Bis(tetramethylammonium) tetrachlorozincate(II), Phase VI

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Abstract

The crystal structure of phase VI of bis(tetramethylammonium) tetrachlorozincate(II) was found to contain three formula units per asymmetric unit of the cell. Several short C–H···Cl contacts were observed, but these contacts were believed to only participate in van der Waals interactions.

Related literature

For related literature, see: Madariaga et al. (1987); Ruiz-Larrea, Lopez-Echarri & Tello (1981); Wiesner et al. (1967); Zuñiga, Madariaga & Pérez-Mato (1989).

Computing details

Data collection: SMART (Bruker, 1998); cell refinement: SMART; data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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Crystal data

\begin{eqnarray*}
2(\text{C}_4\text{H}_{12}\text{N})\cdot\text{Cl}_4\text{Zn} & : & V = 4912.2 (17) \, \text{Å}^3 \\
M_r = 355.46 & : & Z = 12 \\
\text{Orthorhombic, } P2_12_12_1 & : & \mu = 2.13 \, \text{mm}^{-1} \\
\alpha = 8.9114 (18) \, \text{Å} & : & T = 100.0 (2) \, \text{K} \\
b = 15.105 (3) \, \text{Å} & : & 0.36 \times 0.24 \times 0.04 \, \text{mm} \\
c = 36.493 (7) \, \text{Å} & : & 9616 \, \text{independent reflections}
\end{eqnarray*}
Absorption correction: multi-scan
SADABS (Sheldrick, 2007)
$T_{	ext{min}} = 0.512, T_{	ext{max}} = 0.918$
32538 measured reflections

9039 reflections with $I > 2\sigma(I)$
$R_{	ext{int}} = 0.038$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.055$
$S = 1.00$
9616 reflections
407 parameters

H-atom parameters constrained
$\Delta \rho_{\text{max}} = 0.43 \text{ e Å}^3$
$\Delta \rho_{\text{min}} = -0.29 \text{ e Å}^3$
Absolute structure: Flack (1983)
Flack parameter: 0.611 (6)

Selected geometric parameters (Å, °)

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C4E—N1E—C1E 109.4 (2)

Acknowledgements

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References

supplementary materials
Bis(tetramethylammonium) tetrachlorozincate(II), Phase VI

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Comment

Bis(tetramethylammonium) tetrachlorozincate(II) undergoes five solid-solid phase transitions with decreasing temperature according to a calorimetric study by Ruiz-Larrea \textit{et al.} (1981). The room temperature phase I crystallized in the space group \textit{Pnma} with \(a = 12.276\) (2), \(b = 8.998\) (2), and \(c = 15.541\) (2) Å (Wiesner \textit{et al.}, 1967). Weak incommensurate lattice spots in phases II, III, and IV have shown that these two phases are small distortions of the room temperature phase (Madariaga \textit{et al.}, 1987). Similarly, phase V was found to be an incommensurately modulated structure related to phase I (Zúñiga \textit{et al.}, 1989).

No evidence of superlattice spots were observed in the frame data for phase VI. Short C—H···Cl contacts were observed, but because of the very large estimated pK\textsubscript{a} of 42 for the protons of the cations (Zhang & Bordwell, 1994) it is unlikely that any of these contacts are weak hydrogen bonds. There were three formula units in the asymmetric unit of the cell.

Experimental

Single crystals of bis(tetramethylammonium) tetrachlorozincate(II) were grown by slow diffusion of diethyl ether into a methanol solution of ZnCl\textsubscript{2} and N(CH\textsubscript{3})\textsubscript{4}OH in a 1:3 mole ratio, respectively over the course of three days.

Refinement

The methyl H atoms were initially located by geometry. The H atoms were then refined with distances of 0.98 Å and U\textsubscript{iso}(H) = 1.5U\textsubscript{eq}(C), but each methyl group was allowed to rotate freely about its N—C bond.

The refined Flack parameter indicated racemic twinning in the sample.

Figures

Fig. 1. View of the unique atoms showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity.

Fig. 2. The molecular packing of the structure viewed along the \textit{a}-axis. H atoms are omitted for clarity.

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Crystal data

\begin{verbatim}
\begin{tabular}{ll}
2(C\textsubscript{4}H\textsubscript{12}N)\textsubscript{4}Cl\textsubscript{4}Zn & \(F_{000} = 2208 \) \\
\(M_r = 355.46\) & \(D_x = 1.442\) Mg m\textsuperscript{-3} \\
Orthorhombic, \textit{P2\textsubscript{1}2\textsubscript{1}2\textsubscript{1}} & Mo \textit{K\alpha} radiation \\
Hall symbol: P 2ac 2ab & \(\lambda = 0.71073\) Å \\
a = 8.9114 (18) Å & \(0 = 2.5^\circ-28.2^\circ\) \\
b = 15.105 (3) Å & \(\mu = 2.13\) mm\textsuperscript{-1} \\
c = 36.493 (7) Å & \(T = 100.0\) (2) K
\end{tabular}
\end{verbatim}
supplementary materials

\[ V = 4912.2 \text{ (17) } \text{Å}^3 \]
\[ Z = 12 \]
\[ 0.36 \times 0.24 \times 0.04 \text{ mm} \]

Data collection

CCD Bruker APEX
diffractometer 9616 independent reflections
Radiation source: fine-focus sealed tube 9039 reflections with \( I > 2\sigma(I) \)
Monochromator: graphite \( R_{\text{int}} = 0.038 \)
\[ T = 100.0(2) \text{ K} \]
\[ \theta_{\text{max}} = 26.0^\circ \]
\( \omega \) scans \( \theta_{\text{min}} = 1.8^\circ \)
Absorption correction: multi-scan SADABS (Sheldrick, 2007)
\( h = -10 \rightarrow 10 \)
\( k = -18 \rightarrow 18 \)
\( l = -44 \rightarrow 45 \)

Refinement

Refinement on \( F^2 \)
Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full H-atom parameters constrained
\[ R[F^2 > 2\sigma(F^2)] = 0.026 \]
\[ wR(F^2) = 0.055 \]
\[ S = 1.00 \]
9616 reflections
407 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map Absolute structure: Flack (1983)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\( \text{Å}^2 \))

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supplementary materials

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H2E1—C2E—H2E2 109.5  H3H2—C3H—H3H3 109.5
N1E—C2E—H2E3 109.5  N1H—C4H—H4H1 109.5
H2E1—C2E—H2E3 109.5  N1H—C4H—H4H2 109.5
H2E2—C2E—H2E3 109.5  H4H1—C4H—H4H2 109.5
N1E—C3E—H3E1 109.5  N1H—C4H—H4H3 109.5
N1E—C3E—H3E2 109.5  H4H1—C4H—H4H3 109.5
H3E1—C3E—H3E2 109.5  H4H2—C4H—H4H3 109.5
N1E—C3E—H3E3 109.5  C1I—N1I—C3I 109.2 (2)
H3E1—C3E—H3E3 109.5  C1I—N1I—C2I 109.63 (19)
H3E2—C3E—H3E3 109.5  C3I—N1I—C2I 110.0 (2)
N1E—C4E—H4E1 109.5  C1I—N1I—C4I 109.6 (2)
N1E—C4E—H4E2 109.5  C3I—N1I—C4I 109.4 (2)
H4E1—C4E—H4E2 109.5  C2I—N1I—C4I 109.0 (2)
N1E—C4E—H4E3 109.5  N1I—C1I—H1I1 109.5
H4E1—C4E—H4E3 109.5  N1I—C1I—H1I2 109.5
H4E2—C4E—H4E3 109.5  H1I1—C1I—H1I2 109.5
C2F—N1F—C3F 109.9 (2)  N1I—C1I—H1I3 109.5
C2F—N1F—C1F 109.4 (2)  H1I1—C1I—H1I3 109.5
C3F—N1F—C1F 109.4 (2)  H1I2—C1I—H1I3 109.5
C2F—N1F—C4F 109.3 (2)  N1I—C2I—H2I1 109.5
C3F—N1F—C4F 108.9 (2)  N1I—C2I—H2I2 109.5
C1F—N1F—C4F 110.0 (2)  H2I1—C2I—H2I2 109.5
N1F—C1F—H1F1 109.5  N1I—C2I—H2I3 109.5
N1F—C1F—H1F2 109.5  H2I1—C2I—H2I3 109.5
H1F1—C1F—H1F2 109.5  H2I2—C2I—H2I3 109.5
N1F—C1F—H1F3 109.5  N1I—C3I—H3I1 109.5
H1F1—C1F—H1F3 109.5  N1I—C3I—H3I2 109.5
H1F2—C1F—H1F3 109.5  H3I1—C3I—H3I2 109.5
N1F—C2F—H2F1 109.5  N1I—C3I—H3I3 109.5
N1F—C2F—H2F2 109.5  H3I1—C3I—H3I3 109.5
H2F1—C2F—H2F2 109.5  H3I2—C3I—H3I3 109.5
N1F—C2F—H2F3 109.5  N1I—C4I—H4I1 109.5
H2F1—C2F—H2F3 109.5  N1I—C4I—H4I2 109.5
N1F—C3F—H3F1 109.5  N1I—C4I—H4I3 109.5
N1F—C3F—H3F2 109.5  H4I1—C4I—H4I3 109.5
H3F1—C3F—H3F2 109.5  H4I2—C4I—H4I3 109.5