Electronic supplementary information

s-Block Chalcogenoether Chemistry – Thio- and Selenoether Coordination with Hard Group 2

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The crystal structure of [18]aneO_4Se_2 is shown in Fig. S1.

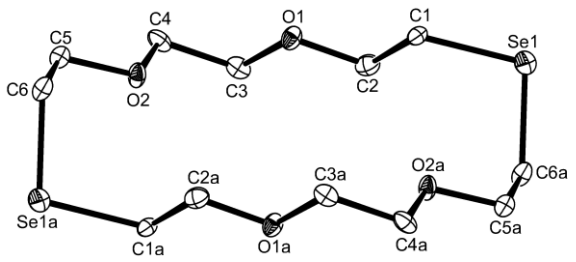

Fig. S1. Structure of the centrosymmetric [18]aneO_4Se_2 showing the atom numbering scheme. Atomic displacement ellipsoids are drawn at the 50% probability level and hydrogen atoms have been omitted for clarity. Symmetry operation: a = 1 – x, 1 – y, –z. Selected bond lengths (Å) and angles (°): Se1–C6a = 1.940(3), Se1–C1 = 1.952(3), O1–C3 = 1.409(4), O1–C2 = 1.425(4), O2–C4 = 1.410(4), O2–C5 = 1.425(4), C6–Se1–C1 = 101.70(14), C3–O1–C2 = 112.1(2), C4–O2–C5 = 112.7(2).

Table S1. Crystallographic data for [18]aneO_4Se_2

Compound	[18]aneO_4Se_2
Formula	$C_{12}H_{24}O_4Se_2$
M	390.23
Crystal system	Monoclinic
Space group	$P2_1/n$ (no. 14)
a /Å	6.933(4)
b /Å	13.419(7)
c /Å	8.573(4)
α /°	90
β /°	102.489(7)
γ /°	90
U /Å^3	778.7(7)
Z	2
μ(Mo-Kα) /mm^{-1}	4.752
Total no. reflections	7115
Unique reflections	1775
R_{int}	0.118
No. of parameters, restraints	82, 0
R_1 [$I_o > 2\sigma(I_o)$]	0.0349
R_1 (all data)	0.084
wR_2 [$I_o > 2\sigma(I_o)$]	0.055
wR_2 (all data)	0.059

Temperature = 120 K; wavelength (Mo-Kα) = 0.71073 Å; θ(max) = 27.5°; $R_1 = \Sigma\,||F_o| - |F_c||\,/\,\Sigma\,|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma\, wF_o^4]^{1/2}$.