Carbonyl Sulphide (COS, $F0_2$) Structure: ABC_hR3_160_a_a_a-001

This structure originally had the label `ABC_hR3_160_a_a_a`. Calls to that address will be redirected here.

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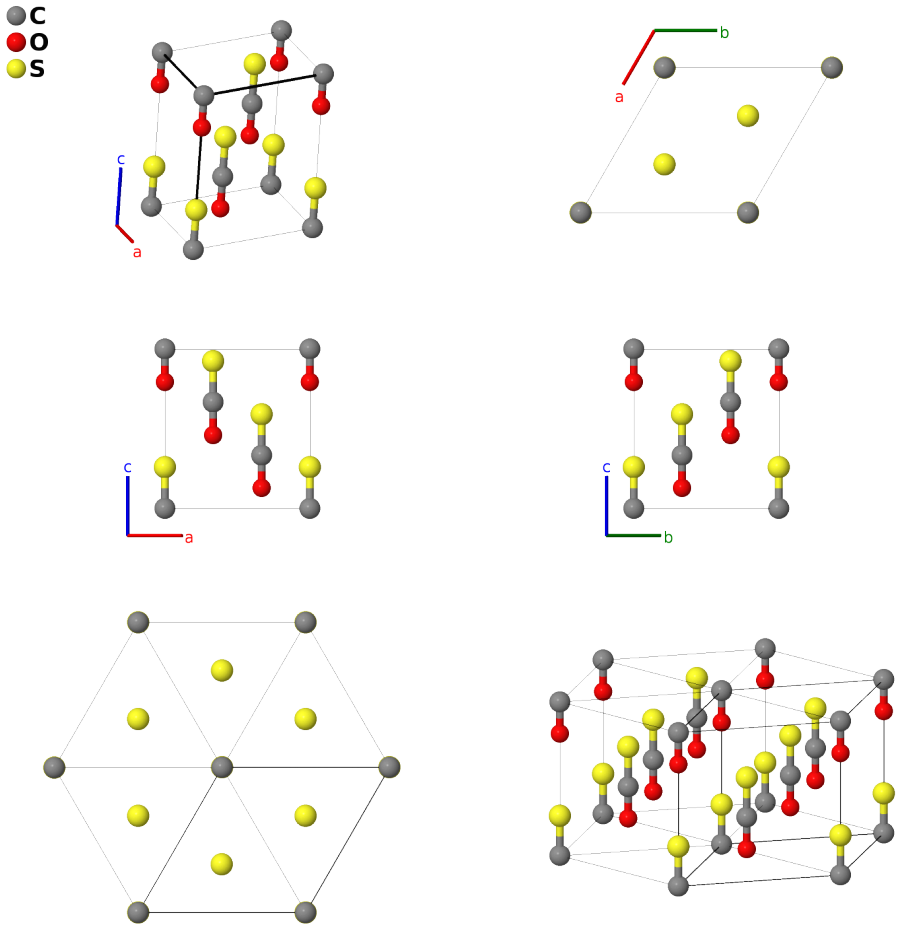
https://aflow.org/p/V77F

https://aflow.org/p/ABC_hR3_160_a_a_a-001



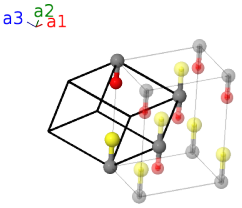
Prototype	COS
AFLOW prototype label	ABC_hR3_160_a_a_a-001
***Strukturbericht* designation**	$F0_2$
ICSD	33540
Pearson symbol	hR3
Space group number	160
Space group symbol	$R3m$

AFLOW prototype command `aflow --proto=ABC_hR3_160_a_a_a-001 --params=`$a, c/a, x_1, x_2, x_3$

- (Overell, 1982) does not explicitly give the Wyckoff positions. We infer them from the C-O and C-S bond lengths. The experimental data was obtained at 90 K.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(1a)	C I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(1a)	O I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(1a)	S I

References

[1] J. S. W. Overell, G. S. Pawley, and B. M. Powell, *Powder refinement of carbonyl sulphide*, Acta Crystallogr. Sect. B **38**, 1121–1123 (1982), doi:10.1107/S0567740882005111.