

Supplementary Material

Synthesis and structural studies of some selenoureas and their metal complexes

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X-Ray crystallography

Compounds 1 and 2

Diffraction data were collected at 150 K using an Oxford Diffraction Gemini E Ultra diffractometer, equipped with an EOS CCD area detector and a four-circle kappa goniometer. For the data collection the Mo source emitting graphite-monochromated Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$) was used. Data integration, scaling and empirical absorption correction was carried out using the CrysAlis Pro program package.¹ The structure was solved using Direct Methods and refined by Full-Matrix-Least-Squares against F². The non-hydrogen atoms were refined anisotropically and hydrogen atoms were placed at idealised positions and refined using the riding model. All calculations were carried out using the program Olex2.²

Compound 6

A single crystal suitable for single crystal X-ray diffraction analysis was mounted on the tip of a MiTeGen MicroMount in perfluoropolyether and cooled using an Oxford Cryosystems 700 series Cryostream. Data were collected using a Bruker AXS APEX II CCD detector mounted on a Mach3 goniometer, which is placed in front of a FR591 rotating anode equipped with an Incoatec graded multilayer mirror. Data collection and integration were controlled by APEX Ver. 2 software, absorption correction was based on SADABS.³ Structure solution was by direct

methods (SHELXS-97)⁴ followed by least-squares refinement (SHELXL-97).⁵ All non-hydrogen atoms were refined anisotropically, for hydrogen atoms a riding model was employed.

Full crystallographic details, atomic co-ordinates together with complete bond distances and angles can be found in the CIF files, which have been deposited at the Cambridge Crystallographic Data Centre with the deposition codes CCDC 791347 - 791349.

Table 1. Important crystallographic and refinement details for compounds **1**, **2** and **6**

	1	2	6
Empirical Formula	C ₁₅ H ₁₄ N ₂ OSe	C ₁₆ H ₁₆ N ₂ OSe	C ₃₁ H ₄₁ F ₆ N ₄ OPSePd
Formula weight	317.24	331.27	816.01
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	P-1	P-1	P21/n
<i>a</i> (Å)	8.5478(11)	8.6923(4)	10.1701(2)
<i>b</i> (Å)	8.8535(14)	8.7563(5)	18.8639(3)
<i>c</i> (Å)	10.8280(11)	11.1219(6)	17.7680(3)
α (°)	90.371(11)	104.426(5)	90.0
β (°)	109.254(11)	90.930(4)	105.2590(10)
γ (°)	113.706(14)	114.391(5)	90.0
<i>V</i> (Å ³)	699.10(16)	739.81(7)	3288.58(10)
<i>Z</i>	2	2	4
ρ_{calc} (mg mm ⁻³)	1.507	1.487	1.648
μ (mm ⁻¹)	2.679	2.535	1.786
<i>F</i> (000)	320	336	1648
θ -range	2.79 to 29.52°	2.81 to 29.38°	2.92 to 33.25°
Reflections collected	5257	5955	92084
Independent reflections	3217	3377	12544
Data/restraints/parameters	3217/0/173	3377/0/187	12544/0/415
Goodness-of-fit on <i>F</i> ²	0.938	0.917	1.073
Final <i>R</i> indices [<i>I</i> >2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0292 w <i>R</i> ₂ = 0.0609	<i>R</i> ₁ = 0.0286 w <i>R</i> ₂ = 0.0565	<i>R</i> ₁ = 0.0361 w <i>R</i> ₂ = 0.0876
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0433 w <i>R</i> ₂ = 0.0627	<i>R</i> ₁ = 0.0412 w <i>R</i> ₂ = 0.0581	<i>R</i> ₁ = 0.0510 w <i>R</i> ₂ = 0.0967
Largest diff. peak and hole (e Å ⁻³)	0.385/-0.450	0.360/-0.288	0.846/-2.000

References

1. CrysAlis Pro 171.33.42, Oxford Diffraction Ltd., 2009.
2. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Cryst.* **2009**, *42*, 339.
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4. Sheldrick, G. M. *SHELXS-97, Program for Crystal Structure Solution*, University of Göttingen, Germany, 1997.
5. Sheldrick, G. M. *SHELXL-97, Program for Crystal Structure Refinement*, University of Göttingen, Germany, 1997.