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$Na_3Cr_2(AsO_4)_3$: trisodium dichromium(III) triarsenate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(As–O) = 0.002 Å
R factor = 0.019
wR factor = 0.039
Data-to-parameter ratio = 12.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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Trisodium dichromium(III) triarsenate, $Na_3Cr_2(AsO_4)_3$, has been synthesized by a solid-state reaction and structurally characterized by single-crystal X-ray diffraction. It has the garnet structure type.

Comment

Until now, in the system Na_2O–Cr_2O_3–As_2O_5, only the structures of compounds formed from two components have been studied: $NaCrO_2$ (Ruedorff & Becker, 1977), $CrAsO_4$ (Attfield *et al.*, 1987), $Na_2As_4O_{11}$ (Driss *et al.*, 1988), $NaAsO_3$ (Liebau, 1956), $Na_4As_2O_7$ (Leung & Calvo, 1973) and Na_3AsO_4 (Palazzi & Remy, 1971).

To our knowledge, only one ternary compound, *viz*. $Na_3Cr_2(AsO_4)_3$ (Schwarz & Schmidt, 1972), has been reported, but its structure has not been determined. On investigating this system, we synthesized this arsenate and report here the synthesis and crystal structure determination.

Experimental

The title compound was prepared as previously described by Schwarz & Schmidt (1972), starting from reagent-grade Na_2CO_3 (Fluka, 99%), $(NH_4)_2Cr_2O_7$ (Prolabo, 99.5%) and As_2O_3 (Hoping & Williams, 99.5%) mixed in stoichiometric ratios. The sample was heated first at 773 K for 6 h, and then at 1173 K for 60 h, and finally quenched to room temperature.

Crystal data

$Na_3Cr_2(AsO_4)_3$
M_r = 589.73
Cubic, $Ia\bar{3}d$
a = 12.188 (2) Å
V = 1810.6 (5) Å^3
Z = 8
D_x = 4.327 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–14°
μ = 13.50 mm^{-1}
T = 293 (2) K
Polyhedron, green
0.10 × 0.08 × 0.06 mm

Data collection

Enarf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.406, T_{max} = 0.508
735 measured reflections
216 independent reflections
194 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 29.9°
$h = 0 \rightarrow 17$
$k = 0 \rightarrow 17$
$l = 0 \rightarrow 10$
2 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.039
S = 1.14
216 reflections
18 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0156P)^2 + 7.0122P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.00326 (17)

Table 1
Selected geometric parameters (Å).

As1—O1^{i}	1.6983 (16)	Cr1—O1^{iii}	1.9942 (15)
As1—O1	1.6984 (16)	Na1—O1^{iv}	2.3919 (17)
Cr1—O1^{ii}	1.9941 (15)	Na1—O1^{v}	2.5337 (17)

Symmetry codes: (i) $\frac{3}{4}-x, z-\frac{1}{4}, \frac{1}{4}-y$; (ii) $z, \frac{1}{2}-x, \frac{1}{2}+y$; (iii) $\frac{1}{2}-x, \frac{1}{2}+y, z$; (iv) $\frac{1}{4}-x, z-\frac{1}{4}, \frac{1}{4}+y$; (v) $\frac{1}{4}+y, x-\frac{1}{4}, \frac{3}{4}-z$.

Data collection: *CAD*-4 *EXPRESS* (Duisenberg, 1992; Enraf–Nonius, 1994; Macíček & Yordanov, 1992); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL*97.

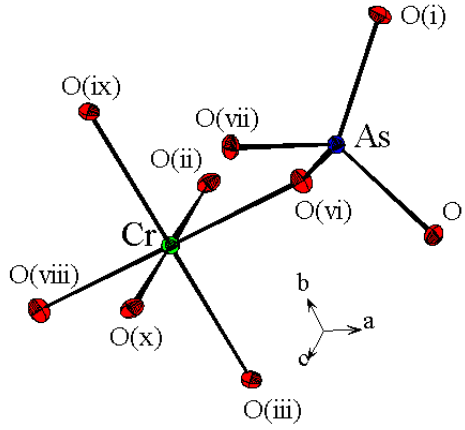

Figure 1
A plot of the asymetric unit. [Symmetry codes: (i) $-x+\frac{3}{4}, z-\frac{1}{4}, -y+\frac{1}{4}$; (ii) $z, -x+\frac{1}{2}, y+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, z$; (vi) $x, -y, -z+\frac{1}{2}$; (vii) $-x+\frac{3}{4}, -z+\frac{1}{4}, y+\frac{1}{4}$; (viii) $y+\frac{1}{2}, z, -x+\frac{1}{2}$; (ix) $-y-1, -z+\frac{1}{2}, x-1$; (x) $-z+\frac{1}{2}, x-1, -y-1$.]

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