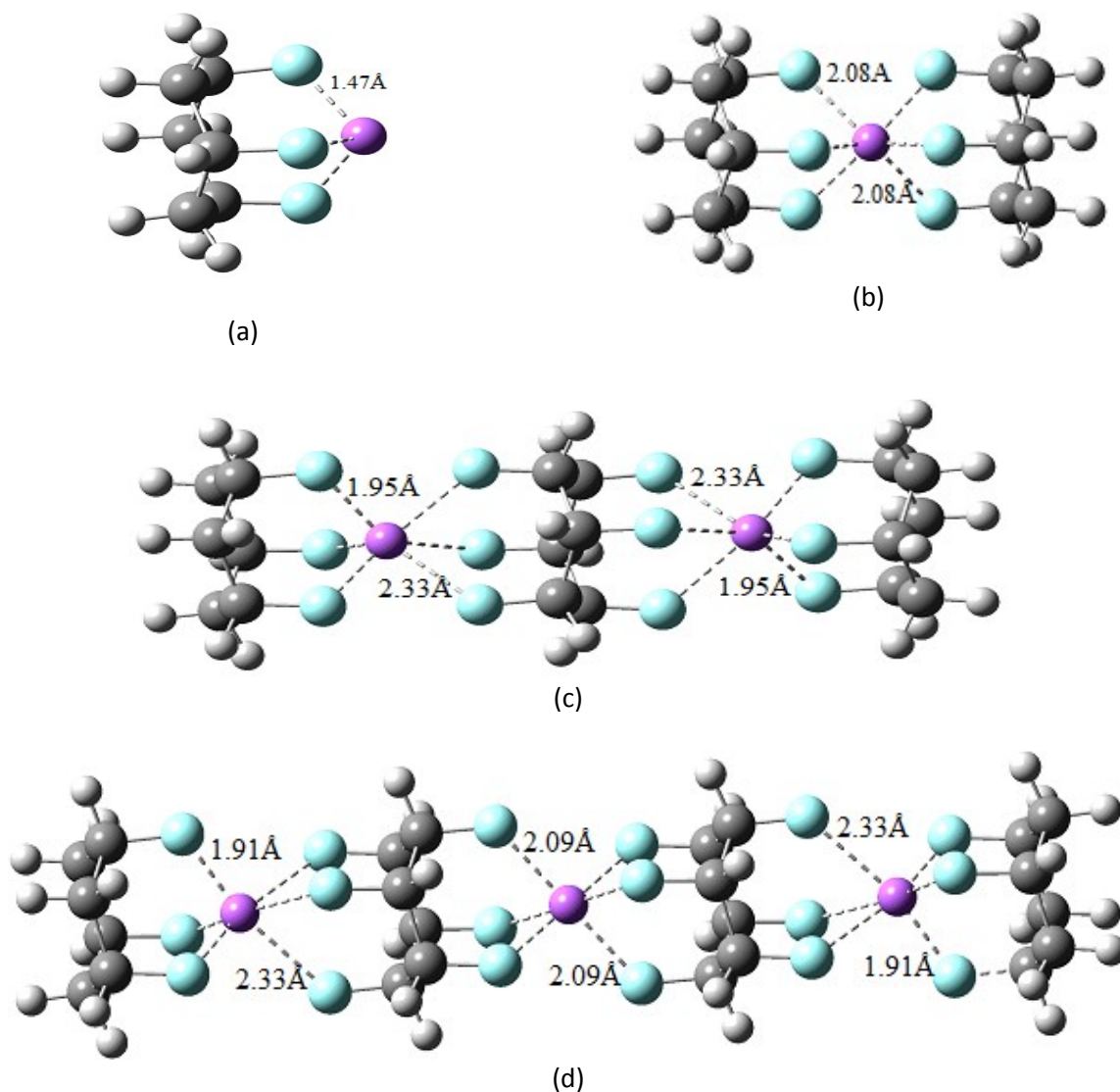


Supplementary information

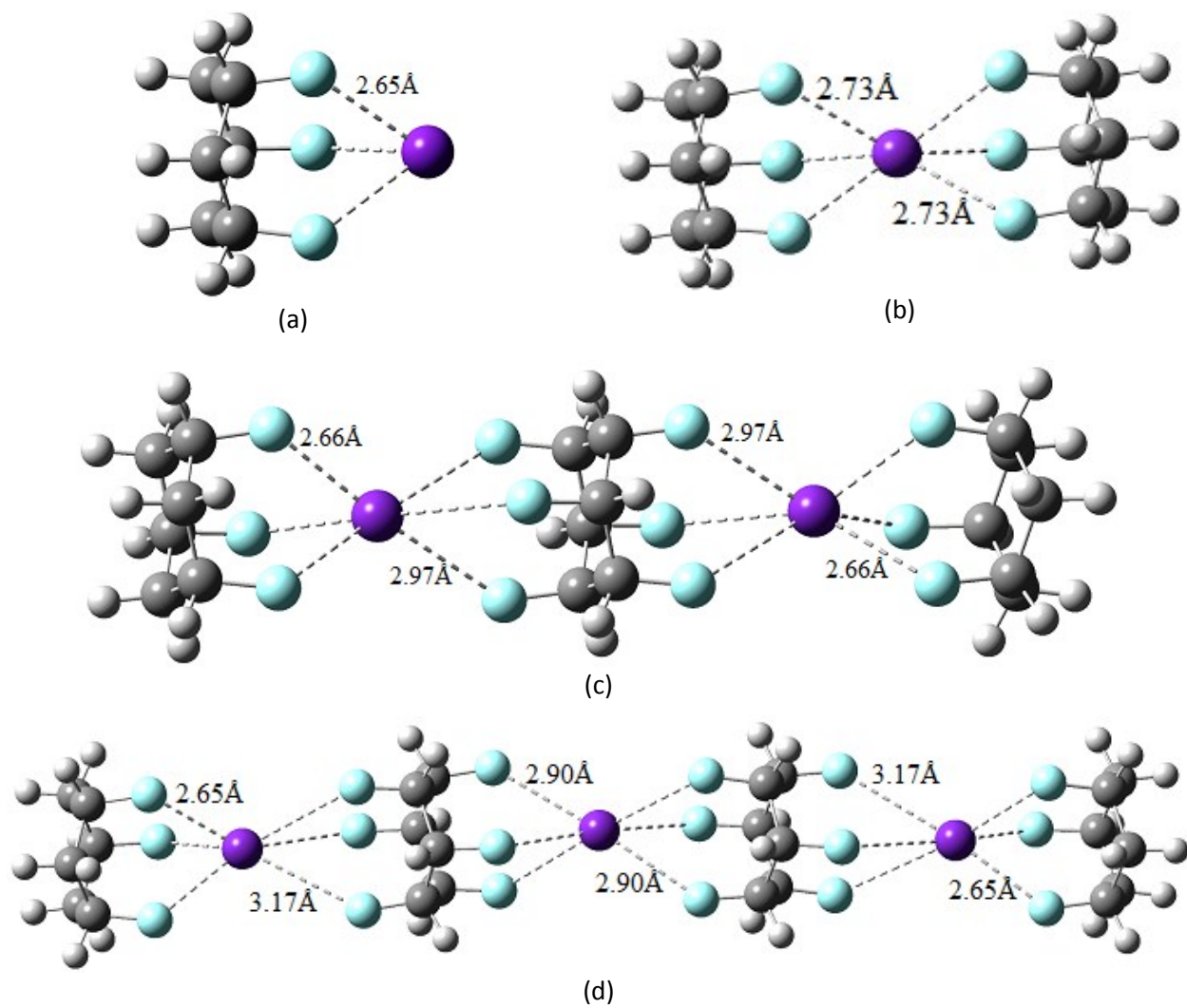
Title: Unique cation-cyclohexane interactions in tri- and hexa-fluorocyclohexane mutlidecker complexes in gas phase: A DFT study

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Name of the Journal: RSC Advances



Supplementary Fig. S1 Optimized structures of the complexes (a) $\text{Li}^+@1$ (b) $\text{Li}^+@2$ (c) $\text{Li}^+@3$ and (d) $\text{Li}^+@4$ obtained at B3LYP/6-31+G (d,p) level of theory.



Supplementary Fig. S2 Optimized structures of the complexes (a) $K^+@1$ (b) $K^+@2$ (c) $K^+@3$ and (d) $K^+@4$ obtained at B3LYP/6-31+G (d,p) level of theory.

Supplementary Table S1: BSSE Correction in kcal/mol for Na⁺, Li⁺, K⁺ complexes obtained at B3LYP/6-31+G(d,p) level of theory

Complex	BSSE Correction	Complex	BSSE Correction	Complex	BSSE Correction
Na ⁺ @1	0.94	Li ⁺ @1	0.61	K ⁺ @1	0.50
Na ⁺ @2	1.73	Li ⁺ @2	1.47	K ⁺ @2	0.86
Na ⁺ @3	3.37	Li ⁺ @3	2.90	K ⁺ @3	1.67
Na ⁺ @4	5.13	Li ⁺ @4	4.33	K ⁺ @4	2.34

Supplementary Table S2: BSSE Correction in kcal/mol for Na⁺ complexes obtained at different level of theory

Complex	B3LYP/6-31+ G(d,p)	B3LYP/6-31++ G(d,p)	M06-2X/ 6-31+G(d,p)	M06-2X/ 6- 31++G(d,p)	ω B97X-D/ 6-31+G(d,p)	ω B97X-D/6- 31++G(d,p)
Na ⁺ @ 1	0.94	0.94	0.85	0.83	0.98	0.97
Na ⁺ @ 2	1.73	1.71	1.66	1.61	1.97	1.92
Na ⁺ @ 3	3.37	3.45	3.17	3.19	3.72	3.74
Na ⁺ @ 4	5.13	5.27	4.71	4.78	5.61	5.67

Supplementary Table S3: E_{HOMO} , E_{LUMO} , global hardness and electrophilicity of the complexes along with TFCH and HFCH obtained at B3LYP/6-31+G(d,p) level of theory.

System	HOMO	LUMO	η	ω
TCHF	-196.89	-11.70	92.60	58.73
HFCH	-216.32	-17.10	99.61	68.37
Na ⁺ @1	-298.78	-105.60	96.59	211.61
Na ⁺ @2	-277.22	-75.58	100.82	154.31
Na ⁺ @3	-320.49	-158.43	81.03	353.84
Na ⁺ @4	-344.05	-202.77	70.64	529.10
Li ⁺ @1	-310.43	-99.42	105.51	199.01
Li ⁺ @2	-278.89	-75.73	101.58	154.76
Li ⁺ @3	-329.68	-155.20	87.24	336.86
Li ⁺ @4	-358.60	-206.01	76.30	522.27
K ⁺ @1	-288.12	-97.71	95.21	195.45
K ⁺ @2	-272.16	-73.67	99.25	150.64
K ⁺ @3	-309.31	-148.43	80.44	325.57
K ⁺ @4	-328.85	-184.70	72.08	457.40