Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Tetraphenylphosphonium 2,4,5-tricarboxybenzoate

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Received 23 December 2006
Accepted 25 January 2007

Key indicators

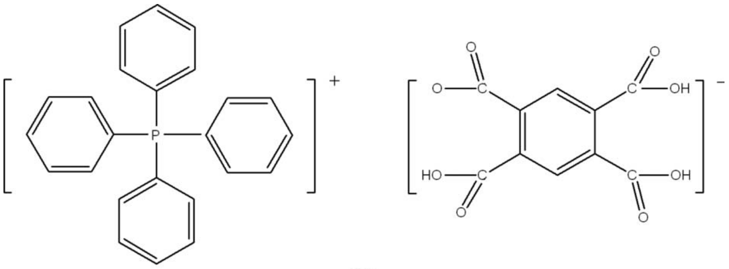
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.109
Data-to-parameter ratio = 16.0

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

The title compound, $C_{24}H_{20}P^+ \cdot C_{10}H_5O_8^-$, is a salt of singly-deprotonated 1,2,4,5-benzenetetracarboxylic acid (pyromellitic acid). The crystal packing is stabilized by intermolecular hydrogen bonds involving the anions, in addition to normal Coulombic forces.

Comment

The title compound, (I), is an air-stable salt at ambient temperature. Its structure contains discrete Ph_4P^+ cations and H_3BTC^- anions (Fig. 1; H_4BTC = 1,2,4,5-benzenetetracarboxylic acid or pyromellitic acid). All bond distances and angles in (I) are normal.



(I)

H_3BTC^- anions are linked together by intermolecular hydrogen bonds between carboxyl and carboxylate groups (Fig. 2 and Table 2), generating a chain of centrosymmetric dimers along the *a* axis. There is also a strong intramolecular O—H···O hydrogen bond between one carboxyl group and the adjacent carboxylate group. The main interaction of the cations with the anions is normal Coulombic attraction.

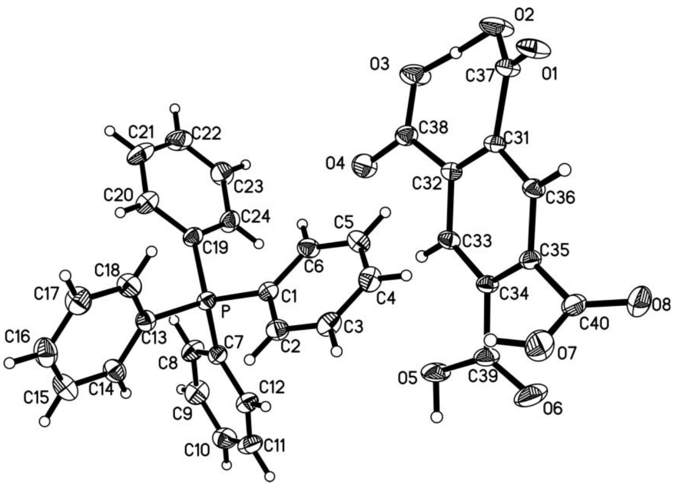


Figure 1
The asymmetric unit of compound (I), with 30% probability displacement ellipsoids. The almost symmetric strong intramolecular hydrogen bond is shown with two full bonds.

Experimental

The title compound was obtained as hexagonal-prismatic colorless crystals in about 50% yield from the hydrothermal reaction of 1,2,4,5-benzenetetracarboxylic acid (0.5 mmol), tetraphenylphosphonium chloride (0.53 mmol) and water (5 ml) heated at 473 K for 5 d, then cooled at a rate of 2 K h^{-1} to 423 K, and finally left to cool naturally to ambient temperature. The crystal structure is consistent with the IR spectrum of (I).

Crystal data

$C_{24}H_{20}P^{+}\cdot C_{10}H_5O_8^{-}$
$M_r = 592.51$
Triclinic, $P\overline{1}$
$a = 9.715\ (3)$ Å
$b = 10.920\ (3)$ Å
$c = 14.268\ (5)$ Å
$\alpha = 90.218\ (4)^\circ$
$\beta = 106.435\ (3)^\circ$
$\gamma = 102.776\ (4)^\circ$

$V = 1412.3\ (8)$ Å^3
$Z = 2$
$D_x = 1.393$ Mg m^{-3}
Mo *Kα* radiation
$\mu = 0.15$ mm^{-1}
$T = 293\ (2)$ K
Prism, colorless
0.60 × 0.35 × 0.25 mm

Data collection

Rigaku Mercury70 diffractometer
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
$T_{\min} = 0.897$, $T_{\max} = 0.963$

11070 measured reflections
6387 independent reflections
5443 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.013$
$\theta_{\max} = 27.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.109$
$S = 1.01$
6387 reflections
400 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 0.383P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.29$ e Å^{-3}
$\Delta\rho_{\min} = -0.22$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1···O1$^{\rm i}$	0.95 (2)	1.64 (2)	2.5832 (17)	172 (2)
O7—H2···O4$^{\rm ii}$	0.90 (2)	1.78 (3)	2.682 (2)	177 (2)
O3—H3···O2	1.16 (3)	1.24 (3)	2.3942 (18)	174 (3)

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y, -z+1$.

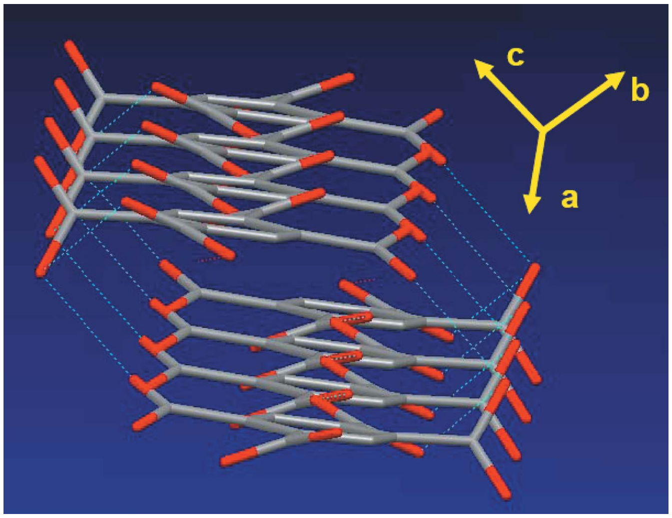


Figure 2
The hydrogen bonding (dashed lines) linking anions into a chain of centrosymmetric dimers. H atoms have been omitted.

C-bound H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). Carboxyl H atoms were located in a difference map and refined freely.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

We are grateful for financial support from the Research Fund of Fujian Province, China (No. 2003F006).

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Acta Cryst. (2007). E**63**, o1010–o1011 Yang *et al.* • $C_{24}H_{20}P^{+}\cdot C_{10}H_5O_8^{-}$ **o1011**