SUPPORTING INFORMATION FOR:

Exploring Binding Chemistry of Alkali/Alkaline Earth Cations in Solution through Modulation of Intramolecular Charge-Transfer in an Excited Ambidentate Organic Fluorophore

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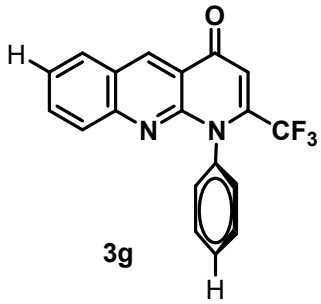
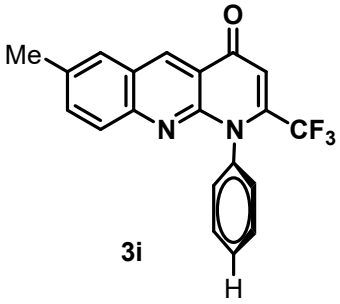
1. Experimental Results

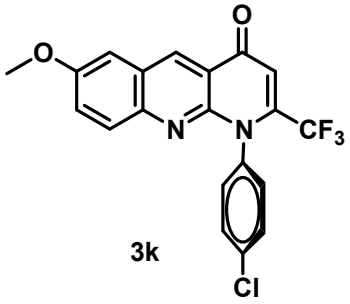
Table S1. Photophysical properties of the N^1-(aryl)-2-(trifluoromethyl) benzo[*b*][1,8]naphthyridin-4(1*H*)-ones **3g**, **3i** and **3k** in ethanol and ethanol/water (8/2).



3g



3i



3k

Probe	λ_{abs} (nm) [ε ($M^{-1}.cm^{-1}$)][a]	λ_{em} (nm)[b] (R.I.)[c]	$\Delta\lambda$ (nm)[d]	$\tau_{1/2}$ ± S.D.[e] (%)[f]	Φ ± S.D.[g]	Φ ± S.D.[j]
3g	332 (15863) 384 (20293) 400 (20179)	426 (1.0) 476 (0.5)	42 92	8.13 ± 0.30 (37.6) 2.27 ± 0.20 (32.3) 0.44 ± 0.02 (30.1)	0.052 ± 0.004[h]	0.062 ± 0.005[h]
3i	332 (< 8000) 374 (21758)	436 (< 0.5) 472 (1.0)	62 98	3.33 ± (66.0) 2.75 ± 0.40 (23.6) 0.93 ± 0.30 (10.4)	0.038 ± 5.5 %[i]	0.044 ± 0.003
3k	332 (< 8000) 402 (12663) 418 (12959)	**472 (1.00)**	36 74	14.20± 0.50 (79.3) 6.73 ± 0.90 (20.7)	0.237 ± 0.016[i]	0.252 ± 0.008[i]

[a]Absorption wavelength and molar absorptivity (in brackets); [b]Emission wavelength at 370 nm excitation; [c]Relative intensity ratio between 426 and 476 emissions; [d]Stoke shift; [e]lifetimes obtained at 370 nm excitation; [f]abundance percentages of excited species; [g]Q.Y. calculated from Rhodamine 6G; [h]Q.Y. for LE-state; [i]Q.Y. for CT-state. [j]Q.Y. in ethanol/water (8/2).

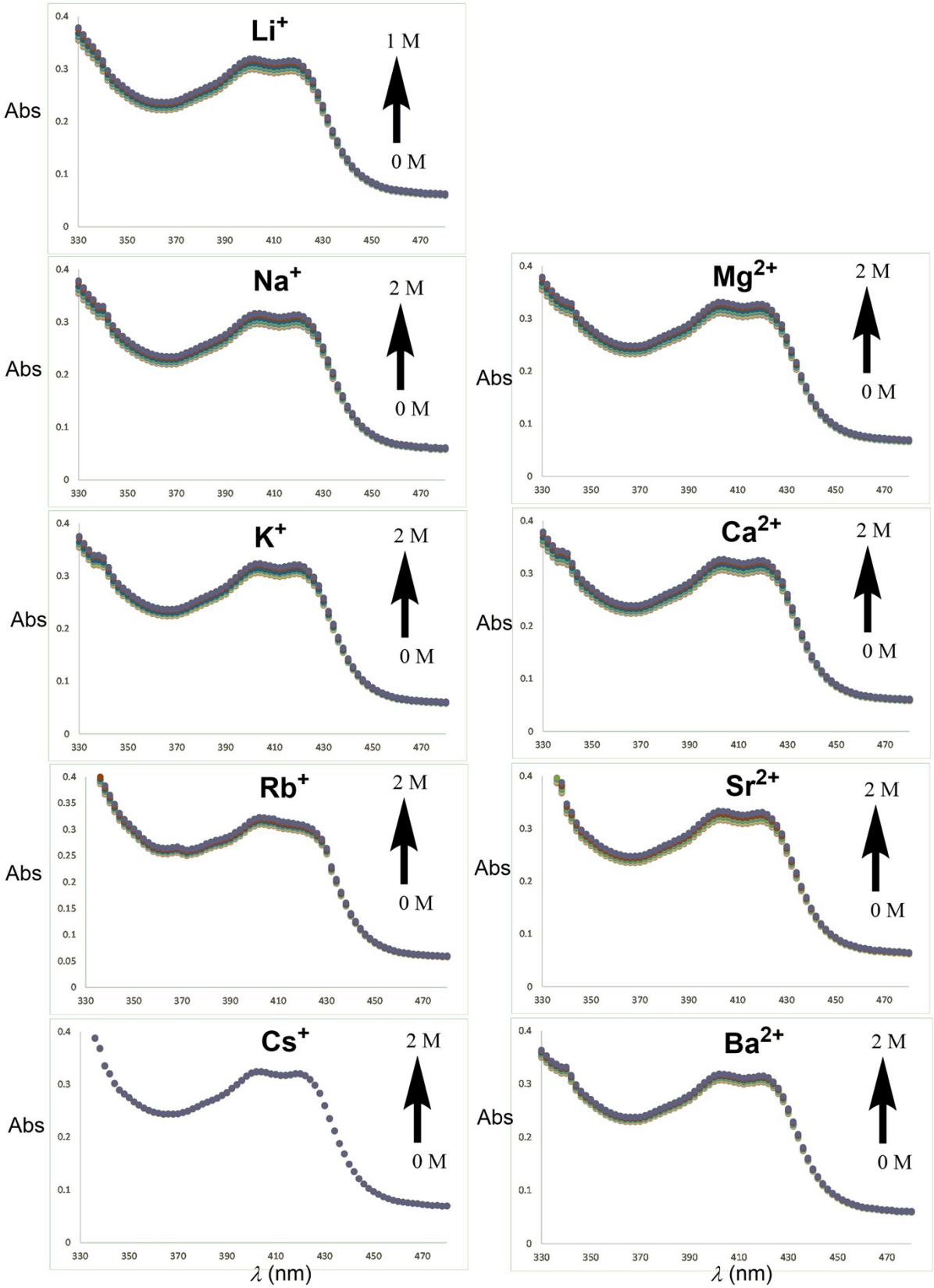


Figure S1. Absorption spectra of the probe **3k** in presence of AM cations.

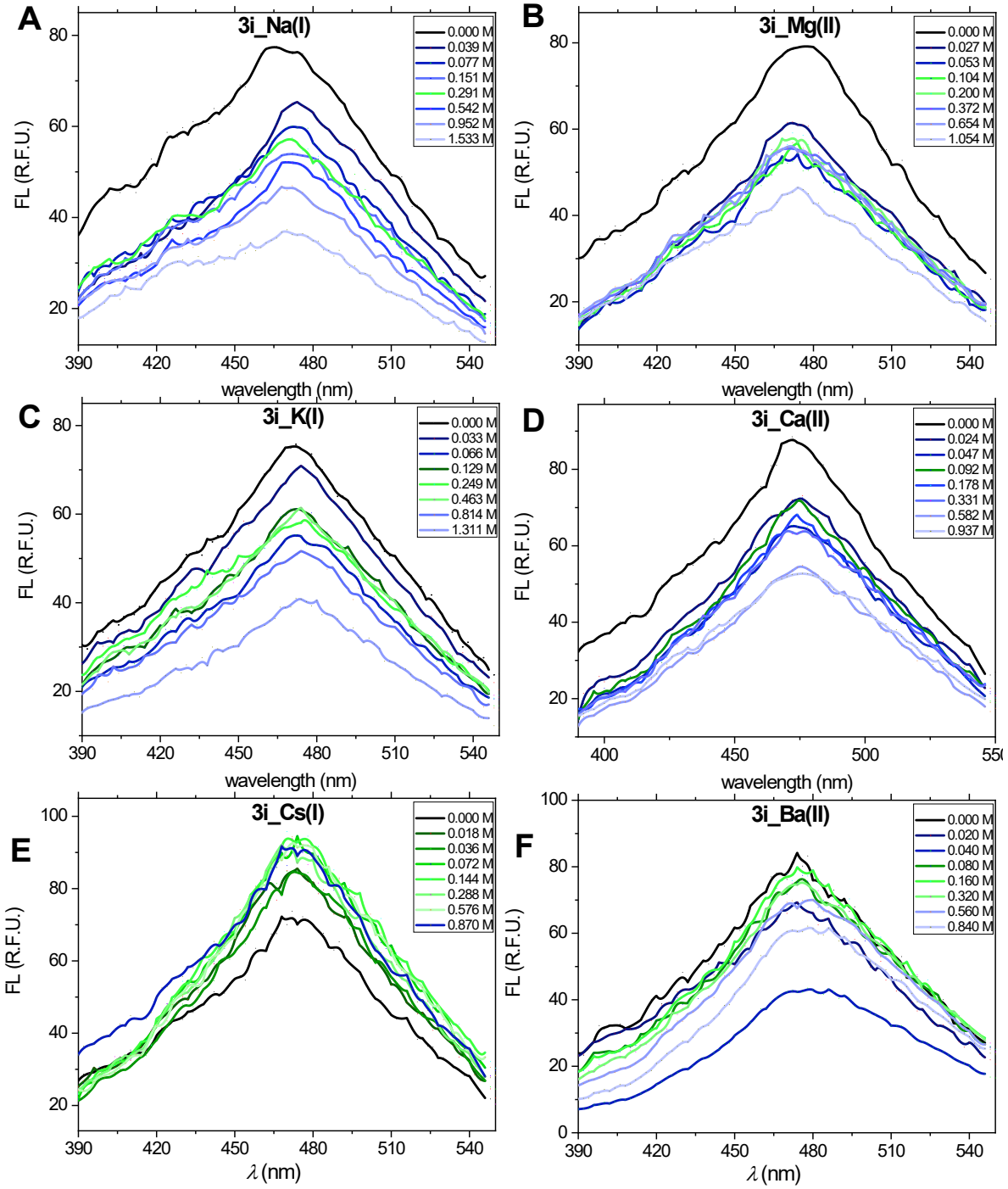


Figure S2. Titration of probe **3i** (50 μM) upon 370 nm excitation in ethanol/water solution (8/2) containing: (**A**) Na^+; (**B**) Mg^{2+}; (**C**) K^+; (**D**) Ca^{2+}; (**E**) Cs^+ and (**F**) Ba^{2+}.

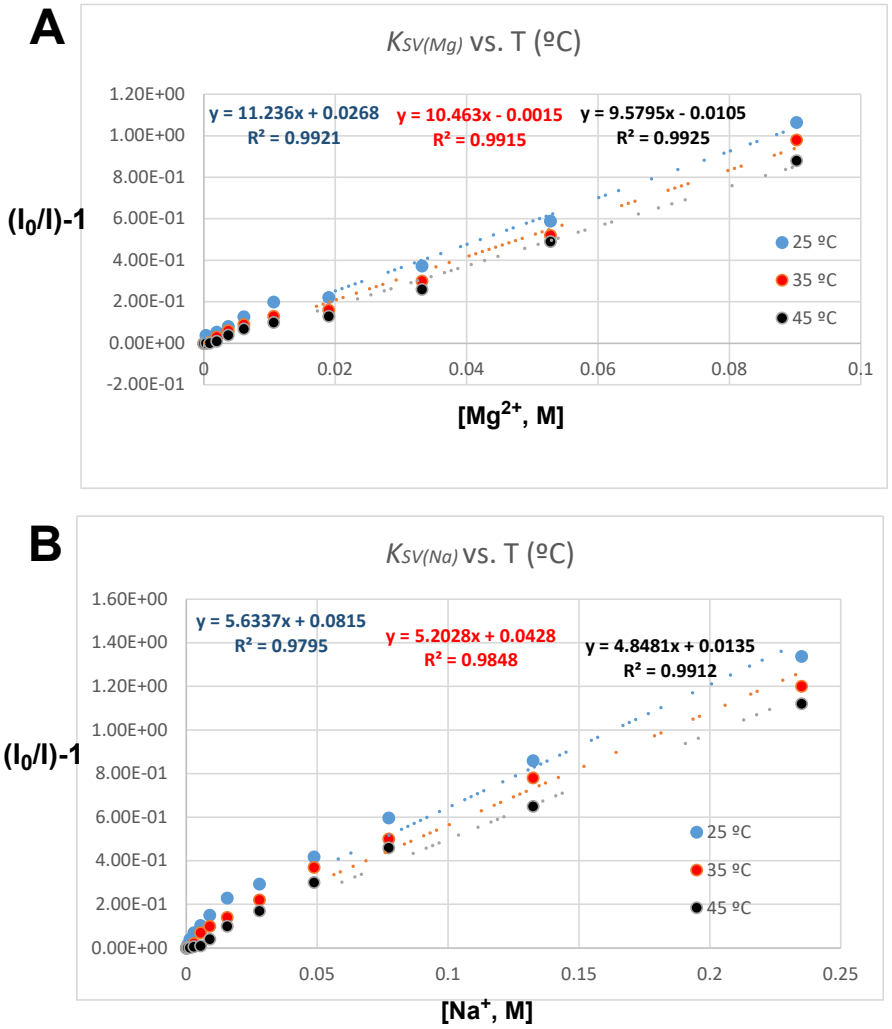


Figure S3. Stern-Volmer constant (K_{SV}) derived from (I_0/I-1) *vs.* cation concentration as function of temperature (25, 35 and 45 ºC) for Mg^{2+} (**A**) and Na^+ (**B**) cations.

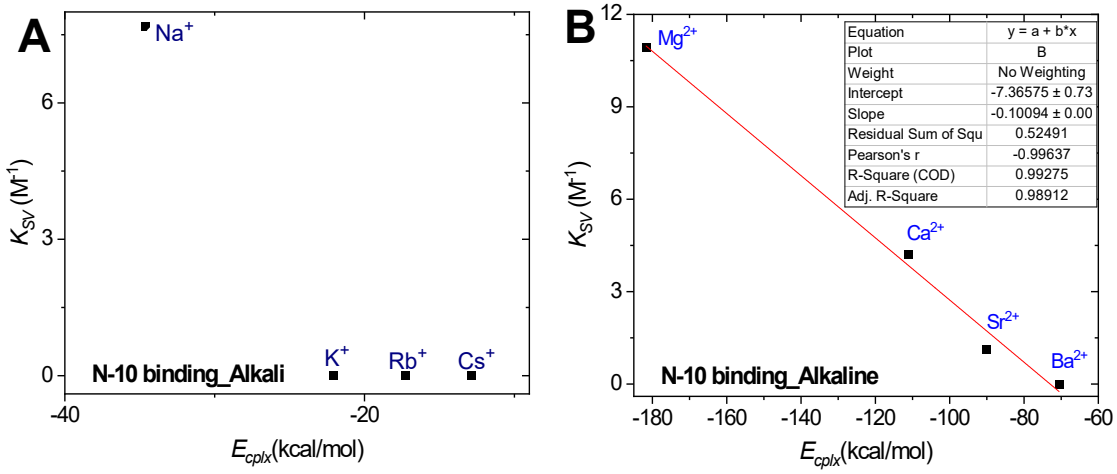


Figure S4. Stern-Volmer constant as function of free complexation energy for [**3k(N-10)**-cation] adduct of alkali (**A**) and alkaline earth (**B**) cations.

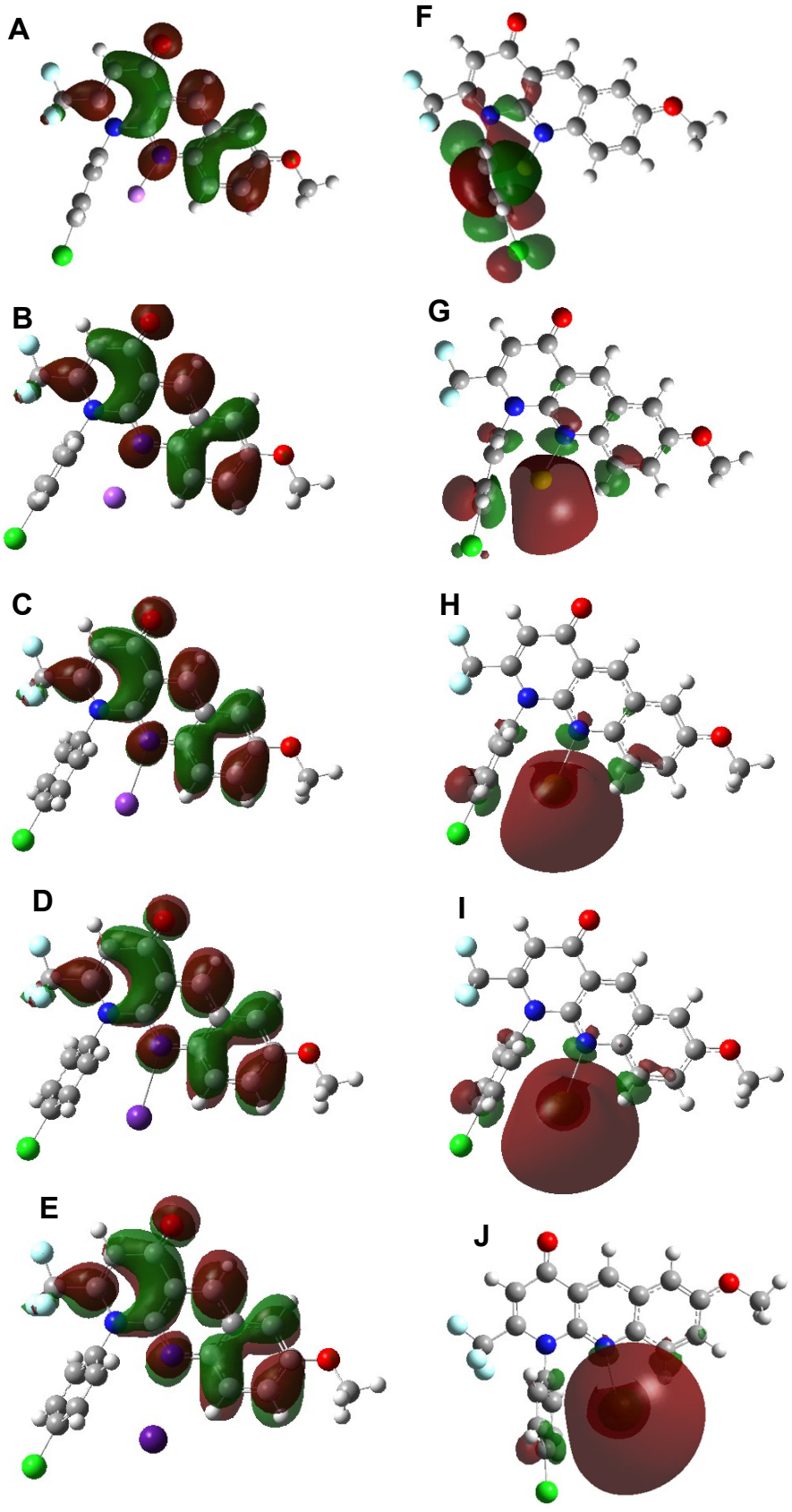
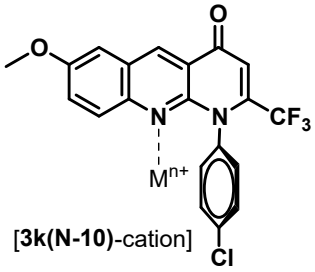


Figure S5. LUMO orbital frontiers for the metal-ligand adduct through nitrogen-10. (A) Li^{+}-**3k**, (B) Na^{+}-**3k**, (C) K^{+}-**3k**, (D) Rb^{+}-**3k**, (E) Cs^{+}-**3k**, (F) Be^{2+}-**3k**, (G) Mg^{2+}-**3k**, (H) Ca^{2+}-**3k**, (I) Sr^{2+}-**3k**, (J) Ba^{2+}-**3k**.

Table S2. Experimental Stern-Volmer constant for **3k** upon transition cation-binding.



[**3k(N-10)**-cation]

Entries	[**3k(N-10)**-M^{n+}]	K_{SV}
1	**3k**-Mn^{2+}	10.29 ±0.04
2	**3k**-Fe^{2+}	16.77 ±0.09
3	**3k**-Co^{2+}	23.11 ±0.14
4	**3k**-Ni^{2+}	14.98 ± 0.08
5	**3k**-Cu^{2+}	39.02 ± 0.21
6	**3k**-Zn^{2+}	1.81±0.03

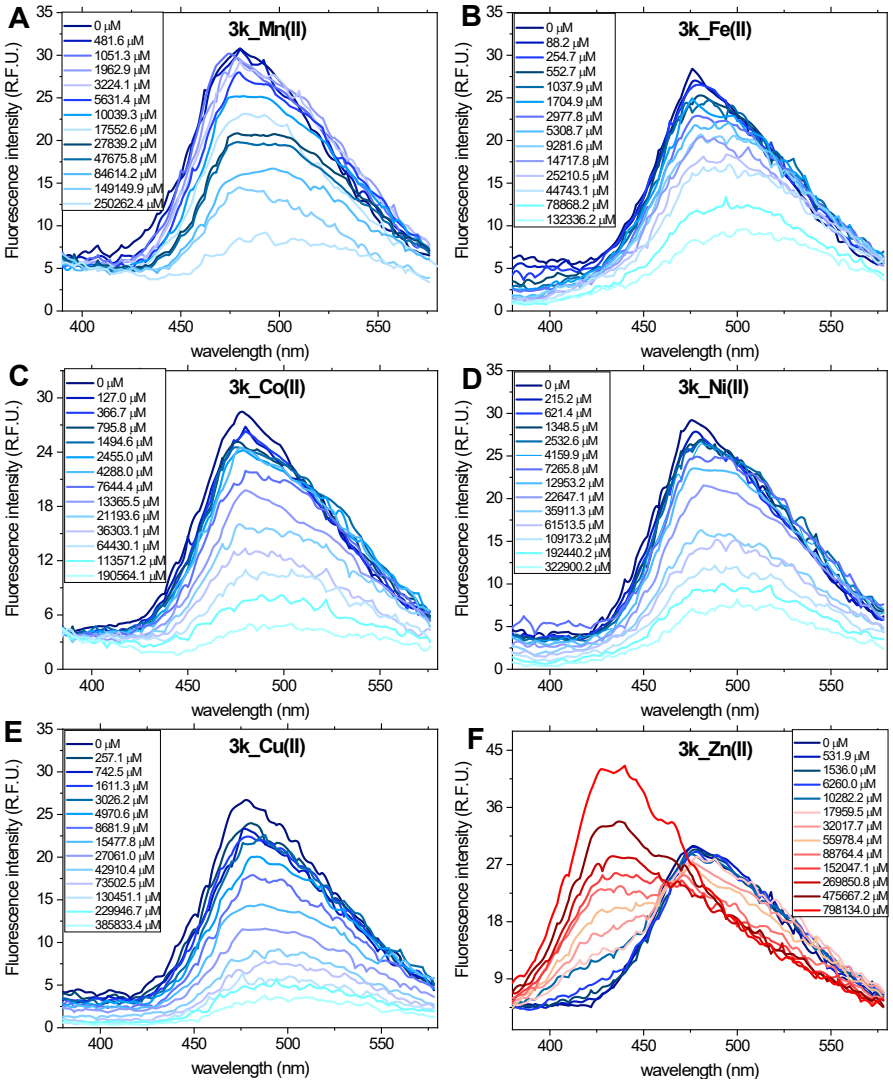


Figure S6. Titration of probe 3k (10 μM) upon 360 nm excitation under different first row transition metal cations in ethanol/water solution (8/2): (A) Mn^{2+}; (B) Fe^{2+}; (C) Co^{2+}; (D) Ni^{2+}; (E) Cu^{2+} and (F) Zn^{2+}.

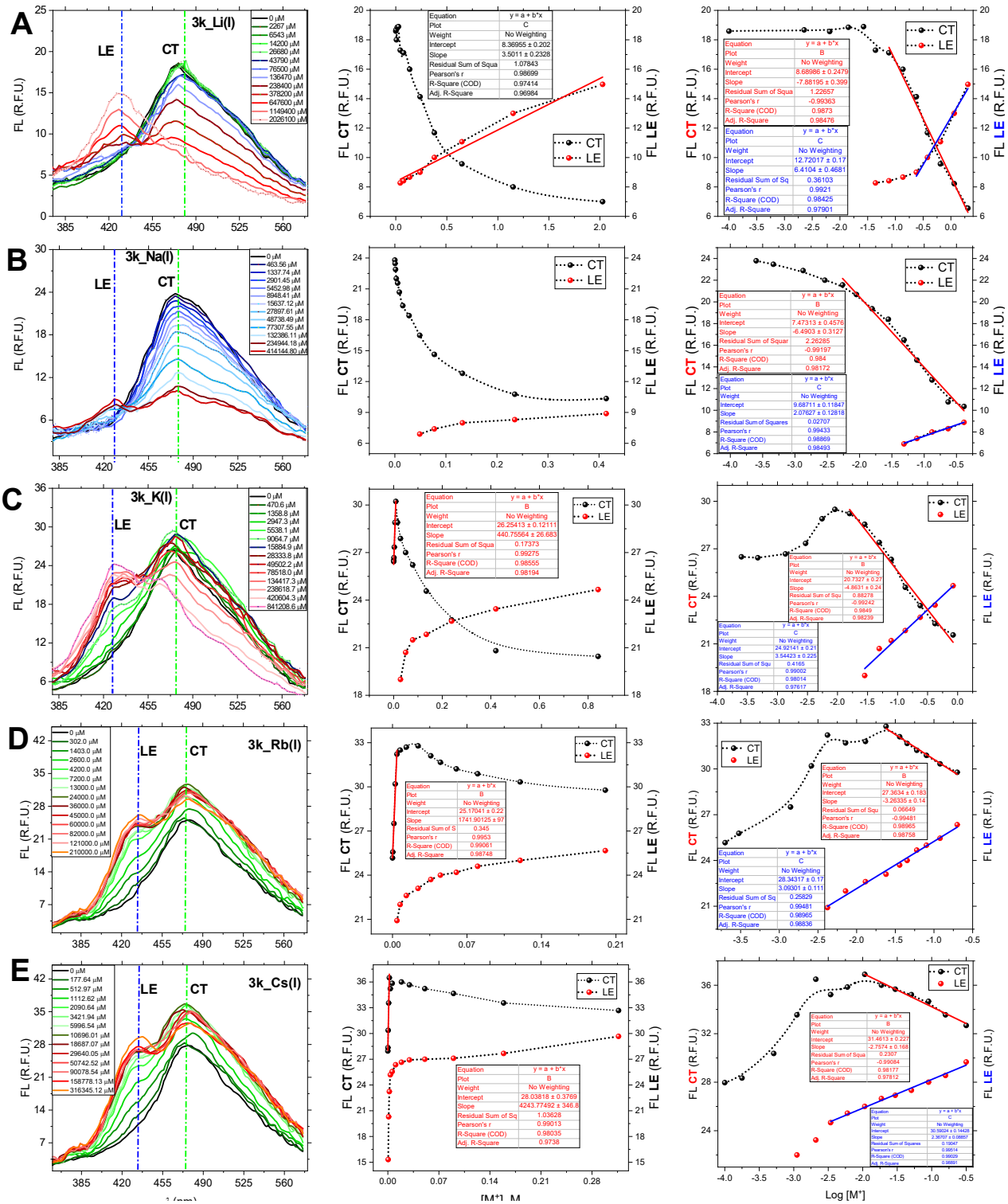


Figure S7. Emission spectra (left side) of the 7-methoxy probe **3k** (c ~8 μM) in presence of the alkali cations (**A:** Li^+, **B:** Na^+, **C:** K^+, **D:** Rb^+ and **E:** Cs^+). LE- (blue vertical line) and CT-states (green vertical line) are placed at 432 and 476 nm, respectively. FL_{max} vs. $[M^+]$ and FL_{max} vs. Log $[M^+]$ plots area placed at central and right side, respectively. Black and red curves are corresponded to CT- and LE-states, respectively.

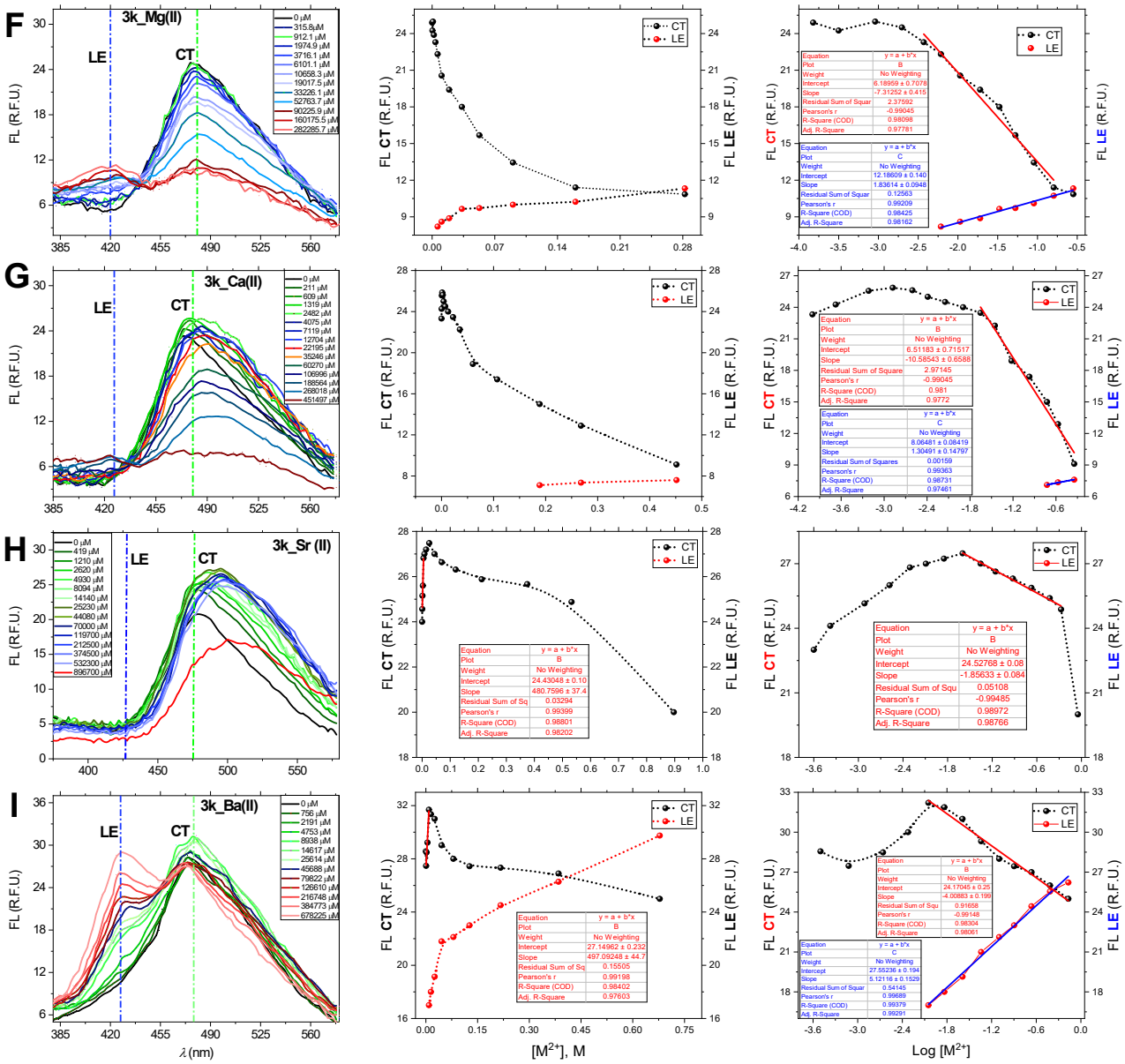


Figure S8. Emission spectra (left side) of the 7-methoxy probe **3k** (c ~ 8 μM) in presence of the alkaline-earth cations (**F:** Mg^{2+}, **G:** Ca^{2+}, **H:** Sr^{2+} and **I:** Ba^{2+}). LE- (blue vertical line) and CT-states (green vertical line) are placed at 432 and 476 nm, respectively. FL_{max} vs. $[M^+]$ and FL_{max} vs. Log $[M^+]$ plots are placed at central and right side, respectively. Black and red curves are corresponded to CT- and LE-states, respectively.

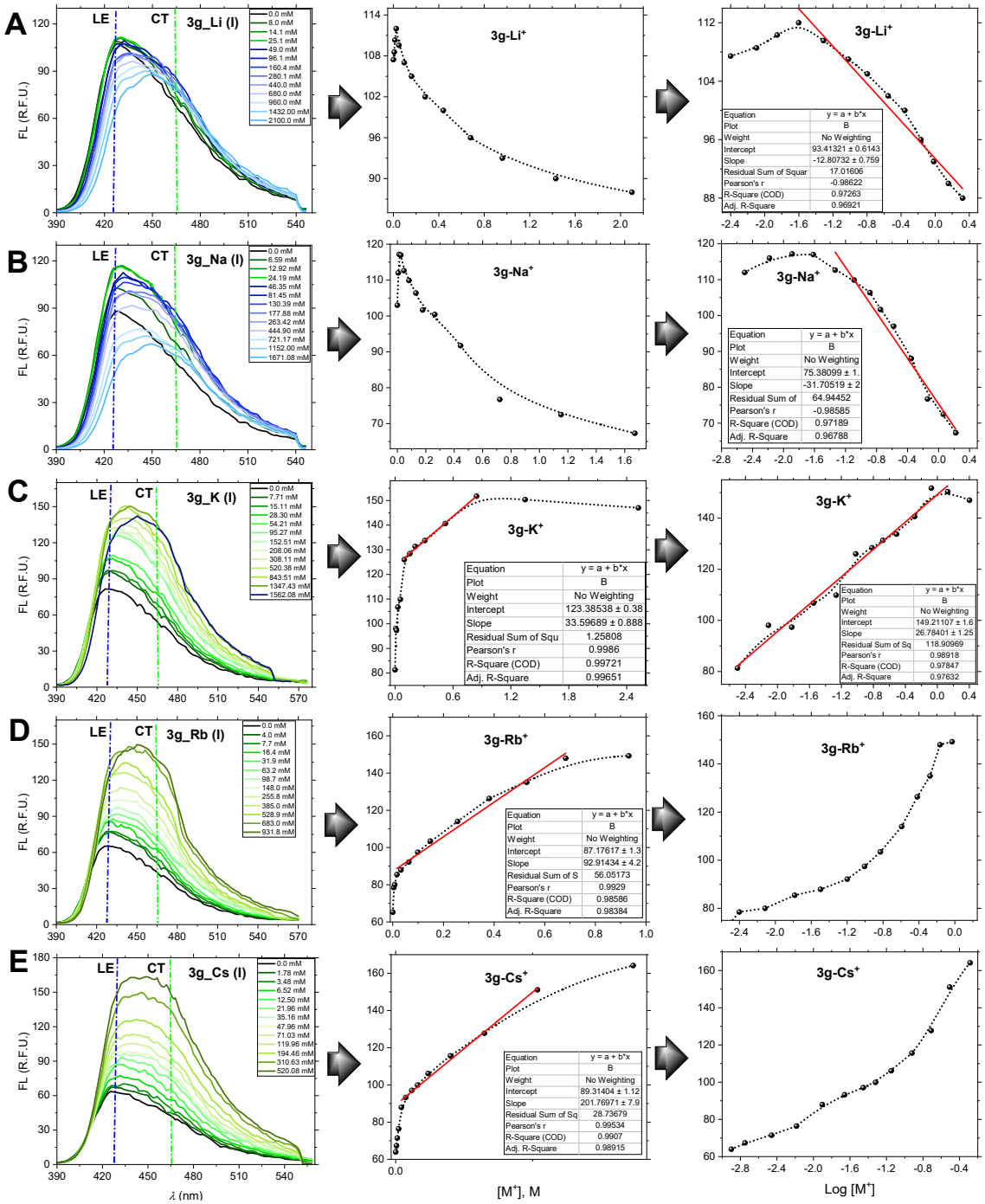


Figure S9. Effect of the alkali cations (**A:** Li^+, **B:** Na^+, **C:** K^+, **D:** Rb^+ and **E:** Cs^+) on the emission spectrum of the 7-methoxy probe **3k** (c = 50 μM). LE- (blue vertical line) and CT-states (green vertical line) are placed at 432 and 476 nm, respectively. Second and third row show FL_{max} vs. [M^+] and FL_{max} vs. Log [M^+] plots, respectively.

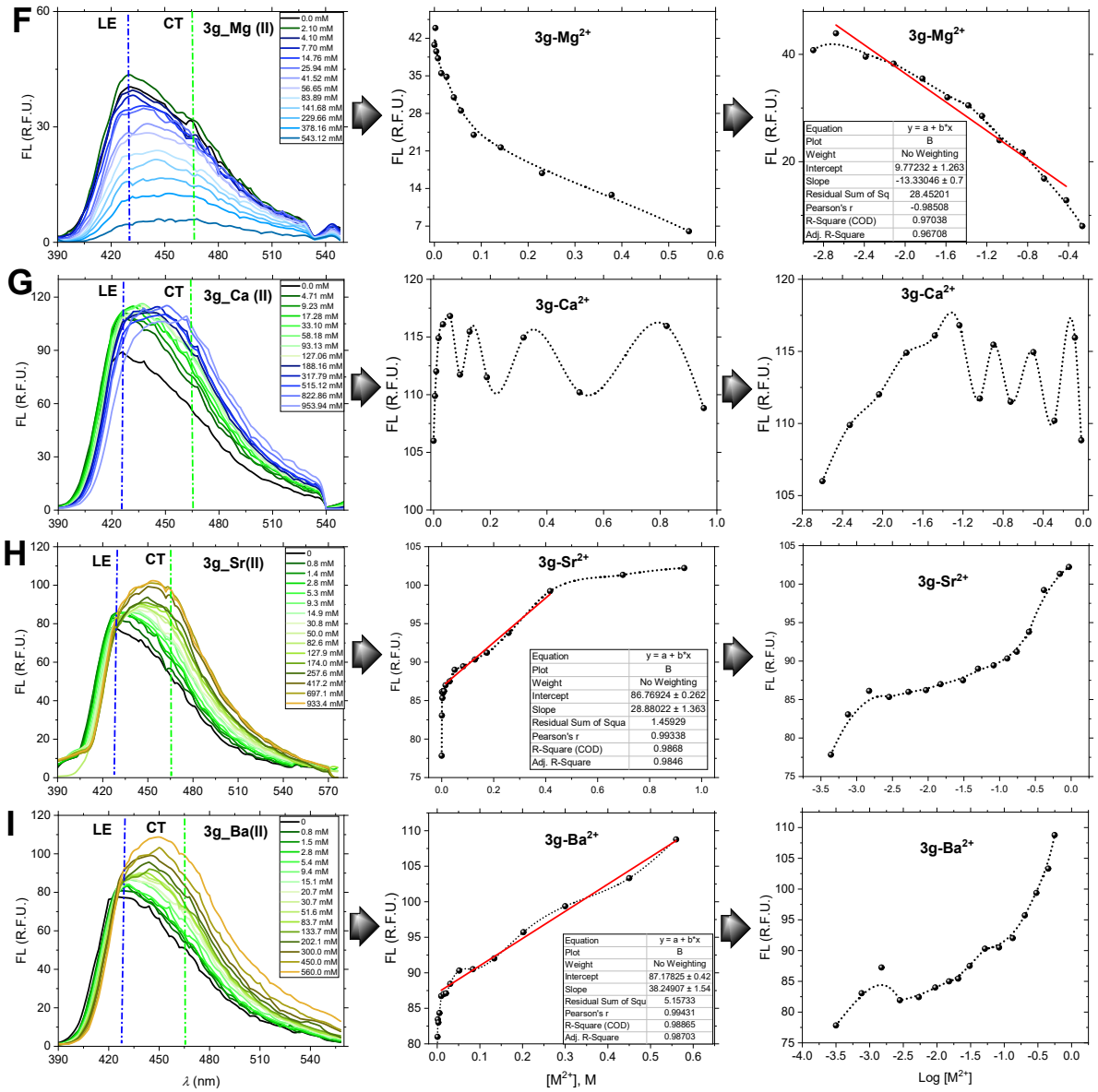


Figure S10. Effect of the alkaline-earth cations (**F:** Mg^{2+}, **G:** Ca^{2+}, **H:** Sr^{2+} and **I:** Ba^{2+}) on the emission spectrum of the 7-methoxy probe **3k** (c = 50 μM). LE- (blue vertical line) and CT-states (green vertical line) are placed at 432 and 476 nm, respectively. Second and third row show FL_{max} vs. $[M^+]$ and FL_{max} vs. Log $[M^+]$ plots, respectively.

Table S3. Relative slopes of the **3k**-cation complexation derived from the FL vs. [cation] or FL vs. Log [cation] plots.

Cation	FL *vs.* [cation]	FL *vs.* Log [cation]	
	Slope CT-enhancement (R^2)-ionic ketonic binding	**Slope CT-decay (R^2)-methoxy or N-10 binding**	**Slope LE-enhancement (R^2)-methoxy binding**	**Δs[a] N-10**
Li^+	~ 0	-7.88±0.40 (0.9873) (A.R)	6.41±0.47 (0.9843)	1.88
Na^+	~ 0	-6.49±0.31 (0.9840) (A.R.)	2.08±0.13 (0.9887) (0.07-0.4)	6.41
K^+	440.76±26.68 (0.9856) (0-0.009)	-4.86±0.24 (0.9849) (0.009-0.8)	3.54±0.23 (0.9801) (0.009-0.8)	1.32
Rb^+	1741.90±97.01(0.9906) (0-0.004)	-3.26±0.14 (0.9897) (0.024-0.2)	3.09±0.11 (0.9897) (0.07-0.2)	0.17
Cs^+	4243.77±346.8(0.9804) (0-0.002)	-2.76±0.17 (0.9818) (0.002-0.3)	2.37±0.09 (0.9903) (0.002-0.3)	0.39
Mg^{2+}	~ 0	-7.31±0.42 (0.9810) (A.R)	1.84±0.09 (0.9843) (0.019-0.28)	4.47
Ca^{2+}	1830. (0-0.001)	-10.59±0.66(0.9810) (0.001-0.4)	1.30±0.14 (0.9873) (0.10-0.45)	9.29
Sr^{2+}	480.76±37.40 (0.9880) (0-0.008)	-1.86±0.08 (0.9897) (0.025-0.9)	~ 0	1.86
Ba^{2+}	497.09±44.7 (0.9840) (0-0.009)	-4.01±0.20 (0.9830) (0.009-0.7)	5.12±0.15 (0.9938) (0.014-0.7)	-1.11

[a]**Δs:** difference between the absolute magnitudes of the slope of the CT-decay with the slope of the LE-enhancement.

[b]Concentration range for Li^+ (0.14-2.0 M). 3.50±0.23(0.9741)[b] A.R.: all concentration range.

Table S4. Relative slopes of the metal-dye complexation derived from the FL vs. [cation] or FL vs. Log [cation] plots for **3g**.

Entries	**Cation**	**Slope FL *vs.* [cation]**	**Slope FL *vs.* Log [cation]**
1	Li^+	~ 0 (slow exp. decay)	-12.81±0.76 (0.9726)
2	Na^+	~ 0 (exp. decay)	-31.71±2.00 (0.9718)
3	K^+	33.60±0.89 (0.9972)	26.78±1.25 (0.9785)
4	Rb^+	92.91±4.20(0.9859)	exp. Enhancement
5	Cs^+	201.77±7.90(0.9907)	exp. Enhancement
6	Mg^{2+}	~ 0 (exp. decay)	-13.33±0.70 (0.9704)
7	Ca^{2+}	Sinosoide	Sinosoide
8	Sr^{2+}	28.88±1.36 (0.9868)	exp. Enhancement
9	Ba^{2+}	38.25±1.54 (0.9887)	exp. Enhancement

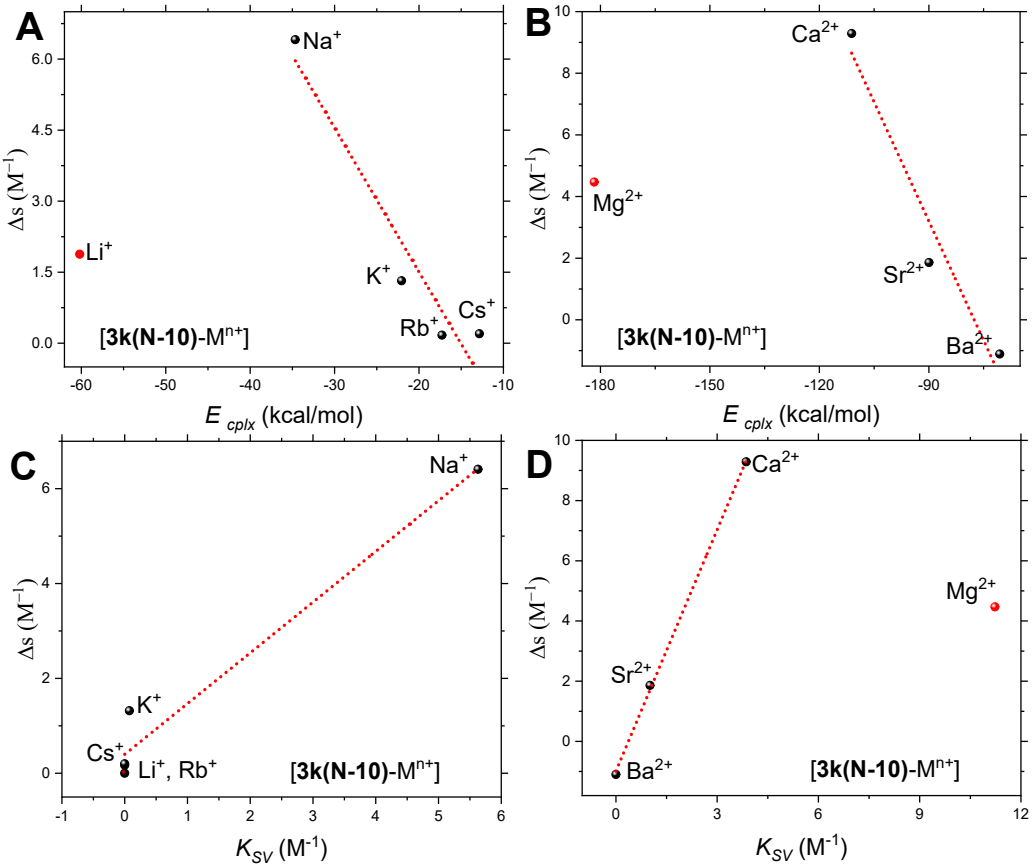
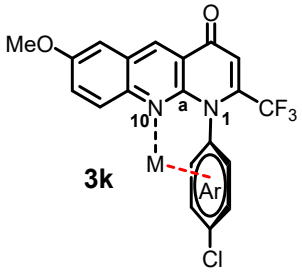


Figure S11. Correlation of slope difference (Δs) *vs.* free complexation energy, E_{cplx}, for alkali (**A**) and alkaline earth (**B**) cations, and slope difference (Δs) *vs.* Stern-Volmer constant for alkali (**C**) and alkaline earth (**D**) cations.

Table S5. Binding affinities, structural parameters derived from [**3k(N-10)**-M^{n+}] adduct.



Entries	Cation	E_{cplx} (kcal/mol)[a]	$d_{M\text{-}N10}$[b]	$d_{M\text{-}Ar}$[c]	$d_{M\text{-}N10\text{-}Ca}$[d]	$d_{M\text{-}N10\text{-}C\text{-}N1}$[e]
1	Li^+	-60.19	1.9801	2.2701	120.3879	-0.0026
2	Na^+	-34.65	2.4166	2.8361	128.3516	6.1424
3	K^+	-22.06	2.8072	3.1703	129.4703	31.3517
4	Rb^+	-17.27	3.049	3.3787	128.5918	41.0289
5	Cs^+	-12.84	3.3402	3.6298	127.3026	49.4469
6	Be^{2+}	-337.14	1.6143	1.8856	112.7465	-0.0037
7	Mg^{2+}	-181.69	2.0183	2.4747	122.7987	0.0042
8	Ca^{2+}	-111.16	2.3801	2.8816	130.321	11.2776
9	Sr^{2+}	-89.97	2.5414	3.0533	131.6779	20.8143
10	Ba^{2+}	-70.57	2.7437	3.2545	131.8667	30.284

[a]Complexation energy calculated by using CP model; [b]M-N binding distance expressed in Å; [c]M-arene distance expressed in Å; [d]M-N_{10}-C_a bond angle; [e]M-N_{10}-C_a-N_1 dihedral angle.

2. Theoretical di-nuclear and tri-nuclear 3k-metal adducts

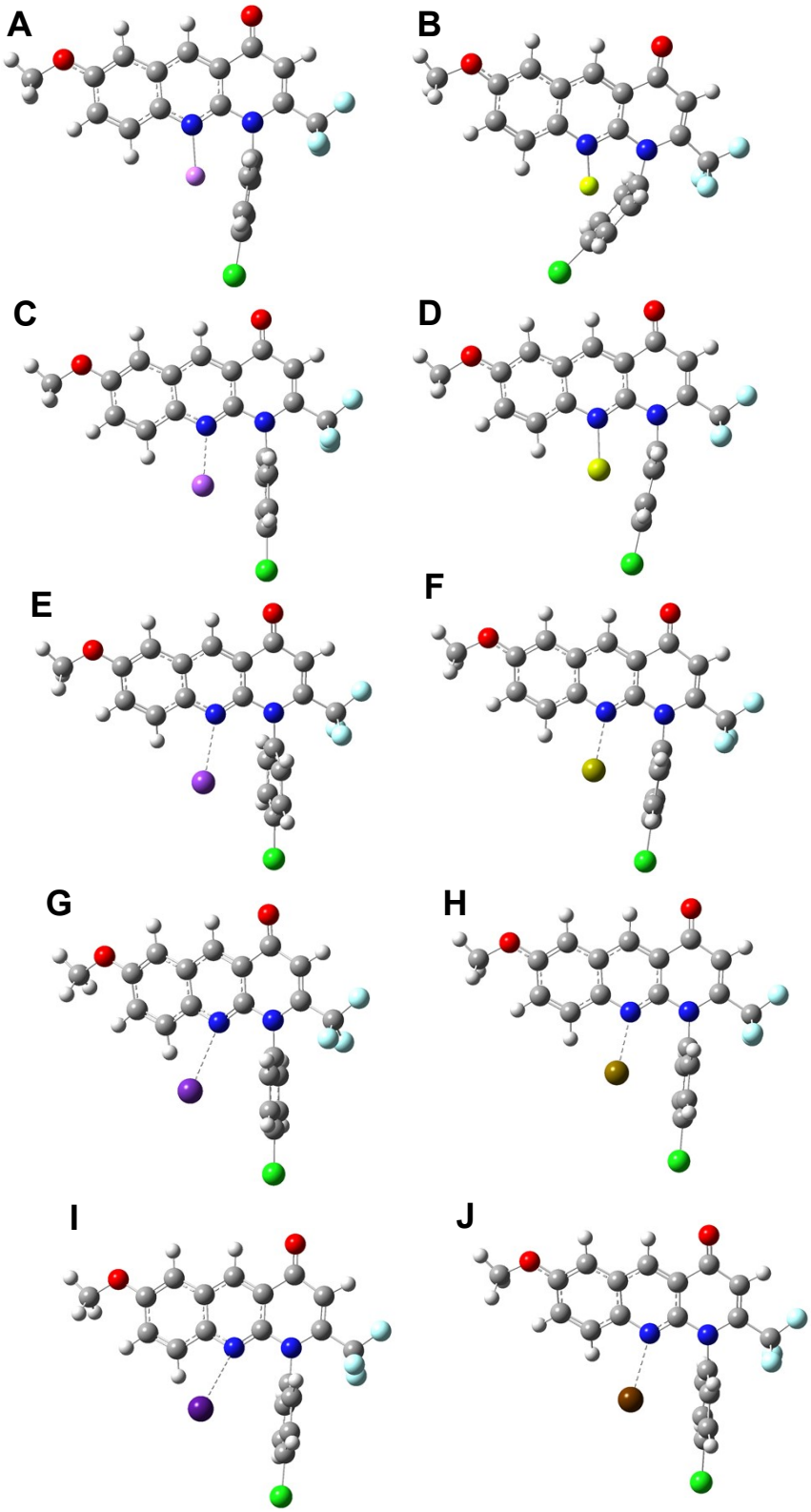


Figure S12. Binding preference of the ambidentate ligand **3k** with one molecule of Li^{+} (**A**), Be^{2+} (**B**), Na^{+} (**C**), Mg^{2+} (**D**), K^{+} (**E**), Ca^{2+} (**F**), Rb^{+} (**G**), Sr^{2+} (**H**), Cs^{+} (**I**) and Ba^{2+} (**J**) upon counter-poise (CP) model.

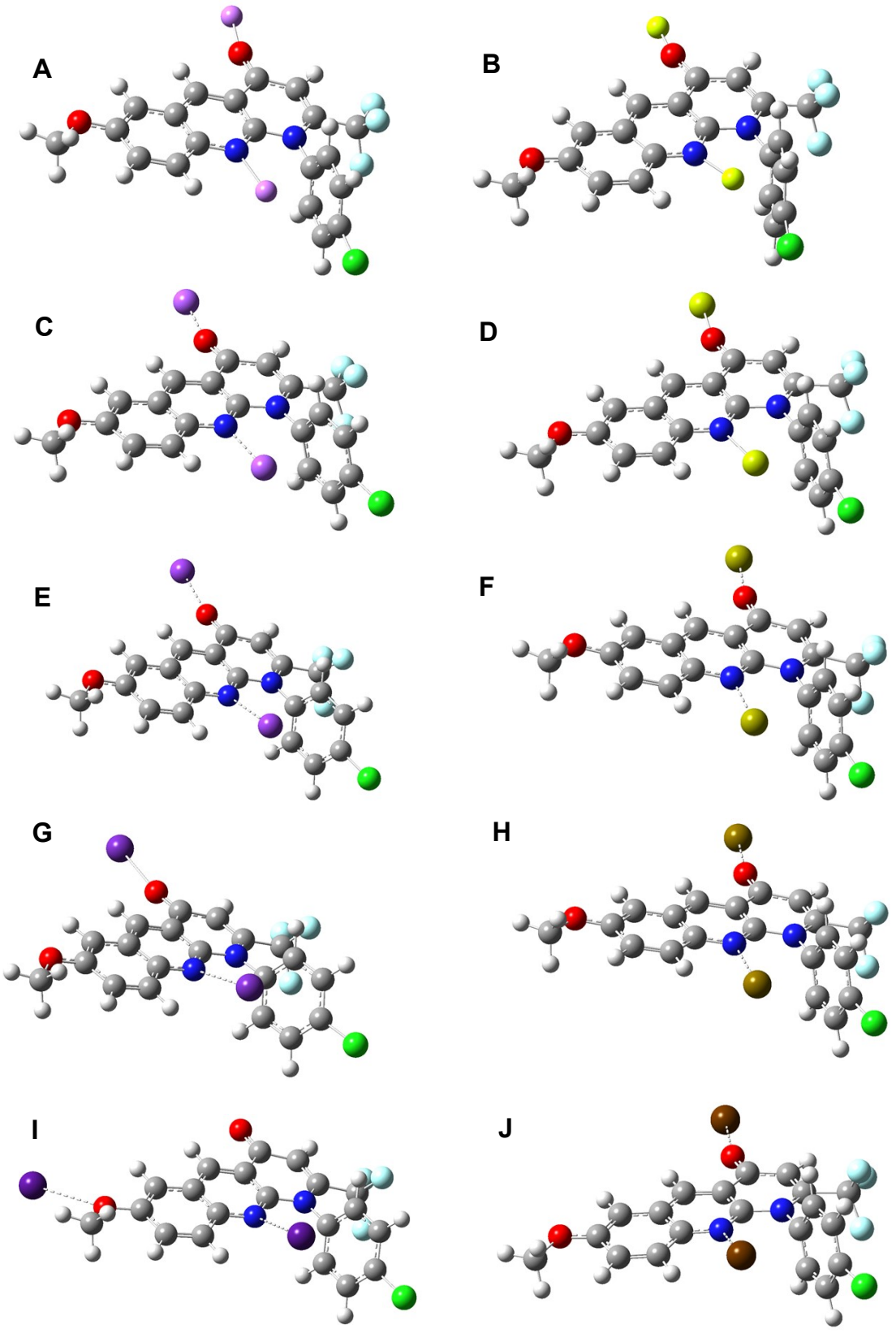


Figure S13. Binding preference of the ambidentate ligand **3k** with two molecule of Li^{+} (**A**), Be^{2+} (**B**), Na^{+} (**C**), Mg^{2+} (**D**), K^{+} (**E**), Ca^{2+} (**F**), Rb^{+} (**G**), Sr^{2+} (**H**), Cs^{+} (**I**) and Ba^{2+} (**J**) upon counter-poise (CP) model.

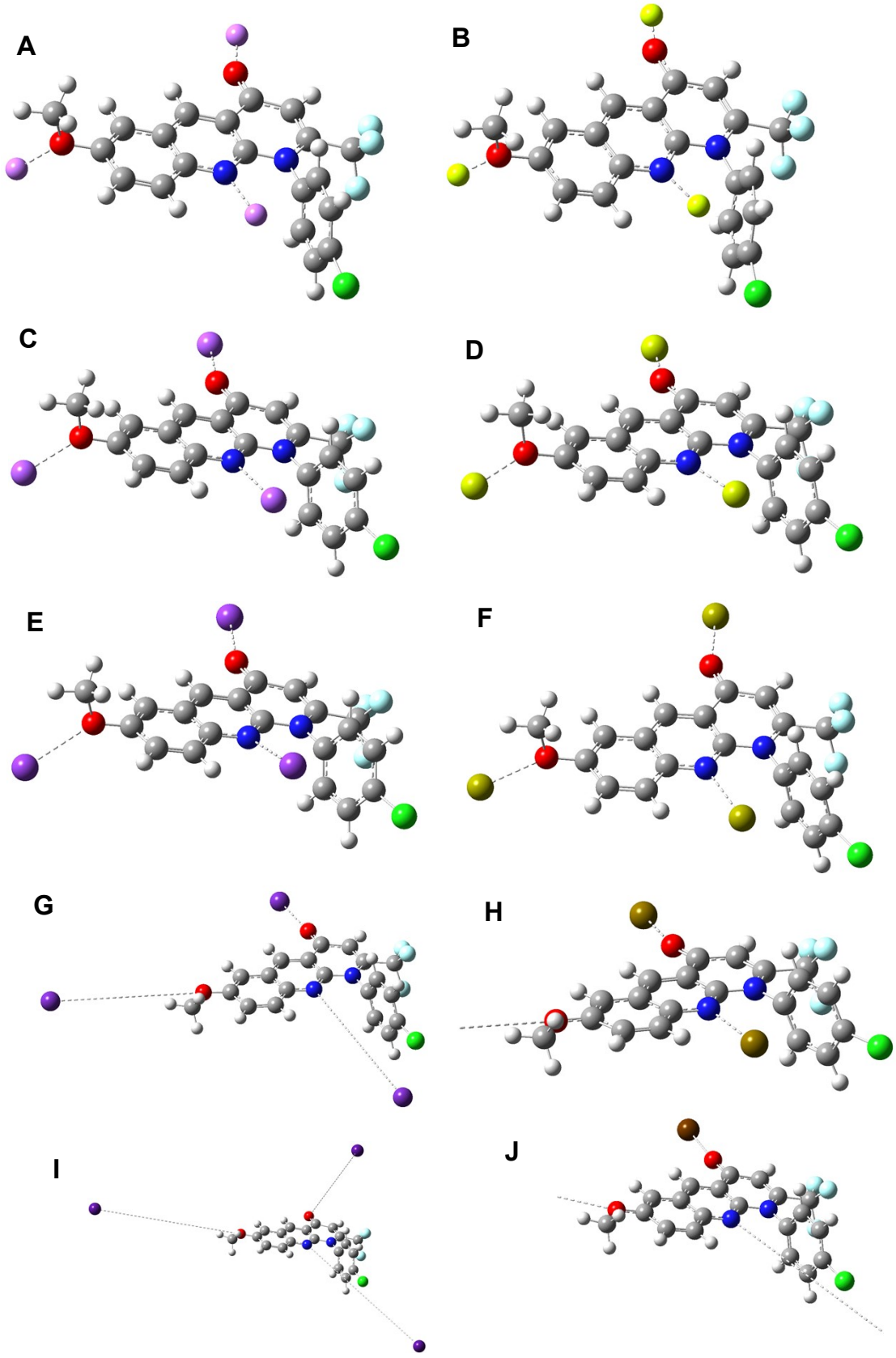


Figure S14. Binding preference of the ambidentate ligand **3k** with three molecule of Li^{+} (**A**), Be^{2+} (**B**), Na^{+} (**C**), Mg^{2+} (**D**), K^{+} (**E**), Ca^{2+} (**F**), Rb^{+} (**G**), Sr^{2+} (**H**), Cs^{+} (**I**) and Ba^{2+} (**J**) upon counter-poise (CP) model.

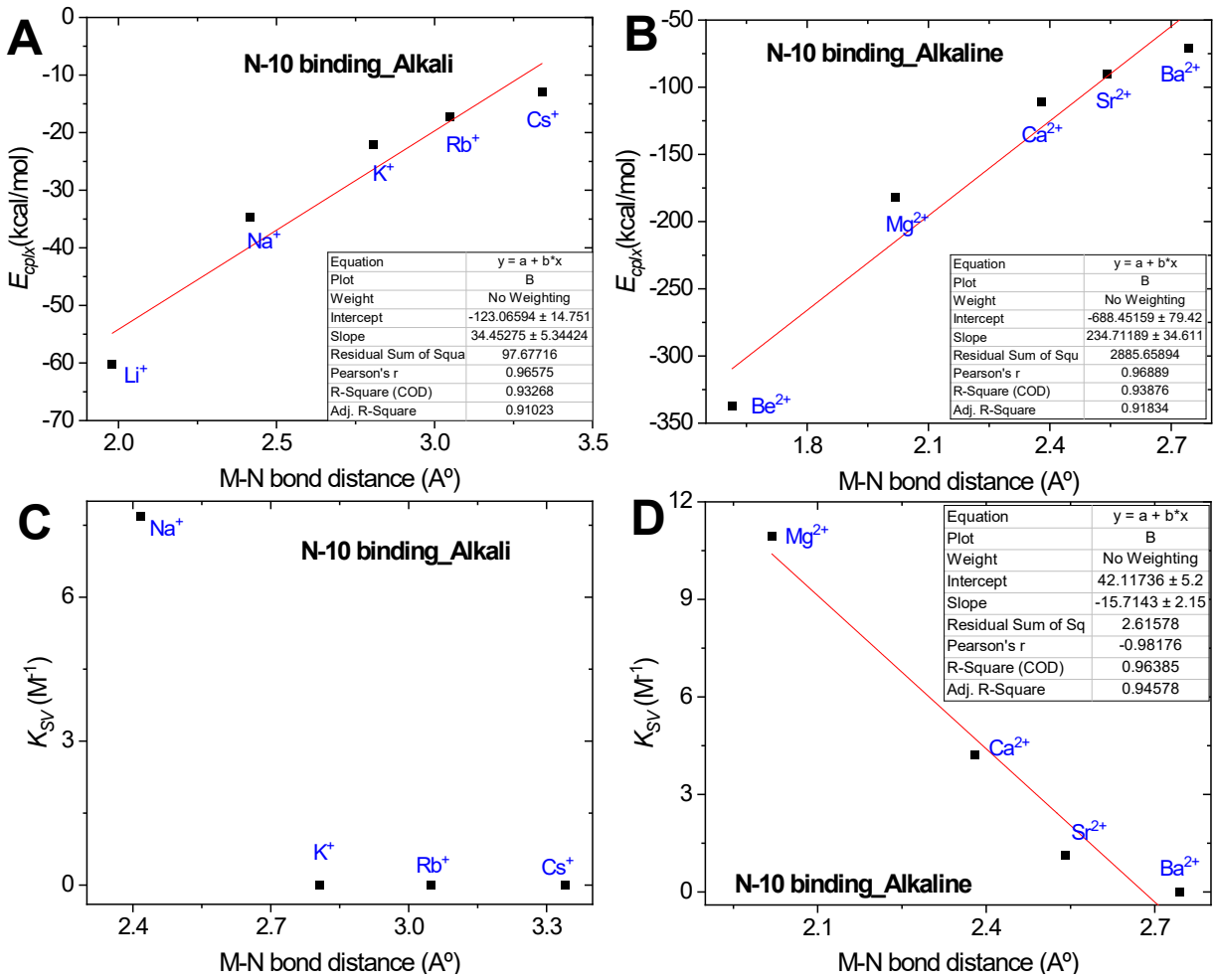


Figure S15. Correlation of the complexation energy (**A-B**) cations and with Stern-Volmer constant (**C-D**) as function of the M-N bond distance.

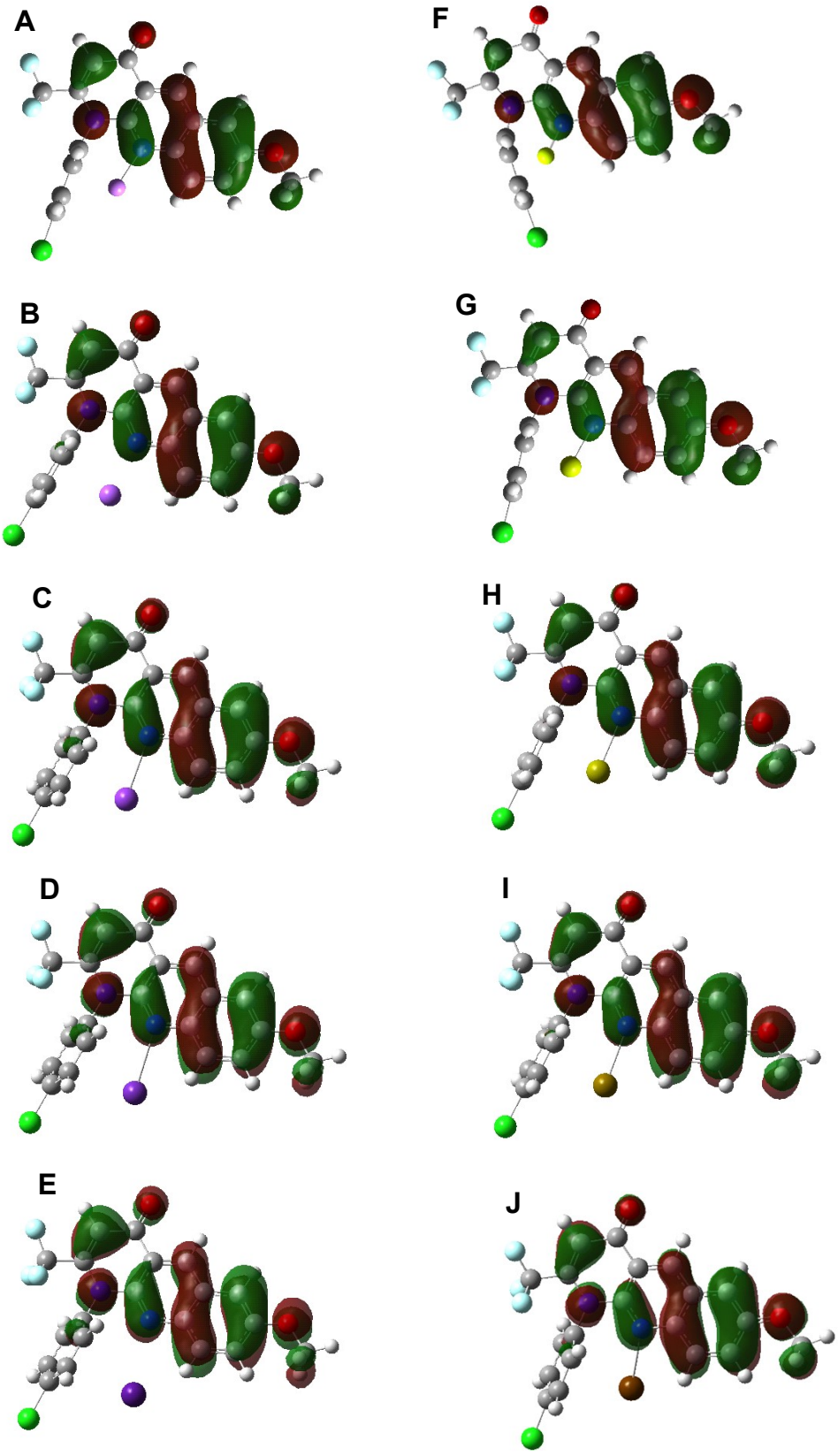


Figure S16. HOMO orbital frontiers for the metal-ligand adduct through nitrogen-10. (A) Li^{+}-**3k**, (B) Na^{+}-**3k**, (C) K^{+}-**3k**, (D) Rb^{+}-**3k**, (E) Cs^{+}-**3k**, (F) Be^{2+}-**3k**, (G) Mg^{2+}-**3k**, (H) Ca^{2+}-**3k**, (I) Sr^{2+}-**3k**, (J) Ba^{2+}-**3k**.

Table S6. Binding affinities, structural parameters and HOMO-LUMO levels derived from the dinuclear interaction of ambidentate ligand **3k** with the indicated cation.

Metal	E_{cplx} (kcal/mol)[a]	$d_{M\text{-}N10}$[b]	$d_{M\text{-}Ar}$[b]	$d_{M\text{-}N10\text{-}Ca}$[d]	$d_{M\text{-}N10\text{-}C\text{-}N1}$[e]	$d_{M\text{-}O}$[f]	$d_{M\text{-}C\text{-}O}$[g]	$d_{M\text{-}C\text{-}C\text{-}O}$[h]
Li^+	-70.07	1.98	2.27	120.388	-0.0026	1.7561	162.554	-0.0501
Na^+	-29.83	2.417	2.836	128.352	6.1424	2.1889	160.3707	0.0493
K^+	-10.45	2.807	3.17	129.47	31.3517	2.5739	162.5025	3.7023
Rb^+	-3.62	3.049	3.379	128.592	41.0289	2.7961	161.8200	6.3506
Cs^+	16.07	3.34	3.63	127.303	49.4469	3.4586	129.3247	29.2392
Be^{2+}	-386.5	1.614	1.886	112.747	-0.0037	1.4121	163.9042	-0.0905
Mg^{2+}	-140.39	2.018	2.475	122.799	0.0042	1.8395	159.3862	-0.9094
Ca^{2+}	-38	2.38	2.882	130.321	11.2776	2.2249	162.4731	-0.0139
Sr^{2+}	-8.65	2.541	3.053	131.678	20.8143	2.4036	162.2132	0.0072
Ba^{2+}	16.17	2.744	3.255	131.867	30.284	2.6182	161.8687	3.4319

[a]Complexation energy calculated by using CP model; [b]M-N binding distance against N-10 (expressed in Å); [c]M-arene distance expressed in Å; [d]M-N_{10}-C_a bond angle; [e]M-N_{10}-C_a-N_1 dihedral angle; [f]M-O binding distance against oxygen ketonic (expressed in Å); [g]M-C-O bond angle for ketonic moiety; [h]M-C-C-O dihedral angle for ketonic moiety.

Table S7. Binding affinities, structural parameters and HOMO-LUMO levels derived from the trinuclear interaction of ambidentate ligand **3k** with the indicated cation.

Metal	E_{cplx} (kcal/mol)[a]	$d_{M\text{-}N10}$[b]	$d_{M\text{-}Ar}$[b]	$d_{M\text{-}N10\text{-}Ca}$[d]	$d_{M\text{-}N10\text{-}C\text{-}N1}$[e]	$d_{M\text{-}O}$[f]	$d_{M\text{-}C\text{-}O}$[g]	$d_{M\text{-}C\text{-}C\text{-}O}$[h]	$d_{M\text{-}N10}$[i]	$d_{M\text{-}C\text{-}O}$[j]
Li^+	-17.98	2.0772	2.3855	118.2828	0.3141	1.7987	153.52	-1.4132	1.8843	129.581
Na^+	29.28	2.5624	2.8208	125.7543	4.0304	2.2437	150.589	-2.5415	2.3555	132.696
K^+	50.24	3.1379	3.1998	128.6861	19.4646	2.6588	151.482	-4.8346	2.8741	136.641
Rb^+	38.21	> 9 Å				2.7712			> 7 Å	
Cs^+	36.2	> 12 Å				> 9 Å			> 12 Å	
Be^{2+}	-202.44	1.7448	1.9731	110.78	0.0301	1.4516	153.146	-0.2048	1.525	133.899
Mg^{2+}	99.02	2.206	2.4125	117.1357	0.358	1.9063	149.018	-0.6995	2.0053	139.772
Ca^{2+}	211.04	2.6871	2.8361	122.8807	2.4881	2.3312	150.423	-1.7397	2.5817	146.008
Sr^{2+}	18.14	2.6928	3.1056	130.717	-5.2090	2.4024	161.913	-1.3283	>>20 Å	
Ba^{2+}	-58.92	>>20 Å				2.4378	170.095	1.7863	>>20 Å	

[a]Complexation energy calculated by using CP model; [b]M-N binding distance against N-10 (expressed in Å); [c]M-arene distance expressed in Å; [d]M-N_{10}-C_a bond angle; [e]M-N_{10}-C_a-N_1 dihedral angle; [f]M-O binding distance against oxygen ketonic (expressed in Å); [g]M-C-O bond angle for ketonic moiety; [h]M-C-C-O dihedral angle for ketonic moiety; [i]M-O binding distance against methoxy (expressed in Å); [j]M-C-O bond angle for methoxy moiety.

3. References

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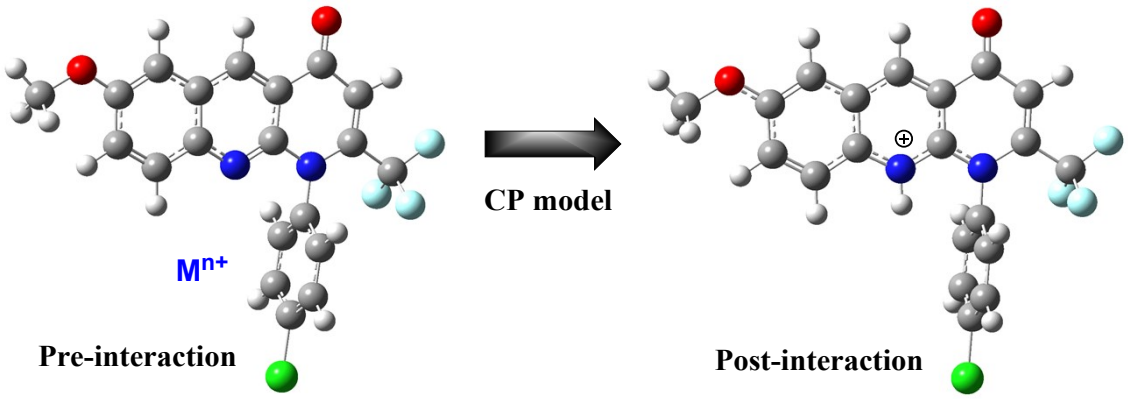
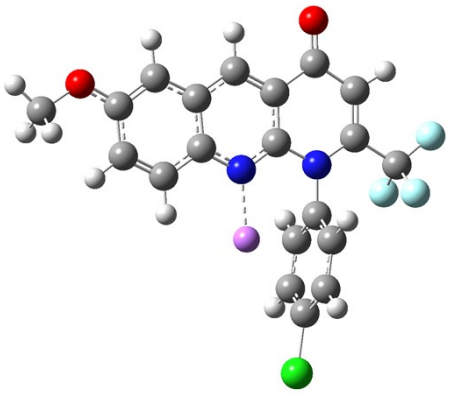
5. Output of Theoretical Calculations for Interacting Model

a. Interaction with a metal ion molecule



i. Ligand 3k-Li



Cartesian coordinates of optimized structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.276519	1.699764	-0.000211
2	6	0	2.906039	1.624293	-0.000140
3	6	0	2.243057	0.381448	-0.000043
4	6	0	3.036096	-0.797954	0.000014
5	6	0	4.440560	-0.707955	-0.000067
6	6	0	5.065156	0.521290	-0.000191
7	6	0	2.350505	-2.030018	0.000184
8	6	0	0.979935	-2.069190	0.000239
9	6	0	0.270335	-0.838925	0.000108
10	6	0	-1.805394	-2.085136	0.000051
11	6	0	-1.184783	-3.274672	0.000205
12	6	0	0.273105	-3.373825	0.000449
13	1	0	2.328713	2.546425	-0.000140

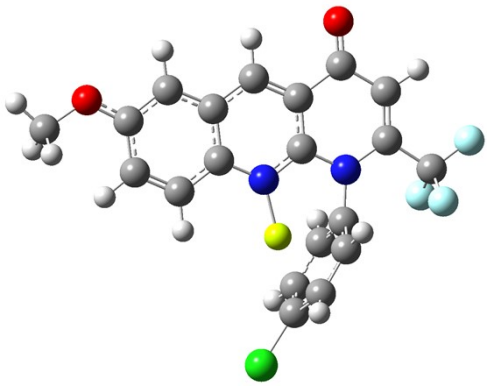
14	1	0	5.046540	-1.606932	-0.000026
15	1	0	2.885208	-2.975569	0.000294
16	1	0	-1.759336	-4.190429	0.000131
17	6	0	-1.798508	0.401327	0.000144
18	6	0	-2.053244	1.050934	1.209512
19	6	0	-2.053674	1.050806	-1.209210
20	6	0	-2.531905	2.359764	1.213261
21	1	0	-1.856365	0.537577	2.144083
22	6	0	-2.532340	2.359635	-1.212929
23	1	0	-1.857146	0.537325	-2.143784
24	6	0	-2.766309	3.013619	0.000173
25	1	0	-2.729444	2.871019	2.148526
26	1	0	-2.730212	2.870789	-2.148179
27	6	0	-3.317066	-2.015553	-0.000333
28	7	0	-1.127551	-0.864384	0.000099
29	9	0	-3.854394	-3.227328	-0.000241
30	9	0	-3.763498	-1.357370	1.082373
31	9	0	-3.762878	-1.357807	-1.083603
32	7	0	0.871141	0.342024	-0.000006
33	8	0	0.874668	-4.431308	0.000754
34	1	0	4.752619	2.672084	-0.000270
35	6	0	7.110934	1.753029	-0.000202
36	1	0	6.886452	2.341083	-0.896449
37	1	0	6.886300	2.341097	0.895997
38	1	0	8.167789	1.492305	-0.000111
39	8	0	6.408847	0.519639	-0.000249
40	17	0	-3.348849	4.637166	0.000187
41	3	0	-0.197041	2.009247	-0.000259

Rotational constants (GHZ): 0.2058485 0.1101392 0.0746133

Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RCAM-B3LYP) = -1788.43364730 A.U. after 8 cycles
NFock= 8 Conv=0.74D-08 -V/T= 2.0049

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.018313722 RMS 0.005039795
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot= 338287 Len1MO= 874561 IndFrg= 4711092
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 338287 Len1MO= 874561 IndFrg= 1212848
Counterpoise corrected energy = -1795.793861102566
BSSE energy = 0.004842665874
sum of monomers = -1795.697939581149
complexation energy = -63.23 kcal/mole (raw)
complexation energy = -60.19 kcal/mole (corrected)

ii. 3k-Be



Cartesian coordinates of optimized structure

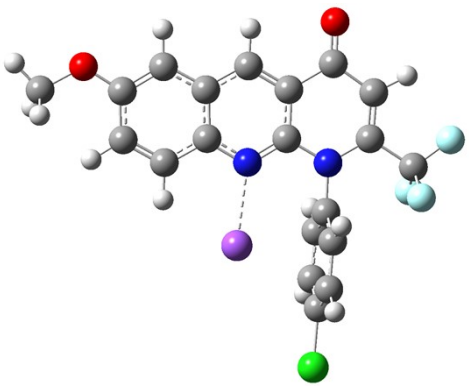
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.263150	0.730014	0.000169
2	6	0	2.905362	0.966679	0.000051
3	6	0	2.001064	-0.097082	-0.000035
4	6	0	2.497928	-1.430438	-0.000034
5	6	0	3.882777	-1.656652	0.000086
6	6	0	4.773263	-0.593173	0.000207
7	6	0	1.559964	-2.485708	-0.000201
8	6	0	0.203190	-2.240946	-0.000308
9	6	0	-0.227295	-0.907161	-0.000265
10	6	0	-2.545222	-1.655784	-0.000112
11	6	0	-2.199139	-2.945166	-0.000203
12	6	0	-0.784385	-3.360992	-0.000435
13	1	0	2.547829	1.995660	0.000024
14	1	0	4.274037	-2.667910	0.000088
15	1	0	1.885130	-3.523609	-0.000249
16	1	0	-2.959778	-3.716676	-0.000044
17	6	0	-1.863571	0.776831	-0.000284
18	6	0	-1.732593	1.475923	1.215948
19	6	0	-1.732601	1.476022	-1.216464
20	6	0	-1.311600	2.812820	1.220283
21	1	0	-1.792308	0.924547	2.149819
22	6	0	-1.311632	2.812938	-1.220691
23	1	0	-1.792287	0.924725	-2.150384
24	6	0	-1.078710	3.491513	-0.000176
25	1	0	-1.107709	3.318987	2.159630
26	1	0	-1.107753	3.319177	-2.160003
27	6	0	-3.969466	-1.162815	0.000471
28	7	0	-1.588174	-0.620332	-0.000325
29	9	0	-4.834822	-2.149206	0.000465
30	9	0	-4.169407	-0.382376	1.081483
31	9	0	-4.170146	-0.381696	-1.079876
32	7	0	0.629970	0.142158	-0.000128
33	8	0	-0.427064	-4.515993	-0.000880

34	1	0	4.944518	1.571630	0.000231
35	6	0	7.053913	0.135463	0.000441
36	1	0	6.973992	0.753175	-0.898848
37	1	0	6.973777	0.753186	0.899704
38	1	0	8.012065	-0.379244	0.000558
39	8	0	6.066109	-0.897109	0.000331
40	17	0	-0.498896	5.086726	-0.000098
41	4	0	-0.128055	1.567456	-0.000156

Rotational constants (GHZ): 0.2042204 0.1221620 0.0797168

Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RCAM-B3LYP) = -1788.40873681 A.U. after 8 cycles
NFock= 8 Conv=0.69D-08 -V/T= 2.0050
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.049195176 RMS 0.012097807
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot= 338287 Len1MO= 874567 IndFrg= 4711122
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 338287 Len1MO= 874567 IndFrg= 1212854
Counterpoise corrected energy = -1802.576290266966
BSSE energy = 0.005472839105
sum of monomers = -1802.039018422297
complexation energy = -340.58 kcal/mole (raw)
complexation energy = -337.14 kcal/mole (corrected)

iii. 3k-Na



Cartesian coordinates of optimized structure

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.329692	1.763460	-0.031963
2	6	0	2.961325	1.653329	-0.029774
3	6	0	2.317495	0.397681	-0.003412

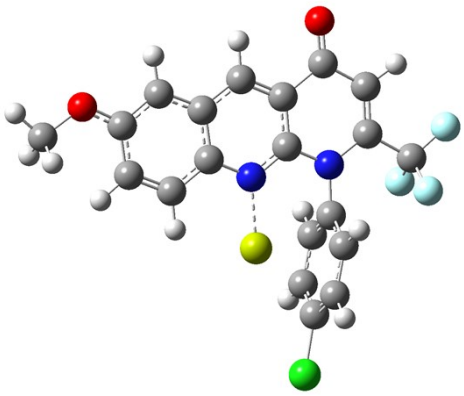
4	6	0	3.146378	-0.757739	0.010904
5	6	0	4.548411	-0.635394	0.010604
6	6	0	5.146348	0.605986	-0.007812
7	6	0	2.495112	-2.007150	0.020322
8	6	0	1.128061	-2.080696	0.012571
9	6	0	0.381038	-0.867726	0.004886
10	6	0	-1.648053	-2.191484	-0.008506
11	6	0	-0.987015	-3.360068	-0.001673
12	6	0	0.469609	-3.409142	0.014788
13	1	0	2.377191	2.570139	-0.067289
14	1	0	5.173375	-1.521307	0.022720
15	1	0	3.053548	-2.938671	0.030311
16	1	0	-1.529358	-4.294744	-0.010276
17	6	0	-1.770397	0.277667	-0.007831
18	6	0	-2.195775	0.841545	1.193673
19	6	0	-2.048243	0.915453	-1.216070
20	6	0	-2.880107	2.055026	1.193640
21	1	0	-1.999143	0.325610	2.126947
22	6	0	-2.729121	2.129013	-1.225946
23	1	0	-1.733532	0.457321	-2.147227
24	6	0	-3.141114	2.696195	-0.018244
25	1	0	-3.229849	2.491567	2.122356
26	1	0	-2.961799	2.624086	-2.161896
27	6	0	-3.164388	-2.202357	-0.026757
28	7	0	-1.017888	-0.944058	0.000045
29	9	0	-3.631870	-3.443907	-0.072229
30	9	0	-3.664599	-1.613634	1.072121
31	9	0	-3.639497	-1.541584	-1.093920
32	7	0	0.947696	0.326377	0.004641
33	8	0	1.109057	-4.445121	0.027255
34	1	0	4.781441	2.747071	-0.056736
35	6	0	7.161882	1.885027	-0.029852
36	1	0	6.925977	2.449071	-0.938730
37	1	0	6.920371	2.486632	0.853121
38	1	0	8.225056	1.651268	-0.021658
39	8	0	6.490823	0.635707	-0.005738
40	17	0	-3.986880	4.206451	-0.025092
41	11	0	-0.112469	2.489249	0.199541

Rotational constants (GHZ): 0.2047844 0.1045882 0.0719047

Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RCAM-B3LYP) = -1788.43444520 A.U. after 8 cycles
NFock= 8 Conv=0.64D-08 -V/T= 2.0049
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.013079569 RMS 0.004089751
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot= 336893 Len1MO=

870766 IndFrg= 4690723
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 336893 Len1MO=
870766 IndFrg= 1207659
Counterpoise corrected energy = -1788.489659924476
BSSE energy = 0.004315386986
sum of monomers = -1788.434445197841
complexation energy = -37.36 kcal/mole (raw)
complexation energy = -34.65 kcal/mole (corrected)

iv. 3k-Mg



Cartesian coordinates of optimized structure

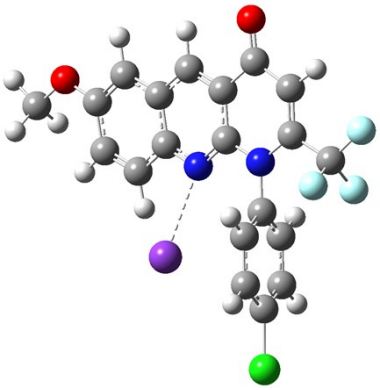
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.283554	1.501285	-0.000183
2	6	0	2.908242	1.448542	-0.000167
3	6	0	2.222884	0.228078	-0.000080
4	6	0	2.979820	-0.971485	-0.000001
5	6	0	4.381696	-0.915280	-0.000022
6	6	0	5.043630	0.303511	-0.000123
7	6	0	2.253932	-2.184754	0.000101
8	6	0	0.880407	-2.193698	0.000100
9	6	0	0.191437	-0.958492	0.000006
10	6	0	-1.917641	-2.171233	0.000017
11	6	0	-1.319917	-3.366082	0.000114
12	6	0	0.143022	-3.489692	0.000226
13	1	0	2.358638	2.401146	-0.000249
14	1	0	4.967947	-1.827582	0.000040
15	1	0	2.763305	-3.145447	0.000188
16	1	0	-1.910625	-4.273535	0.000111
17	6	0	-1.833800	0.324009	0.000022
18	6	0	-2.035061	1.000252	1.212768
19	6	0	-2.035147	1.000281	-1.212668
20	6	0	-2.351002	2.365260	1.218906
21	1	0	-1.901531	0.468301	2.149906
22	6	0	-2.351094	2.365313	-1.218745
23	1	0	-1.901675	0.468374	-2.149839

24	6	0	-2.515199	3.058119	0.000089
25	1	0	-2.508585	2.888362	2.157568
26	1	0	-2.508749	2.888410	-2.157396
27	6	0	-3.422503	-2.031309	-0.000156
28	7	0	-1.200100	-0.954104	-0.000012
29	9	0	-4.018211	-3.204548	-0.000183
30	9	0	-3.818333	-1.335034	1.082012
31	9	0	-3.818064	-1.335113	-1.082479
32	7	0	0.838492	0.214998	-0.000060
33	8	0	0.727666	-4.549607	0.000392
34	1	0	4.783371	2.461725	-0.000238
35	6	0	7.133076	1.471604	0.000046
36	1	0	6.931747	2.061314	-0.899354
37	1	0	6.931335	2.061374	0.899313
38	1	0	8.175240	1.160159	0.000293
39	8	0	6.372753	0.263218	-0.000081
40	17	0	-2.939518	4.712950	0.000161
41	12	0	-0.119271	1.991582	-0.000059

Rotational constants (GHZ): 0.1963547 0.1125281 0.0743929

Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RCAM-B3LYP) = -1788.42488619 A.U. after 8 cycles
NFock= 8 Conv=0.66D-08 -V/T= 2.0050
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.038974000 RMS 0.010071287
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot= 336893 Len1MO= 870766 IndFrg= 4690723
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 336893 Len1MO= 870766 IndFrg= 1207659
Counterpoise corrected energy = -1788.714420709823
BSSE energy = 0.005122031727
sum of monomers = -1788.424886194950
complexation energy = -184.90 kcal/mole (raw)
complexation energy = -181.69 kcal/mole (corrected)

v. 3k-K



Cartesian coordinates of optimized structure

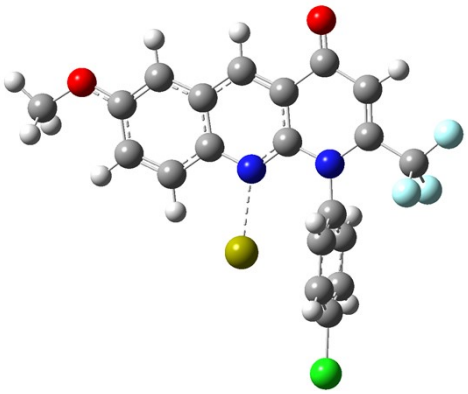
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.331959	-1.636937	-0.283825
2	6	0	-2.962925	-1.527083	-0.279855
3	6	0	-2.319440	-0.282325	-0.096533
4	6	0	-3.149051	0.864537	0.047038
5	6	0	-4.551093	0.738920	0.053517
6	6	0	-5.147947	-0.493598	-0.098624
7	6	0	-2.497069	2.109339	0.155628
8	6	0	-1.130833	2.183786	0.111574
9	6	0	-0.387419	0.972705	-0.004641
10	6	0	1.641581	2.291472	-0.027700
11	6	0	0.983319	3.458538	0.074422
12	6	0	-0.468050	3.506985	0.190365
13	1	0	-2.370681	-2.412663	-0.493357
14	1	0	-5.177459	1.616657	0.167635
15	1	0	-3.053914	3.035880	0.260675
16	1	0	1.524903	4.393503	0.061327
17	6	0	1.764291	-0.178707	-0.070291
18	6	0	2.388974	-0.644936	1.083065
19	6	0	1.863926	-0.899976	-1.258307
20	6	0	3.110891	-1.836023	1.056176
21	1	0	2.332688	-0.064224	1.996952
22	6	0	2.570896	-2.094801	-1.292018
23	1	0	1.388894	-0.519538	-2.155381
24	6	0	3.190918	-2.558740	-0.131440
25	1	0	3.625366	-2.190484	1.942440
26	1	0	2.664957	-2.655017	-2.215315
27	6	0	3.153179	2.317164	-0.163736
28	7	0	1.012819	1.044573	-0.032289
29	9	0	3.595199	3.561107	-0.314460
30	9	0	3.750446	1.803631	0.925232
31	9	0	3.555602	1.603106	-1.224282
32	7	0	-0.952015	-0.216944	-0.077595

33	8	0	-1.100827	4.539071	0.324983
34	1	0	-4.785531	-2.606431	-0.447836
35	6	0	-7.164118	-1.760834	-0.266139
36	1	0	-6.942552	-2.190777	-1.248996
37	1	0	-6.908766	-2.481349	0.518736
38	1	0	-8.227311	-1.533897	-0.208320
39	8	0	-6.493538	-0.526474	-0.076284
40	17	0	4.066756	-4.056291	-0.167653
41	19	0	-0.017674	-2.695600	0.851614

Rotational constants (GHZ): 0.1912934 0.1031963 0.0701724

Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RCAM-B3LYP) = -1788.43401200 A.U. after 8 cycles
NFock= 8 Conv=0.72D-08 -V/T= 2.0049
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.011418490 RMS 0.003413078
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot= 342487 Len1MO= 885786 IndFrg= 4771417
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 342487 Len1MO= 885786 IndFrg= 1228273
Counterpoise corrected energy = -1816.405888449023
BSSE energy = 0.004665835044
sum of monomers = -1816.370737354451
complexation energy = -24.99 kcal/mole (raw)
complexation energy = -22.06 kcal/mole (corrected)

vi. 3k-Ca



Cartesian coordinates of optimized structure

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.323860	-1.606925	-0.146364
2	6	0	-2.949717	-1.502350	-0.169659

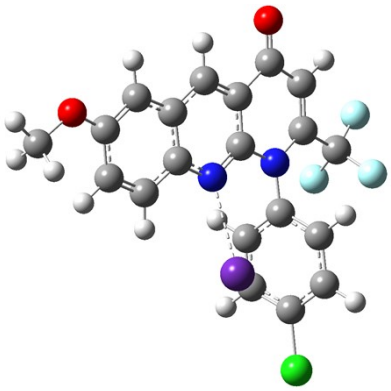
3	6	0	-2.293230	-0.262032	-0.063290
4	6	0	-3.106415	0.897358	0.033758
5	6	0	-4.504628	0.788206	0.063155
6	6	0	-5.125621	-0.448525	-0.010768
7	6	0	-2.436300	2.142052	0.078041
8	6	0	-1.069610	2.207959	0.034261
9	6	0	-0.328597	0.997326	-0.023578
10	6	0	1.717534	2.311019	-0.022140
11	6	0	1.066454	3.478597	0.019356
12	6	0	-0.395726	3.535430	0.066861
13	1	0	-2.401146	-2.430517	-0.381429
14	1	0	-5.121097	1.677410	0.138239
15	1	0	-2.986707	3.077447	0.140264
16	1	0	1.615333	4.411207	0.018025
17	6	0	1.787973	-0.171755	-0.031267
18	6	0	2.197159	-0.742657	1.178597
19	6	0	2.033522	-0.843407	-1.234020
20	6	0	2.796278	-2.006344	1.196355
21	1	0	2.057334	-0.194010	2.104954
22	6	0	2.627110	-2.106593	-1.227751
23	1	0	1.757392	-0.374798	-2.173375
24	6	0	3.011849	-2.691981	-0.010044
25	1	0	3.149661	-2.435064	2.129296
26	1	0	2.845524	-2.616626	-2.160931
27	6	0	3.231103	2.276664	-0.070854
28	7	0	1.061930	1.060096	-0.032084
29	9	0	3.735042	3.494474	-0.121647
30	9	0	3.721714	1.653764	1.016210
31	9	0	3.648343	1.589305	-1.147765
32	7	0	-0.911955	-0.199771	-0.052528
33	8	0	-1.029282	4.566690	0.127066
34	1	0	-4.789004	-2.579048	-0.251531
35	6	0	-7.171229	-1.687499	-0.065351
36	1	0	-6.983692	-2.175881	-1.026658
37	1	0	-6.914592	-2.357823	0.760968
38	1	0	-8.223706	-1.421000	0.002333
39	8	0	-6.456816	-0.457293	0.032030
40	17	0	3.763773	-4.238433	0.001191
41	20	0	0.015966	-2.372526	0.235307

Rotational constants (GHZ): 0.1935916 0.1061998 0.0712686

Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RCAM-B3LYP) = -1788.42846042 A.U. after 8 cycles
NFock= 8 Conv=0.67D-08 -V/T= 2.0049
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.025491334 RMS 0.008238413

CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot= 342487 Len1MO= 885786 IndFrg= 4771417
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 342487 Len1MO= 885786 IndFrg= 1228273
Counterpoise corrected energy = -1824.449063557017
BSSE energy = 0.005412240594
sum of monomers = -1824.271929748913
complexation energy = -114.55 kcal/mole (raw)
complexation energy = -111.15 kcal/mole (corrected)

vii. 3k-Rb



Cartesian coordinates of optimized structure

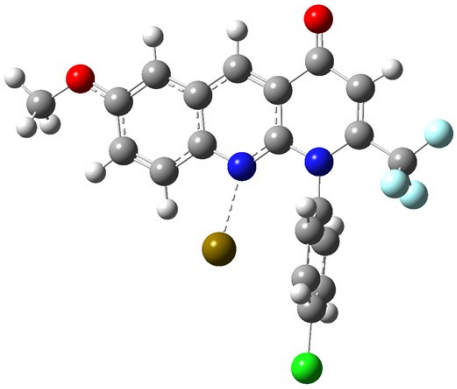
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.326907	-1.348076	-0.528929
2	6	0	-2.957133	-1.249218	-0.514336
3	6	0	-2.306523	-0.028275	-0.223888
4	6	0	-3.127419	1.109285	0.014038
5	6	0	-4.530609	0.992415	0.011122
6	6	0	-5.134866	-0.218808	-0.245136
7	6	0	-2.465220	2.336457	0.219538
8	6	0	-1.098474	2.403513	0.172688
9	6	0	-0.365864	1.198590	-0.041210
10	6	0	1.672159	2.499740	-0.001072
11	6	0	1.024313	3.661438	0.194083
12	6	0	-0.423330	3.711051	0.346229
13	1	0	-2.363044	-2.109817	-0.808107
14	1	0	-5.151742	1.861489	0.197518
15	1	0	-3.013973	3.256118	0.400245
16	1	0	1.571993	4.592297	0.227570
17	6	0	1.776993	0.034016	-0.180775
18	6	0	2.451743	-0.465399	0.928928
19	6	0	1.817956	-0.654934	-1.390818
20	6	0	3.170839	-1.654310	0.834871
21	1	0	2.440621	0.089720	1.860109
22	6	0	2.518689	-1.848854	-1.490005

23	1	0	1.301210	-0.250300	-2.253263
24	6	0	3.191192	-2.344124	-0.373294
25	1	0	3.726997	-2.032754	1.685360
26	1	0	2.565985	-2.384929	-2.430991
27	6	0	3.180129	2.531305	-0.177137
28	7	0	1.035557	1.259873	-0.073625
29	9	0	3.616972	3.781254	-0.295509
30	9	0	3.808864	1.982612	0.876630
31	9	0	3.554239	1.856755	-1.272455
32	7	0	-0.940164	0.023497	-0.200198
33	8	0	-1.044566	4.733815	0.575321
34	1	0	-4.788170	-2.295107	-0.780177
35	6	0	-7.159796	-1.449417	-0.535901
36	1	0	-6.935439	-1.785013	-1.554238
37	1	0	-6.914716	-2.244417	0.177202
38	1	0	-8.221730	-1.220985	-0.462109
39	8	0	-6.481489	-0.244643	-0.224818
40	17	0	4.057681	-3.845123	-0.489681
41	37	0	-0.106102	-2.672707	0.953682

Rotational constants (GHZ): 0.1631683 0.1015622 0.0666449

Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RCAM-B3LYP) = -1788.43385224 A.U. after 8 cycles
NFock= 8 Conv=0.50D-08 -V/T= 2.0049
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.010574819 RMS 0.003106769
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot= 342487 Len1MO= 885792 IndFrg= 4771447
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 342487 Len1MO= 885792 IndFrg= 1228279
Counterpoise corrected energy = -1812.134800760948
BSSE energy = 0.003969212661
sum of monomers = -1812.107283354044
complexation energy = -19.76 kcal/mole (raw)
complexation energy = -17.27 kcal/mole (corrected)

viii. 3k-Sr



Cartesian coordinates of optimized structure

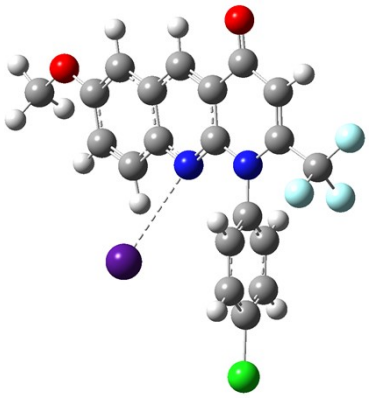
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.338091	-1.403714	-0.314793
2	6	0	-2.961742	-1.304878	-0.335605
3	6	0	-2.300277	-0.075316	-0.133473
4	6	0	-3.113898	1.074881	0.044666
5	6	0	-4.512135	0.965220	0.080725
6	6	0	-5.136556	-0.261753	-0.073657
7	6	0	-2.445933	2.317224	0.145217
8	6	0	-1.081553	2.387183	0.076233
9	6	0	-0.340208	1.179226	-0.043236
10	6	0	1.700877	2.499051	-0.030328
11	6	0	1.048086	3.663399	0.062975
12	6	0	-0.410838	3.713652	0.154696
13	1	0	-2.423019	-2.191729	-0.685461
14	1	0	-5.125937	1.848967	0.217753
15	1	0	-2.996245	3.246958	0.264950
16	1	0	1.593962	4.597519	0.069765
17	6	0	1.787520	0.019974	-0.084996
18	6	0	2.292177	-0.516885	1.102221
19	6	0	1.979375	-0.659865	-1.291508
20	6	0	2.944307	-1.752771	1.096280
21	1	0	2.198909	0.043609	2.027232
22	6	0	2.620519	-1.896800	-1.307210
23	1	0	1.629203	-0.213886	-2.216837
24	6	0	3.102188	-2.446444	-0.110458
25	1	0	3.377578	-2.151857	2.008369
26	1	0	2.797842	-2.413345	-2.245309
27	6	0	3.213775	2.482875	-0.127916
28	7	0	1.050396	1.246426	-0.059124
29	9	0	3.697950	3.708507	-0.206799
30	9	0	3.751372	1.882396	0.949332
31	9	0	3.606715	1.792748	-1.210701
32	7	0	-0.919111	-0.016804	-0.112674

33	8	0	-1.045387	4.739066	0.279982
34	1	0	-4.807458	-2.359332	-0.512881
35	6	0	-7.185600	-1.486509	-0.218477
36	1	0	-7.009690	-1.883215	-1.223266
37	1	0	-6.921226	-2.232374	0.537944
38	1	0	-8.236970	-1.227348	-0.114280
39	8	0	-6.468297	-0.272041	-0.014169
40	17	0	3.895901	-3.976623	-0.125930
41	38	0	-0.047186	-2.348534	0.398797

Rotational constants (GHZ): 0.1734402 0.1045038 0.0679582

Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RCAM-B3LYP) = -1788.42796914 A.U. after 8 cycles
NFock= 8 Conv=0.54D-08 -V/T= 2.0049
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.023775294 RMS 0.007606450
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot= 342487 Len1MO= 885792 IndFrg= 4771447
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 342487 Len1MO= 885792 IndFrg= 1228279
Counterpoise corrected energy = -1818.346904483129
BSSE energy = 0.005001044150
sum of monomers = -1818.203525578751
complexation energy = -93.11 kcal/mole (raw)
complexation energy = -89.97 kcal/mole (corrected)

ix. 3k-Cs



Cartesian coordinates of optimized structure

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.314297	-0.971060	-0.796346
2	6	0	-2.943098	-0.903962	-0.765395

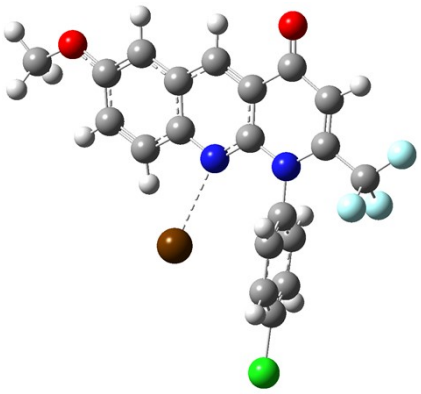
3	6	0	-2.270480	0.272509	-0.361897
4	6	0	-3.067966	1.401600	-0.024225
5	6	0	-4.473628	1.314758	-0.043809
6	6	0	-5.100172	0.145497	-0.414487
7	6	0	-2.379838	2.590493	0.292025
8	6	0	-1.011597	2.631215	0.250230
9	6	0	-0.306029	1.433905	-0.071935
10	6	0	1.758864	2.682463	0.058184
11	6	0	1.137142	3.836930	0.357816
12	6	0	-0.306575	3.902493	0.535946
13	1	0	-2.357434	-1.743085	-1.128618
14	1	0	-5.078540	2.175985	0.217481
15	1	0	-2.908612	3.502186	0.554232
16	1	0	1.703887	4.751646	0.455911
17	6	0	1.810200	0.233505	-0.301178
18	6	0	2.512102	-0.334761	0.756549
19	6	0	1.794405	-0.393184	-1.544798
20	6	0	3.205140	-1.528612	0.575997
21	1	0	2.544498	0.171349	1.714644
22	6	0	2.465905	-1.593091	-1.728950
23	1	0	1.254931	0.063501	-2.366029
24	6	0	3.166577	-2.156218	-0.663834
25	1	0	3.784167	-1.959686	1.385181
26	1	0	2.466918	-2.082512	-2.696107
27	6	0	3.264308	2.704207	-0.142792
28	7	0	1.097302	1.465685	-0.104476
29	9	0	3.715610	3.954001	-0.199076
30	9	0	3.904884	2.091649	0.868019
31	9	0	3.611321	2.088084	-1.279967
32	7	0	-0.905228	0.291329	-0.332294
33	8	0	-0.902778	4.912956	0.865848
34	1	0	-4.794514	-1.880012	-1.137158
35	6	0	-7.148274	-1.002866	-0.846266
36	1	0	-6.915044	-1.238721	-1.890325
37	1	0	-6.933557	-1.872811	-0.215372
38	1	0	-8.205925	-0.757662	-0.764282
39	8	0	-6.448076	0.146588	-0.404160
40	17	0	3.993394	-3.669803	-0.884712
41	55	0	-0.233248	-2.696682	1.000884

Rotational constants (GHZ): 0.1383378 0.0992869 0.0629963

Integral accuracy reduced to 1.0D-05 until final iterations.
DSYEVD-2 returned Info= 105109 IAlg= 4 N= 456 NDim= 456 NE2= 2353113 trying DSYEV.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RCAM-B3LYP) = -1788.43381986 A.U. after 8 cycles
NFock= 8 Conv=0.56D-08 -V/T= 2.0049
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****
Cartesian Forces: Max 0.009615937 RMS 0.002777271
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot= 342487 Len1MO= 885792 IndFrg= 4771447
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 342487 Len1MO= 885792 IndFrg= 1228279
Counterpoise corrected energy = -1808.156268197121
BSSE energy = 0.003380716835
sum of monomers = -1808.135815368074
complexation energy = -14.96 kcal/mole (raw)
complexation energy = -12.83 kcal/mole (corrected)

x. 3k-Ba



Cartesian coordinates of optimized structure

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.344154	-1.160219	-0.518241
2	6	0	-2.966100	-1.076075	-0.515737
3	6	0	-2.295752	0.130204	-0.213731
4	6	0	-3.103834	1.271389	0.037497
5	6	0	-4.503574	1.170786	0.057734
6	6	0	-5.136026	-0.035235	-0.191763
7	6	0	-2.429729	2.501376	0.213595
8	6	0	-1.066162	2.567108	0.136273
9	6	0	-0.332529	1.361673	-0.054368
10	6	0	1.711501	2.675375	-0.017801
11	6	0	1.064390	3.836180	0.144023
12	6	0	-0.389725	3.884212	0.280674
13	1	0	-2.426817	-1.921892	-0.947769
14	1	0	-5.111167	2.048450	0.250446
15	1	0	-2.973707	3.425242	0.392246
16	1	0	1.611926	4.768761	0.170162
17	6	0	1.799601	0.202333	-0.162621
18	6	0	2.406540	-0.325135	0.978169
19	6	0	1.912459	-0.468690	-1.382943
20	6	0	3.095142	-1.537924	0.913100

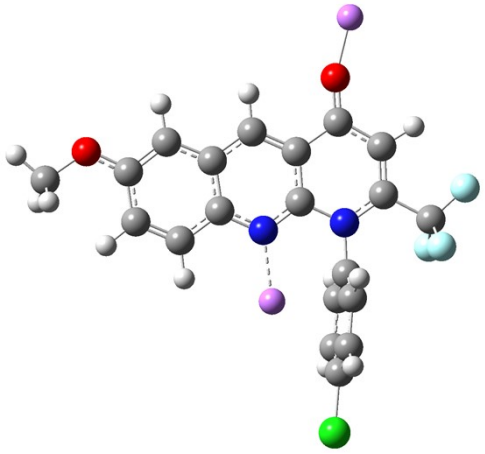
21	1	0	2.374635	0.231003	1.909680
22	6	0	2.584008	-1.685053	-1.454833
23	1	0	1.480030	-0.028860	-2.275491
24	6	0	3.171260	-2.222316	-0.302835
25	1	0	3.610797	-1.927216	1.785566
26	1	0	2.699337	-2.195517	-2.405666
27	6	0	3.221539	2.674136	-0.168465
28	7	0	1.059637	1.425522	-0.078045
29	9	0	3.688487	3.906830	-0.261168
30	9	0	3.806514	2.082079	0.888569
31	9	0	3.585624	1.993005	-1.265489
32	7	0	-0.915079	0.173307	-0.177312
33	8	0	-1.017329	4.901964	0.484672
34	1	0	-4.820408	-2.089601	-0.805587
35	6	0	-7.193175	-1.222140	-0.467790
36	1	0	-7.006170	-1.525734	-1.502637
37	1	0	-6.946045	-2.038674	0.218529
38	1	0	-8.244080	-0.964816	-0.354052
39	8	0	-6.469722	-0.039491	-0.141280
40	17	0	3.988495	-3.742342	-0.384625
41	56	0	-0.109428	-2.345394	0.554049

Rotational constants (GHZ): 0.1537437 0.1024441 0.0646801

Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RCAM-B3LYP) = -1788.42772996 A.U. after 8 cycles
NFock= 8 Conv=0.78D-08 -V/T= 2.0049
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.022083496 RMS 0.006973532
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot= 342487 Len1MO= 885792 IndFrg= 4771447
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 342487 Len1MO= 885792 IndFrg= 1228279
Counterpoise corrected energy = -1813.158594643937
BSSE energy = 0.004767165877
sum of monomers = -1813.046137624002
complexation energy = -73.56 kcal/mole (raw)
complexation energy = -70.57 kcal/mole (corrected)

b. Interaction with two metal ion molecules

i. Li-3k-Li



Cartesian coordinates of optimized structure

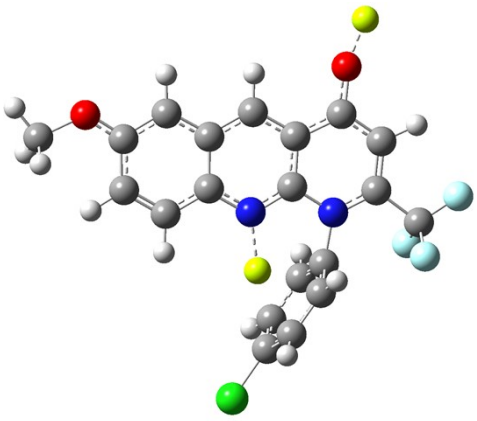
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.207336	1.908926	-0.000655
2	6	0	2.842456	1.796091	-0.000779
3	6	0	2.215126	0.532198	-0.000321
4	6	0	3.050918	-0.628489	0.000121
5	6	0	4.454163	-0.495170	0.000262
6	6	0	5.040607	0.752581	-0.000091
7	6	0	2.408561	-1.872056	0.000271
8	6	0	1.027590	-1.958721	0.000083
9	6	0	0.284442	-0.745981	-0.000163
10	6	0	-1.746418	-2.019436	-0.000082
11	6	0	-1.079359	-3.202595	0.000135
12	6	0	0.347578	-3.245787	0.000224
13	1	0	2.240735	2.701266	-0.001375
14	1	0	5.090042	-1.373101	0.000630
15	1	0	2.986551	-2.789747	0.000497
16	1	0	-1.640930	-4.125888	0.000134
17	6	0	-1.826812	0.449775	-0.000113
18	6	0	-2.104521	1.083082	1.212055
19	6	0	-2.103806	1.083692	-1.212116
20	6	0	-2.642815	2.368450	1.213856
21	1	0	-1.889466	0.581230	2.149183
22	6	0	-2.642085	2.369060	-1.213588
23	1	0	-1.888158	0.582323	-2.149366
24	6	0	-2.911038	3.012419	0.000218
25	1	0	-2.865776	2.868625	2.149743
26	1	0	-2.864475	2.869710	-2.149354
27	6	0	-3.270786	-2.018308	-0.000264

28	7	0	-1.114924	-0.805181	-0.000227
29	9	0	-3.736019	-3.259523	-0.000526
30	9	0	-3.732227	-1.388768	1.084384
31	9	0	-3.731880	-1.388408	-1.084863
32	7	0	0.852318	0.450448	-0.000317
33	8	0	0.988805	-4.324803	0.000288
34	1	0	4.655340	2.894886	-0.001020
35	6	0	7.051507	2.053147	0.000335
36	1	0	6.813423	2.630030	-0.898252
37	1	0	6.812416	2.630416	0.898408
38	1	0	8.112068	1.810867	0.000979
39	8	0	6.372581	0.797818	0.000231
40	17	0	-3.573507	4.597165	0.000413
41	3	0	-0.285315	2.120554	0.000898
42	3	0	1.392082	-6.034016	0.000812

Rotational constants (GHZ): 0.1871392 0.1091970 0.0716082

SCF Done: E(RCAM-B3LYP) = -7.26429228391 A.U. after 1 cycles
NFock= 1 Conv=0.97D-16 -V/T= 2.0092
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 6 LCPTot= 351494 Len1MO= 908642 IndFrg= 6711988
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 351494 Len1MO= 908642 IndFrg= 1260136
Counterpoise corrected energy = -1803.071694871855
BSSE energy = 0.009967404368
sum of monomers = -1802.960033359005
complexation energy = -76.32 kcal/mole (raw)
complexation energy = -70.07 kcal/mole (corrected)

ii. Be-3k-Be



Cartesian coordinates of optimized structure

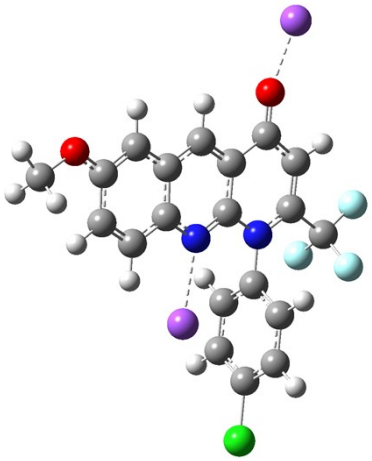
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.259406	-0.961142	-0.000388
2	6	0	-2.894952	-1.155691	-0.000473
3	6	0	-2.024659	-0.064859	-0.000167
4	6	0	-2.587064	1.277530	0.000144
5	6	0	-3.980539	1.450664	0.000256
6	6	0	-4.837568	0.354366	-0.000008
7	6	0	-1.702598	2.352458	0.000137
8	6	0	-0.308728	2.157525	0.000047
9	6	0	0.163690	0.817586	-0.000030
10	6	0	2.436626	1.574305	-0.000065
11	6	0	2.028345	2.892396	-0.000152
12	6	0	0.669320	3.195284	-0.000018
13	1	0	-2.512424	-2.174330	-0.000792
14	1	0	-4.414904	2.444661	0.000525
15	1	0	-2.099927	3.361732	0.000181
16	1	0	2.787240	3.666803	-0.000243
17	6	0	1.854676	-0.848941	0.000050
18	6	0	1.744388	-1.542632	1.221566
19	6	0	1.744160	-1.542597	-1.221451
20	6	0	1.424180	-2.908316	1.221861
21	1	0	1.768576	-1.001399	2.164582
22	6	0	1.423526	-2.908255	-1.221602
23	1	0	1.768175	-1.001415	-2.164500
24	6	0	1.284114	-3.626084	0.000147
25	1	0	1.267355	-3.426569	2.166413
26	1	0	1.266202	-3.426372	-2.166142
27	6	0	3.918861	1.175926	-0.000157
28	7	0	1.534772	0.567533	0.000008
29	9	0	4.675393	2.246074	-0.000382
30	9	0	4.146100	0.435373	1.084383
31	9	0	4.145936	0.434980	-1.084419
32	7	0	-0.658651	-0.252492	-0.000162
33	8	0	0.278754	4.472785	0.000070
34	1	0	-4.913179	-1.827463	-0.000622
35	6	0	-7.117691	-0.459857	0.000025
36	1	0	-7.026742	-1.063122	-0.905545
37	1	0	-7.026375	-1.063744	0.905145
38	1	0	-8.071011	0.062766	0.000402
39	8	0	-6.117981	0.592340	0.000182
40	17	0	0.911600	-5.261429	0.000212
41	4	0	0.171482	-1.699514	-0.000377
42	4	0	0.256476	5.884670	0.000749

Rotational constants (GHZ): 0.1775687 0.1213848 0.0750287

SCF Done: E(RCAM-B3LYP) = -13.6302816171 A.U. after 1 cycles

NFock= 1 Conv=0.24D-15 -V/T= 2.0080
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 6 LCPTot= 351494 Len1MO= 908654 IndFrg= 6712072
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 351494 Len1MO= 908654 IndFrg= 1260148
Counterpoise corrected energy = -1816.263549727275
BSSE energy = 0.013090735724
sum of monomers = -1815.647624265975
complexation energy = -394.71 kcal/mole (raw)
complexation energy = -386.50 kcal/mole (corrected)

iii. Na-3k-Na



Cartesian coordinates of optimized structure

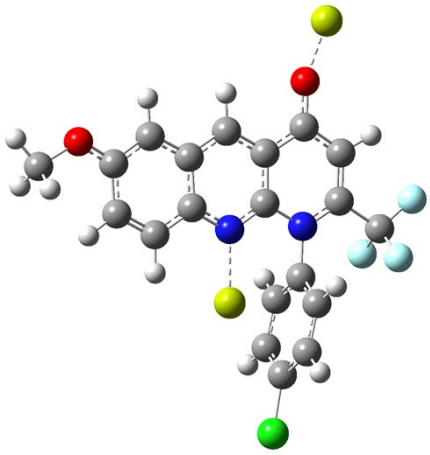
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.956979	-2.615919	0.000168
2	6	0	2.616851	-2.331794	0.000250
3	6	0	2.140106	-1.001134	0.000071
4	6	0	3.118038	0.039599	-0.000121
5	6	0	4.494096	-0.264966	-0.000224
6	6	0	4.925027	-1.573472	-0.000126
7	6	0	2.637697	1.355794	-0.000143
8	6	0	1.284153	1.614139	-0.000064
9	6	0	0.388190	0.504352	0.000031
10	6	0	-1.450513	2.051101	-0.000082
11	6	0	-0.634459	3.132920	-0.000079
12	6	0	0.792205	2.992593	-0.000025
13	1	0	1.920199	-3.165380	0.000473
14	1	0	5.231757	0.529478	-0.000366

15	1	0	3.323846	2.195679	-0.000185
16	1	0	-1.068275	4.122111	-0.000142
17	6	0	-1.902853	-0.365757	0.000029
18	6	0	-2.334660	-0.905514	-1.209690
19	6	0	-2.334921	-0.905257	1.209768
20	6	0	-3.192428	-2.001951	-1.213034
21	1	0	-2.012521	-0.463454	-2.146267
22	6	0	-3.192689	-2.001700	1.213158
23	1	0	-2.012978	-0.463001	2.146319
24	6	0	-3.620981	-2.547720	0.000070
25	1	0	-3.551034	-2.417834	-2.147971
26	1	0	-3.551503	-2.417381	2.148104
27	6	0	-2.959232	2.277279	-0.000275
28	7	0	-0.993131	0.754642	-0.000001
29	9	0	-3.233921	3.577112	-0.000250
30	9	0	-3.517518	1.732558	-1.085525
31	9	0	-3.517882	1.732471	1.084768
32	7	0	0.796925	-0.752119	0.000155
33	8	0	1.568351	3.966494	0.000012
34	1	0	4.278429	-3.649990	0.000335
35	6	0	6.760045	-3.109612	-0.000147
36	1	0	6.451372	-3.653606	0.897837
37	1	0	6.451040	-3.653926	-0.897823
38	1	0	7.842933	-3.003960	-0.000366
39	8	0	6.244712	-1.780920	-0.000291
40	17	0	-4.688243	-3.902395	0.000113
41	11	0	2.278220	6.037065	0.000687
42	11	0	-0.574058	-2.815014	0.000327

Rotational constants (GHZ): 0.1509391 0.1015750 0.0627576

Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RCAM-B3LYP) = -1788.43338827 A.U. after 8 cycles
NFock= 8 Conv=0.58D-08 -V/T= 2.0049
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.034459247 RMS 0.006236749
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 6 LCPTot= 348655 Len1MO= 900916 IndFrg= 6655067
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 348655 Len1MO= 900916 IndFrg= 1249571
Counterpoise corrected energy = -1788.480919246945
BSSE energy = 0.008545552926
sum of monomers = -1788.433388269636
complexation energy = -35.19 kcal/mole (raw)
complexation energy = -29.83 kcal/mole (corrected)

iv. Mg-3k-Mg



Cartesian coordinates of optimized structure

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.935950	-2.452233	0.000488
2	6	0	-2.585466	-2.200223	0.000845
3	6	0	-2.084400	-0.890459	0.000395
4	6	0	-3.033178	0.193001	-0.000394
5	6	0	-4.413078	-0.075376	-0.000761
6	6	0	-4.887582	-1.380949	-0.000334
7	6	0	-2.510247	1.487071	-0.000798
8	6	0	-1.133068	1.721440	-0.000407
9	6	0	-0.267111	0.588811	0.000094
10	6	0	1.632069	2.045474	-0.000859
11	6	0	0.835909	3.159724	-0.001377
12	6	0	-0.566333	3.048554	-0.001109
13	1	0	-1.910638	-3.063353	0.001571
14	1	0	-5.134620	0.734249	-0.001428
15	1	0	-3.186205	2.334623	-0.001581
16	1	0	1.319205	4.128141	-0.002411
17	6	0	1.949140	-0.399563	0.000205
18	6	0	2.259305	-1.023721	1.217702
19	6	0	2.259226	-1.024266	-1.217074
20	6	0	2.838628	-2.300057	1.220778
21	1	0	2.033876	-0.534487	2.161505
22	6	0	2.838556	-2.300574	-1.219660
23	1	0	2.033740	-0.535390	-2.161050
24	6	0	3.161651	-2.944058	0.000686
25	1	0	3.097827	-2.778319	2.162475
26	1	0	3.097697	-2.779228	-2.161179
27	6	0	3.159954	2.187724	-0.001214
28	7	0	1.117783	0.785458	-0.000064
29	9	0	3.494474	3.461499	-0.001332
30	9	0	3.651095	1.590633	1.084142

31	9	0	3.650643	1.590585	-1.086748
32	7	0	-0.729118	-0.667560	0.000511
33	8	0	-1.329664	4.098169	-0.002555
34	1	0	-4.287538	-3.478167	0.000801
35	6	0	-6.793925	-2.861458	-0.000954
36	1	0	-6.515548	-3.408622	-0.904532
37	1	0	-6.516837	-3.408161	0.903303
38	1	0	-7.865099	-2.675395	-0.001768
39	8	0	-6.185914	-1.549991	-0.000866
40	17	0	3.939127	-4.447471	0.000995
41	12	0	0.548809	-2.321226	0.000576
42	12	0	-1.818606	5.871458	0.005219

Rotational constants (GHZ): 0.1467765 0.1087928 0.0646644

No special actions if energy rises.

SCF Done: E(RCAM-B3LYP) = 0.000000000000E+00 A.U. after 1 cycles
NFock= 1 Conv=0.00D+00 -V/T= 0.0000

QCSCF skips out because SCF is already converged.

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

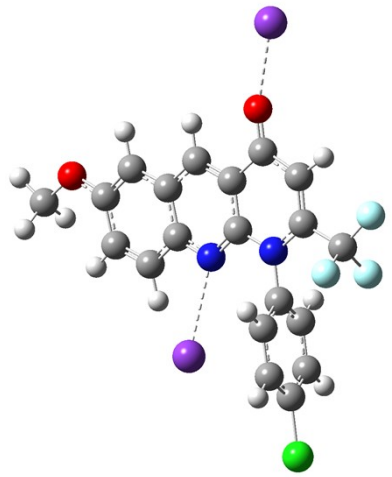
Cartesian Forces: Max 0.000000000 RMS 0.000000000

CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 6 LCPTot= 348655 Len1MO= 900916 IndFrg= 6655067

CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 348655 Len1MO= 900916 IndFrg= 1249571

Counterpoise corrected energy = -1788.638286037795
BSSE energy = 0.010664801063
sum of monomers = -1788.414564464560
complexation energy = -147.08 kcal/mole (raw)
complexation energy = -140.39 kcal/mole (corrected)

v. K-3k-K



Cartesian coordinates of optimized structure

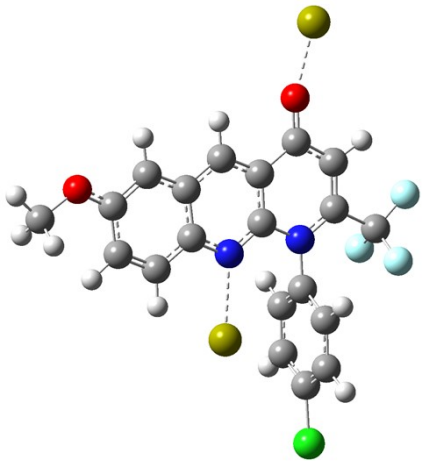
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.989024	-3.694329	0.214805
2	6	0	1.780273	-3.048792	0.203238
3	6	0	1.689716	-1.642711	0.073115
4	6	0	2.916748	-0.918643	-0.011114
5	6	0	4.153346	-1.595078	-0.011185
6	6	0	4.204729	-2.967525	0.090608
7	6	0	2.819760	0.479478	-0.067036
8	6	0	1.593204	1.101654	-0.034748
9	6	0	0.425779	0.281749	0.017231
10	6	0	-0.912800	2.277698	0.061247
11	6	0	0.168692	3.091228	0.020221
12	6	0	1.505645	2.566769	-0.046728
13	1	0	0.879348	-3.633828	0.356785
14	1	0	5.082161	-1.040204	-0.080870
15	1	0	3.709839	1.097073	-0.119982
16	1	0	0.026991	4.161542	0.046586
17	6	0	-2.019851	0.079840	0.062540
18	6	0	-2.758997	-0.099468	-1.102245
19	6	0	-2.430485	-0.507679	1.256571
20	6	0	-3.919083	-0.869639	-1.077411
21	1	0	-2.448854	0.384145	-2.021784
22	6	0	-3.580791	-1.285364	1.286689
23	1	0	-1.857255	-0.346181	2.162717
24	6	0	-4.323482	-1.462478	0.117504
25	1	0	-4.520937	-0.988944	-1.971551
26	1	0	-3.920768	-1.731488	2.214578
27	6	0	-2.293828	2.921902	0.133469
28	7	0	-0.834209	0.902730	0.037753
29	9	0	-2.184373	4.237062	0.299031
30	9	0	-2.976095	2.706942	-0.998395
31	9	0	-3.001379	2.433004	1.154344
32	7	0	0.468004	-1.035947	0.047701
33	8	0	2.512701	3.289083	-0.097951
34	1	0	3.014163	-4.770318	0.334343
35	6	0	5.542505	-4.946856	0.211104
36	1	0	5.143676	-5.294216	1.169406
37	1	0	5.046529	-5.467585	-0.614197
38	1	0	6.610415	-5.152345	0.172766
39	8	0	5.417151	-3.534992	0.080815
40	17	0	-5.754724	-2.433314	0.150836
41	19	0	4.059087	5.346442	-0.127246
42	19	0	-1.514580	-3.026186	-0.775711

Rotational constants (GHZ): 0.1219206 0.0947154 0.0551725

No special actions if energy rises.
SCF Done: E(RCAM-B3LYP) = -27.9367253505 A.U. after 1 cycles

NFock= 1 Conv=0.16D-12 -V/T= 3.7447
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 6 LCPTot= 360083 Len1MO= 931596 IndFrg= 6881255
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 360083 Len1MO= 931596 IndFrg= 1291679
Counterpoise corrected energy = -1844.323621277858
BSSE energy = 0.008255566578
sum of monomers = -1844.306960422741
complexation energy = -15.64 kcal/mole (raw)
complexation energy = -10.45 kcal/mole (corrected)

vi. Ca-3k-Ca



Cartesian coordinates of optimized structure

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.136976	-3.594694	0.000268
2	6	0	-1.902912	-2.993352	0.000253
3	6	0	-1.748000	-1.592534	0.000052
4	6	0	-2.951449	-0.812341	-0.000079
5	6	0	-4.213603	-1.433198	-0.000090
6	6	0	-4.332555	-2.813895	0.000064
7	6	0	-2.796555	0.577554	-0.000150
8	6	0	-1.541660	1.167758	-0.000083
9	6	0	-0.401442	0.305174	-0.000021
10	6	0	1.018442	2.236112	0.000031
11	6	0	-0.044381	3.089575	-0.000027
12	6	0	-1.379149	2.613700	-0.000083
13	1	0	-1.041065	-3.668363	0.000581

14	1	0	-5.120450	-0.838669	-0.000201
15	1	0	-3.673431	1.214736	-0.000240
16	1	0	0.156040	4.151989	-0.000006
17	6	0	2.030254	0.000918	0.000047
18	6	0	2.583755	-0.419892	1.213728
19	6	0	2.584179	-0.419435	-1.213588
20	6	0	3.672979	-1.294639	1.216999
21	1	0	2.184406	-0.053600	2.155082
22	6	0	3.673417	-1.294191	-1.216792
23	1	0	2.185192	-0.052788	-2.154957
24	6	0	4.238244	-1.723409	0.000123
25	1	0	4.134899	-1.589350	2.155371
26	1	0	4.135678	-1.588543	-2.155109
27	6	0	2.438393	2.817702	0.000132
28	7	0	0.877502	0.875190	0.000016
29	9	0	2.385077	4.138048	0.000315
30	9	0	3.092331	2.405701	1.086035
31	9	0	3.092384	2.406012	-1.085850
32	7	0	-0.498220	-1.023686	-0.000009
33	8	0	-2.375184	3.411467	-0.000123
34	1	0	-3.204966	-4.676514	0.000466
35	6	0	-5.777584	-4.740028	0.000205
36	1	0	-5.362721	-5.195198	-0.902557
37	1	0	-5.362836	-5.194987	0.903126
38	1	0	-6.858917	-4.853977	0.000149
39	8	0	-5.547556	-3.317738	0.000053
40	17	0	5.608092	-2.740024	0.000172
41	20	0	1.312723	-2.730472	-0.000719
42	20	0	-3.612271	5.260779	-0.000008

Rotational constants (GHZ): 0.1260398 0.0967990 0.0564136

No special actions if energy rises.

SCF Done: E(RCAM-B3LYP) = -35.8434693286 A.U. after 1 cycles

NFock= 1 Conv=0.41D-15 -V/T= 3.8132

QCSCF skips out because SCF is already converged.

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Cartesian Forces: Max 0.000000000 RMS 0.000000000

CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 6 LCPTot= 360083 Len1MO= 931596 IndFrg= 6881255

CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 360083 Len1MO= 931596 IndFrg= 1291679

Counterpoise corrected energy = -1860.171145663334

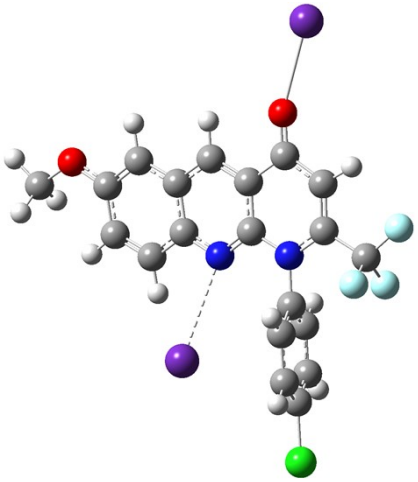
BSSE energy = 0.010034313266

sum of monomers = -1860.110581272526

complexation energy = -44.30 kcal/mole (raw)

complexation energy = -38.00 kcal/mole (corrected)

vii. Rb-3k-Rb



Cartesian coordinates of optimized structure

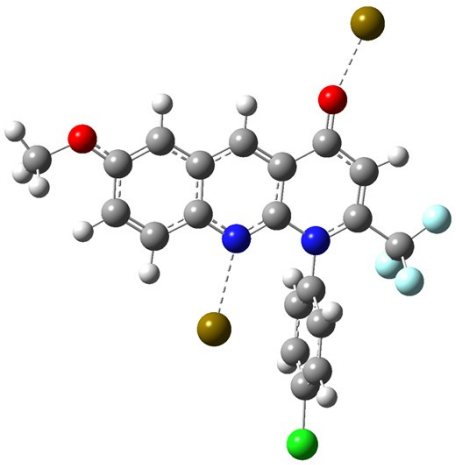
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.349657	4.738053	-0.434528
2	6	0	-0.846781	3.461250	-0.409066
3	6	0	-0.004641	2.340879	-0.212629
4	6	0	1.393616	2.592688	-0.080939
5	6	0	1.890306	3.911958	-0.092384
6	6	0	1.039718	4.982238	-0.256428
7	6	0	2.227550	1.469038	0.025544
8	6	0	1.701810	0.198736	-0.005628
9	6	0	0.283912	0.061335	-0.101928
10	6	0	0.565438	-2.325287	-0.119860
11	6	0	1.913907	-2.239754	-0.038471
12	6	0	2.588990	-0.971388	0.045576
13	1	0	-1.900814	3.302469	-0.611002
14	1	0	2.952863	4.099316	0.014186
15	1	0	3.303166	1.579039	0.113008
16	1	0	2.503063	-3.144679	-0.049455
17	6	0	-1.705591	-1.374537	-0.177819
18	6	0	-2.404283	-1.760974	0.960531
19	6	0	-2.377422	-1.154116	-1.377053
20	6	0	-3.784089	-1.938325	0.902221
21	1	0	-1.871114	-1.957166	1.883897
22	6	0	-3.754588	-1.315073	-1.439414
23	1	0	-1.820811	-0.868083	-2.262286
24	6	0	-4.453148	-1.708686	-0.297351
25	1	0	-4.334424	-2.276134	1.773544
26	1	0	-4.286172	-1.163842	-2.372101
27	6	0	-0.058272	-3.713827	-0.217454
28	7	0	-0.270627	-1.229976	-0.121013
29	9	0	0.886243	-4.636202	-0.386589
30	9	0	-0.725951	-4.016154	0.903697
31	9	0	-0.902960	-3.793085	-1.247862

32	7	0	-0.538808	1.087477	-0.176803
33	8	0	3.819555	-0.865280	0.135100
34	1	0	-1.023917	5.567174	-0.609980
35	6	0	0.772394	7.350220	-0.459278
36	1	0	0.287879	7.323149	-1.440499
37	1	0	0.018779	7.447394	0.328908
38	1	0	1.445517	8.204258	-0.416562
39	8	0	1.589882	6.204252	-0.254724
40	17	0	-6.173153	-1.902006	-0.369640
41	37	0	-3.544453	1.468360	0.931071
42	37	0	6.541997	-1.498378	0.211330

Rotational constants (GHZ): 0.1047180 0.0652803 0.0417483

SCF Done: E(RCAM-B3LYP) = -23.6734311154 A.U. after 1 cycles
NFock= 1 Conv=0.35D-13 -V/T= 4.3225
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 6 LCPTot= 360083 Len1MO= 931608 IndFrg= 6881339
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 360083 Len1MO= 931608 IndFrg= 1291691
Counterpoise corrected energy = -1835.786216641622
BSSE energy = 0.006927503996
sum of monomers = -1835.780440721484
complexation energy = -7.97 kcal/mole (raw)
complexation energy = -3.62 kcal/mole (corrected)

viii. Sr-3k-Sr



Cartesian coordinates of optimized structure

Center Atomic Atomic Coordinates (Angstroms)

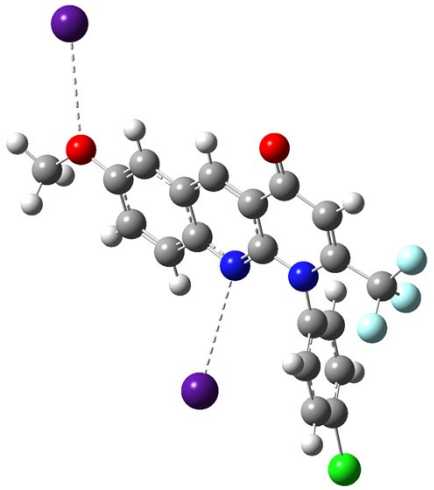
Number	Number	Type	X	Y	Z
1	6	0	0.233499	4.830898	-0.000155
2	6	0	-0.421189	3.624091	-0.000166
3	6	0	0.262566	2.389307	-0.000060
4	6	0	1.694106	2.461239	0.000025
5	6	0	2.361072	3.699758	0.000048
6	6	0	1.657898	4.892081	-0.000023
7	6	0	2.383679	1.244590	0.000058
8	6	0	1.712769	0.035376	0.000020
9	6	0	0.281779	0.066421	-0.000015
10	6	0	0.279765	-2.334227	-0.000021
11	6	0	1.639013	-2.399307	-0.000006
12	6	0	2.442041	-1.227847	0.000018
13	1	0	-1.511017	3.676893	-0.000336
14	1	0	3.444606	3.740596	0.000116
15	1	0	3.467567	1.239639	0.000103
16	1	0	2.103281	-3.375189	-0.000006
17	6	0	-1.859370	-1.144653	-0.000047
18	6	0	-2.553775	-1.172457	1.212260
19	6	0	-2.553744	-1.172269	-1.212376
20	6	0	-3.948694	-1.195995	1.215633
21	1	0	-2.011838	-1.207882	2.152743
22	6	0	-3.948659	-1.195808	-1.215790
23	1	0	-2.011778	-1.207534	-2.152849
24	6	0	-4.653397	-1.222179	-0.000091
25	1	0	-4.493471	-1.266315	2.152978
26	1	0	-4.493410	-1.265976	-2.153162
27	6	0	-0.514465	-3.647481	-0.000004
28	7	0	-0.413063	-1.150775	-0.000024
29	9	0	0.316748	-4.677199	-0.000068
30	9	0	-1.284329	-3.714318	1.086008
31	9	0	-1.284473	-3.714299	-1.085910
32	7	0	-0.422186	1.196994	-0.000041
33	8	0	3.709995	-1.283675	0.000043
34	1	0	-0.341298	5.749658	-0.000260
35	6	0	1.713037	7.296903	-0.000071
36	1	0	1.109791	7.425370	-0.902421
37	1	0	1.109561	7.425380	0.902125
38	1	0	2.523367	8.021973	0.000028
39	8	0	2.355979	6.009755	0.000020
40	17	0	-6.362685	-1.294254	-0.000119
41	38	0	-3.079689	1.615115	0.000200
42	38	0	5.964166	-2.117872	-0.000010

Rotational constants (GHZ): 0.1068633 0.0699955 0.0432776

SCF Done: E(RCAM-B3LYP) = -29.7755564424 A.U. after 1 cycles
NFock= 1 Conv=0.39D-14 -V/T= 4.4694
QCSCF skips out because SCF is already converged.

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 6 LCPTot= 360083 Len1MO= 931608 IndFrg= 6881339
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 360083 Len1MO= 931608 IndFrg= 1291691
Counterpoise corrected energy = -1847.990085297811
BSSE energy = 0.008926138302
sum of monomers = -1847.976308522411
complexation energy = -14.25 kcal/mole (raw)
complexation energy = -8.65 kcal/mole (corrected)

ix. Cs-3k-Cs



Cartesian coordinates of optimized structure

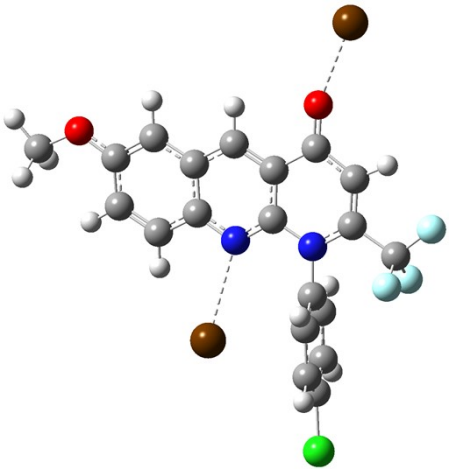
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.448599	-2.147429	0.310612
2	6	0	1.143103	-1.727728	0.345499
3	6	0	0.775357	-0.403145	0.004118
4	6	0	1.820729	0.485567	-0.365807
5	6	0	3.157863	0.034737	-0.417993
6	6	0	3.477619	-1.256212	-0.082638
7	6	0	1.453926	1.814796	-0.648522
8	6	0	0.151260	2.209046	-0.526515
9	6	0	-0.827730	1.238315	-0.152862
10	6	0	-2.472860	3.007314	-0.148928
11	6	0	-1.587209	3.954059	-0.508159
12	6	0	-0.196540	3.629984	-0.773448
13	1	0	0.373545	-2.406275	0.697550
14	1	0	3.935207	0.723617	-0.731677
15	1	0	2.180851	2.564750	-0.946738

16	1	0	-1.895232	4.987019	-0.584503
17	6	0	-3.169089	0.676208	0.293010
18	6	0	-4.100120	0.320723	-0.676600
19	6	0	-3.240071	0.123030	1.568935
20	6	0	-5.116481	-0.580060	-0.370967
21	1	0	-4.057991	0.776259	-1.659276
22	6	0	-4.236816	-0.792171	1.875652
23	1	0	-2.522199	0.421728	2.323970
24	6	0	-5.172633	-1.138450	0.901693
25	1	0	-5.871927	-0.830659	-1.107633
26	1	0	-4.311348	-1.214967	2.871105
27	6	0	-3.900984	3.441544	0.150897
28	7	0	-2.155622	1.651705	-0.015600
29	9	0	-3.984738	4.766411	0.204010
30	9	0	-4.748374	3.020019	-0.800659
31	9	0	-4.318235	2.952286	1.324386
32	7	0	-0.534398	-0.029982	0.065985
33	8	0	0.641289	4.437082	-1.136380
34	1	0	2.685174	-3.161851	0.606223
35	6	0	5.115742	-2.996098	-0.066162
36	1	0	4.916075	-3.417407	0.924197
37	1	0	4.564939	-3.559776	-0.824532
38	1	0	6.181986	-3.084673	-0.278435
39	8	0	4.801921	-1.607829	-0.121511
40	17	0	-6.410611	-2.297053	1.275584
41	55	0	-2.471139	-2.946972	-0.827352
42	55	0	7.605792	0.351580	0.389438

Rotational constants (GHZ): 0.1283497 0.0352046 0.0287929

SCF Done: E(RCAM-B3LYP) = -19.7019955092 A.U. after 1 cycles
NFock= 1 Conv=0.28D-12 -V/T= 5.0390
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 6 LCPTot= 360083 Len1MO= 931608 IndFrg= 6881339
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 360083 Len1MO= 931608 IndFrg= 1291691
Counterpoise corrected energy = -1827.811241769859
BSSE energy = 0.004693813302
sum of monomers = -1827.836844153083
complexation energy = 13.12 kcal/mole (raw)
complexation energy = 16.07 kcal/mole (corrected)

x. Ba-3k-Ba



Cartesian coordinates of optimized structure

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.970100	4.743707	-0.336825
2	6	0	-1.351415	3.424264	-0.314319
3	6	0	-0.424455	2.372216	-0.134227
4	6	0	0.950353	2.755399	-0.019025
5	6	0	1.331318	4.110041	-0.019740
6	6	0	0.393309	5.116904	-0.159580
7	6	0	1.887107	1.717731	0.051464
8	6	0	1.495534	0.394506	0.012213
9	6	0	0.091905	0.115915	-0.046059
10	6	0	0.613208	-2.228095	-0.060389
11	6	0	1.952286	-1.998210	-0.018980
12	6	0	2.487533	-0.679468	0.025116
13	1	0	-2.393549	3.218611	-0.552731
14	1	0	2.375373	4.387328	0.074072
15	1	0	2.944777	1.945902	0.117793
16	1	0	2.617461	-2.849434	-0.027504
17	6	0	-1.734786	-1.534058	-0.113841
18	6	0	-2.405548	-1.917081	1.047580
19	6	0	-2.398431	-1.525925	-1.342481
20	6	0	-3.751904	-2.279320	0.986772
21	1	0	-1.872617	-1.981700	1.991184
22	6	0	-3.743190	-1.878420	-1.408424
23	1	0	-1.859577	-1.274998	-2.250900
24	6	0	-4.422305	-2.265119	-0.243252
25	1	0	-4.265689	-2.634307	1.875626
26	1	0	-4.254421	-1.917528	-2.365831
27	6	0	0.132050	-3.684076	-0.107377
28	7	0	-0.323270	-1.223867	-0.058037
29	9	0	1.170490	-4.499533	-0.218215
30	9	0	-0.525009	-3.982862	1.015659

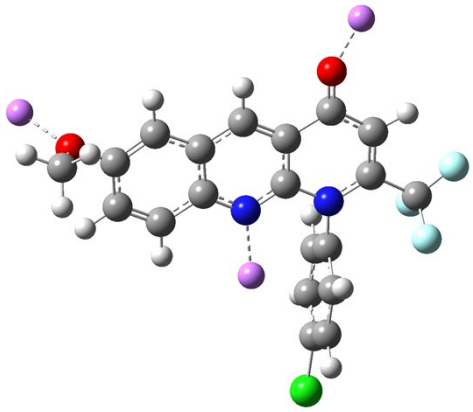
31	9	0	-0.675706	-3.874605	-1.148556
32	7	0	-0.839377	1.063494	-0.088663
33	8	0	3.730775	-0.460643	0.061727
34	1	0	-1.714903	5.511176	-0.511632
35	6	0	-0.065900	7.470667	-0.321683
36	1	0	-0.544342	7.428469	-1.303728
37	1	0	-0.810479	7.495539	0.478438
38	1	0	0.558208	8.359159	-0.261665
39	8	0	0.831590	6.362820	-0.146141
40	17	0	-6.076608	-2.716594	-0.324677
41	56	0	-3.750928	1.011714	0.434414
42	56	0	6.322969	-0.829167	0.070174

Rotational constants (GHZ): 0.1026918 0.0491138 0.0339951

SCF Done: E(RCAM-B3LYP) = -24.6184076656 A.U. after 1 cycles
NFock= 1 Conv=0.20D-13 -V/T= 5.2125
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 6 LCPTot= 360083 Len1MO= 931608 IndFrg= 6881339
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 360083 Len1MO= 931608 IndFrg= 1291691
Counterpoise corrected energy = -1837.636887108778
BSSE energy = 0.008459762774
sum of monomers = -1837.662655724651
complexation energy = 10.86 kcal/mole (raw)
complexation energy = 16.17 kcal/mole (corrected)

c. Interaction with three metal ion molecules

i. Li-3k-Li-Li



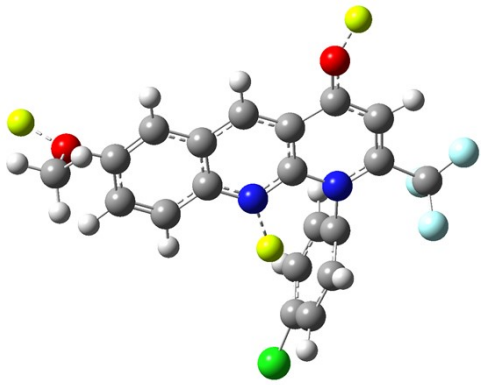
Cartesian coordinates of optimized structure

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.055299	2.088859	-0.164841
2	6	0	2.697180	1.932333	-0.146486
3	6	0	2.114418	0.638466	-0.122219
4	6	0	2.979640	-0.493239	-0.130409
5	6	0	4.391254	-0.309835	-0.154060
6	6	0	4.903434	0.954548	-0.170566
7	6	0	2.383061	-1.761955	-0.098204
8	6	0	1.009261	-1.891161	-0.058512
9	6	0	0.225048	-0.700731	-0.054810
10	6	0	-1.755992	-2.046186	0.020115
11	6	0	-1.054238	-3.207378	0.018664
12	6	0	0.372618	-3.210801	-0.017348
13	1	0	2.061845	2.812071	-0.143841
14	1	0	5.047116	-1.174438	-0.147550
15	1	0	2.986645	-2.664021	-0.099518
16	1	0	-1.592804	-4.144442	0.046788
17	6	0	-1.932527	0.417813	-0.002008
18	6	0	-2.208000	1.045037	1.214700
19	6	0	-2.286316	1.019810	-1.211010
20	6	0	-2.819614	2.297473	1.222218
21	1	0	-1.942293	0.564901	2.150503
22	6	0	-2.898060	2.272249	-1.204988
23	1	0	-2.081685	0.519750	-2.151665
24	6	0	-3.167112	2.913526	0.012022
25	1	0	-3.045490	2.791168	2.161219
26	1	0	-3.184756	2.746417	-2.137423
27	6	0	-3.284228	-2.097080	0.060842
28	7	0	-1.163119	-0.807031	-0.013625
29	9	0	-3.698442	-3.353826	0.087576
30	9	0	-3.730974	-1.470385	1.150266
31	9	0	-3.787225	-1.498021	-1.019832
32	7	0	0.756819	0.517693	-0.087032
33	8	0	1.054567	-4.259846	-0.014277
34	1	0	4.493420	3.081832	-0.174462
35	6	0	6.852331	1.317991	1.158471
36	1	0	6.400398	2.181396	1.649382
37	1	0	6.677817	0.410461	1.737751
38	1	0	7.925067	1.480985	1.043872
39	8	0	6.287334	1.157439	-0.181109
40	17	0	-3.925499	4.448982	0.020670
41	3	0	-0.525168	2.152113	-0.063159
42	3	0	1.260640	-6.046028	0.034891
43	3	0	7.458563	1.369748	-1.641821

Rotational constants (GHZ): 0.1878888 0.0989942 0.0679443

SCF Done: E(RCAM-B3LYP) = -7.26429228391 A.U. after 1 cycles
NFock= 1 Conv=0.54D-16 -V/T= 2.0092
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 8 LCPTot= 364953 Len1MO= 943371 IndFrg= 8855292
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 364953 Len1MO= 943371 IndFrg= 1308324
Counterpoise corrected energy = -1810.248257085240
BSSE energy = 0.013326532944
sum of monomers = -1810.219610155185
complexation energy = -26.34 kcal/mole (raw)
complexation energy = -17.98 kcal/mole (corrected)

ii. Be-3k-Be-Be



Cartesian coordinates of optimized structure

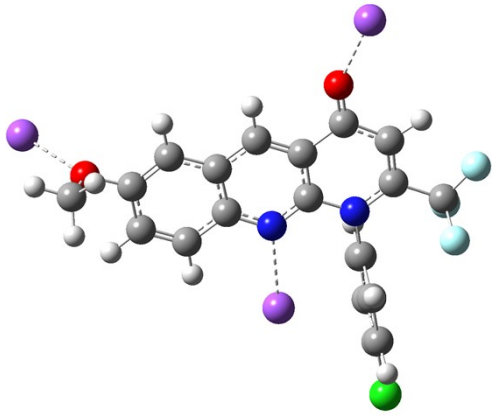
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.046343	-1.558563	-0.192201
2	6	0	-2.671435	-1.564151	-0.161526
3	6	0	-1.938252	-0.353032	-0.138856
4	6	0	-2.651634	0.890085	-0.159693
5	6	0	-4.091861	0.882265	-0.196582
6	6	0	-4.731873	-0.322834	-0.214623
7	6	0	-1.917494	2.089196	-0.128754
8	6	0	-0.515888	2.080152	-0.076229
9	6	0	0.116328	0.802952	-0.058314
10	6	0	2.273309	1.840725	0.031816
11	6	0	1.709432	3.105584	0.015785
12	6	0	0.331333	3.263015	-0.036383
13	1	0	-2.163169	-2.524129	-0.145107
14	1	0	-4.631500	1.825991	-0.198726
15	1	0	-2.439459	3.042666	-0.142721
16	1	0	2.386256	3.955116	0.046529

17	6	0	2.031282	-0.633401	0.013913
18	6	0	1.994637	-1.341004	1.235710
19	6	0	2.095813	-1.333741	-1.210912
20	6	0	1.957299	-2.743981	1.227746
21	1	0	1.884458	-0.814853	2.182469
22	6	0	2.058361	-2.736753	-1.214229
23	1	0	2.064587	-0.801808	-2.160344
24	6	0	2.074503	-3.482509	0.007318
25	1	0	1.875777	-3.283144	2.172295
26	1	0	2.055435	-3.270392	-2.165388
27	6	0	3.812168	1.639761	0.091869
28	7	0	1.505320	0.726252	-0.003550
29	9	0	4.404990	2.802457	0.120219
30	9	0	4.069983	0.934686	1.186729
31	9	0	4.156170	0.943826	-0.985055
32	7	0	-0.558070	-0.372360	-0.089696
33	8	0	-0.209847	4.475283	-0.049352
34	1	0	-4.583380	-2.505054	-0.191962
35	6	0	-6.846591	-0.386480	1.287497
36	1	0	-6.432808	-1.268995	1.774648
37	1	0	-6.566688	0.568113	1.730189
38	1	0	-7.933444	-0.467606	1.145688
39	8	0	-6.208210	-0.370548	-0.178424
40	17	0	2.163335	-5.141150	0.006168
41	4	0	0.547485	-1.721682	-0.050340
42	4	0	-0.139618	5.925080	-0.034822
43	4	0	-7.287341	-0.534379	-1.243503

Rotational constants (GHZ): 0.1733622 0.1058504 0.0689620

SCF Done: E(RCAM-B3LYP) = -13.6302816171 A.U. after 1 cycles
NFock= 1 Conv=0.22D-15 -V/T= 2.0080
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 8 LCPTot= 364953 Len1MO= 943389 IndFrg= 8855454
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 364953 Len1MO= 943389 IndFrg= 1308342
Counterpoise corrected energy = -1829.578211313144
BSSE energy = 0.017463929312
sum of monomers = -1829.255606195869
complexation energy = -213.40 kcal/mole (raw)
complexation energy = -202.44 kcal/mole (corrected)

iii. Na-3k-Na-Na



Cartesian coordinates of optimized structure

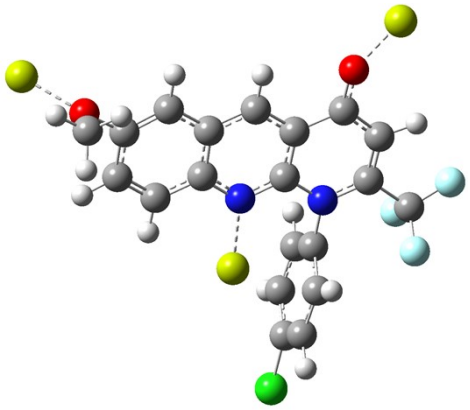
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.870020	-2.198634	-0.082838
2	6	0	2.511226	-2.051529	-0.043356
3	6	0	1.908639	-0.765106	-0.032201
4	6	0	2.771740	0.367544	-0.042240
5	6	0	4.182896	0.195975	-0.079335
6	6	0	4.714350	-1.061585	-0.102121
7	6	0	2.165654	1.632347	-0.031246
8	6	0	0.794781	1.751264	-0.009591
9	6	0	0.012434	0.555241	-0.000428
10	6	0	-1.966321	1.914418	0.049249
11	6	0	-1.265393	3.072374	0.038341
12	6	0	0.166949	3.081965	-0.001363
13	1	0	1.891631	-2.941555	-0.019968
14	1	0	4.829068	1.067568	-0.101182
15	1	0	2.759459	2.540751	-0.042247
16	1	0	-1.802602	4.009447	0.060455
17	6	0	-2.190267	-0.532305	0.020072
18	6	0	-2.640564	-1.056373	-1.190551
19	6	0	-2.534723	-1.137420	1.227592
20	6	0	-3.429907	-2.203745	-1.196986
21	1	0	-2.396766	-0.560824	-2.124274
22	6	0	-3.322496	-2.284982	1.226184
23	1	0	-2.207442	-0.704665	2.166927
24	6	0	-3.773732	-2.815874	0.012872
25	1	0	-3.807526	-2.606103	-2.130684
26	1	0	-3.617524	-2.750724	2.160068
27	6	0	-3.494025	1.993825	0.093534
28	7	0	-1.379146	0.665929	0.023796
29	9	0	-3.883521	3.261672	0.140282
30	9	0	-4.022675	1.431208	-0.994894
31	9	0	-3.962305	1.368836	1.175016

32	7	0	0.549723	-0.657733	-0.015793
33	8	0	0.843679	4.123950	-0.025516
34	1	0	4.315637	-3.187962	-0.099832
35	6	0	6.580207	-1.369899	-1.515504
36	1	0	6.120977	-2.227144	-2.013168
37	1	0	6.366576	-0.455501	-2.072681
38	1	0	7.660124	-1.517908	-1.466251
39	8	0	6.090794	-1.251543	-0.154470
40	17	0	-4.760505	-4.224637	0.009621
41	11	0	0.983994	6.362364	-0.089918
42	11	0	-0.742716	-2.866166	-0.151352
43	11	0	7.721890	-1.583800	1.512088

Rotational constants (GHZ): 0.1455542 0.0776223 0.0530272

SCF Done: E(RCAM-B3LYP) = 0.000000000000E+00 A.U. after 1 cycles
NFock= 1 Conv=0.00D+00 -V/T= 0.0000
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 8 LCPTot= 360618 Len1MO= 931578 IndFrg= 8744820
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 360618 Len1MO= 931578 IndFrg= 1292196
Counterpoise corrected energy = -1788.382094164396
BSSE energy = 0.011181539244
sum of monomers = -1788.428749041155
complexation energy = 22.26 kcal/mole (raw)
complexation energy = 29.28 kcal/mole (corrected)

iv. Mg-3k-Mg-Mg



Cartesian coordinates of optimized structure

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

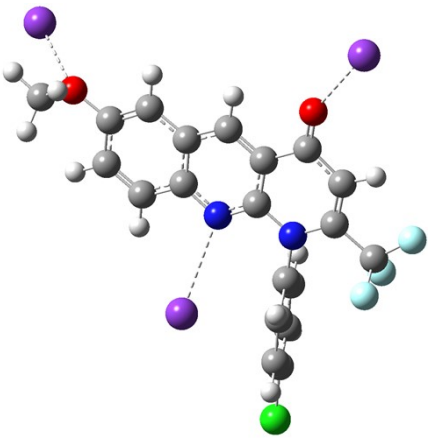
1	6	0	-3.877229	-2.084492	-0.020191
2	6	0	-2.509494	-1.969646	-0.046986
3	6	0	-1.869800	-0.704735	-0.056388
4	6	0	-2.697249	0.458122	-0.062454
5	6	0	-4.125926	0.324623	-0.046062
6	6	0	-4.685803	-0.923601	-0.020995
7	6	0	-2.058004	1.711485	-0.057407
8	6	0	-0.671134	1.815451	-0.043230
9	6	0	0.085491	0.595117	-0.039525
10	6	0	2.108945	1.882729	-0.016203
11	6	0	1.427095	3.067616	-0.018049
12	6	0	0.022325	3.110377	-0.027187
13	1	0	-1.931441	-2.891078	-0.043410
14	1	0	-4.739360	1.220986	-0.032529
15	1	0	-2.646306	2.624386	-0.058830
16	1	0	2.016356	3.976751	-0.010398
17	6	0	2.244992	-0.565002	-0.011276
18	6	0	2.543901	-1.186803	1.215654
19	6	0	2.575535	-1.194273	-1.226010
20	6	0	3.134358	-2.458842	1.228088
21	1	0	2.320953	-0.694806	2.159655
22	6	0	3.165947	-2.466407	-1.214992
23	1	0	2.377459	-0.707882	-2.178385
24	6	0	3.503306	-3.099214	0.013074
25	1	0	3.389176	-2.927980	2.177068
26	1	0	3.445588	-2.941338	-2.153999
27	6	0	3.657039	1.900497	-0.003426
28	7	0	1.477655	0.668226	-0.024195
29	9	0	4.078293	3.145141	-0.000262
30	9	0	4.077499	1.270017	1.087393
31	9	0	4.095045	1.269540	-1.087090
32	7	0	-0.493311	-0.623182	-0.047345
33	8	0	-0.626128	4.224836	-0.020993
34	1	0	-4.327122	-3.072990	0.017001
35	6	0	-6.549041	-1.032977	1.543079
36	1	0	-6.053815	-1.833335	2.093276
37	1	0	-6.307148	-0.048304	1.940684
38	1	0	-7.636631	-1.178930	1.572948
39	8	0	-6.110921	-1.091030	0.096940
40	17	0	4.333653	-4.559273	0.028448
41	12	0	0.847901	-2.374509	-0.022527
42	12	0	-0.600032	6.130753	0.009293
43	12	0	-7.696441	-1.560079	-1.037678

Rotational constants (GHZ): 0.1453320 0.0791892 0.0534348

SCF Done: E(RCAM-B3LYP) = 0.000000000000E+00 A.U. after 1 cycles
NFock= 1 Conv=0.00D+00 -V/T= 0.0000
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 8 LCPTot= 360618 Len1MO= 931578 IndFrg= 8744820
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 360618 Len1MO= 931578 IndFrg= 1292196
Counterpoise corrected energy = -1788.246260161371
BSSE energy = 0.013765434452
sum of monomers = -1788.404059532870
complexation energy = 90.38 kcal/mole (raw)
complexation energy = 99.02 kcal/mole (corrected)

v. K-3k-K-K



Cartesian coordinates of optimized structure

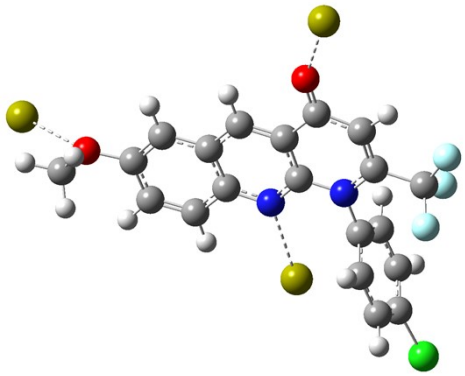
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.657248	-2.165979	-0.226365
2	6	0	2.296922	-2.049342	-0.154719
3	6	0	1.663948	-0.777025	-0.158746
4	6	0	2.500871	0.374308	-0.209153
5	6	0	3.913069	0.233140	-0.285738
6	6	0	4.476184	-1.011483	-0.298555
7	6	0	1.864455	1.624497	-0.181820
8	6	0	0.495054	1.708768	-0.092522
9	6	0	-0.254747	0.492008	-0.049883
10	6	0	-2.259311	1.797508	0.165127
11	6	0	-1.590825	2.972200	0.119932
12	6	0	-0.163309	3.026643	-0.039263
13	1	0	1.690323	-2.942910	-0.061750
14	1	0	4.539197	1.118021	-0.336884
15	1	0	2.432943	2.548213	-0.221863
16	1	0	-2.144401	3.894620	0.215105
17	6	0	-2.429421	-0.653080	0.087652
18	6	0	-3.118176	-1.057190	-1.051898

19	6	0	-2.546933	-1.368752	1.276644
20	6	0	-3.937092	-2.182619	-1.004676
21	1	0	-3.048868	-0.476930	-1.965430
22	6	0	-3.353540	-2.498535	1.327543
23	1	0	-2.029345	-1.029422	2.167218
24	6	0	-4.052507	-2.900065	0.186176
25	1	0	-4.509058	-2.484494	-1.875483
26	1	0	-3.474450	-3.048392	2.254327
27	6	0	-3.777039	1.846008	0.347726
28	7	0	-1.646942	0.563448	0.056164
29	9	0	-4.171375	3.095647	0.570854
30	9	0	-4.398384	1.407580	-0.751361
31	9	0	-4.156170	1.097361	1.383916
32	7	0	0.306258	-0.704912	-0.105104
33	8	0	0.472165	4.086390	-0.112899
34	1	0	4.129283	-3.143038	-0.219360
35	6	0	6.311881	-1.294863	-1.734282
36	1	0	5.867887	-2.168807	-2.218967
37	1	0	6.070168	-0.395610	-2.306485
38	1	0	7.396080	-1.417001	-1.704755
39	8	0	5.850059	-1.171038	-0.374277
40	17	0	-5.059162	-4.301433	0.248469
41	19	0	0.583215	6.739858	-0.240015
42	19	0	-1.007923	-3.454323	-0.853268
43	19	0	8.016599	-1.536305	1.478576

Rotational constants (GHZ): 0.1079116 0.0637180 0.0421561

SCF Done: E(RCAM-B3LYP) = -27.9367253505 A.U. after 1 cycles
NFock= 1 Conv=0.12D-12 -V/T= 3.7447
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 8 LCPTot= 378120 Len1MO= 978558 IndFrg= 9185142
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 378120 Len1MO= 978558 IndFrg= 1356678
Counterpoise corrected energy = -1872.159612347651
BSSE energy = 0.010412232030
sum of monomers = -1872.239679701604
complexation energy = 43.71 kcal/mole (raw)
complexation energy = 50.24 kcal/mole (corrected)

vi. Ca-3k-Ca-Ca



Cartesian coordinates of optimized structure

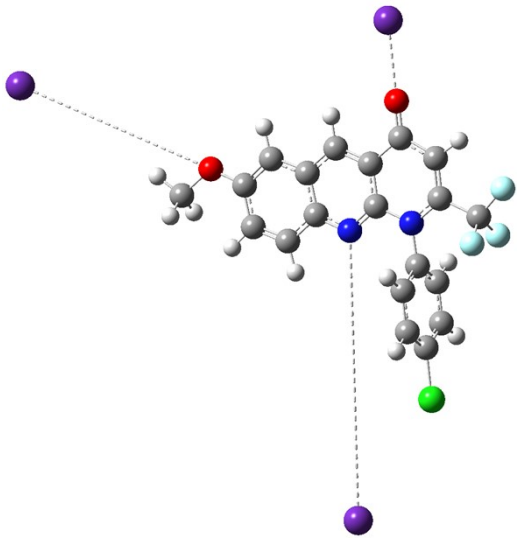
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.781943	-2.072588	0.118674
2	6	0	-2.413444	-2.001638	0.062157
3	6	0	-1.723003	-0.762115	0.033787
4	6	0	-2.519552	0.420205	0.034744
5	6	0	-3.946964	0.332635	0.082549
6	6	0	-4.561116	-0.890668	0.132335
7	6	0	-1.837468	1.650970	0.016067
8	6	0	-0.455290	1.704284	-0.005042
9	6	0	0.263397	0.455696	-0.009444
10	6	0	2.319885	1.693207	-0.078550
11	6	0	1.677570	2.890684	-0.070004
12	6	0	0.264768	2.993087	-0.019682
13	1	0	-1.866494	-2.942336	0.049400
14	1	0	-4.528919	1.249151	0.100827
15	1	0	-2.389327	2.585847	0.021830
16	1	0	2.288035	3.782713	-0.102733
17	6	0	2.430841	-0.742258	-0.025176
18	6	0	2.892887	-1.258382	1.194180
19	6	0	2.815068	-1.339256	-1.234332
20	6	0	3.704659	-2.395824	1.208662
21	1	0	2.655223	-0.761628	2.131246
22	6	0	3.626232	-2.476837	-1.224504
23	1	0	2.516126	-0.905385	-2.184820
24	6	0	4.113149	-2.994901	-0.003708
25	1	0	4.104166	-2.767518	2.149438
26	1	0	3.965384	-2.911569	-2.161848
27	6	0	3.864206	1.699985	-0.138612
28	7	0	1.657470	0.486433	-0.039079
29	9	0	4.294166	2.947335	-0.185113
30	9	0	4.355999	1.105973	0.943909
31	9	0	4.267727	1.054701	-1.228302
32	7	0	-0.348713	-0.737227	0.015974
33	8	0	-0.320565	4.117834	0.008160

34	1	0	-4.267584	-3.042376	0.166366
35	6	0	-6.341839	-0.885765	1.692629
36	1	0	-5.875904	-1.680546	2.277737
37	1	0	-6.055164	0.094159	2.075293
38	1	0	-7.431681	-0.979401	1.775583
39	8	0	-5.968243	-1.009164	0.271220
40	17	0	5.187667	-4.305980	0.005269
41	20	0	0.992859	-3.063516	0.110227
42	20	0	-0.235526	6.447018	0.055178
43	20	0	-8.195750	-1.569925	-0.907206

Rotational constants (GHZ): 0.1163267 0.0618908 0.0418593

SCF Done: E(RCAM-B3LYP) = -35.8434693286 A.U. after 1 cycles
NFock= 1 Conv=0.41D-15 -V/T= 3.8132
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 8 LCPTot= 378120 Len1MO= 978558 IndFrg= 9185142
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 378120 Len1MO= 978558 IndFrg= 1356678
Counterpoise corrected energy = -1895.609107521840
BSSE energy = 0.012587770584
sum of monomers = -1895.945414799272
complexation energy = 203.14 kcal/mole (raw)
complexation energy = 211.04 kcal/mole (corrected)

vii. Rb-3k-Rb-Rb



Cartesian coordinates of optimized structure

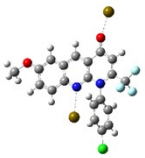
Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000034785	0.002264219	0.000947214
2	6	-0.003906814	-0.008781000	0.000362396
3	6	-0.000823251	-0.000744958	0.000281230
4	6	-0.001159989	0.002902708	-0.000021931
5	6	0.000603034	-0.000194358	-0.000026800
6	6	0.003661788	0.001394080	-0.000008373
7	6	0.002674123	-0.001907046	-0.000110103
8	6	-0.000795737	-0.000525680	0.001833224
9	6	-0.001807189	0.002468530	-0.003617364
10	6	-0.000038833	-0.000389503	-0.001101391
11	6	0.002179047	-0.001879133	0.001626785
12	6	0.001695555	-0.004360329	-0.001858635
13	1	0.000211628	0.004040216	-0.000335526
14	1	0.000285633	0.000003736	0.000041526
15	1	0.000459906	-0.000176474	0.000052591
16	1	0.000095076	0.000671303	-0.000268805
17	6	-0.000936233	0.003812066	0.001316571
18	6	0.000741137	0.001287045	-0.000579680
19	6	0.000448562	0.002690843	-0.000085191
20	6	0.000020509	0.000094736	-0.000424816
21	1	-0.000009315	-0.000746172	-0.000179416
22	6	-0.000081910	0.000732741	-0.000005358
23	1	-0.000169996	-0.000375862	0.000419158
24	6	0.001725765	-0.001839297	0.000338042
25	1	-0.000056982	0.000510041	0.000373609
26	1	-0.000051644	-0.000325992	-0.000174831
27	6	-0.004397106	0.002272107	0.000240886
28	7	0.000366507	0.000204925	0.000387013
29	9	-0.000238336	-0.002302469	0.000209338
30	9	0.000970031	-0.000256180	0.000241051
31	9	0.001415078	-0.001782538	-0.000379765
32	7	0.000715517	-0.002656823	0.000525083
33	8	0.001214005	0.006006431	0.000642820
34	1	0.000166856	0.000096496	-0.000405817
35	6	0.002252503	-0.001683174	-0.000761459
36	1	0.000078389	0.000585099	0.000076165
37	1	-0.000137770	0.000153919	0.000265390
38	1	-0.000250113	0.001237417	-0.000040837
39	8	-0.005620995	-0.001962104	0.000355409
40	17	-0.001844935	0.000376254	-0.000107896
41	37	-0.001053955	-0.000862786	-0.000028503
42	37	0.000397924	-0.002098811	0.000074047
43	37	0.000967742	0.002045779	-0.000087048

Cartesian Forces: Max 0.008781000 RMS 0.001755589

SCF Done: E(RCAM-B3LYP) = -23.6734311154 A.U. after 1 cycles

NFock= 1 Conv=0.34D-13 -V/T= 4.3225
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 8 LCPTot= 378120 Len1MO= 978576 IndFrg= 9185304
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 378120 Len1MO= 978576 IndFrg= 1356696
Counterpoise corrected energy = -1859.394084083040
BSSE energy = 0.003752020806
sum of monomers = -1859.454969235119
complexation energy = 35.85 kcal/mole (raw)
complexation energy = 38.21 kcal/mole (corrected)

viii. Sr-3k-Sr-Sr



Cartesian coordinates of optimized structure

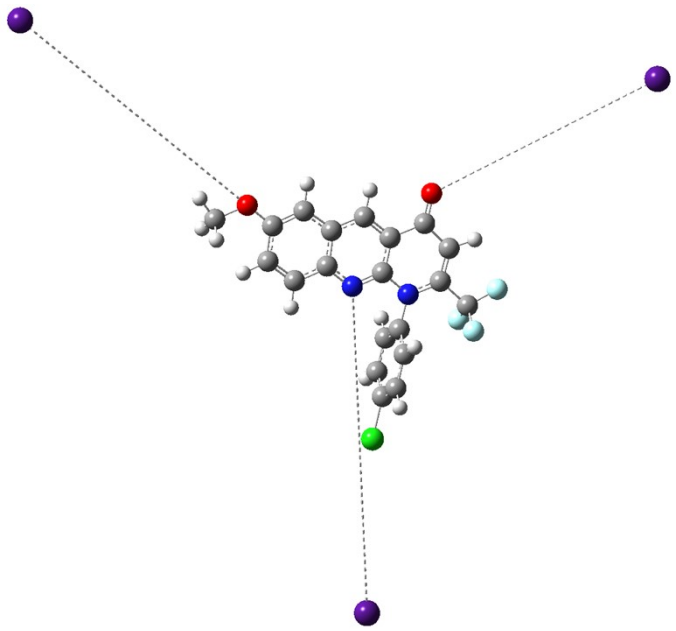
Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000440008	-0.000684018	0.000362102
2	6	-0.000271194	0.000223055	-0.000154922
3	6	-0.000051784	-0.000048238	0.000056234
4	6	0.000232719	-0.000301986	0.000193132
5	6	-0.000635733	0.000877028	0.000024107
6	6	0.000265229	0.000452462	-0.000328562
7	6	-0.000189756	0.000149657	0.000018259
8	6	0.000130020	0.000007869	-0.000049729
9	6	-0.000236516	0.000073744	0.000070540
10	6	0.000048251	-0.000063478	0.000034695
11	6	-0.000056078	0.000040142	0.000028047
12	6	0.000272884	-0.000149940	-0.000166825

13	1	0.000105099	0.000006027	-0.000089856
14	1	0.000180907	-0.000136033	0.000093693
15	1	0.000012283	-0.000043935	0.000034263
16	1	0.000003542	0.000011032	-0.000019268
17	6	-0.000171144	0.000032171	-0.000174763
18	6	0.000005713	-0.000066139	-0.000049768
19	6	-0.000029051	-0.000044470	0.000038606
20	6	-0.000021997	-0.000001264	0.000001941
21	1	0.000033178	0.000013626	0.000026843
22	6	0.000046461	0.000014922	-0.000027825
23	1	0.000020500	-0.000014915	0.000079842
24	6	-0.000004505	0.000085528	0.000047330
25	1	0.000007440	0.000044108	-0.000029431
26	1	0.000032966	0.000003517	0.000003945
27	6	0.000146842	-0.000021703	-0.000002348
28	7	0.000108793	0.000298426	0.000116243
29	9	0.000031572	-0.000003751	-0.000065807
30	9	-0.000069667	0.000087217	-0.000093858
31	9	-0.000018610	-0.000069841	0.000035006
32	7	0.000058142	0.000100093	-0.000022115
33	8	-0.000365024	0.000046269	0.000321209
34	1	-0.000168895	0.000110565	-0.000147130
35	6	0.000370995	0.000626066	0.000100762
36	1	-0.000048484	-0.000060451	-0.000028300
37	1	0.000049846	-0.000073423	-0.000163762
38	1	-0.000089780	0.000130392	0.000024194
39	8	-0.000664895	-0.001805703	0.000174908
40	17	0.000059689	-0.000021070	-0.000054744
41	38	0.000241301	0.000023708	-0.000082577
42	38	0.000082400	-0.000045788	-0.000102554
43	38	0.000106332	0.000198520	-0.000031757

Cartesian Forces: Max 0.001805703 RMS 0.000250883

SCF Done: E(RCAM-B3LYP) = -29.7755564424 A.U. after 1 cycles
NFock= 1 Conv=0.30D-15 -V/T= 4.4694
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 8 LCPTot= 378120 Len1MO= 978576 IndFrg= 9185304
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 378120 Len1MO= 978576 IndFrg= 1356696
Counterpoise corrected energy = -1877.722924607608
BSSE energy = 0.009086538520
sum of monomers = -1877.751828392092
complexation energy = 12.44 kcal/mole (raw)
complexation energy = 18.14 kcal/mole (corrected)

ix. Cs-3k-Cs-Cs



Cartesian coordinates of optimized structure

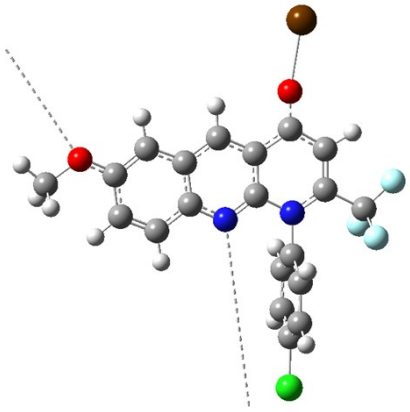
Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000540060	-0.000533253	0.000005769
2	6	0.000231823	-0.000128822	0.000207315
3	6	-0.001137740	0.000595126	-0.000342688
4	6	-0.000509110	0.000613428	-0.000233514
5	6	0.000539590	-0.000806900	0.000125126
6	6	-0.002094397	0.001984636	0.000433302
7	6	0.000597919	-0.000163232	-0.000071050
8	6	-0.000025688	-0.000769318	-0.000121348
9	6	-0.001366191	0.000399328	-0.000060331
10	6	-0.000248379	-0.000101046	0.000031911
11	6	-0.000061823	0.000396166	-0.000041475
12	6	-0.000543251	0.000820731	0.000904335
13	1	-0.000169076	-0.000112655	0.000001367
14	1	-0.000081294	0.000098506	-0.000010413
15	1	-0.000112201	0.000043833	0.000004041
16	1	-0.000021125	-0.000203488	-0.000081230
17	6	0.000398107	-0.000673562	0.000815676
18	6	0.000028008	0.000294502	-0.000095049
19	6	-0.000035499	-0.000754463	-0.000402140
20	6	0.000313361	0.000521494	-0.000571514
21	1	0.000085856	-0.000228848	0.000119283
22	6	0.000405672	0.001046175	-0.000060587
23	1	0.000040416	0.000009155	0.000017253
24	6	-0.000742956	-0.001645532	0.000406896
25	1	-0.000090929	-0.000019845	0.000236001
26	1	0.000043272	-0.000149344	-0.000191226

27	6	0.000038360	0.000273337	-0.000677569
28	7	0.000787521	0.000457195	-0.000346125
29	9	0.000150253	-0.000223318	0.000031361
30	9	-0.000200386	-0.000124134	0.000778395
31	9	-0.000159750	0.000294260	-0.000189817
32	7	0.001374766	-0.001091064	0.000377290
33	8	0.000385057	0.000040778	-0.000525934
34	1	-0.000468699	0.000121828	0.000074633
35	6	0.002045545	-0.000354386	0.000070206
36	1	0.000390102	0.000194166	-0.000141302
37	1	-0.000101300	-0.000132775	0.000060048
38	1	0.000378958	-0.000021481	0.000166100
39	8	0.000873042	-0.000678173	-0.000699066
40	17	-0.000074280	0.000742824	-0.000025362
41	55	0.000306494	0.000432723	0.000019123
42	55	-0.000784128	-0.000058301	0.000024675
43	55	0.000154141	-0.000406250	-0.000022364

Cartesian Forces: Max 0.002094397 RMS 0.000555593

SCF Done: E(RCAM-B3LYP) = -19.7019955092 A.U. after 1 cycles
NFock= 1 Conv=0.75D-12 -V/T= 5.0390
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 8 LCPTot= 378120 Len1MO= 978576 IndFrg= 9185304
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 378120 Len1MO= 978576 IndFrg= 1356696
Counterpoise corrected energy = -1847.485037079681
BSSE energy = 0.000108722425
sum of monomers = -1847.542720773608
complexation energy = 36.13 kcal/mole (raw)
complexation energy = 36.20 kcal/mole (corrected)

x. Ba-3k-Ba-Ba



Cartesian coordinates of optimized structure

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.001116582	0.000217133	-0.000148014
2	6	0.001116012	0.001188038	0.000524990
3	6	0.000578120	-0.000614086	-0.000251506
4	6	0.000174142	-0.000984181	-0.000227017
5	6	-0.000948634	0.000555871	0.000338193
6	6	0.000258323	-0.001411306	-0.000460954
7	6	-0.000635373	0.000007536	0.000070494
8	6	-0.000866417	0.000133242	0.000120652
9	6	-0.001090976	0.000899284	0.000333773
10	6	-0.000152536	0.000450183	0.000496503
11	6	-0.000133504	0.000371679	0.000052621
12	6	-0.000534681	-0.000288982	0.000188274
13	1	-0.000060482	0.000423358	-0.000176556
14	1	-0.000162077	-0.000048734	-0.000002524
15	1	-0.000245448	-0.000103741	-0.000001044
16	1	0.000292965	-0.000387915	-0.000162650
17	6	0.000441681	-0.000461239	0.000094929
18	6	-0.000125752	-0.000272254	0.000247256
19	6	-0.000386377	-0.000186994	-0.000425365
20	6	0.000360882	0.000262282	-0.000523703
21	1	0.000139837	-0.000047070	0.000324281
22	6	0.000167949	0.000104301	-0.000248467
23	1	0.000202532	0.000190172	-0.000443213
24	6	0.000067979	-0.000087598	0.000443694
25	1	-0.000079644	-0.000157412	0.000548256
26	1	-0.000221272	0.000064718	-0.000428480
27	6	-0.000061583	0.000341787	-0.001095682
28	7	-0.000030613	0.000813662	0.000335485
29	9	0.000134446	-0.000686261	-0.000216614
30	9	-0.000315580	-0.000223890	0.000698486
31	9	0.000274320	-0.000187016	0.000154025
32	7	0.001977564	-0.000664571	-0.000463230
33	8	0.000462256	-0.000120559	-0.000233254
34	1	-0.001170295	0.000833209	0.000347682
35	6	-0.000179646	0.000861384	0.000188937
36	1	-0.000430040	0.000004596	-0.000461563
37	1	-0.000214806	-0.000347305	0.000534389
38	1	-0.000330103	0.000254902	0.000012325
39	8	0.000572697	-0.000676153	-0.000155130
40	17	0.000179047	0.000050207	0.000037954
41	56	-0.000057121	-0.000039563	-0.000000490
42	56	-0.000118221	-0.000085901	0.000034366
43	56	0.000033848	0.000055188	-0.000002111

Cartesian Forces: Max 0.001977564 RMS 0.000485585

SCF Done: E(RCAM-B3LYP) = -24.6184076656 A.U. after 1 cycles
NFock= 1 Conv=0.53D-14 -V/T= 5.2125
QCSCF skips out because SCF is already converged.
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
Cartesian Forces: Max 0.000000000 RMS 0.000000000
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 8 LCPTot= 378120 Len1MO= 978576 IndFrg= 9185304
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 378120 Len1MO= 978576 IndFrg= 1356696
Counterpoise corrected energy = -1862.377304852748
BSSE energy = 0.004354600380
sum of monomers = -1862.283405026697
complexation energy = -61.66 kcal/mole (raw)
complexation energy = -58.92 kcal/mole (corrected)