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#### Key indicators

Single-crystal X-ray study

$T = 180$  K

Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å

$R$  factor = 0.028

$wR$  factor = 0.061

Data-to-parameter ratio = 15.0

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

## Tetra- $\mu_2$ -acetato-bis({1-[5-(dimethylamino)naphthyl-sulfonyl]imidazole- $\kappa N^3$ }]rhodium)( $Rh-Rh$ ) acetonitrile disolvate

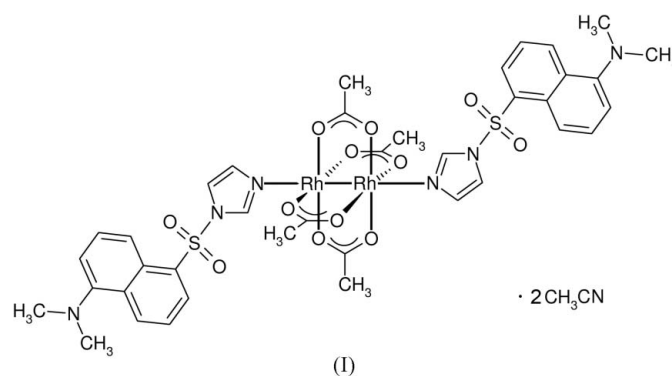
In the title compound,  $[\text{Rh}_2(\mu_2\text{-CH}_3\text{COO})_4(\text{C}_{15}\text{H}_{15}\text{N}_3\text{O}_2\text{S})_2] \cdot 2\text{C}_2\text{H}_3\text{N}$ , the dirhodium tetraacetate complex lies on a centre of inversion. The conformation of the complex differs from that in a previously reported 1:2 chloroform solvate.

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### Comment

The title dirhodium tetraacetate complex has been examined previously as a potential fluorescence-based nitric oxide sensor (Hilderbrand *et al.*, 2004). In that work, the complex was characterized crystallographically as a 1:2 chloroform solvate. Crystallization of the complex from acetonitrile solution yields the title 1:2 acetonitrile solvate, (I).



The conformation of the dirhodium tetraacetate complex in (I) (Fig. 1, Table 1) differs from that in the chloroform solvate. The complex is centrosymmetric in both cases, with the imidazole rings of the two dansylimidazole ligands being approximately coplanar. The central  $[\text{Rh}_2(\text{O}_2\text{CCH}_3)_4]$  unit is twisted with respect to this plane. In (I), the plane through the imidazole ring (N1/N2/C1–C3) forms a dihedral angle of  $65.4(1)^\circ$  with the plane through Rh1, O1, O2 and C4. In the  $\text{CHCl}_3$  solvate, the corresponding angle is  $74.2^\circ$ . The arrangement of the naphthalene rings also differs in the two cases: the angle between the  $\text{Rh} \cdots \text{Rh}$  vector and the normal to the least-squares plane through the naphthalene rings is  $63.5(1)^\circ$  in (I), compared with  $7.0^\circ$  in the  $\text{CHCl}_3$  solvate. Thus, the naphthalene rings in the  $\text{CHCl}_3$  solvate lie approximately perpendicular to the  $\text{Rh} \cdots \text{Rh}$  vector, while in (I) they form an angle to it.

The differences in conformation appear to be driven by differing intermolecular arrangements of the naphthalene rings. In the  $\text{CHCl}_3$  solvate, these adopt centrosymmetric face-to-face arrangements. In (I), the naphthalene rings adopt edge-to-face arrangements with neighbouring imidazole rings (Fig. 2): the C10–C12 edge is directed towards a neighbouring

imidazole ring, and the C3–H3 bond is directed towards the C12–C17 ring of a neighbouring naphthalene unit. The acetonitrile molecules in (I) lie in comparable positions to the  $\text{CHCl}_3$  molecules in the  $\text{CHCl}_3$  solvate: they lie between neighbouring  $[\text{Rh}_2(\text{O}_2\text{CCH}_3)_4]$  units, close to the imidazole rings (Fig. 1).

## Experimental

The title complex was prepared by reaction of rhodium acetate with dansylimidazole, according to the method reported by Hilderbrand *et al.* (2004). In the original report, the crystals used for structure determination were obtained after recrystallization of the crude product by vapour diffusion ( $\text{Et}_2\text{O}-\text{CHCl}_3$ ). In the present case, the crystals were deposited directly from the acetonitrile reaction mixture.

### Crystal data

$[\text{Rh}_2(\text{C}_2\text{H}_3\text{O}_2)_4(\text{C}_{15}\text{H}_{15}\text{N}_3\text{O}_2\text{S})_2] \cdot 2\text{C}_2\text{H}_3\text{N}$	$V = 2314.8 (4) \text{ \AA}^3$
$M_r = 1126.82$	$Z = 2$
Monoclinic, $P2_1/n$	$D_x = 1.617 \text{ Mg m}^{-3}$
$a = 8.8710 (9) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 25.256 (3) \text{ \AA}$	$\mu = 0.87 \text{ mm}^{-1}$
$c = 10.9402 (10) \text{ \AA}$	$T = 180 (2) \text{ K}$
$\beta = 109.195 (4)^\circ$	Block, red
	$0.15 \times 0.12 \times 0.10 \text{ mm}$

### Data collection

Bruker Nonius X8 APEX-II CCD area-detector diffractometer	22091 measured reflections
Thin-slice $\omega$ and $\varphi$ scans	4539 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	3604 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.807$ , $T_{\max} = 0.918$	$R_{\text{int}} = 0.042$
	$\theta_{\text{max}} = 26.4^\circ$

### Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.028$	$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2]$
$wR(F^2) = 0.061$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{\text{max}} = 0.002$
4539 reflections	$\Delta\rho_{\text{max}} = 0.34 \text{ e \AA}^{-3}$
303 parameters	$\Delta\rho_{\text{min}} = -0.50 \text{ e \AA}^{-3}$

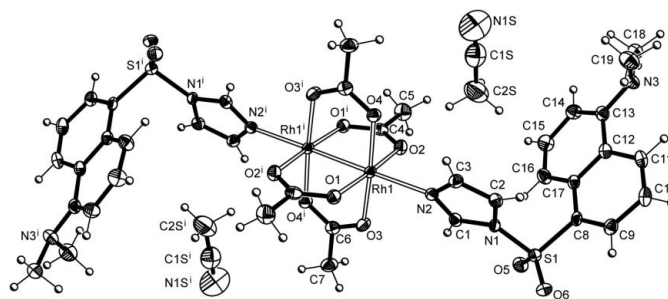
**Table 1**

Selected bond lengths ( $\text{\AA}$ ).

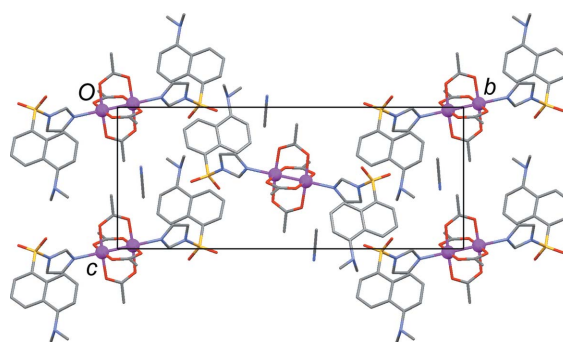
Rh1–Rh1 <sup>i</sup>	2.3997 (4)	Rh1–O3	2.0406 (15)
Rh1–O1	2.0436 (16)	Rh1–O4	2.0378 (15)
Rh1–O2	2.0406 (15)	Rh1–N2	2.2343 (18)

Symmetry code: (i)  $-x + 1, -y + 1, -z + 1$ .

H atoms were positioned geometrically and allowed to ride during subsequent refinement, with  $\text{C}-\text{H} = 0.95 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for  $\text{Csp}^2$ , and  $\text{C}-\text{H} = 0.98 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl groups. The methyl groups were allowed to rotate about their local threefold axes.



**Figure 1**  
The structure of (I), showing displacement ellipsoids at the 50% probability level. [Symmetry code (i):  $1 - x, 1 - y, 1 - z$ ].



**Figure 2**  
A view of (I) along the  $a$  axis, showing the edge-to-face arrangements of neighbouring naphthalene and imidazole rings.

Data collection: APEX2 (Bruker Nonius, 2004); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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