

**Synthetic and Structural Investigations of  
Bis(N-alkyl-benzoselenadiazolium) cations**

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**Supporting Information**

**Table S1. Crystallographic and Refinement Parameters for the salts of the dications 4a-d.**

	[4a]Cl <sub>2</sub> ·4H <sub>2</sub> O	[4a](CF <sub>3</sub> SO <sub>3</sub> ) <sub>2</sub>	[4b](CF <sub>3</sub> SO <sub>3</sub> ) <sub>2</sub>	[4c]Cl <sub>2</sub> ·H <sub>2</sub> O	[4d](BF <sub>4</sub> ) <sub>2</sub>	[4d](BF <sub>4</sub> ) <sub>2</sub> ·(CH <sub>3</sub> CN)
CCDC	1912322	1912323	1912324	1912321	1912325	1914922
Chemical formula	C <sub>14</sub> H <sub>12</sub> N <sub>4</sub> Se <sub>2</sub> Cl <sub>2</sub> ·5·4(H <sub>2</sub> O)	C <sub>14</sub> H <sub>12</sub> N <sub>4</sub> Se <sub>2</sub> (CF <sub>3</sub> O <sub>3</sub> S) <sub>2</sub>	C <sub>15</sub> H <sub>14</sub> N <sub>4</sub> Se <sub>2</sub> (CF <sub>3</sub> O <sub>3</sub> S) <sub>2</sub>	C <sub>18</sub> H <sub>18</sub> N <sub>4</sub> Se <sub>2</sub> Cl <sub>2</sub> ·H <sub>2</sub> O	C <sub>20</sub> H <sub>16</sub> N <sub>4</sub> Se <sub>2</sub> (BF <sub>4</sub> ) <sub>2</sub>	C <sub>20</sub> H <sub>16</sub> N <sub>4</sub> Se <sub>2</sub> (BF <sub>4</sub> ) <sub>2</sub> ·(CH <sub>3</sub> CN)
Crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
a [Å]	7.624(2)	8.3966(16)	11.9799(2)	8.9756(3)	6.4979(3)	10.353(2)
b [Å]	7.942(2)	11.300(2)	29.8901(6)	12.4952(4)	11.9131(6)	7.3989(17)
c [Å]	18.270(5)	11.9466(19)	6.63540(10)	9.3428(3)	14.6745(8)	33.631(7)
α [°]	83.560(5)	90.953(3)	90	90	90	90
β [°]	77.649(5)	90.846(4)	93.9400(10)	108.347(2)	97.399(3)	93.402(5)
γ [°]	71.357(4)	94.122(4)	90	90	90	90
V [Å <sup>3</sup> ]	1022.9(5)	1130.3(4)	2370.39(7)	994.55(6)	1126.50(10)	2571.5(10)
T [K]	296(2)	296(2)	100(2)	100(2)	100(2)	100(2)
Space group	P -1	P -1	P 1 21/c 1	P 1 21 1	P 1 21/n 1	P 1 21/n 1
Z	2	2	4	2	2	4
No. of reflections measured	15656	22047	84681	35869	27865	7022
No. independent reflections	4016	4636	7252	10311	4295	5030
Final R <sub>i</sub> values (I > 2σ(I))	0.0564	0.0252	0.0281	0.0356	0.0294	0.0470
Final wR(F <sup>2</sup> ) values (I > 2σ(I))	0.1387	0.0562	0.0655	0.0583	0.0703	0.1080
Final R1* values (all data)	0.0699	0.0388	0.0325	0.0602	0.0411	0.0883
Final wR2*(F <sup>2</sup> ) values (all data)	0.1459	0.0593	0.0669	0.0635	0.0744	0.1410

\* R1 =  $\sum ||F_o| - |F_c|| / \sum |F_o|$ , wR2 =  $\{\sum [w(F_o^2 - F_c^2)^2] / \sum w(F_o^2)^2\}^{1/2}$