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4,4′-Dichloro-*N*,*N*′-(*o*-phenylene)-dibenzenesulfonamide

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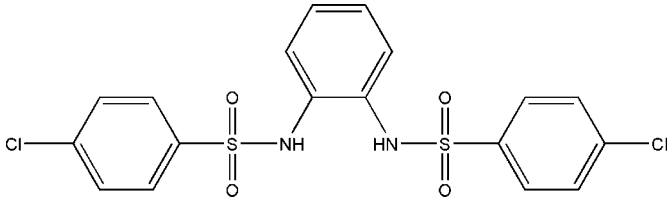
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.122; data-to-parameter ratio = 16.2.

The title compound, $C_{18}H_{14}Cl_2N_2O_4S_2$, is a diamine that is a precursor to a quinonoid bidentate redox-active ligand. The dihedral angles between the central phenyl ring and the end rings are 87.5(1) and 60.7(1)°, while the two end rings make a dihedral angle of 82.5(1)°. The crystal structure is stabilized by two weak intermolecular N—H···O hydrogen bonds, as well as one intramolecular C—H···O and one N—H···N hydrogen bond.

Related literature

For the synthesis of related substituted *o*-phenylenediamines, see: Massacret *et al.* (1999). For background to the use of substituted *o*-benzoquinones as ligands, see: Masui & Lever (1993); Kalinina *et al.* (2008) and references therein.



Experimental

Crystal data

$C_{18}H_{14}Cl_2N_2O_4S_2$
M_r = 457.33
Triclinic, $P\overline{1}$
a = 7.7225 (4) Å
b = 11.1920 (4) Å
c = 11.9325 (5) Å
α = 109.669 (2)°
β = 91.420 (2)°
γ = 101.782 (2)°
V = 945.79 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.59 mm^{-1}
T = 150 (1) K
0.40 × 0.36 × 0.30 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.748, T_{max} = 0.876
8650 measured reflections
4235 independent reflections
3386 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.122
S = 1.08
4235 reflections
261 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O4^{i}	0.87 (3)	2.12 (3)	2.936 (3)	157 (2)
N2—H2···O2^{ii}	0.85 (3)	2.30 (3)	3.107 (3)	159 (2)
N1—H1···N2	0.87 (3)	2.45 (3)	2.811 (3)	106 (2)
C6—H6···O1	0.95	2.22	2.900 (3)	128

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

Data collection: *COLLECT* (Nonius, 2002); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2184).

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