Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Protonation of N_2O and NO_2 in a solid phase

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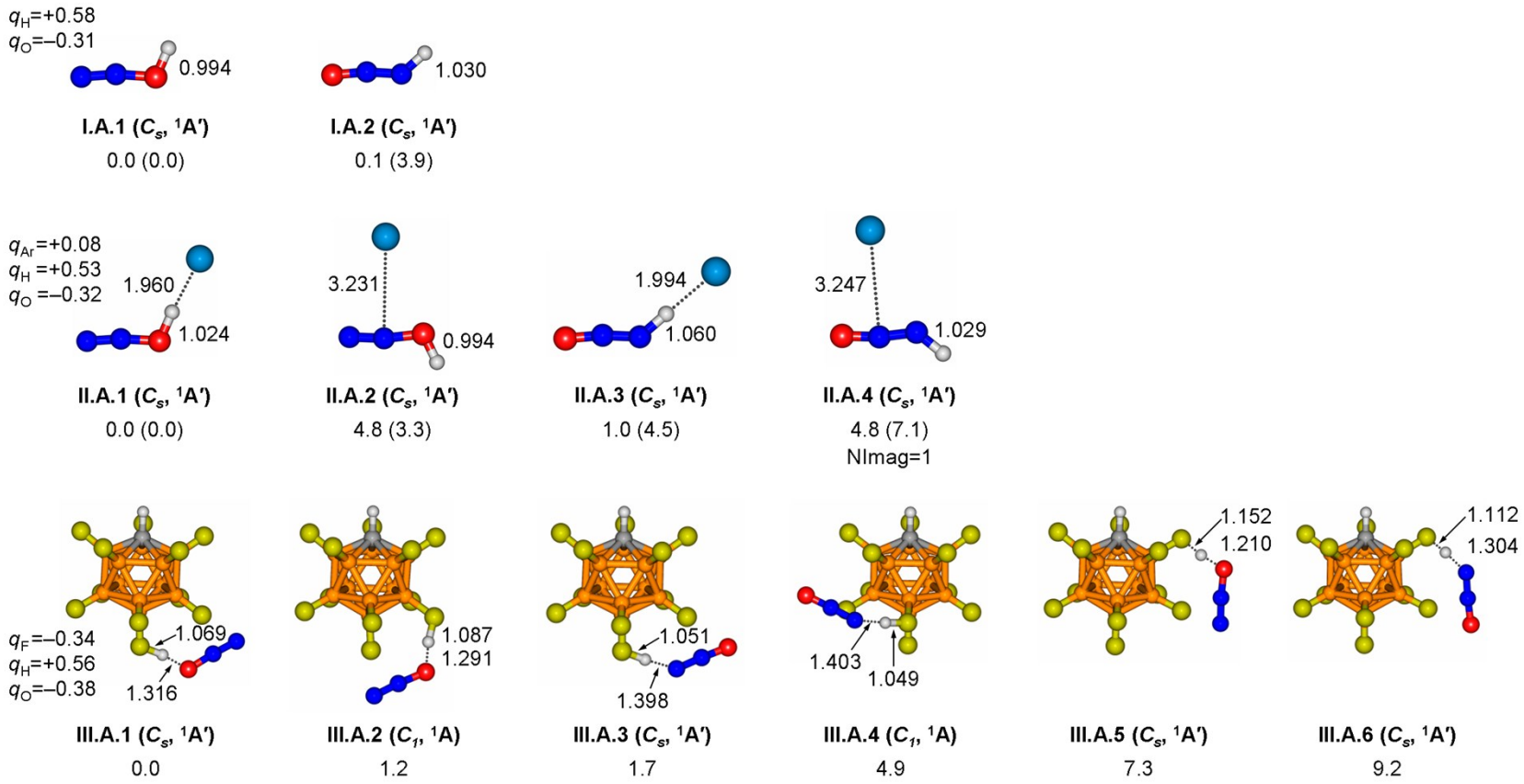


Figure S1. Representative structures of N_2OH^+ (I), $N_2OH^+\cdots Ar$ (II), and $N_2OH\{F_{11}\}$ (III), their point group symmetries and spectroscopic states. Relevant interatomic distances (Å) and natural population analysis (NPA) charges on the corresponding atoms (q, $|e|$) are presented for the structures of interest. Zero-point energy (ZPE)-corrected (B3LYP-D3/def2-TZVPD) relative energies (kcal/mol) are given at the B3LYP-D3/def2-TZVPD and CCSD(T)/def2-TZVPD theoretical levels (in parentheses).

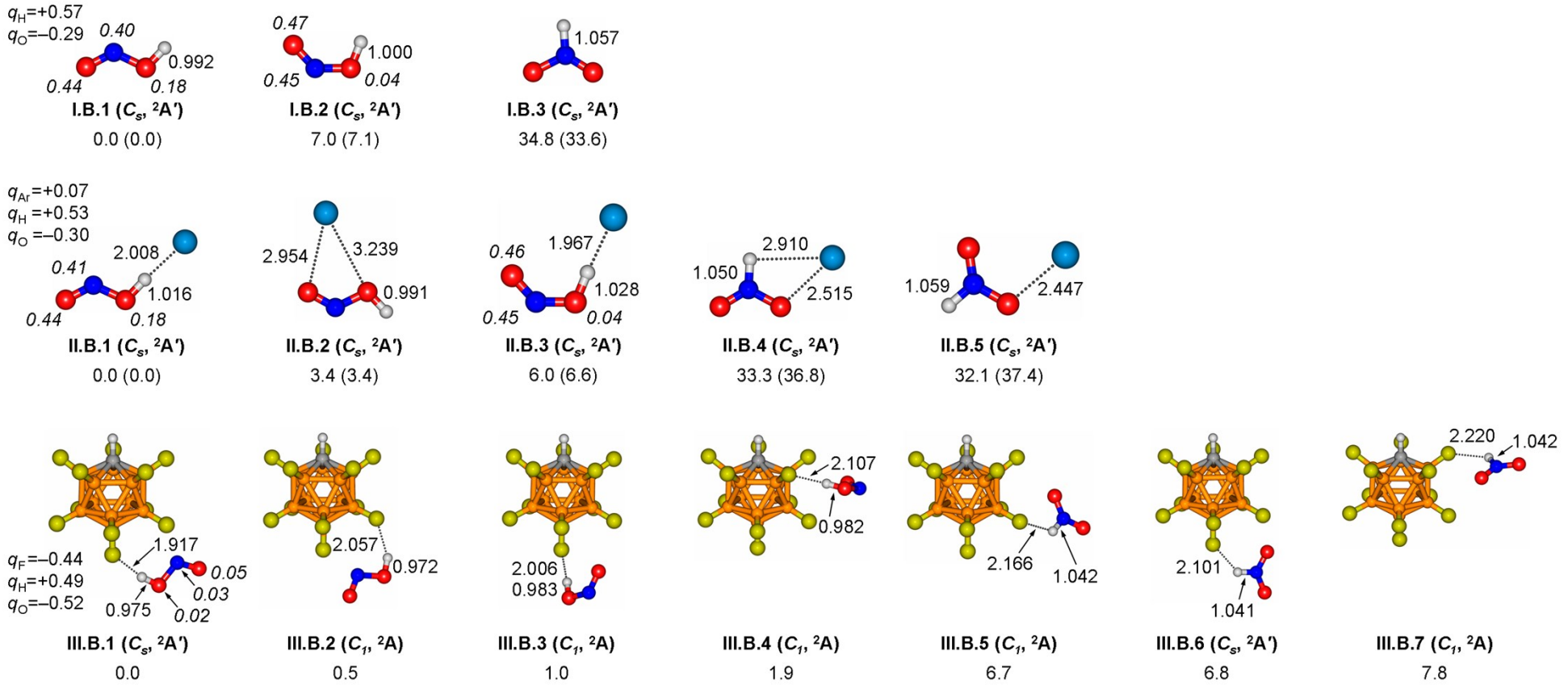


Figure S2. Representative structures of NO_2H^+ (I), $NO_2H^+\cdots Ar$ (II), and $NO_2H\{F_{11}\}$ (III), their point group symmetries and spectroscopic states. Relevant interatomic distances (Å), NPA charges on the corresponding atoms (q, $|e|$), and Mulliken spin densities (*in italics*, $|e|$) are presented for the structures of interest. ZPE-corrected (B3LYP-D3/def2-TZVPD) relative energies (kcal/mol) are given at the B3LYP-D3/def2-TZVPD and CCSD(T)/def2-TZVPD theoretical levels (in parentheses).

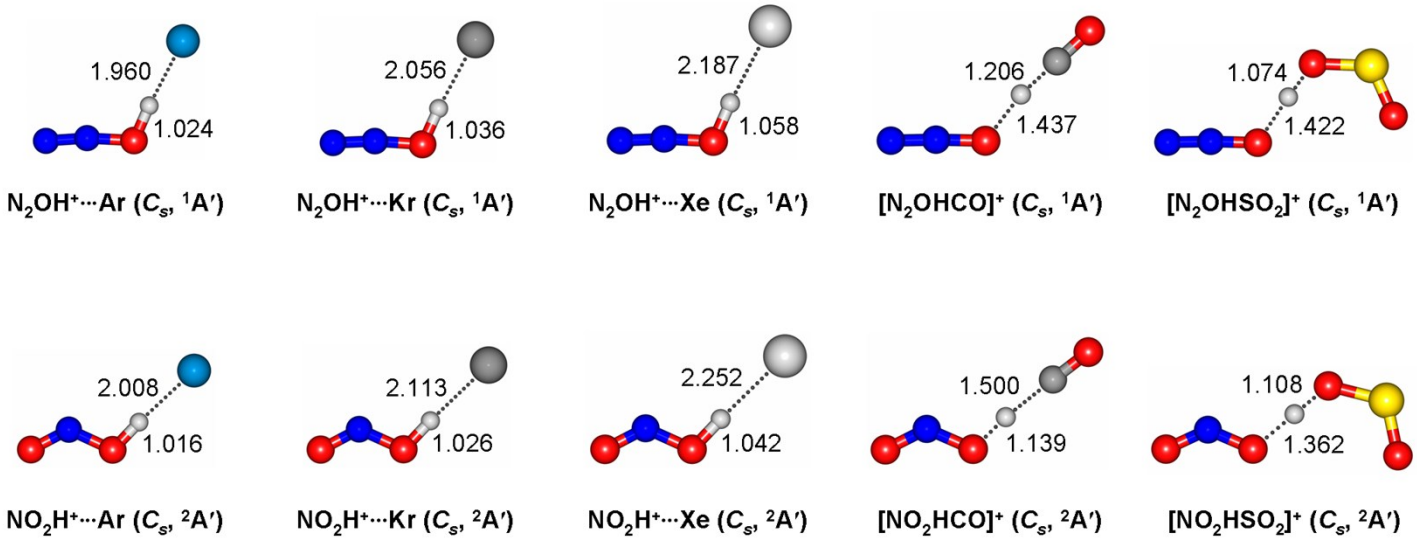


Figure S3. Representative structures of $[N_2OHX]^+$ and $[NO_2HX]^+$ (X=Ar, Kr, Xe, CO, SO_2), their point group symmetries, spectroscopic states, and relevant interatomic distances (Å).

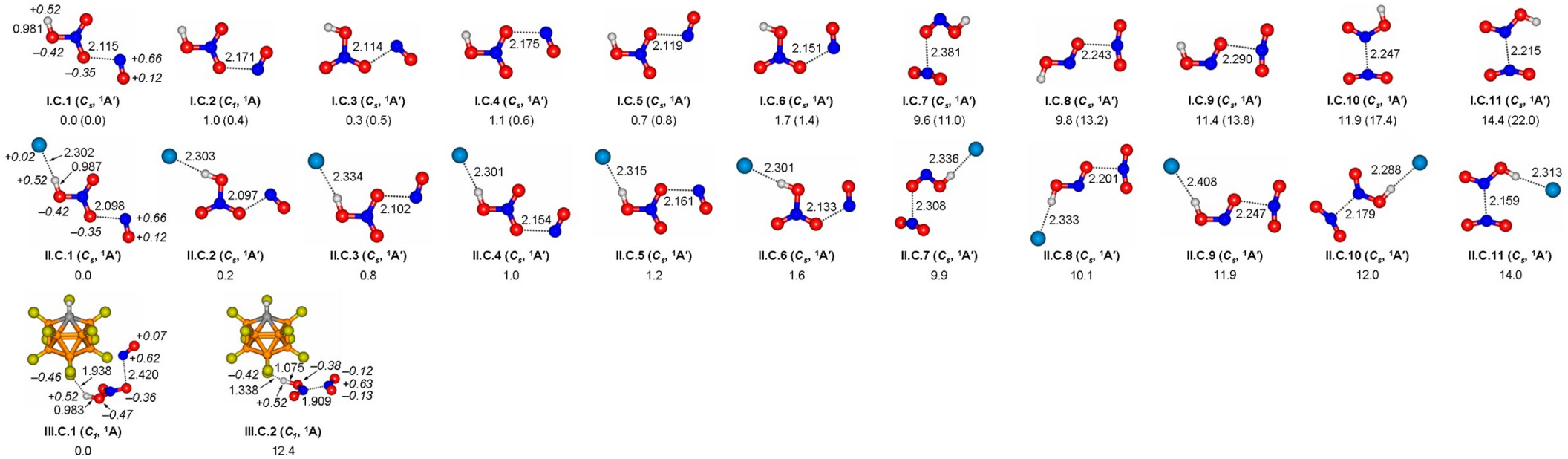


Figure S4. Representative structures of $(NO_2)_2H^+$ (I), $(NO_2)_2H^+\cdots Ar$ (II), and $(NO_2)_2H\{F_{11}\}$ (III), their point group symmetries and spectroscopic states. Relevant interatomic distances (Å) and NPA atomic charges (*q*, *in italics*, |*e*|) are presented for the structures of interest. ZPE-corrected (B3LYP-D3/def2-TZVPD) relative energies (kcal/mol) are given at the B3LYP-D3/def2-TZVPD and CCSD(T)/def2-TZVPD theoretical levels (in parentheses).

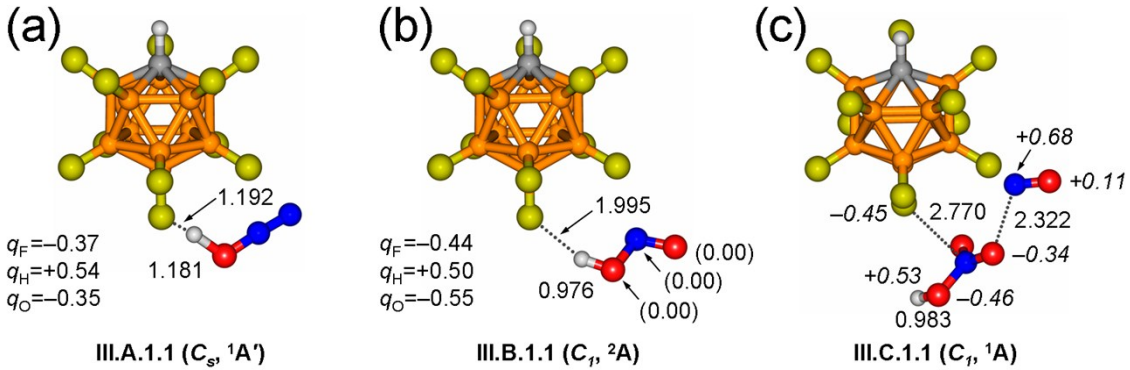


Figure S5. Representative structures of $N_2OH\{F_{11}\}$ (a), $NO_2H\{F_{11}\}$ (b), and $(NO_2)_2H\{F_{11}\}$ (c) optimized in a dichloroethane solution, their point group symmetries and spectroscopic states. Relevant interatomic distances (Å), NPA atomic charges (q, *in italics*, $|e|$), and Mulliken spin densities (in parentheses, $|e|$) are presented for the structures of interest.

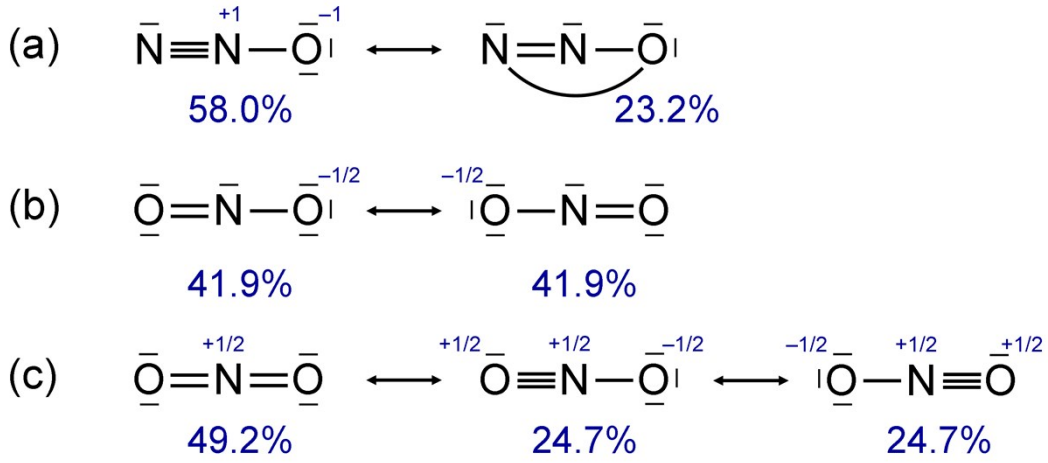


Figure S6. Results of natural resonance theory (NRT) analysis for N_2O (a) and NO_2 (b – α spin density; c – β spin density) calculated at the zero-order regular approximation (ZORA)-B3LYP/TZ2P//B3LYP-D3/def2-TZVPD level of theory. Leading resonance structures and their weighting (>13%) are presented.

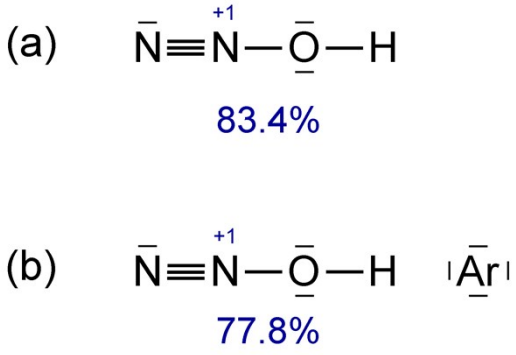


Figure S7. Results of NRT analysis for N_2OH^+ (a; I.A.1) and $N_2OH^+\cdots Ar$ (b; II.A.1) calculated at the ZORA-B3LYP/TZ2P//B3LYP-D3/def2-TZVPD level of theory. Leading resonance structures and their weighting (>10%) are presented.

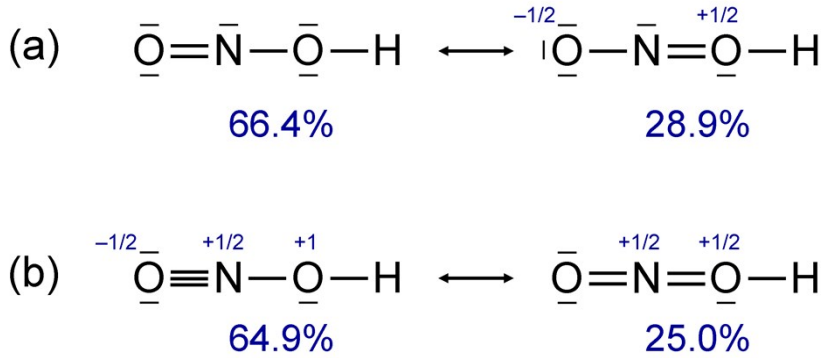


Figure S8. Results of NRT analysis for NO_2H^+ (I.B.1) calculated at the ZORA-B3LYP/TZ2P//B3LYP-D3/def2-TZVPD level of theory. Leading resonance structures and their weighting (>10%) are presented for the α (a) and β (b) spin densities.

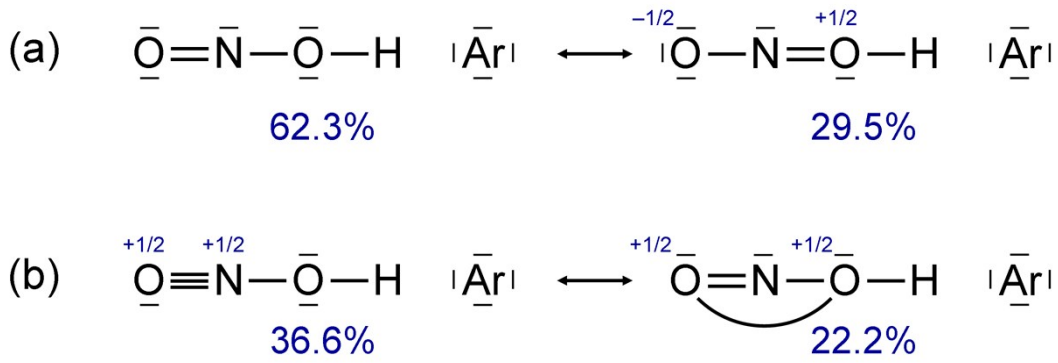


Figure S9. Results of NRT analysis for $NO_2H^+\cdots Ar$ (II.B.1) calculated at the ZORA-B3LYP/TZ2P//B3LYP-D3/def2-TZVPD level of theory. Leading resonance structures and their weighting (>10%) are presented for the α (a) and β (b) spin densities.

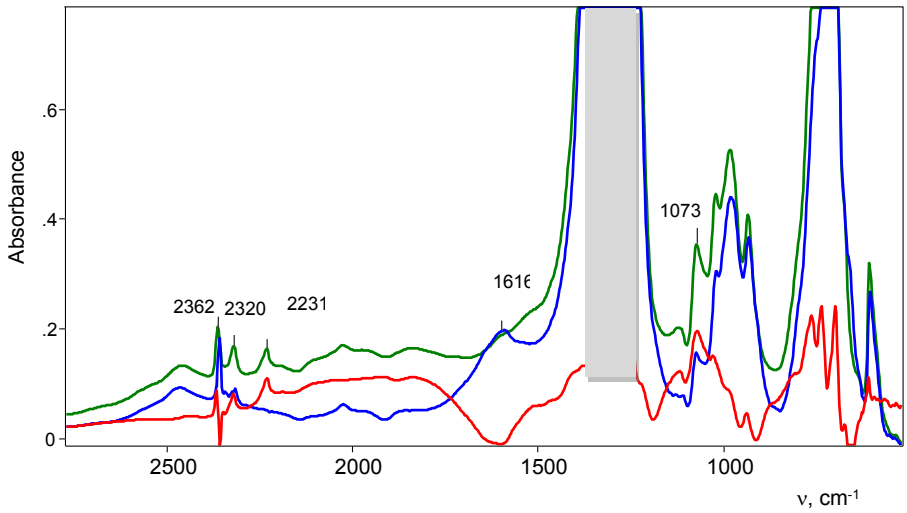


Figure S10. IR spectra of the $N_2OH^+\{F_{11}^-\}$ salt before (green) and after heating at 100 °C (blue) and their difference (red) that allowed to see the broad absorption from OH stretch of the cation (in more detail it can be seen in Figure 5).

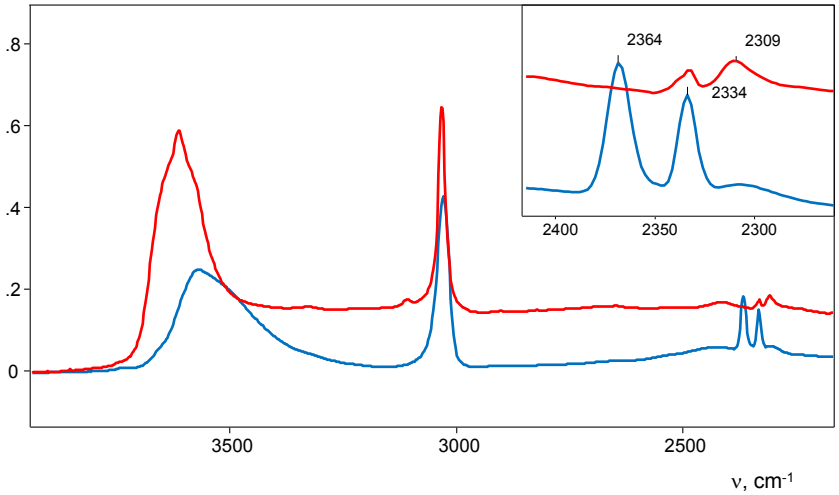


Figure S11. IR spectra of the products formed after 24 h reaction of a gas mixture $NO_2 + N_2O_4$ with an $H\{F_{11}\}$ acid (blue) and after purging with moist air (red).

Table S1. Frequencies (cm^{-1}, scaled by the factor of 0.9674) and their IR intensities (km/mol, in parentheses) calculated at the B3LYP-D3/def2-TZVPD level of theory for the N_2O, NO_2, and NO^+ species.

Compound	Frequency					
N_2O	598	(5)	1285	(70)	2268	(393)
NO_2	741	(5)	1346	(0)	1641	(439)
NO^+					2403	(27)

Table S2. Selected frequencies (cm^{-1}, scaled by the factor of 0.9674) and their IR intensities (km/mol, in parentheses) calculated at the (SMD-)B3LYP-D3/def2-TZVPD level of theory for the N_2OH-containing compounds.

Compound	νNN		νNO(H)		νOH	
N_2OH^+ (I.A.1) [a]	2357	(17)	1034	(84)	3332	(437)
$N_2OH^+\cdots Ar$ (II.A.1) [a]	2350	(76)	1063	(93)	2799	(2224)
$N_2OH^+\cdots Kr$ [a]	2342	(214)	1070	(103)	2592	(2876)
$N_2OH^+\cdots Xe$ [a]	2368	(635)	1079	(131)	2246	(3701)
$[N_2OHCO]^+$ [a]	2309	(182)	1150	(709)	1467	(3204)
$[N_2OHSO_2]^+$ [a]	2326	(41)	1175	(625)	1964	(4893)
$N_2OH\{F_{11}\}$ (III.A.1) [a]	2346	(81)	1181	(147)	1729	(3786)
			1192	(266)		
$N_2OH\{F_{11}\}$ (III.A.1.1) [b]	2356	(109)	1137	(749)	1212	(968)

[a] Gas; [b] Dichloroethane solution.

Table S3. Selected frequencies (cm^{-1}, scaled by the factor of 0.9674) and their IR intensities (km/mol, in parentheses) calculated at the (SMD-)B3LYP-D3/def2-TZVPD level of theory for the NO_2H-containing compounds.

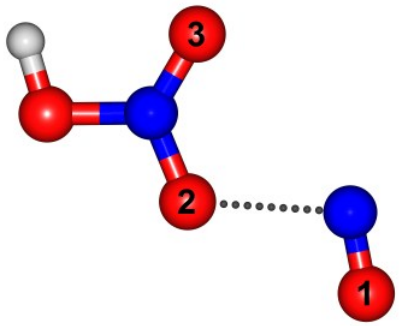
Compound	νNO		νNO(H)		νOH	
NO_2H^+ (I.B.1) [a]	1798	(59)	1011	(107)	3368	(423)
$NO_2H^+\cdots Ar$ (II.B.1) [a]	1786	(101)	1059	(132)	2917	(1972)
$NO_2H^+\cdots Kr$ [a]	1779	(131)	1072	(151)	2746	(2605)
$NO_2H^+\cdots Xe$ [a]	1770	(220)	1086	(197)	2491	(3568)
$[NO_2HCO]^+$ [a]	1759	(44)	1125	(2086)	1215	(1689)
$[NO_2HSO_2]^+$ [a]	1753	(446)	1177	(2412)	1572	(3397)
$NO_2H\{F_{11}\}$ (III.B.1) [a]	1685	(1587)	784	(620)	3518	(245)
$NO_2H\{F_{11}\}$ (III.B.1.1) [b]	1678	(259)	813	(231)	3515	(403)

[a] Gas; [b] Dichloroethane solution.

Table S4. Selected frequencies (cm^{-1}, scaled by the factor of 0.9674) and their IR intensities (km/mol, in parentheses) calculated at the (SMD-)B3LYP-D3/def2-TZVPD level of theory for the $(NO_2)_2H$-containing compounds.

Compound	νNO1		νNO2		νNO3		νNO(H)		νOH	
$(NO_2)_2H^+$ (I.C.1) [a]	2230	(442)	1195	(763)	1623	(436)	953	(79)	3488	(266)
$(NO_2)_2H^+\cdots Ar$ (II.C.1) [a]	2221	(486)	1191	(902)	1618	(387)	962	(67)	3365	(861)
$(NO_2)_2H\{F_{11}\}$ (III.C.1) [a]	2142	(2110)	1267	(250)	1617	(293)	927	(61)	3426	(139)
$(NO_2)_2H\{F_{11}\}$ (III.C.1.1) [b]	2222	(1210)	1248	(798)	1598	(492)	930	(227)	3456	(358)

[a] Gas; [b] Dichloroethane solution.



Atomic labeling for the $(NO_2)_2H$-containing compounds

Table S5. Reaction energy (ΔE), enthalpy at 0 K (ΔH_0°), enthalpy at 298 K (ΔH_{298}°), and Gibbs free energy at 298 K (ΔG_{298}°) calculated at the B3LYP-D3/def2-TZVPD and CCSD(T)/def2-TZVPD theoretical levels (in parentheses) for the dissociation processes under study. All values are given in kcal/mol.

Process	ΔE	ΔH (0 K)	ΔH (298 K)	ΔG (298 K)
N_2OH^+ (I.A.1) = $H^+ + N_2O$ [a]	140.0 (142.1)	133.8 (135.9)	134.9 (136.9)	128.7 (130.8)
NO_2H^+ (I.B.1) = $H^+ + NO_2$ [a]	145.3 (145.9)	138.0 (138.6)	139.3 (139.9)	132.3 (132.9)
$H(NO_2)_2^+$ (I.C.1) = $H^+ + (NO_2)_2$ [a]	193.6 (195.5)	185.8 (187.7)	186.9 (188.8)	180.2 (182.1)
$N_2OH\{F_{11}\}$ (III.A.1) = $H\{F_{11}\} + N_2O$ [a]	18.2	18.1	18.1	8.1
$NO_2H\{F_{11}\}$ (III.B.1) = $H\{F_{11}\} + NO_2$ [a]	34.5	34.8	33.5	27.3
$(NO_2)_2H\{F_{11}\}$ (III.C.1) = $H\{F_{11}\} + (NO_2)_2$ [a]	46.8	44.9	44.2	33.2
$N_2OH\{F_{11}\}$ (III.A.1.1) = $H\{F_{11}\} + N_2O$ [b]	9.8	10.5	10.8	0.1
$NO_2H\{F_{11}\}$ (III.B.1.1) = $H\{F_{11}\} + NO_2$ [b]	23.9	24.7	23.5	17.4
$(NO_2)_2H\{F_{11}\}$ (III.C.1.1) = $H\{F_{11}\} + (NO_2)_2$ [b]	40.9	39.1	38.6	26.9
$H(NO_2)_2^+$ (I.C.1) = $HNO_3 + NO^+$ [a]	24.8 (17.1)	23.8 (16.1)	23.9 (16.2)	15.7 (8.0)
$(NO_2)_2H\{F_{11}\}$ (III.C.1) = $HNO_3\{F_{11}\}^- + NO^+$ [a]	98.8	98.2	98.4	86.7
$(NO_2)_2H\{F_{11}\}$ (III.C.1.1) = $HNO_3\{F_{11}\}^- + NO^+$ [b]	17.9	17.0	17.2	6.9
$(NO_2)_2H\{F_{11}\}$ (III.C.1) = $\{F_{11}\}^- + HNO_3 + NO^+$ [a]	110.1	108.7	108.3	89.4
$(NO_2)_2H\{F_{11}\}$ (III.C.1.1) = $\{F_{11}\}^- + HNO_3 + NO^+$ [b]	23.4	21.6	21.2	2.3

[a] Gas. [b] Dichloroethane solution.

Cartesian coordinates (Å) and total energies (a.u.) for the most relevant species under study.

N2O
E(B3LYP-D3/def2-TZVPD)=-184.7447753 a.u.,
E(CCSD(T)/def2-TZVPD)=-184.4162418 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.011181 a.u.

O	0.000000000	0.000000000	1.109673000
N	0.000000000	0.000000000	-0.073660000
N	0.000000000	0.000000000	-1.194538000

N2OH+ (I.A.1)
E(B3LYP-D3/def2-TZVPD)=-184.9679365 a.u.,
E(CCSD(T)/def2-TZVPD)=-184.6427272 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.021112 a.u.

O	0.049270000	-1.084378000	0.000000000
N	0.000000000	0.177933000	0.000000000
N	-0.198678000	1.259414000	0.000000000
H	0.996581000	-1.386405000	0.000000000

N2OH+Ar (II.A.1)
E(B3LYP-D3/def2-TZVPD)=-712.5302806 a.u.,
E(CCSD(T)/def2-TZVPD)=-711.6856533 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.021738 a.u.

O	-1.013205000	0.659083000	0.000000000
N	-1.614697000	-0.442157000	0.000000000
N	-2.253975000	-1.337857000	0.000000000
H	0.000000000	0.513935000	0.000000000
Ar	1.954797000	0.370750000	0.000000000

N2OH{F11} (III.A.1)
E(B3LYP-D3/def2-TZVPD)=-1596.974302 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.120131 a.u.

B	1.494911000	-1.287774000	0.000000000
B	-0.460064000	0.742409000	0.913679000
B	-1.013304000	-0.845079000	1.473740000
B	0.742958000	-0.507329000	1.493416000
B	0.178850000	-2.092140000	0.908516000
B	0.742958000	-0.507329000	-1.493416000
B	-1.013304000	-0.845079000	-1.473740000
B	-0.460064000	0.742409000	-0.913679000
B	-1.748455000	-0.071879000	0.000000000
B	1.021084000	0.417955000	0.000000000
B	0.178850000	-2.092140000	-0.908516000
C	-1.238669000	-1.710572000	0.000000000
H	-2.022106000	-2.459914000	0.000000000
F	-1.796891000	-1.106176000	2.538008000
F	0.257666000	-3.267740000	1.560977000
F	-3.059726000	0.243270000	0.000000000
F	-1.796891000	-1.106176000	-2.538008000
F	0.257666000	-3.267740000	-1.560977000
F	-0.594905000	1.946428000	1.561866000
F	-0.594905000	1.946428000	-1.561866000
F	1.468909000	-0.299032000	-2.620166000
F	2.784765000	-1.701325000	0.000000000
F	1.468909000	-0.299032000	2.620166000
F	2.039492000	1.512303000	0.000000000
H	1.647793000	2.507276000	0.000000000
O	1.327834000	3.783819000	0.000000000
N	0.160103000	4.117797000	0.000000000
N	-0.880854000	4.491422000	0.000000000

NO2
E(B3LYP-D3/def2-TZVPD)=-205.1687088 a.u.,
E(CCSD(T)/def2-TZVPD)= -204.8127911 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.008778 a.u.

N	0.000000000	0.000000000	0.319960000
O	0.000000000	1.097957000	-0.139983000
O	0.000000000	-1.097957000	-0.139983000

NO2H+ (I.B.1)
E(B3LYP-D3/def2-TZVPD)=-205.4003341 a.u.,
E(CCSD(T)/def2-TZVPD)=-205.0453453 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.020521 a.u.

O	0.901707000	-0.547335000	0.000000000
N	0.000000000	0.378870000	0.000000000
O	-1.125887000	0.229882000	0.000000000
H	1.793441000	-0.112469000	0.000000000

NO2H+Ar (II.B.1)
E(B3LYP-D3/def2-TZVPD)=-732.9613554 a.u.,
E(CCSD(T)/def2-TZVPD)=-732.0874755 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.020842 a.u.

O	-1.010096000	0.344445000	0.000000000
N	-1.286294000	-0.906770000	0.000000000
O	-2.318328000	-1.388759000	0.000000000
H	0.000000000	0.456592000	0.000000000
Ar	1.979525000	0.791406000	0.000000000

NO2H{F11} (III.B.1)
E(B3LYP-D3/def2-TZVPD)=-1617.4241900 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.116984 a.u.

B	1.569117000	-1.231553000	0.000000000
B	-0.518285000	0.641176000	0.934362000
B	-1.024604000	-0.994749000	1.452991000
B	0.792137000	-0.534628000	1.470446000
B	0.275980000	-2.151218000	0.924115000
B	0.792137000	-0.534628000	-1.470446000
B	-1.024604000	-0.994749000	-1.452991000
B	-0.518285000	0.641176000	-0.934362000
B	-1.794988000	-0.306716000	0.000000000
B	1.037862000	0.487061000	0.000000000
B	0.275980000	-2.151218000	-0.924115000
C	-1.178143000	-1.897277000	0.000000000
H	-1.892071000	-2.713360000	0.000000000
F	-1.749098000	-1.301061000	2.533554000
F	0.446584000	-3.305439000	1.563251000
F	-3.109817000	-0.051129000	0.000000000
F	-1.749098000	-1.301061000	-2.533554000
F	0.446584000	-3.305439000	-1.563251000
F	-0.816199000	1.741901000	1.627945000
F	-0.816199000	1.741901000	-1.627945000
F	1.444311000	-0.338303000	-2.627708000
F	2.853120000	-1.638449000	0.000000000
F	1.444311000	-0.338303000	2.627708000
F	1.932660000	1.522334000	0.000000000
H	1.652795000	3.419270000	0.000000000
O	1.323186000	4.337280000	0.000000000
N	-0.067159000	4.175851000	0.000000000
O	-0.632985000	5.194525000	0.000000000

(NO2)2H+ (I.C.1)
E(B3LYP-D3/def2-TZVPD)=-410.650106709 a.u.,
E(CCSD(T)/def2-TZVPD)=-409.950041 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.033505 a.u.

N	1.915628000	-0.260521000	0.000000000
O	0.000000000	0.635376000	0.000000000
O	2.603243000	0.564115000	0.000000000
N	-0.967632000	-0.147033000	0.000000000
O	-2.143938000	0.514246000	0.000000000
O	-0.933788000	-1.334955000	0.000000000
H	-2.840106000	-0.177370000	0.000000000

(NO2)2H+Ar (II.C.1)
E(B3LYP-D3/def2-TZVPD)=-938.205351878 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.033801 a.u.

N	1.900782000	2.585682000	0.000000000
O	0.006457000	1.684678000	0.000000000
O	1.701966000	3.641975000	0.000000000
N	0.000000000	0.437001000	0.000000000
O	-1.250182000	-0.054153000	0.000000000
O	0.946048000	-0.282808000	0.000000000
H	-1.161482000	-1.037241000	0.000000000
Ar	-1.298795000	-3.335505000	0.000000000

(NO2)2H{F11} (III.C.1)
E(B3LYP-D3/def2-TZVPD)=-1822.61659382 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.132756 a.u.

B	-1.669817000	-1.470858000	-0.491100000
B	0.377696000	0.183701000	0.772866000
B	-1.077318000	0.295086000	1.779226000
B	-0.650250000	-1.282989000	1.017993000
B	-2.347373000	-0.718652000	0.991420000
B	-1.224278000	-0.130271000	-1.659912000
B	-1.648419000	1.438376000	-0.873417000
B	0.035971000	0.883207000	-0.842512000
B	-0.665606000	1.613435000	0.622866000
B	0.024257000	-0.904507000	-0.612016000
B	-2.699553000	-0.012006000	-0.647066000
C	-2.231193000	0.981565000	0.690244000
H	-3.008118000	1.600017000	1.124156000
F	-1.138739000	0.569660000	3.097753000
F	-3.366326000	-1.191178000	1.733664000
F	-0.336486000	2.846933000	1.086738000
F	-2.130338000	2.542061000	-1.479803000
F	-3.972821000	0.025055000	-1.082851000
F	1.679984000	0.340958000	1.226132000
F	1.100674000	1.525500000	-1.450650000
F	-1.262480000	-0.306015000	-3.002836000
F	-2.054704000	-2.693994000	-0.931433000
F	-0.219546000	-2.355025000	1.730546000
F	1.023325000	-1.698085000	-1.142226000
H	2.643076000	-2.374392000	-0.321692000
O	3.304399000	-2.082951000	0.345095000
N	3.907728000	-0.998358000	-0.227755000
O	3.808634000	-0.849323000	-1.416165000
O	4.481528000	-0.269513000	0.562878000
N	3.121768000	1.607745000	-0.130864000
O	3.201227000	2.538516000	0.409361000

N2OH{F11} (III.A.1.1)
E(SMD-B3LYP-D3/def2-TZVPD)=-1596.99666739 a.u.,
ZPE(SMD-B3LYP-D3/def2-TZVPD)=0.118529 a.u.

B	1.536113000	-1.165064000	0.000000000
B	-0.555431000	0.712108000	0.916081000
B	-0.987234000	-0.924635000	1.461981000
B	0.735381000	-0.446737000	1.484850000
B	0.286943000	-2.071231000	0.902022000
B	0.735381000	-0.446737000	-1.484850000
B	-0.987234000	-0.924635000	-1.461981000
B	-0.555431000	0.712108000	-0.916081000
B	-1.773331000	-0.210141000	0.000000000
B	0.969929000	0.526760000	0.000000000
B	0.286943000	-2.071231000	-0.902022000
C	-1.152678000	-1.808067000	0.000000000
H	-1.880958000	-2.613798000	0.000000000
F	-1.746458000	-1.242389000	2.538964000
F	0.468892000	-3.239524000	1.565457000
F	-3.110867000	0.011727000	0.000000000
F	-1.746458000	-1.242389000	-2.538964000
F	0.468892000	-3.239524000	-1.565457000
F	-0.836869000	1.865532000	1.602912000
F	-0.836869000	1.865532000	-1.602912000
F	1.438546000	-0.222141000	-2.632879000
F	2.855194000	-1.512168000	0.000000000
F	1.438546000	-0.222141000	2.632879000
F	1.924195000	1.624460000	0.000000000
H	1.588461000	2.768044000	0.000000000
O	1.368073000	3.928149000	0.000000000
N	0.169626000	4.192147000	0.000000000
N	-0.890608000	4.492617000	0.000000000

NO2H{F11} (III.B.1.1)
E(SMD-B3LYP-D3/def2-TZVPD)=-1617.44461629 a.u.,
ZPE(SMD-B3LYP-D3/def2-TZVPD)=0.115957 a.u.

B	-1.177224000	-1.086387000	-1.156174000
B	0.775893000	-0.206960000	0.868185000
B	-0.747520000	-0.515936000	1.733370000
B	-0.246767000	-1.603563000	0.282270000
B	-1.962684000	-1.108732000	0.496571000
B	-0.793454000	0.638886000	-1.534826000
B	-1.290122000	1.698306000	-0.060915000
B	0.446686000	1.234032000	-0.284814000
B	-0.367055000	1.188776000	1.363352000
B	0.500634000	-0.475881000	-0.915089000
B	-2.293493000	0.315664000	-0.641011000
C	-1.912744000	0.542979000	1.035674000
H	-2.733119000	0.856401000	1.675592000
F	-0.878697000	-0.940601000	2.993229000
F	-2.963017000	-1.895476000	0.878790000
F	-0.134440000	2.047086000	2.367662000
F	-1.787693000	2.939964000	-0.145915000
F	-3.537325000	0.505804000	-1.078619000
F	1.972524000	-0.373912000	1.445274000
F	1.390682000	2.126717000	-0.591142000
F	-0.790200000	1.137552000	-2.783092000
F	-1.540565000	-1.949301000	-2.130161000
F	0.161312000	-2.874360000	0.474956000
F	1.526764000	-0.873456000	-1.725721000
H	3.455437000	-1.089402000	-1.263006000
O	4.289422000	-1.022844000	-0.759593000
N	4.261156000	0.285537000	-0.262340000
O	5.201513000	0.514744000	0.398069000

(NO2)2H{F11} (III.C.1.1)
E(SMD-B3LYP-D3/def2-TZVPD)=-1822.64817494 a.u.,
ZPE(SMD-B3LYP-D3/def2-TZVPD)=0.132620 a.u.

B	-1.320253000	-1.670469000	-0.043467000
B	0.130902000	0.729384000	0.780698000
B	-1.462073000	0.758422000	1.563852000
B	-0.608550000	-0.805256000	1.393792000
B	-2.359002000	-0.713321000	1.049514000
B	-0.994440000	-0.666879000	-1.530455000
B	-1.844354000	0.894021000	-1.332520000
B	-0.096490000	0.818503000	-1.004913000
B	-1.153252000	1.748167000	0.089824000
B	0.225564000	-0.770002000	-0.207070000
B	-2.594212000	-0.629832000	-0.736705000
C	-2.553497000	0.787579000	0.232978000
H	-3.494019000	1.308723000	0.381875000
F	-1.782647000	1.379951000	2.727306000
F	-3.358748000	-1.195715000	1.831610000
F	-1.221440000	3.103469000	0.168182000
F	-2.456748000	1.608437000	-2.311340000
F	-3.767828000	-1.050513000	-1.274623000
F	1.271446000	1.297340000	1.331957000
F	0.867906000	1.440836000	-1.765736000
F	-0.788682000	-1.245023000	-2.753300000
F	-1.369926000	-3.037226000	-0.100906000
F	-0.097645000	-1.487035000	2.464064000
F	1.420612000	-1.421604000	-0.396250000
H	4.340397000	-2.704496000	-0.509258000
O	4.279234000	-2.180680000	0.320744000
N	4.120335000	-0.887983000	-0.074208000
O	4.129621000	-0.630331000	-1.246880000
O	3.986195000	-0.110858000	0.855510000
N	2.995887000	1.729488000	-0.157219000
O	3.429346000	2.644349000	0.189136000

(NO2)2
E(B3LYP-D3/def2-TZVPD)=-410.341615285 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.021121 a.u.

N	-1.462504000	0.384680000	0.117172000
O	-0.211674000	-0.636006000	-0.107906000
O	-2.411553000	-0.210216000	-0.015017000
N	1.039377000	0.026328000	-0.012734000
O	1.955017000	-0.740306000	0.076061000
O	1.038445000	1.226896000	-0.044521000

(NO2)2
E(SMD-B3LYP-D3/def2-TZVPD)=-410.343773986 a.u.,
ZPE(SMD-B3LYP-D3/def2-TZVPD)=0.021071 a.u.

N	1.603196000	-0.068262000	0.000000000
O	0.000000000	0.671254000	0.000000000
O	2.335225000	0.763335000	0.000000000
N	-1.012484000	-0.239637000	0.000000000
O	-2.118182000	0.253256000	0.000000000
O	-0.733915000	-1.418433000	0.000000000

H{F11}
E(B3LYP-D3/def2-TZVPD)=-1412.20047176 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.108700 a.u.

B	1.082097000	0.952996000	0.934462000
B	0.350651000	-0.638588000	-1.498614000
B	-0.637136000	0.817734000	-1.475694000
B	1.082097000	0.952996000	-0.934462000
B	-0.198804000	1.784569000	0.000000000
B	0.350651000	-0.638588000	1.498614000
B	-1.332506000	-0.780176000	0.921017000
B	-0.070809000	-1.591468000	0.000000000
B	-1.332506000	-0.780176000	-0.921017000
B	1.306806000	-0.522575000	0.000000000
B	-0.637136000	0.817734000	1.475694000
C	-1.522144000	0.665341000	0.000000000
H	-2.515973000	1.099373000	0.000000000
F	-1.192736000	1.450121000	-2.524044000
F	-0.448761000	3.106157000	0.000000000
F	-2.378484000	-1.309967000	-1.577256000
F	-2.378484000	-1.309967000	1.577256000
F	-1.192736000	1.450121000	2.524044000
F	0.848844000	-1.308292000	-2.568839000
F	0.439199000	-2.909055000	0.000000000
F	0.848844000	-1.308292000	2.568839000
F	2.040379000	1.588737000	1.641722000
F	2.040379000	1.588737000	-1.641722000
F	2.471338000	-1.545481000	0.000000000
H	1.951773000	-2.399093000	0.000000000

H{F11}
E(SMD-B3LYP-D3/def2-TZVPD)=-1412.23916274 a.u.,
ZPE(SMD-B3LYP-D3/def2-TZVPD)=0.108564 a.u.

B	1.326995000	0.791608000	0.662528000
B	-0.633992000	-1.445489000	0.560884000
B	0.370664000	-1.484707000	-0.912735000
B	1.156982000	-1.042365000	0.627728000
B	1.562195000	-0.126960000	-0.849195000
B	-0.361300000	1.519950000	0.617597000
B	-1.122450000	1.029123000	-0.919005000
B	-1.572999000	0.134109000	0.556249000
B	-1.288745000	-0.771287000	-0.955079000
B	-0.044834000	-0.022742000	1.450625000
B	0.638715000	1.426196000	-0.857440000
C	0.055959000	0.026538000	-1.665007000
H	0.091956000	0.042963000	-2.750241000
F	0.646298000	-2.576271000	-1.664674000
F	2.714694000	-0.219966000	-1.553955000
F	-2.240728000	-1.334499000	-1.736231000
F	-1.952899000	1.787598000	-1.672875000
F	1.110621000	2.478977000	-1.566547000
F	-1.128775000	-2.549755000	1.186120000
F	-2.789697000	0.228196000	1.166172000
F	-0.649031000	2.681904000	1.268424000
F	2.336545000	1.392880000	1.350258000
F	2.033498000	-1.844986000	1.292286000
F	-0.045406000	-0.070855000	2.977618000
H	-0.899941000	0.001611000	3.410147000

{F11}⁻
E(B3LYP-D3/def2-TZVPD)=-1411.83060905 a.u.,
ZPE(B3LYP-D3/def2-TZVPD)=0.098616 a.u.

B	0.000000000	1.548986000	0.643815000
B	0.910471000	-1.253156000	0.643815000
B	1.456908000	-0.473378000	-0.863945000
B	1.473173000	0.478663000	0.643815000
B	0.900418000	1.239320000	-0.863945000
B	-1.473173000	0.478663000	0.643815000
B	-1.456908000	-0.473378000	-0.863945000
B	-0.910471000	-1.253156000	0.643815000
B	0.000000000	-1.531883000	-0.863945000
B	0.000000000	0.000000000	1.576931000
B	-0.900418000	1.239320000	-0.863945000
C	0.000000000	0.000000000	-1.641027000
H	0.000000000	0.000000000	-2.723605000
F	2.533401000	-0.823152000	-1.619445000
F	1.565728000	2.155039000	-1.619445000
F	0.000000000	-2.663775000	-1.619445000
F	-2.533401000	-0.823152000	-1.619445000
F	-1.565728000	2.155039000	-1.619445000
F	1.629205000	-2.242409000	1.256908000
F	-1.629205000	-2.242409000	1.256908000
F	-2.636110000	0.856524000	1.256908000
F	0.000000000	2.771770000	1.256908000
F	2.636110000	0.856524000	1.256908000
F	0.000000000	0.000000000	2.944726000

{F11}⁻
E(SMD-B3LYP-D3/def2-TZVPD)=-1411.88955671 a.u.,
ZPE(SMD-B3LYP-D3/def2-TZVPD)=0.098185 a.u.

B	0.000000000	1.545660000	0.638274000
B	0.908516000	-1.250465000	0.638274000
B	1.454476000	-0.472588000	-0.870956000
B	1.470010000	0.477635000	0.638274000
B	0.898916000	1.237251000	-0.870956000
B	-1.470010000	0.477635000	0.638274000
B	-1.454476000	-0.472588000	-0.870956000
B	-0.908516000	-1.250465000	0.638274000
B	0.000000000	-1.529327000	-0.870956000
B	0.000000000	0.000000000	1.568978000
B	-0.898916000	1.237251000	-0.870956000
C	0.000000000	0.000000000	-1.648471000
H	0.000000000	0.000000000	-2.733698000
F	2.539886000	-0.825259000	-1.613301000
F	1.569736000	2.160556000	-1.613301000
F	0.000000000	-2.670594000	-1.613301000
F	-2.539886000	-0.825259000	-1.613301000
F	-1.569736000	2.160556000	-1.613301000
F	1.627100000	-2.239511000	1.260344000
F	-1.627100000	-2.239511000	1.260344000
F	-2.632703000	0.855417000	1.260344000
F	0.000000000	2.768188000	1.260344000
F	2.632703000	0.855417000	1.260344000
F	0.000000000	0.000000000	2.942193000