

Table S1. Components of J(Hz) for complexes with F-Li⁺-F lithium bonds

1J(F-Li)	PSO	DSO	FC	SD	J
Complexes with Li-F-Li ⁺ as the acid					
Base					
FLi	-2.69	0.33	163.08	0.02	160.73
FCH ₃	-3.34	0.32	169.10	0.02	166.10
FH	-3.46	0.28	169.84	0.02	166.69
FCI	-3.59	0.31	171.07	0.02	167.82
F ₂	-3.82	0.32	170.98	0.02	167.50
Monomer	-3.77	0.10	170.76	0.02	167.12
Complexes with CH ₃ F-Li ⁺ as the acid					
Base					
FCH ₃	0.08	0.63	150.39	-0.65	150.45
FH	0.05	0.60	152.14	-0.65	152.14
FCI	0.00	0.63	154.57	-0.65	154.55
F ₂	-0.08	0.63	154.47	-0.65	154.38
Monomer	0.07	0.42	155.77	-0.65	155.60
Complexes with H-F-Li ⁺ as the acid					
Base					
FH	0.12	0.40	135.35	-0.40	135.47
FCI	0.03	0.42	135.35	-0.39	135.41
F ₂	0.13	0.44	141.20	-0.41	141.36
Monomer	0.30	0.23	142.13	-0.41	142.25
Complexes with Cl-F-Li ⁺ as the acid					
Base					
FCI	-1.78	0.66	80.76	-0.15	79.5
F ₂	-1.81	0.68	81.47	-0.19	80.15
Monomer	-1.53	0.47	83.39	-0.25	82.08
F ₂ ...Li ⁺ ...F ₂					
	-1.09	0.30	9.62	-0.08	8.75
Monomer	-0.92	0.11	9.54	-0.09	8.65

1liJ(Li-F)	PSO	DSO	FC	SD	J
Complexes with Li-F-Li+ as the acid					
Base					
FLi	-2.69	0.33	163.08	0.02	160.73
FCH3	0.25	0.63	140.73	-0.64	140.97
FH	-0.04	0.41	118.23	-0.32	118.27
FCI	-1.69	0.65	68.88	-0.01	67.84
FF	-0.93	0.29	8.06	-0.07	7.35
Complexes with CH3F-Li+ as the acid					
Base					
FCH3	0.08	0.63	150.39	-0.65	150.45
FH	0.15	0.43	133.94	-0.40	134.12
FCI	-1.81	0.66	76.15	-0.08	74.92
FF	-1.02	0.29	9.00	-0.08	8.20
Complexes with H-F-Li+ as the acid					
Base					
FH	0.12	0.40	135.35	-0.40	135.47
FCI	-1.79	0.63	78.57	-0.11	77.29
F2	-1.02	0.27	9.13	-0.08	8.30
Complexes with Cl-F-Li+ as the acid					
Base					
FCI	-1.78	0.66	80.76	-0.15	79.50
F2	-1.26	0.30	10.60	0.00	9.64
	-0.83	0.29	8.43	-0.17	7.72
F2...Li+...F2					
	-1.09	0.30	9.62	-0.08	8.75

2liJ(F-F)	PSO	SDO	FC	SD	J
Complexes with Li-F-Li+ as the acid					
Base					
FLi	5.75	-0.28	1.11	1.60	8.19
FCH3	3.25	0.00	1.82	0.62	5.68
FH	2.80	-0.19	1.55	0.51	4.67
FCI	1.24	0.13	1.09	0.40	2.86
F2	0.18	-0.18	0.20	-0.08	0.13
Complexes with CH3F-Li+ as the acid					
Base					
FCH3	1.98	0.25	2.45	0.08	4.76
FH	1.73	0.07	2.31	0.03	4.15
FCI	0.58	0.37	1.48	0.08	2.51
F2	-0.08	0.05	0.15	-0.15	-0.03
Complexes with H-F-Li+ as the acid					
Base					
FH	1.57	-0.10	2.21	0.01	3.70
FCI	0.60	0.20	1.41	0.10	2.31
F2	0.08	-0.11	0.09	-0.07	-0.01
Complexes with Cl-F-Li+ as the acid					
Base					
FCI	-0.16	0.48	0.97	0.21	1.51
F2	-0.15	0.07	0.20	-0.10	0.02
	-0.79	0.34	0.15	0.01	-0.29
F2...Li+...F2					
	-1.99	0.04	0.08	0.40	-1.48
	0.79	-0.30	0.04	-0.22	0.31

Full references:

- (35) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision C.02, Gaussian, Inc., Wallingford CT, 2004.
- (41) *ACES II* is a program product of the Quantum Theory Project, University of Florida. Stanton, J. F.; Gauss, J.; Perera, S. A.; Watts, J. D.; Yau, A. D.; Nooijen, M.; Oliphant, N.; Szalay, P. G.; Lauderdale, W. J.; Gwaltney, S. R.; Beck, S.; Balková, A.; Bernholdt, D. E.; Baeck, K. K.; Rozyczko, P.; Sekino, H.; Huber, C.; Pittner, J.; Cencek, W.; Taylor, D.; Bartlett, R. J. Integral packages included are VMOL (Almlöf, J.; Taylor, P. R.); VPROPS (Taylor, P.); ABACUS (Helgaker, H.; Jensen, H. J. Aa.; Jørgensen, P.; Olsen, J.; Taylor, P. R.); HONDO/GAMESS (Schmidt, M. W.; Baldridge, K. K.; Boatz, J. A.; Elbert, S. T.; Gordon, M. S.; Jensen, J. J.; Koseki, S.; Matsunaga, N.; Nguyen, K. A.; Su, S.; Windus, T. L.; Dupuis, M.; Montgomery, J. A.)