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9,9′-Biacridine *N*,*N*′-dioxide: a novel potential bridging ligand bearing the bulky acridine *N*-oxide skeleton

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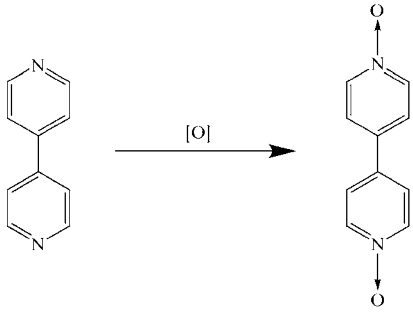
The title compound, $C_{26}H_{16}N_2O_2$, is a potential linear bridging *O*-donor ligand comprising bulky acridine *N*-oxide ring systems. Weak intermolecular C—H$\cdots$O hydrogen-bonding interactions link adjacent molecules to form extended chains. The structure also contains intermolecular C—H$\cdots\pi$ interactions.

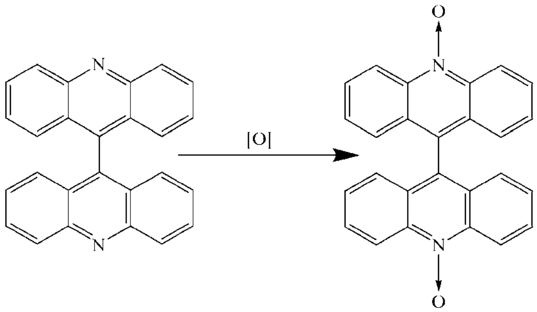
Comment

In recent years, 4,4′-bipyridine, (*A*), and its analogues containing two 4-pyridyl donor units have been used extensively as bridging ligands in coordination and metallosupramolecular chemistry (Kitagawa *et al.*, 2004; Steel, 2005), and this has resulted in a large number of extended assemblies, including helical networks and diamondoid, honeycomb, square-grid, ribbon, grid, T-shaped, ladder, brick wall and octahedral frameworks (Withersby *et al.*, 1999; Yaghi *et al.*, 1998). In comparison with other N-containing heterocyclic ligands, acridine-based ligands have some primary structural characteristics: (*a*) the acridine ring has a larger conjugated π system and therefore π–π stacking interactions may play important roles in the formation of their metal complexes, and (*b*) the larger conjugated π systems and the steric hindrance between H atoms of adjacent benzene rings may affect the coordination abilities of the acridine N-donor atom (Bu *et al.*, 2004; Liu *et al.*, 2006). To explore the influence of the bulky acridine-based ligand with a large conjugated π system on the structures and properties of its complexes, we synthesized a 4,4′-bipyridyl-like linear diamine bridging ligand, 9,9′-biacridine, (*B*), and reported its crystal structure (Liu, 2007). Unfortunately, unlike 4,4′-bipyridine, when we sequentially reacted 9,9′-biacridine with various metal salts in order to construct related metal–organic complexes, no complexes suitable for a crystal structure determination could be obtained; this may be due to the steric hindrance between the H atoms of the adjacent benzene rings.

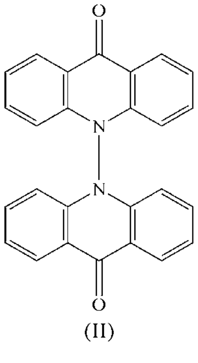
Recently, we also noticed that Long *et al.* (2001) have demonstrated the use of 4,4′-bipyridine *N*,*N*′-dioxide, (*C*), in the construction of lanthanide coordination polymers with unusual two- or three-dimensional networks. Considering all of the aspects stated above, we sequentially synthesized a novel linear bridging ligand with a bulky aromatic skeleton, *viz.* 9,9′-biacridine *N*,*N*′-dioxide, (I), whose coordination sites could potentially mimic those of 4,4′-bipyridyl *N*,*N*′-dioxide in supramolecular chemistry, except for the bulky aromatic skeleton. In comparision with 9,9′-biacridine, the N—O bonds of (I) may reduce the steric hindrance of the H atoms of the adjacent benzene rings so as to facilitate the formation of coordination bonds between metal ions and the oxygen donors of the acridine *N*-oxide rings in the construction of unique supramolecular architectures with potential uses as functional materials. We report here the crystal structure of (I) and compare it with a structurally related compound, 10,10′-biacridinyl-9,9′-dione, (II), whose crystal structure has been reported by Boyer *et al.* (1993).



(*A*) (*C*)



(*B*) (I)



(II)

The bond distances and angles in (I) (Fig. 1) have normal values, and are comparable to those observed for similar

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acridine-based molecules (Boyer *et al.*, 1999; Liu *et al.*, 2006). Each of the acridine *N*-oxide ring systems in the molecule is essentially planar, but the planes are twisted away from one another by an angle of 76.24 (9)°. In comparison with (I), the dihedral angles between the planes of the acridine ring systems in (*B*) and (II) show an even greater degree of perpendicularity, at 84.67 (7) and 85.3 (3)°, respectively (Liu, 2007; Boyer *et al.*, 1993).

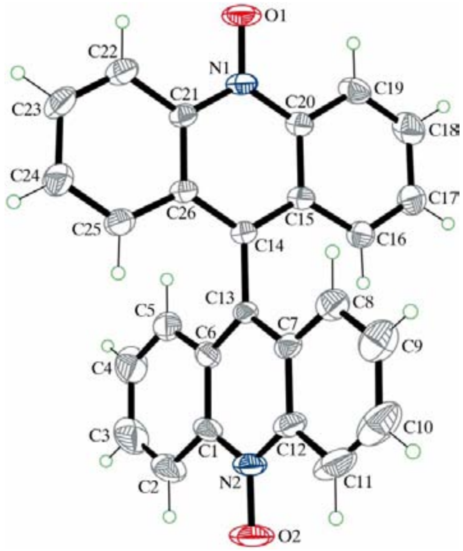

Figure 1
The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

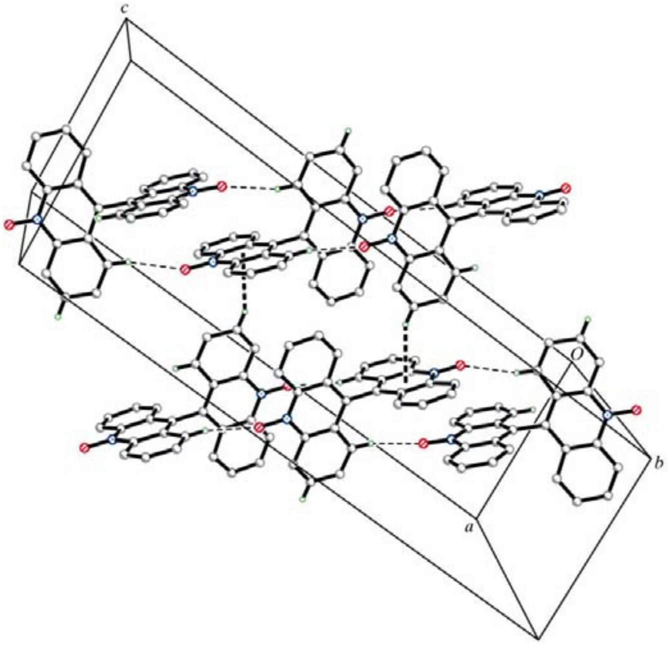

Figure 2
Part of the crystal packing of (I), showing the two-dimensional network in the title compound formed by the co-effects of intermolecular C—H···O hydrogen bonds (thin dashed lines) and C—H···π interactions (thick dashed lines). For clarity, only H atoms involved in these interactions are shown.

In the crystal structure of (I), adjacent molecules are linked into an extended chain along the [201] direction by two distinct intermolecular C—H···O hydrogen-bonding interactions (Fig. 2 and Table 1) (Desiraju & Steiner, 1999). The interaction involving the C8—H8 group as a donor links pairs of molecules into centrosymmetric dimers, and this hydrogen-bond pattern can be described by a graph-set motif of $R_2^2(18)$ (Bernstein *et al.*, 1995). The interaction involving the C16—H16 group links pairs of molecules *via* another $R_2^2(18)$ motif into dimers with C_2 symmetry, but the acceptor molecule for the C16—H16 interaction is not the same as that for the C8—H8 interaction. The combination of both types of C—H···O interactions links these dimers continuously into an extended chain structure. Adjacent chains are crosslinked *via* intermolecular C—H···π interactions (Table 1) involving the C1/C6/C7/C12/C13/N2 pyridine ring. The net result is a two-dimensional network running parallel to the (010) plane (Fig. 2). In adjacent chains, the acridine ring systems are arranged in an edge-to-face orientation (Sony & Ponnuswamy, 2006).

Experimental

Compound (I) was synthesized according to a method reported in the literature (Boyer *et al.*, 1999; Simpson *et al.*, 1963). A mixed solution of (I) (0.1 mmol) in methanol and CH_2Cl_2 (10 ml, *v*/*v* 1:1) was filtered and the resulting solution was kept at room temperature. Yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of the solvent after several days (yield 30%, m.p. > 573 K). Analysis calculated for $C_{26}H_{16}N_2O_2$: C 80.40, H 4.15, N 7.21%; found: C 80.55, H 4.09, N 7.07%.

Crystal data

$C_{26}H_{16}N_2O_2$
$M_r = 388.41$
Monoclinic, $C2/c$
$a = 9.251$ (3) Å
$b = 14.972$ (5) Å
$c = 27.350$ (10) Å
$\beta = 98.791$ (6)°
$V = 3744$ (2) Å^3
$Z = 8$
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
0.30 × 0.25 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
9593 measured reflections
3304 independent reflections
1532 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.087$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.183$
$S = 1.00$
3304 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max} = 0.17$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.18$ e Å^{-3}

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

*Cg*1 is the centroid of the C1/C6/C7/C12/C13/N2 pyridine ring.

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1$^{\rm i}$	0.93	2.38	3.272 (5)	161
C16—H16···O2$^{\rm ii}$	0.93	2.55	3.456 (5)	165
C18—H18···*Cg*1$^{\rm iii}$	0.93	2.71	3.579 (5)	156

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, y, -z+\frac{1}{2}$; (iii) $x+1, y, z$.

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms [C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C)].

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: LN3064). Services for accessing these data are described at the back of the journal.

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