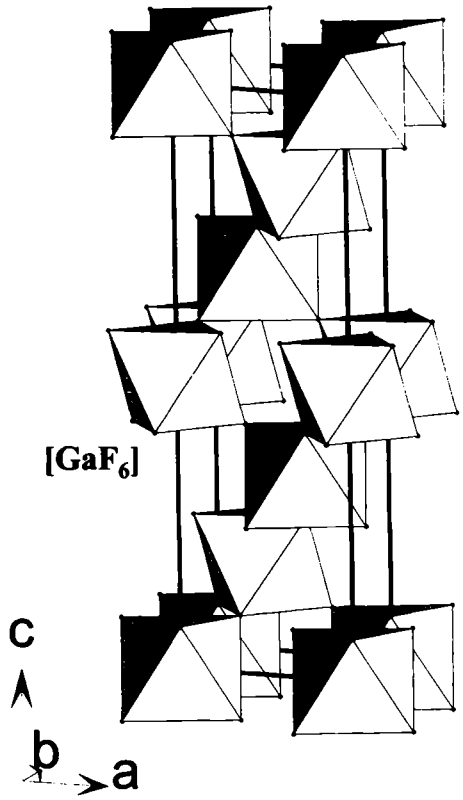
Refinement of the crystal structure of gallium trifluoride, GaF_3

M. Roos and G. Meyer*

Universität zu Köln, Institut für Anorganische Chemie, Greinstraße 6, D-50939 Köln, Germany

Received July 14, 2000, CSD-No. 409507



Abstract

F_3Ga, trigonal, $R\bar{3}c$ (No. 167), a = 5.012(4) Å, c = 12.99(1) Å, V = 282.6 Å^3, Z = 6, $R_{gt}(F)$ = 0.022, $wR_{ref}(F^2)$ = 0.053, T = 293 K.

Source of material

GaF_3 may be obtained through the reaction of gallium metal (Ventron 4 N) with NH_4F (Merck, 99,8 %, recrystallized from CH_3OH to remove traces of water) in the molar ratio of 1:3 in a sealed Monel container. The reaction temperature is 748 K with a crystallization time of six weeks. Colourless square shaped nearly cubic crystals are obtained [1].

Discussion

GaF_3 crystallizes in the VF_3 type of structure with the hexagonal space group $R\bar{3}c$ [1]. A previous description of the crystal structure [2] uses the rhombohedral setting of the space group. The cell parameters obtained by powder diffraction refinement are a = 4.995(1) Å and c = 13.063(4) Å. GaF_3 is built of a three-dimensional network of $[GaF_6]$ octahedra sharing common corners with a Ga–F–Ga angle of 147.79(8)°.

Table 1. Data collection and handling.

Crystal:	colourless, square-formed, nearly cubic, size 0.16 × 0.20 × 0.20 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	143.37 cm^{-1}
Diffractometer, scan mode:	STOE IPDS, φ
$2\theta_{max}$:	55.7°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	726, 77
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 74
$N(param)_{refined}$:	8
Programs:	SHELXS-97 [3], SHELXL-97 [4], DIAMOND [5]

Acknowledgment. We are grateful to the Deutsche Forschungsgemeinschaft, Bonn, for financial support.

References

1. Roos, M.: Aufbau und Abbau komplexer Ammoniumfluorometallate der Elemente Aluminium, Gallium und Indium unter Ammoniakatmosphäre. Dissertation, Universität zu Köln, Germany 1999.
2. Brewer, F. M.; Garton, G.; Goodgame, D. M. L.: The preparation and crystal structure of gallium trifluoride. J. Inorg. Nucl. Chem. **9** (1959) 56.
3. Sheldrick, G. M.: SHELXS-97-2, Program for the Solution of Crystal Structures. University of Göttingen, Germany 1997.
4. Sheldrick, G. M.: SHELXL-97-2, Program for Crystal Structure Refinement. University of Göttingen, Germany 1997.
5. Brandenburg, K.: Diamond (Version 2.1a). Crystal Impact GbR, Germany 1996-1999.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ga	6*b*	0	0	0	0.0033(4)	U_{11}	0.0030(5)	0.0016(2)	0	0
F	18*e*	0.0591(3)	x–1/3	1/12	0.0090(7)	U_{11}	0.0083(7)	0.0057(7)	–0.0020(3)	$-U_{13}$

* Correspondence author (e-mail: gerd.meyer@uni-koeln.de)