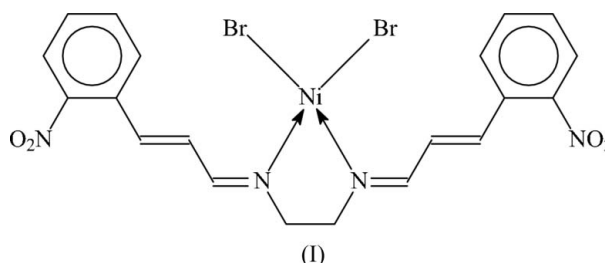


[*N,N'*-Bis(*trans*-2-nitroprop-2-enylidene)ethylenediamine- κ^2 *N,N'*]dibromonickel(II)Saeed Dehghanpour,^{a*} Ali Mahmoudi,^b Fatemeh Sepaveh^b and Seik Weng Ng^c^aDepartment of Chemistry, Alzahra University, Vanak, Tehran, Iran, ^bDepartment of Chemistry, Islamic Azad University, Karaj Branch, Karaj, Iran, and ^cDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

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Key indicatorsSingle-crystal X-ray study
T = 293 K
Mean σ (C–C) = 0.005 Å
Disorder in main residue
R factor = 0.039
wR factor = 0.107
Data-to-parameter ratio = 20.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.The Ni^{II} center in the monomeric complex, [NiBr₂·(C₂₀H₁₈N₄O₄)], is covalently bonded to two Br atoms and datively bonded to two N atoms of the Schiff base in a tetrahedral geometry.Received 12 May 2006
Accepted 26 May 2006**Comment**Cinnamaldehyde and its substituted derivatives condense with ethylenediamine to furnish a range of Schiff base compounds; a small number of such bis(cinnamaldehyde)ethylenediimine ligands have been used to furnish adducts with transition metals. Among such complexes whose structures have been described are, for example, the copper(I) iodide (Kickelbick *et al.*, 2002), (triphenylphosphine)(halogen/pseudohalogeno)-copper(I) (Kickelbick *et al.*, 2003), copper(I) perchlorate (Meghdadi *et al.*, 2002), and the cobalt(II) chloride, cobalt(II) bromide and nickel bromide (Amirnasr *et al.*, 2003) adducts. The 2-nitro-substituted Schiff base forms a 1:1 adduct, (I), with nickel bromide. The Ni atom is four-coordinated in a tetrahedral geometry (Fig. 1). The Ni–Br and Ni–N bond dimensions compare well with the values found in other tetrahedral Schiff base adducts of nickel bromide (Amirnasr *et al.*, 2002; Amort *et al.*, 2003; Cherian *et al.*, 2003; Feldman *et al.*, 1997; Gates *et al.*, 2000; Jin & Zhang, 2004; Horrocks *et al.*, 1971; Maldanis *et al.*, 2002).**Experimental**To a solution of bis(2-nitrocinnamaldehyde)ethylenediimine (37.8 mg, 0.1 mmol) in 20 ml acetonitrile was added nickel bromide (28.9 mg, 0.1 mmol). The mixture was heated to dissolve the reactants. The solution was filtered and the volume of the solvent was reduced under vacuum to about 5 ml. The diffusion of diethyl ether vapor into the solution gave violet crystals. The crystals were collected and washed with diethyl ether–dichloromethane (9:1 *v/v*) (yield 85%). Analysis calculated for C₂₀H₁₈Br₂N₄NiO₄: C 40.23, H 3.01, N 9.38%; found: C 40.25, H 3.02, N 9.37%.

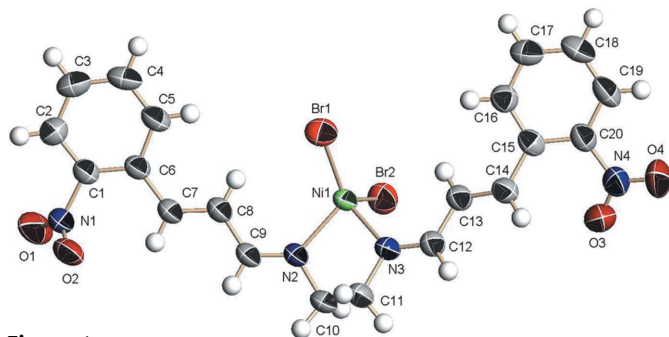


Figure 1
ORTEP plot of the title complex, $\text{NiBr}_2(\text{C}_{20}\text{H}_{18}\text{N}_4\text{O}_4)$. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are shown as spheres of arbitrary radii. The minor disordered components are not shown.

Crystal data

$[\text{NiBr}_2(\text{C}_{20}\text{H}_{18}\text{N}_4\text{O}_4)]$
 $M_r = 596.91$
 Monoclinic, $P2_1/n$
 $a = 7.6644$ (3) Å
 $b = 16.3219$ (6) Å
 $c = 18.5582$ (7) Å
 $\beta = 98.204$ (1)°
 $V = 2297.8$ (3) Å³

$Z = 4$
 $D_x = 1.725$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 4.36$ mm⁻¹
 $T = 293$ (2) K
 Thick plate, purple
 $0.45 \times 0.30 \times 0.15$ mm

Data collection

Bruker SMART area-detector
 diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.231$, $T_{\max} = 0.522$

25133 measured reflections
 6270 independent reflections
 3365 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.058$
 $\theta_{\text{max}} = 29.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.107$
 $S = 1.00$
 6270 reflections
 309 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0431P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.51$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.37$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ni1—N2	1.985 (2)	Ni1—Br1	2.349 (2)
Ni1—N3	1.990 (2)	Ni1—Br2	2.369 (1)
N2—Ni1—N3	84.2 (1)	N3—Ni1—Br1	112.5 (1)
N2—Ni1—Br1	113.4 (1)	N3—Ni1—Br2	102.4 (1)
N2—Ni1—Br2	106.4 (1)	Br1—Ni1—Br2	128.5 (1)

One of the two Br atoms (Br1) is disordered over two positions, with the occupancy factors refined to 0.63 (3) and 0.37 (3). The Ni1—Br1 and Ni1—Br1' distances were restrained to within 0.01 Å of each other. One of the nitro groups is also disordered; the occupancy factors were refined to 0.65 (1) and 0.35 (1). The four N—O distances were restrained to within 0.01 Å of each other, and the —CNO₂ unit was restrained to be nearly planar in the refinement. H atoms were positioned geometrically and refined as riding atoms, with C—H distances of 0.93 (CH) and 0.97 Å (CH₂) and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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: ORTEPII (Johnson, 1976) and SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXL97.

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