

Complex	1 (E = S)	2 (E = Se)
Empirical formula	C ₉₇ H ₁₃₄ LiN ₆ O ₄ S ₉ V	C ₉₇ H ₁₃₄ LiN ₆ O ₄ S ₆ Se ₃ V
Formula weight	1794.51	1935.21
Crystal size [mm]	0.28 × 0.28 × 0.11	0.3 × 0.23 × 0.22
Wavelength [Å]	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic,
Space group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> [Å]	15.4498 (12)	15.4863 (5)
<i>b</i> [Å]	26.372 (2)	26.4050 (9)
<i>c</i> [Å]	24.676 (2)	24.7686 (9)
α [°]	90	90
β [°]	91.465 (2)	91.593 (1)
γ [°]	90	90
<i>V</i> [Å ³]	10050.6 (14)	10124.4 (6)
<i>Z</i>	4	4
Temperature [K]	100	100
<i>r</i> [Mg m ⁻³]	2-1.186	1.27
<i>m</i> [mm ⁻¹]	0.34	1.35
<i>F</i> (000)	3840	4056
θ -area [°]	2.2–22.7	2.3–28.7
Reflections collected	486516	137675
Independent reflections	17368	17892
Reflections with <i>I</i> > 2σ(<i>I</i>)	13163	15115
<i>R</i> _{int}	0.105	0.050
Number of restraints	0	12
Parameters	1087	1097
<i>R</i> 1 [<i>I</i> > 2σ(<i>I</i>)]	0.051	0.081
<i>wR</i> 2 [<i>I</i> > 2σ(<i>I</i>)]	0.125	0.251
<i>R</i> 1 [all data]	0.076	0.091
<i>wR</i> 2 [all data]	0.142	0.264
GooF	1.03	1.08
Largest diff. peak / hole / e Å ⁻³	1.06 / -0.56	2.17 / -2.75
CCDC number	2424329	2427545