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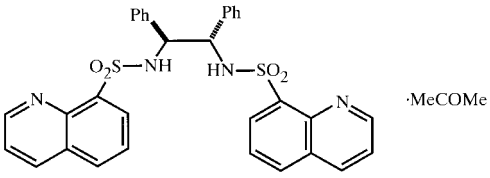
The crystal structure of the new chiral complex (1*R*,2*R*)-1,2-diphenyl-1,2-bis(8-quinolinesulfonylamino)-ethylenediamine–acetone (1/1), $C_{32}H_{26}N_4O_4S_2{\cdot}C_3H_6O$, is reported. The conformation of the $C_{32}H_{26}N_4O_4S_2$ (BQSDA) molecule is determined by a bifurcated N—H···N hydrogen-bond system. The acetone of solvation is linked to the BQSDA molecule by an N—H···O hydrogen bond.

Comment

The structure of the title compound, (I), has been determined as part of a study into asymmetric catalysis in transfer hydrogenation reaction and addition of dialkylzinc to aldehydes. Further study shows that BQSDA as chiral catalyst has high enantioselectivity. Therefore the structure of this new ligand can help us know of its catalytic mechanism in asymmetric reaction.



(I)

Experimental

A mixture of 1 mmol (1*R*,2*R*)-diphenylethylenediamine and 2 mmol 8-quinolinesulfonyl chloride in 10 ml dichloroethane was stirred for 24 h at room temperature. Then the resulting white solid was collected by evaporation of the solution. The yield of analytically pure product was 100%. The single-crystal was obtained from acetone at room temperature.

Crystal data

$C_{32}H_{26}N_4O_4S_2{\cdot}C_3H_6O$	D_x = 1.350 Mg m^{-3}
M_r = 652.77	Mo $K\alpha$ radiation
Monoclinic, $P2_1$	Cell parameters from 33 reflections
a = 9.717 (2) Å	θ = 3.18–16.51°
b = 9.4950 (10) Å	μ = 0.215 mm^{-1}
c = 17.542 (3) Å	T = 296 (2) K
β = 97.130 (10)°	Flake, colorless
V = 1606.0 (5) Å^3	0.48 × 0.40 × 0.36 mm
Z = 2	

Data collection

*P*4 diffractometer	θ_{max} = 27°
ω scans	$h = -1 \rightarrow 12$
Absorption correction: none	$k = -1 \rightarrow 12$
5056 measured reflections	$l = -22 \rightarrow 22$
4159 independent reflections	3 standard reflections
3405 reflections with $I > 2\sigma(I)$	every 97 reflections
R_{int} = 0.012	intensity decay: 1.42%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2]$ where $P = F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.0319	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.0742	$\Delta\rho_{max}$ = 0.211 e Å^{-3}
S = 0.944	$\Delta\rho_{min}$ = −0.179 e Å^{-3}
4159 reflections	Extinction correction: *SHELXL*
426 parameters	Extinction coefficient: 0.0146 (11)
H atoms treated by a mixture of independent and constrained refinement	Absolute structure: Flack (1983), 433 Friedel pairs
	Flack parameter = −0.05 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O5	0.80 (3)	2.22 (3)	2.905 (4)	145 (3)
N3—H3N···N1	0.78 (3)	2.42 (3)	2.806 (3)	112 (2)
N3—H3N···N4	0.78 (3)	2.39 (3)	2.956 (3)	130 (3)

The H atoms bonded to N1 and N3 were refined isotropically; all other H atoms were allowed for as riding atoms. N—H dimensions are 0.78 (3) and 0.80 (3) Å.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS* (Siemens, 1994); data reduction: *SHELXTL*/*PC* (Sheldrick, 1994); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*b*); molecular graphics: *SHELXTL*/*PC* (Sheldrick, 1994); software used to prepare material for publication: *SHELXTL*/*PC* (Sheldrick, 1994).

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