

M17 Sb₂S₃, Stibnite**Table M17-001.** Sb₂S₃. Fractional coordinates and temperature parameters [72Bay]. Temperature parameters are defined by Eq. (a) in Introduction.

Atom	Fractional coordinates			Temperature parameters · 10 ³			
	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> ₁₁	<i>B</i> ₂₂	<i>B</i> ₃₃	<i>B</i> ₁₂
Sb _I	0.3261 (1)	0.0293 (1)	1/4	2.5 (2)	3.0 (2)	14.4 (15)	0.6 (1)
Sb _{II}	0.0360 (1)	0.1495 (1)	3/4	3.6 (2)	2.7 (2)	23.0 (15)	1.3 (1)
S _I	0.8769 (3)	0.0497 (3)	1/4	2.7 (3)	3.2 (2)	18.0 (25)	0.4 (3)
S _{II}	0.4386 (3)	0.1251 (3)	3/4	2.4 (3)	3.5 (3)	17.7 (25)	0.8 (3)
S _{III}	0.1917 (3)	0.2079 (3)	1/4	2.3 (3)	3.1 (3)	26.7 (26)	0.2 (3)