

AM-95-581

The crystal structure of pararealgar, As_4S_4

Paola Bonazzi, Silvio Menchetti, Giovanni Pratesi

For deposit: Tables 3 and 4

American Mineralogist, 80, 3-4, 400-403.

Table 3. Anisotropic thermal parameters for pararealgar

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
As1	.0331(21)	.0428(24)	.0359(22)	-.0096(18)	.0004(18)	.0105(21)
As2	.0331(20)	.0421(21)	.0326(22)	.0064(18)	.0121(18)	.0000(20)
As3	.0506(23)	.0525(25)	.0496(26)	.0152(22)	.0153(20)	.0216(23)
As4	.0423(21)	.0283(21)	.0532(25)	-.0114(19)	.0147(19)	-.0065(22)
S1	.0465(50)	.0234(49)	.0476(61)	.0035(44)	.0026(47)	-.0050(42)
S2	.0523(53)	.0552(61)	.0324(54)	.0128(52)	.0095(46)	.0039(50)
S3	.0240(49)	.0721(67)	.0582(70)	-.0043(48)	.0027(51)	.0214(55)
S4	.0407(52)	.0459(57)	.0363(53)	-.0028(47)	-.0024(43)	-.0159(50)