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#### Key indicators

Single-crystal X-ray study

$T = 220\text{ K}$

Mean  $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$

$R$  factor = 0.052

$wR$  factor = 0.138

Data-to-parameter ratio = 16.6

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

## [1,2-Bis(diphenylphosphino)ethane]dibromonickel(II) tetrahydrofuran solvate

The title complex,  $[\text{Ni}(\text{dppe})\text{Br}_2]\cdot\text{THF}$ , where dppe is bis(diphenylphosphino)ethane ( $\text{C}_{26}\text{H}_{24}\text{P}_2$ ) and THF is tetrahydrofuran ( $\text{C}_4\text{H}_8\text{O}$ ), consists of a square-planar Ni center coordinated by the chelating phosphine ligand and by two *cis*-Br atoms. One molecule of THF is included in the asymmetric unit.

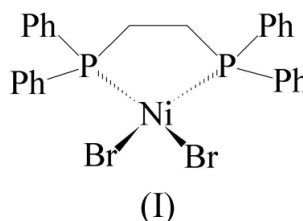
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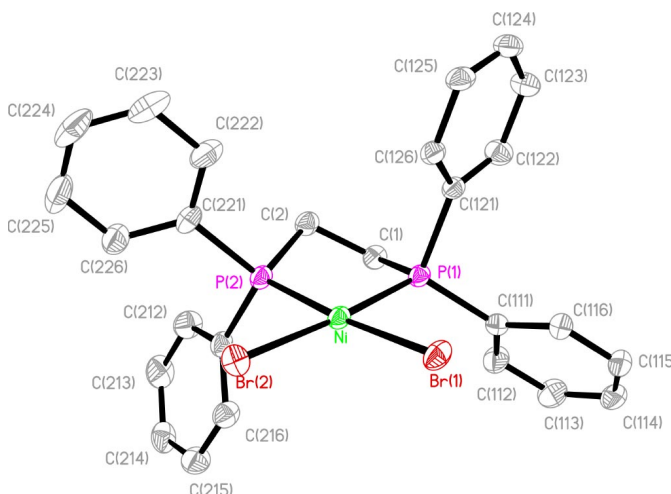
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#### Comment

In the course of our studies, the formation of  $\text{Ni}(\text{dppe})\text{Br}_2$  was observed as a by-product for the reaction of  $\text{Ni}(\text{dppe})_2$  with *N*-bromophthalimide. Even though this compound is well known as a good starting product, only the  $\text{CH}_2\text{Cl}_2$  adduct has been previously characterized using X-ray crystallography (Rahn *et al.*, 1989). The structure of the THF adduct, (I) (Fig. 1), is



isostructural with the one previously reported for the  $\text{CH}_2\text{Cl}_2$  analog, having a slightly larger volume (about  $20\text{ \AA}^3$ ), presumably because of the larger volume of THF compared to  $\text{CH}_2\text{Cl}_2$ . The THF adduct adopts a pseudo-square planar geometry with a  $\text{P}-\text{Ni}-\text{P}$  bite angle of  $89.97(5)^\circ$  and an angle of  $93.93(4)^\circ$  between the Br atoms. We note that the  $\text{Ni}-\text{P}$  bond lengths [ $2.1573(14)$  and  $2.1603(14)\text{ \AA}$ ] are also



**Figure 1**

*SHELXTL* (Bruker, 1997) drawing of the title molecule, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

slightly longer in the THF adduct than the corresponding distances in the  $\text{CH}_2\text{Cl}_2$  adduct [2.141 (1) and 2.156 (1) Å], but both Ni—Br bonds are very similar. In this structure, there is a stacking interaction between the THF ring and the C121—C126 phenyl ring, as shown in Fig. 2.

## Experimental

Using Schlenk techniques, THF (10 ml) was added to a mixture of  $\text{Ni}(\text{dppe})_2$  (40 mg, 0.047 mmol) and *N*-bromophthalimide (13 mg, 0.058 mmol) and stirred for 5 min. A large excess of hexanes was then added to the solution, resulting, after 12 h, in the formation of dark-red crystals. The filtrate was removed and the solid dried under  $\text{N}_2$ .

### Crystal data

$[\text{NiBr}_2(\text{C}_{26}\text{H}_{24}\text{P}_2)] \cdot \text{C}_4\text{H}_8\text{O}$   
 $M_r = 689.03$   
 Monoclinic,  $P2_1/c$   
 $a = 11.709$  (5) Å  
 $b = 14.551$  (4) Å  
 $c = 17.558$  (6) Å  
 $\beta = 107.38$  (3)°  
 $V = 2854.9$  (17) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.603$  Mg m<sup>-3</sup>  
 Cu  $K\alpha$  radiation  
 Cell parameters from 25 reflections  
 $\theta = 20.0$ – $21.0$ °  
 $\mu = 5.48$  mm<sup>-1</sup>  
 $T = 220$  (2) K  
 Block, dark red  
 $0.57 \times 0.15 \times 0.12$  mm

### Data collection

Nonius CAD-4 diffractometer  
 $\omega/2\theta$  scans  
 Absorption correction: by integration (*ABSORP* in *NRCVAX*; Gabe *et al.*, 1989)  
 $T_{\text{min}} = 0.234$ ,  $T_{\text{max}} = 0.573$   
 6651 measured reflections  
 5425 independent reflections  
 4582 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$   
 $\theta_{\text{max}} = 70.0$ °  
 $h = -14 \rightarrow 14$   
 $k = -17 \rightarrow 17$   
 $l = -21 \rightarrow 21$   
 5 standard reflections  
 frequency: 60 min  
 intensity decay: none

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.052$   
 $wR(F^2) = 0.138$   
 $S = 1.08$   
 5425 reflections  
 326 parameters  
 H-atom parameters constrained

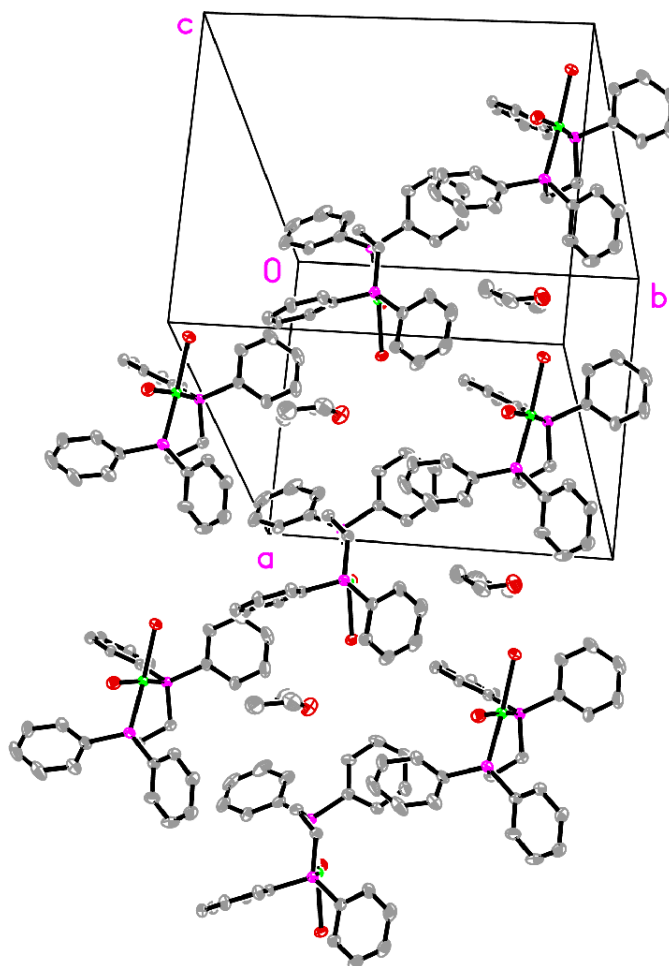
$w = 1/[\sigma^2(F_o^2) + (0.1052P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 1.80$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.12$  e Å<sup>-3</sup>  
 Extinction correction: *SHELXL96* (Sheldrick, 1996)  
 Extinction coefficient: 0.00115 (13)

**Table 1**

Selected geometric parameters (Å, °).

Ni—P2	2.1573 (14)	Ni—Br1	2.3212 (12)
Ni—P1	2.1603 (14)	Ni—Br2	2.3419 (12)
P2—Ni—P1	86.97 (5)	P2—Ni—Br2	88.92 (5)
P2—Ni—Br1	175.13 (4)	P1—Ni—Br2	175.46 (4)
P1—Ni—Br1	90.02 (5)	Br1—Ni—Br2	93.95 (4)

The space group was confirmed by the *PLATON* program (Spek, 1995). Data reduction was performed using a locally modified version of the *NRC-2* program (Ahmed *et al.*, 1973). The structure was solved by direct methods using *SHELXS97* (Sheldrick, 1997) and difmap synthesis using *SHELXTL* (Bruker, 1997) and *SHELXL96* (Sheldrick, 1996). H atoms were constrained to ride on the attached atoms; *SHELXL96* defaults, C—H = 0.94–0.98 Å. The isotropic displacement parameters,  $U_{\text{iso}}$ , were set to values 20% higher than those of the attached atoms. A final verification of possible voids was performed using the *VOID* routine of the *PLATON* program (Spek, 1995).



**Figure 2**

*SHELXTL* (Bruker, 1997) drawing of the unit-cell contents showing the interaction between THF and phenyl rings. Ellipsoids are drawn at the 30% probability level.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRC-2* and *NRC-2A* (Ahmed *et al.*, 1973); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL96* (Sheldrick, 1996); molecular graphics: *SHELXTL* (Bruker, 1997).

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