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2,5-Dibromo-6-isopropyl-3-methyl-*p*-benzoquinone

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
R factor = 0.024
wR factor = 0.064
Data-to-parameter ratio = 16.4

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

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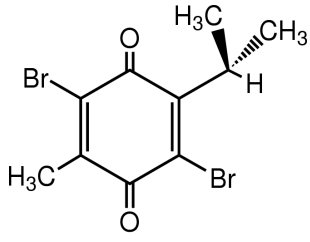
The title compound, $C_{10}H_{10}Br_2O_2$, is a well known inhibitor of respiratory and photosynthetic processes. The methyl groups of the isopropyl group assume approximately equal distances from the ring plane and maximum distances from the neighboring Br atom, possibly to avoid unfavourable steric interactions.

Comment

As one of the Qo-II/III-type inhibitors, dibromothymoquinone, *i.e.* the title compound, (I), is known to interact with the iron–sulfur protein (ISP) of the cytochrome *bc*1 complex in respiratory chains (Degli Esposti *et al.*, 1984) and with that of the chloroplast *b6f* complex in photosynthetic chains (Schoepp *et al.*, 1999). We have analysed the anomalous signal of the four redox centers in the crystal structures of bovine mitochondrial *bc*1 complex with and without bound inhibitors (Kim *et al.*, 1998; Xia *et al.*, 1998), and found that dibromothymoquinone promotes the fixed conformational state of the complex, confirming its interaction with the ISP.



(I)

The methyl groups of the isopropyl group assume approximately equal distances from the ring plane and maximum distances from the neighboring Br2 atom (Fig. 1), possibly to avoid unfavourable steric interactions. This orientation is opposite to that in the majority of known isopropyl quinones including didehydro-12-*O*-methyl royleanone (King *et al.*, 1990), where a methoxy group is in a position equivalent to the Br2 atom in (I).

Experimental

The title compound was purchased from Sigma Co. (*D*-3769) and used without further purification. Crystallization at room temperature from methanol afforded amber crystals suitable for X-ray structure analysis.

Crystal data

$C_{10}H_{10}Br_2O_2$
M_r = 322.00
Monoclinic, *Cc*
a = 5.4507 (2) Å
b = 18.5945 (9) Å
c = 11.4256 (6) Å
β = 100.941 (3)°
V = 1136.97 (9) Å^3
Z = 4
D_x = 1.881 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 15747 reflections
θ = 0.9–27.1°
μ = 7.10 mm^{-1}
T = 295 (2) K
Rod, amber
0.54 × 0.21 × 0.12 mm

Data collection

Nonius KappaCCD diffractometer
φ scans
Absorption correction: empirical (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.180, T_{max} = 0.426
2145 measured reflections
2145 independent reflections
2042 reflections with $I > 2\sigma(I)$
θ_{max} = 26.4°
h = −5 → 5
k = −22 → 22
l = −14 → 14

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.064
S = 1.04
2145 reflections
131 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 1.0226P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0105 (8)
Absolute structure: (Flack, 1983), 976 Friedel pairs
Flack parameter = 0.026 (12)

Table 1
Selected interatomic distances (Å).

O1—C1	1.218 (5)	C4—O2	1.208 (5)
C1—C2	1.485 (5)	C4—C5	1.485 (5)
C1—C6	1.496 (6)	C5—C6	1.338 (5)
C2—C3	1.332 (6)	C5—Br2	1.890 (4)
C2—Br1	1.893 (4)	C6—C8	1.519 (6)
C3—C4	1.494 (6)	C8—C10	1.510 (6)
C3—C7	1.502 (6)	C8—C9	1.540 (7)

The data collection was incomplete (92%), due to the loss of the crystal about three frames before the projected end.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2001) and *ORTEP*-3 (Farrugia, 1997).

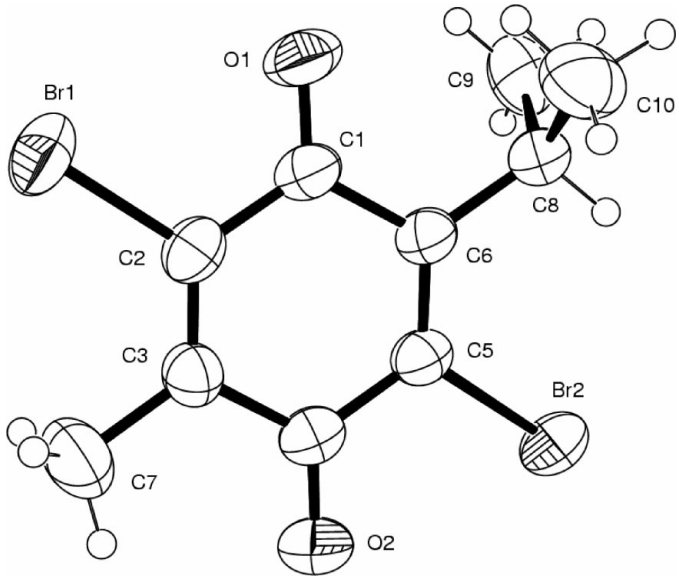


Figure 1
The structure of (I) showing 50% probability displacement ellipsoids for non-H atoms.

References

Degli Esposti, M., Rotilio, G. & Lenaz, G. (1984). *Biochim. Biophys. Acta*, **767**, 10–20.
Farrugia, L. J. (1997). *J. Appl. Cryst*, **30**, 565.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Kim, H., Xia, D., Yu, C.-A., Xia, J. Z., Kachurin, A. M., Zhang, L., Yu, L. & Deisenhofer, J. (1998). *Proc. Natl Acad. Sci. USA*, **95**, 8026–8033.
King, J., Quayle, P. & Malone, J. F. (1990). *Tetrahedron Lett.* **31**, 5221–5224.
Nonius (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter and R. M. Sweet, pp. 307–326. London: Academic Press.
Schoepp, B., Brugna, M., Riedel, A., Nitschke, W. & Kramer, D. M. (1999). *FEBS Lett.* **450**, 245–250.
Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.
Spek, A. L. (2001). *PLATON*. Utrecht University, The Netherlands.
Xia, D., Kim, H., Yu, C.-A., Yu, L., Kachurin, A. M., Zhang, L. & Deisenhofer, J. (1998). *Biochem. Cell Biol.* **76**, 673–679.