Supporting Information of

Probing the Mechanism of Electron Capture and Electron Transfer Dissociation Using Tags with Variable Electron Affinity

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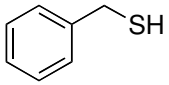
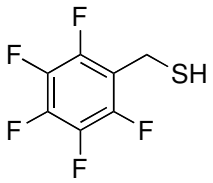
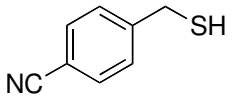
1. ^{1}H-NMR peaks of thiol compounds



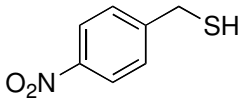
^{1}H-NMR ($CDCl_3$) δ 7.34-7.26 (m, 5H), 3.75 (d, *J* = 7.5 Hz, 2H), 1.77 (t, *J* = 7.5 Hz, 1H).



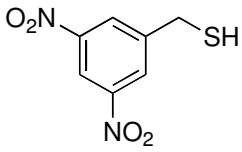
^{1}H-NMR ($CDCl_3$) δ 3.77 (dt, *J* = 8.5, 1.4 Hz, 2H), 2.07 (s, 1H).



^{1}H-NMR ($CDCl_3$) δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 3.75 (d, *J* = 7.8 Hz, 2H), 1.80 (s, 1H).

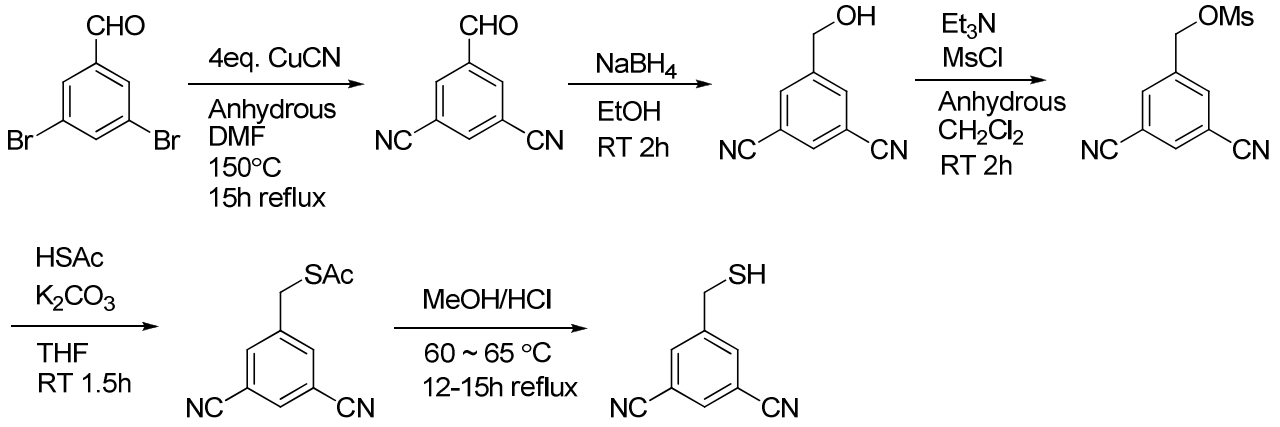


^{1}H-NMR ($CDCl_3$) δ 8.16 (d, *J* = 8.7 Hz, 2H), 7.48 (d, *J* = 8.7 Hz, 2H), 3.80 (d, *J* = 8.1 Hz, 2H), 1.83 (t, *J* = 8.1 Hz, 1H).



^{1}H-NMR (DMSO-d_6) δ 8.71-8.68 (m, 3H), 4.01 (d, *J* = 8.2 Hz, 2H), 3.41 (t, *J* = 8.2 Hz, 2H).

2. Synthesis of 3,5-dicyanobenzyl thiol



Scheme S1

a) Synthesis of 3,5-dicyanobenzaldehyde

The literature procedure was followed with a minor modification.[1] A solution of 3,5-dibromobenzaldehyde in anhydrous DMF (~0.25 M) was added copper cyanide (4 equiv.), and the resulting mixture was stirred at 150 °C for 15 h. The solvent was removed under vacuum and the residue was reconstituted in CH_2Cl_2 and filtered 3 times using Celite. The solvent was removed under vacuum and the residue was washed with diethyl ether 3 times. The filtrate was evaporated under vacuum to give the title compound as a yellow solid. The spectral data were in accordance with the literature.

b) Synthesis of 3,5-dicyanobenzyl alcohol

A solution of 3,5-dicyanobenzaldehyde in EtOH was added sodium borohydride (1.2 equiv.) slowly at 0°C and the resulting solution was stirred while it was slowly warmed to room temperature for 2h. After the solvent was removed, the residue was dissolved in ethyl acetate, and washed with HCl (aq. 1N). The organic layer was separated, dried over anhydrous magnesium sulfate, and evaporated under vacuum. The crude product was purified by flash column chromatography (silica gel, eluent: EtOAc/Hexanes =1/1 ~ 4/1) to give 3,5-dicyanobenzyl alcohol as a white solid. ^{1}H-NMR ($CDCl_3$) δ 7.91 (s, 2H), 7.86 (s, 1H), 4.83 (d, J = 5.5 Hz, 2H), 2.03 (t, J = 5.5 Hz, 1H).

c) Synthesis of 3,5-dicyanobenzyl methane sulfonate

A mixture of 3,5-dicyanobenzyl alcohol, methanesulfonyl chloride (1.2 equiv.), and triethyl amine (1.5 equiv.) in anhydrous methylene chloride was stirred for 2 h at room temperature, after which time, the mixture was diluted with methylene chloride and washed successively with an aqueous solution of ammonium chloride, brine and water. The organic layer was dried over anhydrous magnesium sulfate. The crude product thus obtained was pure enough to use for the next reaction. ^{1}H-NMR ($CDCl_3$) δ 7.96 (s, 1H), 7.93 (s, 2H), 5.28 (s, 2H), 3.13 (s, 3H).

d) Synthesis of 3,5-dicyanobenzyl thioacetate and 3,5-dicyanobenzyl thiol

The procedures in the main text were followed without any modification. 3,5-dicyanobenzyl thioacetate ^{1}H-NMR ($CDCl_3$) δ 7.83-7.81 (m, 3H), 4.11 (s, 2H), 2.39 (s, 3H), 3,5-dicyanobenzyl thiol ^{1}H-NMR ($CDCl_3$) δ 7.96-7.92 (m, 3H), 3.79 (d, J = 8.0 Hz, 2H), 1.85 (t, J = 8.0 Hz, 2H). Final product was derivatized to the model peptide via β-elimination under alkaline condition and subsequent Michael addition reaction. The exact mass of the derivatized peptide was determined by ESI-LTQ-FTMS at m/z 1069.4432 for $[M+2H]^{2+}$ (theoretical m/z: 1069.4420).

3. ECD and IRMPD/ECD spectra of 2-nitrobenzyl and 4-nitrobenzyl containing model peptides

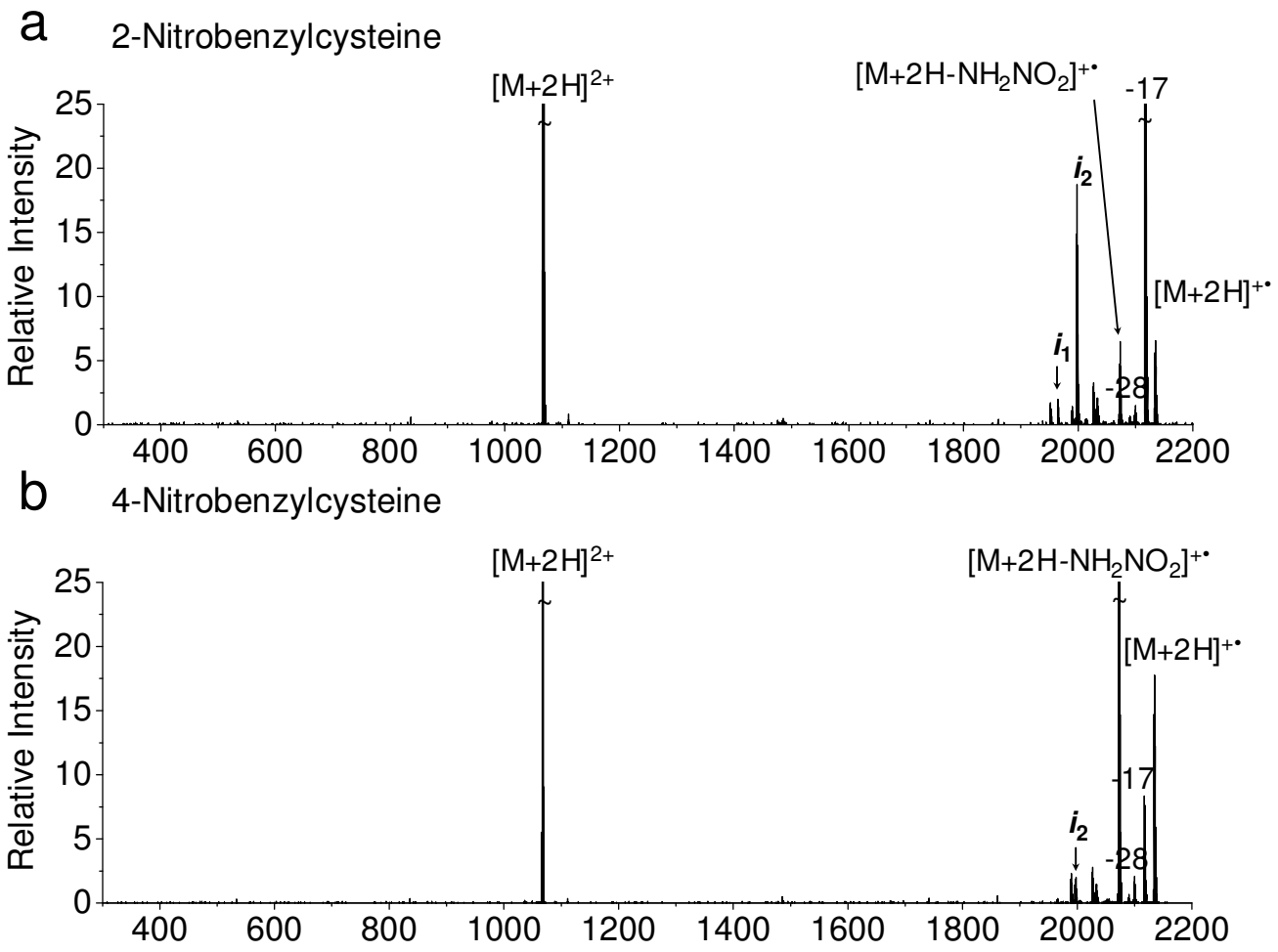


Figure S1-a and b. ECD of 2-nitrobenzyl and 4-nitrobenzyl containing model peptides.

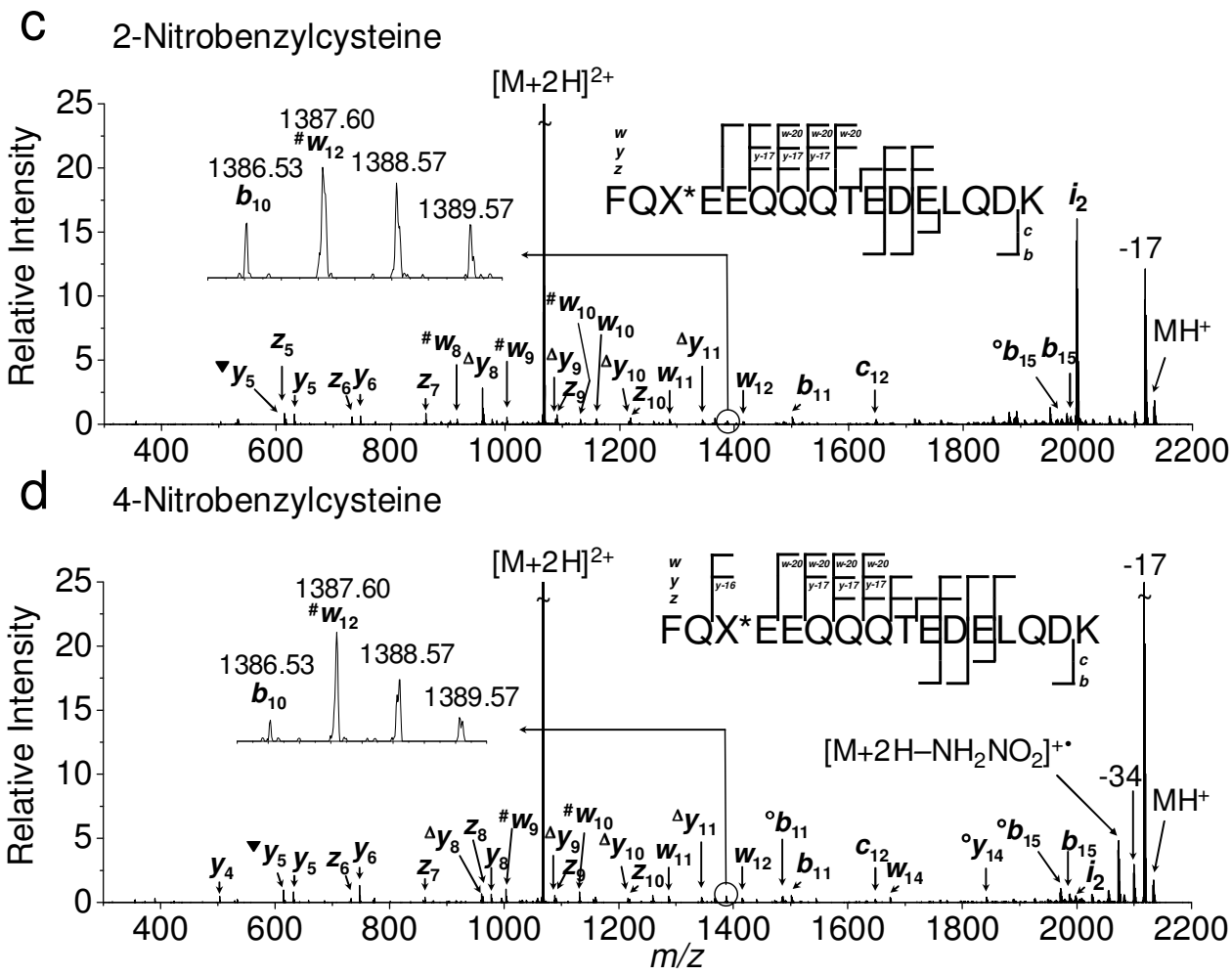


Figure S1-c and d. IRMPD/ECD of 2-nitrobenzyl and 4-nitrobenzyl containing model peptides.

4. ECD, IRMPD/ECD spectra of N_{α}-3,5-dinitrophenyl derivatized peptides

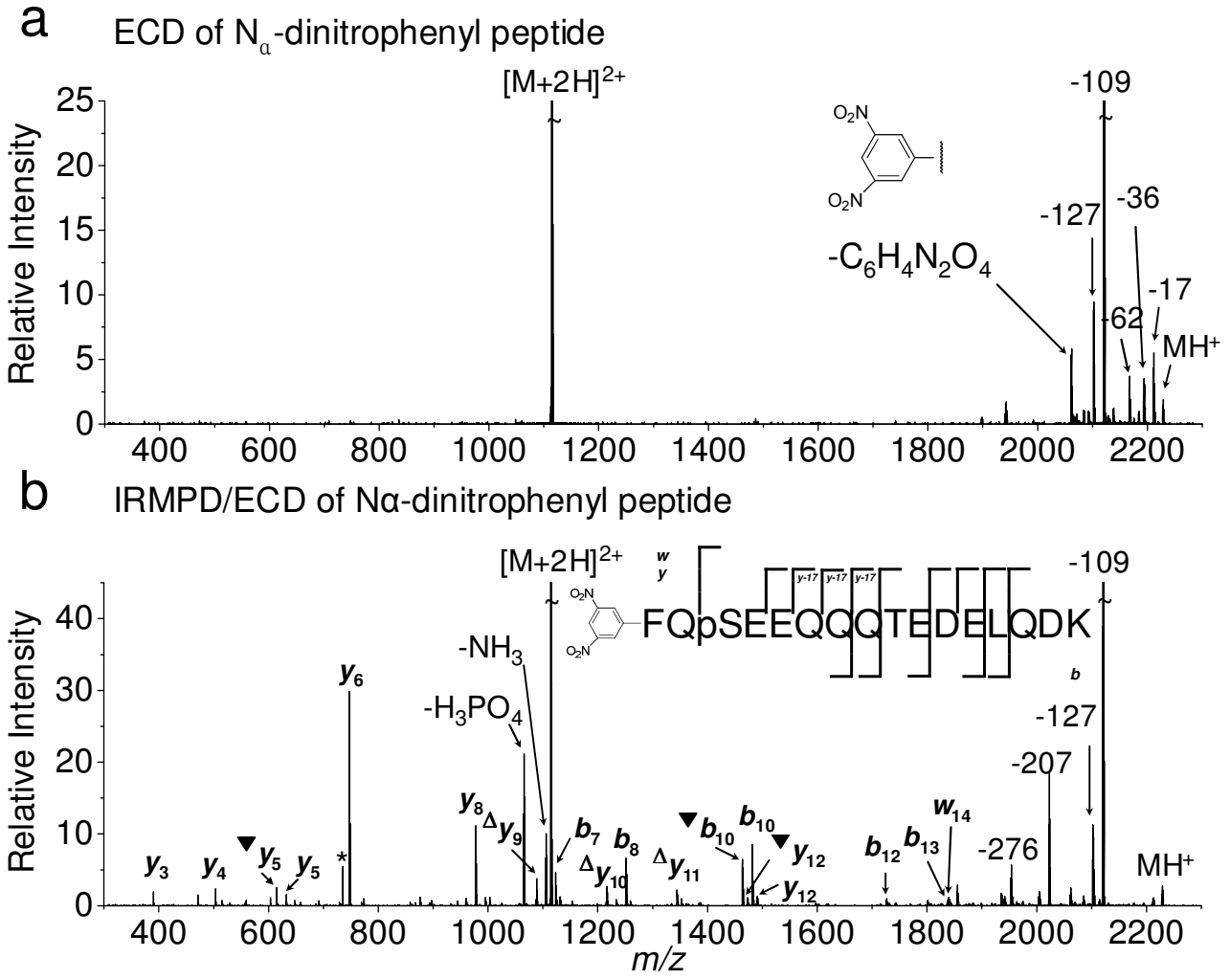


Figure S2. ECD, IRMPD/ECD spectra of N_{α}-3,5-dinitrophenyl derivatized peptides

5. Energies and geometries of dicyanobenzene, protonated dicyanobenzene, dicyanobenzene anion radical and a hydrogen attached dicyanobenzene radical optimized at the (U)B3LYP/6-31+G(d,p) level of theory

Table S1. B3LYP/6-31+G(d,p) optimized geometry and energetics of dicyanobenzene (**DCB**).

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000000000	0.0000000000	2.0417300000
C	6.0	0.0000000000	1.2099500000	1.3488000000
C	6.0	0.0000000000	1.2104600000	-0.0574400000
C	6.0	0.0000000000	-1.2099500000	1.3488000000
C	6.0	0.0000000000	-1.2104600000	-0.0574400000
C	6.0	0.0000000000	0.0000000000	-0.7649100000
H	1.0	0.0000000000	0.0000000000	3.1267100000
H	1.0	0.0000000000	2.1532400000	1.8842100000
H	1.0	0.0000000000	-2.1532400000	1.8842100000
H	1.0	0.0000000000	0.0000000000	-1.8488500000
C	6.0	0.0000000000	-2.4549600000	-0.7742300000
C	6.0	0.0000000000	2.4549600000	-0.7742300000
N	7.0	0.0000000000	3.4651800000	-1.3509200000
N	7.0	0.0000000000	-3.4651800000	-1.3509200000

E[B3LYP/6-31+G(d,p)] = -416.7529215558 hartree
E[B3LYP/6-311+(2df,p)] = -416.871199001 hartree
E[MP2/6-311+G(2df,p)] = -415.8866585981 hartree
ZPE[B3LYP/6-31+G(d,p)] = 256.001 kJ/mol
Enthalpy Correction[B3LYP/6-31+G(d,p)] = 279.286 kJ/mol

Table S2. B3LYP/6-31+G(d,p) optimized geometry and energetics of protonated dicyanobenzene (**DCBH$^+$**).

ATOM	CHARGE	X	Y	Z
C	6.0	-0.2270469337	-2.0607377696	0.0000000000
C	6.0	1.0389940607	-1.4889952163	0.0000000000
C	6.0	1.1407715811	-0.0762608828	0.0000000000
C	6.0	-1.3679435821	-1.2526800966	0.0000000000
C	6.0	-1.2598715714	0.1537308066	0.0000000000
C	6.0	-0.0000947970	0.7563754893	0.0000000000
H	1.0	-0.3301262847	-3.1403103784	0.0000000000
H	1.0	1.9301166709	-2.1073371915	0.0000000000
H	1.0	-2.3541937602	-1.7053546596	0.0000000000
H	1.0	0.0928424105	1.8367128207	0.0000000000
C	6.0	-2.4382846445	0.9725433811	0.0000000000
C	6.0	2.4133962570	0.5201803991	0.0000000000
N	7.0	3.4606743120	1.0088567345	0.0000000000
N	7.0	-3.3906790100	1.6383182065	0.0000000000
H	1.0	4.3732452915	1.4374883570	0.0000000000

E[B3LYP/6-31+G(d,p)] = -417.0628515 hartree
E[B3LYP/6-311+(2df,p)] = -417.1823338 hartree
E[MP2/6-311+G(2df,p)] = -416.1857521 hartree
ZPE[B3LYP/6-31+G(d,p)] = 283.606 kJ/mol
Enthalpy Correction[B3LYP/6-31+G(d,p)] = 308.484 kJ/mol

Table S3. UB3LYP/6-31+G(d,p) optimized geometry and energetics of dicyanobenzene anion (**DCB**$^{-\bullet}$).

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000000000	-0.0000000001	2.0961482218
C	6.0	0.0000000000	1.2246717477	1.4282494957
C	6.0	0.0000000000	1.2259394174	-0.0298578321
C	6.0	0.0000000000	-1.2246717378	1.4282494997
C	6.0	0.0000000000	-1.2259394133	-0.0298578225
C	6.0	0.0000000000	0.0000000063	-0.7124031644
H	1.0	0.0000000000	-0.0000000033	3.1856841429
H	1.0	0.0000000000	2.1650218994	1.9680970353
H	1.0	0.0000000000	-2.1650218949	1.9680970291
H	1.0	0.0000000000	-0.0000000014	-1.7991413383
C	6.0	0.0000000000	-2.4395336105	-0.7562397348
C	6.0	0.0000000000	2.4395335370	-0.7562396933
N	7.0	0.0000000000	3.4630527486	-1.3353163831
N	7.0	0.0000000000	-3.4630526952	-1.3353163532

E[UB3LYP/6-31+G(d,p)] = -416.7883736 hartree
E[UB3LYP/6-311+(2df,p)] = -416.9074846 hartree
E[ROMP2/6-311+G(2df,p)] = -415.9113402 hartree
ZPE[UB3LYP/6-31+G(d,p)] = 244.453 kJ/mol
Enthalpy Correction[UB3LYP/6-31+G(d,p)] = 268.831 kJ/mol

Table S4. UB3LYP/6-31+G(d,p) optimized geometry and energetics of hydrogen atom attached dicyanobenzene (**DCBH•**).

ATOM	CHARGE	X	Y	Z
C	6.0	-0.0921524176	2.0542348981	0.0473576881
C	6.0	1.1280600132	1.3932372497	-0.0535294093
C	6.0	1.1697412859	-0.0209686527	-0.1190331531
C	6.0	-1.2926928872	1.3406758715	0.0713593888
C	6.0	-1.2590629696	-0.0651749865	-0.0053830155
C	6.0	-0.0411332194	-0.7465759691	-0.1079338505
H	1.0	-0.1106002572	3.1377380878	0.1108245600
H	1.0	2.0562217720	1.9548096780	-0.0739898616
H	1.0	-2.2447295104	1.8539877941	0.1460385932
H	1.0	-0.0283683119	-1.8288266984	-0.1715689126
C	6.0	-2.4867984018	-0.8107000874	0.0205591816
C	6.0	2.4124345303	-0.7003679125	-0.2988903953
N	7.0	3.3383288723	-1.1862099809	0.3617374011
N	7.0	-3.4838374863	-1.4102963135	0.0405183280
H	1.0	4.1157019876	-1.6082169783	-0.1538685428

E[UB3LYP/6-31+G(d,p)] = -417.3020565 hartree
E[UB3LYP/6-311+(2df,p)] = -417.4191066 hartree
E[ROMP2/6-311+G(2df,p)] = -416.4088129 hartree
ZPE[UB3LYP/6-31+G(d,p)] = 279.983 kJ/mol
Enthalpy Correction[UB3LYP/6-31+G(d,p)] = 305.064 kJ/mol

6. Energies and geometries of N-phenethylacetamide, N-(4-cyanophenethyl)acetamide, N-(perfluorophenethyl)acetamide, N-(3,5-dicyanophenethyl)acetamide, N-(3-nitrophenethyl)acetamide, N-(3,5-dinitrophenethyl)acetamide and their methyl ammonium complexes optimized at the (U)B3LYP/6-31++G(d,p) level of theory

Table S5. B3LYP/6-31++G(d,p) optimized geometry of N-phenethylacetamide (**A1**) and electronic energy of N-phenethylacetamide (**A1**) neutral and anion formed by vertical electron attachment.

ATOM	ATOMIC	COORDINATES (BOHR)		
CHARGE	X	Y	Z	
C	6.0	4.1717212960	-3.9922540189	-1.4798444210
C	6.0	4.1742346315	-1.4584149283	-0.1260636206
O	8.0	5.5493882328	-1.0550907107	1.7024919369
N	7.0	2.5848427950	0.3363712258	-1.0937922990
C	6.0	2.2814850822	2.8208884682	0.0503611976
C	6.0	0.0599232111	2.9761861498	1.9392179113
C	6.0	-2.4878998519	2.4416771542	0.7531313951
C	6.0	-3.6417098482	0.0685214643	1.0038035474
C	6.0	-5.9621988748	-0.4456351824	-0.1511969763
C	6.0	-3.7307159422	4.2940054646	-0.6850256705
C	6.0	-6.0478412566	3.7899777492	-1.8426718106
C	6.0	-7.1721526302	1.4132693744	-1.5814171928
H	1.0	-6.8267485142	-2.2939005820	0.0770441285
H	1.0	6.0772642902	-4.3614875797	-2.1901735225
H	1.0	2.8355716391	-4.0943370168	-3.0538727852
H	1.0	3.7226468123	-5.4749708234	-0.1121363401
H	1.0	1.3724323958	-0.1727209553	-2.4757867083
H	1.0	4.0463001822	3.2519349660	1.0303164030
H	1.0	2.0208918685	4.2055284939	-1.4667297226
H	1.0	0.0696741972	4.8803118496	2.7598125242
H	1.0	0.4235064911	1.6477087805	3.4832374269
H	1.0	-2.7212621141	-1.3830715532	2.1290030923
H	1.0	-2.8824557409	6.1557824050	-0.8870562759
H	1.0	-6.9816871479	5.2543642116	-2.9376168424
H	1.0	-8.9781448594	1.0202063690	-2.4740103659

E[B3LYP/6-31++G(d,p)] = -518.6105774 hartree
E[B3LYP/6-311++G(2df,p)] = -518.7518539 hartree
E[M06/6-31++G(d,p)] = -518.5539733 hartree
E[M06/6-311++G(2df,p)] = -518.6945007 hartree
E[MP2/6-311++G(2df,p)]= -517.7913924 hartree

E[UB3LYP/6-31++G(d,p)] = -518.595006 hartree
E[UB3LYP/6-311++G(2df,p)] = -518.7373883 hartree
E[UM06/6-31++G(d,p)] = -518.5317336 hartree
E[UM06/6-311++G(2df,p)] = -518.6754261 hartree
E[ROMP2/6-311++G(2df,p)]= -517.7697563 hartree

Table S6. B3LYP/6-31++G(d,p) optimized geometry of N-(4-cyanophenethyl)acetamide (**A2**) and electronic energy of N-(4-cyanophenethyl)acetamide (**A2**) neutral and anion formed by vertical electron attachment.

ATOM	ATOMIC CHARGE	COORDINATES (BOHR) X	Y	Z
C	6.0	4.6869739838	-3.8386948852	-1.1660932152
C	6.0	4.4794631731	-1.3867754161	0.3130898016
O	8.0	5.3589038532	-1.1622381742	2.4515226266
N	7.0	3.2781832599	0.5643855635	-0.8839571253
C	6.0	2.9517519928	3.0304401830	0.2955531445
C	6.0	0.7195131698	3.1674453171	2.1786839885
C	6.0	-1.8170660235	2.6138500890	0.9903486984
C	6.0	-2.9166408840	0.2081344203	1.1881085230
C	6.0	-5.2231837328	-0.3373160888	0.0413849991
C	6.0	-3.1082779964	4.4759104882	-0.3936677178
C	6.0	-5.4136492151	3.9635490812	-1.5522209263
C	6.0	-6.4866356309	1.5418463306	-1.3439920197
C	6.0	-8.8608684646	0.9960556709	-2.5320816455
H	1.0	-6.0572709893	-2.2021543853	0.2171484132
H	1.0	6.6888174144	-4.2668501022	-1.4527079558
H	1.0	3.7430180584	-3.7852156397	-3.0041729917
H	1.0	3.8829711651	-5.3697319832	-0.0353756705
H	1.0	2.4918682764	0.2522028303	-2.5920615483
H	1.0	4.6944572987	3.4821980776	1.3099013629
H	1.0	2.6998137241	4.4204848250	-1.2150938101
H	1.0	0.7132959713	5.0727048524	2.9959526837
H	1.0	1.0952095934	1.8417269476	3.7188673603
H	1.0	-1.9600237945	-1.2496380012	2.2710348975
H	1.0	-2.3052956297	6.3601751678	-0.5527070569
H	1.0	-6.3971193109	5.4216049615	-2.6061400069
N	7.0	-10.7834567873	0.5447135160	-3.5013787964

E[B3LYP/6-31++G(d,p)] = -610.8102408 hartree
E[B3LYP/6-311++G(2df,p)] = -610.9805241 hartree
E[M06/6-31++G(d,p)] = -610.744172 hartree
E[M06/6-311++G(2df,p)] = -610.9126094 hartree
E[MP2/6-311++G(2df,p)]= -609.8814478 hartree

E[UB3LYP/6-31++G(d,p)] = -610.8129436 hartree
E[UB3LYP/6-311++G(2df,p)] = -610.9855354 hartree
E[UM06/6-31++G(d,p)] = -610.7504557 hartree
E[UM06/6-311++G(2df,p)] = -610.9227138 hartree
E[ROMP2/6-311++G(2df,p)]= -609.8671179 hartree

Table S7. B3LYP/6-31++G(d,p) optimized geometry of N-(perfluorophenethyl)acetamide (**A3**) and electronic energy of N-(perfluorophenethyl)acetamide (**A3**) neutral and anion formed by vertical electron attachment.

ATOM	ATOMIC	COORDINATES (BOHR)		
CHARGE	X	Y	Z	
C	6.0	4.2723869993	-4.0666903256	-1.3418755266
C	6.0	4.0577708189	-1.5297331871	-0.0207302941
O	8.0	5.0004228334	-1.1411488322	2.0644500525
N	7.0	2.7451104561	0.3102930072	-1.2845601374
C	6.0	2.3703777927	2.8148413450	-0.2097028929
C	6.0	0.2064336669	2.9435694793	1.7494705249
C	6.0	-2.3768784501	2.4094195316	0.6516342123
C	6.0	-3.5679349456	0.0657624644	0.8986591935
C	6.0	-5.9512573614	-0.4266434362	-0.1107568401
C	6.0	-3.7116297097	4.2533952532	-0.6894287321
C	6.0	-6.0937238036	3.8261093101	-1.7204443337
C	6.0	-7.2198871087	1.4634793939	-1.4305603672
F	9.0	-2.6735276356	6.5654749991	-1.0002319653
F	9.0	-7.3058885384	5.6594080798	-2.9834615949
F	9.0	-9.5078539511	1.0151041088	-2.4148052507
F	9.0	-7.0267004210	-2.7041222994	0.1765193045
F	9.0	-2.4190382369	-1.8127952428	2.1790241392
H	1.0	6.2686557383	-4.5861193078	-1.4552023941
H	1.0	3.4558364000	-4.0889890922	-3.2407099936
H	1.0	3.3218359303	-5.4931877819	-0.1865537495
H	1.0	1.9810942392	-0.0968484569	-2.9825167319
H	1.0	4.1219270162	3.3672082512	0.7371254160
H	1.0	2.0236319712	4.1374794611	-1.7592215110
H	1.0	0.2062068998	4.8402118641	2.5766035897
H	1.0	0.6108539255	1.6003333500	3.2621205890

E[B3LYP/6-31++G(d,p)] = -1014.62137 hartree
E[B3LYP/6-311++G(2df,p)] = -1014.937722 hartree
E[M06/6-31++G(d,p)] = -1014.608053 hartree
E[M06/6-311++G(2df,p)] = -1014.906433 hartree
E[MP2/6-311++G(2df,p)]= -1013.425995 hartree

E[UB3LYP/6-31++G(d,p)] = -1014.620447 hartree
E[UB3LYP/6-311++G(2df,p)] = -1014.936681 hartree
E[UM06/6-31++G(d,p)] = -1014.600937 hartree
E[UM06/6-311++G(2df,p)] = -1014.90127 hartree
E[ROMP2/6-311++G(2df,p)]= -1013.410628 hartree

Table S8. B3LYP/6-31++G(d,p) optimized geometry of N-(3,5-dicyanophenethyl)acetamide (**A4**) and electronic energy of N-(3,5-dicyanophenethyl)acetamide (**A4**) neutral and anion formed by vertical electron attachment.

ATOM	ATOMIC	COORDINATES (BOHR)		
CHARGE	X	Y	Z	
C	6.0	4.7098396682	-4.0539157779	-0.8678944544
C	6.0	4.4130015101	-1.5213428037	0.4468257098
O	8.0	5.1434750906	-1.1652050440	2.6227506984
N	7.0	3.2908633213	0.3599739034	-0.9319939599
C	6.0	2.9954235604	2.9116331101	0.0616995535
C	6.0	0.7994296818	3.2033501108	1.9686409450
C	6.0	-1.7767203737	2.6549138347	0.8624709408
C	6.0	-2.8828336860	0.2657899602	1.1195114696
C	6.0	-5.2550256157	-0.2622561726	0.0462793894
C	6.0	-3.0973175857	4.5126845559	-0.4832596268
C	6.0	-5.4697740769	3.9965247997	-1.5572287002
C	6.0	-6.5662119923	1.6002766582	-1.3006228083
C	6.0	-6.7832470220	5.9396922383	-2.9205337195
C	6.0	-6.3451518462	-2.7297658810	0.3356909245
H	1.0	6.7267253177	-4.4772899882	-1.0318470811
H	1.0	3.8557591108	-4.1209443587	-2.7487198327
H	1.0	3.8638660353	-5.5226675073	0.3131842879
H	1.0	2.7109064157	-0.0152122942	-2.7084497719
H	1.0	4.7503553934	3.4411343319	1.0183922320
H	1.0	2.7266667304	4.1844958437	-1.5459281388
H	1.0	0.8489971945	5.1466498303	2.6847526080
H	1.0	1.1740867562	1.9524648905	3.5697868771
H	1.0	-1.9118735763	-1.1999571049	2.1747911530
H	1.0	-2.2982658490	6.3911477768	-0.6954380607
H	1.0	-8.3988115634	1.1989177557	-2.1220866952
N	7.0	-7.8344071026	7.5207503832	-4.0287257305
N	7.0	-7.2176383348	-4.7342171335	0.5671445634

E[B3LYP/6-31++G(d,p)] = -703.0052326 hartree
E[B3LYP/6-311++G(2df,p)] = -703.2044955 hartree
E[M06/6-31++G(d,p)] = -702.9293438 hartree
E[M06/6-311++G(2df,p)] = -703.1258404 hartree
E[MP2/6-311++G(2df,p)]= -701.9673638 hartree

E[UB3LYP/6-31++G(d,p)] = -703.0346715 hartree
E[UB3LYP/6-311++G(2df,p)] = -703.2366543 hartree
E[UM06/6-31++G(d,p)] = -702.9641359 hartree
E[UM06/6-311++G(2df,p)] = -703.1640454 hartree
E[ROMP2/6-311++G(2df,p)]= -701.9577306 hartree

Table S9. B3LYP/6-31++G(d,p) optimized geometry of N-(3-nitrophenethyl)acetamide (**A5**) and electronic energy of N-(3-nitrophenethyl)acetamide (**A5**) neutral and anion formed by vertical electron attachment.

ATOM	ATOMIC CHARGE	COORDINATES (BOHR) X	Y	Z
C	6.0	-5.0640429382	-4.8476304294	1.2094350640
C	6.0	-5.1340828463	-1.9829747823	1.0431260640
O	8.0	-5.3023227589	-0.6534312236	2.9373886296
H	1.0	-3.4583415794	-5.4014916809	2.3865728769
H	1.0	-4.9085286121	-5.7878549880	-0.6250528771
H	1.0	-6.7820583769	-5.4960952950	2.1579120197
N	7.0	-5.0065113020	-0.9922072243	-1.3488528912
C	6.0	-5.0535287034	1.7081790816	-1.8581859312
C	6.0	-2.5484259026	2.7336390104	-2.9504700962
O	8.0	7.1895329438	-1.9092427946	1.0237552988
O	8.0	5.0808844895	-3.0800710898	-2.3128093813
H	1.0	-4.8902655619	-2.1975679258	-2.8231738555
H	1.0	-6.5881451333	2.1342834292	-3.1854585919
H	1.0	-5.4923658791	2.6267609158	-0.0626231337
H	1.0	-2.8355349924	4.7417116697	-3.3815030254
H	1.0	-2.1515893612	1.7964267163	-4.7553558824
C	6.0	-0.3062707633	2.4275253804	-1.2017824578
C	6.0	1.5032001593	0.5550837078	-1.6385214359
C	6.0	3.5219580943	0.2808438064	0.0358033605
C	6.0	-0.0197126335	3.9873700654	0.9263366450
C	6.0	2.0138160109	3.6909186682	2.5793149855
C	6.0	3.8194253116	1.8200814481	2.1497563970
N	7.0	5.4012286070	-1.7130733484	-0.4532326479
H	1.0	1.3765020377	-0.6899255882	-3.2589704974
H	1.0	-1.4150528999	5.4468503152	1.3017916485
H	1.0	2.1922532032	4.9162569298	4.2138376733
H	1.0	5.4149328195	1.5432224913	3.4002830947

E[B3LYP/6-31++G(d,p)] = -723.035315 hartree
E[B3LYP/6-311++G(2df,p)] = -723.246068 hartree
E[M06/6-31++G(d,p)] = -722.9761272 hartree
E[M06/6-311++G(2df,p)] = -723.1808133 hartree
E[MP2/6-311++G(2df,p)]= -722.016958 hartree

E[UB3LYP/6-31++G(d,p)] = -723.0653981 hartree
E[UB3LYP/6-311++G(2df,p)] = -723.277387 hartree
E[UM06/6-31++G(d,p)] = -723.0114837 hartree
E[UM06/6-311++G(2df,p)] = -723.2182506 hartree
E[ROMP2/6-311++G(2df,p)]= -722.002523 hartree

Table S10. B3LYP/6-31++G(d,p) optimized geometry of N-(3,5-dinitrophenethyl)acetamide (**A6**) and electronic energy of N-(3,5-dinitrophenethyl)acetamide (**A6**) neutral and anion formed by vertical electron attachment.

ATOM	ATOMIC CHARGE	COORDINATES (BOHR) X	Y	Z
C	6.0	-5.0072825387	-4.7598607151	0.9187469807
C	6.0	-4.9509498070	-1.8914267411	0.9061803029
O	8.0	-4.6273909234	-0.6597222396	2.8449257827
H	1.0	-3.2442248839	-5.4549775225	1.7413824977
H	1.0	-5.2535894239	-5.5984077249	-0.9544061101
H	1.0	-6.5506028556	-5.3829033733	2.1441775920
N	7.0	-5.2952011902	-0.7642240867	-1.4058616486
C	6.0	-5.3682202024	1.9638977327	-1.7390959292
C	6.0	-2.8912240694	3.0960136747	-2.8038242425
O	8.0	6.5513398488	-1.9288811102	1.4146866689
O	8.0	4.3080650260	-3.1869472893	-1.8055953867
H	1.0	-5.5650729585	-1.8784254263	-2.9307193426
H	1.0	-6.9209135602	2.4379732913	-3.0239962173
H	1.0	-5.7887031319	2.7836419690	0.1088293196
H	1.0	-3.2201497749	5.1120489475	-3.1495685092
H	1.0	-2.4810212493	2.2321632340	-4.6411859231
C	6.0	-0.6458516508	2.7714910309	-1.0671471625
C	6.0	1.0288802113	0.7502968062	-1.3766086903
C	6.0	3.0350700116	0.4373392853	0.3046994183
C	6.0	-0.2356677279	4.4557660092	0.9344883982
C	6.0	1.7980553801	4.0865135512	2.5625251311
C	6.0	3.4754517558	2.0801347782	2.3040484105
N	7.0	4.7646417219	-1.7221639844	-0.0548398482
H	1.0	0.8016406613	-0.5887441315	-2.9082127061
H	1.0	-1.4803168525	6.0514128387	1.2516600080
N	7.0	2.2048566934	5.8993465885	4.6474976079
H	1.0	5.0429038736	1.8186722906	3.5889486986
O	8.0	3.9900808340	5.5055087954	6.0811004340
O	8.0	0.7341963407	7.6928477289	4.8127919400

E[B3LYP/6-31++G(d,p)] = -927.4559891 hartree
E[B3LYP/6-311++G(2df,p)] = -927.7365305 hartree
E[M06/6-31++G(d,p)] = -927.394532 hartree
E[M06/6-311++G(2df,p)] = -927.6636976 hartree
E[MP2/6-311++G(2df,p)]= -926.2398478 hartree

E[UB3LYP/6-31++G(d,p)] = -927.5141941 hartree
E[UB3LYP/6-311++G(2df,p)] = -927.7954118 hartree
E[UM06/6-31++G(d,p)] = -927.4579133 hartree
E[UM06/6-311++G(2df,p)] = -927.728107 hartree
E[ROMP2/6-311++G(2df,p)] is not available due to failure of SCF convergence.

Table S11. B3LYP/6-31++G(d,p) optimized geometry of N-phenethylacetamide with the methyl ammonium ion complex (**B1**) and electronic energy of the complex and the charge-neutralized radical formed by vertical electron attachment.

ATOM	ATOMIC CHARGE	COORDINATES (BOHR) X	Y	Z
C	6.0	4.0815435718	-3.9344095064	-1.6651320541
C	6.0	4.3449335800	-1.3116399108	-0.5695823100
O	8.0	6.4822514666	-0.3951417040	-0.0484147798
N	7.0	2.2391363229	0.0081636163	-0.1688659143
C	6.0	2.1414374893	2.5822349732	0.8556490300
C	6.0	-0.2574562686	2.9652635336	2.4564170169
C	6.0	-2.6724504918	2.4142761274	1.0151985951
C	6.0	-4.0013624982	0.1537481064	1.4105292718
C	6.0	-6.1905533632	-0.3904740808	0.0308970199
C	6.0	-3.5937486026	4.1264623586	-0.7912471683
C	6.0	-5.7775159540	3.5883061918	-2.1687818243
C	6.0	-7.0793292897	1.3237719517	-1.7654387095
H	1.0	-7.2081897048	-2.1379414962	0.3803451495
N	7.0	11.2405059147	-1.2892844524	0.0713938478
C	6.0	12.4051818354	1.2692155624	-0.2996160554
H	1.0	5.0851392494	-4.0227164018	-3.4713321531
H	1.0	2.1177403254	-4.4842819743	-1.9786564927
H	1.0	4.9512143687	-5.3035726763	-0.3824049509
H	1.0	0.5612108238	-0.7691940660	-0.6740085680
H	1.0	3.8424743371	2.8747078643	1.9846658213
H	1.0	2.1794020844	3.9295340134	-0.7185683068
H	1.0	-0.2455320976	4.9279518417	3.1144385031
H	1.0	-0.1476820859	1.7643804630	4.1390479336
H	1.0	-3.3550762104	-1.1662065988	2.8485918512
H	1.0	-2.6134721438	5.9061873965	-1.1032031344
H	1.0	-6.4747681517	4.9425594236	-3.5438031448
H	1.0	-8.7848825827	0.9124919877	-2.8286552420
H	1.0	11.6793947753	-2.0033930059	1.8123039140
H	1.0	11.8922346133	-2.5468782000	-1.2416444602
H	1.0	11.8751892849	1.9573781781	-2.1663629751
H	1.0	14.4554211486	1.1408653733	-0.1397452368
H	1.0	11.6518425704	2.5346516728	1.1387866747
H	1.0	9.1761881430	-1.1620303044	-0.0697686835

E[B3LYP/6-31++G(d,p)] = -614.8260779 hartree
E[B3LYP/6-311++G(2df,p)] = -614.9919194 hartree
E[M06/6-31++G(d,p)] = -614.7529275 hartree
E[M06/6-311++G(2df,p)] = -614.9169829 hartree
E[MP2/6-311++G(2df,p)]= -613.8405171 hartree

E[UB3LYP/6-31++G(d,p)] = -614.9344925 hartree
E[UB3LYP/6-311++G(2df,p)] = -615.1001801 hartree
E[UM06/6-31++G(d,p)] = -614.8520682 hartree
E[UM06/6-311++G(2df,p)] = -615.0176261 hartree
E[ROMP2/6-311++G(2df,p)]= -613.9412151 hartree

Table S12. B3LYP/6-31++G(d,p) optimized geometry of N-(4-cyanophenethyl)acetamide with the methyl ammonium ion complex (**B2**) and electronic energy of the complex and the charge-neutralized radical formed by vertical electron attachment.

ATOM	ATOMIC CHARGE	COORDINATES (BOHR) X	Y	Z
C	6.0	4.4973021864	-3.7974610641	-1.5920374529
C	6.0	4.8094282278	-1.1696647974	-0.5210163521
O	8.0	6.9567427649	-0.2992003156	0.0206736023
N	7.0	2.7227927921	0.2021817834	-0.1651998458
C	6.0	2.6646648208	2.7951881947	0.8112215720
C	6.0	0.3735610333	3.2119483641	2.5577252271
C	6.0	-2.1302125169	2.6336733146	1.2915899181
C	6.0	-3.4485042632	0.4021147929	1.8537833994
C	6.0	-5.7106574486	-0.1874986125	0.6352124935
C	6.0	-3.1502488106	4.2871835538	-0.5179549960
C	6.0	-5.4057123660	3.7249522780	-1.7487524290
C	6.0	-6.6949212293	1.4701690239	-1.1857274683
N	7.0	11.7181530553	-1.3224491435	0.0929745186
C	6.0	12.9422797557	1.2291722687	0.2894115350
C	6.0	-9.0089473930	0.8693684407	-2.4661869003
N	7.0	-10.8735778197	0.3723705059	-3.5192178097
H	1.0	-6.7219254137	-1.9103806928	1.0951717989
H	1.0	5.5165825897	-3.9260002258	-3.3871826549
H	1.0	2.5260156250	-4.3093689369	-1.9227961925
H	1.0	5.3239439225	-5.1721989257	-0.2871627611
H	1.0	1.0434122041	-0.5599258102	-0.6816052665
H	1.0	4.4290074892	3.1186525921	1.8277051808
H	1.0	2.5995070687	4.1104374822	-0.7888661136
H	1.0	0.4230718541	5.1894521239	3.1704688786
H	1.0	0.5915598232	2.0464976557	4.2537354038
H	1.0	-2.7236998606	-0.8730534063	3.2920538487
H	1.0	-2.1839752213	6.0457814553	-0.9575808498
H	1.0	-6.1845251373	5.0193011960	-3.1345640849
H	1.0	12.1318140741	-2.4093250453	1.6362570410
H	1.0	12.3506254462	-2.2772143015	-1.4630825515
H	1.0	12.4403307388	2.3178623075	-1.3846778202
H	1.0	14.9874735004	1.0181654649	0.4201805734
H	1.0	12.2101054217	2.1680259339	1.9690188902
H	1.0	9.6677058724	-1.1252184421	-0.0287427323

E[B3LYP/6-31++G(d,p)] = -707.0192877 hartree
E[B3LYP/6-311++G(2df,p)] = -707.2141321 hartree
E[M06/6-31++G(d,p)] = -706.9364181 hartree
E[M06/6-311++G(2df,p)] = -707.1284837 hartree
E[MP2/6-311++G(2df,p)]= -705.9236485 hartree

E[UB3LYP/6-31++G(d,p)] = -707.1363112 hartree
E[UB3LYP/6-311++G(2df,p)] = -707.3315977 hartree
E[UM06/6-31++G(d,p)] = -707.0455363 hartree
E[UM06/6-311++G(2df,p)] = -707.2399301 hartree
E[ROMP2/6-311++G(2df,p)]= -706.0291795 hartree

Table S13. B3LYP/6-31++G(d,p) optimized geometry of N-(perfluorophenethyl)acetamide with the methyl ammonium ion complex (**B3**) and electronic energy of the complex and the charge-neutralized radical formed by vertical electron attachment.

ATOM	ATOMIC CHARGE	COORDINATES (BOHR) X	Y	Z
C	6.0	3.5929171232	-4.9150450132	0.4898169760
C	6.0	3.6600779848	-2.1774367694	1.2917977879
O	8.0	5.5022773639	-0.7688539154	0.7677578743
N	7.0	1.6833679099	-1.2817633430	2.5833499115
C	6.0	1.4721343390	1.3335607323	3.4834452967
C	6.0	-1.3041188014	2.1259039417	3.8084781666
C	6.0	-2.8178460093	2.1122601200	1.3815786696
C	6.0	-4.1180530779	-0.0305757665	0.5618533307
C	6.0	-5.5447773014	-0.0801621764	-1.6465371504
C	6.0	-2.9984660192	4.2484252738	-0.1593227980
C	6.0	-4.4085606540	4.2726704582	-2.3826421144
C	6.0	-5.6916845997	2.0945344903	-3.1281390165
N	7.0	9.9053200181	-0.4800659899	-1.3239798215
C	6.0	10.1670659646	2.2717718907	-1.9644268560
F	9.0	-1.7712779628	6.3782787428	0.5122102290
F	9.0	-4.5323943980	6.3581720583	-3.8010704407
F	9.0	-7.0408922631	2.0847646069	-5.2559893760
F	9.0	-6.7487217282	-2.1854870021	-2.3561292588
F	9.0	-3.9880210327	-2.1784950159	1.9619135205
H	1.0	3.7820597973	-5.0267278191	-1.5662993849
H	1.0	1.8544637008	-5.8791832122	1.0422972658
H	1.0	5.1960472676	-5.9124990813	1.3337686021
H	1.0	0.2437935497	-2.4804921260	2.9748066499
H	1.0	2.4527698458	1.5178090161	5.2992641011
H	1.0	2.4366693803	2.5477474739	2.1219544144
H	1.0	-1.3126792601	4.0327130523	4.6007646842
H	1.0	-2.2252090423	0.9011347345	5.1986550895
H	1.0	11.2389941339	-1.0209055676	-0.0339772733
H	1.0	10.1463734651	-1.5841572955	-2.8910539941
H	1.0	8.7059298309	2.7604172366	-3.3303585945
H	1.0	12.0350223090	2.6316891023	-2.7551637983
H	1.0	9.8953233676	3.3636177718	-0.2403542484
H	1.0	8.0514610296	-0.8541939410	-0.5192022151

E[B3LYP/6-31++G(d,p)] = -1110.830942 hartree
E[B3LYP/6-311++G(2df,p)] = -1111.172204 hartree
E[M06/6-31++G(d,p)] = -1110.800526 hartree
E[M06/6-311++G(2df,p)] = -1111.122906 hartree
E[MP2/6-311++G(2df,p)]= -1109.469031 hartree

E[UB3LYP/6-31++G(d,p)] = -1110.945597 hartree
E[UB3LYP/6-311++G(2df,p)] = -1111.286553 hartree
E[UM06/6-31++G(d,p)] = -1110.906748 hartree
E[UM06/6-311++G(2df,p)] = -1111.230569 hartree
E[ROMP2/6-311++G(2df,p)]= -1109.574072 hartree

Table S14. B3LYP/6-31++G(d,p) optimized geometry of N-(3,5-dicyanophenethyl)acetamide with the methyl ammonium ion complex (**B4**) and electronic energy of the complex and the charge-neutralized radical formed by vertical electron attachment.

ATOM	ATOMIC CHARGE	COORDINATES (BOHR) X	Y	Z
C	6.0	4.6701932170	-4.0142693267	-1.3996822446
C	6.0	4.8894770206	-1.3809739573	-0.3229730686
O	8.0	7.0001497708	-0.4284386759	0.2109879065
N	7.0	2.7514221409	-0.0857746626	0.0539516769
C	6.0	2.6277773695	2.4953075777	1.0544859984
C	6.0	0.2748984394	2.8814352888	2.7200337922
C	6.0	-2.1972033032	2.4681711126	1.3274947119
C	6.0	-3.6396311496	0.2933988569	1.7445194428
C	6.0	-5.8995355611	-0.1192795043	0.4047037175
C	6.0	-3.0573309838	4.2424159452	-0.4406085113
C	6.0	-5.3142118336	3.8428333851	-1.7746794696
C	6.0	-6.7499878446	1.6531322941	-1.3633239166
N	7.0	11.8426859979	-1.1431897363	0.2166381872
C	6.0	12.9334736326	1.4192031140	-0.3265257534
C	6.0	-6.1419307135	5.6841067985	-3.5865676439
C	6.0	-7.3204961203	-2.3846074294	0.8582001601
H	1.0	5.6865823395	-4.1018770235	-3.1986635904
H	1.0	2.7185220114	-4.6021819787	-1.7208978680
H	1.0	5.5550007190	-5.3572030999	-0.1000420938
H	1.0	1.1052629357	-0.8967694675	-0.4896469007
H	1.0	4.3456705731	2.8178082148	2.1482782974
H	1.0	2.6235443833	3.8357847071	-0.5263264821
H	1.0	0.3526795611	4.8167414674	3.4504128865
H	1.0	0.3818191358	1.6176999318	4.3546845661
H	1.0	-3.0485815524	-1.0903907922	3.1394962697
H	1.0	-1.9951538006	5.9638996282	-0.7857669630
H	1.0	-8.4928254313	1.3441998896	-2.3928088402
H	1.0	12.3498506585	-1.7537035111	1.9790722324
H	1.0	12.4851550392	-2.4547729553	-1.0480042383
H	1.0	12.3274385083	1.9965144033	-2.2078802550
H	1.0	14.9898167606	1.3391921157	-0.2310567965
H	1.0	12.2024520315	2.7415010794	1.0719281693
H	1.0	9.7934104451	-1.0826618129	0.1353232780
N	7.0	-6.7820564946	7.1837744451	-5.0591555171
N	7.0	-8.4298408641	-4.2453261232	1.2269990838

E[B3LYP/6-31++G(d,p)] = -799.2096641 hartree
E[B3LYP/6-311++G(2df,p)] = -799.4335119 hartree
E[M06/6-31++G(d,p)] = -799.1168022 hartree
E[M06/6-311++G(2df,p)] = -799.3370771 hartree
E[MP2/6-311++G(2df,p)]= -798.0047667 hartree

E[UB3LYP/6-31++G(d,p)] = -799.3380498 hartree
E[UB3LYP/6-311++G(2df,p)] = -799.5629747 hartree
E[UM06/6-31++G(d,p)] = -799.2398239 hartree
E[UM06/6-311++G(2df,p)] = -799.4629314 hartree
E[ROMP2/6-311++G(2df,p)]= -798.1130718 hartree

Table S15. B3LYP/6-31++G(d,p) optimized geometry of N-(3-nitrophenethyl)acetamide with the methyl ammonium ion complex (**B5**) and electronic energy of the complex and the charge-neutralized radical formed by vertical electron attachment.

ATOM	ATOMIC CHARGE	COORDINATES (BOHR) X	Y	Z
C	6.0	4.3758305999	-3.4290589828	-1.7661945999
C	6.0	4.6392206081	-0.8062893872	-0.6706448558
O	8.0	6.7765384947	0.1102088196	-0.1494773256
N	7.0	2.5334233509	0.5135141399	-0.2699284601
C	6.0	2.4357245174	3.0875854968	0.7545864842
C	6.0	0.0368307595	3.4706140573	2.3553544711
C	6.0	-2.3781634638	2.9196266510	0.9141360493
C	6.0	-3.7070754701	0.6590986300	1.3094667259
C	6.0	-5.8962663351	0.1148764428	-0.0701655259
C	6.0	-3.2994615746	4.6318128822	-0.8923097141
C	6.0	-5.4832289260	4.0936567154	-2.2698443702
C	6.0	-6.7850422617	1.8291224753	-1.8665012553
N	7.0	11.2405059147	-1.2892844524	0.0713938478
C	6.0	12.4051818354	1.2692155624	-0.2996160554
N	7.0	-7.2276160880	-2.2861716027	0.3662288964
H	1.0	5.3794262775	-3.5173658782	-3.5723946990
H	1.0	2.4120273535	-3.9789314507	-2.0797190385
H	1.0	5.2455013967	-4.7982221527	-0.4834674967
H	1.0	0.8554978519	-0.2638435424	-0.7750711139
H	1.0	4.1367613652	3.3800583879	1.8836032755
H	1.0	2.4736891124	4.4348845370	-0.8196308527
H	1.0	0.0487549305	5.4333023654	3.0133759573
H	1.0	0.1466049421	2.2697309866	4.0379853878
H	1.0	-3.0607891823	-0.6608560752	2.7475293053
H	1.0	-2.3191851157	6.4115379202	-1.2042656802
H	1.0	-6.1804811237	5.4479099473	-3.6448656906
H	1.0	-8.4905955546	1.4178425113	-2.9297177878
H	1.0	11.6793947753	-2.0033930059	1.8123039140
H	1.0	11.8922346133	-2.5468782000	-1.2416444602
H	1.0	11.8751892849	1.9573781781	-2.1663629751
H	1.0	14.4554211486	1.1408653733	-0.1397452368
H	1.0	11.6518425704	2.5346516728	1.1387866747
H	1.0	9.1761881430	-1.1620303044	-0.0697686835
O	8.0	-9.2198030188	-2.6308954174	-0.7727467509
O	8.0	-6.2435223826	-3.8012594133	1.8355286464

E[B3LYP/6-31++G(d,p)] = -819.2464238 hartree
E[B3LYP/6-311++G(2df,p)] = -819.4818931 hartree
E[M06/6-31++G(d,p)] = -819.170015 hartree
E[M06/6-311++G(2df,p)] = -819.3982571 hartree
E[MP2/6-311++G(2df,p)]= -818.0618472 hartree

E[UB3LYP/6-31++G(d,p)] = -819.3758248 hartree
E[UB3LYP/6-311++G(2df,p)] = -819.6116289 hartree
E[UM06/6-31++G(d,p)] = -819.2950838 hartree
E[UM06/6-311++G(2df,p)] = -819.525209 hartree
E[ROMP2/6-311++G(2df,p)]= -818.1659839 hartree

Table S16. B3LYP/6-31++G(d,p) optimized geometry of N-(3,5-dicyanophenethyl)acetamide with the methyl ammonium ion complex (**C4**) and electronic energy of the complex and the charge-neutralized radical formed by vertical electron attachment.

ATOM	ATOMIC CHARGE	COORDINATES (BOHR) X	Y	Z
C	6.0	-3.4316479074	-6.4293769335	3.3369915327
C	6.0	-4.0105465665	-4.9855506898	0.9264381655
O	8.0	-2.9984093275	-5.5214013909	-1.1010299495
N	7.0	-5.7135109348	-3.0564428125	1.1490100923
C	6.0	-6.8587415752	-1.7285134637	-0.9903486984
C	6.0	-4.9856451761	-0.5173880782	-2.8774668642
C	6.0	-2.9088552129	1.0422405740	-1.6846907181
C	6.0	-0.4664977573	0.0507202455	-1.4777846197
C	6.0	1.4817341470	1.5029557698	-0.3984109300
C	6.0	-3.3558698953	3.4903238993	-0.7838772370
C	6.0	-1.4137984977	4.9364556087	0.3132220825
C	6.0	1.0333399646	3.9531366910	0.5110574961
C	6.0	-1.9297881787	7.4401913643	1.2238054469
C	6.0	3.9705032728	0.4632096341	-0.2520894468
N	7.0	-2.3443940604	9.4650327602	1.9694724244
N	7.0	5.9926423605	-0.3899071630	-0.1528410379
H	1.0	-1.3964319159	-6.7500256391	3.4573670781
H	1.0	-4.3449146827	-8.2828201823	3.2266882268
H	1.0	-4.0806365034	-5.4775030562	5.0524469898
H	1.0	-6.5531539857	-2.8205483175	2.8462296937
H	1.0	-8.0703204949	-3.0236371694	-2.0643366690
H	1.0	-8.0778793989	-0.2707599395	-0.1773507839
H	1.0	-6.1051377485	0.6778447118	-4.1468336047
H	1.0	-4.1381030707	-2.0121424372	-4.0145716828
H	1.0	-0.0961114637	-1.8554274610	-2.1383950304
H	1.0	-5.2285694519	4.3150570121	-0.9413103090
H	1.0	2.5375051591	5.0693222429	1.3394188828
N	7.0	10.6883657756	-2.6541579443	-0.2121217421
C	6.0	12.7272667328	-0.6969498415	0.0733024711
H	1.0	10.8658677376	-3.6177292254	-1.8797482345
H	1.0	8.8646668139	-1.8048961881	-0.1817916400
H	1.0	12.4474928003	0.2733110696	1.8677484745
H	1.0	12.5613676883	0.6430359591	-1.4812995100
H	1.0	14.5711290708	-1.6133724593	0.0347898554
H	1.0	10.7598541097	-3.9590515333	1.2136198238

E[B3LYP/6-31++G(d,p)] = -799.2067168 hartree
E[B3LYP/6-311++G(2df,p)] = -799.4311592 hartree
E[M06/6-31++G(d,p)] = -799.1170901 hartree
E[M06/6-311++G(2df,p)] = -799.3375442 hartree
E[MP2/6-311++G(2df,p)]= -798.0028924 hartree

E[UB3LYP/6-31++G(d,p)] = -799.3378863 hartree
E[UB3LYP/6-311++G(2df,p)] = -799.5639059 hartree
E[UM06/6-31++G(d,p)] = -799.2481694 hartree
E[UM06/6-311++G(2df,p)] = -799.4719508 hartree
E[ROMP2/6-311++G(2df,p)]= -798.1101728 hartree

Table S17. B3LYP/6-31++G(d,p) optimized geometry of N-(3-nitrophenethyl)acetamide with the methyl ammonium ion complex (**C5**) and electronic energy of the complex and the charge-neutralized radical formed by vertical electron attachment.

ATOM	ATOMIC CHARGE	COORDINATES (BOHR) X	Y	Z
C	6.0	3.7663561743	-5.7200304895	-2.6053652193
C	6.0	4.3549869223	-3.9129422192	-0.4621702848
O	8.0	3.4156230310	-4.1244781463	1.6435135888
N	7.0	5.9780158813	-2.0377671216	-1.0791847171
C	6.0	7.0999084057	-0.2802274667	0.7456102857
C	6.0	5.1940063636	1.0079231501	2.5460467205
O	8.0	-5.4034446948	2.1768320570	-1.5512193715
O	8.0	-3.8249754745	-1.1423393596	0.3629218759
C	6.0	3.0443485662	2.3016484585	1.1726883589
C	6.0	0.7423032652	1.0905230730	0.9047252139
C	6.0	-1.2183063443	2.3307691360	-0.2997483362
C	6.0	3.3069070950	4.7242393803	0.1974574685
C	6.0	1.3280616297	5.9379914849	-1.0269904853
C	6.0	-0.9672373496	4.7473129346	-1.2799681033
N	7.0	-3.5968855478	1.0907309429	-0.5241532972
H	1.0	5.4489870911	-6.7748377413	-3.1102433114
H	1.0	3.1221674824	-4.6996918397	-4.2604628284
H	1.0	2.3237771498	-7.0208611677	-1.9893145473
H	1.0	6.6630226546	-1.9844012597	-2.8335307350
H	1.0	8.4863247739	-1.2572535969	1.8953573712
H	1.0	8.0784463167	1.1463077842	-0.3433821092
H	1.0	6.2311824719	2.3883301896	3.6495711083
H	1.0	4.4502858038	-0.4023415600	3.8091962625
H	1.0	0.4990388388	-0.7869952848	1.6052466375
H	1.0	5.0752181880	5.6915712161	0.4114878338
H	1.0	1.5785070148	7.8069871786	-1.7575585521
H	1.0	-2.5303997893	5.6390368337	-2.1920443512
N	7.0	-8.7726938501	-2.1154537570	-0.4732440791
C	6.0	-10.2193735800	-2.3013461024	2.0161864508
H	1.0	-9.2659879219	-0.5393655914	-1.4530481065
H	1.0	-9.0804735217	-3.6547678548	-1.5728567341
H	1.0	-9.5723314018	-3.9635868757	2.9981825603
H	1.0	-12.2115605107	-2.4268428052	1.6141850415
H	1.0	-9.8067330133	-0.6296378018	3.1030056609
H	1.0	-6.8377656167	-1.9294858225	-0.1302588123

E[B3LYP/6-31++G(d,p)] = -819.236232 hartree
E[B3LYP/6-311++G(2df,p)] = -819.4728518 hartree
E[M06/6-31++G(d,p)] = -819.1644663 hartree
E[M06/6-311++G(2df,p)] = -819.3932871 hartree
E[MP2/6-311++G(2df,p)]= -818.0532317 hartree

E[UB3LYP/6-31++G(d,p)] = -819.4077703 hartree
E[UB3LYP/6-311++G(2df,p)] = -819.6455717 hartree
E[UM06/6-31++G(d,p)] = -819.3408058 hartree
E[UM06/6-311++G(2df,p)] = -819.571629 hartree
E[ROMP2/6-311++G(2df,p)]= -818.2114235 hartree

Table S18. B3LYP/6-31++G(d,p) optimized geometry of N-(3-nitrophenethyl)acetamide with the methyl ammonium ion complex (**D5**) and electronic energy of the complex and the charge-neutralized radical formed by vertical electron attachment.

ATOM	ATOMIC CHARGE	COORDINATES (BOHR) X	Y	Z
C	6.0	4.6615571693	0.9345450900	4.4003214487
C	6.0	4.4568809475	0.1196385523	1.6653021294
O	8.0	4.0650651612	1.6942338343	-0.0568618550
N	7.0	4.6949108329	-2.3623653545	1.1926060709
C	6.0	4.6963848192	-3.6008350751	-1.2961441577
C	6.0	2.3751776967	-3.0903822913	-2.9978613069
O	8.0	-7.0696349954	1.6678154650	1.3633428138
O	8.0	-3.7179036000	3.6094144311	0.0086927395
C	6.0	-0.1568661542	-3.1203533454	-1.6655099993
C	6.0	-1.4053892171	-0.8357691126	-1.2459719327
C	6.0	-3.7159760795	-0.8018674284	0.0188972599
C	6.0	-1.3200680887	-5.3538393876	-0.8246197293
C	6.0	-3.6566953753	-5.2985649025	0.4109398133
C	6.0	-4.8891368700	-3.0105224710	0.8563671259
N	7.0	-4.9331674855	1.6406601025	0.4979616950
H	1.0	6.1477888641	2.3616472586	4.5623087604
H	1.0	5.0912052698	-0.6159183912	5.6925349764
H	1.0	2.8783550355	1.7968459554	4.9974937581
H	1.0	5.0484029762	-3.4864688583	2.6945602859
H	1.0	6.4016546533	-3.0477122785	-2.3313171565
H	1.0	4.8476951790	-5.6207820806	-0.8965049058
H	1.0	2.4162981342	-4.5290306857	-4.4882881934
H	1.0	2.6195948560	-1.2634141036	-3.9230900478
H	1.0	-0.5843221727	0.9048385974	-1.9250071719
H	1.0	-0.4089744983	-7.1641590893	-1.1595358661
H	1.0	-4.5276511858	-7.0490558794	1.0277652729
H	1.0	-6.6943165170	-2.9264485618	1.8177652221
N	7.0	1.2139599745	5.9094566225	-0.1267817165
C	6.0	1.5964027199	7.3091577644	-2.5594637750
H	1.0	-0.5815064809	5.1381649606	-0.0305379720
H	1.0	1.4247967030	7.0889290977	1.3875691010
H	1.0	3.5077282757	8.0750826044	-2.5969559386
H	1.0	0.2120083586	8.8277226708	-2.6999649022
H	1.0	1.3467132251	5.9861039086	-4.1168625506
H	1.0	2.5058711460	4.3798746135	0.0557658139

E[B3LYP/6-31++G(d,p)] = -819.2545141 hartree
E[B3LYP/6-311++G(2df,p)] = -819.4897993 hartree
E[M06/6-31++G(d,p)] = -819.1827694 hartree
E[M06/6-311++G(2df,p)] = -819.4109761 hartree
E[MP2/6-311++G(2df,p)]= -818.0732093 hartree

E[UB3LYP/6-31++G(d,p)] = -819.4037156 hartree
E[UB3LYP/6-311++G(2df,p)] = -819.6403233 hartree
E[UM06/6-31++G(d,p)] = -819.3374324 hartree
E[UM06/6-311++G(2df,p)] = -819.5676875 hartree
E[ROMP2/6-311++G(2df,p)]= -818.2054566 hartree

Table S19. B3LYP/6-31++G(d,p) optimized geometry of N-(3,5-dinitrophenethyl)acetamide with the methyl ammonium ion complex (**B6**) and electronic energy of the complex and the charge-neutralized radical formed by vertical electron attachment.

ATOM	ATOMIC CHARGE	COORDINATES (BOHR) X	Y	Z
C	6.0	3.9604310333	-1.4819042223	-4.8946926644
C	6.0	4.5267819118	1.0346627728	-3.6758949913
O	8.0	6.0861460024	1.2389232548	-1.8946581725
N	7.0	3.3107621360	3.0709181136	-4.5553356715
C	6.0	3.6569221424	5.6400194912	-3.5704104867
C	6.0	2.1042854764	6.1884557673	-1.1627861948
C	6.0	-0.7128991289	5.8277070763	-1.5038061465
C	6.0	-1.9232875213	3.6747800530	-0.5603415499
C	6.0	-4.5106436519	3.3485188612	-0.9384190282
C	6.0	-2.1583883314	7.6155012442	-2.8181672627
C	6.0	-4.7379209964	7.2195280608	-3.1524408927
C	6.0	-5.9851023538	5.1003137491	-2.2237161588
N	7.0	9.3209789481	-1.2639054324	0.8201410787
C	6.0	9.6521912220	0.3301162328	3.1450142696
N	7.0	-5.7246225236	1.0334344509	0.0547453619
H	1.0	5.7134353458	-2.2890061917	-5.6373927721
H	1.0	2.5975795482	-1.3488675128	-6.4379940840
H	1.0	3.2106633504	-2.7785586060	-3.4685731532
H	1.0	2.0433418133	2.8117988862	-5.9606681968
H	1.0	5.6646237235	5.9055448897	-3.1704121869
H	1.0	3.1301232288	6.9381856557	-5.0878037630
H	1.0	2.5065703446	8.1431883290	-0.6082838982
H	1.0	2.7856072840	4.9738721832	0.3644336567
H	1.0	-0.8932167826	2.2476022953	0.4861131131
H	1.0	-1.3209940545	9.3250418590	-3.5778371098
N	7.0	-6.2074853080	9.1325165754	-4.5719274657
H	1.0	-7.9948448390	4.8309522068	-2.4930021120
H	1.0	8.7681207132	-3.0575199564	1.2807617882
H	1.0	10.9810276393	-1.4128347375	-0.1589637501
H	1.0	10.2349827166	2.2152879809	2.5572150011
H	1.0	11.0778571989	-0.5108685235	4.3714086411
H	1.0	7.8428919723	0.4349960251	4.1220781943
H	1.0	7.9189156488	-0.4342401347	-0.4258686486
O	8.0	-8.0167089687	0.8304967771	-0.2039770231
O	8.0	-4.3391321212	-0.5434285023	1.0637456557
O	8.0	-8.4978521024	8.8164410067	-4.7285668528
O	8.0	-5.0168823467	10.8961789425	-5.5055087954

E[B3LYP/6-31++G(d,p)] = -1023.660433 hartree
E[B3LYP/6-311++G(2df,p)] = -1023.965968 hartree
E[M06/6-31++G(d,p)] = -1023.582483 hartree
E[M06/6-311++G(2df,p)] = -1023.875477 hartree
E[MP2/6-311++G(2df,p)]= -1022.27865 hartree

E[UB3LYP/6-31++G(d,p)] = -1023.806167 hartree
E[UB3LYP/6-311++G(2df,p)] = -1024.112007 hartree
E[UM06/6-31++G(d,p)] = -1023.729469 hartree
E[UM06/6-311++G(2df,p)] = -1024.023608 hartree
E[ROMP2/6-311++G(2df,p)]= -1022.388559 hartree

7. Energies and molecular orbitals of excited states of anionic radicals of N-phenethylacetamide, N-(4-cyanophenethyl)acetamide, N-(perfluorophenethyl)acetamide, N-(3,5-dicyanophenethyl)acetamide, N-(3-nitrophenethyl)acetamide, N-(3,5-dinitrophenethyl)acetamide and neutralized radicals of their methyl ammonium complexes obtained by the time-dependent density functional calculations at the UB3LYP/6-31++G(d,p) and UB3LYP/6-311++G(2df,p) level of theories.

Table S20. TDDFT excited electronic energy of N-phenethylacetamide (**A1**) anion formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-518.5950060334	0.000				
1	-518.5842656774	0.292	0.9003	2.9264	1.0912	0.076
2	-518.5804542548	0.396	2.4222	-3.2444	1.2356	0.174
3	-518.5788747535	0.439	3.9224	0.7771	-0.9748	0.182
4	-518.5779226784	0.465	-0.2359	-0.9299	1.0713	0.024
5	-518.5736007102	0.582	0.0702	-0.2625	-1.7687	0.046
6	-518.5703701482	0.670	0.2074	-0.1638	-1.2479	0.027
7	-518.5651875614	0.811	-0.5850	0.1396	-0.8043	0.020
8	-518.5621222404	0.895	0.4629	0.1734	0.3378	0.008
9	-518.5591802602	0.975	0.5636	0.1339	0.1133	0.008
10	-518.5544157754	1.105	-0.1271	-0.8579	-0.5750	0.029
11	-518.5476654053	1.288	0.0171	-0.5356	-0.6277	0.021
12	-518.5402508867	1.490	0.1680	-0.0740	0.3113	0.005
13	-518.5327174359	1.695	-0.1992	0.1166	0.5679	0.016
14	-518.5289791740	1.797	-0.2024	-0.2080	0.1928	0.005
15	-518.5245009812	1.919	-0.2216	-0.3174	-0.0726	0.007

Table S21. TDDFT excited electronic energy of N-(4-cyanophenethyl)acetamide (**A2**) anion formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-610.8129435541	0.000				
1	-610.8108974679	0.056	-0.7876	0.9216	0.8124	0.003
2	-610.7977600628	0.413	-1.5654	0.8886	-0.4904	0.035
3	-610.7899668749	0.625	0.8142	1.0666	-0.2970	0.029
4	-610.7882659256	0.672	0.0125	0.0335	0.1669	0.000
5	-610.7866971104	0.714	0.1638	0.2819	-0.2276	0.003
6	-610.7811095255	0.866	-0.9308	-0.1674	-0.3482	0.022
7	-610.7747671869	1.039	-0.4159	1.0605	0.9090	0.054
8	-610.7704473726	1.156	0.6261	-0.0558	0.7643	0.028
9	-610.7638551444	1.336	-0.6079	-0.6431	-0.0950	0.026
10	-610.7597494615	1.447	0.4293	-0.1437	0.2376	0.009
11	-610.7511475314	1.682	0.5787	0.0130	-0.0208	0.014
12	-610.7464061471	1.811	0.2373	0.5210	-0.1442	0.015

13	-610.7424692268	1.918	0.1977	0.3276	-0.3722	0.013
14	-610.7310685057	2.228	0.2244	-0.0912	0.0888	0.004
15	-610.7276418865	2.321	0.0718	0.0522	0.0352	0.001

Table S22. TDDFT excited electronic energy of N-(perfluorophenethyl)acetamide (**A3**) anion formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-1014.6204474469	0.000				
1	-1014.6085379802	0.324	-0.6261	-0.5672	-0.4075	0.007
2	-1014.5998223749	0.561	-2.1605	2.4883	1.4873	0.180
3	-1014.5966336102	0.648	-0.0071	0.0688	-0.1406	0.000
4	-1014.5915406742	0.787	1.0414	1.7368	-1.8450	0.145
5	-1014.5894383989	0.844	2.2817	0.8567	1.0519	0.146
6	-1014.5807302286	1.081	0.2893	-0.8480	0.0222	0.021
7	-1014.5744099810	1.253	0.4364	-0.5350	0.1036	0.015
8	-1014.5680483215	1.426	-0.3045	0.7243	-0.7563	0.042
9	-1014.5660234699	1.481	-0.3399	-0.6485	-0.6677	0.036
10	-1014.5575483069	1.712	0.0786	0.2589	-0.5612	0.016
11	-1014.5509148026	1.892	-0.3414	-0.2264	0.1442	0.009
12	-1014.5480986761	1.969	0.2071	-0.2283	-0.0222	0.005
13	-1014.5407704611	2.168	0.6808	0.1324	0.2520	0.029
14	-1014.5359552016	2.299	-0.2094	0.3593	0.6202	0.031
15	-1014.5299176064	2.463	-0.2351	-0.0495	0.3104	0.009

Table S23. TDDFT excited electronic energy of N-(3,5-dicyanophenethyl)acetamide (**A4**) anion formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-703.0346715024	0.000				
1	-703.0208283171	0.377	0.3926	-0.3871	-0.0112	0.003
2	-703.0155638863	0.520	0.0856	0.2909	-0.2202	0.002
3	-703.0032729295	0.854	0.3223	-0.3987	-0.1094	0.006
4	-702.9944263559	1.095	0.2068	0.1469	-0.0960	0.002
5	-702.9929145981	1.136	0.0162	-0.2532	-0.0445	0.002
6	-702.9831336024	1.402	0.0479	-0.1292	-0.0651	0.001
7	-702.9744803589	1.638	-0.0204	-0.0407	-0.2088	0.002
8	-702.9734264813	1.667	0.0358	0.3895	-0.2743	0.009
9	-702.9666123626	1.852	0.0905	0.0391	-0.0504	0.001
10	-702.9646999058	1.904	-0.0553	-0.1337	-0.0923	0.001
11	-702.9496139618	2.315	-0.0455	-0.0635	-0.1159	0.001
12	-702.9475173057	2.372	0.0441	0.0375	-0.1708	0.002
13	-702.9470682083	2.384	-0.3631	-0.1371	-0.1534	0.010
14	-702.9460180734	2.412	0.1184	-0.0349	0.1785	0.003
15	-702.9382895153	2.623	-0.2312	-0.2772	0.0362	0.008

Table S24. TDDFT excited electronic energy of N-(3-nitrophenethyl)acetamide (**A5**) anion formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE	OSCILLATOR

	HARTREE	EV	X	Y	Z	STRENGTH
0	-723.0653980895	0.000				
1	-723.0532665733	0.330	-1.4568	-0.3353	-0.4518	0.020
2	-723.0413116417	0.655	-0.0612	-0.9730	0.1773	0.016
3	-723.0289231187	0.993	0.2342	-0.2166	-0.3479	0.005
4	-723.0234772894	1.141	-0.1985	0.1099	0.0084	0.001
5	-723.0155619171	1.356	0.2695	0.0756	0.1541	0.003
6	-723.0145528862	1.384	-0.0670	-0.0162	-0.1242	0.001
7	-723.0085857153	1.546	0.1442	-0.3474	0.2212	0.007
8	-723.0061786411	1.611	0.0947	-0.1752	0.2450	0.004
9	-722.9958239686	1.893	-0.1419	-0.1007	-0.1726	0.003
10	-722.9895905935	2.063	-0.2488	0.3588	-0.1380	0.011
11	-722.9863244783	2.152	0.5654	-0.2376	-0.1676	0.021
12	-722.9813624509	2.287	0.1395	-0.2488	-0.0372	0.005
13	-722.9756797268	2.441	-0.8732	0.8226	0.2855	0.091
14	-722.9734309941	2.503	-0.3032	0.3966	0.0436	0.015
15	-722.9673042641	2.669	-0.0611	-0.0017	0.0206	0.000

Table S25. TDDFT excited electronic energy of N-(3,5-dinitrophenethyl)acetamide (**A6**) anion formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-927.5141941037	0.000				
1	-927.4931097678	0.574	-0.3382	1.1055	0.6701	0.025
2	-927.4788787928	0.961	-0.3293	0.1175	0.1367	0.003
3	-927.4615874087	1.432	-0.1131	-0.5134	-0.2155	0.011
4	-927.4472551955	1.822	-0.0707	0.1919	0.0232	0.002
5	-927.4423774962	1.954	-0.0640	0.0859	-0.0252	0.001
6	-927.4378082953	2.079	-0.2572	0.5819	0.4367	0.030
7	-927.4295828218	2.302	0.2597	-0.6117	-0.2572	0.029
8	-927.4240463907	2.453	-0.0732	0.0048	-0.3847	0.009
9	-927.4205187908	2.549	0.0639	-0.0396	-0.0761	0.001
10	-927.4131701349	2.749	0.2652	-0.2136	0.2849	0.013
11	-927.4098294701	2.840	-0.1607	0.0075	-0.1460	0.003
12	-927.4074281209	2.905	-0.6263	-0.0417	-0.3069	0.035
13	-927.4004526538	3.095	-0.0158	0.0220	0.1030	0.001
14	-927.3965177762	3.202	0.1482	0.0907	-0.0807	0.003
15	-927.3884062968	3.423	0.0208	0.1254	0.0095	0.001

Table S26. TDDFT excited electronic energy of N-phenethylacetamide with the methyl ammonium complex radical (**B1**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-614.9344924561	0.000				
1	-614.9218296043	0.345	0.0679	0.4267	-0.0240	0.002
2	-614.9208358885	0.372	-0.9438	0.3345	0.1251	0.009
3	-614.9141723214	0.553	0.5112	-0.1789	-0.8625	0.014
4	-614.9063503860	0.766	2.5788	0.0847	0.5068	0.130
5	-614.9012666196	0.904	0.3049	1.9526	-0.0978	0.087
6	-614.8946352212	1.085	0.0355	-0.2354	-2.5672	0.177
7	-614.8911470875	1.179	1.4478	-0.2183	0.1470	0.063
8	-614.8895999984	1.222	-0.6364	-0.3865	0.4268	0.022
9	-614.8854199076	1.335	-0.3620	0.2349	0.9610	0.036
10	-614.8760935992	1.589	-0.9952	0.2134	-0.1769	0.042
11	-614.8723636544	1.691	-0.0942	0.7706	0.0589	0.025

12	-614.8704328226	1.743	-0.0874	-0.0489	0.3271	0.005
13	-614.8670936800	1.834	-0.0728	0.5532	-0.2260	0.016
14	-614.8635481988	1.930	-0.0385	-0.1069	-0.1427	0.002
15	-614.8601224522	2.024	0.2203	-0.3743	0.1617	0.011

Table S27. TDDFT excited electronic energy of N-(4-cyanophenethyl)acetamide with the methyl ammonium complex radical (**B2**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-707.1363112354	0.000				
1	-707.1285651336	0.211	2.3991	-0.7678	0.0443	0.033
2	-707.1153349327	0.571	-0.9153	0.0477	0.3929	0.014
3	-707.1105285338	0.702	-0.2846	0.0920	0.7868	0.012
4	-707.1007956361	0.966	2.3088	0.4796	0.6257	0.141
5	-707.0987625911	1.022	0.2305	-1.5579	-0.1194	0.062
6	-707.0941636327	1.147	-0.3187	-0.2489	2.3890	0.165
7	-707.0831433377	1.447	0.1464	0.0512	-0.0699	0.001
8	-707.0805336233	1.518	-1.0489	0.1008	-0.1911	0.043
9	-707.0798108181	1.537	0.2488	-0.0413	-0.1789	0.004
10	-707.0675356101	1.871	-0.4862	0.6821	0.0471	0.032
11	-707.0631471434	1.991	0.2240	0.3751	-0.0799	0.010
12	-707.0608507473	2.053	0.3091	-0.0807	0.1164	0.006
13	-707.0560899569	2.183	-0.0824	0.2467	0.0502	0.004
14	-707.0544476569	2.228	-0.2713	0.1043	-0.0716	0.005
15	-707.0512292773	2.315	-0.1510	0.1767	0.1220	0.004

Table S28. TDDFT excited electronic energy of N-(perfluorophenethyl)acetamide with the methyl ammonium complex radical (**B3**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-1110.9455974862	0.000				
1	-1110.9349876477	0.289	1.1021	-0.4573	-0.3210	0.011
2	-1110.9298857435	0.428	-2.6703	0.6584	0.1374	0.079
3	-1110.9279169790	0.481	-0.7426	0.0341	0.3269	0.008
4	-1110.9217968396	0.648	0.5891	0.1962	-0.6736	0.013
5	-1110.9099848549	0.969	1.1297	2.0256	-0.1275	0.128
6	-1110.9056010943	1.088	0.0028	0.2407	2.3130	0.144
7	-1110.9027005380	1.167	1.2836	-0.2227	1.4143	0.106
8	-1110.8956600472	1.359	-0.1139	-0.1473	-0.2025	0.003
9	-1110.8945625153	1.389	-1.0311	-0.1244	0.5182	0.046
10	-1110.8791321096	1.809	0.6263	-0.6017	-0.1224	0.034
11	-1110.8756772907	1.903	0.0183	0.1997	0.2578	0.005
12	-1110.8737216505	1.956	0.3390	-0.0618	0.1147	0.006
13	-1110.8696569777	2.066	-0.0701	-0.0945	-0.0657	0.001
14	-1110.8668635754	2.142	-0.5015	-0.2469	0.2837	0.021
15	-1110.8603041372	2.321	0.1157	-0.2168	0.0487	0.004

Table S29. TDDFT excited electronic energy of N-(3,5-dicyanophenethyl)acetamide with the methyl ammonium complex radical (**B4**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY HARTREE	EXCITATION EV	TRANSITION DIPOLE X	Y	Z	OSCILLATOR STRENGTH
0	-799.3380497965	0.000				
1	-799.3304428405	0.207	2.6116	-0.6665	0.0770	0.037
2	-799.3192441200	0.512	-0.5695	0.0179	0.0880	0.004
3	-799.3085210749	0.804	-0.0513	-0.2520	0.8790	0.017
4	-799.2987182486	1.070	-0.8176	-1.2084	-1.1864	0.093
5	-799.2949900346	1.172	0.4021	-0.6842	1.2063	0.060
6	-799.2932620975	1.219	1.3648	-0.2295	-0.9564	0.084
7	-799.2770958489	1.659	-0.7906	0.3797	-0.1800	0.033
8	-799.2727763773	1.776	0.6169	-0.0542	-0.0739	0.017
9	-799.2684224084	1.895	0.1213	0.2720	0.0781	0.004
10	-799.2605215179	2.110	0.1656	-0.5943	0.2099	0.022
11	-799.2551485116	2.256	-0.0745	-0.0268	-0.1189	0.001
12	-799.2511461057	2.365	-0.1597	-0.3909	0.2193	0.013
13	-799.2498204115	2.401	-0.1327	-0.1864	0.0819	0.003
14	-799.2407019787	2.649	-0.1090	0.1527	-0.1013	0.003
15	-799.2398935215	2.671	-0.0796	0.0926	0.0197	0.001

Table S30. TDDFT excited electronic energy of N-(3-nitrophenethyl)acetamide with the methyl ammonium complex radical (**B5**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY HARTREE	EXCITATION EV	TRANSITION DIPOLE X	Y	Z	OSCILLATOR STRENGTH
0	-819.3758247932	0.000				
1	-819.3667843673	0.246	-2.7875	0.4324	-0.0124	0.048
2	-819.3436963692	0.874	-0.1056	-0.2017	-1.0017	0.023
3	-819.3363221215	1.075	0.4655	1.0750	-1.1184	0.069
4	-819.3321044206	1.190	-0.1917	-0.4687	-1.3675	0.062
5	-819.3293345753	1.265	1.2527	-0.0898	-0.2646	0.051
6	-819.3250092640	1.383	0.8716	-0.3444	0.3312	0.033
7	-819.3072219416	1.867	0.4682	-0.5509	0.0029	0.024
8	-819.3070649938	1.871	0.4604	0.0590	-0.0523	0.010
9	-819.3023830259	1.998	-0.1015	0.1057	-0.0031	0.001
10	-819.2924923029	2.268	0.2060	0.8047	0.2594	0.042
11	-819.2917998190	2.286	-0.4052	-0.6743	0.0294	0.035
12	-819.2888323516	2.367	0.0640	-0.2524	-0.1032	0.005
13	-819.2882804203	2.382	0.3350	0.5069	0.1954	0.024
14	-819.2841028928	2.496	0.0521	0.0359	-0.0006	0.000
15	-819.2749954846	2.744	0.2124	-0.5230	-0.0313	0.021

Table S31. TDDFT excited electronic energy of N-(3,5-dicyanophenethyl)acetamide with the methyl ammonium complex radical (**C4**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE	OSCILLATOR

	HARTREE	EV	X	Y	Z	STRENGTH
0	-799.3378863397	0.000				
1	-799.3331418925	0.129	-1.5580	0.8639	-0.0417	0.010
2	-799.3140698206	0.648	-0.4670	0.2250	0.0711	0.004
3	-799.2981574535	1.081	-0.9060	-0.5877	-0.5754	0.040
4	-799.2964648525	1.127	-0.7889	-0.1831	1.6520	0.093
5	-799.2847558059	1.446	-0.5705	0.4152	-0.0432	0.018
6	-799.2782197559	1.624	-1.0303	0.7811	-0.0870	0.067
7	-799.2714025304	1.809	0.3949	0.0256	0.0965	0.007
8	-799.2651806184	1.978	-0.2802	0.2369	-0.1398	0.007
9	-799.2598366939	2.124	-0.1603	-0.2851	-0.0855	0.006
10	-799.2564932257	2.215	-0.1996	-0.0297	0.0429	0.002
11	-799.2546940229	2.264	0.5365	-0.2594	0.0033	0.020
12	-799.2514947659	2.351	-0.1849	-0.0789	-0.0284	0.002
13	-799.2440356938	2.554	0.6555	0.4201	0.0453	0.038
14	-799.2396720234	2.673	-0.1591	-0.0423	-0.1315	0.003
15	-799.2385742727	2.702	-0.2168	0.5392	0.0096	0.022

Table S32. TDDFT excited electronic energy of N-(3-nitrophenethyl)acetamide with the methyl ammonium complex radical (**C5**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-819.4077702748	0.000				
1	-819.3731312720	0.943	-0.3012	-0.0412	0.1724	0.003
2	-819.3392730134	1.864	-0.5970	-0.2648	0.1100	0.020
3	-819.3266496404	2.207	0.0414	-0.0550	-0.0934	0.001
4	-819.3244095000	2.268	0.1184	-0.0831	-0.0645	0.001
5	-819.3176243206	2.453	0.0646	-0.2842	0.0603	0.005
6	-819.3123693658	2.596	-0.0526	0.1161	0.2963	0.007
7	-819.3072227445	2.736	0.0679	0.0917	0.1251	0.002
8	-819.3012656397	2.898	0.5426	0.2272	0.1416	0.026
9	-819.2964821249	3.028	-0.3716	-0.1150	-0.0382	0.011
10	-819.2958539624	3.045	-0.5333	-0.1365	0.0211	0.023
11	-819.2912648761	3.170	0.3956	0.1230	-0.0995	0.014
12	-819.2893930146	3.221	-0.3699	-0.3316	-0.1175	0.021
13	-819.2824156675	3.411	0.1172	0.0603	0.1247	0.003
14	-819.2814253884	3.438	0.0954	0.0324	0.0115	0.001
15	-819.2760877973	3.583	-0.0316	0.0437	-0.1565	0.002

Table S33. TDDFT excited electronic energy of N-(3-nitrophenethyl)acetamide with the methyl ammonium complex radical (**D5**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-819.4037155691	0.000				
1	-819.3845377943	0.522	0.4535	0.5072	0.3360	0.007
2	-819.3686284152	0.955	0.1863	-0.1072	0.0014	0.001
3	-819.3659058184	1.029	0.1702	-0.0872	0.0024	0.001
4	-819.3571590889	1.267	0.2700	0.5903	0.0497	0.013

5	-819.3440963239	1.622	-0.1249	-0.0878	-0.0270	0.001
6	-819.3406084467	1.717	-0.0857	0.1439	-0.2001	0.003
7	-819.3334482360	1.912	0.2766	-0.0354	-0.2988	0.008
8	-819.3277100536	2.068	0.1117	-0.0541	0.2262	0.003
9	-819.3236931202	2.178	-0.0633	-0.1179	-0.0481	0.001
10	-819.3205472622	2.263	-0.2737	0.4097	0.0694	0.014
11	-819.3132618982	2.461	-0.1585	0.5042	0.1895	0.019
12	-819.3107475706	2.530	-0.4284	0.8195	0.2102	0.056
13	-819.3073704881	2.622	-0.2812	0.5090	-0.0893	0.022
14	-819.3033536667	2.731	0.2411	-0.4211	0.0744	0.016
15	-819.2993620752	2.840	0.0150	0.1106	-0.1049	0.002

Table S34. TDDFT excited electronic energy of N-(3,5-dinitrophenethyl)acetamide with the methyl ammonium complex radical (**B6**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-1023.8061672182	0.000				
1	-1023.8013014568	0.132	1.8250	-0.9868	0.3009	0.014
2	-1023.7853272337	0.567	0.1012	0.8987	-0.5382	0.015
3	-1023.7729650521	0.903	0.3418	0.0751	-0.5531	0.009
4	-1023.7646098653	1.131	-0.9952	-1.0041	-0.0021	0.055
5	-1023.7606083681	1.240	0.2460	0.2919	-1.1052	0.042
6	-1023.7549806592	1.393	0.8191	-0.6193	0.3279	0.040
7	-1023.7422638132	1.739	-0.4179	0.7171	-0.5272	0.041
8	-1023.7351786760	1.932	-0.2769	-0.3261	-0.0728	0.009
9	-1023.7291211632	2.097	-0.3577	0.2095	0.5070	0.022
10	-1023.7235252481	2.249	-0.1132	0.5906	-0.1194	0.021
11	-1023.7158272243	2.458	0.0730	-0.4448	-0.0126	0.012
12	-1023.7106977667	2.598	0.0574	0.1501	0.0439	0.002
13	-1023.7065253913	2.711	-0.3057	-0.0257	-0.3026	0.012
14	-1023.7031754264	2.803	0.4398	-0.0460	-0.0907	0.014
15	-1023.7020007189	2.835	0.4830	0.1948	0.0853	0.019

Table S35. TDDFT excited electronic energy of N-phenethylacetamide (**A1**) anion formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-518.7373883443	0.000				
1	-518.7272245117	0.277	0.9071	2.7572	1.0916	0.065
2	-518.7236248943	0.375	1.6095	-3.4751	1.1728	0.147
3	-518.7220964495	0.416	3.7948	-0.4963	0.0957	0.149
4	-518.7216674700	0.428	-2.2704	-1.3344	1.3218	0.091
5	-518.7169395310	0.556	-0.1826	0.2483	1.9197	0.052
6	-518.7134414323	0.652	0.3186	-0.1684	-1.3229	0.030
7	-518.7082863743	0.792	-0.5548	0.1908	-0.8753	0.022
8	-518.7049566252	0.883	-0.4236	-0.0953	-0.3334	0.006
9	-518.7024093312	0.952	-0.6667	-0.2210	-0.2647	0.013
10	-518.6976601828	1.081	0.1310	0.8535	0.5510	0.028
11	-518.6904747457	1.277	-0.0245	-0.5444	-0.6253	0.022
12	-518.6835365049	1.465	0.1797	-0.0681	0.3236	0.005
13	-518.6770435263	1.642	0.1975	-0.0791	-0.6247	0.018

14	-518.6727348320	1.759	-0.2128	-0.2458	0.1697	0.006
15	-518.6689278690	1.863	0.2273	0.3263	0.0985	0.008

Table S36. TDDFT excited electronic energy of N-(4-cyanophenethyl)acetamide (**A2**) anion formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-610.9855353685	0.000				
1	-610.9824770176	0.083	-1.3136	1.1139	0.7011	0.007
2	-610.9720532158	0.367	-0.5262	-2.2579	-0.2366	0.049
3	-610.9622148667	0.635	0.5405	-0.1565	-1.2647	0.030
4	-610.9603393303	0.686	-0.9428	-0.3548	0.1867	0.018
5	-610.9581449266	0.745	-2.2175	-0.5506	-0.8644	0.109
6	-610.9543069157	0.850	-1.1215	0.1077	-0.4053	0.030
7	-610.9483798276	1.011	0.4149	-0.3052	0.0153	0.007
8	-610.9439188608	1.132	0.2320	0.2564	0.7963	0.021
9	-610.9367834740	1.327	-0.2831	0.3327	-0.2024	0.008
10	-610.9359509970	1.349	0.4227	0.1100	-0.2632	0.009
11	-610.9260634727	1.618	0.0592	-0.1182	-0.2670	0.004
12	-610.9204678488	1.771	-0.2417	0.2836	0.3123	0.010
13	-610.9194577586	1.798	0.0746	0.3411	-0.0375	0.005
14	-610.9076352636	2.120	-0.0785	-0.2840	0.1494	0.006
15	-610.9021727642	2.268	-0.0793	-0.1061	0.1271	0.002

Table S37. TDDFT excited electronic energy of N-(perfluorophenethyl)acetamide (**A3**) anion formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-1014.9366808122	0.000				
1	-1014.9257760619	0.297	0.5891	0.5706	0.4098	0.006
2	-1014.9166335438	0.546	2.1488	-2.6115	-1.4670	0.182
3	-1014.9139427640	0.619	-0.0066	0.0175	-0.0857	0.000
4	-1014.9085170417	0.766	-1.2827	-1.7908	1.8576	0.156
5	-1014.9065720470	0.819	-2.2299	-0.7317	-1.2237	0.141
6	-1014.8975285651	1.065	0.2661	-0.8384	-0.0700	0.020
7	-1014.8918283724	1.220	0.4209	-0.5670	0.1564	0.016
8	-1014.8858804100	1.382	0.3075	-0.7329	0.7372	0.040
9	-1014.8833157538	1.452	-0.4380	-0.6170	-0.7369	0.040
10	-1014.8756732636	1.660	0.1322	0.2585	-0.5429	0.015
11	-1014.8696438349	1.824	0.3613	0.2021	-0.1826	0.009
12	-1014.8665418526	1.909	-0.2040	0.2403	-0.0447	0.005
13	-1014.8588077281	2.119	0.6424	0.1577	0.3342	0.029
14	-1014.8551500453	2.219	-0.1702	0.3259	0.5925	0.026
15	-1014.8490032489	2.386	-0.2755	-0.0331	0.4144	0.015

Table S38. TDDFT excited electronic energy of N-(3,5-dicyanophenethyl)acetamide (**A4**) anion formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-703.2366543280	0.000				

1	-703.2201542153	0.449	-0.3254	0.4049	-0.0404	0.003
2	-703.2173477636	0.525	-0.1237	-0.2501	0.2043	0.002
3	-703.2031132834	0.913	0.2768	-0.3694	-0.1116	0.005
4	-703.1940035023	1.161	0.2117	0.1238	-0.1004	0.002
5	-703.1924281046	1.203	0.0131	0.2545	0.0239	0.002
6	-703.1832620986	1.453	-0.0498	0.1409	0.0522	0.001
7	-703.1747298621	1.685	0.0050	-0.0357	0.2497	0.003
8	-703.1732436486	1.725	-0.0388	-0.3753	0.1979	0.008
9	-703.1667814467	1.901	0.0974	0.0730	-0.0294	0.001
10	-703.1644430317	1.965	-0.0518	-0.1226	-0.0885	0.001
11	-703.1498385186	2.362	-0.0312	-0.0279	-0.1504	0.001
12	-703.1482194941	2.406	0.2174	0.1257	-0.0953	0.004
13	-703.1475129932	2.426	0.3141	0.0633	0.2236	0.009
14	-703.1456428870	2.477	0.0405	-0.0841	0.0954	0.001
15	-703.1401663313	2.626	0.2028	0.2895	-0.0225	0.008

Table S39. TDDFT excited electronic energy of N-(3-nitrophenethyl)acetamide (**A5**) anion formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-723.2773869793	0.000				
1	-723.2645522461	0.349	-0.1986	0.2486	-1.3763	0.017
2	-723.2523457567	0.681	0.5554	0.6996	-0.1447	0.014
3	-723.2399450923	1.019	0.3889	-0.1321	-0.0149	0.004
4	-723.2345116157	1.167	-0.1690	-0.0150	-0.1137	0.001
5	-723.2276808787	1.353	-0.0123	0.0545	0.3275	0.004
6	-723.2265442194	1.384	0.0175	-0.0620	0.0073	0.000
7	-723.2204709816	1.549	0.2057	0.3124	0.1260	0.006
8	-723.2174385948	1.631	-0.0450	-0.2439	-0.1374	0.003
9	-723.2077818267	1.894	-0.0658	0.0542	0.2324	0.003
10	-723.2016735085	2.060	0.3134	0.2655	0.1910	0.010
11	-723.1987641906	2.139	0.5300	-0.0908	0.3637	0.022
12	-723.1936144342	2.280	0.2576	0.0836	0.0483	0.004
13	-723.1885632539	2.417	-1.1538	-0.0889	-0.4474	0.091
14	-723.1864222846	2.475	0.3962	0.1491	0.1314	0.012
15	-723.1804578318	2.638	-0.1203	0.0460	-0.0460	0.001

Table S40. TDDFT excited electronic energy of N-(3,5-dinitrophenethyl)acetamide (**A6**) anion formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-927.7954117827	0.000				
1	-927.7745218484	0.568	-0.3398	1.0964	0.6657	0.025
2	-927.7590731111	0.989	0.3152	-0.1092	-0.1284	0.003
3	-927.7420469770	1.452	0.1011	0.5088	0.2080	0.011
4	-927.7277582160	1.841	0.0729	-0.1863	-0.0048	0.002
5	-927.7232058279	1.965	-0.0766	0.0967	-0.0050	0.001
6	-927.7192889191	2.071	-0.2660	0.6152	0.4559	0.033
7	-927.7111656644	2.292	0.2360	-0.5615	-0.2431	0.024
8	-927.7048995067	2.463	0.0955	-0.0357	0.3495	0.008
9	-927.7018413502	2.546	-0.0415	0.0205	0.1203	0.001
10	-927.6943602756	2.750	0.2958	-0.1968	0.2916	0.014
11	-927.6916974798	2.822	0.1223	-0.0086	0.1093	0.002

12	-927.6892491507	2.889	-0.6173	-0.0434	-0.2965	0.033
13	-927.6824071979	3.075	-0.0109	0.0196	0.1213	0.001
14	-927.6779236705	3.197	-0.1594	-0.0860	0.0603	0.003
15	-927.6710301665	3.385	-0.0172	-0.1063	-0.0304	0.001

Table S41. TDDFT excited electronic energy of N-phenethylacetamide with the methyl ammonium complex radical (**B1**) neutral formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-615.1001801202	0.000				
1	-615.0897829565	0.283	0.2374	0.2996	-0.0323	0.001
2	-615.0889133250	0.307	1.0093	-0.4487	-0.0978	0.009
3	-615.0812095836	0.516	0.4768	-0.1612	-0.8020	0.011
4	-615.0721650165	0.762	2.6176	0.0961	0.4581	0.132
5	-615.0674953715	0.889	-0.2701	-1.9758	0.0488	0.087
6	-615.0608421418	1.070	-0.0601	0.1949	2.5897	0.177
7	-615.0569820291	1.175	1.4061	-0.2196	0.1813	0.059
8	-615.0557705581	1.208	-0.6710	-0.4047	0.3499	0.022
9	-615.0515452134	1.323	0.3625	-0.2431	-1.0171	0.040
10	-615.0422699943	1.576	0.9837	-0.2552	0.1815	0.041
11	-615.0389766847	1.665	-0.0931	0.8037	0.0478	0.027
12	-615.0370452553	1.718	-0.0464	-0.1201	0.2990	0.004
13	-615.0341001723	1.798	0.0572	-0.5017	0.2350	0.014
14	-615.0300945863	1.907	-0.0052	0.1834	0.1239	0.002
15	-615.0268457562	1.996	-0.2419	0.4110	-0.1665	0.012

Table S42. TDDFT excited electronic energy of N-(4-cyanophenethyl)acetamide with the methyl ammonium complex radical (**B2**) neutral formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-707.3315976629	0.000				
1	-707.3238232489	0.212	2.4227	-0.7612	0.0505	0.033
2	-707.3116357206	0.543	0.8807	-0.0620	-0.3531	0.012
3	-707.3063984978	0.686	0.3071	-0.0889	-0.7227	0.010
4	-707.2956994202	0.977	-2.2057	-0.6903	-0.6499	0.138
5	-707.2938832073	1.026	-0.5420	1.4451	0.0365	0.060
6	-707.2898785992	1.135	-0.3529	-0.2533	2.3709	0.162
7	-707.2778315742	1.463	0.1193	0.0144	-0.0480	0.001
8	-707.2752225980	1.534	1.0360	-0.1175	0.1739	0.042
9	-707.2746630776	1.549	0.1449	-0.0355	-0.1460	0.002
10	-707.2633946988	1.856	-0.4615	0.7426	0.0375	0.035
11	-707.2579448101	2.004	-0.1807	-0.3426	0.0698	0.008
12	-707.2557173299	2.065	-0.3252	0.0922	-0.0789	0.006
13	-707.2515720454	2.178	0.0158	-0.2440	-0.0394	0.003
14	-707.2498031228	2.226	0.2568	-0.0884	0.0533	0.004
15	-707.2462803368	2.322	-0.1559	0.1781	0.1104	0.004

Table S43. TDDFT excited electronic energy of N-(perfluorophenethyl)acetamide with the methyl ammonium complex radical (**B3**) neutral formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-1111.2865533885	0.000				
1	-1111.2761603396	0.283	-1.2550	0.5016	0.3062	0.013
2	-1111.2708815307	0.426	2.2405	-0.5814	-0.0277	0.056
3	-1111.2695672576	0.462	1.4414	-0.1966	-0.3600	0.025
4	-1111.2636633302	0.623	0.6723	0.1348	-0.6059	0.013
5	-1111.2512189747	0.961	1.1015	2.0287	-0.1538	0.126
6	-1111.2469075195	1.079	-0.0283	-0.2268	-2.3511	0.147
7	-1111.2439611647	1.159	-1.3087	0.1914	-1.3732	0.103
8	-1111.2368196696	1.353	-0.0634	-0.1451	-0.2347	0.003
9	-1111.2358114483	1.381	1.0290	0.1302	-0.4999	0.045
10	-1111.2211548476	1.780	0.6408	-0.6455	-0.1282	0.037
11	-1111.2172457472	1.886	-0.0316	-0.1607	-0.2244	0.004
12	-1111.2152952896	1.939	-0.3523	0.1031	-0.1003	0.007
13	-1111.2111719760	2.051	-0.0586	-0.0796	-0.0564	0.001
14	-1111.2083557839	2.128	-0.4881	-0.2221	0.2735	0.019
15	-1111.2021262978	2.297	-0.1062	0.2849	-0.0405	0.005

Table S44. TDDFT excited electronic energy of N-(3,5-dicyanophenethyl)acetamide with the methyl ammonium complex radical (**B4**) neutral formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-799.5629746952	0.000				
1	-799.5555592043	0.202	2.5892	-0.6567	0.0779	0.035
2	-799.5444182005	0.505	-0.5560	0.0035	0.0897	0.004
3	-799.5338589899	0.792	-0.0102	0.2543	-0.8078	0.014
4	-799.5236112629	1.071	0.6960	1.1817	1.2461	0.090
5	-799.5201163227	1.166	-0.0062	0.6234	-1.3547	0.064
6	-799.5179079936	1.226	1.4462	-0.3001	-0.5434	0.074
7	-799.5013630139	1.677	-0.7666	0.4108	-0.1730	0.032
8	-799.4970744340	1.793	0.5690	-0.0817	-0.0429	0.015
9	-799.4926070580	1.915	-0.1118	-0.2825	-0.0444	0.004
10	-799.4862289236	2.088	-0.1236	0.6177	-0.2132	0.023
11	-799.4797908445	2.264	0.0690	0.0229	0.0770	0.001
12	-799.4761851487	2.362	0.1500	0.3197	-0.1946	0.009
13	-799.4739148342	2.423	-0.1241	-0.2599	0.1191	0.006
14	-799.4647145127	2.674	-0.0151	-0.0166	0.0445	0.000
15	-799.4642673610	2.686	0.3050	-0.2605	0.0554	0.011

Table S45. TDDFT excited electronic energy of N-(3-nitrophenethyl)acetamide with the methyl ammonium complex radical (**B5**) neutral formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH

0	-819.6116288709	0.000				
1	-819.6027943565	0.240	2.6131	-0.9538	0.2823	0.046
2	-819.5801846901	0.856	-0.2116	-0.2129	0.8747	0.018
3	-819.5723645826	1.068	0.4597	0.8915	1.2815	0.069
4	-819.5686388760	1.170	-0.5240	-0.5076	1.2668	0.061
5	-819.5654806346	1.256	-1.0592	0.2709	-0.4496	0.043
6	-819.5612309422	1.371	-0.9262	0.5240	0.1677	0.039
7	-819.5434034822	1.857	-0.3369	0.6830	-0.0248	0.026
8	-819.5428236248	1.872	-0.4238	0.0404	-0.1128	0.009
9	-819.5386267677	1.986	0.0493	-0.1401	0.0263	0.001
10	-819.5297966109	2.227	-0.2749	-0.6314	0.1878	0.028
11	-819.5281584903	2.271	-0.6272	-0.7573	-0.0463	0.054
12	-819.5249106241	2.360	0.1229	0.2875	-0.1039	0.006
13	-819.5242854614	2.377	-0.3717	-0.2790	0.0822	0.013
14	-819.5204570028	2.481	-0.0658	-0.0950	0.0026	0.001
15	-819.5117185812	2.719	0.1106	-0.5287	-0.0175	0.019

Table S46. TDDFT excited electronic energy of N-(3,5-dicyanophenethyl)acetamide with the methyl ammonium complex radical (**C4**) neutral formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-799.5639059153	0.000				
1	-799.5589753445	0.134	1.6155	-0.8795	0.0280	0.011
2	-799.5402132011	0.645	-0.4509	0.2177	0.0610	0.004
3	-799.5239300314	1.088	0.7887	0.5165	0.7397	0.038
4	-799.5228449579	1.117	-0.8401	-0.2415	1.4902	0.082
5	-799.5091167354	1.491	0.6258	-0.4752	0.0549	0.023
6	-799.5035114829	1.643	0.9043	-0.7276	0.0988	0.055
7	-799.4963643314	1.838	-0.3922	0.0154	-0.0671	0.007
8	-799.4898834495	2.014	-0.3106	0.2449	-0.1083	0.008
9	-799.4855724953	2.132	0.2679	0.2753	0.0813	0.008
10	-799.4818805471	2.232	-0.2518	-0.0073	0.0744	0.004
11	-799.4805342591	2.269	0.5708	-0.2869	-0.0410	0.023
12	-799.4765947398	2.376	0.1482	0.1224	0.0084	0.002
13	-799.4707352265	2.535	0.6040	0.4548	0.0553	0.036
14	-799.4660053484	2.664	0.1565	-0.2652	-0.0838	0.007
15	-799.4647212398	2.699	0.2015	-0.2728	0.1001	0.008

Table S47. TDDFT excited electronic energy of N-(3-nitrophenethyl)acetamide with the methyl ammonium complex radical (**C5**) neutral formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-819.6455716552	0.000				
1	-819.6087854554	1.001	0.3006	0.0420	-0.1683	0.003
2	-819.5752466764	1.914	0.5720	0.2549	-0.1035	0.019
3	-819.5624669976	2.261	-0.0272	0.0417	0.0926	0.001
4	-819.5604469995	2.316	0.1016	-0.0758	-0.0698	0.001
5	-819.5557769892	2.443	-0.0754	0.2742	-0.0625	0.005

6	-819.5484719985	2.642	-0.0411	0.1222	0.2830	0.006
7	-819.5437017412	2.772	0.1187	0.1217	0.1165	0.003
8	-819.5383731721	2.917	0.6354	0.2599	0.1348	0.035
9	-819.5337769006	3.042	-0.4507	-0.1502	-0.0193	0.017
10	-819.5327704643	3.069	0.4527	0.1217	-0.0490	0.017
11	-819.5280241518	3.199	0.3943	0.1764	-0.0671	0.015
12	-819.5259164029	3.256	-0.1791	-0.2519	-0.1433	0.009
13	-819.5193395571	3.435	-0.1360	-0.0581	-0.1129	0.003
14	-819.5187183574	3.452	-0.1126	-0.0481	-0.0180	0.001
15	-819.5140364842	3.579	0.0403	-0.0485	0.1798	0.003

Table S48. TDDFT excited electronic energy of N-(3-nitrophenethyl)acetamide with the methyl ammonium complex radical (**D5**) neutral formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-819.6403232784	0.000				
1	-819.6191136373	0.577	0.3803	0.4337	0.3043	0.006
2	-819.6044371484	0.977	-0.1770	0.0930	-0.0055	0.001
3	-819.6002815817	1.090	0.1573	-0.0490	-0.0053	0.001
4	-819.5923777150	1.305	-0.2368	-0.5611	-0.0326	0.012
5	-819.5804108651	1.630	-0.1008	-0.1008	-0.0445	0.001
6	-819.5753801771	1.767	-0.0717	0.1245	-0.1862	0.002
7	-819.5690161229	1.940	0.2860	-0.0697	-0.2699	0.008
8	-819.5629378603	2.106	0.1058	-0.0317	0.2355	0.003
9	-819.5587803748	2.219	-0.0540	-0.1260	-0.0533	0.001
10	-819.5561031491	2.292	-0.3008	0.4687	0.0861	0.018
11	-819.5490614802	2.483	0.2785	-0.7375	-0.2122	0.041
12	-819.5469011537	2.542	-0.4036	0.7183	0.1063	0.043
13	-819.5427963925	2.654	0.2188	-0.3705	0.1205	0.013
14	-819.5390537562	2.756	-0.1872	0.2856	-0.0847	0.008
15	-819.5347162411	2.874	0.0294	0.0891	-0.1064	0.001

Table S49. TDDFT excited electronic energy of N-(3,5-dinitrophenethyl)acetamide with the methyl ammonium complex radical (**B6**) neutral formed by vertical electron attachment at the UB3LYP/6-311++G(2df,p) level.

STATE	ENERGY	EXCITATION	TRANSITION DIPOLE			OSCILLATOR
	HARTREE	EV	X	Y	Z	STRENGTH
0	-1024.1120067160	0.000				
1	-1024.1071969221	0.131	-1.8178	0.9795	-0.3030	0.014
2	-1024.0912773687	0.564	0.0943	0.8854	-0.5328	0.015
3	-1024.0794523913	0.886	0.3014	0.0552	-0.4991	0.007
4	-1024.0708269134	1.121	0.9927	1.0084	-0.1030	0.055
5	-1024.0670465079	1.223	-0.2300	-0.1494	1.0706	0.037
6	-1024.0607716299	1.394	0.7909	-0.6235	0.4000	0.040
7	-1024.0481955472	1.736	0.3855	-0.7313	0.4980	0.040
8	-1024.0413371004	1.923	0.3152	0.2803	0.0156	0.008
9	-1024.0359718620	2.069	-0.3043	0.2701	0.5149	0.022
10	-1024.0303388094	2.222	0.1207	-0.5760	0.1053	0.019
11	-1024.0228069949	2.427	0.0055	-0.4134	-0.0105	0.010

12	-1024.0171377952	2.582	0.1060	0.0799	0.0451	0.001
13	-1024.0129650313	2.695	0.2843	-0.0025	0.3003	0.011
14	-1024.0101518237	2.772	-0.3389	0.0783	0.0639	0.008
15	-1024.0084435515	2.818	0.5782	0.1766	0.0457	0.025

Figure S3. TDDFT excited molecular orbitals of N-phenethylacetamide (**A1**) anion formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

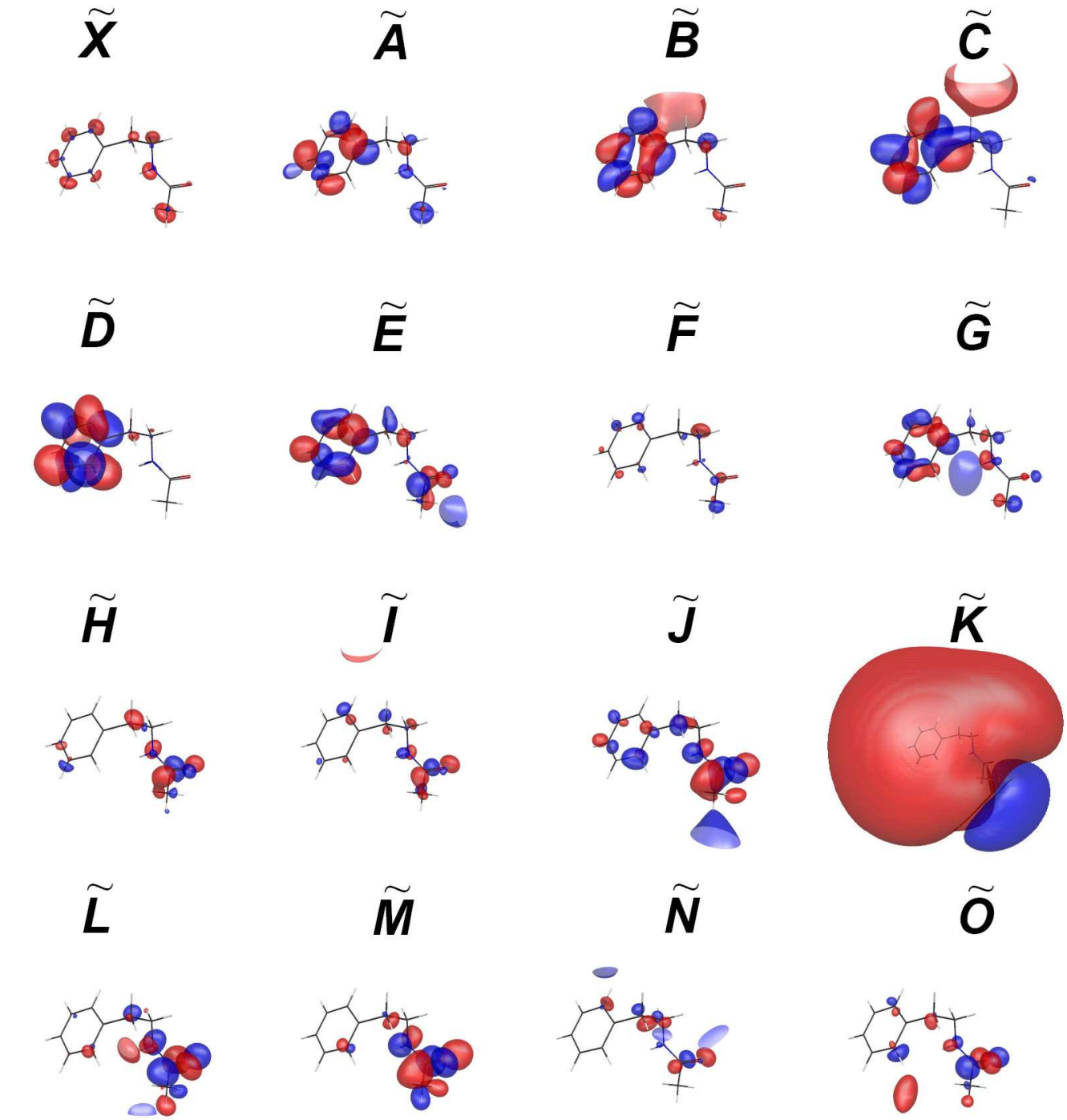


Figure S4. TDDFT excited molecular orbitals of N-(4-cyanophenethyl)acetamide (**A2**) anion formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

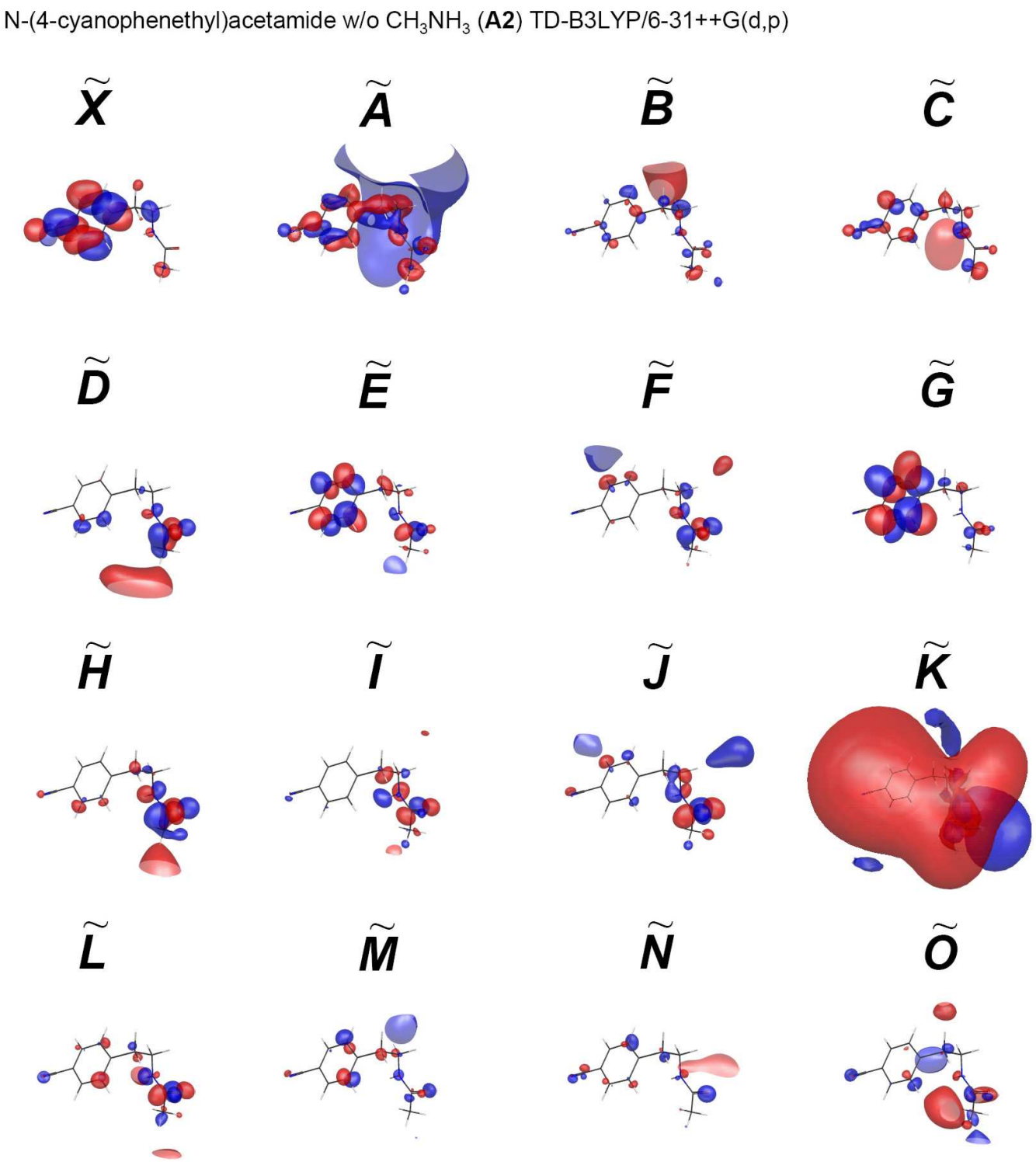


Figure S5. TDDFT excited molecular orbitals of N-(perfluorophenethyl)acetamide (**A3**) anion formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

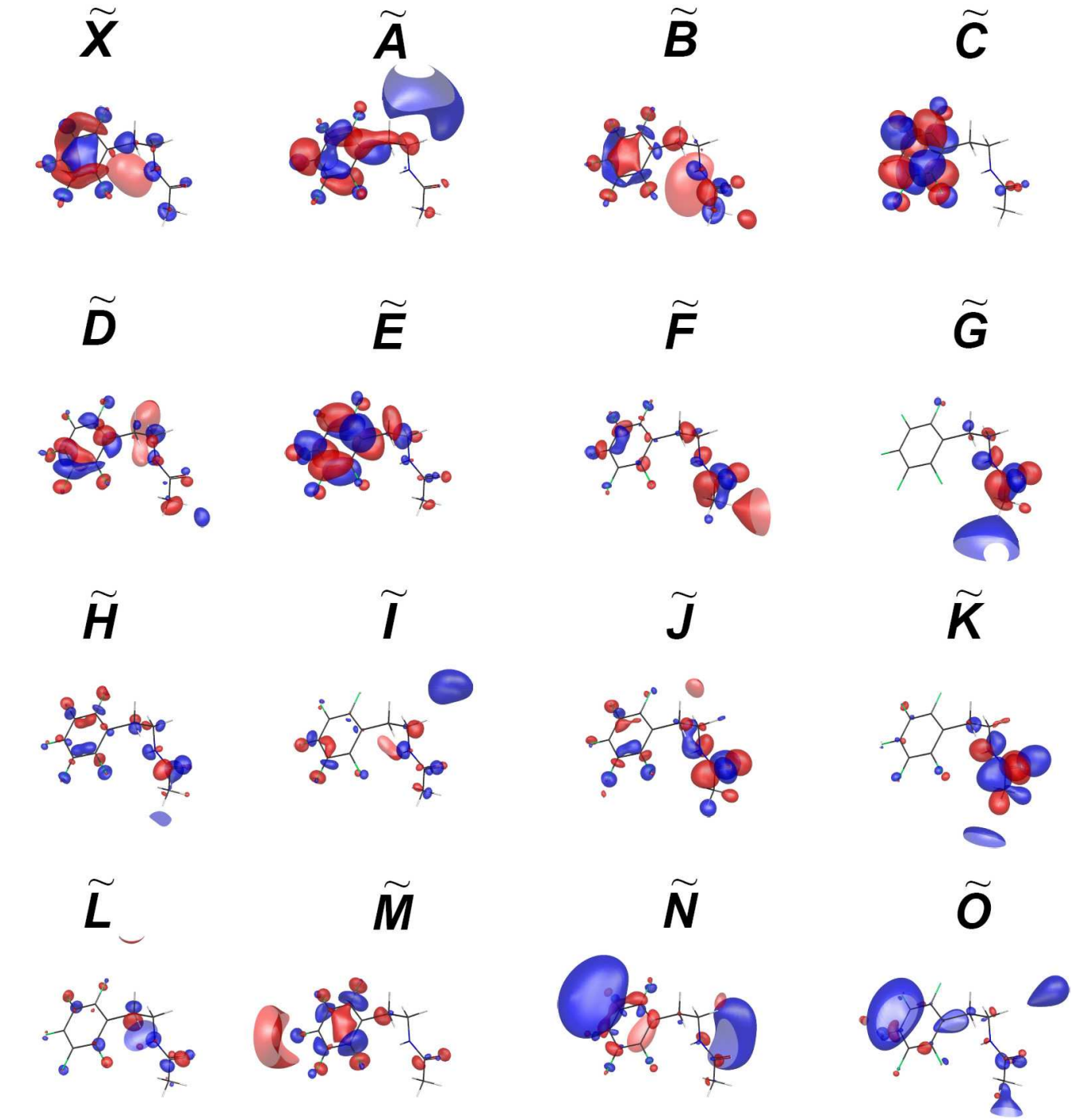


Figure S6. TDDFT excited molecular orbitals of N-(3,5-dicyanophenethyl)acetamide (**A4**) anion formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

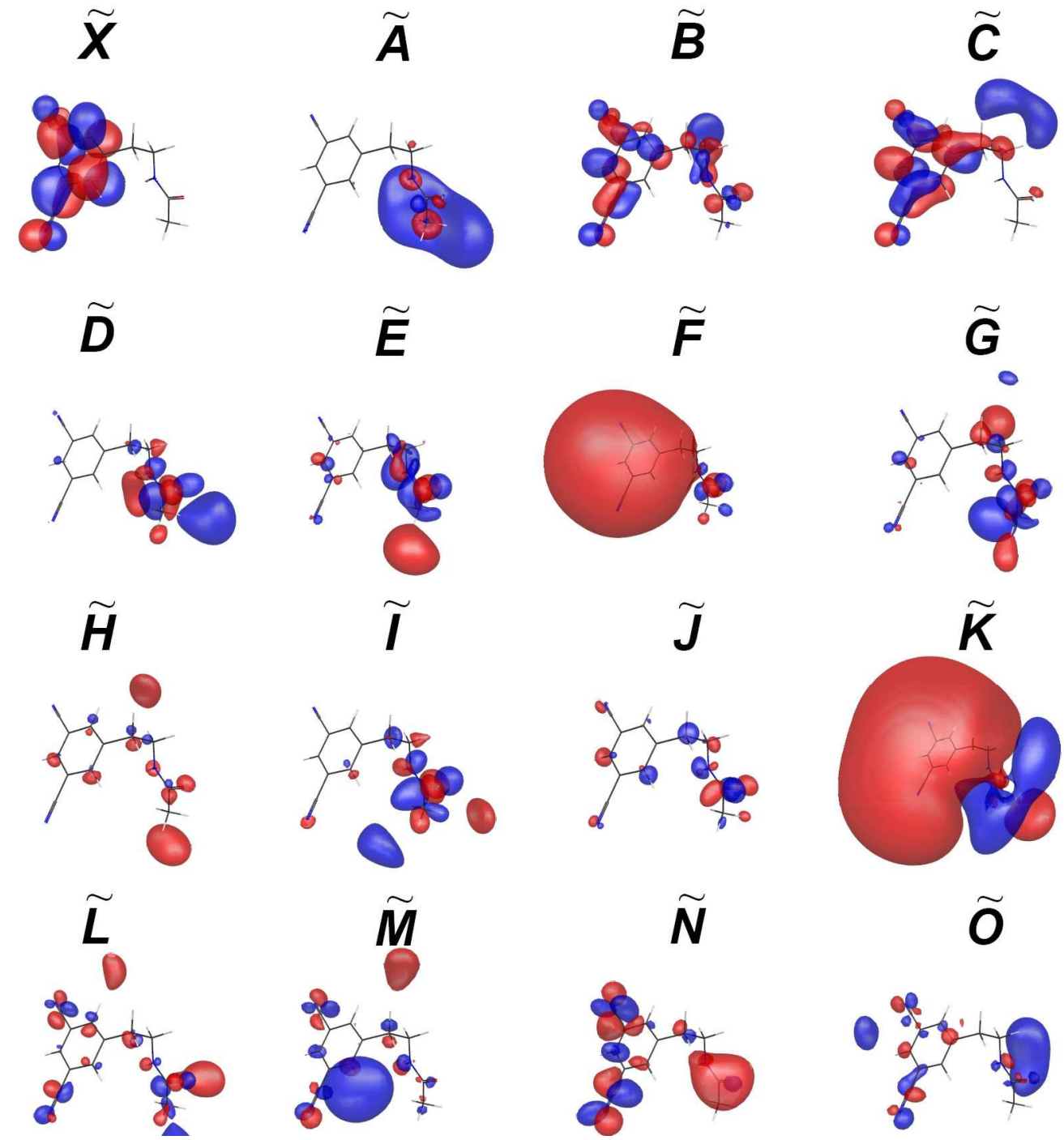


Figure S7. TDDFT excited molecular orbitals of N-(3-nitrophenethyl)acetamide (**A5**) anion formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

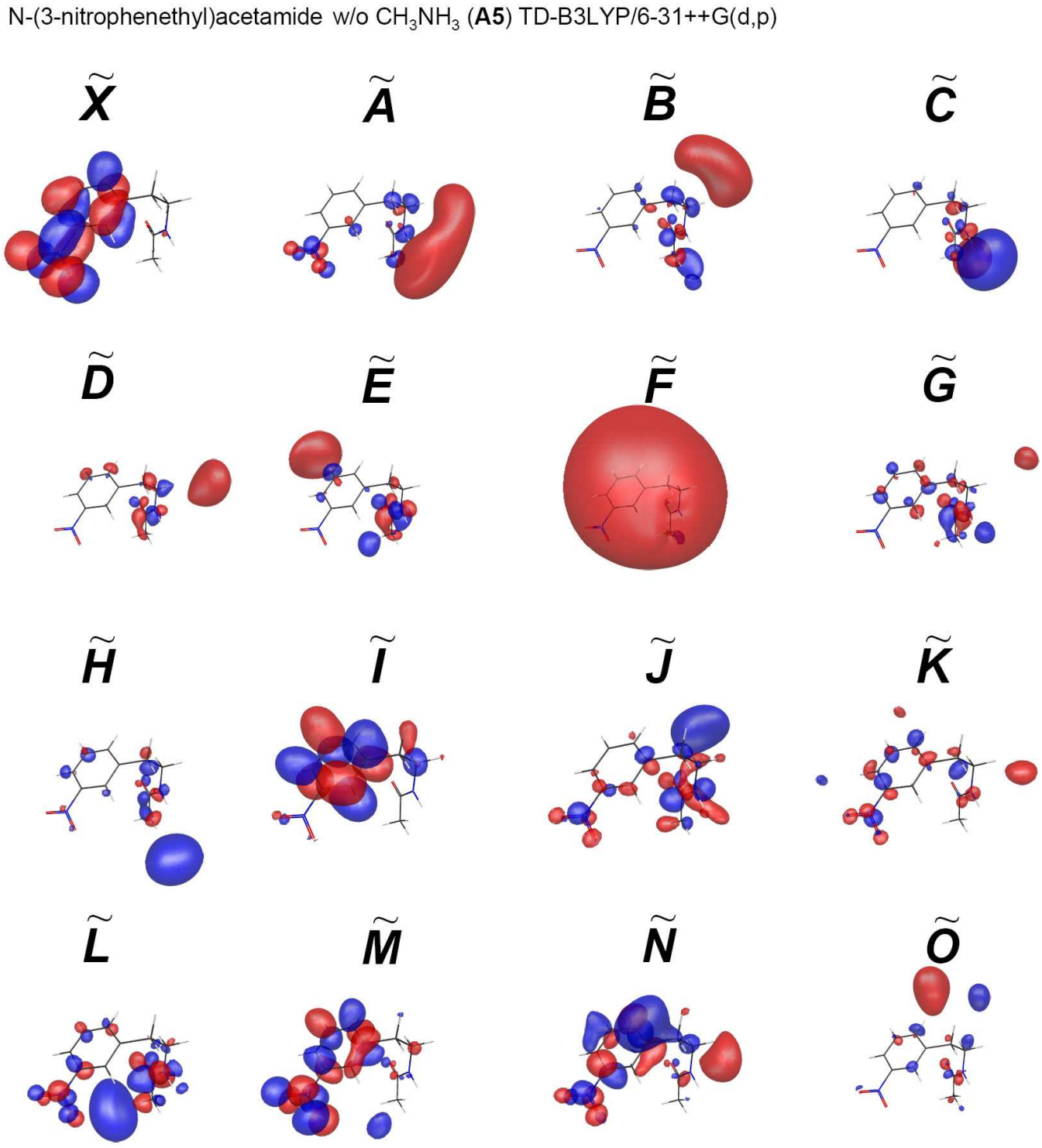


Figure S8. TDDFT excited molecular orbitals of N-(3,5-dinitrophenethyl)acetamide (**A6**) anion formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

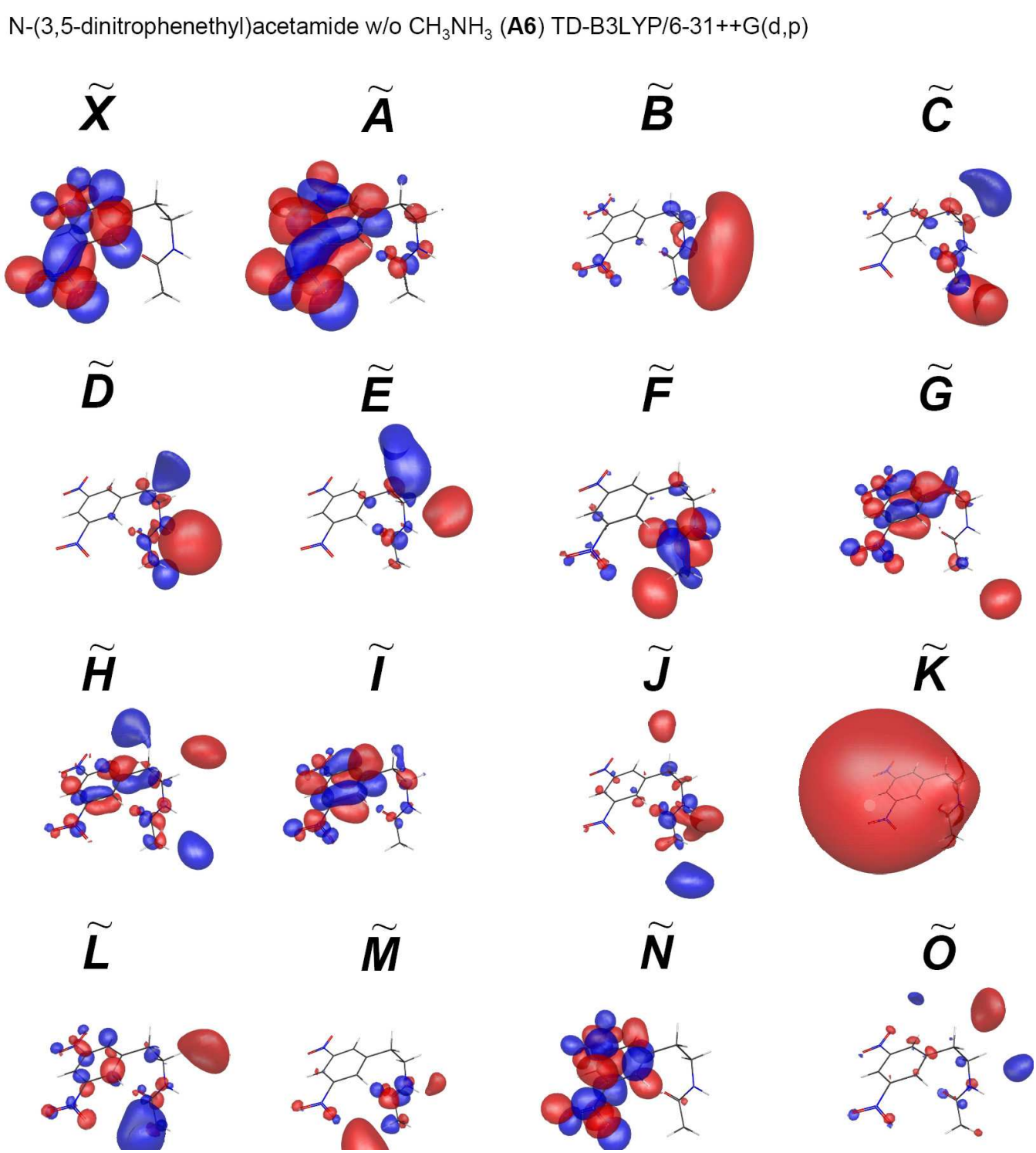


Figure S9. TDDFT excited molecular orbitals of N-phenethylacetamide with the methyl ammonium complex radical (**B1**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

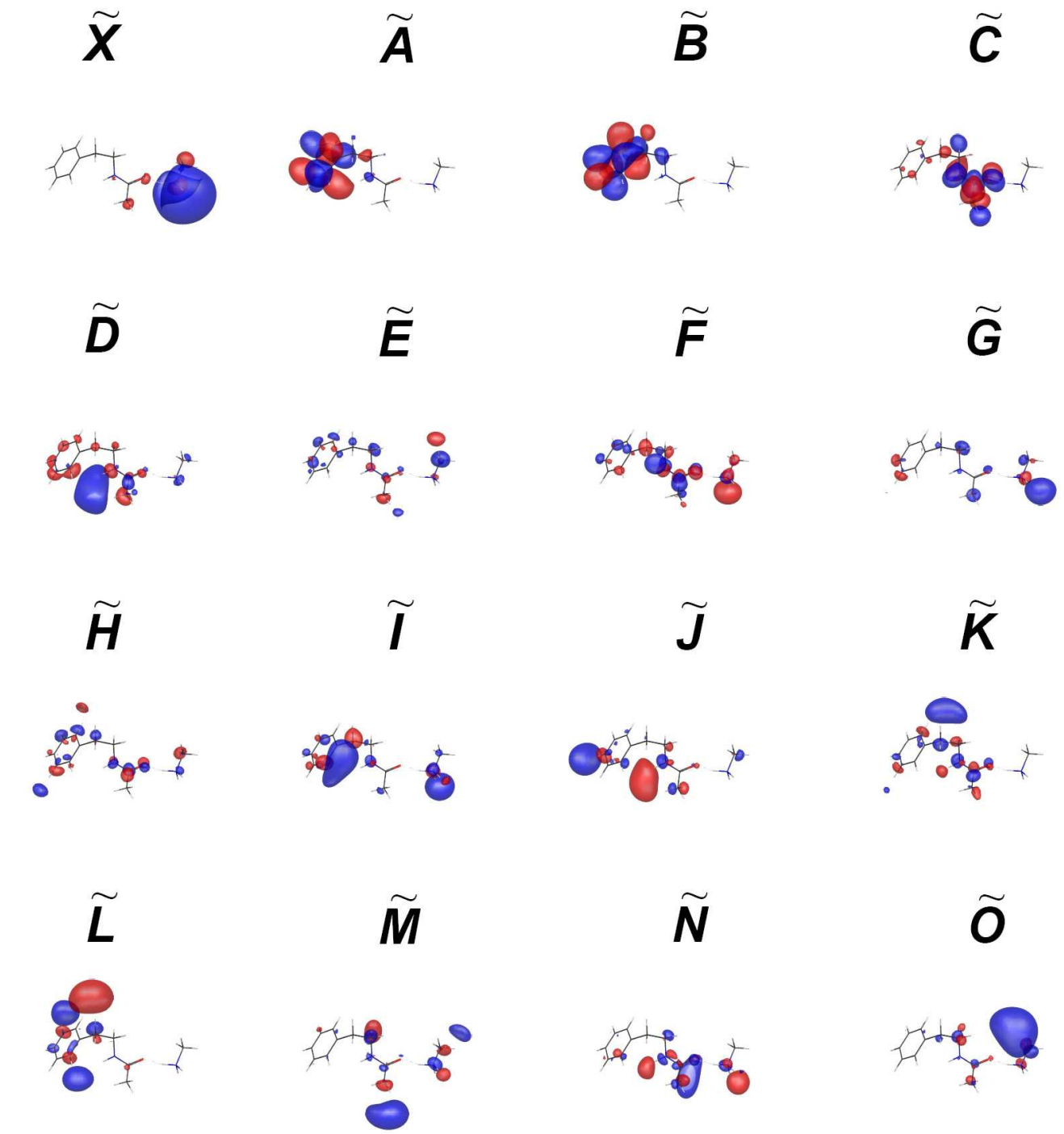


Figure S10. TDDFT excited molecular orbitals of N-(4-cyanophenethyl)acetamide with the methyl ammonium complex radical (**B2**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

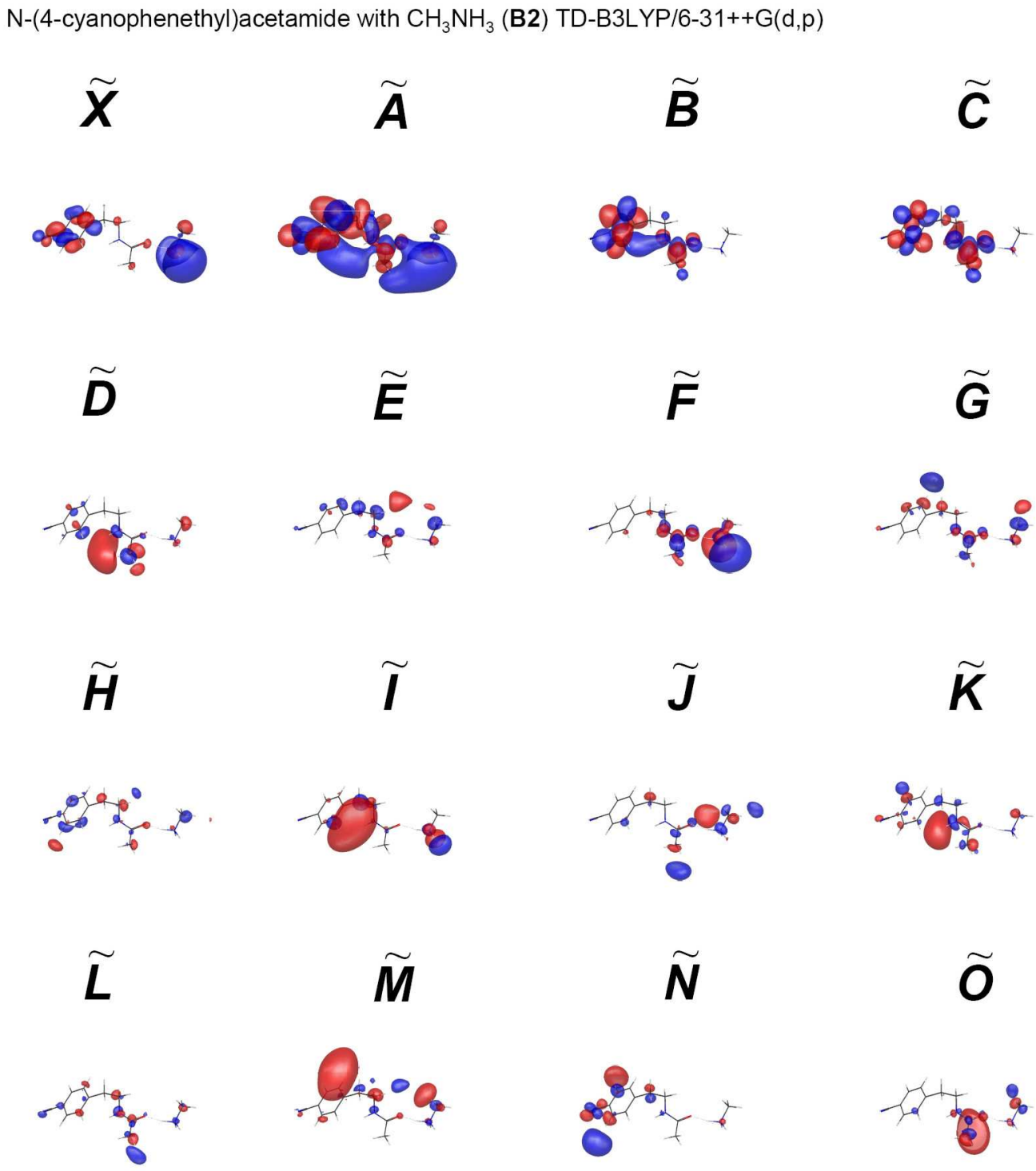


Figure S11. TDDFT excited molecular orbitals of N-(perfluorophenethyl)acetamide with the methyl ammonium complex radical (**B3**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

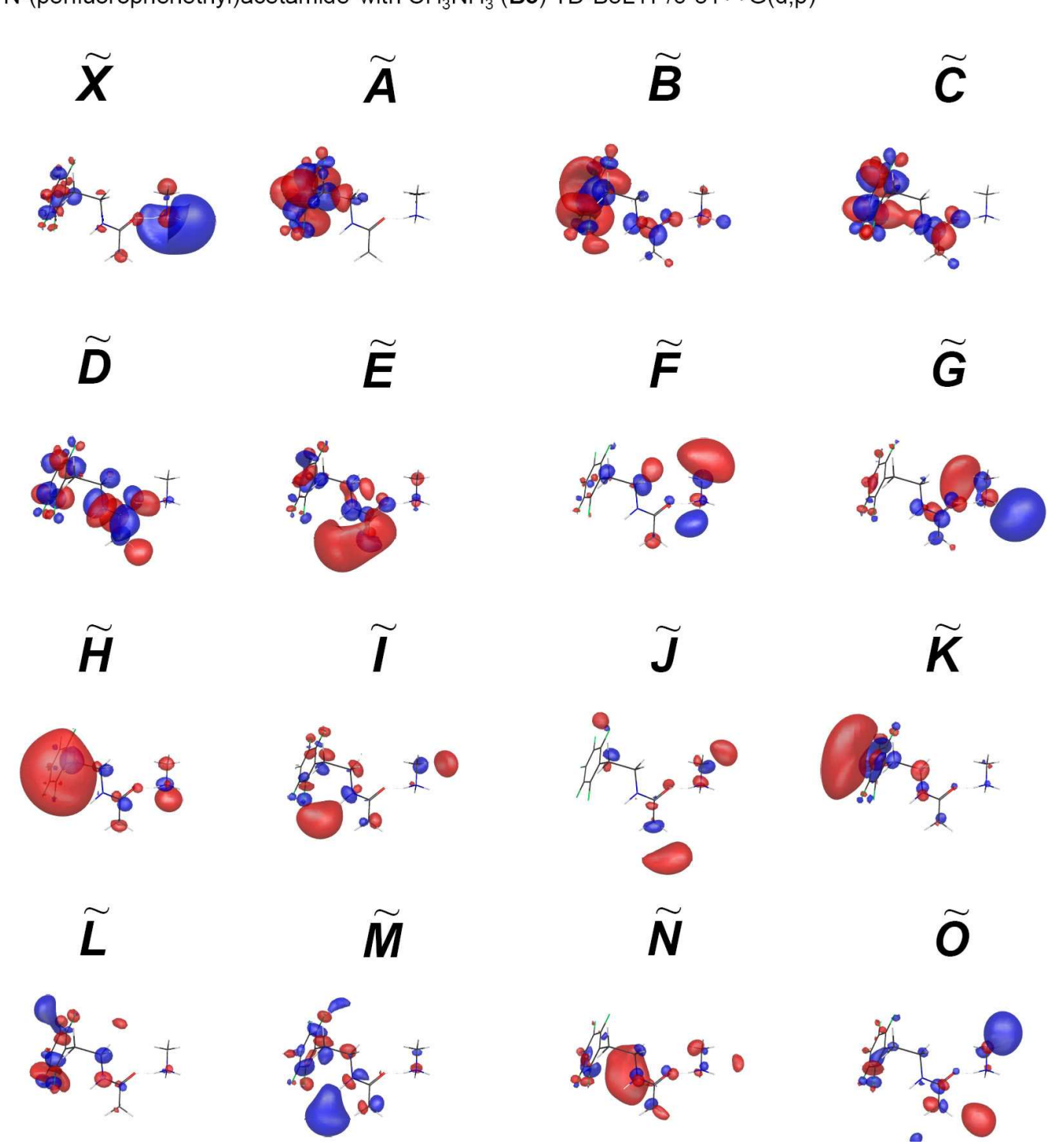


Figure S12. TDDFT excited molecular orbitals of N-(3,5-dicyanophenethyl)acetamide with the methyl ammonium complex radical (**B4**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

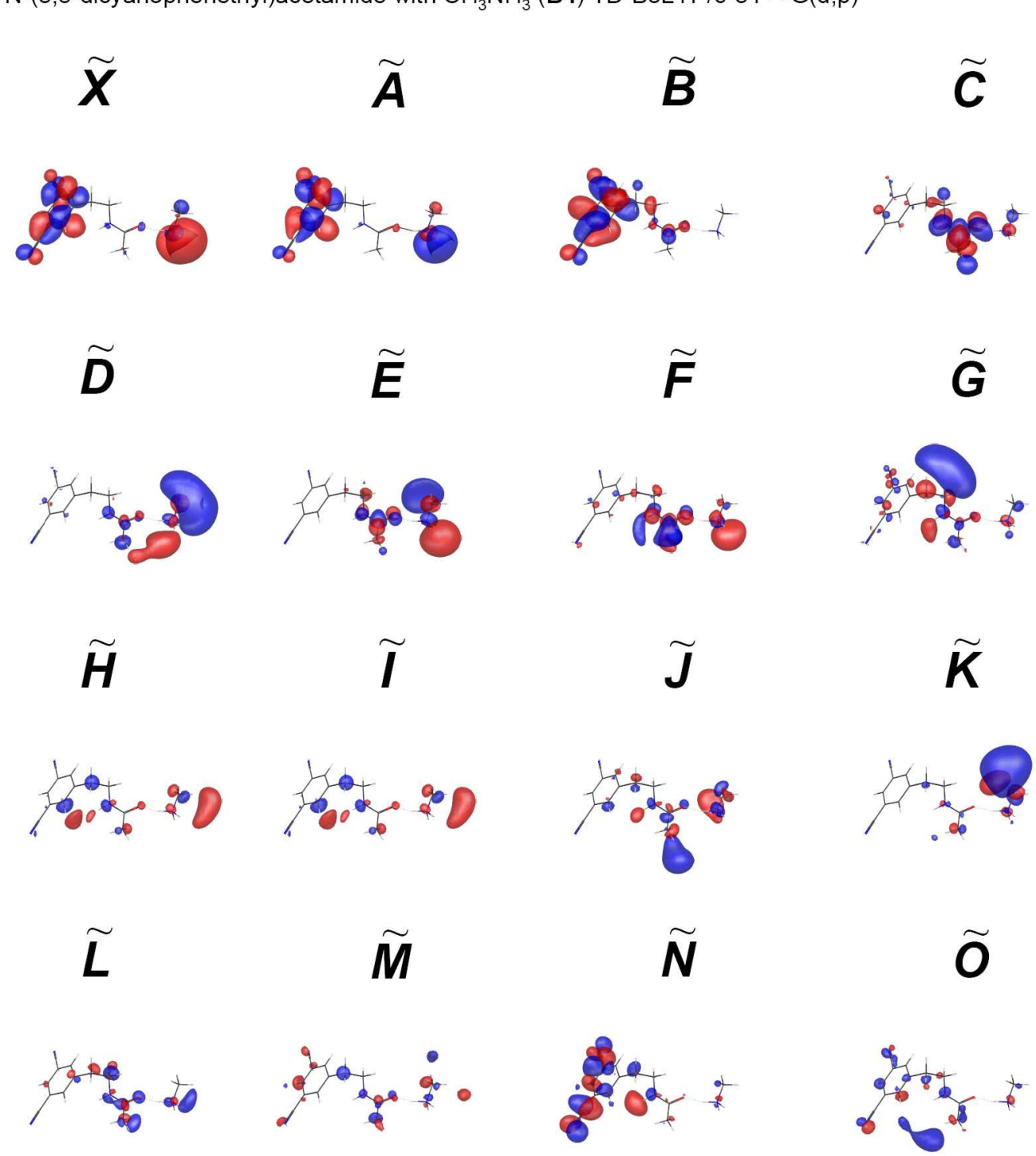


Figure S13. TDDFT excited molecular orbitals of N-(3-nitrophenethyl)acetamide with the methyl ammonium complex radical (**B5**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

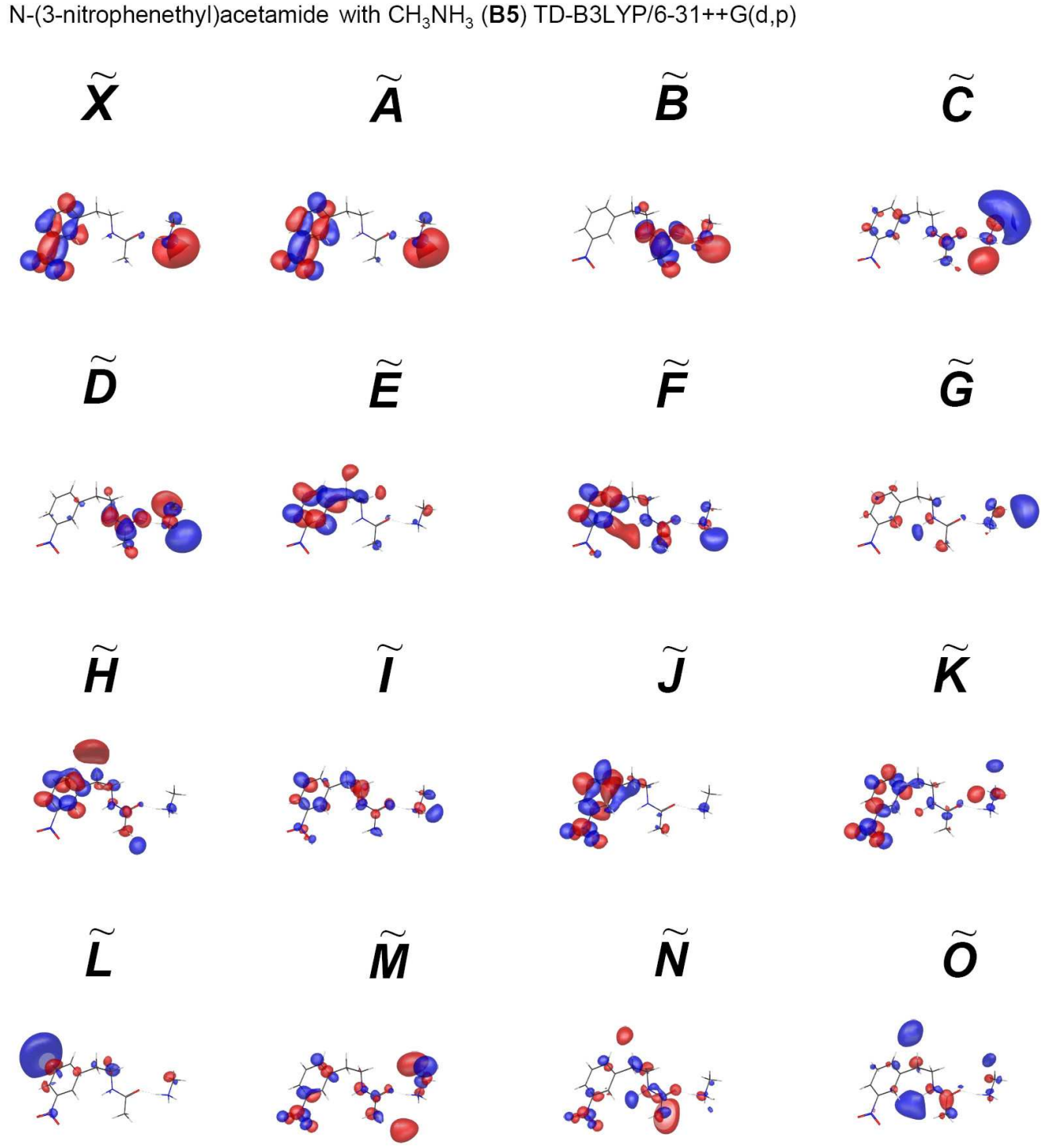


Figure S14. TDDFT excited molecular orbitals of N-(3,5-dicyanophenethyl)acetamide with the methyl ammonium complex radical (**C4**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

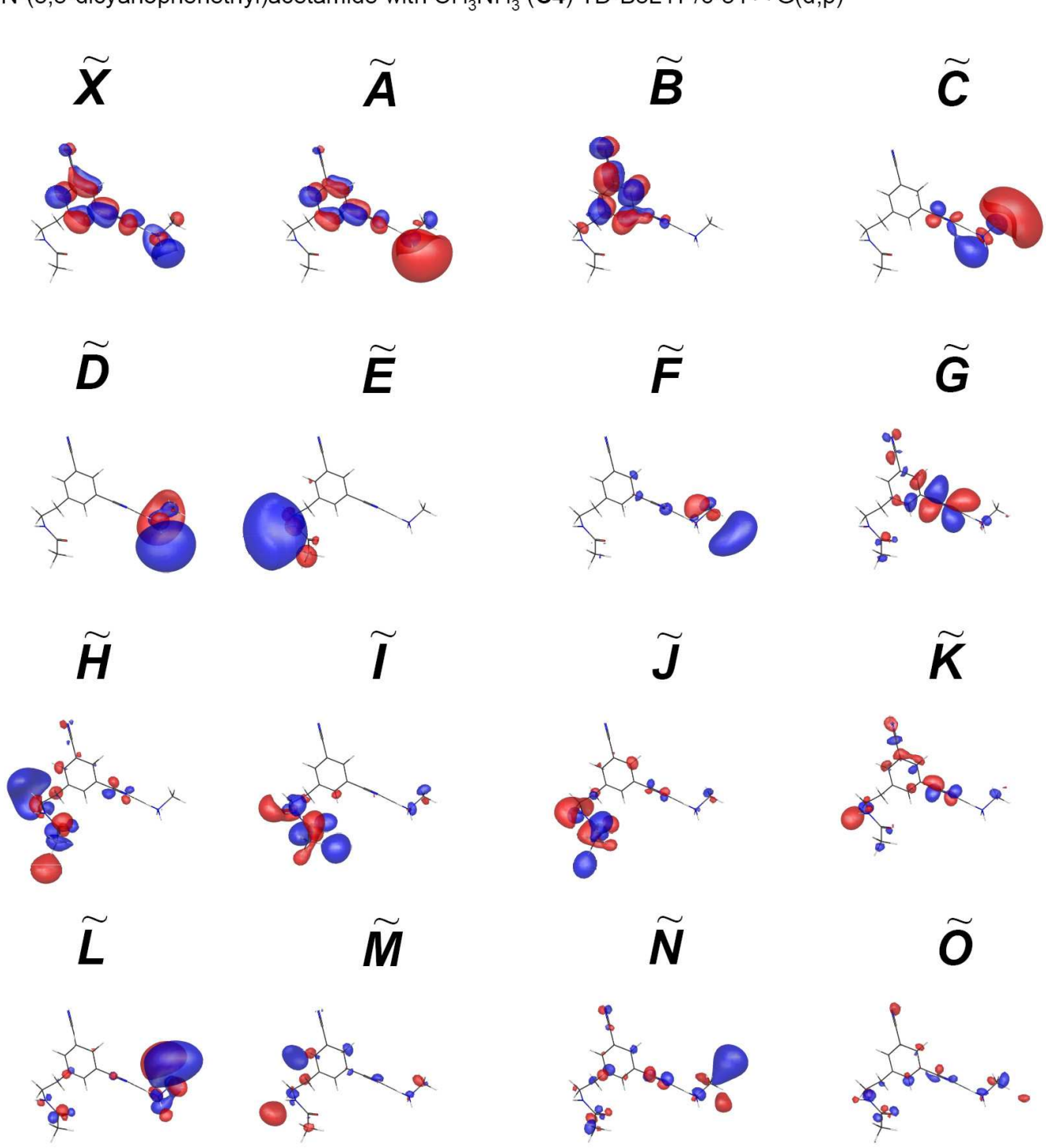


Figure S15. TDDFT excited molecular orbitals of N-(3-nitrophenethyl)acetamide with the methyl ammonium complex radical (**C5**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

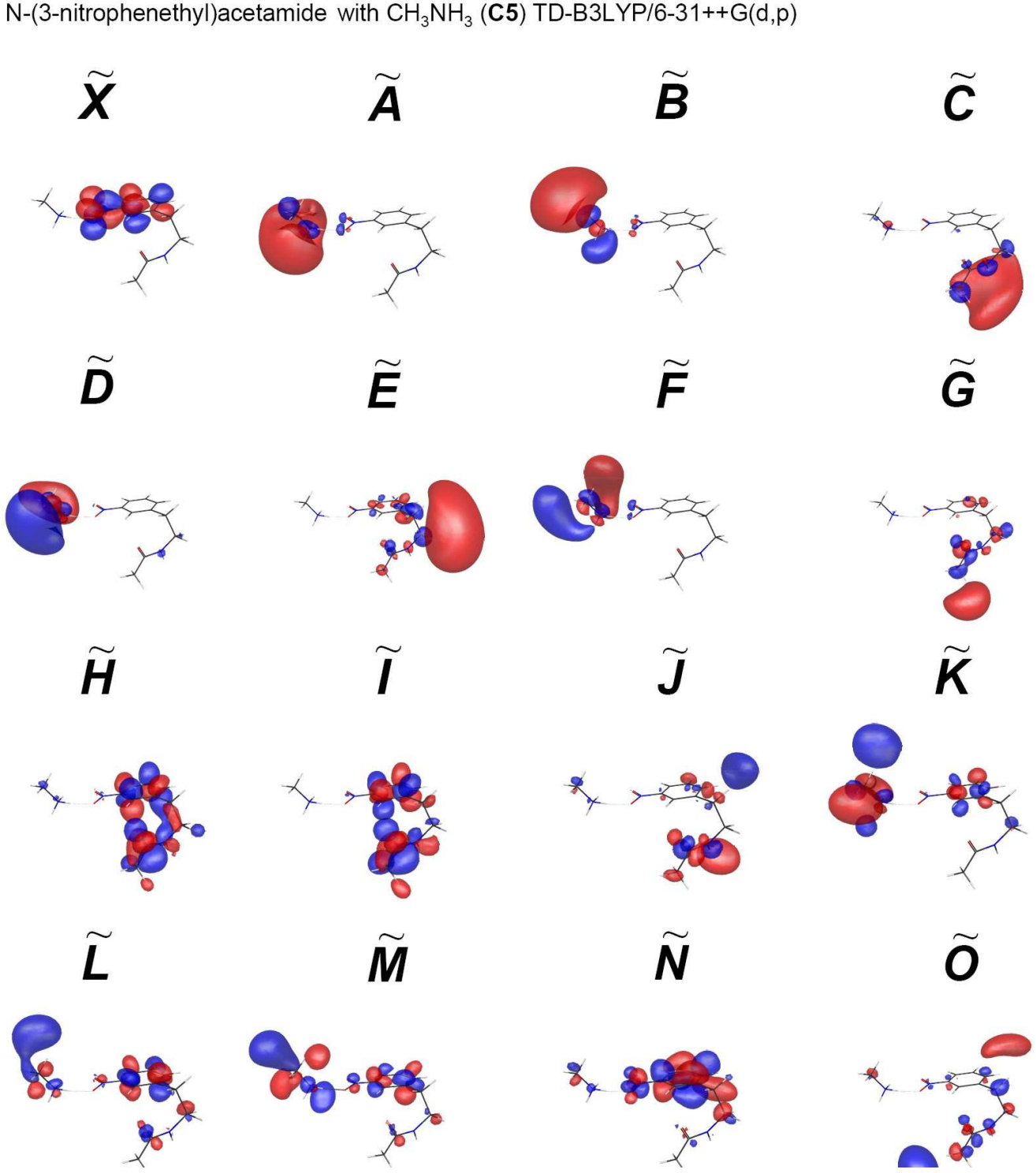


Figure S16. TDDFT excited molecular orbitals of N-(3-nitrophenethyl)acetamide with the methyl ammonium complex radical (**D5**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.

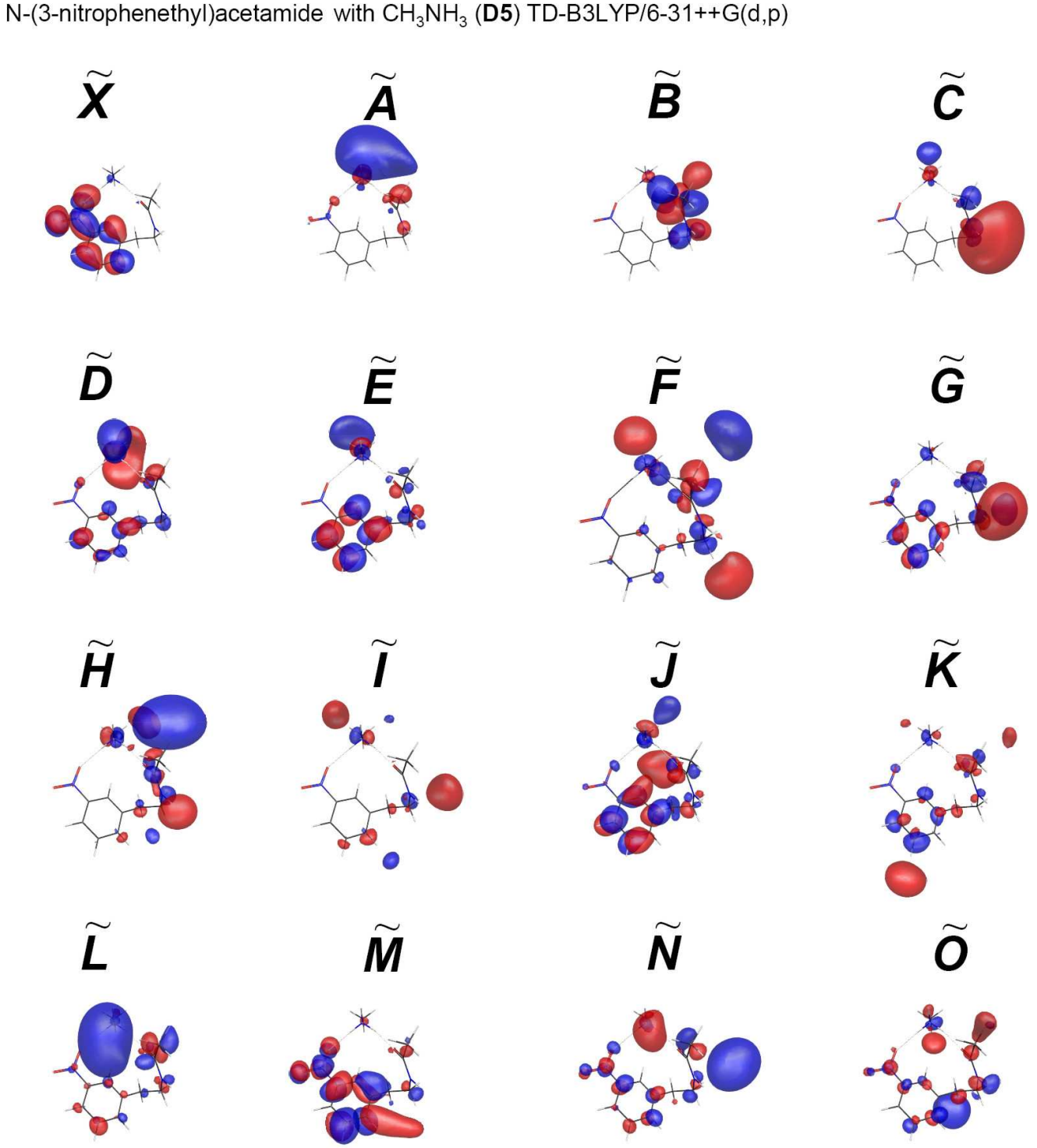
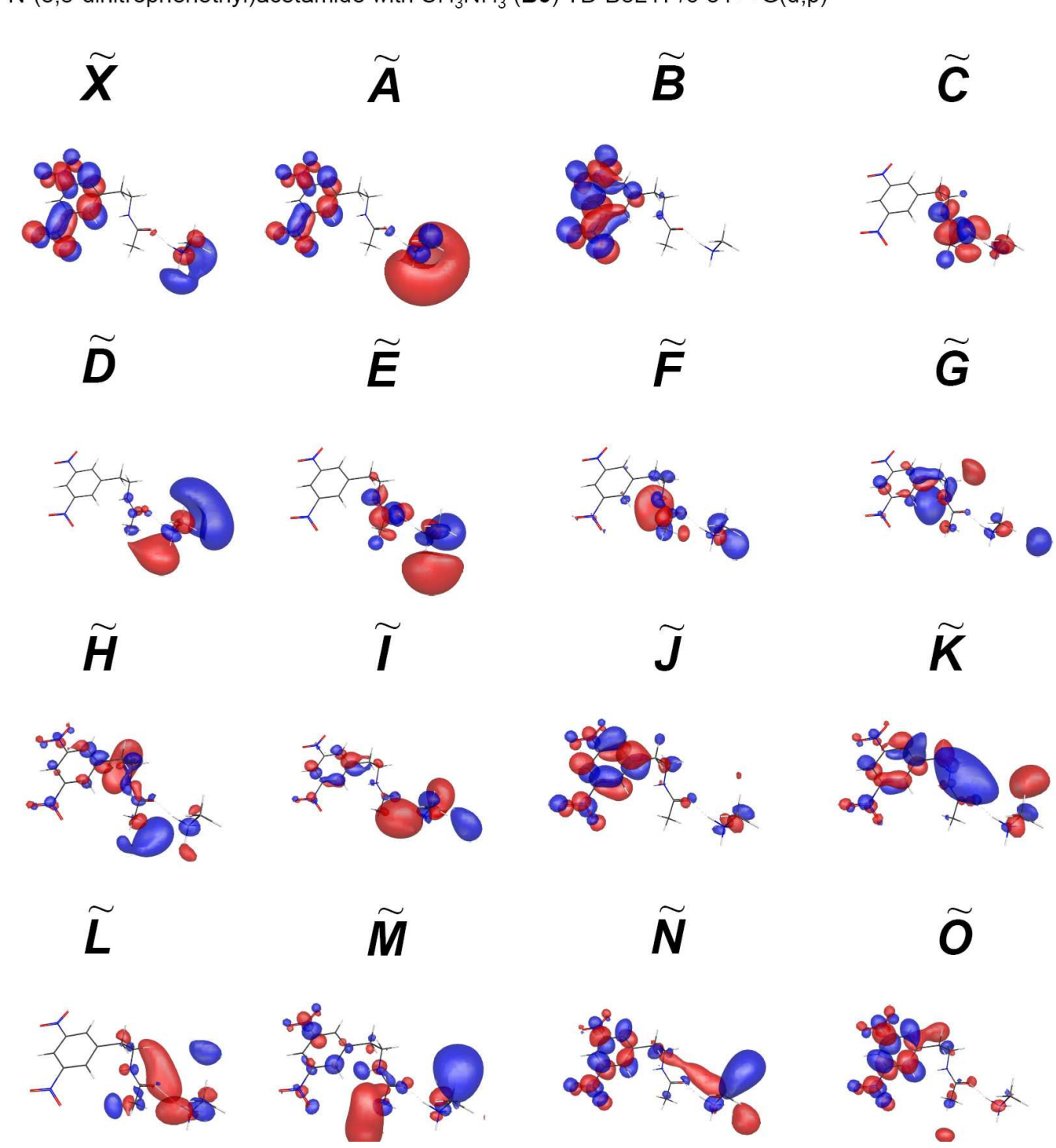


Figure S17. TDDFT excited molecular orbitals of N-(3,5-dinitrophenethyl)acetamide with the methyl ammonium complex radical (**B6**) neutral formed by vertical electron attachment at the UB3LYP/6-31++G(d,p) level.



NOTE: TDDFT excited molecular orbitals of the model compounds described in Figure 8 at the UB3LYP/6-311++G(2df,p) level are omitted due to their similarity with those of orbitals at the UB3LYP/6-31++G(d,p) level. Figure 9, however, is generated by TDDFT orbitals at the UB3LYP/6-311++(2df,p) level.

References

(1) Schweikart, K. H.; Hanack, M.; Luer, L.; Oelkrug, D. *Eur. J. Org. Chem.* **2001**, 293-302.