metal-organic compounds

Acta Crystallographica Section E **Structure Reports** Online

ISSN 1600-5368

Di-*u*-thiocyanato-bis{[1,2-bis(diisopropylphosphanyl)-1,2-dicarba-closododecaborane]silver(I)}

Liguo Yang, Chengchen Zhu and Dacheng Li*

School of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059 People's Republic of China Correspondence e-mail: lidacheng@lcu.edu.cn

Received 1 November 2010; accepted 25 November 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ (C–C) = 0.008 Å; R factor = 0.052; wR factor = 0.099; data-to-parameter ratio = 16.9.

The title compound, $[Ag_2(NCS)_2(C_{14}H_{38}B_{10}P_2)_2]$, was synthesized by the reaction of 1,2-bis(diisopropylphosphanyl)-1,2dicarba-closo-dodecaborane with AgSCN. The diisopropylphosphanyl-closo-carborane ligand is coordinated in a bidentate manner to the Ag^I atom through the two P atoms. The coordination of the Ag^I atom is distorted tetrahedral, in which two vertices are formed by the P atoms of the chelating diphosphine ligand, and the other two are occupied by the S and N atoms of the two bridging thiocyanate anions, leading to a centrosymmetric binuclear complex. The distance between the two C atoms in the carborane skeleton is 1.851 (6) Å.

Related literature

For related structures, see: Zhang et al. (2006); Paavola et al. (2002, 2002*a*,*b*). For the synthesis and structure of 1,2-bis(diisopropylphosphanyl)-1,2-dicarba-closo-dodecaborane, see: Kivekäs et al. (1995).



Experimental

Crystal data $[Ag_2(NCS)_2(C_{14}H_{38}B_{10}P_2)_2]$

 $M_r = 1084.87$

Monoclinic, $P2_1/n$	Z = 2
a = 7.8075 (9) Å	Mo $K\alpha$ radiation
b = 34.220 (3) Å	$\mu = 0.95 \text{ mm}^{-1}$
c = 10.6886 (12) Å	$T = 298 { m K}$
$\beta = 110.074 \ (1)^{\circ}$	$0.41 \times 0.18 \times 0.08 \text{ mm}$
V = 2682.2 (5) Å ³	
Data collection	
Bruker SMART 1000 CCD	13386 measured reflections
diffractometer	4714 independent reflections
Absorption correction: multi-scan	3238 reflections with $I > 2\sigma($

tions with $I > 2\sigma(I)$ (SADABS; Sheldrick, 1996) $R_{\rm int} = 0.050$ $T_{\min} = 0.696, \ T_{\max} = 0.928$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.052$ 2 restraints $wR(F^2) = 0.099$ H-atom parameters constrained $\Delta \rho_{\rm max} = 0.82 \text{ e} \text{ Å}^-$ S = 1.06 $\Delta \rho_{\rm min} = -0.92 \text{ e} \text{ Å}^{-3}$ 4714 reflections 279 parameters

Table 1

Selected geometric parameters (Å, °).

Ag1-N1	2.251 (5)	Ag1-P2	2.4981 (14)
Ag1-P1	2.4566 (14)	Ag1-S1	2.5693 (17)
P1-Ag1-P2	90.97 (4)	N1-Ag1-S1	97.27 (14)

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

This work was supported by the National Natural Science Foundation of China (project No. 20971063), the Natural Science Foundation of Shandong Province (Y2007B01) and the Shandong Tai-Shan Scholar Research Fund.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2319).

References

- Kivekäs, R., Sillanpää, R., Teixidor, F., Viñas, C., Nuñez, R. & Abad, M. (1995). Acta Cryst. C51, 1864-1868.
- Paavola, S., Kivekäs, R., Teixidor, F. & Vinas, C. (2002). J. Organomet. Chem. 606, 183-187.
- Paavola, S., Teixidor, F., Vinas, C. & Kivekäs, R. (2002a). Acta Cryst. C58, m237-m239
- Paavola, S., Teixidor, F., Vinas, C. & Kivekas, R. (2002b). J. Organomet. Chem. 645, 39-46.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
- Siemens (1996). SMART and SAINT. Siemens Analytical X-ray Instruments Inc. Madison Wisconsin USA
- Zhang, D.-P., Dou, J.-M., Li, D.-C. & Wang, D.-Q. (2006). Acta Cryst. E62, 0418-0419



Acta Cryst. (2011). E67, m2 [https://doi.org/10.1107/S1600536810049263]

Di-µ-thiocyanato-bis{[1,2-bis(diisopropylphosphanyl)-1,2-dicarba-*closo*-dodecaborane]silver(I)}

Liguo Yang, Chengchen Zhu and Dacheng Li

S1. Comment

The synthesis and structure of $1,2-(P^iPr_2)_2-1,2-C_2B_{10}H_{10}$ was reported by Kivekäs *et al.* (1995). Since then, only a few complexes of this ligand with Pt(II) and Pd(II) have been described (Paavola *et al.*, 2002, 2002*a*,b). Here we report the structure of this ligand combined with Ag and thiocyanate ion.

As shown in Fig. 1, the coordination of the Ag atom is distorted tetrahedral, formed by one S atom and one N atom of the two SCN anions and the P atoms of diisopropylphosphanyl-*closo*-carborane ligand (Table 1). The two P—Ag bond lengths are slightly shorter than the corresponding bond lengths in the complex $[Ag_2Cl_2(C_{26}H_{30}B_{10}P_2)_2]$.2CH₂Cl₂ [2.5052 (14) Å; Zhang *et al.*, 2006]). The P—Ag—P angle is slightly larger than the corresponding value of 89.80 Å for the complex $[Ag_2Cl_2(C_{26}H_{30}B_{10}P_2)_2]$.2CH₂Cl₂ (Zhang *et al.*, 2006). The five-membered chelate ring fomed by the silver atom, two phosphorus atoms and two carbon atoms of the carborane skeleton is strongly flattened with a maximum deviation of 0.322 Å for C2. The torsion angle P1—C1—C2—P2 is -0.4 (5)°, *viz.* smaller than that of 12.1 (2)° in the free ligand (Kivekäs *et al.*, 1995).

S2. Experimental

The title compound was synthesizd by the reaction of 1 mmol AgSCN and 1 mmol $1,2-(P^iPr_2)_2-1,2-C_2B_{10}H_{10}$ in 10 ml dichloromethane under the protection of N₂, refluxed for 4 h, then a colorless solution formed, and crystals suitable for Xray diffraction were obtained from a dichloromethane- n-hexane solution.(61.7%, m.p. 553–558 K). FTIR (KBr) v (cm⁻¹): 2989, 2966, 2930, 2872 (C—H); 2614, 2602, 2585, 2556 (B—H); 1071 (C—P).

S3. Refinement

All H atoms were placed geometrically and treated as riding on their parent atoms, with B—H 1.10, C—H 0.96 (methyl), C—H 0.98 Å (isopropyl), with $U_{iso}(H) = 1.2U_{eq}(B)$, $U_{iso}(H) = 1.5U_{eq}(C)$. A rigid bond restraints were applied to the Uij values of Ag1,P1 and Ag1,P2 atoms *via* DELU instruction of SHELXL97 (Sheldrick, 2008).



Figure 1

The molecular structure of the title compound with atom labels and 40% probability displacement ellipsoids for non-H atoms. Symmetry code for atoms with the A label: -x + 1, -y, -z + 2. H atoms have been omitted for clarity.

Di-µ-thiocyanato-bis{[1,2-bis(diisopropylphosphanyl)-1,2-dicarba- closo-dodecaborane]silver(I)}

Crystal data

 $[Ag_{2}(NCS)_{2}(C_{14}H_{38}B_{10}P_{2})_{2}]$ $M_{r} = 1084.87$ Monoclinic, $P2_{1}/n$ Hall symbol: -P 2yn a = 7.8075 (9) Å b = 34.220 (3) Å c = 10.6886 (12) Å $\beta = 110.074$ (1)° V = 2682.2 (5) Å³ Z = 2

Data collection

Bruker SMART 1000 CCD diffractometer Radiation source: fine-focus sealed tube Graphite monochromator φ and ω scans Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $T_{\min} = 0.696, T_{\max} = 0.928$

Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.052$ $wR(F^2) = 0.099$ S = 1.064714 reflections 279 parameters 2 restraints Primary atom site location: structure-invariant direct methods F(000) = 1112 $D_x = 1.343 \text{ Mg m}^{-3}$ Mo K α radiation, $\lambda = 0.71073 \text{ Å}$ Cell parameters from 3831 reflections $\theta = 2.4-25.8^{\circ}$ $\mu = 0.95 \text{ mm}^{-1}$ T = 298 KBlock, yellow $0.41 \times 0.18 \times 0.08 \text{ mm}$

13386 measured reflections 4714 independent reflections 3238 reflections with $I > 2\sigma(I)$ $R_{int} = 0.050$ $\theta_{max} = 25.0^{\circ}, \ \theta_{min} = 2.1^{\circ}$ $h = -8 \rightarrow 9$ $k = -36 \rightarrow 40$ $l = -12 \rightarrow 10$

Secondary atom site location: difference Fourier map Hydrogen site location: inferred from neighbouring sites H-atom parameters constrained $w = 1/[\sigma^2(F_o^2) + (0.0185P)^2 + 6.4963P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} = 0.001$ $\Delta\rho_{max} = 0.82$ e Å⁻³ $\Delta\rho_{min} = -0.92$ e Å⁻³

	X	У	Ζ	$U_{\rm iso} * / U_{\rm eq}$	
Ag1	0.61123 (6)	0.074944 (11)	0.96399 (4)	0.04357 (15)	
P1	0.77035 (19)	0.13609 (4)	1.05474 (12)	0.0319 (3)	
P2	0.62319 (19)	0.09058 (4)	0.73885 (13)	0.0335 (3)	
S1	0.2929 (2)	0.06561 (4)	0.9800 (2)	0.0638 (5)	
C2	0.7012 (7)	0.14225 (13)	0.7460 (4)	0.0309 (12)	
N1	0.7232 (7)	0.01564 (15)	1.0410 (5)	0.0634 (16)	
C1	0.7792 (7)	0.16616 (13)	0.9114 (5)	0.0311 (12)	
C3	0.4009 (7)	0.08761 (15)	0.6024 (5)	0.0443 (14)	
H3A	0.4158	0.0956	0.5187	0.053*	
C9	1.0151 (7)	0.13069 (15)	1.1608 (5)	0.0398 (13)	
H9A	1.0841	0.1309	1.0995	0.048*	
B1	0.5741 (8)	0.17712 (16)	0.7899 (5)	0.0327 (14)	
H1	0.4439	0.1695	0.8022	0.039*	
B2	0.9279 (8)	0.15162 (17)	0.8327 (6)	0.0342 (14)	
H2	1.0248	0.1276	0.8725	0.041*	
C4	0.7877 (8)	0.06395 (14)	0.6774 (5)	0.0423 (14)	
H4A	0.9030	0.0783	0.7119	0.051*	
B3	0.9813 (9)	0.19488 (18)	0.7612 (6)	0.0420 (16)	
Н3	1.1164	0.1997	0.7530	0.050*	
B4	0.8264 (9)	0.16041 (18)	0.6591 (6)	0.0401 (16)	
H4	0.8620	0.1431	0.5848	0.048*	
B5	0.7755 (9)	0.21104 (18)	0.6369 (6)	0.0469 (18)	
Н5	0.7765	0.2270	0.5478	0.056*	
C10	0.6616 (8)	0.16743 (16)	1.1476 (5)	0.0459 (15)	
H10A	0.7314	0.1917	1.1744	0.055*	
B6	0.6018 (9)	0.17690 (17)	0.6309 (6)	0.0371 (15)	
H6	0.4882	0.1708	0.5381	0.044*	
B7	0.7247 (9)	0.21373 (16)	0.8895 (6)	0.0379 (16)	
H7	0.6898	0.2313	0.9636	0.045*	
B8	0.9487 (9)	0.19743 (16)	0.9160 (6)	0.0370 (15)	
H8	1.0633	0.2041	1.0077	0.044*	
B9	0.6147 (10)	0.22145 (17)	0.7165 (6)	0.0440 (17)	
H9	0.5083	0.2439	0.6792	0.053*	
C11	0.4625 (8)	0.17704 (17)	1.0711 (6)	0.0542 (16)	
H11A	0.3993	0.1537	1.0310	0.081*	
H11B	0.4556	0.1958	1.0029	0.081*	
H11C	0.4072	0.1877	1.1312	0.081*	
C5	0.8260 (9)	0.02295 (16)	0.7408 (6)	0.0586 (18)	
H5A	0.7171	0.0074	0.7089	0.088*	
H5B	0.8637	0.0253	0.8359	0.088*	
H5C	0.9209	0.0106	0.7169	0.088*	
B10	0.8498 (9)	0.23347 (17)	0.7945 (6)	0.0426 (17)	
H10	0.8978	0.2639	0.8068	0.051*	
C12	0.6691 (9)	0.1440 (2)	1.2724 (5)	0.069 (2)	
H12A	0.6220	0.1596	1.3277	0.104*	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\hat{A}^2)

H12B	0.7932	0.1369	1.3213	0.104*
H12C	0.5968	0.1207	1.2460	0.104*
C6	0.2489 (8)	0.11169 (17)	0.6243 (6)	0.0529 (16)
H6A	0.1335	0.1040	0.5607	0.079*
H6B	0.2694	0.1389	0.6131	0.079*
H6C	0.2481	0.1073	0.7128	0.079*
C7	0.3449 (9)	0.04416 (17)	0.5935 (6)	0.0640 (19)
H7A	0.3260	0.0366	0.6742	0.096*
H7B	0.4397	0.0284	0.5813	0.096*
H7C	0.2340	0.0405	0.5193	0.096*
C8	0.7401 (9)	0.06209 (17)	0.5261 (6)	0.0611 (18)
H8A	0.8417	0.0517	0.5059	0.092*
H8B	0.7129	0.0879	0.4894	0.092*
H8C	0.6357	0.0455	0.4883	0.092*
C13	1.0984 (8)	0.16309 (17)	1.2634 (5)	0.0591 (18)
H13A	1.0457	0.1620	1.3324	0.089*
H13B	1.0736	0.1881	1.2202	0.089*
H13C	1.2278	0.1593	1.3018	0.089*
C15	0.7150 (8)	-0.01747 (17)	1.0327 (6)	0.0467 (15)
C14	1.0478 (8)	0.09062 (17)	1.2272 (6)	0.0565 (17)
H14A	1.1762	0.0867	1.2715	0.085*
H14B	1.0012	0.0707	1.1608	0.085*
H14C	0.9864	0.0892	1.2910	0.085*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0537 (3)	0.0293 (2)	0.0454 (2)	-0.0062 (2)	0.0139 (2)	0.0046 (2)
P1	0.0414 (9)	0.0266 (7)	0.0250 (7)	-0.0005 (6)	0.0079 (6)	0.0023 (5)
P2	0.0384 (9)	0.0254 (7)	0.0320 (6)	-0.0020 (6)	0.0060 (6)	-0.0047 (6)
S1	0.0635 (12)	0.0317 (9)	0.1096 (14)	0.0047 (7)	0.0469 (11)	0.0074 (8)
C2	0.040 (3)	0.023 (3)	0.025 (3)	0.001 (2)	0.005 (2)	0.000 (2)
N1	0.051 (4)	0.039 (3)	0.093 (4)	0.003 (3)	0.015 (3)	0.023 (3)
C1	0.035 (3)	0.021 (3)	0.032 (3)	-0.002 (2)	0.005 (2)	0.001 (2)
C3	0.044 (4)	0.039 (3)	0.042 (3)	-0.006 (3)	0.005 (3)	-0.009 (3)
C9	0.039 (3)	0.042 (3)	0.032 (3)	-0.001 (3)	0.004 (3)	0.007 (2)
B1	0.037 (4)	0.032 (3)	0.025 (3)	0.005 (3)	0.006 (3)	0.002 (2)
B2	0.038 (4)	0.029 (3)	0.034 (3)	0.000 (3)	0.011 (3)	-0.001 (3)
C4	0.050 (4)	0.030 (3)	0.045 (3)	-0.001 (3)	0.014 (3)	-0.010 (2)
B3	0.049 (4)	0.035 (4)	0.045 (4)	0.000 (3)	0.021 (3)	0.006 (3)
B4	0.047 (4)	0.043 (4)	0.030 (3)	0.002 (3)	0.012 (3)	0.005 (3)
B5	0.057 (5)	0.039 (4)	0.043 (4)	-0.002 (3)	0.015 (3)	0.017 (3)
C10	0.060 (4)	0.039 (3)	0.036 (3)	-0.002 (3)	0.014 (3)	-0.004 (3)
B6	0.046 (4)	0.035 (3)	0.027 (3)	0.005 (3)	0.008 (3)	0.010 (3)
B7	0.054 (4)	0.016 (3)	0.034 (3)	0.007 (3)	0.003 (3)	-0.001 (2)
B8	0.043 (4)	0.025 (3)	0.039 (4)	-0.010 (3)	0.009 (3)	0.001 (3)
B9	0.056 (5)	0.026 (3)	0.044 (4)	0.004 (3)	0.011 (3)	0.009 (3)
C11	0.064 (4)	0.058 (4)	0.047 (4)	0.007 (3)	0.028 (3)	-0.009 (3)

C5	0.064 (5)	0.038 (4)	0.069 (4)	0.010 (3)	0.017 (4)	-0.006 (3)
B10	0.056 (5)	0.022 (3)	0.050 (4)	-0.003 (3)	0.019 (4)	0.004 (3)
C12	0.088 (5)	0.088 (5)	0.034 (4)	0.016 (4)	0.025 (4)	0.006 (3)
C6	0.039 (4)	0.060 (4)	0.053 (4)	-0.006 (3)	0.006 (3)	-0.005 (3)
C7	0.056 (5)	0.058 (4)	0.066 (4)	-0.017 (3)	0.006 (3)	-0.021 (3)
C8	0.081 (5)	0.053 (4)	0.056 (4)	-0.006 (3)	0.032 (4)	-0.015 (3)
C13	0.057 (4)	0.058 (4)	0.045 (4)	-0.017 (3)	-0.005 (3)	0.001 (3)
C15	0.039 (4)	0.046 (4)	0.058 (4)	0.006 (3)	0.020 (3)	0.026 (3)
C14	0.059 (4)	0.055 (4)	0.044 (4)	0.006 (3)	0.004 (3)	0.017 (3)

Geometric parameters (Å, °)

A al N1	2 251 (5)		1 1000
Agi—Ni	2.231(3)	В4—П4 D5 D10	1.1000
Agi—Pi	2.4500 (14)	B5—B10	1.759 (9)
Ag1—P2	2.4981 (14)	B5—B6	1.775 (9)
Agl—Sl	2.5693 (17)	B5—B9	1.778 (10)
PI-Cl0	1.853 (6)	B5—H5	1.1000
P1—C1	1.866 (5)	C10—C11	1.524 (8)
P1—C9	1.867 (5)	C10—C12	1.541 (7)
P2—C3	1.847 (5)	C10—H10A	0.9800
P2—C2	1.863 (5)	B6—B9	1.763 (8)
P2—C4	1.868 (5)	B6—H6	1.1000
S1-C15 ⁱ	1.652 (6)	B7—B8	1.763 (9)
C2—B4	1.682 (8)	B7—B10	1.767 (9)
C2—B6	1.693 (7)	B7—B9	1.771 (8)
C2—B1	1.717 (7)	B7—H7	1.1000
C2—B2	1.723 (8)	B8—B10	1.765 (8)
C2—C1	1.851 (6)	B8—H8	1.1000
N1-C15	1.137 (7)	B9—B10	1.784 (9)
C1—B7	1.678 (7)	В9—Н9	1.1000
C1—B8	1.689 (7)	C11—H11A	0.9600
C1—B1	1.722 (7)	C11—H11B	0.9600
C1—B2	1.725 (8)	C11—H11C	0.9600
C3—C6	1.527 (7)	С5—Н5А	0.9600
C3—C7	1.543 (7)	С5—Н5В	0.9600
С3—НЗА	0.9800	С5—Н5С	0.9600
C9—C14	1.525 (7)	B10—H10	1.1000
C9—C13	1.538 (7)	C12—H12A	0.9600
С9—Н9А	0.9800	C12—H12B	0.9600
B1—B6	1.786 (8)	C12—H12C	0.9600
B1—B9	1.786 (8)	C6—H6A	0.9600
B1—B7	1.796 (8)	C6—H6B	0.9600
B1—H1	1.1000	C6—H6C	0.9600
B2—B4	1.775 (8)	С7—Н7А	0.9600
B2—B3	1.780 (8)	С7—Н7В	0.9600
B2—B8	1.783 (8)	C7—H7C	0.9600
B2—H2	1.1000	C8—H8A	0.9600
C4—C8	1.531 (7)	C8—H8B	0.9600

a. a.	1 5 4 9 (5)	60 H06	0.0700
C4—C5	1.542 (7)	С8—Н8С	0.9600
C4—H4A	0.9800	C13—H13A	0.9600
B3—B8	1.761 (9)	C13—H13B	0.9600
B3—B4	1.772 (9)	C13—H13C	0.9600
B3—B10	1.782 (9)	C15—S1 ⁱ	1.652 (6)
B3—B5	1 785 (9)	C14—H14A	0.9600
B3—H3	1 1000	C14—H14B	0.9600
P4 P6	1.767 (0)	C14 $H14C$	0.9600
D4 - D0	1.707(9)	014—11140	0.9000
В4—ВЭ	1.775 (9)		
N1—Ag1—P1	122.90 (14)	B9—B5—B3	108.0 (4)
N1—Ag1—P2	114.03 (15)	B10—B5—H5	121.0
P1—Ag1—P2	90.97 (4)	B4—B5—H5	122.2
N1—Ag1—S1	97.27 (14)	B6—B5—H5	121.9
P1—Ag1—S1	116.70 (5)	B9—B5—H5	122.0
P2—Ag1—S1	116.60 (6)	B3—B5—H5	121.8
10 - P1 - C1	105.9(2)	$C_{11} - C_{10} - C_{12}$	107.8 (5)
C_{10} P_1 C_0	107.1(3)	$\begin{array}{cccc} C11 & C10 & C12 \\ \end{array}$	107.0(3)
C10-F1-C9	107.1(3)	C_{11} C_{10} P_{1}	114.1(4)
	103.6 (2)		105.9 (4)
CI0—PI—Agi	116.2 (2)	CII—CI0—HI0A	109.6
C1—P1—Ag1	107.57 (15)	C12—C10—H10A	109.6
C9—P1—Ag1	115.41 (17)	P1—C10—H10A	109.6
C3—P2—C2	106.9 (2)	C2—B6—B9	107.3 (4)
C3—P2—C4	105.6 (2)	C2—B6—B4	58.1 (3)
C2—P2—C4	102.9 (2)	B9—B6—B4	108.1 (5)
C3—P2—Ag1	114.4 (2)	C2—B6—B5	106.3 (4)
C2—P2—Ag1	106.46 (15)	B9—B6—B5	60.4 (4)
C4— $P2$ — $Ag1$	119 45 (17)	B4—B6—B5	60 2 (4)
C_{15}^{i} S_{1} Δg_{1}	97.4(2)	C_{2} B6 B1	59.1(3)
\mathbf{P}_{4} \mathbf{C}_{2} \mathbf{P}_{6}	63.1(2)	R0 R6 R1	59.1(3)
$B_{4} = C_{2} = B_{0}$	(3,1,0)	$D_{4} D_{4} D_{4} D_{1}$	106.4(3)
B4	(2,1,(2))	D4-D0-D1	100.0 (4)
B6-C2-B1	63.1 (3)	B2—B6—B1	107.7 (4)
B4—C2—B2	62.9 (3)	С2—В6—Н6	123.3
B6—C2—B2	113.0 (4)	B9—B6—H6	121.1
B1—C2—B2	107.9 (4)	B4—B6—H6	122.6
B4—C2—C1	107.6 (4)	B5—B6—H6	121.8
B6—C2—C1	107.6 (3)	B1—B6—H6	122.4
B1—C2—C1	57.6 (3)	C1—B7—B8	58.7 (3)
B2—C2—C1	57.6 (3)	C1—B7—B10	106.7 (4)
B4—C2—P2	124.9 (4)	B8—B7—B10	60.0 (4)
B6-C2-P2	124 9 (3)	C1—B7—B9	1074(4)
$B_1 = C_2 = P_2$	1173(4)	B8	107.1(1) 108.3(5)
$P_2 = P_2$	117.5(4) 117.4(3)	B10 B7 B0	60.5(3)
$D_2 = C_2 = C_2$	117.4(3)	$D_1 - D_7 - D_7$	50.2(2)
$C_1 = C_2 = \Gamma_2$	117.0(3)	$C_1 \longrightarrow D_1 \longrightarrow D_1$	10(((A)
CID—NI—Agi	150.0(5)	B9-B/-B1	100.0 (4)
B/CIB8	63.2 (3)	R10—R/—R1	107.7 (4)
B7—C1—B1	63.8 (3)	B9—B7—B1	60.1 (3)
B8—C1—B1	113.6 (4)	С1—В7—Н7	122.9

B7—C1—B2	113.1 (4)	B8—B7—H7	122.3
B8—C1—B2	62.9 (3)	B10—B7—H7	121.8
B1—C1—B2	107.6 (4)	B9—B7—H7	121.2
B7—C1—C2	108.1 (3)	B1—B7—H7	122.3
B8—C1—C2	107.8 (4)	C1—B8—B7	58.1 (3)
B1—C1—C2	57.3 (3)	C1—B8—B3	107.8 (4)
B2—C1—C2	57.5 (3)	B7—B8—B3	108.7 (4)
B7—C1—P1	124.8 (4)	C1—B8—B10	106.3 (4)
B8—C1—P1	125.1 (3)	B7—B8—B10	60.1 (4)
B1—C1—P1	116.9 (3)	B3—B8—B10	60.7 (3)
B2-C1-P1	117.5 (3)	C1—B8—B2	59.5 (3)
C2—C1—P1	116.6 (3)	B7—B8—B2	106.4 (4)
C6—C3—C7	108.1 (5)	B3—B8—B2	60.3 (3)
C6—C3—P2	114.7 (4)	B10—B8—B2	107.7(4)
C7—C3—P2	105.8 (4)	C1—B8—H8	123.1
C6-C3-H3A	109.4	B7—B8—H8	122.4
C7—C3—H3A	109.4	B3—B8—H8	120.8
P2-C3-H3A	109.1	B10—B8—H8	120.0
C14-C9-C13	110 7 (4)	B2—B8—H8	121.9
C14-C9-P1	110.1 (4)	B6—B9—B7	109.5(4)
C13 - C9 - P1	117.1(4)	B6—B9—B5	60.1(4)
C14 $C9$ $H9A$	106.0	B7-B9-B5	107.5(5)
C13 - C9 - H9A	106.0	B6-B9-B10	107.5(5) 108.0(5)
Р1С9Н9А	106.0	B7-B9-B10	59 6 (4)
$C_2 = B_1 = C_1$	65 1 (3)	B5	59.0 (4) 59.2 (4)
$C_2 = B_1 = B_6$	57 8 (3)	B6B1	57.2(4)
$C_1 = B_1 = B_0$	100 A (A)	B7 B0 B1	60.7(3)
$C_{1} = B_{1} = B_{0}$	105.3 (4)	B5B9B1	107.5(4)
$C_2 = B_1 = B_2$	103.3(4) 104.9(4)	$B_3 - B_3 - B_1$ B10 B0 B1	107.5(4)
B6 B1 B9	50 2 (3)	B6 B0 H0	120.0
$C_2 = B_1 = B_7$	108.0(4)	В0—В9—П9 В7 В0 Ц0	120.9
$C_2 \longrightarrow D_1 \longrightarrow D_7$	108.9 (4) 56 0 (2)	D/D/	121.2
$C_1 - B_1 - B_7$	30.9(3)	$B_3 - B_9 - B_9$	122.4
$B_0 = B_1 = B_7$	107.4(4)	B10 - B9 - H9	122.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	39.3 (3) 120.9	BI = B9 = H9	121.7
$C_2 \longrightarrow B_1 \longrightarrow H_1$	120.8	CIQ CI1 HIIR	109.5
CI-BI-HI	121.1		109.5
	122.1		109.5
B9—B1—H1	124.5		109.5
B / - BI - HI	122.0	HIIA—CII—HIIC	109.5
$C_2 = B_2 = C_1$	65.0 (3)	HIIB—CII—HIIC	109.5
$C_2 = B_2 = B_4$	5/.4 (3)	C4—C5—H5A	109.5
$C_1 - B_2 - B_4$	109.1 (4)		109.5
C2—B2—B3	105.8 (4)	нэа—Сэ—Нэв	109.5
C1—B2—B3	105.4 (4)		109.5
B4—B2—B3	59.8 (<i>3</i>)	H5A—C5—H5C	109.5
C2—B2—B8	109.4 (4)	нэв—С5—Н5С	109.5
C1—B2—B8	57.6 (3)	B8—B10—B5	108.5 (4)
B4—B2—B8	107.7 (4)	B8—B10—B7	59.9 (3)

B3—B2—B8	59.2 (3)	B5—B10—B7	108.6 (4)
$C_2 = B_2 = H_2$	120.8	B8—B10—B3	59.5 (3)
C1 - B2 - H2	121.1	B5-B10-B3	60.5(4)
B4—B2—H2	122.1	B7—B10—B3	107.5(4)
B3—B2—H2	122.1	B8-B10-B9	107.6(4)
B8—B2—H2	122.9	B5-B10-B9	60 3 (4)
C8-C4-C5	111 5 (4)	B7-B10-B9	59 8 (3)
C_{8} C_{4} P_{2}	116.4 (4)	B3-B10-B9	107.9(4)
C_{5} C_{4} P_{2}	110.4(4)	B8-B10-H10	107.9 (4)
C8 - C4 - H4A	106.1	B5B10H10	121.9
$C_5 C_4 H_{4A}$	106.1	B7 B10 H10	121.0
$P_2 = C_4 = H_4 \Lambda$	106.1	B3 B10 H10	121.0
$P_{2} = C_{4} = H_{4}$	108.0 (4)	B0 B10 H10	122.0
$B_0 = B_3 = B_4$ $B_2 = B_2$	100.9(4)	$C_{10} C_{12} H_{12A}$	121.9
$D_0 - D_3 - D_2$ $D_4 - D_2 - D_2$	60.0(3)	$C_{10} = C_{12} = H_{12}$	109.5
D4 - D3 - D2 D8 D2 D10	50.8(3)	H_{12} H	109.5
$B_0 - B_3 - B_{10}$	39.0(3)	$\begin{array}{cccc} \mathbf{H}\mathbf{I}\mathbf{Z}\mathbf{A} & \mathbf{H}\mathbf{I}\mathbf{Z}\mathbf{D} \\ \mathbf{G}\mathbf{I}0 & \mathbf{G}\mathbf{I}2 & \mathbf{H}\mathbf{I}2\mathbf{G} \\ \end{array}$	109.5
B4 - B3 - B10 B2 - B2 - B10	107.3(3) 107.1(4)	U12A C12 U12C	109.5
B2 - B3 - B10 $B^{\circ} B^{\circ} B^{\circ}$	107.1(4) 107.5(5)	H12A - C12 - H12C	109.5
$B_0 - B_3 - B_3$	107.3(3)	H12B - C12 - H12C	109.5
B4—B3—B3	59.9 (4) 107.1 (5)	$C_3 = C_0 = HOA$	109.5
B2 - B3 - B3	107.1(3)		109.5
B10—B3—B3	59.1 (4) 121.2	H0A - C0 - H0B	109.5
B8—B3—H3	121.2		109.5
B4—B3—H3	121.4	H6A—C6—H6C	109.5
B2—B3—H3	122.1	H6B - C6 - H6C	109.5
B10—B3—H3	122.6	$C_3 - C_7 - H_7 A$	109.5
B5—B3—H3	122.5	$C_3 - C_7 - H_7 B$	109.5
C2—B4—B6	58.8 (3)	H/A - C / - H/B	109.5
C2—B4—B3	108.0 (4)	C3—C7—H7C	109.5
B6—B4—B3	108.7 (5)	H/A—C/—H/C	109.5
C2—B4—B5	106.8 (4)	H/B - C/ - H/C	109.5
B6—B4—B5	60.1 (4)	C4—C8—H8A	109.5
B3—B4—B5	60.4 (4)	C4—C8—H8B	109.5
C2—B4—B2	59.7 (3)	H8A—C8—H8B	109.5
B6—B4—B2	107.1 (4)	C4—C8—H8C	109.5
B3—B4—B2	60.2 (3)	H8A—C8—H8C	109.5
B5—B4—B2	107.7 (4)	H8B—C8—H8C	109.5
C2—B4—H4	122.6	С9—С13—Н13А	109.5
B6—B4—H4	122.0	C9—C13—H13B	109.5
B3—B4—H4	121.0	H13A—C13—H13B	109.5
B5—B4—H4	121.9	С9—С13—Н13С	109.5
B2—B4—H4	122.1	H13A—C13—H13C	109.5
B10—B5—B4	108.2 (4)	H13B—C13—H13C	109.5
B10—B5—B6	108.6 (5)	$N1$ — $C15$ — $S1^i$	178.8 (6)
B4—B5—B6	59.7 (3)	C9—C14—H14A	109.5
B10—B5—B9	60.6 (4)	C9—C14—H14B	109.5
B4—B5—B9	107.1 (4)	H14A—C14—H14B	109.5
B6—B5—B9	59.5 (4)	C9—C14—H14C	109.5

B10—B5—B3	60.4 (4)	H14A—C14—H14C	109.5
B4—B5—B3	59.7 (3)	H14B—C14—H14C	109.5
B6—B5—B3	107.7 (4)		
NI—AgI—PI—C10	-111.6 (3)	Ag1—P2—C2—C1	8.3 (3)
P2—Ag1—P1—C10	128.6 (2)	P1—Ag1—N1—C15	-172.8 (9)
S1—Ag1—P1—C10	8.0 (2)	P2—Ag1—N1—C15	-64.7 (10)
N1—Ag1—P1—C1	130.0 (2)	S1—Ag1—N1—C15	58.7 (10)
P2—Ag1—P1—C1	10.24 (17)	P2—C2—C1—P1	-0.4 (5)
S1—Ag1—P1—C1	-110.41 (18)	C10—P1—C1—C2	-132.8 (3)
N1—Ag1—P1—C9	15.0 (3)	C9—P1—C1—C2	114.7 (3)
P2—Ag1—P1—C9	-104.8 (2)	Ag1—P1—C1—C2	-7.9 (4)
S1—Ag1—P1—C9	134.6 (2)	C2—P2—C3—C6	-64.1 (5)
N1—Ag1—P2—C3	104.8 (2)	C4—P2—C3—C6	-173.2 (4)
P1—Ag1—P2—C3	-128.15 (19)	Ag1—P2—C3—C6	53.4 (5)
S1—Ag1—P2—C3	-7.42 (19)	C2—P2—C3—C7	176.9 (4)
N1—Ag1—P2—C2	-137.4 (2)	C4—P2—C3—C7	67.8 (4)
P1—Ag1—P2—C2	-10.35 (17)	Ag1—P2—C3—C7	-65.6 (4)
S1—Ag1—P2—C2	110.38 (17)	C10—P1—C9—C14	103.2 (4)
N1—Ag1—P2—C4	-21.7 (3)	C1—P1—C9—C14	-145.2 (4)
P1—Ag1—P2—C4	105.3 (2)	Ag1—P1—C9—C14	-28.0 (4)
S1—Ag1—P2—C4	-133.9 (2)	C10—P1—C9—C13	-24.5 (5)
C3—P2—C2—B4	-88.9 (4)	C1—P1—C9—C13	87.1 (4)
C4—P2—C2—B4	22.0 (5)	Ag1—P1—C9—C13	-155.7 (4)
Ag1—P2—C2—B4	148.4 (4)	C3—P2—C4—C8	25.7 (5)
C3—P2—C2—B6	-9.6 (5)	C2—P2—C4—C8	-86.2 (4)
C4—P2—C2—B6	101.4 (4)	Ag1—P2—C4—C8	156.3 (3)
Ag1—P2—C2—B6	-132.2 (4)	C3—P2—C4—C5	-102.3 (4)
C3—P2—C2—B1	65.4 (4)	C2—P2—C4—C5	145.8 (4)
C4—P2—C2—B1	176.3 (3)	Ag1—P2—C4—C5	28.3 (4)
Ag1—P2—C2—B1	-57.3 (3)	C1—P1—C10—C11	66.3 (5)
C3—P2—C2—B2	-163.5 (4)	C9—P1—C10—C11	176.3 (4)
C4—P2—C2—B2	-52.6 (4)	Ag1-P1-C10-C11	-53.0 (4)
Ag1—P2—C2—B2	73.8 (4)	C1—P1—C10—C12	-175.3 (4)
C3—P2—C2—C1	130.9 (3)	C9—P1—C10—C12	-65.3 (4)
C4—P2—C2—C1	-118.1 (3)	Ag1—P1—C10—C12	65.4 (4)

Symmetry code: (i) -x+1, -y, -z+2.