

Supporting Information

Crystal growth of a 2D Janus rhodiumchalcogenide RhSeCl

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Synthesis process

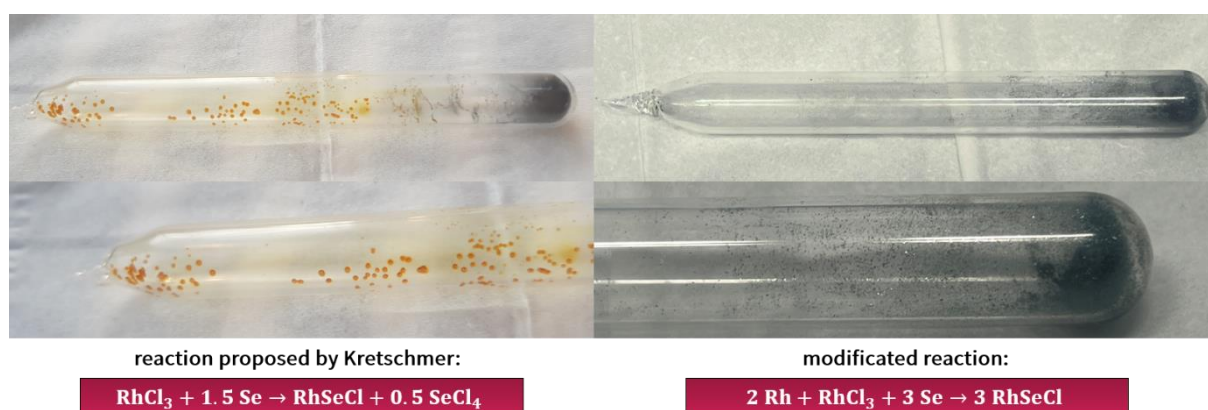


Fig. S1: Proposed and modified solid state reaction for the synthesis of RhSeCl.¹ While in the initial reaction an excess of Se was present, yellow crystals of SeCl₄ have been formed. To counteract this factor, we have reformulated the reaction equation and added rhodium so that no by-products are formed.

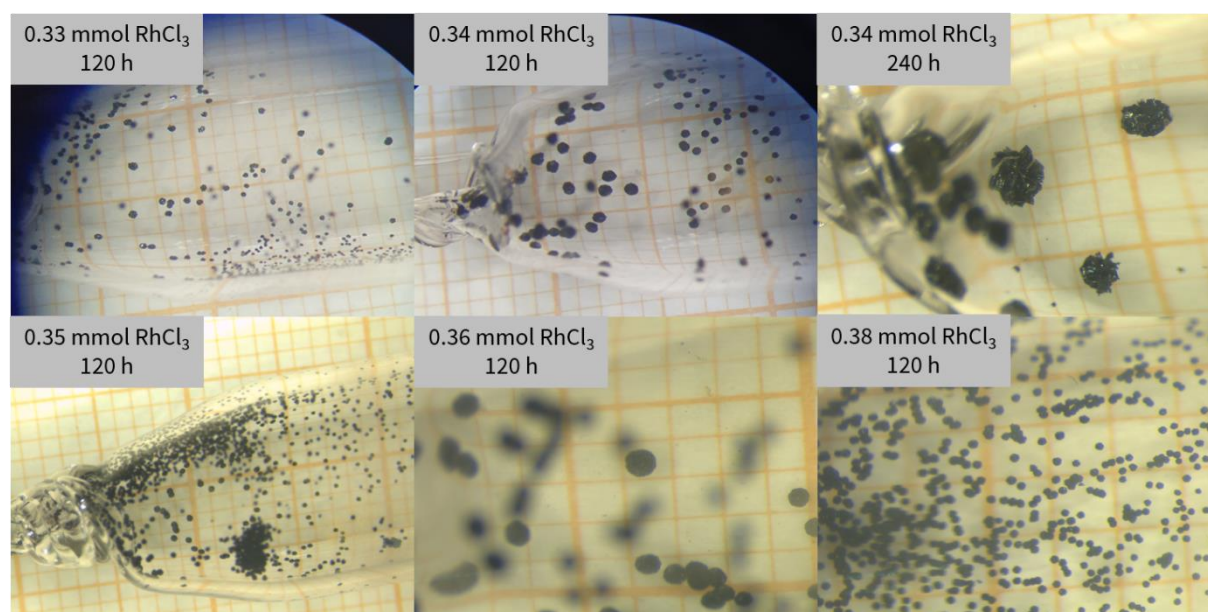


Fig. S2: Overview of the CVT growth experiments. All experiments were done with the same starting materials, only an excess RhCl₃ was used. The temperature gradient [$\Delta T = 100 \text{ K}$ ($T_1 = 900 \text{ }^\circ\text{C}$, $T_2 = 1000 \text{ }^\circ\text{C}$)] and the heating rate of 2,5 K/min were the same. The temperature was hold for 5 (10) days and then cooled down to room temperature. Till a certain excess (0.04 mmol) of RhCl₃ the crystals were growing larger, but after exceeding it the impact of the raised amount was minor on the crystal growth.

Energy dispersive X-ray spectroscopy

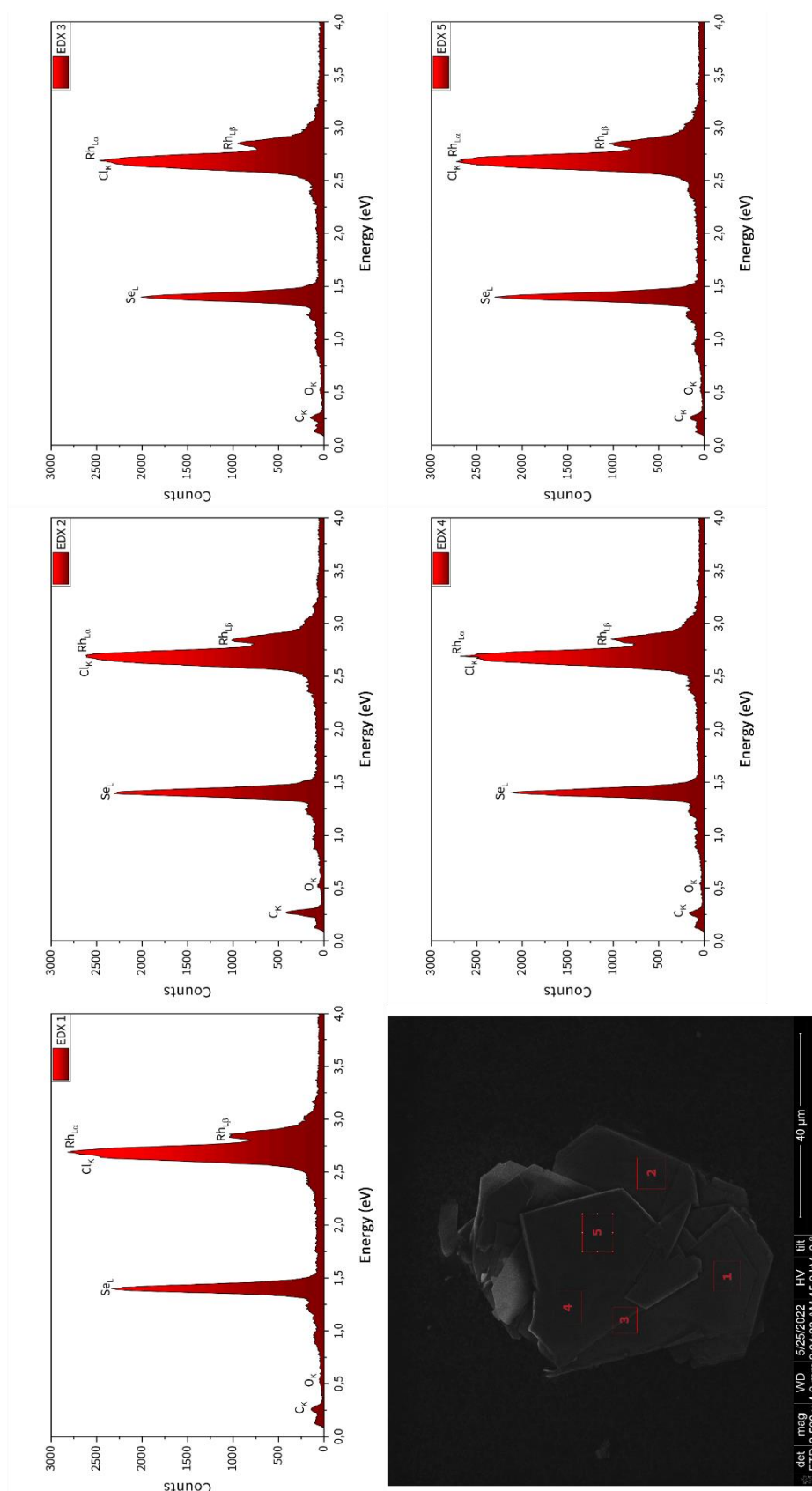


Fig. S3: EDX-spectra of an RhSeCl crystal are showing a strong overlap between the Cl_K and the Rh_{Lα} energy line.

Tab. S1: Atomic distribution of the elements in the measured areas according to the EDX spectra.

	Rh / At-%	Cl / At-%	Se / At-%
1	35.9	30.8	33.3
2	36.0	30.8	33.1
3	35.3	30.3	34.4
4	35.2	30.2	34.6
5	35.4	30.4	34.2
Average	35.6	30.5	33.9

Crystal structure

Tab. S2: Listing of measured atomic distances and the octahedra angle with the DIAMOND Software² as well as the calculated mono- and interlayer height in RhSeCl, RhTeCl, RhCl₃ and Rh₂Se₃.³⁻⁵

RhSeCl						
$d_{Rh-Cl} / \text{\AA}$	$d_{Rh-Se} / \text{\AA}$	$d_{Rh-Rh} / \text{\AA}$	$\angle_{octa} / \text{\AA}$	$l_{octa} / \text{\AA}$	$h_{mono} / \text{\AA}$	$h_{inter} / \text{\AA}$
2.51	2.38	3.49	175.5	4.89	2.78	5.79
RhTeCl						
$d_{Rh-Cl} / \text{\AA}$	$d_{Rh-Te} / \text{\AA}$	$d_{Rh-Rh} / \text{\AA}$	$\angle_{octa} / \text{\AA}$	$l_{octa} / \text{\AA}$	$h_{mono} / \text{\AA}$	$h_{inter} / \text{\AA}$
2.51	2.56	3.87	177.4	5.08	2.73	5.69
2.54	2.57	—	178.1	5.11	—	—
—	2.54	—	—	—	—	—
—	2.58	—	—	—	—	—
RhCl ₃						
$d_{Rh-Cl} / \text{\AA}$	$d_{Rh-Se} / \text{\AA}$	$d_{Rh-Rh} / \text{\AA}$	$\angle_{octa} / \text{\AA}$	$l_{octa} / \text{\AA}$	$h_{mono} / \text{\AA}$	$h_{inter} / \text{\AA}$
2.31	—	3.43	175.8	4.58	2.49	5.70
2.29	—	—	175.9	4.61	—	—
Rh ₂ Se ₃						
$d_{Rh-Cl} / \text{\AA}$	$d_{Rh-Se} / \text{\AA}$	$d_{Rh-Rh} / \text{\AA}$	$\angle_{octa} / \text{\AA}$	$l_{octa} / \text{\AA}$	$h_{mono} / \text{\AA}$	$h_{inter} / \text{\AA}$
—	2.46	3.35	161.5	4.92	—	—
—	2.50	—	169.4	4.98	—	—
—	2.42	—	160.7	4.85	—	—
—	2.53	—	—	—	—	—

References

- 1 J. Kretschmer, *PhD Thesis*, Rheinischen Friedrich–Wilhelms–Universität Bonn, 2018.
- 2 Dr. H. Putz & Dr. K. Brandenburg GbR, *Diamond - Crystal and Molecular Structure Visualization*, 2022.
- 3 J. Köhler and W. Urland, *Zeitschrift für anorganische und allgemeine Chemie*, 1997, **623**, 583–586.
- 4 H. Bärnighausen and B. Handa, *Journal of the Less Common Metals*, 1964, **6**, 226–231.
- 5 E. Parthé, E. Hohnke and F. Hulliger, *Acta Crystallographica*, 1967, **23**, 832–840.