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Electronic Supporting Information

Photoelectron Spectra of Functionalized Adamantanes

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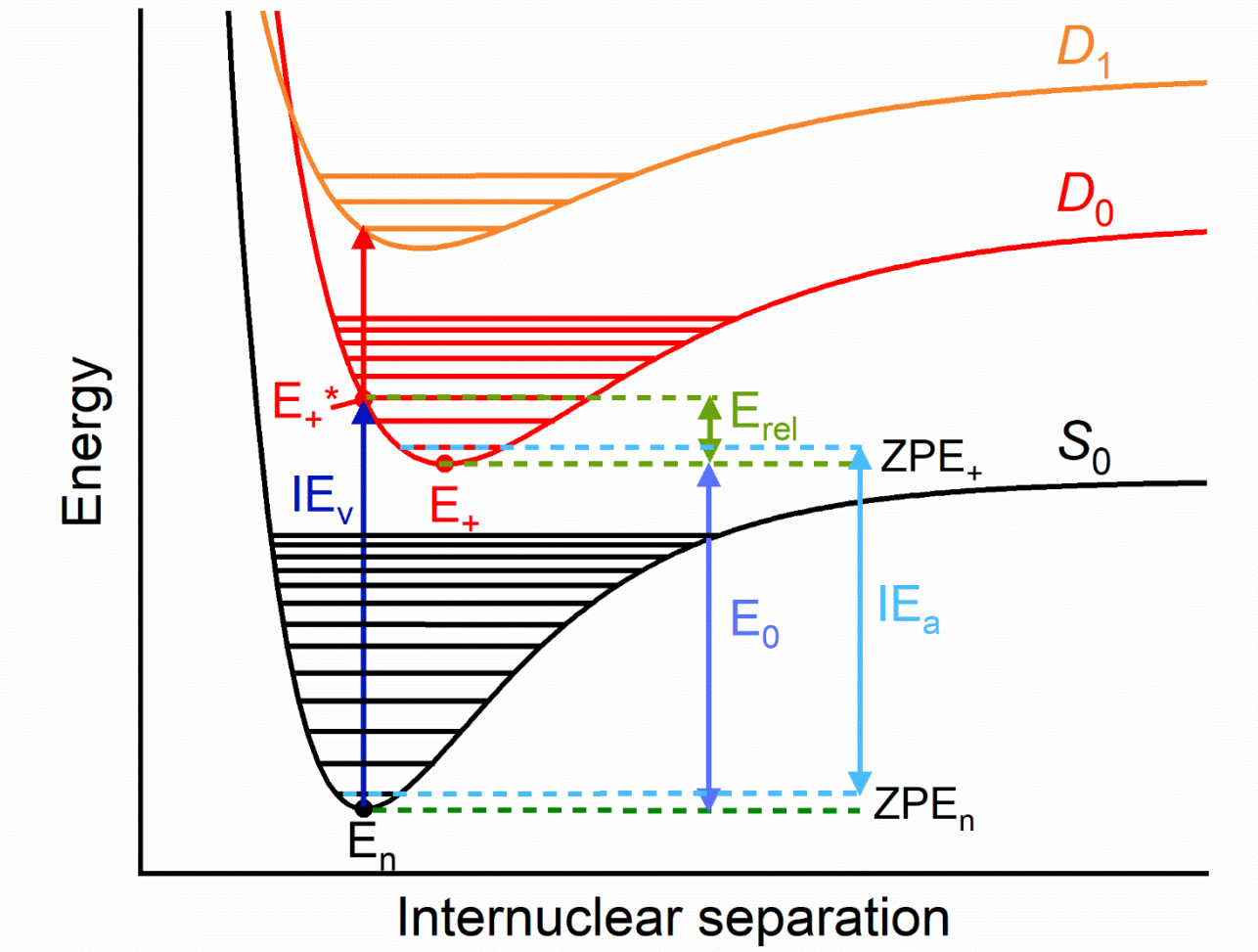


Figure S1. Schematic of the Franck-Condon principle illustrating the energy quantities described in section 2.2.

ADAMANTANE

Table S1. Assignment of the PES spectrum of Ada using MO eigenvalues of neutral Ada vs. vertical transition energies of Ada^+ computed at the M06-2X(D3)/cc-pVTZ level.

Ada MOs[a] T_d			Ada^+ TD-DFT							
			Neutral geom.[b] $T_d \rightarrow C_{3v}$				Opt. geom.[c] C_{3v}			
MO #	IE_v / eV	Sym	State	IE_v / eV	Sym	Assign.	State	IE_v / eV	Sym	Assign.
38	9.83		D_0	9.83	A_1		D_0	9.30	A_1	
37	9.83	$7t_2$	D_1	9.89	E	$7t_2$	D_1	10.46	E	$7t_2$
36	9.83			9.89	E			10.46	E	
35	11.18		D_2	11.07	A_2	$3e$	D_2	11.22	E	$3e$
34	11.18	$2t_1$	D_3	11.12	A_2	$2t_1$		11.22	E	
33	11.18		D_4	11.14	A_1	$3e$	D_3	11.79	E	
32	11.25	$3e$	D_5	11.15	E	$2t_1$		11.79	E	$2t_1$
31	11.25			11.15	E	$2t_1$	D_4	11.90	A_2	
30	13.15		D_6	13.06	E		D_5	13.25	A_1	
29	13.15	$6t_2$		13.06	E	$6t_2$	D_6	13.50	E	$6t_2$
28	13.15		D_7	13.13	A_1			13.50	E	
27	13.60		D_8	13.56	E		D_7	13.98	E	
26	13.60	$1t_1$		13.56	E	$1t_1$		13.98	E	$1t_1$
25	13.60		D_9	13.58	A_2		D_8	14.06	A_2	
24	14.92		D_{10}	14.93	E		D_9	15.34	E	
23	14.92	$5t_2$		14.93	E	$5t_2$		15.34	E	$5t_2$
22	14.92		D_{11}	14.94	A_1		D_{10}	15.47	A_1	
21	15.17	$5a_1$	D_{12}	15.28	A_1	$5a_1$	D_{11}	15.59	A_1	$5a_1$

[a] Energies are the negative MO eigenenergies ($-\varepsilon$) shifted by +0.85 eV ($IE_v + \varepsilon_{HOMO}$).

[b] Energies are shifted to match D_0 to the calculated first IE_v (9.83 eV).

[c] Energies are shifted to match D_0 to the experimental first IE_a (9.30 eV).

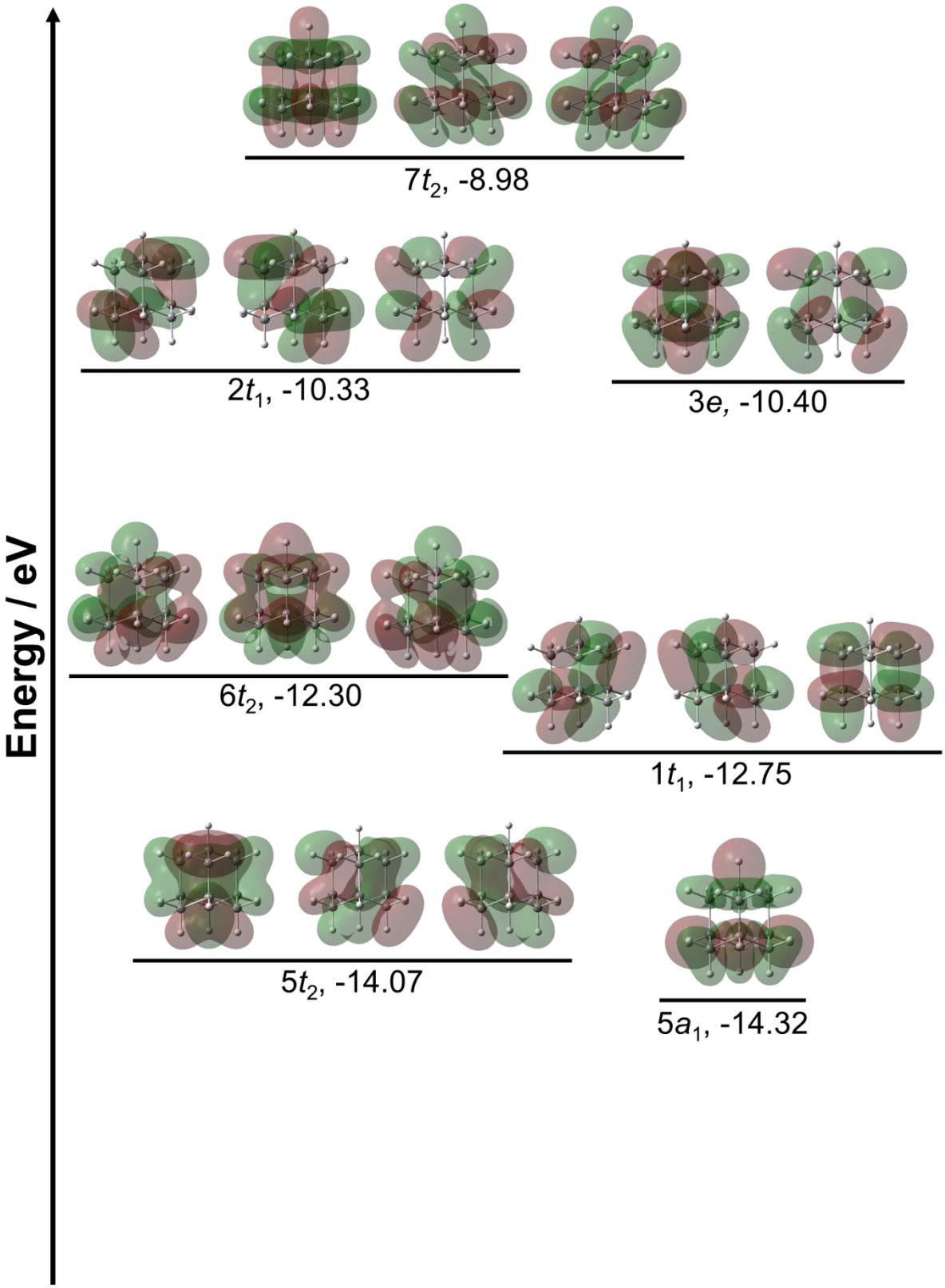


Figure S2. Canonical MOs of Ada at the M06-2X(D3)/cc-pVTZ level with symmetry labels and eigenenergies (ε), given in units of eV.

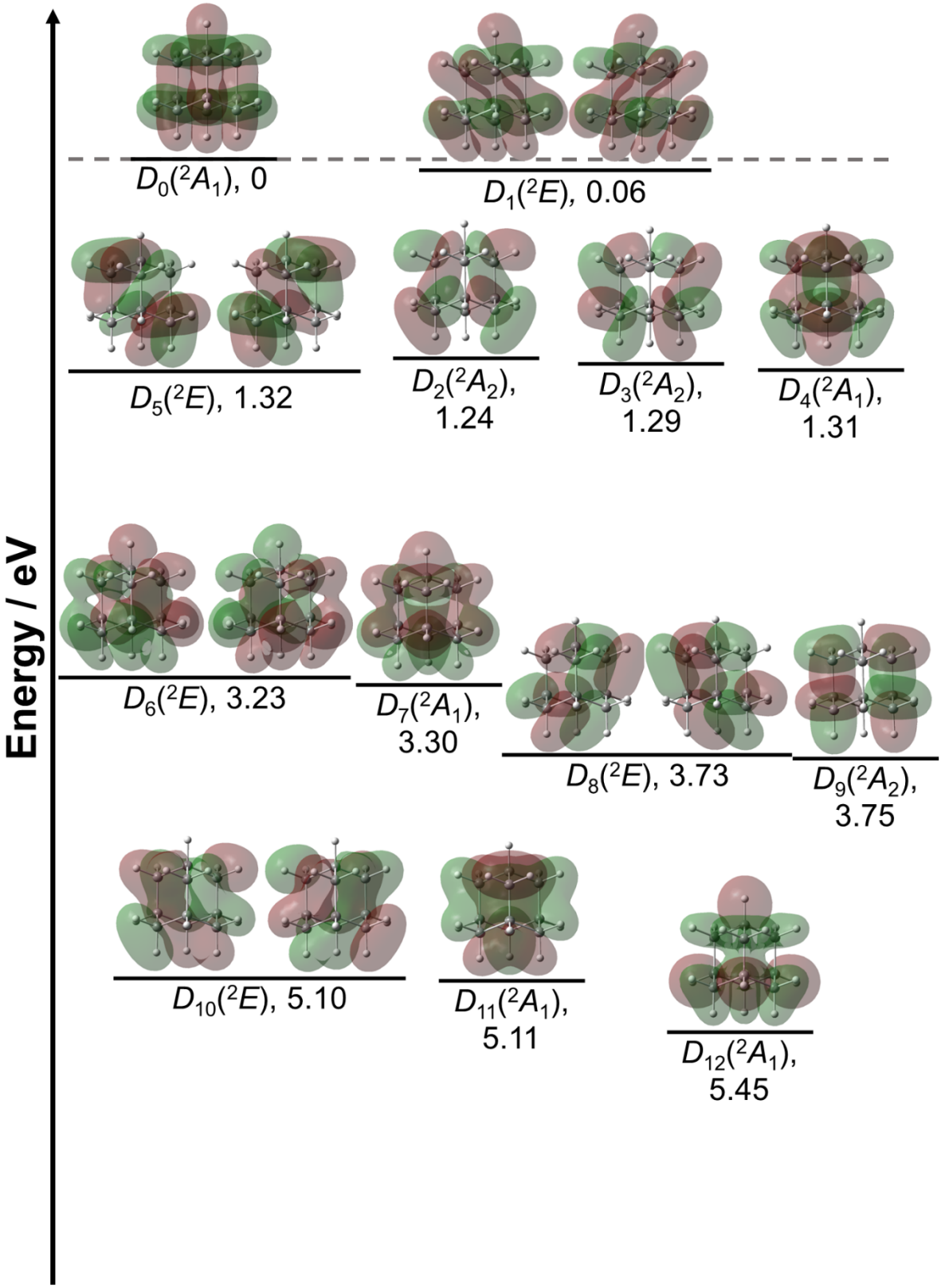


Figure S3. NTOs of Ada^+ at the M06-2X(D3)/cc-pVTZ level in the optimized neutral geometry for the first 12 excited electronic states. All transitions are in the form of SOMO ← SOMO – *n*, where *n* is the number of the excited state. Energies are given in units of eV.

Table S2. Intense FC Excitations of the Ada $D_0(^2A_1)\leftarrow S_0(^1A_1)$ Transition.

Transition Energy / cm^{-1} [a]	Mode	Intensity $\cdot 10^{-5}$ / $dm^3\ mol^{-1}\ cm^{-1}$
0	0–0	6.73
464	ν_{16}	1.91
751	ν_{14}	1.73
886	ν_{12}	5.56
1080	ν_{10}	1.82
1270	ν_9	10.01
1350	$\nu_{12} + \nu_{16}$	1.55
1636	$\nu_{12} + \nu_{14}$	1.25
1734	$\nu_9 + \nu_{16}$	2.86
1772	$2\nu_{12}$	2.06
1966	$\nu_{10} + \nu_{12}$	1.48
2020	$\nu_9 + \nu_{14}$	2.42
2156	$\nu_9 + \nu_{12}$	8.04
2349	$\nu_9 + \nu_{10}$	2.66
2540	$2\nu_9$	7.21
2620	$\nu_9 + \nu_{12} + \nu_{16}$	2.26
2906	$\nu_9 + \nu_{12} + \nu_{14}$	1.70
3004	$\nu_9 + \nu_{16}$	2.07
3042	$\nu_9 + 2\nu_{12}$	2.88
3235	$\nu_9 + \nu_{10} + \nu_{12}$	2.09
3290	$2\nu_9 + \nu_{14}$	1.64
3426	$2\nu_9 + \nu_{12}$	5.62
3619	$2\nu_9 + \nu_{10}$	1.87
3809	$3\nu_9$	3.35
3890	$2\nu_9 + \nu_{12} + \nu_{16}$	1.59
4311	$2\nu_9 + 2\nu_{12}$	1.95
4505	$2\nu_9 + \nu_{10} + \nu_{12}$	1.43
4695	$3\nu_9 + \nu_{12}$	2.53

[a] Energies are expressed in relation to the 0-0 band located at 71096 cm^{-1}.

CYANOADAMANTANE

Table S3. Assignment of the AdCN PES spectrum using MO eigenvalues of neutral AdCN vs. vertical transition energies of $AdCN^+$ computed at the M06-2X(D3)/cc-pVTZ level.

AdCN MOs[a] C_{3v}			$AdCN^+$ TD-DFT					
			Neutral geom.[b] $C_{3v} \rightarrow C_s$				Opt. geom.[c] $C_s \rightarrow C_1$	
MO #	IE_v / eV	Sym	State	IE_v / eV	Sym	Assign.	IE_v / eV	Sym
44	10.34	13*e*	D_0	10.34	*A*'	13*e*	9.78	*A*
43	10.34		D_1	10.37	*A*''		11.00	*A*
42	10.76	15a_1	D_2	10.62	*A*'	15a_1	11.49	*A*
41	11.23	12*e*	D_3	11.21	*A*''	12*e*	11.57	*A*
40	11.23		D_4	11.28	*A*'		11.88	*A*
39	11.76	2a_2	D_5	11.67	*A*''	11*e*	11.93	*A*
38	11.84	11*e*	D_6	11.70	*A*'		12.36	*A*
37	11.84		D_7	11.73	*A*''	2a_2	12.46	*A*
36	12.36	10*e*	D_8	12.38	*A*''	10*e*	12.92	*A*
35	12.36		D_9	12.46	*A*'		13.04	*A*
34	12.68	14a_1	D_{10}	12.80	*A*'	14a_1	13.39	*A*
33	13.70	9*e*	D_{11}	13.62	*A*''	9*e*	13.85	*A*
32	13.70		D_{12}	13.66	*A*'		14.04	*A*
31	14.18	1a_2	D_{13}	14.14	*A*''	1a_2	14.64	*A*
30	14.41	13a_1	D_{14}	14.36	*A*'	13a_1	14.80	*A*
29	14.50	8*e*	D_{15}	14.43	*A*''	8*e*	14.97	*A*
28	14.50		D_{16}	14.44	*A*'		15.03	*A*
27	15.46	12a_1	D_{17}	15.45	*A*'	12a_1	15.89	*A*
26	15.54	7*e*	D_{18}	15.52	*A*''	7*e*	16.05	*A*
25	15.54		D_{19}	15.52	*A*'		16.12	*A*
24	16.51	11a_1	D_{20}	16.52	*A*'	11a_1	17.01	*A*

[a] Energies are the negative MO eigenenergies ($-\varepsilon$) shifted by +0.82 eV ($IE_v + \varepsilon_{HOMO}$).

[b] Energies are shifted to match D_0 to the calculated first IE_v (10.34 eV).

[c] Energies are shifted to match D_0 to the experimental first IE_a (9.78 eV).

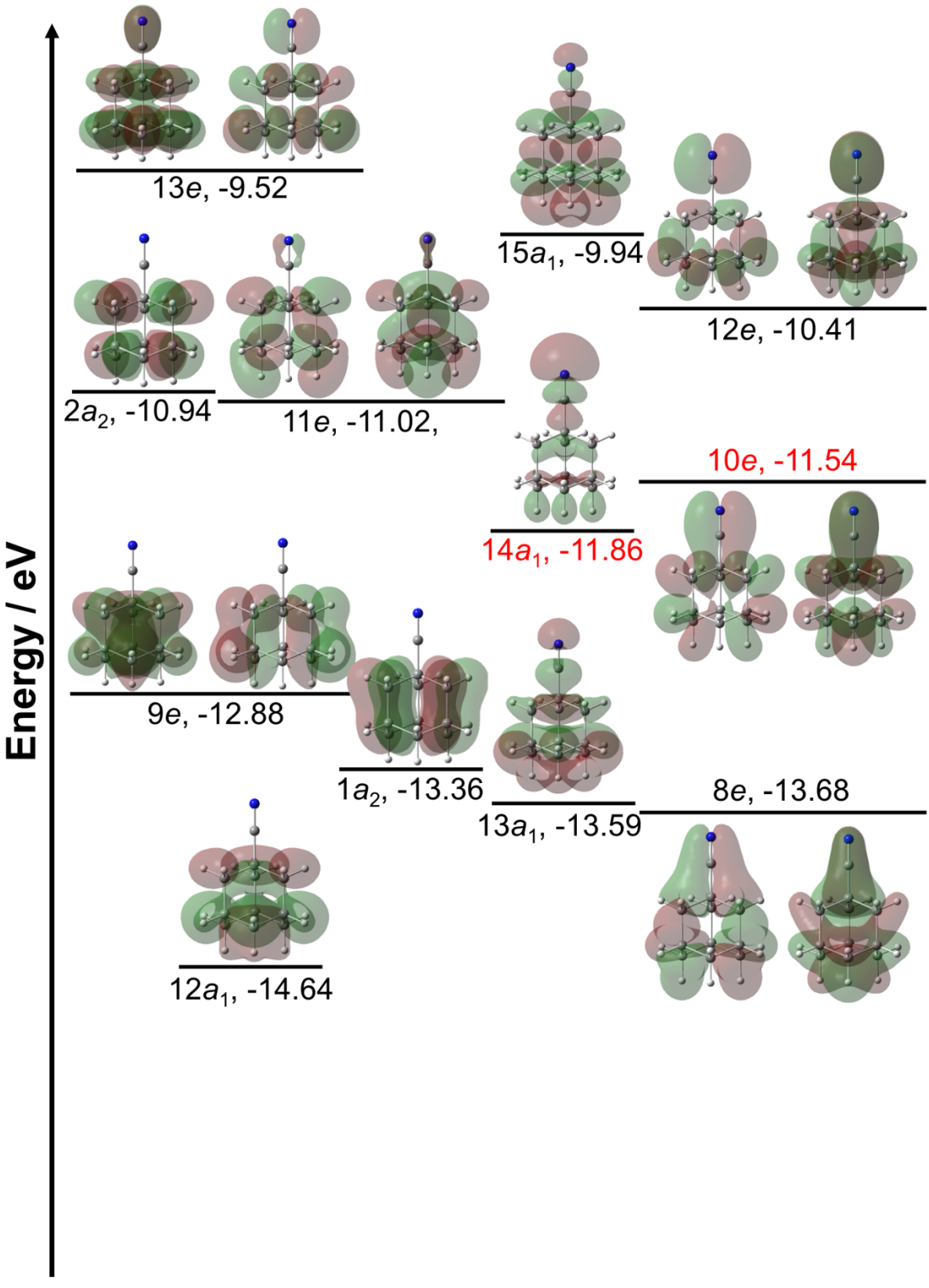


Figure S4. Canonical MOs of AdCN at the M06-2X(D3)/cc-pVTZ level with symmetry labels and eigenenergies (ε), given in units of eV. Orbitals in red are primarily attributed to the nitrile group.

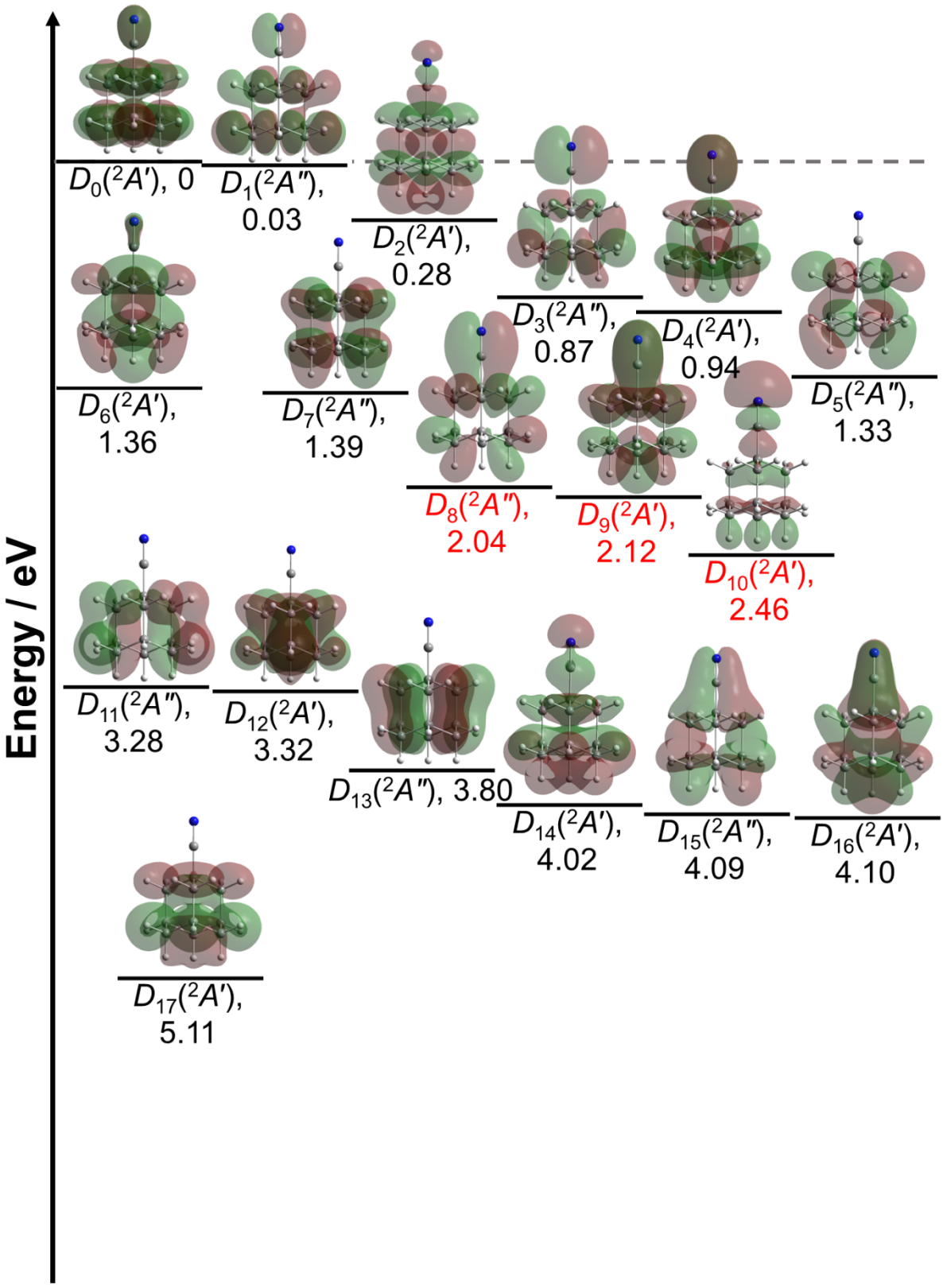


Figure S5. NTOs of $AdCN^+$ at the M06-2X(D3)/cc-pVTZ level in the optimized neutral geometry for the first 17 excited electronic states. All transitions are in the form of SOMO ← SOMO – *n*, where *n* is the number of the excited state. Energies are given in units of eV. NTOs labeled in red indicate transitions originating from orbitals primarily attributed to the nitrile group.

Table S4. Intense FC Excitations of the AdCN $D_0(^2A)\leftarrow S_0(^1A_1)$ Transition.

Transition Energy / cm^{-1} [a]	Mode	Intensity $\cdot 10^{-4}$ / $dm^3\ mol^{-1}\ cm^{-1}$
0	0–0	3.74
361	ν_{69}	0.34
447	ν_{66}	0.60
764	ν_{56}	0.54
795	ν_{55}	0.31
844	ν_{53}	0.38
848	ν_{52}	1.07
890	ν_{50}	1.28
903	ν_{49}	0.59
1077	ν_{40}	0.31
1127	ν_{37}	0.64
1221	ν_{33}	3.26
1286	ν_{30}	0.35
1303	ν_{29}	0.32
1667	$\nu_{33} + \nu_{66}$	0.52
1734	$\nu_{33} + \nu_{53}$	0.40
1985	$\nu_{33} + \nu_{56}$	0.46
2064	$\nu_{33} + \nu_{53}$	0.94
2068	$\nu_{33} + \nu_{52}$	1.22
2111	$\nu_{33} + \nu_{50}$	1.31
2123	$\nu_{33} + \nu_{49}$	0.49
2348	$\nu_{20} + \nu_{37}$	0.56
2441	$2\nu_{33}$	1.35
2507	$\nu_{33} + \nu_{30}$	0.30
3662	$3\nu_{33}$	0.35

[a] Energies are expressed in relation to the 0-0 band located at 75105 cm^{-1}

AMANTADINE

Table S5. Assignment of the $AdNH_2$ PES spectrum using MO eigenvalues of neutral $AdNH_2$ vs. vertical transition energies of $AdNH_2^+$ computed at the M06-2X(D3)/cc-pVTZ level.

$AdNH_2$ MOs[a] C_s			$AdNH_2^+$ TD-DFT						
			Neutral geom.[b] C_s				Opt. geom.[c] C_s		
MO #	IE_v / eV	Sym	State	IE_v / eV	Sym	Assign.	IE_v / eV	Sym	Assign.
42	8.88	27*a*'	D_0	8.88	*A*'	27*a*'	8.27	*A*'	27*a*'
41	9.84	15*a*''	D_1	9.69	*A*''	15*a*''	10.63	*A*''	15*a*''
40	10.02	26*a*'	D_2	9.91	*A*'	26*a*'	10.78	*A*'	26*a*'
39	10.36	25*a*'	D_3	10.22	*A*'	25*a*'	11.02	*A*'	25*a*'
38	11.11	14*a*''	D_4	10.94	*A*''	14*a*''	11.84	*A*'	24*a*'
37	11.18	13*a*''	D_5	11.09	*A*''	13*a*''	11.89	*A*''	14*a*''
36	11.25	24*a*'	D_6	11.12	*A*'	24*a*'	11.93	*A*''	13*a*''
35	11.26	12*a*''	D_7	11.14	*A*''	12*a*''	11.99	*A*''	12*a*''
34	11.53	23*a*'	D_8	11.45	*A*'	23*a*'	12.22	*A*'	23*a*'
33	13.08	11*a*''	D_9	12.97	*A*''	11*a*''	13.72	*A*'	11*a*''
32	13.15	22*a*'	D_{10}	13.05	*A*'	22*a*'	13.72	*A*''	22*a*'
31	13.28	10*a*''	D_{11}	13.13	*A*'	21*a*'	14.02	*A*'	21*a*'
30	13.35	21*a*'	D_{12}	13.21	*A*''	10*a*''	14.07	*A*''	10*a*''
29	13.59	9*a*''	D_{13}	13.50	*A*''	9*a*''	14.35	*A*''	9*a*''
28	14.01	20*a*'	D_{14}	13.90	*A*'	20*a*'	14.51	*A*'	20*a*'
27	14.89	8*a*''	D_{15}	14.82	*A*''	8*a*''	15.53	*A*''	8*a*''
26	14.91	19*a*'	D_{16}	14.84	*A*'	19*a*'	15.56	*A*'	19*a*'
25	14.94	18*a*'	D_{17}	14.85	*A*'	18*a*'	15.71	*A*'	18*a*'
24	15.33	17*a*'	D_{18}	15.21	*A*'	17*a*'	15.75	*A*'	17*a*'
23	15.59	16*a*'	D_{19}	15.45	*A*'	16*a*'	16.29	*A*'	16*a*'

[a] Energies are the negative MO eigenenergies ($-\varepsilon$) shifted by +0.79 eV ($IE_v + \varepsilon_{HOMO}$).

[b] Energies are shifted to match D_0 to the calculated first IE_v (8.88 eV).

[c] Energies are shifted to match D_0 to the experimental first IE_a (8.27 eV).

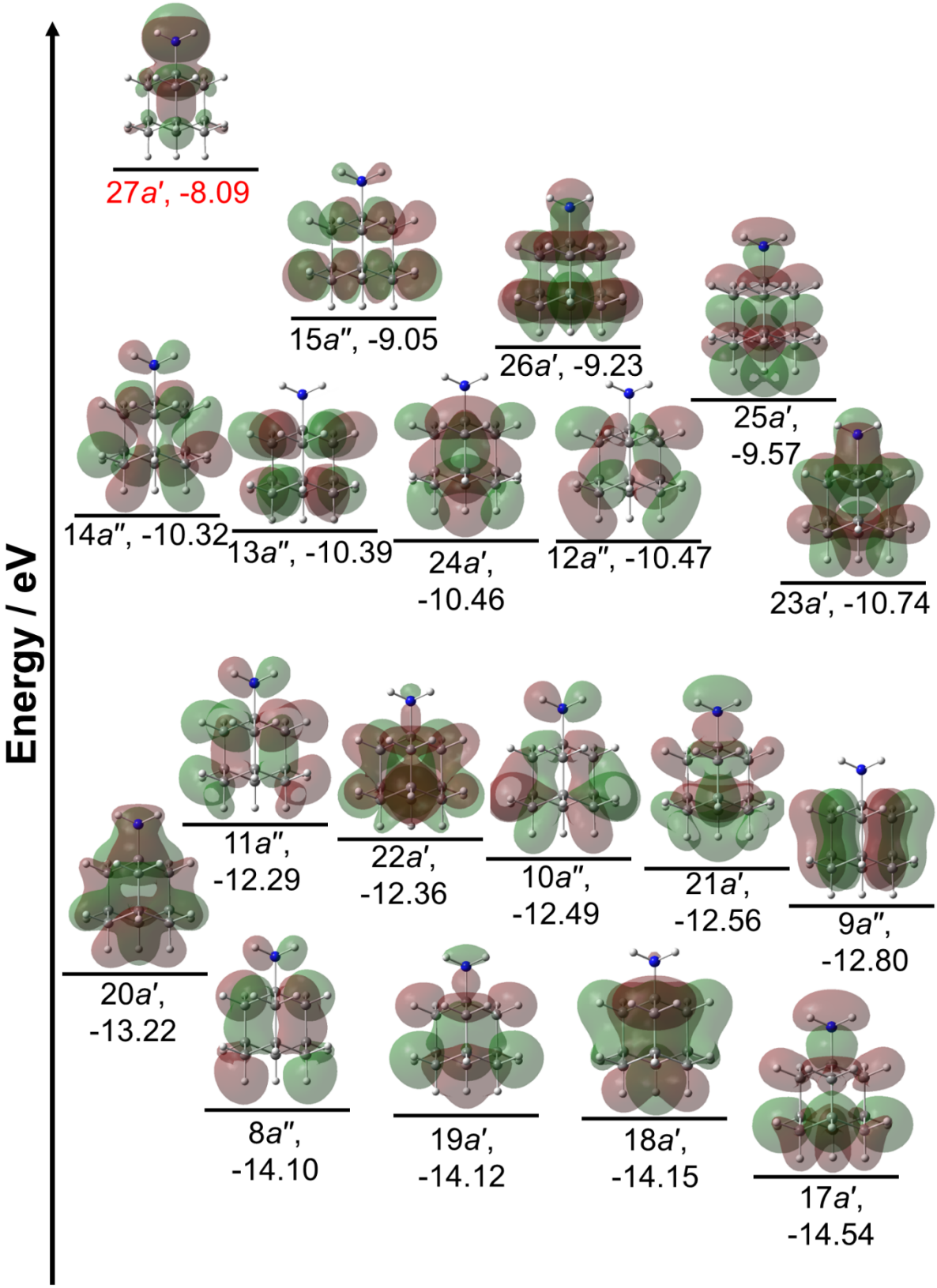


Figure S6. Canonical MOs of $AdNH_2$ at the M06-2X(D3)/cc-pVTZ level with symmetry labels and eigenenergies (ε), given in units of eV. The HOMO (red) is primarily attributed to the nitrogen lone pair (n_N) of the amino group.

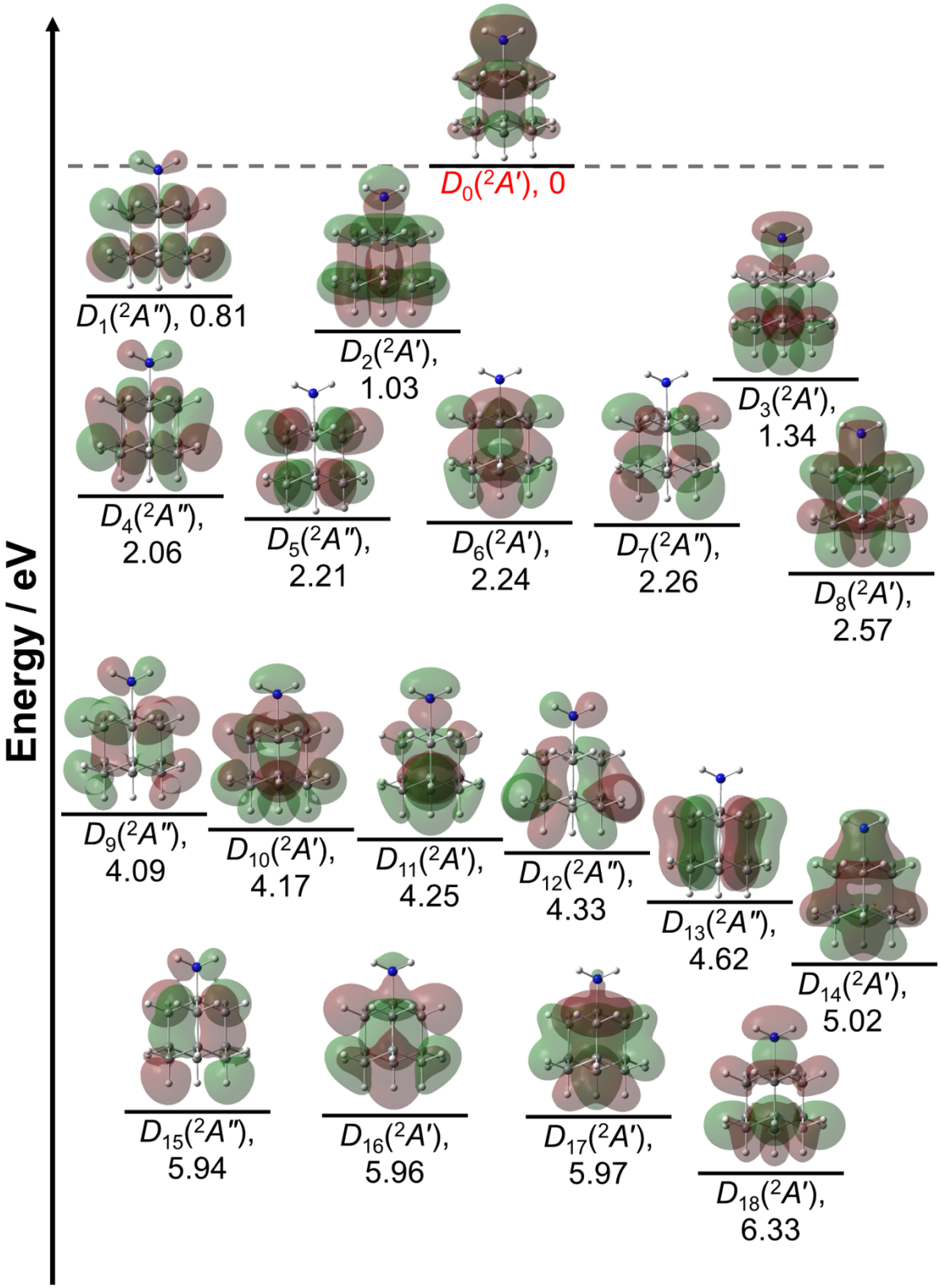


Figure S7. NTOs of $AdNH_2^+$ at the M06-2X(D3)/cc-pVTZ level in the optimized neutral geometry for the first 18 excited electronic states. All transitions are in the form of SOMO ← SOMO – *n*, where *n* is the number of the excited state and the SOMO (red) is primarily attributed to the nitrogen lone pair (n_N) of the amino group. Energies are given in units of eV.

Table S6. Intense FC Excitations of the $AdNH_2$ $D_0(^2A')\leftarrow S_0(^1A')$ Transition.

Transition Energy / cm^{-1} [a]	Mode	Intensity $\cdot 10^{-4}$ / $dm^3\ mol^{-1}\ cm^{-1}$
0	0–0	0.76
615	ν_{36}	3.54
1229	$2\nu_{36}$	7.46
1279	$\nu_{35} + \nu_{36}$	3.81
1731	$2\nu_{36} + \nu_{37}$	3.04
1844	$3\nu_{36}$	9.32
1894	$\nu_{35} + 2\nu_{36}$	7.49
1993	$\nu_{34} + 2\nu_{36}$	3.02
2346	$3\nu_{36} + \nu_{37}$	4.13
2396	$\nu_{35} + 2\nu_{36} + \nu_{37}$	2.79
2458	$4\nu_{36}$	7.58
2508	$\nu_{35} + 3\nu_{36}$	8.63
2558	$2\nu_{35} + 2\nu_{36}$	3.49
2608	$\nu_{34} + 3\nu_{36}$	3.48
2658	$\nu_{34} + \nu_{35} + 2\nu_{36}$	2.73
2960	$4\nu_{36} + \nu_{37}$	3.70
3010	$\nu_{35} + 3\nu_{36} + \nu_{37}$	3.52
3073	$5\nu_{36}$	4.13
3123	$\nu_{35} + 4\nu_{36}$	6.36
3173	$2\nu_{35} + 3\nu_{36}$	3.67
3222	$\nu_{34} + 4\nu_{36}$	2.57
3272	$\nu_{34} + \nu_{35} + 3\nu_{36}$	2.87
3625	$\nu_{35} + 4\nu_{36} + \nu_{37}$	2.87
3737	$\nu_{35} + 5\nu_{36}$	3.05
4735	$\nu_1 + 2\nu_{36}$	2.39
5350	$\nu_1 + 3\nu_{36}$	4.09
5400	$\nu_1 + \nu_{35} + 2\nu_{36}$	2.85
5964	$\nu_1 + 4\nu_{36}$	4.55
6014	$\nu_1 + \nu_{35} + 3\nu_{36}$	4.47
6579	$\nu_1 + 5\nu_{36}$	3.43
6629	$\nu_1 + \nu_{35} + 4\nu_{36}$	4.52
7243	$\nu_1 + \nu_{35} + 5\nu_{36}$	3.03

[a] Energies are expressed in relation to the 0-0 band located at 65721cm^{-1}.

1-ADAMANTANOL

Table S7. Assignment of the 1-AdOH PES spectrum using MO eigenvalues of neutral 1-AdOH vs. vertical transition energies of 1-AdOH$^+$ computed at the M06-2X(D3)/cc-pVTZ level.

1-AdOH MOs[a] C_s			1-AdOH$^+$ TD-DFT					
			Neutral geom.[b] C_s				Opt. geom.[c] $C_s \rightarrow C_1$	
MO #	IE_v / eV	Sym	State	IE_v / eV	Sym	Assign.	IE_v / eV	Sym
42	9.54	15*a*''	D_0	9.54	*A*''	15*a*''	9.07	*A*
41	9.89	27*a*'	D_1	9.89	*A*''	27*a*'	11.21	*A*
40	10.49	14*a*''	D_2	10.50	*A*''	26*a*'	11.63	*A*
39	10.54	26*a*'	D_3	10.52	*A*'	14*a*''	11.88	*A*
38	11.05	25*a*'	D_4	11.05	*A*''	25*a*'	12.31	*A*
37	11.26	13*a*''	D_5	11.35	*A*'	13*a*''	12.50	*A*
36	11.35	24*a*'	D_6	11.36	*A*''	24*a*'	12.53	*A*
35	11.35	12*a*''	D_7	11.37	*A*'	12*a*''	12.58	*A*
34	12.02	11*a*''	D_8	12.11	*A*'	11*a*''	13.34	*A*
33	12.73	23*a*'	D_9	12.68	*A*''	23*a*'	13.89	*A*
32	13.25	10*a*''	D_{10}	13.34	*A*'	10*a*''	14.24	*A*
31	13.27	22*a*'	D_{11}	13.34	*A*''	22*a*'	14.53	*A*
30	13.67	9*a*''	D_{12}	13.72	*A*''	21*a*'	14.86	*A*
29	13.72	21*a*'	D_{13}	13.75	*A*'	9*a*''	14.93	*A*
28	14.24	8*a*''	D_{14}	14.30	*A*'	8*a*''	15.32	*A*
27	14.71	20*a*'	D_{15}	14.77	*A*''	20*a*'	16.03	*A*
26	15.01	19*a*'	D_{16}	15.11	*A*''	19*a*'	16.06	*A*
25	15.05	7*a*''	D_{17}	15.14	*A*'	7*a*''	16.11	*A*
24	15.08	18*a*'	D_{18}	15.16	*A*''	18*a*'	16.27	*A*
23	16.23	17*a*'	D_{19}	16.24	*A*''	17*a*'	16.43	*A*

[a] Energies are the negative MO eigenenergies ($-\varepsilon$) shifted by +0.79 eV ($IE_v + \varepsilon_{HOMO}$).

[b] Energies are shifted to match D_0 to the calculated first IE_v (9.54 eV).

[c] Energies are shifted to match D_0 to the experimental first IE_a (9.07 eV).

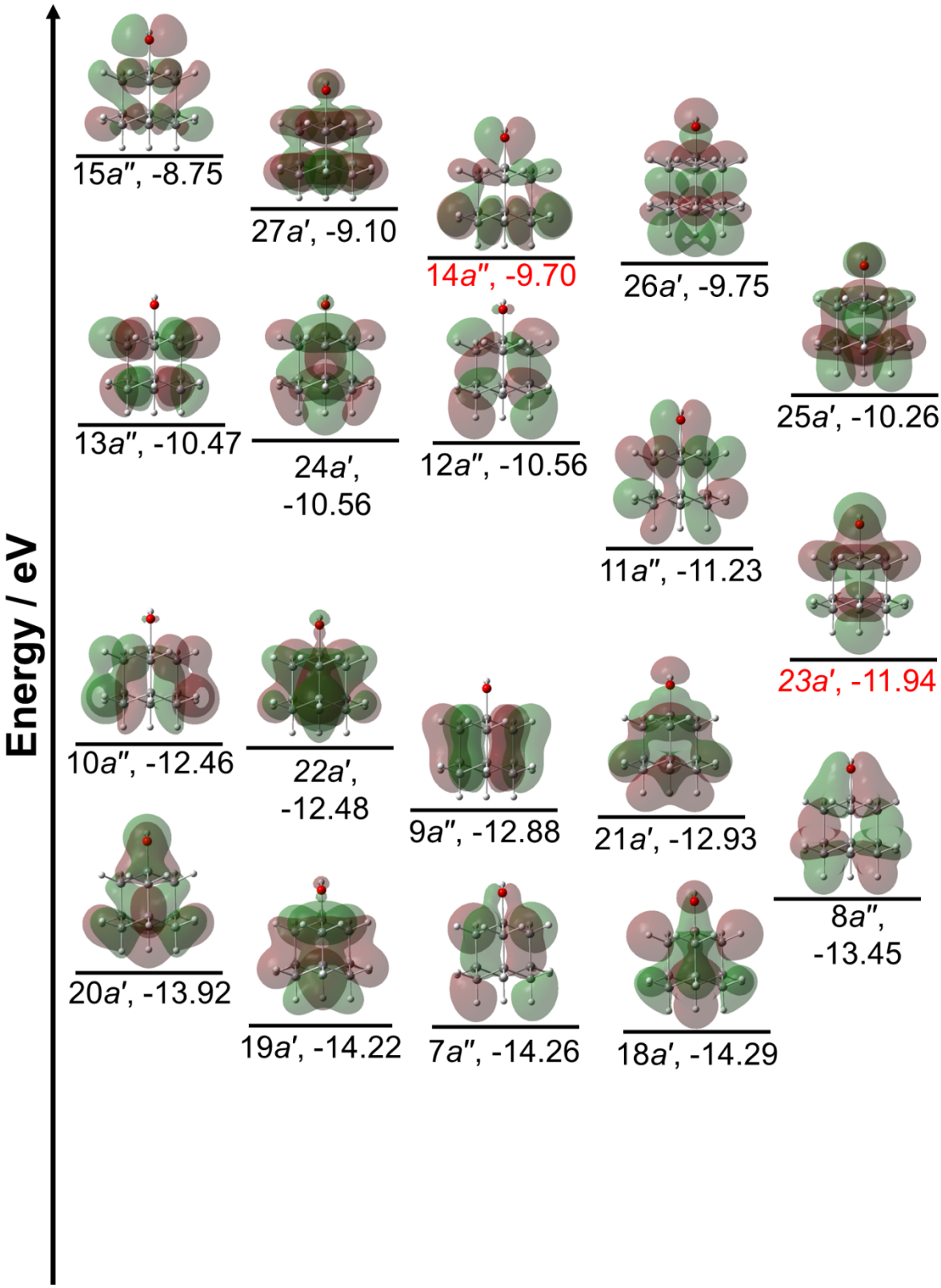


Figure S8. Canonical MOs of 1-AdOH at the M06-2X(D3)/cc-pVTZ level with symmetry labels and eigenenergies (ε), given in units of eV. Orbitals in red are primarily attributed to the oxygen lone pairs (n_O) of the hydroxy group.

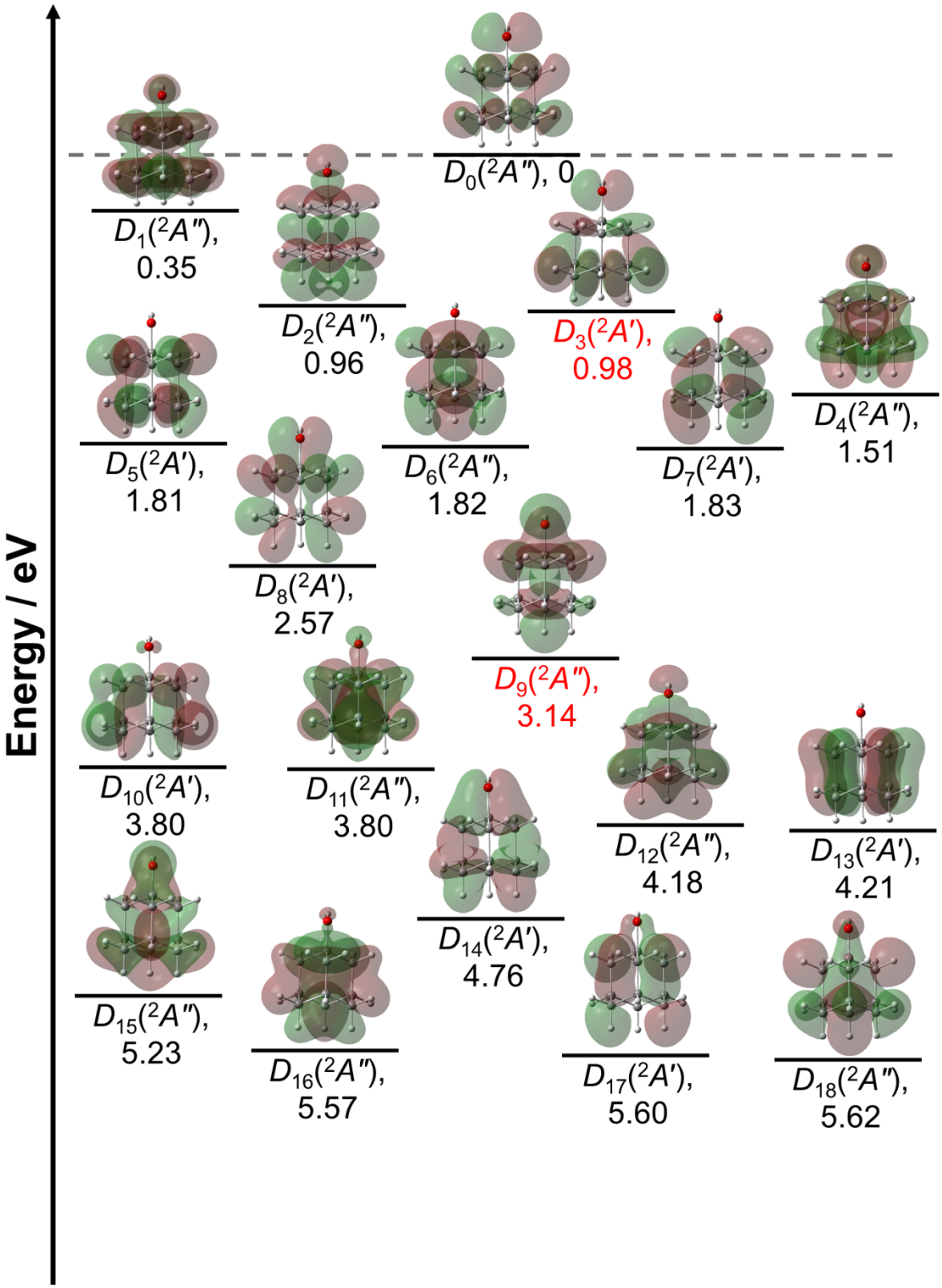


Figure S9. NTOs of 1-AdOH$^+$ at the M06-2X(D3)/cc-pVTZ level in the optimized neutral geometry for the first 18 excited electronic states. All transitions are in the form of SOMO ← SOMO – *n*, where *n* is the number of the excited state. NTOs labeled in red indicate transitions originating from orbitals primarily attributed to the hydroxy group. Energies are given in units of eV.

Table S8. Intense FC Excitations of the 1-AdOH $D_0(^2A)\leftarrow S_0(^1A')$ Transition.

Transition Energy / cm^{-1} [a]	Mode	Intensity $\cdot 10^{-3}$ / $dm^3\ mol^{-1}\ cm^{-1}$
0	0-0	2.90
330	ν_{72}	2.83
393	ν_{70}	1.99
407	ν_{69}	2.83
487	ν_{65}	5.93
533	ν_{64}	5.13
817	$\nu_{65} + \nu_{72}$	5.04
863	$\nu_{64} + \nu_{72}$	4.87
879	$\nu_{65} + \nu_{70}$	3.49
893	$\nu_{65} + \nu_{69}$	5.32
926	$\nu_{64} + 2\nu_{70}$	3.40
940	$\nu_{64} + \nu_{69}$	4.93
974	$2\nu_{65}$	5.49
1020	$\nu_{64} + \nu_{65}$	10.42
1067	$2\nu_{64}$	3.95
1207	ν_{37}	2.88
1223	$\nu_{65} + \nu_{69} + \nu_{72}$	3.91
1270	$\nu_{64} + \nu_{69} + \nu_{72}$	4.12
1304	$2\nu_{65} + \nu_{72}$	3.97
1350	$\nu_{64} + \nu_{65} + \nu_{72}$	8.60
1380	$2\nu_{65} + \nu_{69}$	4.47
1397	$2\nu_{64} + \nu_{72}$	3.62
1427	$\nu_{64} + \nu_{65} + \nu_{69}$	9.20
1507	$2\nu_{64} + \nu_{65}$	7.95
1694	$\nu_{37} + \nu_{65}$	5.77
1740	$\nu_{37} + \nu_{64}$	3.61
1820	$\nu_{64} + \nu_{65} + \nu_{69} + \nu_{70}$	4.29

[a] Energies are expressed in relation to the 0-0 band located at 71559 cm^{-1}.

2-ADAMANTANOL

Table S9. Assignment of the 2-AdOH PES spectrum using MO eigenvalues of neutral 2-AdOH vs. vertical transition energies of 2-AdOH$^+$ computed at the M06-2X(D3)/cc-pVTZ level.

2-AdOH MOs[a] C_1			2-AdOH$^+$ TD-DFT						
			Neutral geom.[b] C_1				Opt. geom.[c] C_1		
MO #	IE_v / eV	Sym	State	IE_v / eV	Sym	Assign.	IE_v / eV	Sym	Assign.
42	9.67	42*a*	D_0	9.67	*A*	42*a*	9.07	*A*	42*a*
41	9.86	41*a*	D_1	9.76	*A*	41*a*	11.23	*A*	41*a*
40	9.97	40*a*	D_2	9.93	*A*	40*a*	11.28	*A*	40*a*
39	10.34	39*a*	D_3	10.29	*A*	39*a*	11.61	*A*	39*a*
38	11.00	38*a*	D_4	10.95	*A*	38*a*	12.27	*A*	38*a*
37	11.22	37*a*	D_5	11.22	*A*	36*a*	12.33	*A*	36*a*
36	11.29	36*a*	D_6	11.26	*A*	37*a*	12.54	*A*	37*a*
35	11.69	35*a*	D_7	11.66	*A*	35*a*	13.08	*A*	35*a*
34	12.14	34*a*	D_8	12.06	*A*	34*a*	13.50	*A*	34*a*
33	12.69	33*a*	D_9	12.68	*A*	33*a*	13.89	*A*	33*a*
32	13.20	32*a*	D_{10}	13.17	*A*	32*a*	14.07	*A*	32*a*
31	13.27	31*a*	D_{11}	13.25	*A*	31*a*	14.24	*A*	31*a*
30	13.36	30*a*	D_{12}	13.36	*A*	30*a*	14.65	*A*	30*a*
29	13.64	29*a*	D_{13}	13.66	*A*	29*a*	14.74	*A*	29*a*
28	14.04	28*a*	D_{14}	14.03	*A*	28*a*	15.27	*A*	28*a*
27	14.58	27*a*	D_{15}	14.60	*A*	27*a*	15.58	*A*	27*a*
26	14.95	26*a*	D_{16}	14.99	*A*	26*a*	16.00	*A*	26*a*
25	15.19	25*a*	D_{17}	15.27	*A*	25*a*	16.19	*A*	25*a*
24	15.41	24*a*	D_{18}	15.45	*A*	24*a*	16.22	*A*	24*a*
23	16.43	23*a*	D_{19}	16.39	*A*	23*a*	16.39	*A*	23*a*

[a] Energies are the negative MO eigenenergies (-ε) shifted by +0.82 eV (IE_v + ε_{HOMO}).

[b] Energies are shifted to match D_0 to the calculated first IE_v (9.67 eV).

[c] Energies are shifted to match D_0 to the experimental first IE_a (9.07 eV).

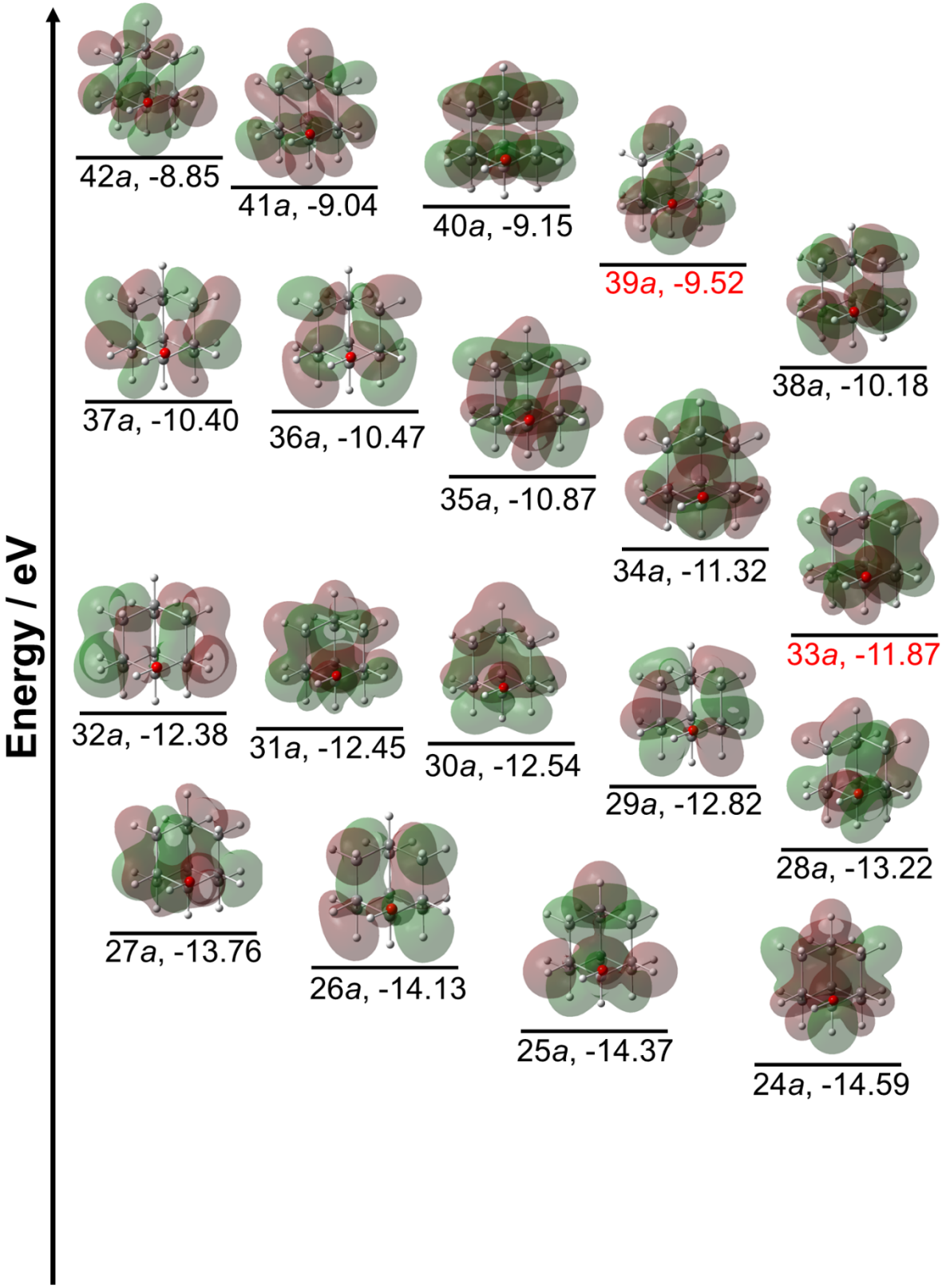


Figure S10. Canonical MOs of 2-AdOH at the M06-2X(D3)/cc-pVTZ level with symmetry labels and eigenenergies (ε), given in units of eV Orbitals in red are primarily attributed to the oxygen lone pairs (n_O) of the hydroxy group.

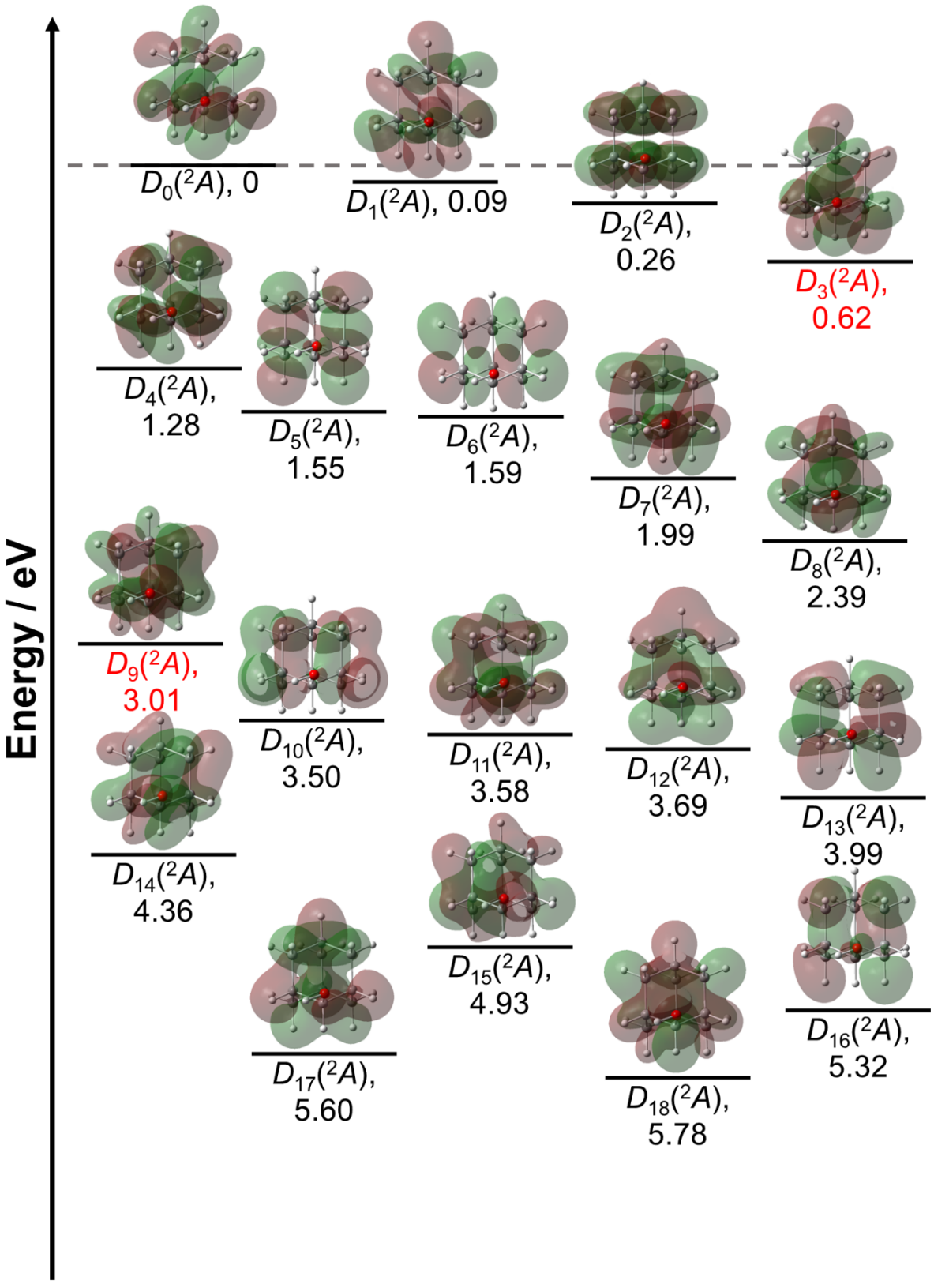


Figure S11. NTOs of 2-AdOH$^+$ at the M06-2X(D3)/cc-pVTZ level in the optimized neutral geometry for the first 18 excited electronic states. All transitions are in the form of SOMO ← SOMO – *n*, where *n* is the number of the excited state. NTOs labeled in red indicate transitions originating from orbitals primarily attributed to the hydroxy group. Energies are given in units of eV.

Table S10. Intense FC Excitations of the 2-AdOH $D_0(^2A)\leftarrow S_0(^1A)$ Transition.

Transition Energy / cm^{-1} [a]	Mode	Intensity $\cdot 10^{-4}$ / $dm^3\ mol^{-1}\ cm^{-1}$
0	0–0	0.67
68	ν_{75}	2.06
135	$2\nu_{75}$	1.70
504	$\nu_{67} + \nu_{75}$	0.72
506	ν_{65}	1.02
574	$\nu_{65} + \nu_{75}$	3.16
641	$\nu_{65} + 2\nu_{75}$	2.66
844	$\nu_{65} + 5\nu_{75}$	0.85
848	$\nu_{65} + \nu_{73} + \nu_{75}$	0.72
935	$\nu_{65} + \nu_{70} + \nu_{75}$	0.75
1011	$\nu_{65} + \nu_{67} + \nu_{75}$	1.03
1017	$\nu_{50} + \nu_{75}$	1.03
1078	$\nu_{65} + \nu_{67} + 2\nu_{75}$	2.78
1080	$2\nu_{65} + \nu_{75}$	1.80
1085	$\nu_{50} + 2\nu_{75}$	0.78
1147	$2\nu_{65} + 2\nu_{75}$	1.56
1263	$\nu_{38} + \nu_{75}$	1.32
1331	$\nu_{38} + 2\nu_{75}$	1.03
1524	$\nu_{50} + \nu_{65} + \nu_{75}$	1.63
1591	$\nu_{50} + \nu_{65} + 2\nu_{75}$	1.26
1770	$\nu_{38} + \nu_{65} + \nu_{75}$	1.90
1829	$\nu_{35} + \nu_{65} + \nu_{75}$	0.83
1837	$\nu_{38} + \nu_{65} + 2\nu_{75}$	1.52

[a] Energies are expressed in relation to the 0-0 band located at 70958 cm^{-1}.

UROTROPINE

Table S11. Assignment of the Uro PES spectrum using MO eigenvalues of neutral Uro vs. vertical transition energies of Uro^+ computed at the M06-2X(D3)/cc-pVTZ level.

Uro MOs[a] T_d			Uro^+ TD-DFT							
			Neutral geom.[b] $T_d \rightarrow C_{3v}$				Opt. geom.[c] C_{2v}			
MO #	IE_v / eV	Sym	State	IE_v / eV	Sym	Assign.	State	IE_v / eV	Sym	Assign.
38	8.60		D_0	8.60	A_1		D_0	8.03	B_1	
37	8.60	$7t_2$	D_1	8.79	E	$7t_2$	D_1	8.68	B_1	$7t_2$
36	8.60			8.79	E		D_2	8.92	A_2	
35	12.39		D_2	12.45	A_2		D_3	12.87	B_2	$3e$
34	12.39	$2t_1$	D_3	12.45	E	$2t_1$	D_4	12.90	A_1	$2t_1$
33	12.39			12.45	E		D_5	12.92	B_1	$3e$
32	12.84	$3e$	D_4	12.76	A_1	$3e$	D_6	13.15	A_2	$2t_1$
31	12.84		D_5	12.77	A_2		D_7	13.27	B_2	$2t_1$
30	12.92	$5a_1$	D_6	12.82	A_1	$5a_1$	D_8	13.61	B_1	$5a_1$
29	13.23		D_7	13.19	A_1		D_9	13.62	A_1	
28	13.23	$6t_2$	D_8	13.19	E	$6t_2$	D_{10}	13.92	A_2	$6t_2$
27	13.23			13.19	E		D_{11}	13.98	B_1	
26	15.68		D_9	15.55	A_2		D_{12}	15.61	A_1	
25	15.68	$1t_1$	D_{10}	15.57	E	$1t_1$	D_{13}	15.82	B_2	$1t_1$
24	15.68			15.57	E		D_{14}	16.14	A_2	
23	16.27		D_{11}	16.32	A_1		D_{15}	16.81	A_1	
22	16.27	$5t_2$	D_{12}	16.33	E	$5t_2$	D_{16}	16.81	A_2	$5t_2$
21	16.27			16.33	E		D_{17}	17.01	B_1	

[a] Energies are the negative MO eigenenergies ($-\varepsilon$) shifted by +0.83 eV ($IE_v + \varepsilon_{HOMO}$).

[b] Energies are shifted to match D_0 to the calculated first IE_v (8.60 eV).

[c] Energies are shifted to match D_0 to the experimental first IE_a (8.03 eV).

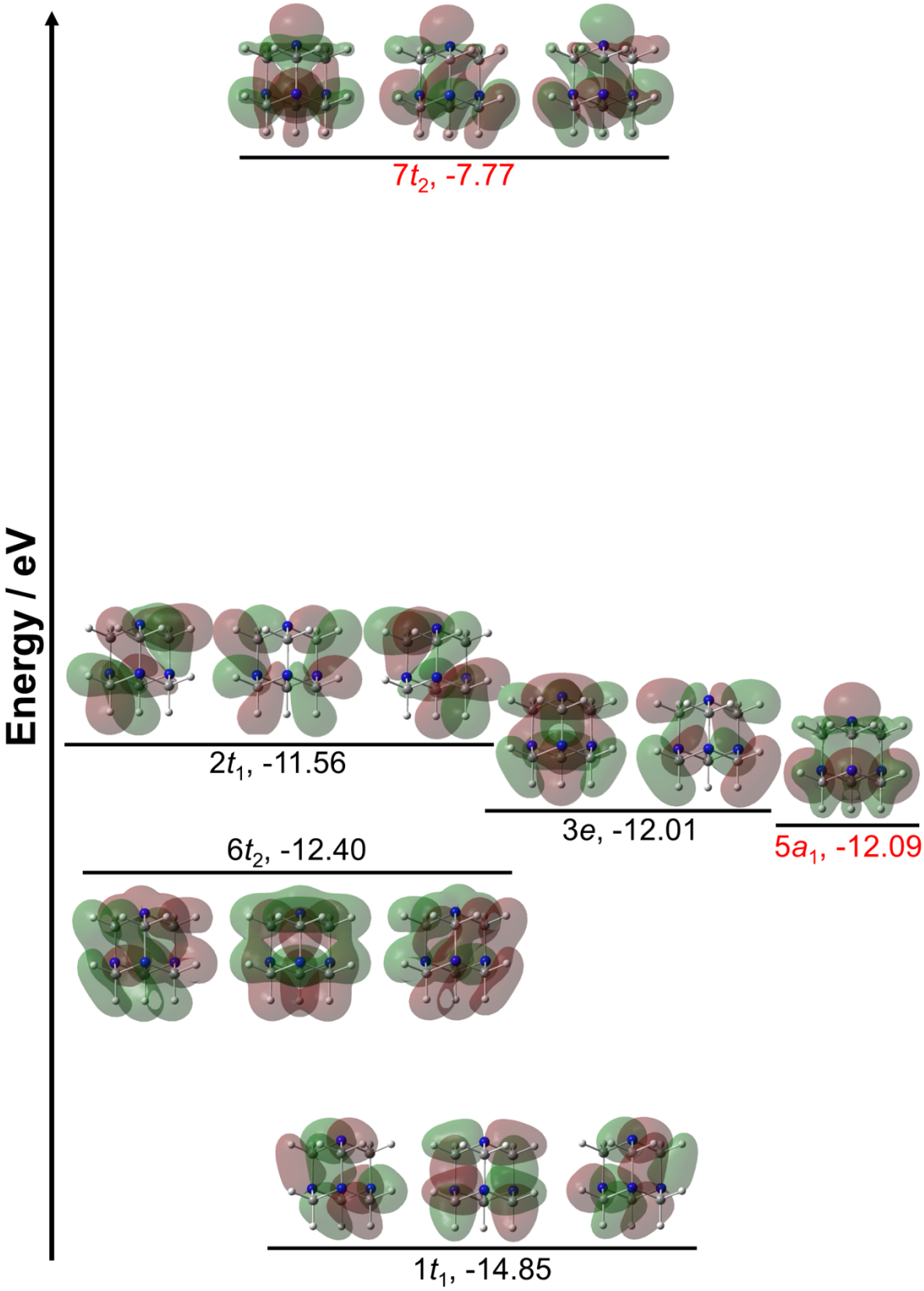


Figure S12. Canonical MOs of Uro at the M06-2X(D3)/cc-pVTZ level with symmetry labels and eigenenergies (ε), given in units of eV. Orbitals in red are primarily attributed to the four nitrogen lone pairs (n_N).

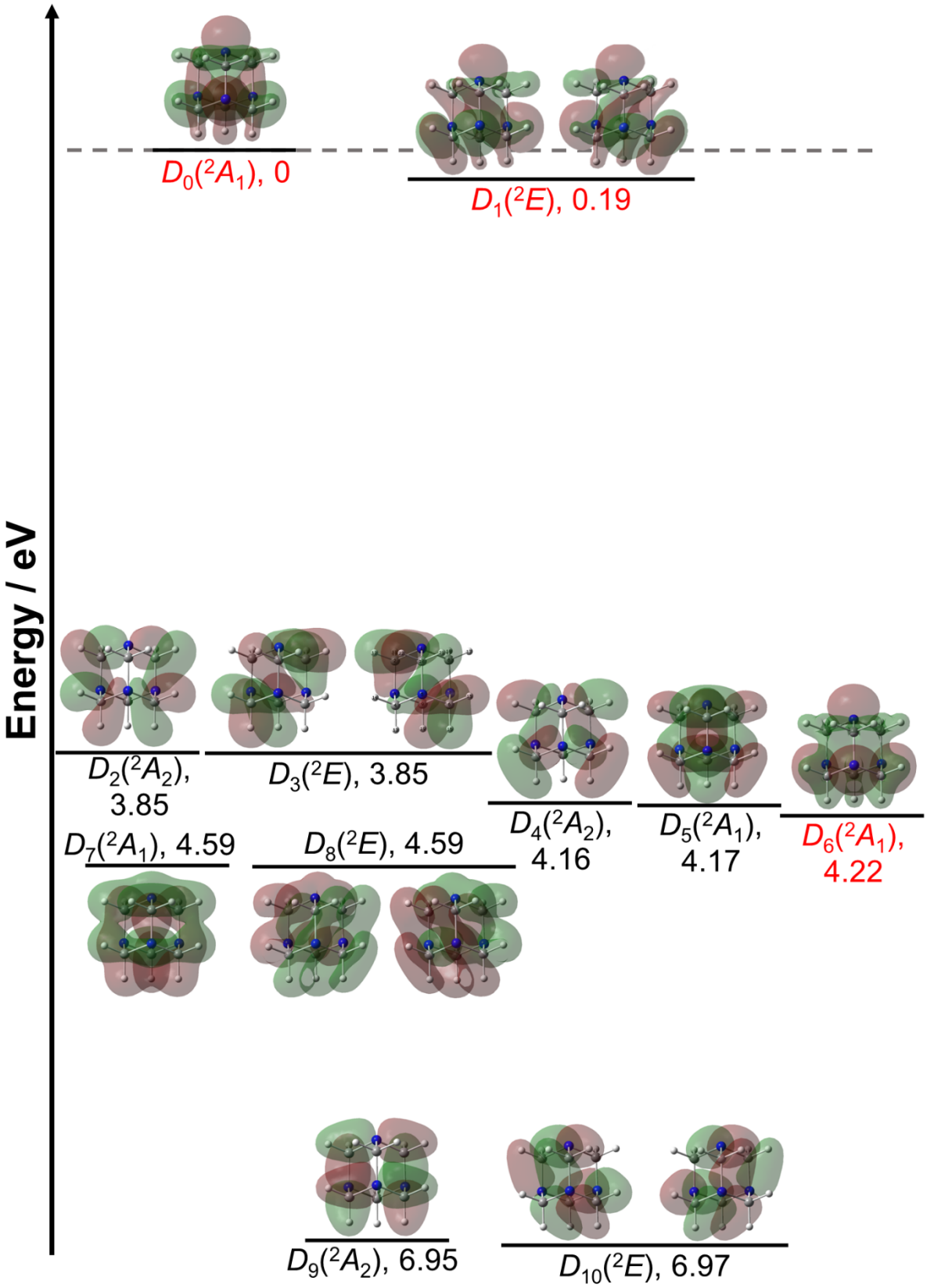


Figure S13. NTOs of Uro at the M06-2X(D3)/cc-pVTZ level in the optimized neutral geometry for the first 10 excited electronic states. All transitions are in the form of SOMO ← SOMO – *n*, where *n* is the number of the excited state. NTOs labeled in red indicate transitions originating from orbitals primarily attributed to the N atoms. Energies are given in units of eV.

Table S12. Intense Calculated FC Excitations of the Uro $D_0(^1B_1) \leftarrow S_0(^2A_1)$ Transition.

Transition Energy / cm^{-1} [a]	Mode	Intensity $\cdot 10^{-5}$ / $dm^3\ mol^{-1}\ cm^{-1}$
0	0–0	1.93
451	ν_{18}	2.17
518	ν_{17}	1.48
647	ν_{16}	2.86
969	$\nu_{17} + \nu_{18}$	1.64
1019	ν_{12}	1.51
1099	$\nu_{16} + \nu_{17}$	3.11
1165	$2\nu_{16}$	2.04
1470	$\nu_{12} + \nu_{18}$	1.68
1550	$\nu_{16} + 2\nu_{18}$	1.62
1617	$\nu_{16} + \nu_{17} + \nu_{18}$	2.28
1666	$\nu_{12} + \nu_{16}$	2.20
1712	$\nu_{11} + \nu_{16}$	1.33
1746	$2\nu_{16} + \nu_{18}$	2.15
1813	$2\nu_{16} + \nu_{17}$	1.46
1988	$\nu_{13} + \nu_{17} + \nu_{18}$	1.28
2118	$\nu_{13} + \nu_{16} + \nu_{18}$	2.37
2164	$\nu_{11} + \nu_{16} + \nu_{18}$	1.41
2184	$\nu_{12} + \nu_{16} + \nu_{17}$	1.64
2264	$2\nu_{16} + \nu_{17} + \nu_{18}$	1.52
2314	$\nu_{12} + 2\nu_{16}$	1.54
2569	$\nu_{12} + \nu_{16} + 2\nu_{18}$	1.22
2636	$\nu_{12} + \nu_{16} + \nu_{17} + \nu_{18}$	1.74
2765	$\nu_{12} + 2\nu_{16} + \nu_{18}$	1.60

[a] Energies are expressed in relation to the 0-0 band located at 62079 cm^{-1}.

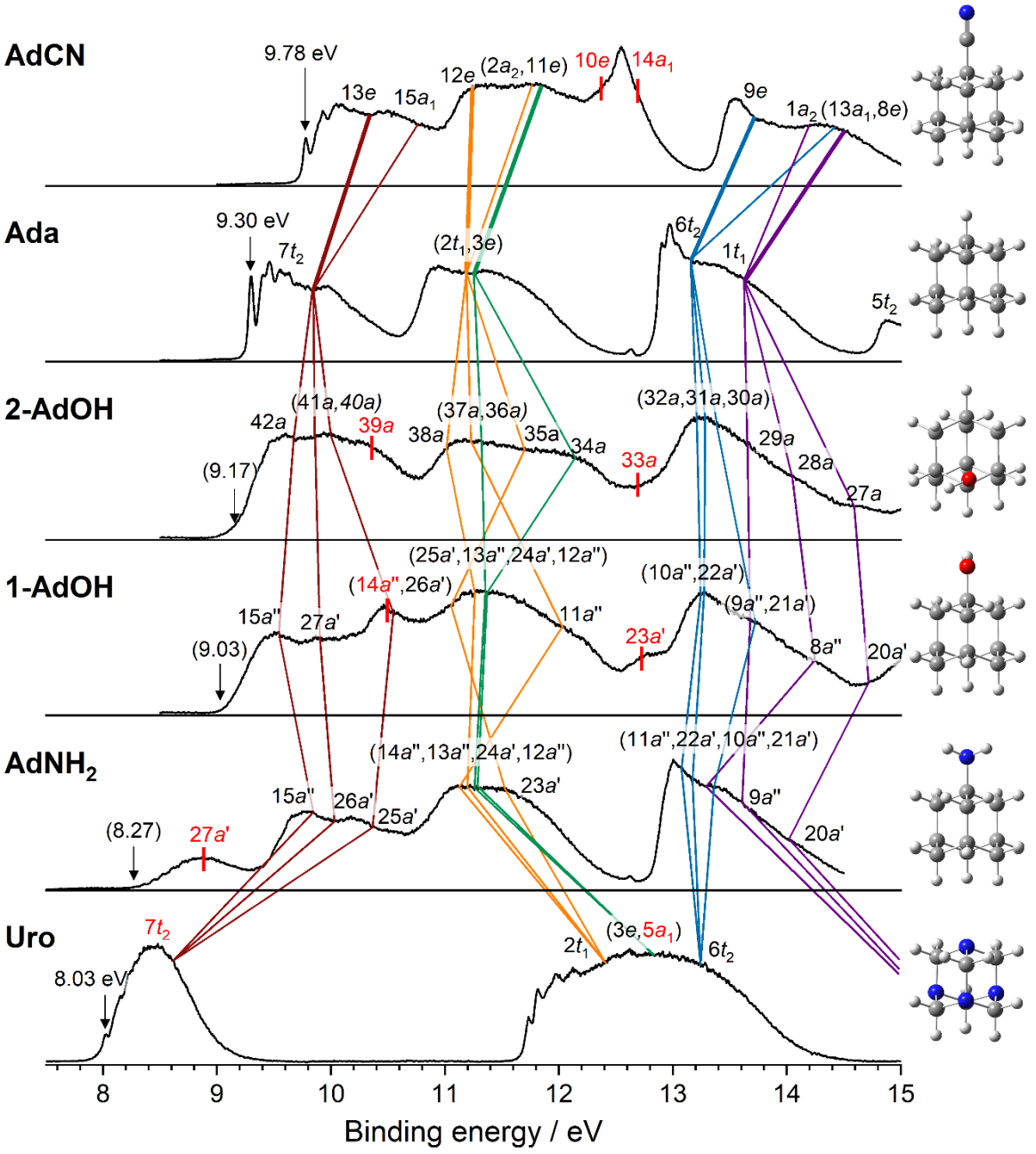


Figure 14. All PES spectra (from Figure 1) with illustrated orbital correlations. Lines cross the spectral bands at the energies predicted by KT-DFT at the M06-2X(D3)/cc-pVTZ level and are colored according to how the MOs of each molecule correlate with the MOs of Ada ($7t_2$, $2t_1$, etc.).

Figure S15. Correlation of MOs of Ada with MOs of its functionalized derivatives. MO number is indicated in bold and eigenenergies are given in eV.

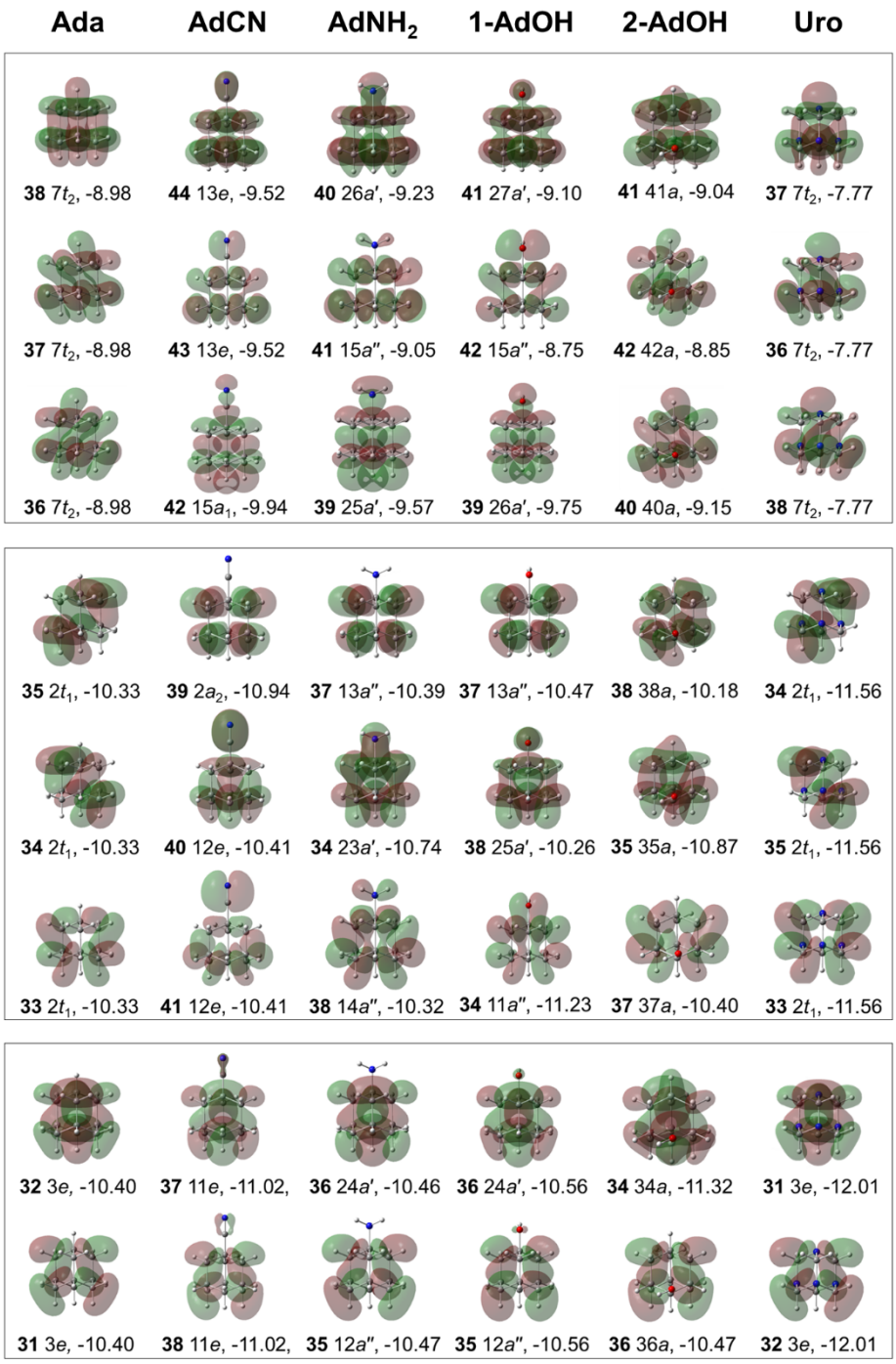
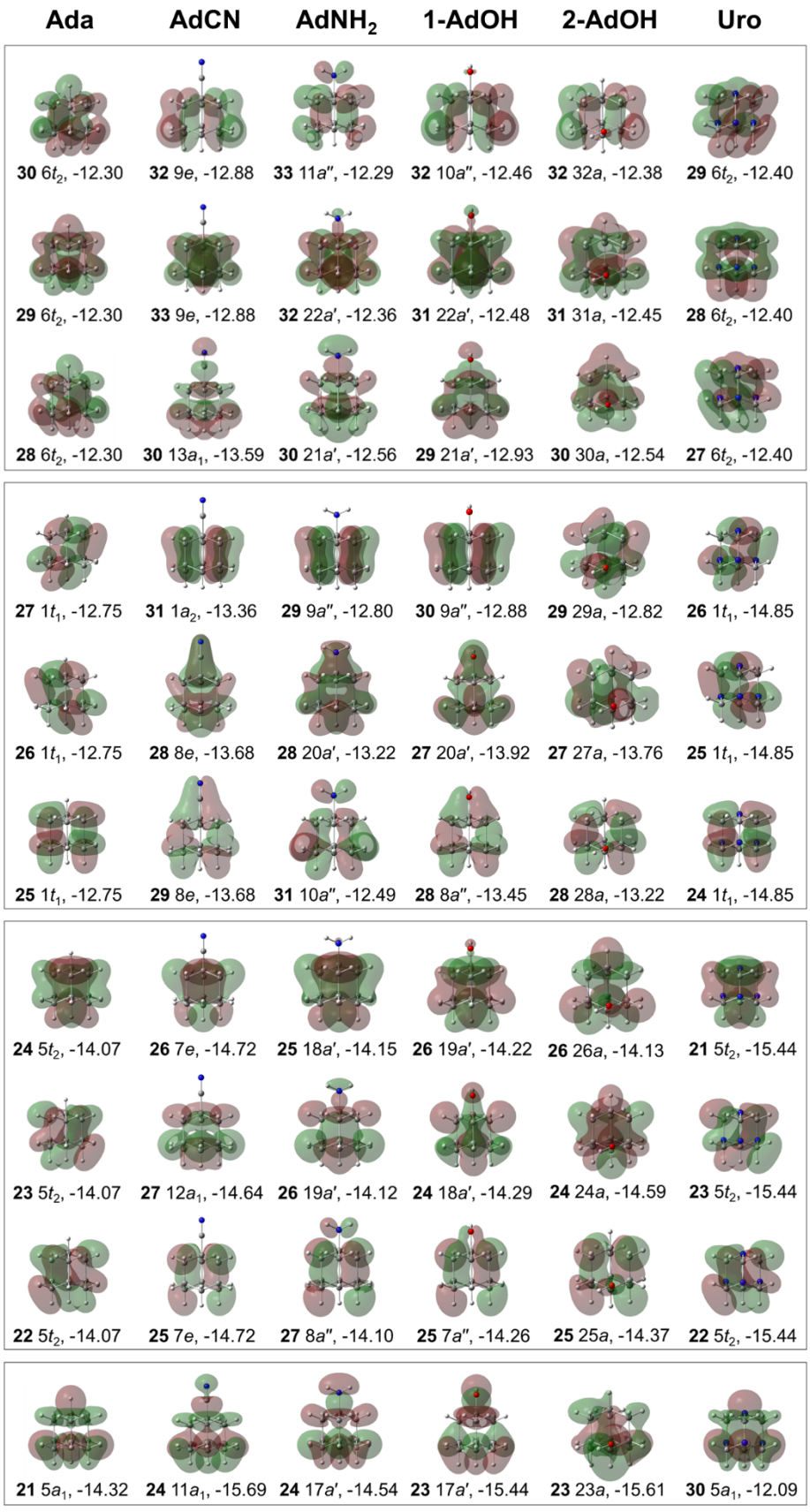


Figure S15. (Continued)



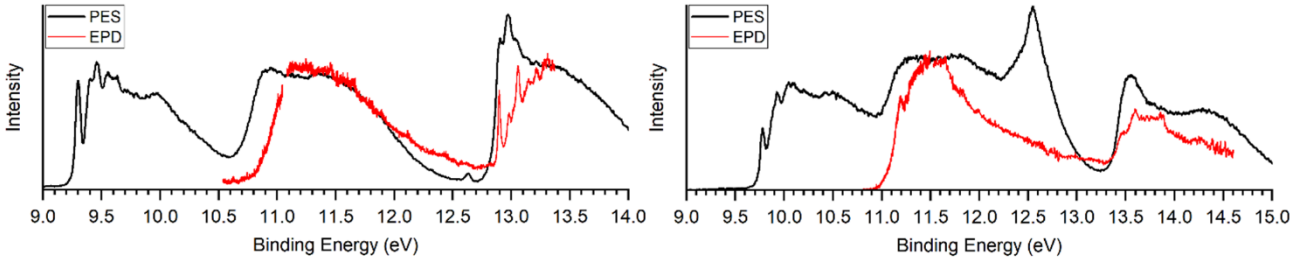


Figure S16. Comparison of PES spectra (black) with EPD spectra (red) of Ada/Ada$^+$ (left) and AdCN/AdCN$^+$ (right). The EPD spectra are taken from ref. 34 and 36 and have been shifted by the experimentally determined IE_a for direct comparison of the ionic states.

Cartesian coordiantes (Å) and energies (hartree) of relevant structures (M06-2X(D3)/cc-pVTZ)

Ada (S_0, D_0*)

1	6	0.000000	1.769062	0.000000
2	1	0.622799	2.416831	-0.622799
3	1	-0.622799	2.416831	0.622799
4	6	0.886717	0.886717	0.886717
5	1	1.517000	1.517000	1.517000
6	6	-0.886717	0.886717	-0.886717
7	1	-1.517000	1.517000	-1.517000
8	6	0.000000	0.000000	-1.769062
9	1	0.622799	0.622799	-2.416831
10	1	-0.622799	-0.622799	-2.416831
11	6	1.769062	0.000000	0.000000
12	1	2.416831	-0.622799	0.622799
13	1	2.416831	0.622799	-0.622799
14	6	0.886717	-0.886717	-0.886717
15	1	1.517000	-1.517000	-1.517000
16	6	0.000000	-1.769062	0.000000
17	1	-0.622799	-2.416831	-0.622799
18	1	0.622799	-2.416831	0.622799
19	6	0.000000	0.000000	1.769062
20	1	-0.622799	0.622799	2.416831
21	1	0.622799	-0.622799	2.416831
22	6	-1.769062	0.000000	0.000000
23	1	-2.416831	0.622799	0.622799
24	1	-2.416831	-0.622799	-0.622799
25	6	-0.886717	-0.886717	0.886717
26	1	-1.517000	-1.517000	1.517000

Electronic energy E_n: -390.680696
ZPE_n: 0.245654
Electronic energy E_+*: -390.319338

Ada$^+$ (D_0)

1	6	-1.260116	0.727528	-0.997643
2	1	-1.308798	0.755635	-2.094489
3	1	-2.153255	1.243182	-0.642562
4	6	0.000000	1.443712	-0.550461
5	1	0.000000	2.492766	-0.847096
6	6	-1.250291	-0.721856	-0.550461
7	1	-2.158798	-1.246383	-0.847096
8	6	0.000000	-1.455057	-0.997643
9	1	0.000000	-1.511269	-2.094489
10	1	0.000000	-2.486365	-0.642562
11	6	1.260116	0.727528	-0.997643
12	1	2.153255	1.243182	-0.642562
13	1	1.308798	0.755635	-2.094489
14	6	1.250291	-0.721856	-0.550461
15	1	2.158798	-1.246383	-0.847096
16	6	1.256512	-0.725448	1.054956
17	1	1.268305	-1.760065	1.393263
18	1	2.158413	-0.218352	1.393263
19	6	0.000000	1.450895	1.054956
20	1	-0.890108	1.978417	1.393263
21	1	0.890108	1.978417	1.393263
22	6	-1.256512	-0.725448	1.054956
23	1	-2.158413	-0.218352	1.393263
24	1	-1.268305	-1.760065	1.393263
25	6	0.000000	0.000000	1.448732
26	1	0.000000	0.000000	2.577139

Electronic energy E_+: -390.335772
ZPE_+: 0.235062

AdCN (S_0, D_0*)

1	6	-1.252060	0.722877	-1.525888
2	1	-2.150291	1.241471	-1.181481
3	1	-1.268767	0.732523	-2.618317
4	6	-1.252781	-0.723294	-1.017408
5	1	-2.145590	-1.238757	-1.374502
6	6	0.000000	1.446587	-1.017408
7	1	0.000000	2.477514	-1.374502
8	6	0.000000	1.453132	0.514282
9	1	-0.880935	1.972919	0.896655
10	1	0.880935	1.972919	0.896655
11	6	-1.258450	-0.726566	0.514282
12	1	-1.268130	-1.749372	0.896655
13	1	-2.149065	-0.223547	0.896655
14	6	1.258450	-0.726566	0.514282
15	1	2.149065	-0.223547	0.896655
16	1	1.268130	-1.749372	0.896655
17	6	0.000000	-1.445754	-1.525888
18	1	0.000000	-1.465046	-2.618317
19	1	0.000000	-2.482942	-1.181481
20	6	1.252060	0.722877	-1.525888
21	1	1.268767	0.732523	-2.618317
22	1	2.150291	1.241471	-1.181481
23	6	1.252781	-0.723294	-1.017408
24	1	2.145590	-1.238757	-1.374502
25	6	0.000000	0.000000	1.031848
26	6	0.000000	0.000000	2.495530
27	7	0.000000	0.000000	3.642991

Electronic energy E_n: -482.930848
ZPE_n: 0.243890
Electronic energy E_+*: -482.550812

$AdCN^+$ (D_0)

1	6	-0.796889	-1.533822	1.257851
2	1	-1.256402	-1.150104	2.167490
3	1	-0.801167	-2.621321	1.268129
4	6	0.734785	-1.013671	1.248052
5	1	1.158229	-1.423779	2.166583
6	6	-1.388461	-0.958060	0.000000
7	1	-2.443176	-1.355085	0.000000
8	6	-1.440476	0.546495	0.000000
9	1	-1.936877	0.939952	0.885940
10	1	-1.936877	0.939952	-0.885940
11	6	0.734785	0.499101	1.265990
12	1	1.765334	0.866773	1.303358
13	1	0.239110	0.883288	2.158241
14	6	0.734785	0.499101	-1.265990
15	1	0.239110	0.883288	-2.158241
16	1	1.765334	0.866773	-1.303358
17	6	1.369021	-1.587296	0.000000
18	1	1.346018	-2.676623	0.000000
19	1	2.431916	-1.296393	0.000000
20	6	-0.796889	-1.533822	-1.257851
21	1	-0.801167	-2.621321	-1.268129
22	1	-1.256402	-1.150104	-2.167490
23	6	0.734785	-1.013671	-1.248052
24	1	1.158229	-1.423779	-2.166583
25	6	0.060014	1.049547	0.000000
26	6	0.057135	2.506961	0.000000
27	7	0.044744	3.653329	0.000000

Electronic energy E_+: -482.566706
ZPE_+: 0.235225

$AdNH_2$ (S_0, D_0*)

1	6	-1.007207	-0.410630	1.252734
2	6	-1.729898	-0.919899	0.000000
3	6	-1.007207	-0.410630	-1.252734
4	6	-1.007207	1.122591	-1.251523
5	6	-0.286017	1.636125	0.000000
6	6	-1.007207	1.122591	1.251523
7	6	0.436585	-0.923696	-1.245202
8	6	0.436585	-0.923696	1.245202
9	6	1.175449	-0.423928	0.000000
10	6	1.155167	1.113766	0.000000
11	7	2.523402	-0.988783	0.000000
12	1	-1.517968	-0.776826	2.145118
13	1	-1.751326	-2.012616	0.000000
14	1	-2.766251	-0.572311	0.000000
15	1	-1.517968	-0.776826	-2.145118
16	1	-2.034437	1.495793	-1.269582
17	1	-0.508786	1.497109	-2.149619
18	1	-0.281265	2.727794	0.000000
19	1	-0.508786	1.497109	2.149619
20	1	-2.034437	1.495793	1.269582
21	1	0.461560	-2.015731	-1.252070
22	1	0.964825	-0.578350	-2.140280
23	1	0.964825	-0.578350	2.140280
24	1	0.461560	-2.015731	1.252070
25	1	1.691334	1.478663	0.882046
26	1	1.691334	1.478663	-0.882046
27	1	3.033864	-0.659138	-0.813160
28	1	3.033864	-0.659138	0.813160

Electronic energy E_n: -446.031143
ZPE_n: 0.261907
Electronic energy E_+*: -445.704666

$AdNH_2^+$ (D_0)

1	6	-1.006428	-0.419592	1.255756
2	6	-1.716175	-0.941222	0.000000
3	6	-1.006428	-0.419592	-1.255756
4	6	-1.006428	1.112858	-1.256917
5	6	-0.292746	1.606848	0.000000
6	6	-1.006428	1.112858	1.256917
7	6	0.436055	-0.928521	-1.278577
8	6	0.436055	-0.928521	1.278577
9	6	1.162741	-0.507174	0.000000
10	6	1.166676	1.181703	0.000000
11	7	2.503374	-0.821396	0.000000
12	1	-1.510191	-0.786035	2.149500
13	1	-1.731336	-2.033051	0.000000
14	1	-2.753892	-0.605818	0.000000
15	1	-1.510191	-0.786035	-2.149500
16	1	-2.031138	1.484883	-1.263305
17	1	-0.515111	1.495899	-2.153583
18	1	-0.245595	2.703436	0.000000
19	1	-0.515111	1.495899	2.153583
20	1	-2.031138	1.484883	1.263305
21	1	0.453786	-2.020703	-1.312349
22	1	0.970361	-0.557283	-2.157026
23	1	0.970361	-0.557283	2.157026
24	1	0.453786	-2.020703	1.312349
25	1	1.704884	1.486432	0.895298
26	1	1.704884	1.486432	-0.895298
27	1	3.030331	-0.869529	-0.865247
28	1	3.030331	-0.869529	0.865247

Electronic energy E_+: -445.728544
ZPE_+: 0.259657

1-AdOH (S_0, D_0*)

1	6	0.718901	0.726889	1.247927
2	1	0.214478	1.120642	2.133429
3	1	1.746800	1.105601	1.256168
4	6	0.000104	1.244697	0.000000
5	6	0.718901	-0.806829	1.253742
6	1	1.232106	-1.168912	2.146231
7	6	-0.730255	-1.308328	1.251377
8	1	-1.246691	-0.961022	2.149735
9	1	-0.745412	-2.401083	1.267780
10	6	-1.439404	0.739406	0.000000
11	1	-1.949784	1.134064	-0.881555
12	1	-1.949784	1.134064	0.881555
13	6	-1.451952	-0.793423	0.000000
14	1	-2.484105	-1.147394	0.000000
15	6	-0.730255	-1.308328	-1.251377
16	1	-0.745412	-2.401083	-1.267780
17	1	-1.246691	-0.961022	-2.149735
18	6	0.718901	0.726889	-1.247927
19	1	1.746800	1.105601	-1.256168
20	1	0.214478	1.120642	-2.133429
21	6	1.437925	-1.319487	0.000000
22	1	2.477140	-0.980126	0.000000
23	1	1.452430	-2.412307	0.000000
24	6	0.718901	-0.806829	-1.253742
25	1	1.232106	-1.168912	-2.146231
26	8	-0.068448	2.662931	0.000000
27	1	0.828532	3.009867	0.000000

Electronic energy E_n: -465.913164
ZPE_n: 0.249139
Electronic energy E_+*: -465.562534

1-AdOH$^+$ (D_0)

1	6	-0.759568	-1.322908	-0.603661
2	1	-1.147829	-1.460201	-1.620501
3	1	-1.161658	-2.133660	0.009969
4	6	-1.303575	0.013428	-0.150143
5	6	0.769677	-1.325322	-0.617532
6	1	1.105771	-2.266484	-1.050923
7	6	1.282465	-0.144184	-1.451094
8	1	0.928319	-0.225902	-2.480431
9	1	2.372053	-0.168437	-1.485655
10	6	-0.711508	1.234137	-0.815561
11	1	-1.097342	2.141512	-0.349459
12	1	-1.107879	1.210480	-1.838269
13	6	0.813935	1.178076	-0.831461
14	1	1.180989	2.019300	-1.418171
15	6	1.343043	1.298148	0.605791
16	1	2.432600	1.284197	0.603474
17	1	1.025313	2.239889	1.055623
18	6	-0.667399	0.154294	1.558871
19	1	-1.130535	-0.706363	2.035462
20	1	-1.106212	1.098470	1.868258
21	6	1.292721	-1.216454	0.822354
22	1	0.939650	-2.054615	1.425505
23	1	2.381890	-1.246953	0.823089
24	6	0.815656	0.110965	1.407381
25	1	1.156046	0.194932	2.457497
26	8	-2.622297	0.116959	0.029754
27	1	-3.045488	-0.742907	0.176819

Electronic energy E_+: -465.584038
ZPE_+: 0.246060

2-AdOH (S_0, D_0*)

1	6	0.749579	-1.553609	-0.706602
2	1	1.315291	-1.703282	-1.629439
3	1	0.522050	-2.543374	-0.301229
4	6	-0.548198	-0.795999	-1.012301
5	1	-1.150940	-1.370159	-1.723555
6	6	1.584133	-0.754499	0.301466
7	1	2.508905	-1.292855	0.517280
8	6	1.912013	0.623566	-0.286203
9	1	2.499730	0.507353	-1.200940
10	1	2.520292	1.193533	0.421207
11	6	-0.220501	0.582276	-1.597873
12	1	-1.142530	1.119284	-1.825663
13	1	0.332546	0.460740	-2.532954
14	6	0.613673	1.381072	-0.589081
15	1	0.850550	2.361199	-1.007061
16	6	-0.194060	1.553929	0.702936
17	1	0.380782	2.133441	1.429994
18	1	-1.117456	2.097192	0.500169
19	6	-1.341327	-0.633081	0.289626
20	1	-1.535029	-1.627197	0.714214
21	6	0.777533	-0.579226	1.593607
22	1	0.553984	-1.556366	2.030310
23	1	1.363367	-0.022337	2.328878
24	6	-0.521707	0.177149	1.292977
25	1	-1.113400	0.292830	2.202743
26	8	-2.571755	0.046080	0.089651
27	1	-3.080933	-0.428105	-0.572478

Electronic energy E_n: -465.908502
ZPE_n: 0.249708
Electronic energy E_+*: -465.553113

2-AdOH$^+$ (D_0)

1	6	0.763989	-1.053193	-1.343775
2	1	1.380890	-0.777510	-2.211904
3	1	0.473639	-2.094287	-1.490926
4	6	-0.416156	-0.135342	-1.394699
5	1	-1.139698	-0.337684	-2.183105
6	6	1.569272	-0.855181	-0.056111
7	1	2.467212	-1.468819	-0.098438
8	6	1.940392	0.622665	0.108403
9	1	2.574366	0.946638	-0.718988
10	1	2.520114	0.755127	1.023090
11	6	-0.140020	1.307944	-1.116180
12	1	-1.058373	1.892790	-1.102341
13	1	0.451544	1.660578	-1.973683
14	6	0.673151	1.481734	0.170858
15	1	0.936642	2.531438	0.289258
16	6	-0.206298	1.045782	1.353548
17	1	0.336671	1.183149	2.289080
18	1	-1.112085	1.649149	1.409704
19	6	-1.471803	-0.689751	0.023465
20	1	-1.623331	-1.729385	-0.271780
21	6	0.693138	-1.307431	1.118706
22	1	0.423458	-2.360769	1.018285
23	1	1.247478	-1.207526	2.052760
24	6	-0.553166	-0.434046	1.199906
25	1	-1.178694	-0.752467	2.048113
26	8	-2.565107	0.067713	0.003423
27	1	-3.293974	-0.331208	-0.491243

Electronic energy E_+: -465.581508
ZPE_+: 0.246351

Uro (S_0, D_0*)

1	7	-0.861281	-0.861281	0.861281
2	6	0.000000	0.000000	1.678142
3	7	0.861281	0.861281	0.861281
4	6	0.000000	1.678142	0.000000
5	7	-0.861281	0.861281	-0.861281
6	6	0.000000	0.000000	-1.678142
7	7	0.861281	-0.861281	-0.861281
8	6	0.000000	-1.678142	0.000000
9	6	1.678142	0.000000	0.000000
10	6	-1.678142	0.000000	0.000000
11	1	0.627050	-0.627050	2.313762
12	1	-0.627050	0.627050	2.313762
13	1	0.627050	2.313762	-0.627050
14	1	-0.627050	2.313762	0.627050
15	1	-0.627050	-0.627050	-2.313762
16	1	0.627050	0.627050	-2.313762
17	1	-0.627050	-2.313762	-0.627050
18	1	0.627050	-2.313762	0.627050
19	1	2.313762	0.627050	-0.627050
20	1	2.313762	-0.627050	0.627050
21	1	-2.313762	-0.627050	-0.627050
22	1	-2.313762	0.627050	0.627050

Electronic energy E_n: -454.812884
ZPE_n: 0.200555
Electronic energy E_+*: -454.496711

Uro+ (D_0)

1	7	0.000000	1.223314	-0.886194
2	6	0.000000	0.000000	-1.704241
3	7	0.000000	-1.223314	-0.886194
4	6	-1.164724	-1.210730	-0.000650
5	7	-1.113471	0.000000	0.833667
6	6	0.000000	0.000000	1.779373
7	7	1.113471	0.000000	0.833667
8	6	1.164724	1.210730	-0.000650
9	6	1.164724	-1.210730	-0.000650
10	6	-1.164724	1.210730	-0.000650
11	1	0.883046	0.000000	-2.340364
12	1	-0.883046	0.000000	-2.340364
13	1	-1.164638	-2.091753	0.638291
14	1	-2.081161	-1.182578	-0.587654
15	1	0.000000	0.899433	2.389188
16	1	0.000000	-0.899433	2.389188
17	1	1.164638	2.091753	0.638291
18	1	2.081161	1.182578	-0.587654
19	1	1.164638	-2.091753	0.638291
20	1	2.081161	-1.182578	-0.587654
21	1	-1.164638	2.091753	0.638291
22	1	-2.081161	1.182578	-0.587654

Electronic energy E_+: -454.514464
ZPE_+: 0.198925