Strong Halogen Bonding of 1,2-Diiodoperfluoroethane and 1,6-Diiodoperfluorohexane with Halide Anions Revealed by UV-Vis, FT-IR, NMR Spectroscopes and Crystallography†

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Supplemtentary information

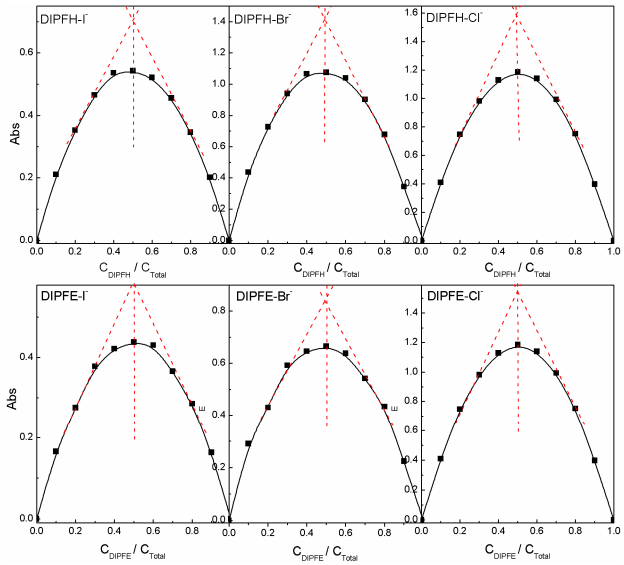

Fig. S1 Job's plots indicated the formation of 1:1 DIPFAlkane···X^- complexes.

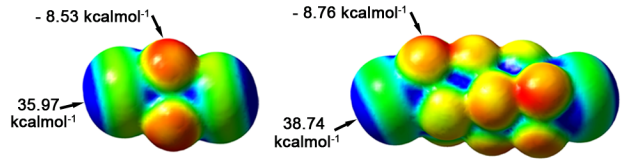

Fig. S2 The computed electrostatic potentials on the surface of DIPFE and DIPFH. (Blue indicates sites of positive charge and red sites of negative charge. Values at the maxima and minima are indicated.)

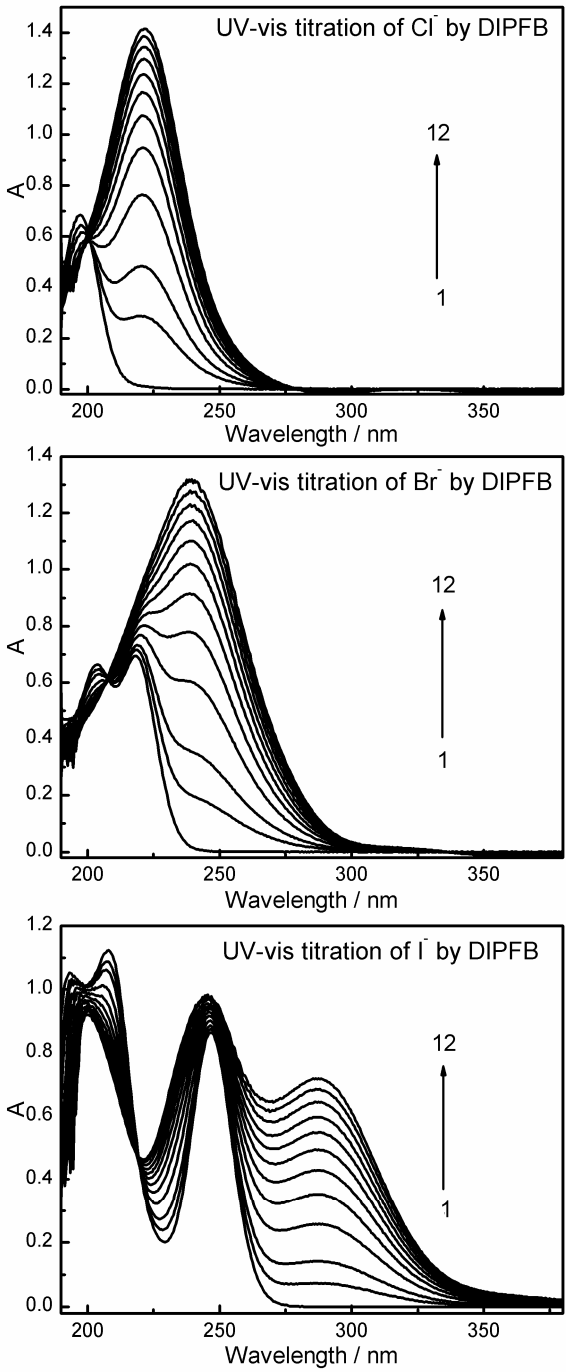

Fig. S3 The subtracted UV titration spectra of 0.5 mM halide anions by diiodoperfluorobutane (DIPFB) in acetonitrile. (From line 1 to 12, [DIPFB] = 0, 1.0, 2.0, 4.0, 6.0, 8.0, 10.0, 12.0, 14.0, 16.0, 18.0, 20.0 mM, respectively.)

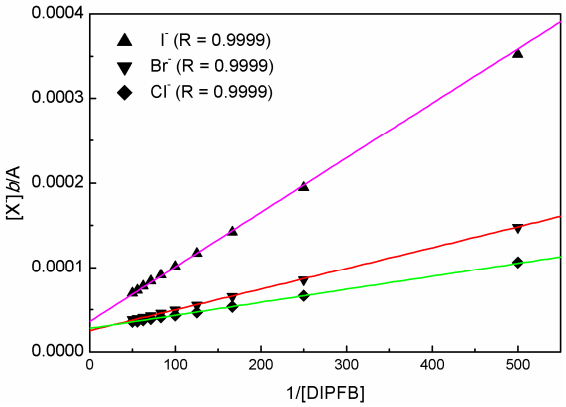

Fig. S4 Benesi-Hildebrand fitting of [halide]*b*/A *vs* 1/[DIPFB]. (R means the correlation coefficient.)

Table S1 Spectroscopic and energetic characteristics of the DIPFB···X^- complexes in acetonitrile

	λ/nm	$h\nu$/eV	$\varepsilon/10^4 M^{-1}cm^{-1}$	K/M^{-1}
DIPFB···Cl^-	221	5.62	3.60 ± 0.01	173.4 ± 7.3
DIPFB···Br^-	242	5.12	3.43 ± 0.26	121.9 ± 18.9
DIPFB···I^-	287	4.33	2.81 ± 0.05	68.6 ± 11.9

ε and *K* are the average results of triplicated experiments.

Table S2 Crystal data and structure refinement

Compound reference	DIPFE···I^-	DIPFH···I^-	DIPFE···Cl^-
Chemical formula	C18 H36 F4 I3 N	C22 H36 F12 I3 N	C18 H36 Cl F4 I2 N
Formula Mass	723.18	923.22	631.73
Crystal system	Monoclinic	Trigonal	Tetragonal
a/Å	8.2768(11)	16.3619(5)	15.8925(2)
b/Å	13.3801(18)	16.3619(5)	15.8925(2)
c/Å	23.548(3)	21.5050(14)	42.2287(11)
α/°	90.00	90.00	90.00
β/°	94.103(2)	90.00	90.00
γ/°	90.00	120.00	90.00
Unit cell volume/$Å^3$	2601.1(6)	4985.8(4)	10665.8(3)
Temperature/K	150(2)	150(2)	296(2)
Space group	*P2(1)/n*	*P3(1)*21	*I4(1)/acd*
No. of formula units per unit cell, *Z*	4	6	16
No. of reflections measured	14252	31251	31963
No. of independent reflections	5892	8903	3142
R_{int}	0.0197	0.0377	0.0506
Final R_1 values ($I > 2\sigma(I)$)	0.0244	0.1003	0.0764
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.0443	0.2305	0.2503
Final R_1 values (all data)	0.0311	0.1024	0.1367
Final $wR(F^2)$ values (all data)	0.0462	0.2314	0.3228