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1,1,1,2,2-Pentaiododiphosphanium tetraiodogallate(III)

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1,1,1,2,2-Pentaiododiphosphanium tetraiodogallate(III), $(P_2I_5)[GaI_4]$, crystallizes in the orthorhombic space group *Pbca*. The structure is isotypic with $(P_2I_5)[AlI_4]$. Short I···I interatomic distances indicate weak interactions between cations and anions.

Key indicators

Single-crystal X-ray study
T = 201 K
Mean σ(P–P) = 0.003 Å
R factor = 0.027
wR factor = 0.076
Data-to-parameter ratio = 28.4

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

Comment

The 2:1 adduct of PI_3 and AlI_3 was structurally characterized by X-ray crystallography and identified as $(P_2I_5)[AlI_4]$ (Pohl, 1983). Recently, the 1,1,1,2,2-pentaiododiphosphanium cation species $(P_2I_5)[EI_4]$ (E = Al, Ga, In) have been characterized by solid-state ^{31}P MAS NMR and vibrational spectroscopy (Aubauer *et al.*, 1999). The crystal structure of $(P_2I_5)[GaI_4]$ is isotypic with the structure found for $(P_2I_5)[AlI_4]$. The P1—P2 bond distance is comparable with the P—P bond length of 2.218 (13) Å in $(P_2I_5)[AlI_4]$ (Pohl, 1983) and 2.230 (3) Å in P_2I_4 (Zak & Cernik, 1996). The $P_2I_5^+$ cation displays a staggered configuration (Fig. 1), with an I1—P1—P2—I4 torsion angle of −52.3 (1)°. The P2—I4 and P2—I5 bond lengths of the PI_2 unit are significantly longer than the P1—I1, P1—I2 and P1—I3 bond lengths found for the PI_3 unit. The GaI_4^- unit has a slightly distorted tetrahedral geometry. The Ga—I bond distances range between 2.521 (1) and 2.577 (1) Å, and the I—Ga—I bond angles between 105.15 (4) and 112.18 (4)°, similar to the bond lengths and angles found in $(TeI_3)[GaI_4]$ (Schulz-Lang *et al.*, 1998). Similar to $(P_2I_5)[AlI_4]$ (Pohl, 1983), the structure of $(P_2I_5)[GaI_4]$ shows weak interatomic I···I distances in the range 3.4002 (8)–3.9168 (8) Å between the $P_2I_5^+$ and the GaI_4^- units (Fig. 2), which are significantly shorter than the sum of the van der Waals radii (*ca* 4.3 Å), indicating weak cation–anion interactions.

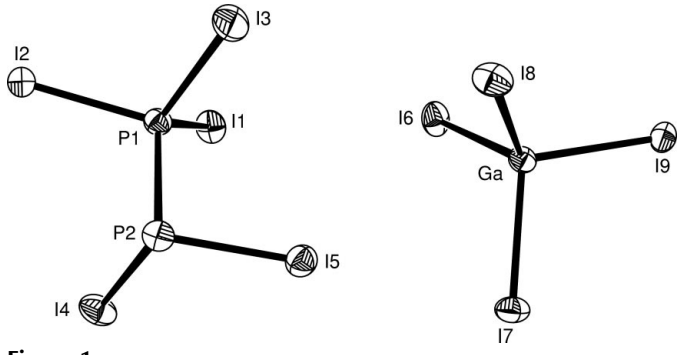

Figure 1
The molecular structure of $(P_2I_5)[GaI_4]$ showing 50% probability displacement ellipsoids.

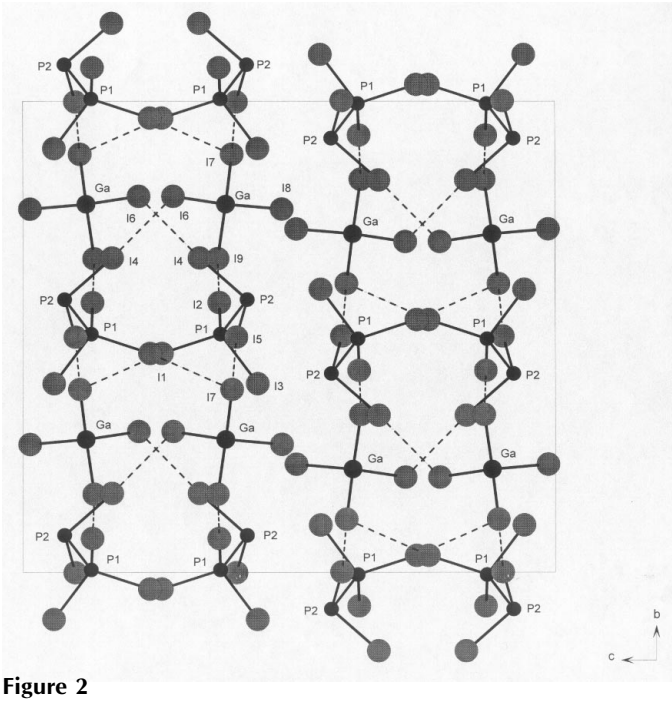

Figure 2
Packing diagram viewed down the *a* axis.

Experimental

$(P_2I_5)[GaI_4]$ was prepared by the reaction of PI_3 (0.84 g, 2.00 mmol) and GaI_3 (0.45 g, 1.00 mmol) in CS_2 (20 ml) at room temperature. The solvent was slowly removed under static vacuum, yielding red crystals.

Crystal data

$(P_2I_5)[GaI_4]$
M_r = 1273.81
Orthorhombic, *Pbca*
a = 10.7960 (5) Å
b = 18.1687 (8) Å
c = 20.1886 (10) Å
V = 3960.0 (3) Å^3
Z = 8
D_x = 4.273 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5000 reflections
θ = 2.4–24.0°
μ = 15.55 mm^{-1}
T = 200 (3) K
Irregular, red
0.19 × 0.12 × 0.10 mm

Data collection

Stoe IPDS image-plate diffractometer
φ scans
Absorption correction: numerical crystal faces optimized with Stoe *XSHAPE* (Stoe, 1997) then a numerical absorption correction with *XRED* (revision 1.09; Stoe, 1997)
T_{min} = 0.194, T_{max} = 0.395
10 907 measured reflections
3094 independent reflections
2570 reflections with $I > 2\sigma(I)$
R_{int} = 0.097
θ_{max} = 24°
$h = -12 \rightarrow 12$
$k = -16 \rightarrow 20$
$l = -19 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.076
S = 0.96
3094 reflections
109 parameters
$w = 1/[\sigma^2(F_o^2) + (0.035P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.38 e Å^{-3} (0.82 Å from I3)
$\Delta\rho_{min}$ = -1.23 e Å^{-3} (0.90 Å from I3)

Table 1
Selected geometric parameters (Å, °).

Ga—I6	2.5210 (10)	P1—I3	2.391 (2)
Ga—I8	2.5330 (10)	P1—I1	2.401 (2)
Ga—I9	2.5549 (10)	P1—I2	2.413 (2)
Ga—I7	2.5771 (10)	P2—I4	2.421 (2)
P1—P2	2.227 (3)	P2—I5	2.442 (2)
I6—Ga—I8	110.60 (4)	I3—P1—I1	108.72 (8)
I6—Ga—I9	109.75 (4)	P2—P1—I2	105.98 (10)
I8—Ga—I9	109.71 (4)	I3—P1—I2	109.04 (9)
I6—Ga—I7	112.18 (4)	I1—P1—I2	109.09 (9)
I8—Ga—I7	109.30 (4)	P1—P2—I4	95.56 (10)
I9—Ga—I7	105.15 (4)	P1—P2—I5	95.05 (10)
P2—P1—I3	106.25 (11)	I4—P2—I5	103.13 (9)
P2—P1—I1	117.50 (11)		

Table 2
Selected contact distancess (Å).

I1···I7^{i}	3.4420 (9)	I4···I6^{iii}	3.7264 (8)
I2···I9^{ii}	3.4002 (8)	I5···I7^{iv}	3.6598 (8)

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

Data collection: *IPDS Software Manual* (Stoe, 1997); cell refinement: *IPDS Software Manual*; data reduction: *IPDS Software Manual*; program(s) used to solve structure: *SIR*97 (Cascarano *et al.*, 1996); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997). *SCHAKAL* (Keller, 1995) and *DIAMOND* (Bergerhoff, 1996); software used to prepare material for publication: *PLATON*95 (Spek, 1995).

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