Electronic Supplementary Information:

Toward a uniform description of hydrogen bond and halogen bond: correlations of interaction energies with various geometric, electronic and topological parameters†

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Table S1. The halogen-bonded and hydrogen-bonded complexes studied, the interaction energies without and with BSSE-corrections (ΔE and ΔE^{cor}), interatomic distance ($r_{A\cdots N}$), electrostatic potential corresponding to the 0.002 a.u. electron density along R–A bond vector ($ESP_{0.002}$), the amount of charge transfer (Q_{CT}), the second-order perturbation stabilization energies of $n(NH_3)\rightarrow\sigma^*(R–A)$ ($E^{(2)}$), electron densities at bond critical points of A⋯N (ρ_b(BCP)) and its Laplacians $\nabla^2\rho_b$(BCP)) calculated at the MP2(full)/aug-cc-PVDZ level of theory

Table S2 Calculated results at the MP2(full)/aug-cc-PVTZ level of theory for two complex series (R–H⋯NH3 and R–Br⋯NH3)

Table S3. Electrostatic potentials (ESPs) at the nuclei of electron donor and acceptor atoms (V_N) in the complexe and monomer, the difference of the change of ESPs at the sites of donor and acceptor atoms due to complex formation ($\Delta\Delta V_N$)

Figure S1 Relationships between the calculated results with mp2(full)/aug-cc-PVDZ method and those with mp2(full)/aug-cc-PVTZ method

Figure S2 Dependence of ΔE^{cor} and $\Delta\Delta V_N$

Table S1. The halogen-bonded and hydrogen-bonded complexes studied, the interaction energies without and with BSSE-corrections (ΔE and ΔE^{cor}), interatomic distance ($r_{A\cdots N}$), electrostatic potential corresponding to the 0.002 a.u. electron density along R–A bond vector ($ESP_{0.002}$), the amount of charge transfer (Q_{CT}), the second-order perturbation stabilization energies of $n(NH_3)\rightarrow\sigma^*(R–A)$ ($E^{(2)}$), electron densities at bond critical points of A⋯N (ρ_b(BCP)) and its Laplacians $\nabla^2\rho_b$(BCP)) calculated at the MP2(full)/aug-cc-PVDZ level of theory [a]

No.	Complexes	ΔE	ΔE^{cor}	$r_{A\cdots N}$	$ESP_{0.002}$	Q_{CT}	$E^{(2)}$	ρ_b(BCP)	$\nabla^2\rho_b$(BCP)
	R–Cl⋯NH_3								
1	F–Cl⋯NH_3	12.46	11.75	2.2694	60.88	0.1376	51.70	0.0536	0.1585
2	Cl–Cl⋯NH_3	6.81	6.07	2.5375	39.15	0.0572	18.27	0.0305	0.1081
3	HO–Cl⋯NH_3	5.43	4.05	2.6490	33.55	0.0330	12.00	0.0236	0.0871
4	NH_2–Cl⋯NH_3	2.29	1.45	2.9607	15.67	0.0086	3.55	0.0129	0.0472
5	H–Cl⋯NH_3	1.20	0.69	3.2245	14.62	0.0015	1.16	0.0080	0.0285
6	CH_3–Cl⋯NH_3	0.52	0.07	3.2771	3.84	0.0016	0.86	0.0073	0.0258
7	CH_2F–Cl⋯NH_3	1.50	0.92	3.1911	13.81	0.0015	0.80	0.0079	0.0281
8	CHF_2–Cl⋯NH_3	2.19	1.52	3.1153	23.33	0.0036	1.51	0.0098	0.0351
9	CF_3–Cl⋯NH_3	3.19	2.37	3.0291	33.59	0.0053	2.18	0.0115	0.0415
10	$(CF_3)_3$C-Cl⋯NH_3	4.14	2.98	2.9298	34.96	0.0099	3.60	0.0140	0.0508
11	$MeCH_2$–Cl⋯NH_3	0.38	-0.09	3.3125	0.60	0.0015	0.75	0.0069	0.0241
12	Me_2CH–Cl⋯NH_3	0.27	-0.23	3.3359	1.99	0.0016	0.75	0.0066	0.0151
13	Me_3C–Cl⋯NH_3	0.26	-0.26	3.3490	3.96	0.0019	0.77	0.0065	0.0225
14	H_2C=CH–Cl⋯NH_3	1.18	0.61	3.2094	10.74	0.0024	1.26	0.0082	0.0293
15	HC≡C–Cl⋯NH_3	3.20	2.34	3.0181	31.72	0.0056	2.66	0.0115	0.0427
16	Ph–Cl⋯NH_3	1.36	0.66	3.1808	10.33	0.0030	1.43	0.0087	0.0311
17	4-NH_2-Ph–Cl⋯NH_3	1.05	0.38	3.2088	5.13	0.0026	1.28	0.0082	0.0295
18	4-F-Ph–Cl⋯NH_3	1.60	0.87	3.1623	13.64	0.0033	1.54	0.0090	0.0322
19	4-NO_2-Ph–Cl⋯NH_3	2.15	1.38	3.1199	22.77	0.0042	1.83	0.0097	0.0350
20	C_6F_5-Cl⋯NH_3	3.18	2.22	3.0098	28.54	0.0064	2.65	0.0119	0.0434
21	4-Pyridine–Cl⋯NH_3	1.87	1.15	3.1383	17.83	0.0038	1.70	0.0094	0.0338
22	HC(O)–Cl⋯NH_3	1.60	1.02	3.2196	18.90	0.0018	0.86	0.0078	0.0270
23	CH_3C(O)–Cl⋯NH_3	1.30	0.68	3.2757	11.38	0.0001	0.42	0.0064	0.0224
24	3-F-PhCl⋯NH_3	1.69	0.96	3.1493	15.06	0.0035	1.61	0.0092	0.0330
	R–Br⋯NH_3								
25	F–Br⋯NH_3	17.20	14.16	2.3221	74.90	0.1492	61.15	0.0538	0.1472
26	Cl–Br⋯NH_3	11.74	8.69	2.4535	51.55	0.1079	39.05	0.0417	0.1238
27	Br–Br⋯NH_3	10.08	6.94	2.5062	44.20	0.0916	31.83	0.0378	0.1155
28	HO–Br⋯NH_3	9.16	6.83	2.5816	45.85	0.0628	23.77	0.0312	0.1029
29	NH_2–Br⋯NH_3	4.80	3.02	2.8681	24.99	0.0204	8.28	0.0180	0.0618
30	H–Br⋯NH_3	2.84	1.67	3.1398	24.37	0.0048	2.76	0.0109	0.0373
31	CH_3–Br⋯NH_3	2.17	0.92	3.1371	11.11	0.0063	2.82	0.0111	0.0373
32	CH_2F–Br⋯NH_3	2.98	1.65	3.0998	19.82	0.0074	3.16	0.0119	0.0397
33	CHF_2–Br⋯NH_3	3.89	2.43	3.0412	28.94	0.0098	4.01	0.0132	0.0444
34	CF_3–Br⋯NH_3	5.21	3.53	2.9560	39.98	0.0139	5.59	0.0154	0.0519
35	$(CF_3)_3$C-Br⋯NH_3	6.69	4.63	2.8404	42.88	0.0253	8.69	0.0193	0.0649

36	$MeCH_2$–Br···NH_3	1.88	0.66	3.1660	7.15	0.0058	2.54	0.0107	0.0354
37	Me_2CH–Br···NH_3	1.68	0.48	3.1794	4.13	0.0058	2.45	0.0105	0.0345
38	Me_3C–Br···NH_3	1.54	0.36	3.1797	1.72	0.0062	2.61	0.0106	0.0345
39	H_3C=CH–Br···NH_3	2.83	1.46	3.1049	17.66	0.0073	3.37	0.0117	0.0397
40	HC≡C–Br···NH_3	5.42	3.64	2.9426	40.24	0.0144	6.10	0.0155	0.0540
41	Ph–Br···NH_3	2.98	1.56	3.0846	17.12	0.0085	3.66	0.0122	0.0414
42	4-NH_2-Ph–Br···NH_3	2.53	1.16	3.1013	11.99	0.0074	3.42	0.0118	0.0402
43	4-F-Ph–Br···NH_3	3.24	1.78	3.0659	20.74	0.0089	3.91	0.0126	0.0430
44	4-NO_2-Ph–Br···NH_3	3.92	2.43	3.0366	29.50	0.0112	4.37	0.0133	0.0452
45	C_6F_5-Br···NH_3	5.32	3.56	2.9347	36.52	0.0164	6.11	0.0160	0.0547
46	4-Pyridine–Br···NH_3	3.55	2.09	3.0541	15.18	0.0099	4.09	0.0122	0.0412
47	HC(O)–Br···NH_3	2.76	1.49	3.1568	24.53	0.0067	2.72	0.0109	0.0354
48	CH_3C(O)–Br···NH_3	2.32	0.97	3.2420	23.46	0.0020	0.91	0.0083	0.0276
49	2-F-PhBr···NH_3	3.59	2.06	3.0328	21.04	0.0104	4.21	0.0133	0.0454
50	3-F-PhBr···NH_3	3.34	1.89	3.0631	21.89	0.0092	3.96	0.0126	0.0431
	R–I···NH_3								
51	F–I···NH_3	19.90	16.54	2.4694	92.12	0.1303	54.64	0.0466	0.1320
52	Cl–I···NH_3	15.69	12.41	2.5323	69.43	0.1202	47.50	0.0422	0.1151
53	Br–I···NH_3	14.00	10.65	2.5675	61.56	0.1179	42.48	0.0398	0.1079
54	I–I···NH_3	11.36	7.96	2.6356	50.79	0.0905	32.47	0.0354	0.0966
55	OH–I···NH_3	12.33	9.75	2.6340	63.83	0.0812	32.05	0.0341	0.0995
56	NH_2–I···NH_3	7.25	5.30	2.8657	40.52	0.0379	15.09	0.0223	0.0676
57	H–I···NH_3	4.59	3.16	3.1579	36.71	0.0124	5.31	0.0133	0.0413
58	CH_3–I···NH_3	3.91	2.40	3.1636	22.57	0.0126	5.39	0.0132	0.0408
59	CH_2F–I···NH_3	4.64	3.06	3.1244	30.69	0.0164	6.31	0.0142	0.0434
60	CHF_2–I···NH_3	5.63	3.92	3.0565	39.78	0.0212	7.98	0.0160	0.0484
61	CF_3–I···NH_3	7.34	5.41	2.9401	51.90	0.0315	11.69	0.0197	0.0587
62	$(CF_3)_3C$-I···NH_3	9.78	7.36	2.8136	57.24	0.0525	16.56	0.0250	0.0727
63	$MeCH_2$–I···NH_3	3.50	2.01	3.1943	18.12	0.0125	4.96	0.0126	0.0388
64	Me_2CH–I···NH_3	3.25	1.76	3.2148	14.53	0.0119	4.62	0.0123	0.0375
65	Me_3C–I···NH_3	3.14	1.61	3.2205	11.89	0.0121	4.72	0.0122	0.0371
66	H_2C=CH–I···NH_3	4.49	2.90	3.1286	28.74	0.0158	6.23	0.0140	0.0433
67	HC≡C–I···NH_3	7.61	5.64	2.9434	53.23	0.0302	11.29	0.0191	0.0594
68	Ph–I···NH_3	4.64	2.97	3.1042	28.25	0.0176	6.63	0.0146	0.0452
69	4-NH_2-Ph–I···NH_3	4.35	2.71	3.1157	24.61	0.0165	6.35	0.0143	0.0444
70	4-F-Ph–I···NH_3	5.02	3.33	3.0863	32.01	0.0189	7.03	0.0151	0.0466
71	4-NO_2-Ph–I···NH_3	5.71	3.98	3.0553	40.98	0.0219	7.84	0.0160	0.0488
72	C_6F_5–I···NH_3	7.67	5.67	2.9267	49.67	0.0333	11.58	0.0201	0.0608
73	HC(O)–I···NH_3	3.82	2.41	3.2146	31.85	0.0134	4.97	0.0123	0.0368
74	CH_3C(O)–I···NH_3	3.02	1.70	3.2636	23.21	0.0102	4.16	0.0113	0.0339
	R–H···NH_3								
75	H_2O···NH_3	7.04	5.80	1.9630	59.60	0.0208	16.31	0.0263	0.0946
76	NH_3···NH_3	3.69	2.73	2.2757	34.86	0.0087	6.01	0.0147	0.0434
77	CH_2F_2···NH_3	3.85	2.76	2.3832	37.57	0.0099	7.03	0.0131	0.0357

78	$CHF_3\cdots NH_3$	5.42	4.05	2.2715	50.67	0.0148	10.49	0.0161	0.0449
79	$(CF_3)_3CH\cdots NH_3$	8.37	5.99	2.0890	57.56	0.0324	17.64	0.0233	0.0683
80	$H_2C{=}CH_2\cdots NH_3$	2.01	1.13	2.5459	20.93	0.0067	3.83	0.0094	0.0267
81	$HCCH\cdots NH_3$	4.81	3.39	2.2493	47.31	0.0154	9.08	0.0156	0.0465
82	$CH_3CH{=}NH\cdots NH_3$	4.26	3.10	2.2145	33.40	0.0137	8.82	0.0171	0.0496
83	$CH_3C{=}NOH\cdots NH_3$	9.62	7.78	1.8329	57.66	0.0374	27.85	0.0357	0.1238
84	$NCH\cdots NH_3$	7.50	6.01	2.1037	70.73	0.0261	15.56	0.0211	0.0641
85	$CH_3OH\cdots NH_3$	7.77	6.30	1.9204	57.52	0.0302	21.33	0.0293	0.1044
86	$CHF_2OH\cdots NH_3$	12.38	10.54	1.7798	82.39	0.0532	37.35	0.0408	0.1326
87	$CH_3CH_2OH\cdots NH_3$	7.40	5.91	1.9426	55.36	0.0279	19.83	0.0279	0.0992
88	$CF_3CH_2OH\cdots NH_3$	9.99	8.23	1.8630	72.78	0.0386	27.08	0.0334	0.1166
89	$PhOH\cdots NH_3$	10.35	8.20	1.8475	68.69	0.0437	29.41	0.0347	0.1196
90	$HCOOH\cdots NH_3$	11.86	10.09	1.8000	85.04	0.0504	35.52	0.0390	0.1281
91	$CH_3NH_2\cdots NH_3$	3.93	2.81	2.2549	32.82	0.0115	7.25	0.0155	0.0458
92	$Ph{-}H\cdots NH_3$	2.65	1.43	2.4821	22.79	0.0097	4.96	0.0106	0.0302
93	$4\text{-}NH_2\text{-}Ph\cdots NH_3$	2.38	1.19	2.4963	18.94	0.0093	4.73	0.0103	0.0295
94	$4\text{-}F\text{-}Ph\cdots NH_3$	2.95	1.71	2.4574	26.94	0.0104	5.37	0.0111	0.0315
95	$3\text{-}F\text{-}Ph\cdots NH_3$	3.09	1.84	2.4520	28.37	0.0107	5.49	0.0112	0.0318
96	$4\text{-}NO2\text{-}Ph\cdots NH_3$	3.64	2.34	2.4245	37.49	0.0115	5.93	0.0118	0.0333
97	$C_6F_5{-}H\cdots NH_3$	5.49	3.79	2.2536	46.14	0.0187	10.27	0.0163	0.0470
98	$4\text{-}Pyridine{-}H\cdots NH_3$	3.28	2.06	2.4404	31.53	0.0109	5.57	0.0115	0.0324
99	$H_2S\cdots NH_3$	4.49	3.25	2.1822	34.23	0.0193	11.64	0.0193	0.0519
100	$CH_3SH\cdots NH_3$	4.38	2.99	2.2002	29.38	0.0205	12.04	0.0188	0.0504
101	$(pyrrole)N{-}H\cdots NH_3$	8.20	6.53	1.9965	60.08	0.0313	21.44	0.0258	0.0853
102	$(imidazole)N{-}H\cdots NH_3$	9.18	7.49	1.9662	68.25	0.0349	23.78	0.0276	0.0910
103	$F{-}H\cdots NH_3$	13.26	11.63	1.6890	98.17	0.0556	42.26	0.0483	0.1506
104	$Cl{-}H\cdots NH_3$	10.12	8.22	1.7239	59.27	0.0790	49.21	0.0497	0.1164
105	$Br{-}H\cdots NH_3$	9.35	7.04	1.7044	50.74	0.0914	54.97	0.0533	0.1127
106	$ClO{-}H\cdots NH_3$	11.83	9.94	1.7657	76.87	0.0518	38.85	0.0425	0.1333
107	$BrO{-}H\cdots NH_3$	11.65	9.60	1.7718	73.54	0.0492	37.14	0.0419	0.1326
108	$IO{-}H\cdots NH_3$	11.13	9.06	1.7887	67.78	0.0451	33.77	0.0402	0.1306

[a] In units of kcal/mol for ΔE, ΔE^{cor}, $ESP_{0.002}$ and $E^{(2)}$; Å for $r_{A\cdots N}$; a.u. for Q_{CT}, ρ_b(BCP) and $\nabla^2\rho_b$(BCP);.

Table S2 Calculated results at the MP2(full)/aug-cc-PVTZ level of theory for two complex series (R–H···NH3 and R–Br···NH3) [a]

No.	Complexes	ΔE	ΔE^{cor}	$ESP_{0.002}$	Q_{CT}	ρ_b(BCP)
	R–Br···NH_3					
25	F–Br···NH_3	18.67	14.78	74.92	0.13949	0.0574
26	Cl–Br···NH_3	11.57	8.16	49.77	0.10279	0.0447
27	Br–Br···NH_3	9.98	6.50	41.10	0.08700	0.0401
28	HO–Br···NH_3	9.63	7.19	47.52	0.05686	0.0329
29	NH_2–Br···NH_3	4.87	3.30	26.93	0.01615	0.0183
30	H–Br···NH_3	2.99	1.84	24.50	0.00268	0.0109
31	CH_3–Br···NH_3	2.25	1.09	11.97	0.00537	0.0110
32	CH_2F–Br···NH_3	3.02	1.77	20.84	0.00647	0.0118
33	CHF_2–Br···NH_3	3.85	2.48	30.04	0.00871	0.0132
34	CF_3–Br···NH_3	5.13	3.55	40.85	0.01248	0.0156
35	$(CF_3)_3$C-Br···NH_3	6.29	4.74	44.92	0.02271	0.0198
36	$MeCH_2$–Br···NH_3	1.88	0.86	8.43	0.00487	0.0105
37	Me_2CH–Br···NH_3	1.62	0.71	5.66	0.00472	0.0102
38	Me_3C–Br···NH_3	1.50	0.60	3.47	0.00548	0.0103
39	H_3C=CH–Br···NH_3	2.61	1.64	18.41	0.00641	0.0116
40	HC≡C–Br···NH_3	5.34	3.76	40.84	0.01260	0.0157
41	Ph–Br···NH_3	2.71	1.69	18.15	0.00702	0.0121
42	4-NH_2-Ph–Br···NH_3	2.28	1.29	13.06	0.00633	0.0117
43	4-F-Ph–Br···NH_3	2.85	1.90	21.62	0.00763	0.0125
44	4-NO_2-Ph–Br···NH_3	3.62	2.53	30.77	0.00902	0.0133
45	C_6F_5-Br···NH_3	5.02	3.63	37.48	0.01362	0.0162
46	4-Pyridine–Br···NH_3	3.32	2.25	25.75	0.00827	0.0128
47	HC(O)–Br···NH_3	2.90	1.72	24.30	0.00582	0.0107
48	CH_3C(O)–Br···NH_3	2.38	1.28	16.22	0.00145	0.0081
49	2-F-PhBr···NH_3	3.28	2.17	22.13	0.00839	0.0133
50	3-F-PhBr···NH_3	3.08	2.01	22.94	0.00782	0.0126
	R–H···NH_3					
75	H_2O···NH_3	7.18	6.25	60.50	0.0178	0.0282
76	NH_3···NH_3	3.64	3.00	36.16	0.00499	0.0145
77	CH_2F_2···NH_3	3.70	2.80	37.65	0.0048	0.0126
78	CHF_3···NH_3	5.45	4.03	50.66	0.00891	0.0159
79	$(CF_3)_3CH$···NH_3	8.19	6.24	57.99	0.02017	0.0238
80	H_2C=CH_2···NH_3	1.85	1.23	21.38	0.00354	0.0090
81	HCCH···NH_3	5.08	3.49	47.41	0.01146	0.0157
82	CH_3CH=NH···NH_3	4.51	3.43	34.67	0.0087	0.0171
83	CH_3C=NOH···NH_3	9.85	8.55	57.95	0.03339	0.0382
84	NCH···NH_3	7.90	6.22	71.87	0.02187	0.0217
85	CH_3OH···NH_3	7.88	6.81	58.35	0.02425	0.0314
86	CHF_2OH···NH_3	12.31	10.96	84.91	0.04727	0.0436

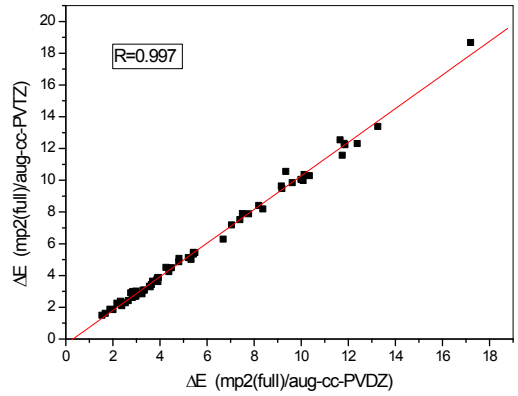
87	$CH_3CH_2OH\cdots NH_3$	7.51	6.39	55.94	0.02271	0.0299
88	$CF_3CH_2OH\cdots NH_3$	10.05	8.79	67.70	0.03289	0.0359
89	$PhOH\cdots NH_3$	10.28	8.76	69.07	0.03625	0.0371
90	$HCOOH\cdots NH_3$	12.23	10.78	85.77	0.04483	0.0418
91	$CH_3NH_2\cdots NH_3$	3.87	3.09	34.23	0.00637	0.0154
92	$Ph–H\cdots NH_3$	2.41	1.52	22.60	0.00499	0.0102
93	$4\text{-}NH_2\text{-}Ph\cdots NH_3$	2.10	1.26	18.58	0.00474	0.0099
94	$4\text{-}F\text{-}Ph\cdots NH_3$	2.69	1.79	26.57	0.00533	0.0108
95	$3\text{-}F\text{-}Ph\cdots NH_3$	2.86	1.93	28.06	0.00552	0.0109
96	$4\text{-}NO2\text{-}Ph\cdots NH_3$	3.42	2.48	37.11	0.00604	0.0115
97	$C_6F_5–H\cdots NH_3$	5.44	3.86	45.80	0.01044	0.0162
98	$4\text{-}Pyridine–H\cdots NH_3$	3.08	2.18	31.36	0.00566	0.0111
99	$H_2S\cdots NH_3$	4.49	3.47	34.58	0.01534	0.0194
100	$CH_3SH\cdots NH_3$	4.24	3.25	29.56	0.01391	0.0188
101	$(pyrrole)N–H\cdots NH_3$	8.41	6.83	61.15	0.02414	0.0270
102	$(imidazole)N–H\cdots NH_3$	9.48	7.81	69.55	0.0277	0.0290
103	$F–H\cdots NH_3$	13.39	12.26	94.08	0.05505	0.0521
104	$Cl–H\cdots NH_3$	10.36	8.42	59.91	0.07464	0.0524
105	$Br–H\cdots NH_3$	10.55	7.31	50.55	0.08799	0.0564
106	$ClO–H\cdots NH_3$	12.32	10.78	77.30	0.04698	0.0454
107	$BrO–H\cdots NH_3$	12.54	10.54	74.05	0.04547	0.0448

[a] In units of kcal/mol for ΔE, ΔE^{cor}, $ESP_{0.002}$ and a.u. for Q_{CT} and ρ_b(BCP).

Table S3. Electrostatic potentials (ESPs) at the nuclei of electron donor and acceptor atoms (V_N) in the complexe and monomer, the difference of the change of ESPs at the sites of donor and acceptor atoms due to complex formation ($\Delta\Delta V_N$)

No.	Complexes	V_N(H or Br) In complex	V_N(H or Br) In monomer	V_N(N) In complex	$\Delta\Delta V_N$
	R–Br···NH_3				
25	F–Br···NH_3	-175.775059	-175.730315	-18.284218	0.11489
26	Cl–Br···NH_3	-175.796569	-175.761832	-18.302334	0.08677
27	Br–Br···NH_3	-175.792128	-175.772475	-18.313069	0.06095
28	HO–Br···NH_3	-175.801650	-175.773273	-18.329065	0.05368
29	NH_2–Br···NH_3	-175.829216	-175.807737	-18.354194	0.02165
30	H–Br···NH_3	-175.830731	-175.808447	-18.359336	0.01731
31	CH_3–Br···NH_3	-175.853214	-175.834657	-18.366202	0.00672
32	CH_2F–Br···NH_3	-175.834660	-175.816400	-18.359326	0.0133
33	CHF_2–Br···NH_3	-175.818055	-175.799043	-18.351990	0.02139
34	CF_3–Br···NH_3	-175.80003	-175.779237	-18.343433	0.03173
35	$(CF_3)_3$C-Br···NH_3	-175.79137	-175.770553	-18.337366	0.03782
36	$MeCH_2$–Br···NH_3	-175.858610	-175.841528	-18.368031	0.00342
37	Me_2CH–Br···NH_3	-175.863184	-175.847310	-18.369244	9.96E-4
38	Me_3C–Br···NH_3	-175.867065	-175.852160	-18.370063	-7.92E-4
39	H_3C=CH–Br···NH_3	-175.839734	-175.821445	-18.361835	0.01082
40	HC≡C–Br···NH_3	-175.799100	-175.775605	-18.347513	0.03035
41	Ph–Br···NH_3	-175.839656	-175.822521	-18.361491	0.01001
42	4-NH_2-Ph–Br···NH_3	-175.849650	-175.833013	-18.366048	0.00496
43	4-F-Ph–Br···NH_3	-175.833202	-175.815598	-18.358021	0.01395
44	4-NO_2-Ph–Br···NH_3	-175.814705	-175.797024	-18.349423	0.02262
45	C_6F_5-Br···NH_3	-175.802732	-175.782609	-18.345866	0.02862
46	4-Pyridine–Br···NH_3	-175.824677	-175.806785	-18.354711	0.01755
47	HC(O)–Br···NH_3	-175.818436	-175.80246	-18.354823	0.01552
48	CH_3C(O)–Br···NH_3	-175.824796	-175.819091	-18.364832	-0.00476
49	2-F-PhBr···NH_3	-175.831946	-175.814174	-18.359766	0.01237
50	3-F-PhBr···NH_3	-175.830385	-175.812819	-18.357372	0.01456
	R–H···NH_3				
75	H_2O···NH_3	-1.029310	-0.99055	-18.339583	0.05354
76	NH_3···NH_3	-1.081083	-1.0552	-18.354366	0.02588
77	CH_2F_2···NH_3	-1.083107	-1.0579	-18.347551	0.03202
78	CHF_3···NH_3	-1.049398	-1.021754	-18.337753	0.04426
79	$(CF_3)_3CH$···NH_3	-1.014194	-0.985161	-18.330433	0.05297
80	H_2C=CH_2···NH_3	-1.116781	-1.09584	-18.357927	0.01738
81	HCCH···NH_3	-1.034874	-1.008185	-18.346940	0.03411
82	CH_3CH=NH···NH_3	-1.082789	-1.058557	-18.350165	0.02843
83	CH_3C=NOH···NH_3	-1.018576	-0.984659	-18.346021	0.04226
84	NCH···NH_3	-0.975641	-0.94367	-18.326798	0.05954
85	CH_3OH···NH_3	-1.035216	-1.00088	-18.336865	0.05184

86	$CHF_2OH\cdots NH_3$	-0.968697	-0.919832	-18.311361	0.09187
87	$CH_3CH_2OH\cdots NH_3$	-1.037788	-1.005475	-18.338669	0.04801
88	$CF_3CH_2OH\cdots NH_3$	-0.965717	-0.957727	-18.309912	0.05244
89	$PhOH\cdots NH_3$	-0.999448	-0.968164	-18.322255	0.0634
90	$HCOOH\cdots NH_3$	-0.998313	-0.919012	-18.327000	0.10667
91	$CH_3NH_2\cdots NH_3$	-1.090012	-1.06558	-18.353648	0.02515
92	$Ph–H\cdots NH_3$	-1.114287	-1.09423	-18.355466	0.01896
93	$4\text{-}NH_2\text{-}Ph\cdots NH_3$	-1.122842	-1.10372	-18.358562	0.01493
94	$4\text{-F-}Ph\cdots NH_3$	-1.105832	-1.08531	-18.351426	0.02346
95	$3\text{-F-}Ph\cdots NH_3$	-1.101235	-1.08067	-18.351001	0.02393
96	$4\text{-NO2-}Ph\cdots NH_3$	-1.08125	-1.06061	-18.342159	0.03285
97	$C_6F_5–H\cdots NH_3$	-1.042765	-1.021335	-18.342130	0.03367
98	$4\text{-Pyridine–H}\cdots NH_3$	-1.093819	-1.07277	-18.348345	0.02707
99	$H_2S\cdots NH_3$	-1.019836	-1.00012	-18.345304	0.02878
100	$CH_3SH\cdots NH_3$	-1.038377	-1.01971	-18.346337	0.0267
101	$(pyrrole)N–H\cdots NH_3$	-1.021988	-0.99467	-18.332166	0.04952
102	$(imidazole)N–H\cdots NH_3$	-1.001894	-0.97348	-18.324030	0.05875
103	$F–H\cdots NH_3$	-0.961554	-0.90147	-18.317645	0.09681
104	$Cl–H\cdots NH_3$	-0.946982	-0.92352	-18.317292	0.06054
105	$Br–H\cdots NH_3$	-0.942211	-0.93148	-18.313911	0.05119
106	$ClO–H\cdots NH_3$	-0.976450	-0.932700	-18.321150	0.07697
107	$BrO–H\cdots NH_3$	-0.981902	-0.941176	-18.322686	0.07241



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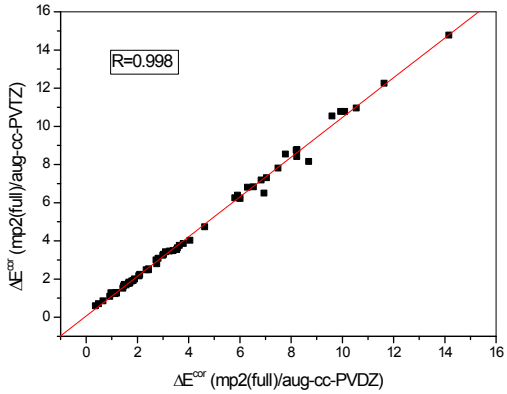

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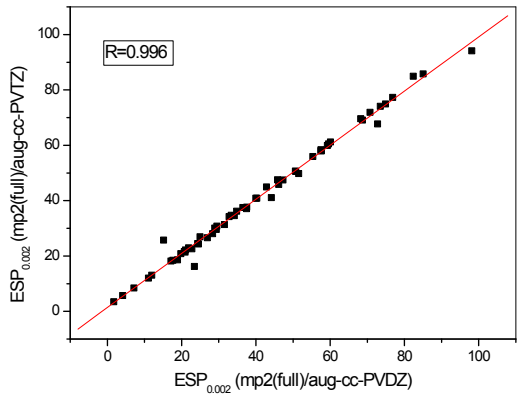

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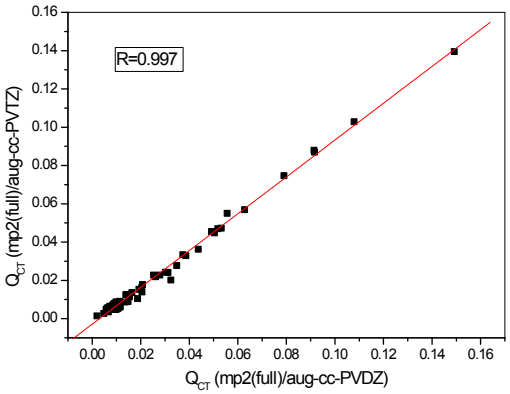

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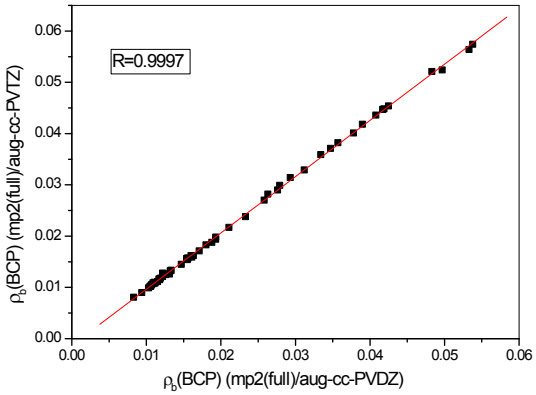

(e)

Figure S1 Relationships between the calculated results with mp2(full)/aug-cc-PVDZ method and those with mp2(full)/aug-cc-PVTZ method (a) ΔE^{cor} (b) ΔE^{cor} (c) $ESP_{0.002}$ (d) Q_{CT} (e) ρ_b(BCP)

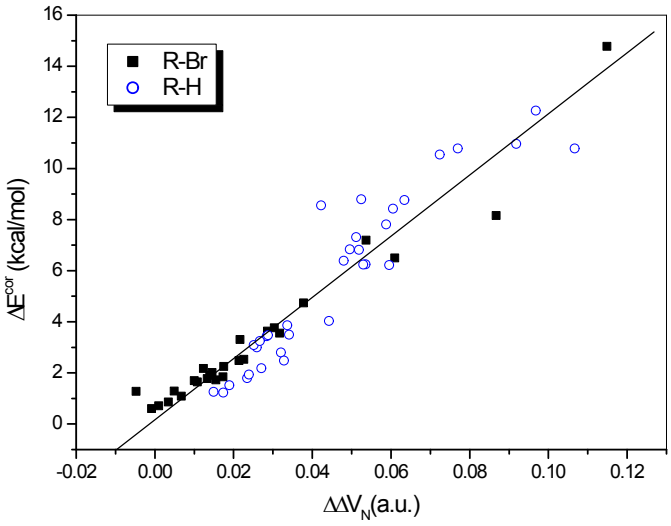

Figure S2 Dependence of ΔE^{cor} and $\Delta\Delta V_N$

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