Electronic Supplementary Material (ESI) for New Journal of Chemistry.
This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2015

Exploring the specific halogen bond solvent effects in halogenated solvent systems by ESR probe

*Xue Pang and Wei Jun Jin**

College of Chemistry, Beijing Normal University, Beijing 100875 (P. R. China)

E-mail: wjjin@bnu.edu.cn Tel/Fax: (+86)10-58802146

Supporting Information

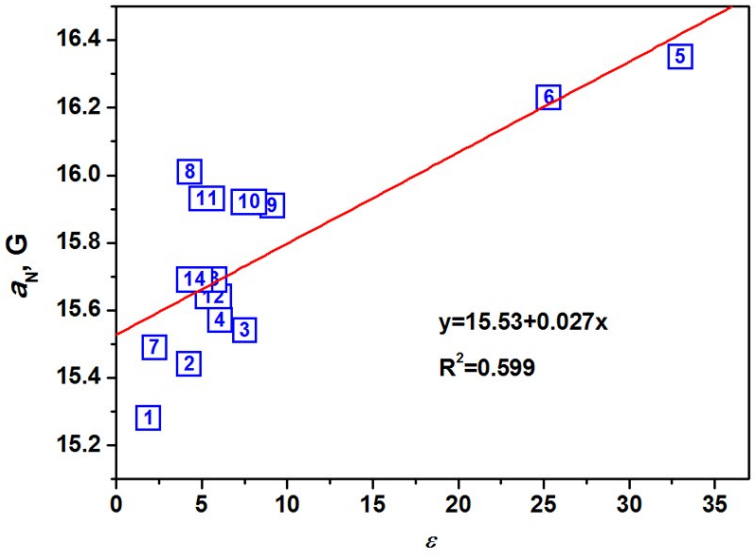

Figure S1 Relationship between a_N and ε (dielectric constant).

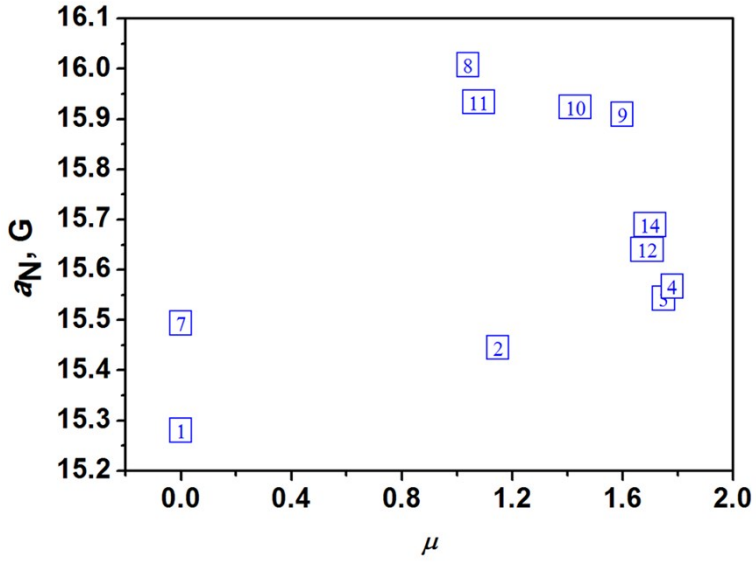

Figure S2 Relationship between a_N and μ (dipole moment).

Table S1. SP, SdP, SA, and SB Data Values for Each of the Solvents Studied in the MS.

No.	solvents	SP	SdP	SA	SB	a_N
1	n-Hexane	0.616	0	0	0.056	15.28
2	Diethyl ether	0.617	0.385	0	0.562	15.44
3	Tetrahydrofuran	0.714	0.634	0	0.591	15.54
4	Ethyl acetate	0.656	0.603	0	0.542	15.57
5	Methanol	0.608	0.904	0.605	0.545	16.35
6	Ethanol	0.633	0.783	0.4	0.658	16.23
7	Tetrachloromethane	0.768	0	0	0.044	15.49
8	Chloroform	0.783	0.614	0.047	0.071	16.01
9	Dichloromethane	0.761	0.769	0.04	0.178	15.91
10	Dibromomethane	/	/	/	/	15.92
11	Diiodomethane	/	/	/	/	15.93
12	Chlorobenzene (Cl-Ben)	0.833	0.537	0	0.182	15.64
13	Bromobenzene (Br-Ben)	0.875	0.497	0	0.192	15.69
14	Iodobenzene (I-Ben)	/	/	/	/	15.69
15	Pentafluorochlorobenzene (Cl-5FBen)	/	/	/	/	15.60
16	Pentafluorobromobenzene (Br-5FBen)	/	/	/	/	15.69
17	Pentafluoroiodobenzene (I-5FBen)	/	/	/	/	16.03
18	1,4-Dibromoperfluorobutane (1,4-DBrPFB)	/	/	/	/	15.65
19	1,4-Diiodoperfluorobutane (1,4-DIPFB)	/	/	/	/	16.07
20	1-Iodoperfluorobutane (I-PFB)	/	/	/	/	16.14

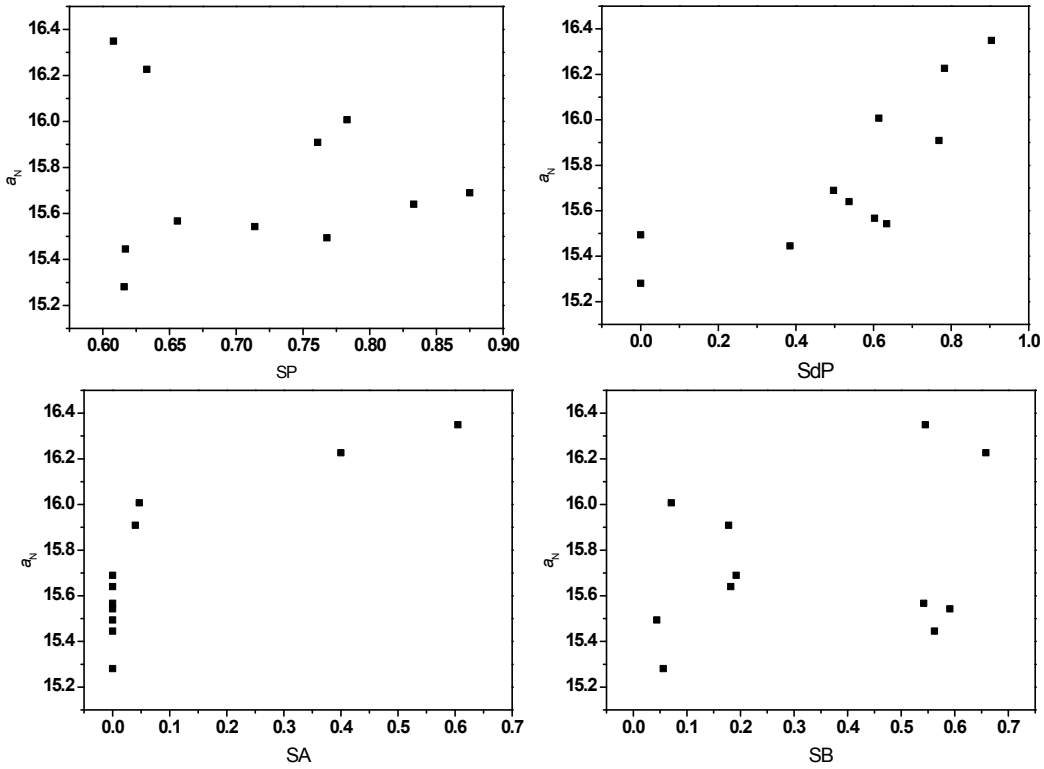

Figure S3 The correlation of a_N with Catalans four parameter scales.

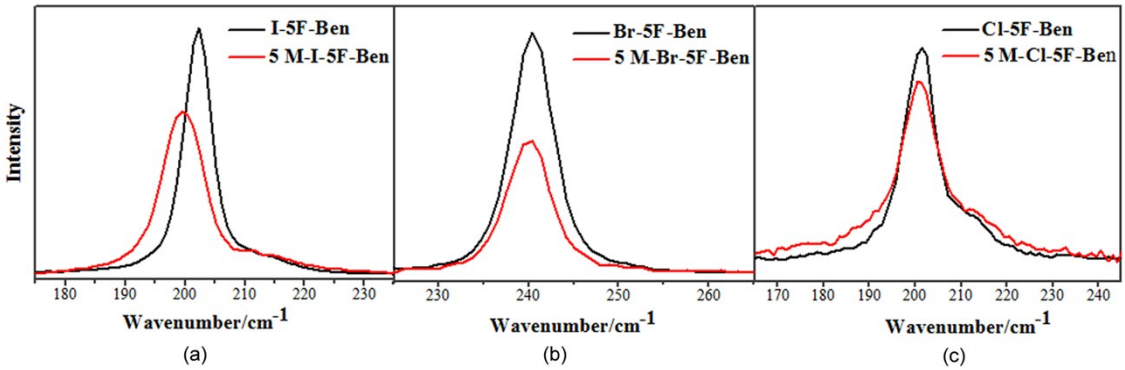

Figure S4 The Raman spectra of (a) pure I-5F-Ben and with TEMPO added 5 M; (b) pure Br-5F-Ben and with TEMPO added 5 M; (c) pure Cl-5F-Ben and with TEMPO added 5 M.

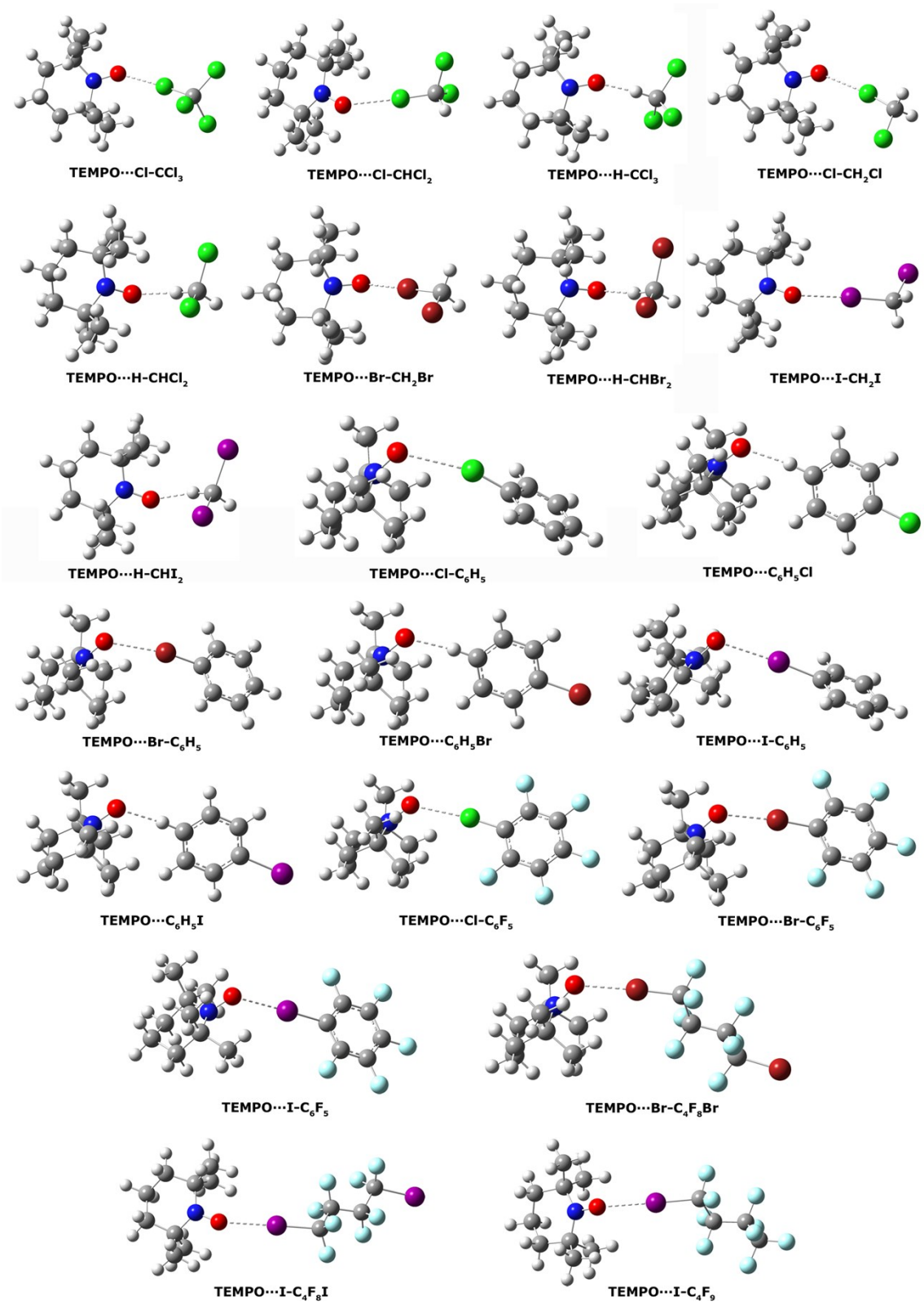

Figure S5 MP2/aug-cc-pVDZ(-PP) optimised XB or HB structures of TEMPO and solvent molecules. (Colour code: green, chlorine; red brown, bromine; purple, iodine; cyan, fluorine; red, oxygen; blue, nitrogen; white, hydrogen; grey, carbon).