

Table 40A-8-001. CsHSeO₄. Structure of phase II [87Bar]. $T = 299(1)$ K. Fractional coordinates and isotropic temperature parameters. B is defined by Eq. (e) in Introduction.

	x	y	z	$B [\text{\AA}^2]$
Cs	0.2099(1)	0.1285(2)	0.2062(2)	1.55
Se	0.7452(2)	0.1261(2)	0.2786(2)	1.15
O(1)	0.5689(13)	0.2182(14)	0.1125(16)	2.67
O(2)	0.8965(14)	0.2599(13)	0.3653(15)	2.48
O(3)	0.6505(13)	0.0644(12)	0.4186(14)	2.13
O(4)	0.8112(16)	−0.0191(13)	0.1876(16)	3.20

Table 40A-8-002. CsHSeO₄. Structure of phase II [87Bar]. $T = 299(1)$ K. Interatomic distances [\AA] and bond angles [$^\circ$].

Se–O(1)	1.711(11)	O(1)–Se–O(2)	106.6(6)
Se–O(2)	1.608(11)	O(1)–Se–O(3)	101.5(6)
Se–O(3)	1.623(10)	O(1)–Se–O(4)	108.8(6)
Se–O(4)	1.595(11)	O(2)–Se–O(3)	113.7(6)
O(1)⋯O(3 ⁱ)	2.603(15)	O(2)–Se–O(4)	113.8(6)
		O(3)–Se–O(4)	111.4(6)

Symmetry code: (i) $x, 0.5 - y, z - 0.5$.

Cs–O(1)	3.291(11)	Cs–O(1 ⁱ)	3.899(11)
–O(1 ⁱⁱ)	3.647(11)	–O(2 ⁱⁱⁱ)	3.358(11)
–O(2 ⁱ)	3.208(10)	–O(2 ^{iv})	3.059(11)
–O(3)	3.339(11)	–O(3 ^v)	4.052(10)
–O(3 ^{vi})	3.173(10)	–O(4 ^{vii})	3.368(13)
–O(4 ^v)	3.099(10)	–O(4 ^{viii})	3.152(12)

Symmetry code: (i) $1 - x, y - 0.5, 0.5 - z$; (ii) $x, 0.5 - y, 0.5 + z$; (iii) $x - 1, y, z$; (iv) $x - 1, 0.5 - y, z - 0.5$; (v) $1 - x, 0.5 + y, 0.5 - z$; (vi) $1 - x, -y, 1 - z$; (vii) $1 - x, -y, -z$.