Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Phenylethyl phenyldithioacetate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.143
Data-to-parameter ratio = 20.8

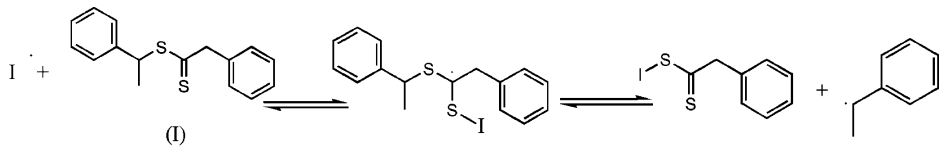
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 13 January 2006
Accepted 12 May 2006

The overall shape of the title compound, $C_{16}H_{16}S_2$, is like a capital 'M', with both planar benzene rings projecting to one side of the central thioacetate portion.

Comment

The title compound, (I), is commonly used as a chain-transfer agent in living-radical polymerizations. The S atom adjacent to the carbon with a double bond can be attacked by radicals and, in a reverse process, yields styrene radicals as shown in the scheme, in which *I* may indicate either an initiator-born radical or a long-chain propagating radical. The mediation of this compound in free-radical polymerizations leads to a well controlled molecular weight, a narrow molecular-weight distribution and an improvement in the extent of conversion.



radical adduct radicals

Overall, the shape of molecule (I) is like a capital 'M', with both planar benzene rings projecting to one side of the central thioacetate portion (Fig. 1). The dihedral angle between the two benzene planes is 126.5 (1)°. There are no unusually short intermolecular contact distances.

Experimental

Compound (I) was synthesized by the authors, using a literature procedure (Quinn, *et al.*, 2001). Briefly, a simple Grignard reagent

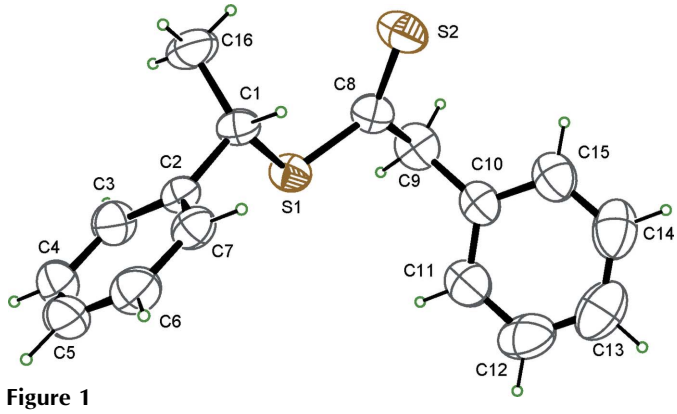


Figure 1
The structure of (I), showing 50% probability ellipsoids and the atom-labelling scheme.

was first synthesized from benzyl chloride and magnesium. The Grignard reagent and carbon disulfide then were used to produce a dithiocarboxylic acid salt, which was then acidified and subsequently underwent an addition reaction with styrene. The product (I) was crystallized by evaporation of a cold (268 K) methanol solution.

Crystal data

$C_{16}H_{16}S_2$
M_r = 272.41
Monoclinic, $P2_1/c$
a = 11.311 (2) Å
b = 6.019 (2) Å
c = 22.003 (4) Å
β = 98.188 (10)°
V = 1482.7 (6) Å^3
Z = 4
D_x = 1.220 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 298 (1) K
Chunk, yellow
0.23 × 0.20 × 0.13 mm

Data collection

Rigaku RAXIS-RAPID diffractometer
ω scans
Absorption correction: multi-scan *ABSCOR* (Higashi, 1995)
T_{min} = 0.916, T_{max} = 0.957
13414 measured reflections
3398 independent reflections
2251 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.143
S = 0.99
3398 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0814P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

All H atoms were positioned geometrically and refined with riding constraints (C—H = 0.93–0.98 Å). The U_{iso}(H) values were set equal to $1.2U_{eq}$(carrier atom).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge Professor Jianming Gu from the Zhejiang University for help in determining the crystal structure.

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