Supporting Information

Supramolecular association of 1,2,5-chalcogenadiazoles : design of a self-assembled dissymetric $[Se^{\cdots}N]_2$ four-membered ring.

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1. Experimental Procedure

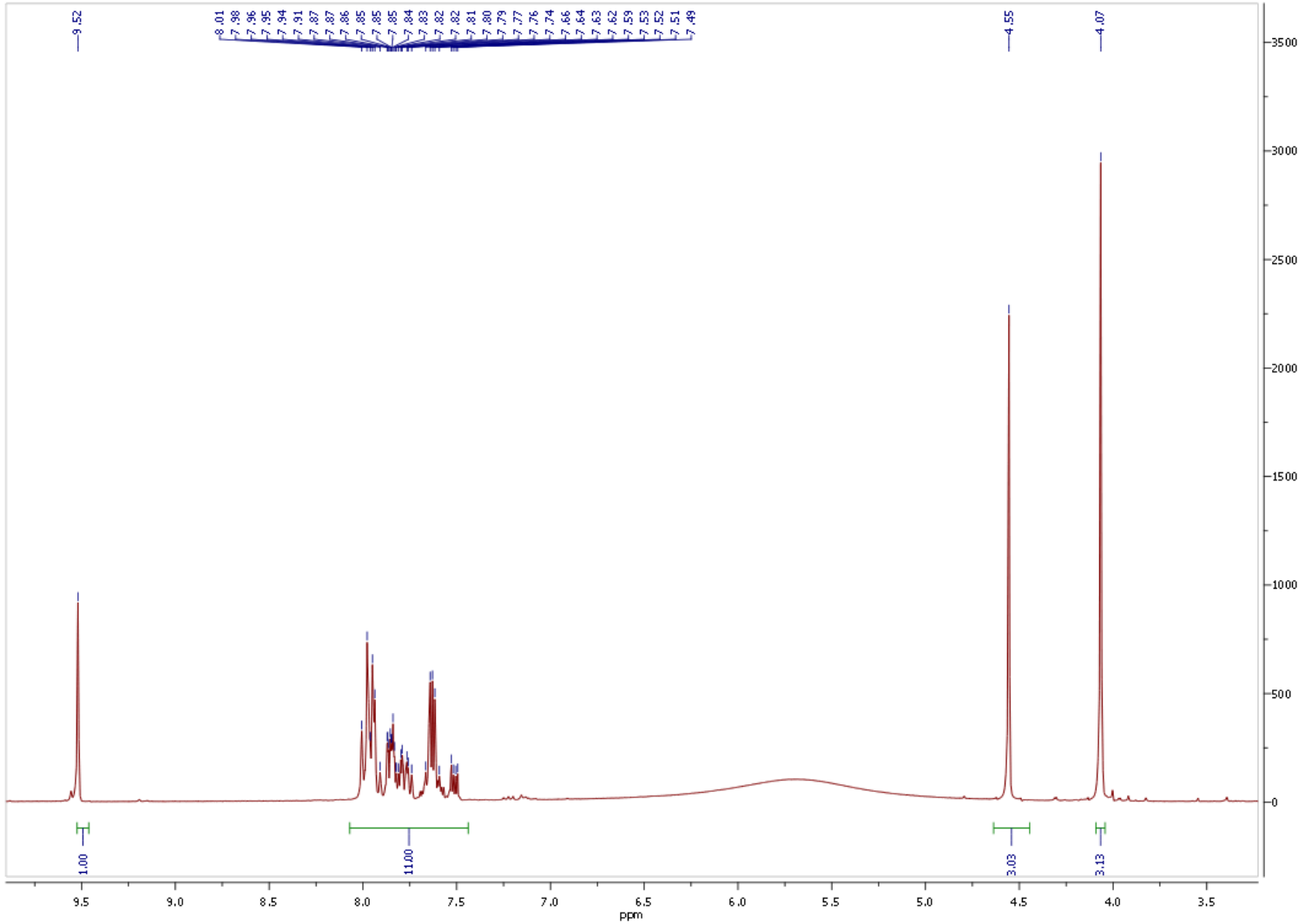
General data

General: Melting points were determined on a Reichert-type microscope and are uncorrected. ^{1}H, ^{19}F spectra and ^{13}C NMR spectra were recorded on a 300 MHz spectrometer. Internal reference was the residual peak of $CHCl_3$ (7.27 ppm) for ^{1}H (300 MHz) NMR spectra, central peak of $CDCl_3$ (77 ppm) for ^{13}C (75 MHz) NMR spectra, internal $CFCl_3$ (0 ppm) for ^{19}F (282 MHz) NMR spectra. Chemical shifts are reported in parts per million (ppm). Electronic Impact mass spectra (EI, 70eV) were obtained using a HEWLETT PACKARD 5989B and a NERMAG R10-10C spectrometer

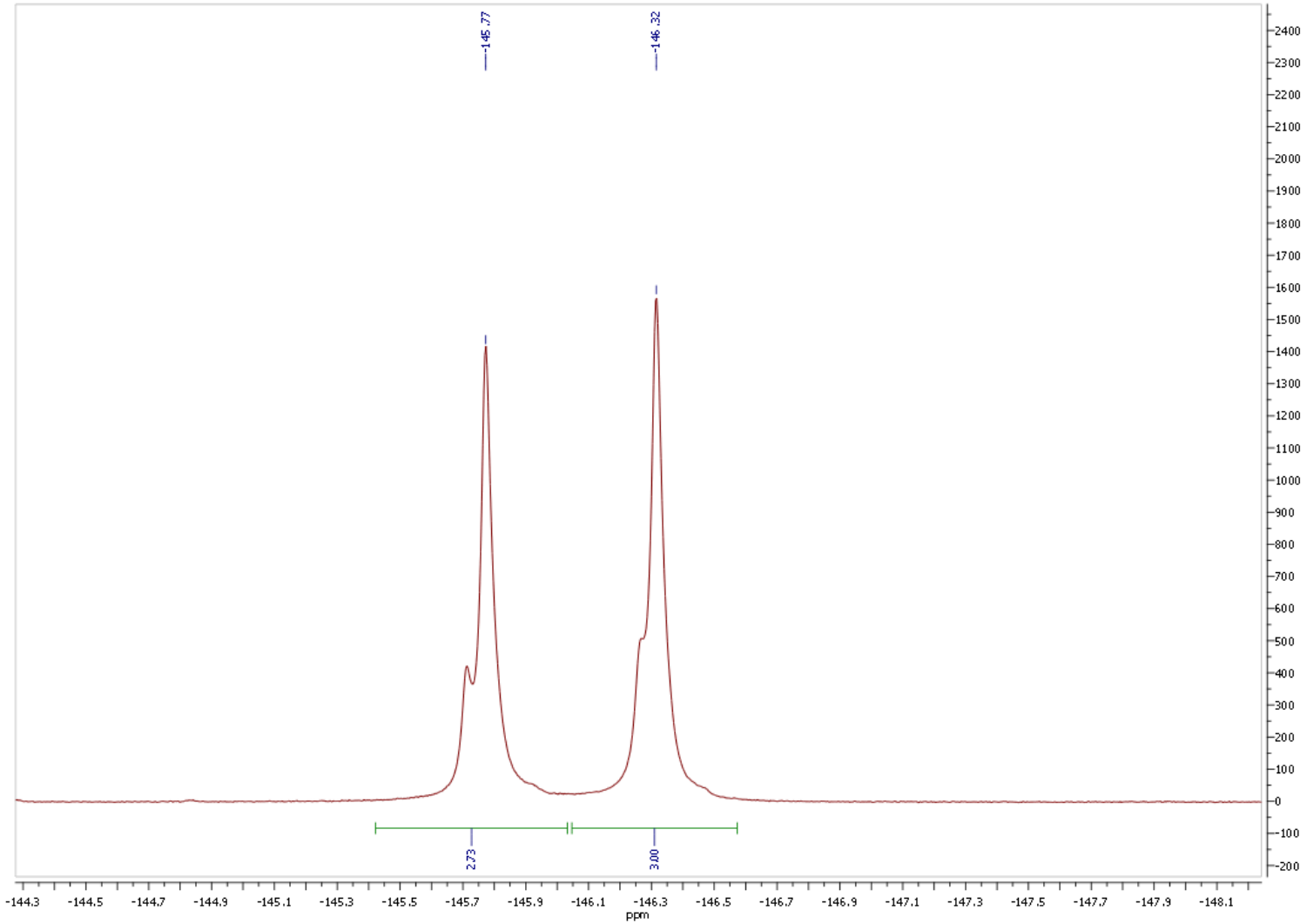
equipped with a quadrupole.

NMR spectra:

^{1}H NMR spectra oh [3-Se]$^{2+}$ in CD_3CN :



^{19}F NMR spectra of $[3\text{-}Se]^{2+}$ in CD_3CN :



2. Density functional theory calculations at the B3LYP/6-31G(d) level of theory.

Electrostatic potential (ESP)

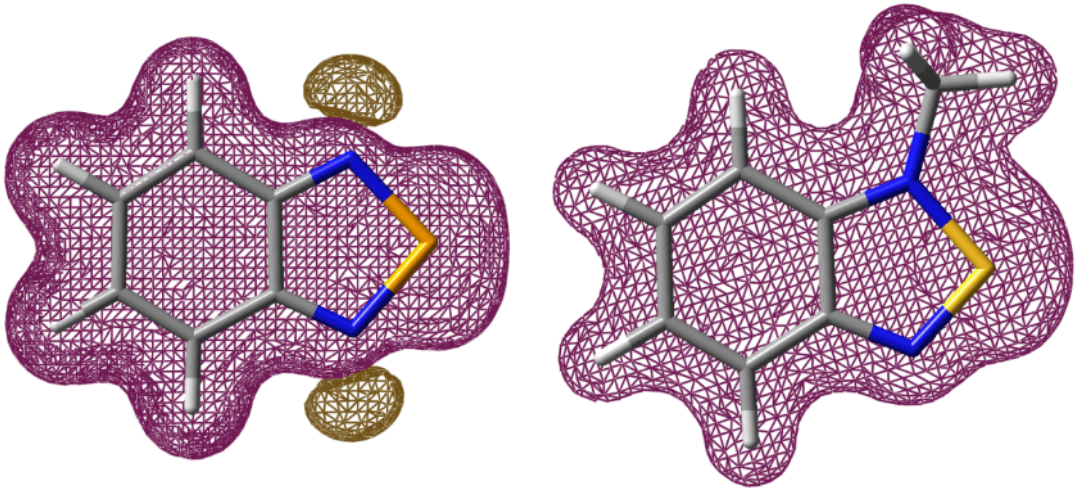


Figure S1 : Calculated 3D electrostatic potential (Isovalue = 0.05) onto the total electron density isosurface for the **2-Se** (left) and **[2-Se]**$^+$ (right) compounds in the gas phase using GAUSSIAN 03 package.[1] Brown indicates regions of net negative charge.

Natural Bond Orbital (NBO)

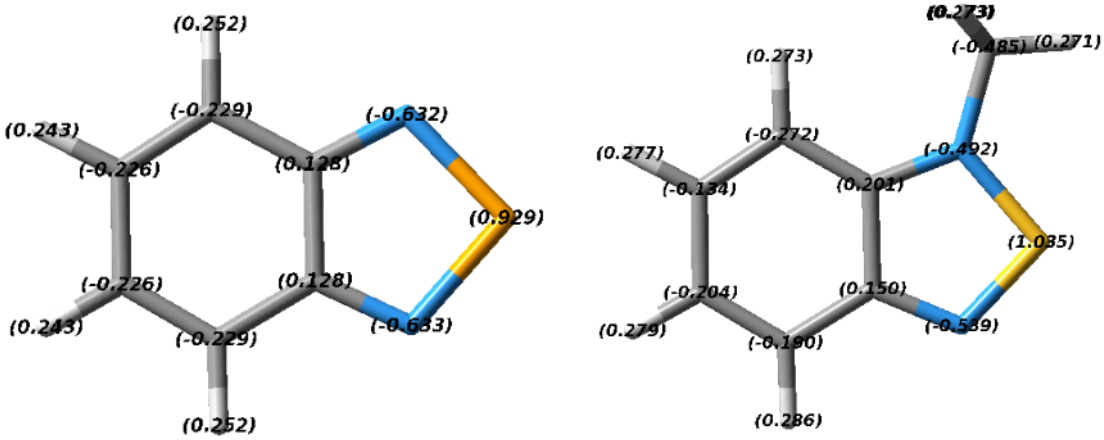
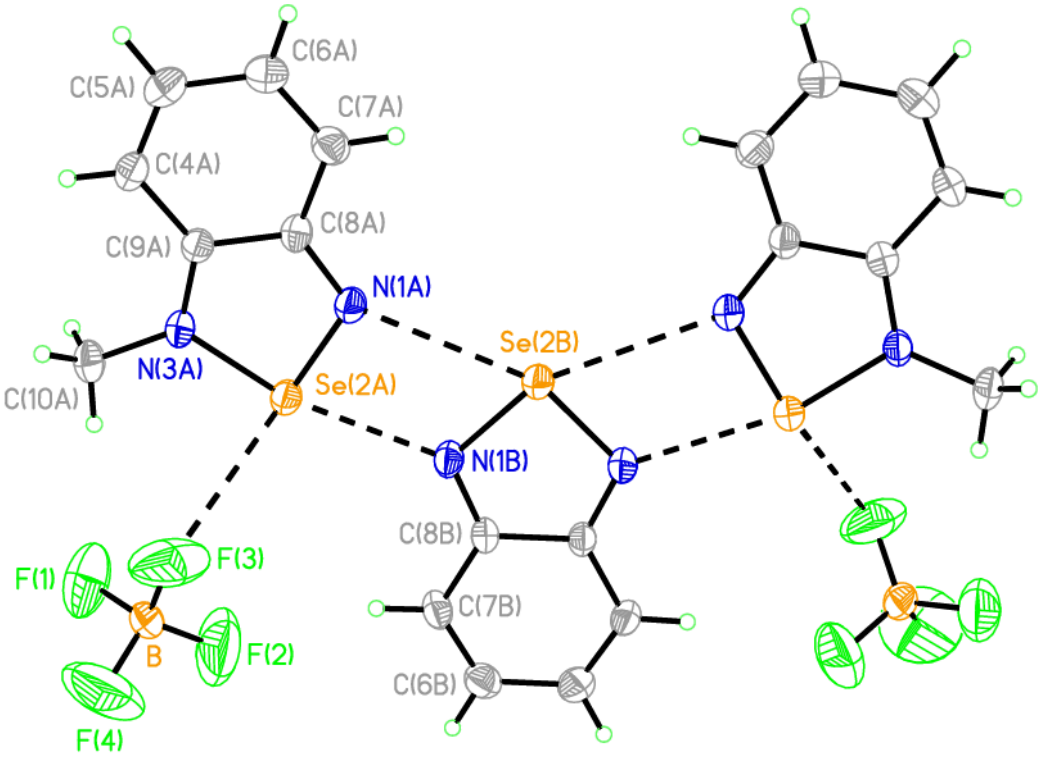


Figure S2 : Atomic charges were determined by the Natural Bond Orbital (NBO) analysis.

3. X-ray crystallographic data

ORTEP view of [3-Se]$^{2+}$



Bond lengths [Å] for [3-Se]$^{2+}$

Se(2A)-N(1A)	1.767(2)
Se(2A)-N(3A)	1.8504(19)
Se(2A)···N(1B)	2.5732(19)
Se(2B)···N(1A)	2.9666(9)
Se(2B)-N(1B)	1.800(2)
N(1A)-C(8A)	1.329(3)
C(8A)-C(9A)	1.410(4)
C(8A)-C(7A)	1.447(3)
C(7A)-C(6A)	1.358(4)
C(7A)-H(3A)	0.9300
C(6A)-C(5A)	1.439(4)
C(6A)-H(6A)	0.9300
C(5A)-C(4A)	1.355(4)
C(5A)-H(5A)	0.9300
C(6A)-C(7A)	1.419(3)
C(4A)-H(4A)	0.9300
C(9A)-N(3A)	1.333(3)
N(3A)-C(10A)	1.471(3)
C(10A)-H(10A1)	0.9600
C(10A)-H(10A2)	0.9600
C(10A)-H(10A3)	0.9600
N(1B)-C(8B)	1.322(3)
C(8B)-C(7B)	1.423(3)
C(8B)-C(8B')	1.458(4)
C(7B)-C(6B)	1.345(4)
C(7B)-H(7B)	0.9300
C(6B)-C(6B')	1.431(6)
C(6B)-H(6B)	0.9300
H(7B)···F(2)	2.460(5)
Se(2A)···F(3)	2.970(1)
B-F(4)	1.273(5)
B-F(3)	1.311(4)
B-F(2)	1.323(5)
B-F(1)	1.391(4)

Angles [deg] for [3-Se]$^{2+}$.

N(1A)-Se2A-N(3A)	88.88(9)
N(1A)-Se2A-N(1B)	77.30(8)
N(3A)-Se2A-N(1B)	166.07(8)
N(1B)-Se2B-N(1B′)	91.60(13)
C(8A)-N(1A)-Se2A	111.76(15)
N(1A)-C(8A)-C(7A)	123.8(2)
N(1A)-C(8A)-C(9A)	116.1(2)
C(7A)-C(8A)-C(9A)	120.1(2)
C(6A)-C(7A)-C(8A)	118.6(2)
C(6A)-C(7A)-H(7A)	120.7
C(8A)-C(7A)-H(7A)	120.7
C(7A)-C(6A)-C(5A)	121.1(3)
C(7A)-C(6A)-H(6A)	119.4
C(5A)-C(6A)-H(6A)	119.4
C(4A)-C(5A)-C(6A)	122.3(2)
C(4A)-C(5A)-H(5A)	118.8
C(6A)-C(5A)-H(5A)	118.8
C(5A)-C(4A)-C(9A)	117.8(2)
C(5A)-C(4A)-H(4A)	121.1
C(9A)-C(4A)-H(4A)	121.1
N(3A)-C(9A)-C(4A)	127.8(2)
N(3A)-C(9A)-C(8A)	112.1(2)
C(4A)-C(9A)-C(8A)	120.1(2)
C(9A)-N(3A)-C(10A)	125.6(2)
C(9A)-N(3A)-Se2A	111.14(15)
C(10A)-N(3A)-Se2A	123.26(17)
N(3A)-C(10A)-H(10A1)	109.5
N(3A)-C(10A)-H(10A2)	109.5
H(9A1)-C(10A)-H(10A2)	109.5
N(3A)-C(10A)-H(10A3)	109.5
H(10A1)-C(10A)-H(10A3)	109.5
H(10A2)-C(10A)-H(10A3)	109.5
C(8B)-N(1B)-Se2B	109.09(14)
C(8B)-N(1B)-Se2A	135.31(15)
Se2B-N(1B)-Se2A	115.60(10)
N(1B)-C(8B)-C(7B)	125.41(19)
N(1B)-C(8B)-C(8B′)	115.11(12)
C(7B)-C(8B)-C(8B′)	119.48(13)
C(6B)-C(7B)-C(8B)	118.5(2)
C(6B)-C(7B)-H(7B)	120.8
C(8B)-C(7B)-H(7B)	120.8
C(7B)-C(6B)-C(6B′)	122.05(15)
C(7B)-C(6B)-H(6B)	119.0
C(6B′)-C(6B)-H(6B)	119.0
F(4)-B-F(3)	112.2(4)
F(4)-B-F(2)	108.9(4)
F(3)-B-F(2)	111.5(4)
F(4)-B-F(1)	103.8(4)
F(3)-B-F(1)	109.7(3)
F(2)-B-F(1)	110.4(4)

[1] Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W.Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, **2004**.