–21.7	–18.3	–8.7	18.5	–0.1	4.9
XeN^-(S) + O_2 (S)	14.2	18.2	12.6	36.7	21.9	26.0
XeN^-(T) + O_2 (T)	–59.9	–59.8	–58.4	–22.9	–41.1	–35.3
Xe + O(T) + NO^-(T)	–90.8	–91.9	–91.2	–54.7	–72.7	–66.6
Xe + O(S) + NO^-(S)	1.0	8.0	2.4	35.0	2.6	7.8

[a]Single point calculation using CCSD(T)/ aug-cc-pVTZ structure.

SI47: Dissociation energies (in kcal/mol) of $XeNO_3^-$ by various channels.

Method	B3LYP/aptz	MPW1PW91/aptz	MP2/apdz	MP2/aptz	CCSD(T)/aptz	CCSD(T)/apqz[a]
Xe + N(Q) + 2O(T) + O^-(D)	74.8	74.8	58.8	119.0	87.0	100.7
XeO_2 + NO^-(S)	–19.5	–11.9	–7.6	13.4	–3.4	1.4
XeO_2 + NO^-(T)	–47.9	–43.1	–33.3	–10.2	–27.9	–22.7
Xe + NO_3^-	–260.7	–261.4	–271.3	–232.5	–235.4	–230.4
XeO + NO_2^-	–158.1	–153.8	–160.0	–127.3	–136.9	–131.3
Xe + NO^-(S) + O_2(S)	–104.9	–97.4	–114.9	–73.5	–87.2	–80.4
Xe + NO^-(T) + O_2(T)	–171.7	–169.2	–171.1	–126.1	–141.5	–134.0
XeO + N^-(S) + O_2(S)	77.5	89.7	79.8	115.3	87.6	95.1
XeO + N^-(T) + O_2(T)	-3.3	1.6	5.4	46.9	21.1	29.5
XeO + N(D) + O_2^-(D)	52.3	62.7	63.3	101.0	68.4	77.0
Xe + NO(D) + O_2^-(D)	–176.5	–170.9	–177.8	–135.5	–149.8	–142.8
XeN^-(S) + O(S) + O_2(S)	119.9	130.9	120.0	158.3	118.9	126.9
XeN^-(S) + O(T) + O_2(T)	18.0	21.4	21.5	63.2	38.3	47.1
XeN^-(T) + O(S) + O_2(T)	45.8	52.9	49.1	98.7	56.0	65.6
XeN^-(T) + O(T) + O_2(S)	20.8	24.8	11.8	61.6	34.9	44.8
XeN^-(T) + O(T) + O_2(T)	–17.7	–15.8	–18.9	32.6	5.1	15.3
XeN^-(S) + O_3(S)	1.3	8.2	–7.7	26.1	17.2	24.0
XeN^-(T) + O_3(T)	–15.5	–10.3	–1.9	42.5	14.4	22.3
XeN (D) + O_3^-(D)	–44.8	–38.2	–26.2	9.8	–15.0	–7.4

[a]Single point calculation using CCSD(T)/aptz structure.

[b]Single point calculation using MP2/aug-cc-pVDZ structure.