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Dependence of the structure of alkali metal−trifluoride ion pairs $F_3^-M^+$ on the counterion M^+ (M = Li, Na, K)

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Table S1 Data* obtained by CCSD(T)/6-311+G(3df) calculations for structures **1-13**.

Structure, Symmetry	E_{tot}, a.u.	E_{ZPE}, a.u.	ΔE, kcal·mol^{-1}	ΔE_{ZPE}, kcal·mol^{-1}	$\omega_1/i\omega_1$, cm^{-1}
1, C_{2v}	-306.639733	-306.635105	6.65	6.33	103
2, C_s	-306.639711	-306.635153	6.66	6.30	i106
3, C_s	-306.650326	-306.645186	0	0	59
4, C_s	-306.647384	-306.642588	1.85	1.63	i32
5, $C_{\infty v}$	-306.647493	-306.642530	1.78	1.67	31
6, C_{2v}	-461.170647	-461.166398	0	0	79
7, C_s	-461.170350	-461.166156	0.19	0.15	i52
8, C_s	-461.170417	-461,166146	0.14	0.16	58
9, C_s	-461.165392	-461.161397	3.30	3.14	i20
10, $C_{\infty v}$	-461.165472	-461.161386	3.25	3.15	15
11, C_{2v}	-898.699674	-898.695505	0	0	72
12, C_s	-898.691912	-898.688186	4.87	4.59	i14
13, $C_{\infty v}$	-898.691937	-898.688166	4.86	4.61	10

* E_{tot} (in a.u.) - total energy (1a.u.=627.5095 kcal·mol^{-1}); E_{ZPE} (in a.u.) – energy with harmonic zero-point correction; ω_1 or $i\omega_1$ (in cm^{-1}) - the lowest or imaginary harmonic vibration frequency; ΔE (in kcal·mol^{-1}) - relative energy (1a.u.=627.5095 kcal·mol^{-1}); ΔE_{ZPE} (in kcal·mol^{-1}) - relative energy including harmonic zero-point correction.

Optimized Cartesian coordinates

Structure 1 [CCSD(T)/6-311+G(3df)]

9	0.000000000	0.000000000	0.579338000
9	0.000000000	1.694011000	-0.105855000
9	0.000000000	-1.694011000	-0.105855000
3	0.000000000	0.000000000	-1.102888000

Structure 2 [CCSD(T)/6-311+G(3df)]

9	0.000000000	0.560856000	0.000000000
9	1.706683000	-0.028516000	0.000000000
9	-1.689739000	-0.158764000	0.000000000
3	-0.050832000	-1.120728000	0.000000000

Structure 3 [CCSD(T)/6-311+G(3df)]

9	1.220104000	-1.602170000	0.000000000
9	0.000000000	0.582592000	0.000000000
9	-1.099787000	1.499260000	0.000000000
3	-0.360951000	-1.439042000	0.000000000

Structure 4 [CCSD(T)/6-311+G(3df)]

9	0.377191000	-1.715513000	0.000000000
9	0.000000000	0.674945000	0.000000000
9	-0.256028000	2.078053000	0.000000000
3	-0.363489000	-3.112455000	0.000000000

Structure 5 [CCSD(T)/6-311+G(3df)]

9	0.000000000	0.000000000	2.125524000
9	0.000000000	0.000000000	0.699960000
9	0.000000000	0.000000000	-1.724280000
3	0.000000000	0.000000000	-3.303610000

Structure 6 [CCSD(T)/6-311+G(3df)]

9	0.000000000	0.000000000	-0.793060000
9	0.000000000	1.725660000	-0.350346000
9	0.000000000	-1.725660000	-0.350346000
11	0.000000000	0.000000000	1.222161000

Structure 7 [CCSD(T)/6-311+G(3df)]

9	-1.688190000	0.058230000	0.000000000
9	0.000000000	0.741522000	0.000000000
9	1.714266000	0.791998000	0.000000000
11	-0.021335000	-1.302341000	0.000000000

Structure 8 [CCSD(T)/6-311+G(3df)]

9	0.000000000	0.709011000	0.000000000
9	1.648570000	-0.129029000	0.000000000
9	-1.626584000	1.106357000	0.000000000
11	-0.017988000	-1.379732000	0.000000000

Structure 9 [CCSD(T)/6-311+G(3df)]

9	0.000000000	1.052637000	0.000000000
9	-0.762504000	-1.147490000	0.000000000
9	-1.207361000	-2.511165000	0.000000000
11	1.611708000	2.132196000	0.000000000

Structure 10 [CCSD(T)/6-311+G(3df)]

9	0.000000000	0.000000000	-2.881260000
9	0.000000000	0.000000000	-1.447968000
9	0.000000000	0.000000000	0.881804000
11	0.000000000	0.000000000	2.820619000

Structure 11 [CCSD(T)/6-311+G(3df)]

9	0.000000000	0.000000000	-1.085539000
9	0.000000000	1.734518000	-0.759107000
9	0.000000000	-1.734518000	-0.759107000
19	0.000000000	0.000000000	1.233356000

Structure 12 [CCSD(T)/6-311+G(3df)]

9	0.000000000	0.583165000	0.000000000
9	1.736322000	-0.918586000	0.000000000
9	2.811089000	-1.875289000	0.000000000
19	-2.154037000	1.047179000	0.000000000

Structure 13 [CCSD(T)/6-311+G(3df)]

9	0.000000000	0.000000000	-3.465948000
9	0.000000000	0.000000000	-2.027875000
9	0.000000000	0.000000000	0.271703000
19	0.000000000	0.000000000	2.473636000