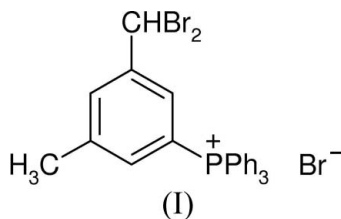


**[5-(Dibromomethyl)-3-methylbenzyl]tri-phenylphosphonium bromide****Ai-Yun Fu,<sup>a\*</sup> Yu Li,<sup>a</sup> Da-Qi Wang,<sup>b</sup> Lian-Wen Zhou<sup>a</sup> and Shi-Zhou Fu<sup>b</sup>**<sup>a</sup>Department of Chemistry, Dezhou University, Shandong Dezhou 253023, People's Republic of China, and <sup>b</sup>Department of Chemistry, Liaocheng University, Shandong Liaocheng 252059, People's Republic of ChinaCorrespondence e-mail:  
aiyunfu@yahoo.com.cn**Key indicators**Single-crystal X-ray study  
*T* = 298 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.011 \text{ \AA}$   
*R* factor = 0.056  
*wR* factor = 0.138  
Data-to-parameter ratio = 16.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.The asymmetric unit of the title structure,  $\text{C}_{27}\text{H}_{24}\text{Br}_2\text{P}^+\cdot\text{Br}^-$ , comprises two  $[(\text{CH}_3\text{C}_6\text{H}_3\text{CHBr}_2)(\text{C}_6\text{H}_5)_3\text{P}]^+$  cations and two bromide anions. The cations exhibit closely comparable conformations, with a slight distortion from tetrahedral geometry around P.**Comment**The title compound includes two  $\text{C}_{27}\text{H}_{24}\text{Br}_2\text{P}^+$  cations and two bromide anions in the asymmetric unit (Fig. 1). The two independent cations have closely comparable conformations. The average C–P bond length is 1.793 and 1.790 Å in the two cations, comparable to the corresponding value of 1.792 Å in the compound  $[\text{PPh}_4]\text{Cl}\cdot\text{H}_2\text{O}$  (Blake *et al.*, 2003), for example. The C–P–C angles span the range 107.5 (3)–111.5 (3)°, demonstrating a slight distortion from tetrahedral geometry around P.**Experimental**

A tetrahydrofuran solution (10 ml) of 3-methyl-5-dibromomethyl-phenyl bromide (0.17 g, 0.5 mmol) was added dropwise to a stirred tetrahydrofuran solution (10 ml) of triphenylphosphine (0.12 g, 0.5 mmol). Refluxing for 5 h gave a clear mixture from which yellow crystals of (I) were obtained in 65% yield after standing at room temperature for several days. Elemental analysis found: C 52.31, H 3.77, Br 38.69, P 4.86%; calculated: C 52.37, H 3.91, Br 38.72, P 5.00%.

**Crystal data** $\text{C}_{27}\text{H}_{24}\text{Br}_2\text{P}^+\cdot\text{Br}^-$   
*M<sub>r</sub>* = 619.16  
Monoclinic,  $P2_1/c$   
*a* = 12.307 (3) Å  
*b* = 21.789 (4) Å  
*c* = 19.849 (3) Å  
 $\beta$  = 91.387 (2)°  
*V* = 5321.2 (17) Å<sup>3</sup>*Z* = 8  
*D<sub>x</sub>* = 1.546 Mg m<sup>-3</sup>  
Mo *K*α radiation  
 $\mu$  = 4.62 mm<sup>-1</sup>  
*T* = 298 (2) K  
Block, yellow  
0.43 × 0.37 × 0.29 mm**Data collection**Bruker SMART CCD  
diffractometer  
 $\varphi$  and  $\omega$  scans  
Absorption correction: multi-scan  
(*SADABS*; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.182, *T<sub>max</sub>* = 0.26227500 measured reflections  
9287 independent reflections  
4405 reflections with  $I > 2\sigma(I)$   
*R<sub>int</sub>* = 0.082  
 $\theta_{\text{max}}$  = 25.0°

Refinement

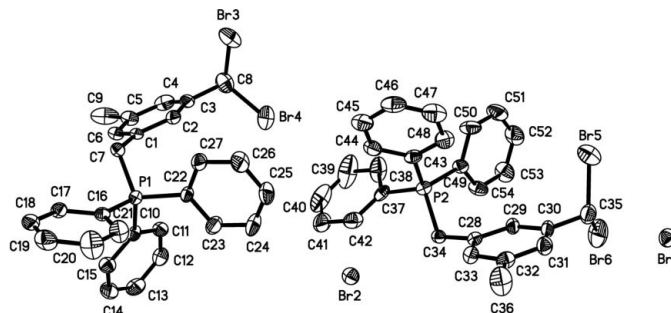
Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.056$   
 $wR(F^2) = 0.138$   
 $S = 1.01$   
 9287 reflections  
 559 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0549P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 1.12 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.84 \text{ e } \text{Å}^{-3}$

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C–H = 0.93 Å for aromatic H, 0.98 Å for CHBr<sub>2</sub>, 0.97 Å for CH<sub>2</sub>, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . For the methyl groups, C–H = 0.96 Å and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ . The highest peak in the residual electron density lies 1.66 Å from the C36 methyl group.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

We are grateful for financial support from the National Natural Science Foundation of Shangdong (Grant No. Y2005B20), and from the Technology Office of Dezhou City, Shandong Province (Grant No. 030701).



**Figure 1**  
 The asymmetric unit of (I), showing displacement ellipsoids at the 30% probability level. H atoms are omitted.

References

Blake, A. J., Garner, C. D. & Tunney, J. M. (2003). *Acta Cryst.* **E59**, o9–o10.  
 Bruker (1997). *SMART, SAINT and SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997). *SHELXL97 and SHELXS97*. University of Göttingen, Germany.