Table 40A-3-001. $CsHSO_4$. Fractional coordinates and isotropic temperature parameters of phase II at 296 K [90Ito]. For Cs, S and O, the temperature parameters are reduced by $(U_{11} + U_{22} + U_{33} + 2U_{13}\cos\beta)/3$. U_{ij} is defined by Eq. (d) in Introduction. u^2 for H is defined by Eq. (e) in Introduction.

Atom	x	y	z	$\overline{u^2}$ [10^{-2} Å^2]
Cs	0.28808(4)	0.74303(5)	0.15233(3)	2.34(1)
S	0.2459(2)	0.2359(2)	0.3974(1)	1.84(3)
O(1)	0.3008(8)	0.2480(6)	0.2917(6)	3.2(1)
O(2)	0.3929(8)	0.2404(6)	0.5392(5)	3.4(1)
O(3)	0.1158(7)	0.0444(8)	0.3707(5)	3.3(1)
O(4)	0.1304(7)	0.4599(8)	0.3820(5)	3.4(2)
$H^{0.3-}$	0.026(7)	0.494(7)	0.276(6)	0.5(17)

Table 40A-3-002. $CsHSO_4$. Interatomic distances [Å] and bond angles [°] of phase II at 296 K [90Ito].

Cs–O(1)	3.235(5)	O(1)–O(2^{vii})	3.639(6)
–O(1^{i})	3.122(7)	–O(3)	2.399(10)
–O(2^{ii})	3.350(5)	–O(3^{iv})	3.444(7)
–O(2^{iii})	3.105(4)	–O(4)	2.412(10)
–O(3^{ii})	3.172(5)	–O(4^{viii})	3.515(7)
–O(3^{iv})	3.402(6)	O(2)–O(2^{iii})	3.798(7)
–O(3^{v})	3.763(7)	–O(2^{vii})	3.623(8)
–O(4)	3.736(7)	–O(3)	2.402(6)
–O(4^{iv})	3.503(6)	–O(4)	2.367(6)
–O(4^{vi})	3.114(5)	O(3)–O(3^{iv})	3.760(6)
S–O(1)	1.439(8)	–O(4)	2.416(6)
–O(2)	1.428(4)	–O(4^{ix})	3.398(6)
–O(3)	1.469(5)	–O(4^{viii})	2.555(6)
–O(4)	1.570(5)	–H^{viii}	1.479(47)
O(1)–O(2)	2.438(8)	O(4)–O(4^{iv})	3.917(6)
–O(2^{ii})	3.214(10)	O(4)–H	1.075(47)
–O(2^{iii})	3.745(6)		
O(1)–S–O(2)	116.6(4)	O(2)–S–O(4)	104.2(3)
O(1)–S–O(3)	111.2(3)	O(3)–S–O(4)	105.3(3)
O(1)–S–O(4)	106.5(3)	O(3)–H^{viii}–O(4^{viii})	179.2(41)
O(2)–S–O(3)	112.0(3)		

Symmetry code: (i) $1-x, 0.5+y, 0.5-z$; (ii) $x, 0.5-y, z-0.5$; (iii) $1-x, 1-y, 1-z$; (iv) $-x, 0.5+y, 0.5-z$; (v) $x, 1+y, z$; (vi) $x, 1.5-y, z-0.5$; (vii) $1-x, -y, 1-z$; (viii) $-x, y-0.5, 0.5-z$; (ix) $x, -1+y, z$.

Table 40A-3-003. $CsDSO_4$. Fractional coordinates and isotropic temperature parameters [Å^2] at RT [86Mer]. B is defined by Eq. (e) in Introduction.

Atom	x	y	z	B
Cs	0.78433(4)	0.12914(4)	0.79359(4)	2.467(4)
S	0.2478(2)	0.1273(2)	0.7205(2)	2.13(1)
O_1	0.3340(6)	0.0711(6)	0.5923(6)	2.95(6)
O_2	0.4102(7)	0.2207(7)	0.8685(7)	3.59(9)
O_3	0.8072(7)	0.0047(6)	0.1869(6)	3.47(8)
O_4	0.1039(6)	0.2454(5)	0.6409(6)	3.12(7)

Table 40A-3-004. $CsDSO_4$. Interatomic distances [Å] at RT [86Mer].

Cs polyhedron (11 vertices)		SO_4 tetrahedron	
Cs $-O_4^*$	3.112(4)	S $-O_4$	1.438(4)
$-O_3^*$	3.116(5)	$-O_3^*$	1.439(6)
$-O_3^*$	3.148(5)	$-O_1$	1.454(6)
$-O_1^*$	3.231(5)	$-O_2$	1.567(5)
$-O_4^*$	3.236(4)	O_1-O_2	2.343(7)
$-O_4^*$	3.252(5)	O_1-O_4	2.418(7)
$-O_2$	3.253(6)	$O_1-O_3^*$	2.416(8)
$-O_3^*$	3.315(5)	O_2-O_4	2.416(6)
$-O_1$	3.325(4)	$O_2-O_3^*$	2.430(7)
$-O_2^*$	3.685(5)	$O_4-O_3^*$	2.397(6)
$-O_2^*$	3.736(4)		

Table 40A-3-005. $CsHSO_4$. $c_{\lambda\mu}$ at 20 °C [87Lus]. $c_{\lambda\mu}$: elastic stiffness constants obtained by Brillouin scattering.

$c_{\lambda\mu}$ [10^9 N m^{-2}]		$c_{\lambda\mu}$·[10^9 N m^{-2}]	
c_{11}	28.79	c_{12}	15.74
c_{22}	30.72	c_{13}	13.76
c_{33}	30.65	c_{23}	20.43
c_{44}	6.64	c_{15}	5.66
c_{55}	8.62	c_{25}	–5.45
c_{66}	6.64	c_{35}	1.18
		c_{46}	0