ESI

Macrocycles Containing 1,1'-Ferrocenyl Diselenolato Ligands on Group 14 Metallocenes

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Table S1. Selected bond lengths (Å) and angles (°) in **1**-**3** and **5**.

Parameter	**1** **M = Ti**	**2** **M = Zr**	**3** **M = Hf**	**5** **M = Hf**
M1-Se1	2.5471(11)	2.6434(11)	2.6219(5)	2.6438(11)
M1-Se3	2.5242(12)	2.6396(12)	2.6145(5)	2.6180(10)
M2-Se2	2.5414(11)	2.6284(15)	2.6197(5)	2.6368(11)
M2-Se4	2.5517(10)	2.6521(14)	2.6301(5)	2.6253(10)
Se1-M1-Se3	97.80(4)	102.52(4)	102.947(16)	98.53(3)
Se2-M2-Se4	99.40(4)	100.98(5)	101.800(16)	98.37(3)
M1-Se1-C111	108.33(14)	105.1(2)	107.63(13)	104.5(3)
C111-Se1-M1-Se3	61.7(3)	63.5(3)	58.41(14)	61.29(2)
C211-Se3-M1-Se1	62.0(3)	63.7(3)	63.32(14)	59.97(2)
Se1-C111	1.907(4)	1.918(7)	1.918(4)	1.923(8)
Se2-C121	1.907(4)	1.907(7)	1.913(4)	1.902(8)
Se3-C211	1.902(4)	1.908(7)	1.912(5)	1.906(9)
Se4-C221	1.904(5)	1.921(7)	1.916(5)	1.894(9)
M1-Se3-C211	107.94(13)	103.3(2)	105.95(13)	106.6(3)
M2-Se2-C121	107.34(14)	105.8(2)	105.94(13)	107.5(3)
M2-Se4-C221	107.74(14)	105.1(2)	107.28(13)	104.5(2)
C121-Se2-M2-Se4	61.3(3)	65.9(3)	61.55(13)	59.04(2)
C221-Se4-M2-Se2	60.7(3)	63.6(3)	56.46(15)	61.46(2)

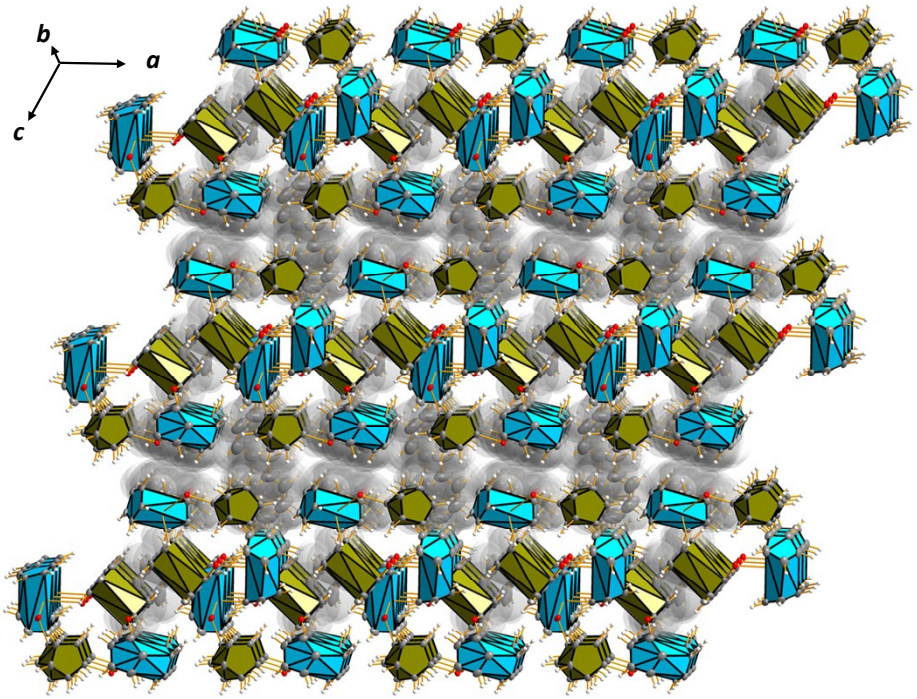

Figure S1. Packing of complexes in **1**·3$CH_3C_6H_5$ into quasi-2D layers. The $Fe(C_5H_4Se)_2$ polyhedra have been shown in green and the $Ti(C_5H_5)_2$ polyhedra in light blue. The solvent molecules have been displayed in grey using van der Waals-surfaces.

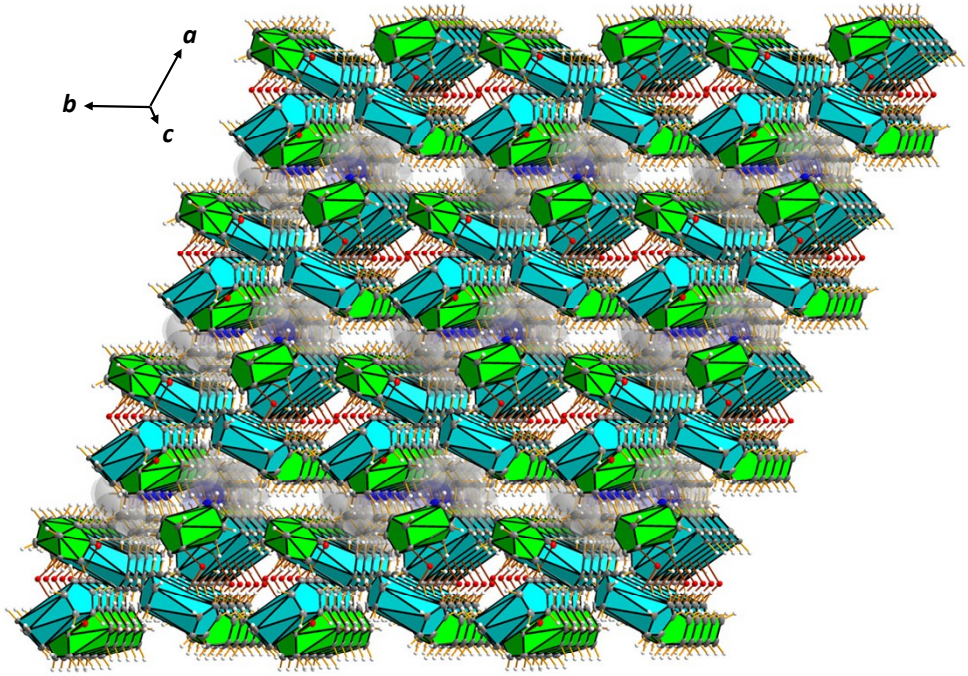

Figure S2. Packing of complexes in **2**·C_2H_4O into quasi-2D layers. The $Fe(C_5H_4Se)_2$ polyhedra have been shown in green and the $Zr(C_5H_5)_2$ polyhedra in light blue. The solvent molecules have been displayed in grey using van der Waals-surfaces.

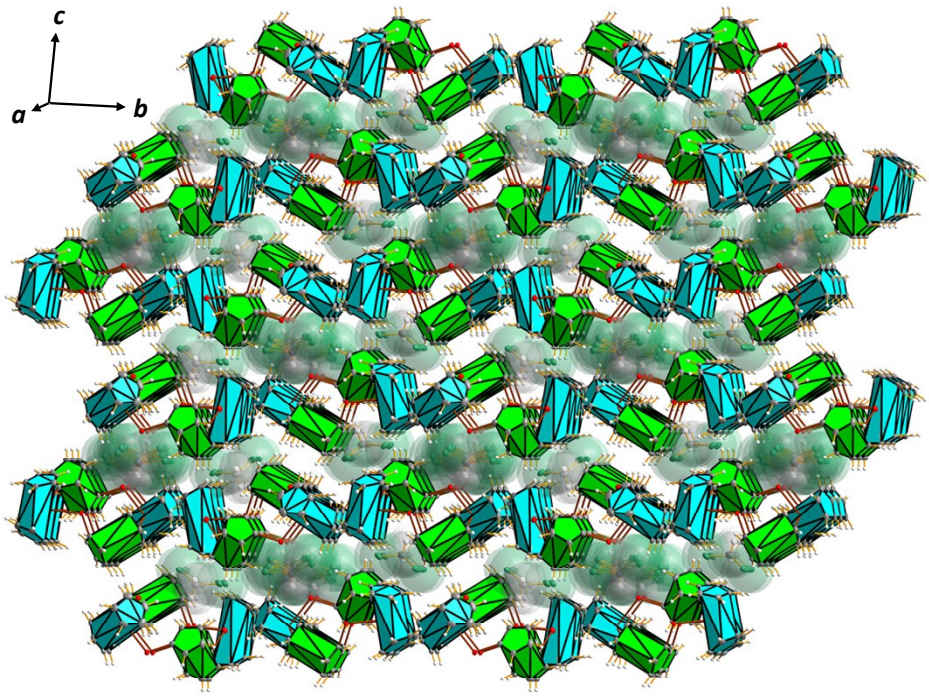

Figure S3. Packing of complexes in **3**·1.90CH_2Cl_2 into quasi-2D layers. The $Fe(C_5H_4Se)_2$ polyhedra have been shown in green and the $Hf(C_5H_5)_2$ polyhedra in light blue. The solvent molecules have been displayed in grey using van der Waals-surfaces.

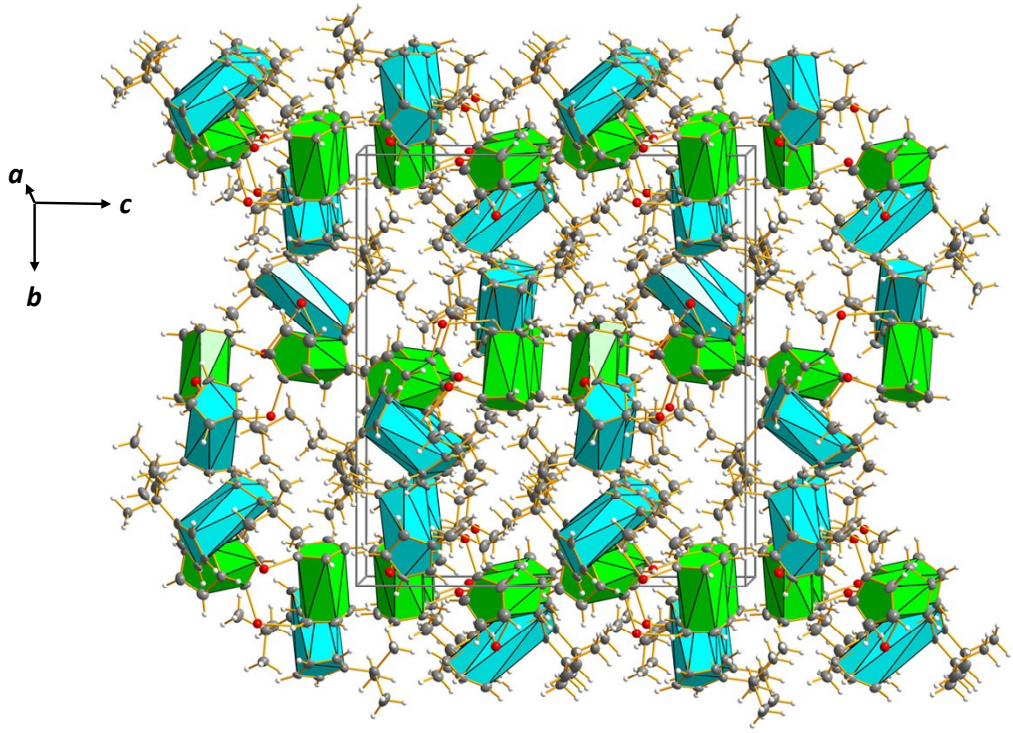

Figure S4. Weak H···Se hydrogen bonds link the macrocyclic complexes of **5** into a three-dimensional network. The $Fe(C_5H_4Se)_2$ polyhedra have been shown in green and the $Hf(C_5H_4{}^tBu)_2$ polyhedra in light blue.

References

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