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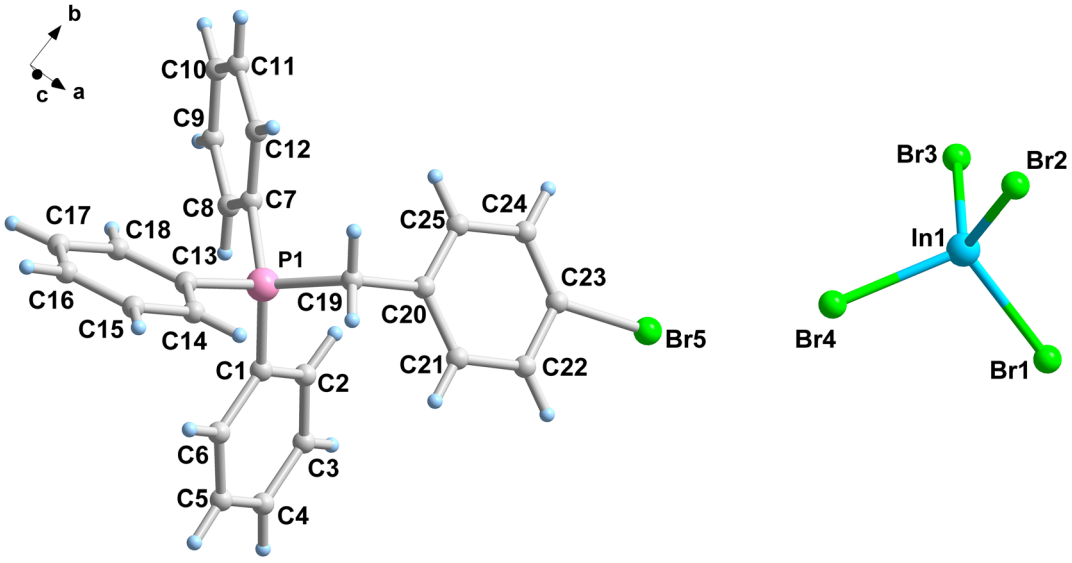
# Crystal structure of [(4-bromobenzyl) triphenylphosphonium] tetrabromidoindium(III), $[C_{25}H_{21}BrP]^{+}[InBr_4]^{-}$

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**Abstract**

$C_{25}H_{21}Br_5PIn$, monoclinic, $P2_1/c$ (no. 14), $a$ = 10.5887(2) Å, $b$ = 14.7713(2) Å, $c$ = 18.9737(3) Å, $\beta$ = 102.300(2)°, $V$ = 2899.53(8) Å$^3$, $Z$ = 4, $R_{gt}(F)$ = 0.0450, $wR_{ref}(F^2)$ = 0.1205, T = 293(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Clear light colourless block |
| Size: | 0.12 × 0.10 × 0.09 mm |
| Wavelength: | Cu $K\alpha$ radiation (1.54184 Å) |
| $\mu$: | 15.2 mm$^{-1}$ |
| Diffractometer, scan mode: | Rigaku Synergy, $\omega$ scans |
| $\theta_{max}$, completeness: | 66.6°, 100 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 29219, 5137, 0.079 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 4,462 |
| $N(param)_{refined}$: | 301 |
| Programs: | Rigaku,[1] SHELX,[2] Olex2[3] |

## 1 Source of materials

The 0.5 mmol of (4-bromobenzyl)triphenylphosphonium bromide and 0.5 mmol of $InBr_3$ were dissolved in 5 mL ethanol/dichloromethane (2:3, *v*/*v*). And the 0.5 mL of aqueous hydrobromic acid was added. The solution was then left at room temperature for 10 days, the well-shaped single crystals were obtained.

## 2 Experimental details

Crystal data were collected on a Rigaku.[1] The crystal structure was determined using the SHELXT program within the Olex2 and subsequently refined with SHELXL.[2–4] The structural picture was finished using Diamond.[5]

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**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| In1 | 1.29064 (3) | 0.84882 (2) | 0.38592 (2) | 0.05273 (15) |
| Br1 | 1.52311 (6) | 0.80484 (6) | 0.42340 (4) | 0.0849 (2) |
| Br2 | 1.23438 (8) | 0.95841 (5) | 0.47351 (4) | 0.0834 (2) |
| Br3 | 1.25291 (8) | 0.91719 (5) | 0.26444 (3) | 0.0827 (2) |
| Br4 | 1.16394 (8) | 0.70507 (5) | 0.37790 (5) | 0.0904 (3) |
| P1 | 0.29418 (10) | 0.33206 (8) | 0.35609 (6) | 0.0429 (2) |
| C1 | 0.4035 (4) | 0.2458 (3) | 0.3407 (2) | 0.0475 (9) |
| C2 | 0.5002 (4) | 0.2661 (4) | 0.3042 (3) | 0.0580 (11) |
| H2 | 0.507900 | 0.324367 | 0.287052 | 0.070* |
| C3 | 0.5856 (5) | 0.1986 (5) | 0.2936 (4) | 0.0738 (16) |
| H3 | 0.648174 | 0.210994 | 0.267141 | 0.089* |
| C4 | 0.5781 (6) | 0.1146 (5) | 0.3216 (4) | 0.0828 (19) |
| H4 | 0.636427 | 0.069994 | 0.314926 | 0.099* |
| C5 | 0.4845 (6) | 0.0950 (4) | 0.3600 (4) | 0.0804 (18) |
| H5 | 0.481504 | 0.037757 | 0.379954 | 0.097* |
| C6 | 0.3951 (5) | 0.1598 (4) | 0.3691 (3) | 0.0618 (13) |
| H6 | 0.330447 | 0.146107 | 0.393779 | 0.074* |
| C7 | 0.2311 (4) | 0.3945 (3) | 0.2753 (2) | 0.0487 (10) |
| C8 | 0.2479 (6) | 0.3658 (4) | 0.2081 (3) | 0.0649 (13) |
| H8 | 0.300690 | 0.316580 | 0.204249 | 0.078* |
| C9 | 0.1851 (7) | 0.4116 (5) | 0.1472 (3) | 0.0820 (18) |
| H9 | 0.197681 | 0.393893 | 0.102166 | 0.098* |
| C10 | 0.1047 (6) | 0.4824 (5) | 0.1523 (4) | 0.087 (2) |
| H10 | 0.061404 | 0.511650 | 0.110753 | 0.104* |
| C11 | 0.0880 (7) | 0.5101 (6) | 0.2180 (5) | 0.101 (3) |
| H11 | 0.033000 | 0.558342 | 0.221051 | 0.121* |
| C12 | 0.1523 (6) | 0.4670 (5) | 0.2807 (4) | 0.0752 (16) |
| H12 | 0.142175 | 0.487071 | 0.325595 | 0.090* |
| C13 | 0.1566 (4) | 0.2851 (3) | 0.3844 (3) | 0.0474 (9) |
| C14 | 0.1553 (5) | 0.2715 (5) | 0.4559 (3) | 0.0705 (14) |
| H14 | 0.228072 | 0.284874 | 0.491309 | 0.085* |
| C15 | 0.0452 (6) | 0.2378 (5) | 0.4749 (4) | 0.0808 (17) |
| H15 | 0.044984 | 0.227745 | 0.523276 | 0.097* |
| C16 | −0.0630 (5) | 0.2190 (4) | 0.4235 (4) | 0.0784 (18) |
| H16 | −0.137881 | 0.198690 | 0.436635 | 0.094* |
| C17 | −0.0595 (7) | 0.2307 (6) | 0.3528 (4) | 0.100 (3) |
| H17 | −0.131605 | 0.215410 | 0.317445 | 0.120* |
| C18 | 0.0482 (6) | 0.2645 (5) | 0.3325 (3) | 0.0810 (19) |
| H18 | 0.047949 | 0.273403 | 0.283921 | 0.097* |
| C19 | 0.3752 (5) | 0.4073 (4) | 0.4275 (3) | 0.0567 (11) |
| H19A | 0.316878 | 0.456352 | 0.432532 | 0.068* |
| H19B | 0.393177 | 0.373957 | 0.472632 | 0.068* |
| C20 | 0.5007 (4) | 0.4473 (3) | 0.4152 (2) | 0.0506 (10) |
| C21 | 0.6159 (5) | 0.4053 (4) | 0.4450 (3) | 0.0656 (13) |
| H21 | 0.615545 | 0.351947 | 0.471045 | 0.079* |
| C22 | 0.7331 (5) | 0.4423 (5) | 0.4365 (4) | 0.0784 (18) |
| H22 | 0.810999 | 0.413618 | 0.455819 | 0.094* |
| C23 | 0.7306 (6) | 0.5216 (5) | 0.3991 (4) | 0.0779 (19) |
| C24 | 0.6186 (7) | 0.5644 (4) | 0.3696 (4) | 0.0758 (17) |
| H24 | 0.619353 | 0.618315 | 0.344306 | 0.091* |
| C25 | 0.5026 (6) | 0.5262 (4) | 0.3778 (3) | 0.0646 (13) |
| H25 | 0.425113 | 0.554772 | 0.357580 | 0.078* |
| Br5 | 0.9024 (6) | 0.5556 (6) | 0.3986 (4) | 0.0995 (13) |
| Br5A | 0.8798 (5) | 0.5878 (4) | 0.3818 (3) | 0.1010 (12)[a] |

[a]Occupancy: 0.589 (12).

# 3 Comment

In this study, a zero-dimensional indium(III)-based compound was reported, including a (4-bromobenzyl)triphenylphosphonium (**4BBTP**) cation, and a [$InBr_4$]$^-$ anion. The **4BBTP** cation carries a positive charge, tetrahedron [$InBr_4$]$^-$ anion carries a negative charge. The bond lengths of In–Br are 2.470, 2.482, 2.498, 2.499 Å, which are in the normal range.[6–8]

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**Conflict of interest:** The authors declare no conflicts of interest regarding this article.

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