

Supplementary materials for Article

2D, or not 2D: an Almost Perfect Mock of Symmetry

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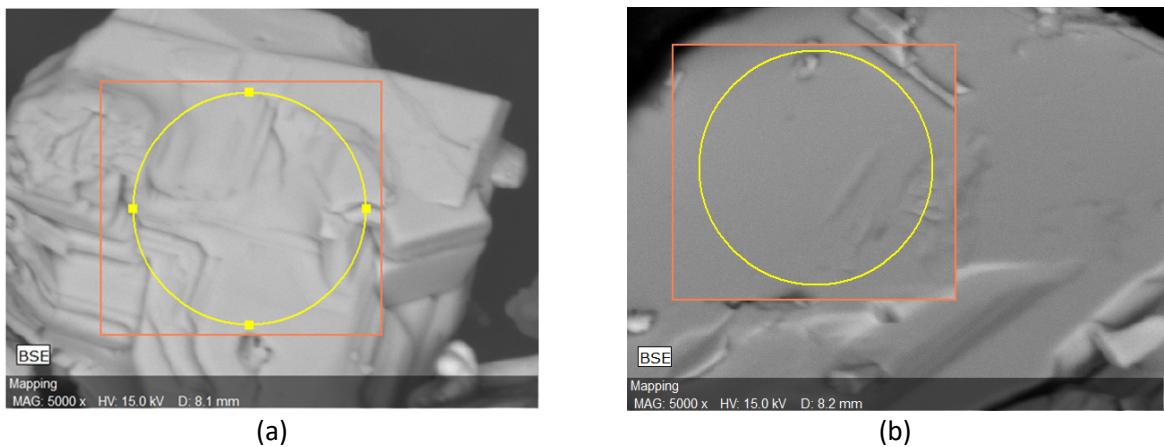


Figure S1. SEM picture of two specimens from a product of synthesis, described in section 2.1.2 of the article. (a) a stick, V : Se : I = 4 : 6.9 : 9.5; (b) a plate, V : Se : I = 4 : 6.6 : 9.1.

Table S1. Crystal data and structure refinement details for **M2**, **C** and **L** (three variants)

	M2	C	L		
Identification code	spplate_rt_s3	sp54need_s3_rt	sp54plate_rt_s2		
Empirical formula	I ₁₀ O ₀ Se ₈ V ₄	I ₅ OSe ₈ V ₄	I ₆ O ₂ Se ₁₂ V ₈	I ₆ O _{1.02} Se _{14.38} V _{3.74}	I ₁₀ OSe ₈ V ₄
Formula weight	2104.44	1485.94	2148.44	2103.68	2120.44
Temperature/K	298(3)	298(3)	298(3)	298(3)	298(3)
Crystal system	monoclinic	monoclinic	orthorhombic	orthorhombic	orthorhombic
Space group	C2/c	C2/c	Pccm	Pccm	Pccm
a/Å	20.22(12)	21.19(3)	5.919(12)	5.919(12)	5.919(12)
b/Å	11.81(9)	5.941(10)	10.15(2)	10.15(2)	10.15(2)
c/Å	12.12(7)	18.17(4)	12.13(3)	12.13(3)	12.13(3)
α/°	90	90	90	90	90
β/°	90.5(3)	123.55(3)	90	90	90
γ/°	90	90	90	90	90
Volume/Å ³	2892(32)	1906(6)	729(3)	729(3)	729(3)
Z	4	4	1	1	1
ρ _{calc} g/cm ³	4.833	5.177	4.895	4.793	4.831
μ/mm ⁻¹	21.986	25.255	23.786	25.471	21.817
F(000)	3576.0	2548.0	926.0	901.0	902.0
Crystal size/mm ³	0.54 × 0.52 × 0.28	0.29 × 0.16 × 0.14	0.54 × 0.52 × 0.28	0.54 × 0.52 × 0.28	0.54 × 0.52 × 0.28
Radiation	MoKα (λ = 0.71073)				
2θ range for data collection/°	5.21 to 46.52	4.614 to 46.76	6.72 to 46.51	6.72 to 46.51	6.72 to 46.51
Index ranges	-15 ≤ h ≤ 20, -7 ≤ k ≤ 7, -13 ≤ l ≤ 8	-23 ≤ h ≤ 17, -3 ≤ k ≤ 5, -12 ≤ l ≤ 20	-6 ≤ h ≤ 6, -10 ≤ k ≤ 10, -13 ≤ l ≤ 13	-6 ≤ h ≤ 6, -10 ≤ k ≤ 10, -13 ≤ l ≤ 13	-6 ≤ h ≤ 6, -10 ≤ k ≤ 10, -13 ≤ l ≤ 13
Reflections collected	1410	1271	3423	3423	3423
Independent reflections	928 [R _{int} = 0.1464, R _{sigma} = 0.2516]	936 [R _{int} = 0.0918, R _{sigma} = 0.3141]	519 [R _{int} = 0.1423, R _{sigma} = 0.1131]	519 [R _{int} = 0.1423, R _{sigma} = 0.1131]	519 [R _{int} = 0.1423, R _{sigma} = 0.1131]
Data / restraints / parameters	928/36/71	936/12/80	519/0/35	519/0/37	519/0/39
Goodness-of-fit on F ²	1.148	0.915	1.504	1.038	1.082
Final R indexes [I>=2σ (I)]	R ₁ = 0.1567, wR ₂ = 0.3614	R ₁ = 0.0837, wR ₂ = 0.1351	R ₁ = 0.1301, wR ₂ = 0.3583	R ₁ = 0.0942, wR ₂ = 0.2457	R ₁ = 0.0830, wR ₂ = 0.1956
Final R indexes [all data]	R ₁ = 0.2530, wR ₂ = 0.4530	R ₁ = 0.2383, wR ₂ = 0.1933	R ₁ = 0.1611, wR ₂ = 0.3988	R ₁ = 0.1224, wR ₂ = 0.2840	R ₁ = 0.1091, wR ₂ = 0.2190
Largest diff. peak/hole / e Å ⁻³	4.22/-4.59	1.83/-1.68	5.27/-3.21	3.81/-3.12	4.03/-1.97
CIF file name*	M2_spplate_rt_s3	C_sp54need_s3_rt	L_sp54plate_rt_s2	L_sp54plate_rt_s2_(sof_ref)	L_sp54plate_rt_s2_(se_i_overlay)
HTML file name*	M2_spplate_rt_s3_tbl	C_sp54need_s3_rt_tbl	L_sp54plate_rt_s2_tbl	L_sp54plate_rt_s2_(sof_ref)_tbl	L_sp54plate_rt_s2_(se_i_overlay)_tbl

*The files are available in the attached SC_XRD_models_archive.zip

Table S2. Main indicators of unrestricted Kohn-Sham DFT with periodic boundary conditions for structures of **M1**, **M2** and **L**

	M1	M2	L				
a, Å	11.8384	20.22	11.838				
b, Å	11.8384	11.81	12.15				
c, Å	18.6888	12.12	12.13				
α, Å	90	90	90				
β, Å	90	90.5	90				
γ, Å	90	90	90				
N atoms	84	92	56				
formula unit	V ₄ O ₁ Se ₈ I ₈	V ₄ O ₁ Se ₈ I ₁₀	V ₄ O ₁ Se ₆ I ₃				
Z	4	4	4				
spin multiplicity per periodic unit	17	17	5	13	21	39	37
spin per f.u.	2	2	1/2	3/2	5/2	7/2	9/2
E total, Ha	-1875.99301	-1967.81140	-1570.63528	-1570.64630	-1570.62564	-1570.57831	-1570.52612
CP2K project name*	02_M1_11 1aaaa	03_M2_111	05_L_211_m5	06_L_211_m13	07_L_211_m21	08_L_211_m29	09_L_211_m37

*The files are available in the attached CP2K_UKS_DFT_archive.zip