Acta Cryst. (1999). C**55**, IUC9900107 [**doi:10.1107/S0108270199098893**]

Bromo(1,10-phenanthroline-*N*,*N*')(triphenylphosphine)copper(I)

Q.-H. Jin, X.-L. Xin and F.-J. Zhu

Abstract

In the structure of the title complex [Cu(phen)(PPh_3)Br], (I), the coordination polyhedron with Cu as the center atom is a distorted tetrahedron, with two N atoms of phenathroline, one Br atom and one P atom of PPh_3 occupying the four corners.

Comment

Cu^I and Cu^{II} complexes are noted because of their important roles in the field of chemistry simulation of the metalloenzyme, metabolism, and homo-phase catalysis. Because of the difficulty of the synthesis, Cu^I complexes are few compared with Cu^{II} complexes. In previous work, we have reported three Cu^I complexes, $[CuX(PPh_3)(C_9H_7N)]_2$ (*X* = Br, I; Jin, Long *et al.*, 1998; Jin, Wang & Xin, 1999), [CuI(PPh_3)(phen)], (II) (Jin, Xin *et al.*, 1998). Here we report a new Cu^I complex [CuBr(PPh_3)(phen)](I).

The crystal structure of the title complex (I) has been detertermined by X-ray diffraction. Phenanthroline acts as a bidentate ligand coordinating *via* two N atoms to Cu. The coordinated polyhedron with Cu as the center atom is a distorted tetrahedron, with the Cu—P distance of 2.1856 (12) Å, an average Cu—N distance of 2.092 (3)Å and Cu—Br distance of 2.4436 (10) Å.

[CuBr(PPh_3)(phen)] can be regarded as the analogue of [CuI(PPh_3)(phen)] with the I atom replaced by a Br atom. Most bond distances in (I) are very similar to those in (II), but the range of N—Cu—P in (I) [118.57 (8)–123.73 (8)°] is smaller than that in (II).

It is noted that an excess of PPh_3 in the synthesis is the key to obtaining stable single crystals of this Cu^I complex. The reducing property of PPh_3 prevents the Cu(I) from being oxidized to Cu^{II} complexes in the air and also improves the solubility of Cu(I) complexes in the organic solvent. The reducing property of PPh_3 has been shown by the fact that it can reduce Cu(II) to Cu(I) (Mülleret al., 1983) and that it can be oxidized to a P(V) compound, such as $SPPh_3$ (Lang *et al.*, 1993; Jin, Xin *et al.*, 1999).

Experimental

[CuBr(PPh_3)($C_{12}H_8N_2$)] was obtained by the reaction of CuBr, PPh_3 and phen in a molar ratio of 2:1:1 in DMF solution at room temperature. The orange columnar prism crystals were obtained by slowly evaporating the solvent.

CIF access

Refinement

All non-H atoms were refined anisotropically. H atoms were placed at calculated positions with C—H distance of 0.93 Å. Final difference Fourier maps showed the highest and lowest electron densities of 0.630 and −0.930 e $Å^{-3}$, respectively.

Data collection: *XSCANS* (Fait, 1991). Cell refinement: *XSCANS* (Fait, 1991). Data reduction: *XSCANS* (Fait, 1991). Program(*s*) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(*s*) used to refine structure: *SHELXL93* (Sheldrick, 1993). Software used to prepare material for publication: *SHELXL93*. Software used to prepare material for publication: *SHELXL93*.

Computing details

Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993).

Bromo (1,10-Phenanthroline-N,N') (Triphenylphosphine) Copper(I)

Crystal data

$[CuBr(C_{12}H_8N_2)(C_{18}H_{15}P_1)]$	γ = 70.50 (2)°
M_r = 585.92	V = 1294.5 (10) $Å^3$
Triclinic, $P\bar{1}$	Z = 2
a = 8.409 (4) Å	Mo $K\alpha$
b = 9.327 (4) Å	μ = 2.47 mm^{-1}
c = 18.144 (7) Å	T = 293 (2) K
α = 78.555 (14)°	0.4 × 0.4 × 0.2 mm
β = 76.85 (2)°	

Data collection

Siemens P4 diffractometer	3947 reflections with $I > 2\sigma(I)$
Absorption correction: ψ scan (Siemens, 1990)	R_{int} = 0.042
T_{min} = 0.360, T_{max} = 0.610	3 standard reflections
7496 measured reflections	every 97 reflections
6237 independent reflections	intensity decay: 5.1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037	387 parameters
$wR(F^2)$ = 0.086	Only H-atom displacement parameters refined
S = 0.95	$\Delta\rho_{max}$ = 0.63 e $Å^{-3}$
6237 reflections	$\Delta\rho_{min}$ = −0.93 e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °)

Br—Cu	2.4436 (10)	Cu—N2	2.104 (2)
Cu—N1	2.079 (3)	Cu—P	2.1856 (12)
N1—Cu—N2	79.89 (10)	N1—Cu—Br	102.96 (8)
N1—Cu—P	123.76 (8)	N2—Cu—Br	105.84 (8)
N2—Cu—P	118.59 (8)	P—Cu—Br	118.63 (3)

Acknowledgements

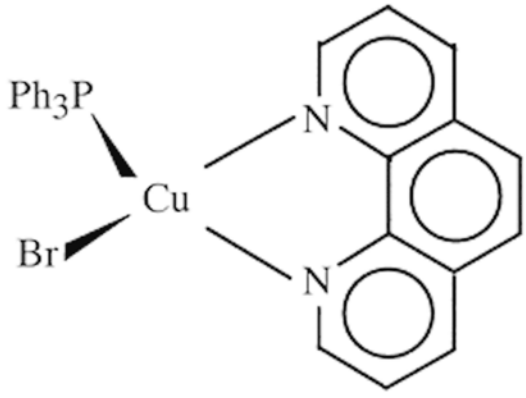
We are very grateful the support of the project of the Beijing Science and Technology Commission of China.

References

Fait, J. (1991). *XSCANS* Users Manual. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Lang, J. P., Bao, S. A., Zhu, H. Z., Xin, X. Q. & Yu, K. B. (1993). *Chin. J. Chem.* . **11**, 126–136.
+fr1096+Jin, Q. H., Long, D. L., Wang, Y. X. & Xin, X. Q., (1998*a*). *Acta Cryst.* C**54**, 948–949.
+bm1209+Jin, Q. H., Xin, X. L., Dong, C. J. & Zhu, H. J. (1998*b*). *Acta Cryst.* C**54**, 1087–1089.
+jz1317+Jin, Q. H., Wang, Y. X. & Xin, X. L. (1999). *Acta Cryst.* C**55**, 341–343.
+ta1221+Jin, Q. H., Xin, X. L., Deng, Y. H. & Yu, K. B. (1999). *Acta Cryst.* C**55**, 860–863.
Müller, A., Bögger, H. & Schimanski, U. (1983). *Inorg. Chim. Acta*, **69**, 5–16.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1993). *SHELXL93*. Program for the Refinement of Crystal Structures. University of Göttingen, Germany.
Siemens (1990). *XPREP*. Data preparation & reciprocal space exploration. Version 5.03. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1991). *XEMP*. Empirical Absorption Correction Program. Siemens Analytical X-ray Instrument Inc., Madison, Wisconsin, USA.

CIF access

Scheme 1



supplementary materials

Bromo (1,10-Phenanthroline-N,N') (Triphenylphosphine) Copper(I)

Crystal data

$[CuBr(C_{12}H_8N_2)(C_{18}H_{15}P_1)]$	$Z = 2$
$M_r = 585.92$	$F_{000} = 592$
Triclinic, $P\bar{1}$	$D_x = 1.503$ Mg m^{-3}
$a = 8.409$ (4) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 9.327$ (4) Å	Cell parameters from 30 reflections
$c = 18.144$ (7) Å	$\theta = 5.2$–14.8º
$\alpha = 78.555$ (14)º	$\mu = 2.47$ mm^{-1}
$\beta = 76.85$ (2)º	$T = 293$ (2) K
$\gamma = 70.50$ (2)º	Prism, orange
$V = 1294.5$ (10) Å^3	0.4 × 0.4 × 0.2 mm

Data collection

Siemens P4 diffractometer	$R_{int} = 0.042$
Radiation source: fine-focus sealed tube	$\theta_{max} = 28$º
Monochromator: graphite	$\theta_{min} = 1.2$º
$T = 293$(2) K	$h = -1 \rightarrow 11$
θ–2θ scans	$k = -11 \rightarrow 12$
Absorption correction: ψ scan (Siemens, 1990)	$l = -23 \rightarrow 23$
$T_{min} = 0.360$, $T_{max} = 0.610$	3 standard reflections
7496 measured reflections	every 97 reflections
6237 independent reflections	intensity decay: 5.1%
3947 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	Only H-atom displacement parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.037$	Calculated $w = 1/[\sigma^2(F_o^2) + (0.0601P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$?
$wR(F^2) = 0.086$	$(\Delta/\sigma)_{max} = 0.003$
$S = 0.95$	$\Delta\rho_{max} = 0.63$ e Å^{-3}
6237 reflections	$\Delta\rho_{min} = -0.93$ e Å^{-3}
387 parameters	Extinction correction: SHELXL93, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0403 (16)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement on F^2 for ALL reflections except for 0 with very negative F^2 or flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\mathrm{sigma}(F^2)$ is used only for calculating observed *R*-factors *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br	0.93526 (5)	0.93314 (4)	0.32558 (2)	0.04722 (13)
Cu	0.77266 (5)	0.76632 (4)	0.31549 (2)	0.04211 (13)
P	0.71397 (11)	0.76717 (9)	0.20406 (4)	0.0367 (2)
N1	0.5927 (3)	0.7830 (3)	0.41570 (14)	0.0392 (6)
N2	0.8794 (3)	0.5540 (3)	0.37886 (14)	0.0385 (6)
H1	0.430 (5)	0.988 (4)	0.390 (2)	0.063 (2)*
H2	0.271 (5)	0.967 (4)	0.513 (2)	0.063 (2)*
H3	0.321 (5)	0.778 (4)	0.610 (2)	0.063 (2)*
H5	0.521 (5)	0.526 (4)	0.646 (2)	0.063 (2)*
H6	0.768 (5)	0.316 (4)	0.610 (2)	0.063 (2)*
H8	1.022 (5)	0.211 (4)	0.515 (2)	0.063 (2)*
H9	1.169 (5)	0.232 (4)	0.395 (2)	0.063 (2)*
H10	1.085 (5)	0.460 (4)	0.313 (2)	0.063 (2)*
H14	0.858 (5)	0.451 (4)	0.229 (2)	0.063 (2)*
H15	0.801 (5)	0.230 (4)	0.223 (2)	0.063 (2)*
H16	0.534 (5)	0.253 (4)	0.191 (2)	0.063 (2)*
H17	0.353 (5)	0.493 (4)	0.158 (2)	0.063 (2)*
H18	0.422 (5)	0.703 (4)	0.170 (2)	0.063 (2)*
H20	0.384 (5)	0.927 (4)	0.270 (2)	0.063 (2)*
H21	0.156 (5)	1.129 (4)	0.234 (2)	0.063 (2)*
H22	0.169 (5)	1.270 (4)	0.120 (2)	0.063 (2)*
H23	0.425 (5)	1.185 (4)	0.030 (2)	0.063 (2)*
H24	0.639 (5)	0.985 (4)	0.065 (2)	0.063 (2)*
H26	0.839 (5)	0.641 (4)	0.060 (2)	0.063 (2)*
H27	1.074 (5)	0.638 (4)	−0.029 (2)	0.063 (2)*
H28	1.263 (5)	0.765 (4)	−0.032 (2)	0.063 (2)*
H29	1.220 (5)	0.896 (4)	0.073 (2)	0.063 (2)*
H30	0.979 (5)	0.892 (4)	0.167 (2)	0.063 (2)*
C1	0.4533 (5)	0.8967 (4)	0.4344 (2)	0.0546 (9)
C2	0.3503 (6)	0.8963 (4)	0.5057 (2)	0.0641 (12)
C3	0.3909 (5)	0.7742 (4)	0.5603 (2)	0.0552 (9)

C4	0.5360 (4)	0.6509 (4)	0.5433 (2)	0.0412 (7)
C5	0.5894 (5)	0.5171 (4)	0.5967 (2)	0.0496 (8)
C6	0.7303 (5)	0.4036 (4)	0.5785 (2)	0.0526 (9)
C7	0.8348 (4)	0.4088 (3)	0.5038 (2)	0.0427 (7)
C8	0.9839 (5)	0.2926 (4)	0.4812 (2)	0.0616 (11)
C9	1.0757 (5)	0.3076 (4)	0.4104 (2)	0.0621 (11)
C10	1.0199 (5)	0.4406 (4)	0.3607 (2)	0.0508 (9)
C11	0.7866 (4)	0.5378 (3)	0.4499 (2)	0.0355 (6)
C12	0.6348 (4)	0.6602 (3)	0.4700 (2)	0.0354 (6)
C13	0.6497 (4)	0.6021 (3)	0.1971 (2)	0.0418 (7)
C14	0.7594 (5)	0.4575 (4)	0.2156 (2)	0.0502 (9)
C15	0.7176 (6)	0.3269 (4)	0.2143 (2)	0.0595 (10)
C16	0.5653 (7)	0.3397 (5)	0.1954 (3)	0.0702 (12)
C17	0.4540 (7)	0.4815 (5)	0.1772 (3)	0.0822 (15)
C18	0.4974 (6)	0.6122 (4)	0.1778 (3)	0.0659 (12)
C19	0.5396 (4)	0.9311 (3)	0.1723 (2)	0.0379 (7)
C20	0.3891 (5)	0.9785 (4)	0.2241 (2)	0.0546 (9)
C21	0.2546 (5)	1.1017 (5)	0.2036 (3)	0.0629 (11)
C22	0.2684 (6)	1.1823 (5)	0.1316 (3)	0.0643 (11)
C23	0.4165 (6)	1.1372 (5)	0.0798 (2)	0.0605 (10)
C24	0.5497 (5)	1.0127 (4)	0.0995 (2)	0.0478 (8)
C25	0.8922 (4)	0.7629 (3)	0.1245 (2)	0.0380 (7)
C26	0.9169 (5)	0.6875 (4)	0.0627 (2)	0.0535 (9)
C27	1.0553 (6)	0.6883 (5)	0.0048 (2)	0.0659 (12)
C28	1.1665 (5)	0.7642 (5)	0.0071 (2)	0.0643 (11)
C29	1.1416 (5)	0.8430 (5)	0.0667 (2)	0.0615 (10)
C30	1.0063 (5)	0.8399 (4)	0.1262 (2)	0.0499 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.0569 (2)	0.0468 (2)	0.0388 (2)	−0.0208 (2)	−0.0054 (2)	−0.00202 (13)
Cu	0.0489 (3)	0.0450 (2)	0.0299 (2)	−0.0150 (2)	−0.0029 (2)	−0.0024 (2)
P	0.0427 (5)	0.0388 (4)	0.0292 (4)	−0.0171 (4)	−0.0028 (3)	−0.0013 (3)
N1	0.043 (2)	0.0352 (12)	0.0350 (13)	−0.0099 (12)	−0.0017 (12)	−0.0049 (10)
N2	0.0365 (15)	0.0404 (13)	0.0340 (13)	−0.0075 (11)	−0.0026 (11)	−0.0057 (10)
C1	0.058 (2)	0.042 (2)	0.049 (2)	−0.003 (2)	0.003 (2)	−0.007 (2)
C2	0.059 (3)	0.052 (2)	0.058 (2)	0.008 (2)	0.008 (2)	−0.018 (2)
C3	0.050 (2)	0.065 (2)	0.046 (2)	−0.015 (2)	0.009 (2)	−0.018 (2)
C4	0.042 (2)	0.049 (2)	0.034 (2)	−0.0179 (15)	−0.0003 (14)	−0.0075 (13)
C5	0.048 (2)	0.067 (2)	0.032 (2)	−0.023 (2)	−0.001 (2)	0.001 (2)
C6	0.058 (2)	0.058 (2)	0.040 (2)	−0.022 (2)	−0.012 (2)	0.011 (2)
C7	0.044 (2)	0.044 (2)	0.039 (2)	−0.0117 (15)	−0.0129 (15)	0.0020 (13)
C8	0.061 (3)	0.053 (2)	0.057 (2)	−0.001 (2)	−0.020 (2)	0.007 (2)
C9	0.051 (2)	0.054 (2)	0.064 (3)	0.009 (2)	−0.011 (2)	−0.013 (2)
C10	0.046 (2)	0.059 (2)	0.040 (2)	−0.006 (2)	−0.002 (2)	−0.012 (2)
C11	0.035 (2)	0.042 (2)	0.033 (2)	−0.0153 (13)	−0.0067 (13)	−0.0051 (12)
C12	0.038 (2)	0.0387 (15)	0.0322 (15)	−0.0160 (13)	−0.0049 (13)	−0.0049 (12)

C13	0.053 (2)	0.042 (2)	0.032 (2)	−0.021 (2)	−0.0031 (15)	−0.0002 (12)
C14	0.059 (2)	0.043 (2)	0.048 (2)	−0.015 (2)	−0.009 (2)	−0.0054 (15)
C15	0.082 (3)	0.044 (2)	0.048 (2)	−0.018 (2)	−0.007 (2)	−0.005 (2)
C16	0.097 (4)	0.052 (2)	0.073 (3)	−0.041 (2)	−0.007 (3)	−0.011 (2)
C17	0.080 (3)	0.074 (3)	0.117 (4)	−0.041 (3)	−0.037 (3)	−0.014 (3)
C18	0.069 (3)	0.045 (2)	0.091 (3)	−0.023 (2)	−0.030 (2)	0.002 (2)
C19	0.040 (2)	0.0380 (15)	0.039 (2)	−0.0178 (14)	−0.0030 (14)	−0.0048 (12)
C20	0.050 (2)	0.056 (2)	0.049 (2)	−0.018 (2)	0.007 (2)	0.000 (2)
C21	0.040 (2)	0.066 (2)	0.075 (3)	−0.013 (2)	0.003 (2)	−0.013 (2)
C22	0.056 (3)	0.058 (2)	0.076 (3)	−0.009 (2)	−0.022 (2)	−0.005 (2)
C23	0.066 (3)	0.061 (2)	0.050 (2)	−0.013 (2)	−0.023 (2)	0.005 (2)
C24	0.054 (2)	0.048 (2)	0.038 (2)	−0.014 (2)	−0.008 (2)	−0.0015 (14)
C25	0.041 (2)	0.043 (2)	0.0267 (14)	−0.0121 (14)	−0.0034 (13)	−0.0009 (12)
C26	0.059 (2)	0.062 (2)	0.045 (2)	−0.028 (2)	0.004 (2)	−0.017 (2)
C27	0.077 (3)	0.068 (2)	0.048 (2)	−0.022 (2)	0.012 (2)	−0.024 (2)
C28	0.053 (2)	0.084 (3)	0.048 (2)	−0.023 (2)	0.011 (2)	−0.010 (2)
C29	0.058 (3)	0.089 (3)	0.046 (2)	−0.042 (2)	0.002 (2)	−0.007 (2)
C30	0.054 (2)	0.068 (2)	0.034 (2)	−0.027 (2)	−0.003 (2)	−0.009 (2)

Geometric parameters (Å, °)

Br—Cu	2.4436 (10)	C9—C10	1.391 (5)
Cu—N1	2.079 (3)	C11—C12	1.430 (4)
Cu—N2	2.104 (2)	C13—C18	1.372 (5)
Cu—P	2.1856 (12)	C13—C14	1.383 (5)
P—C25	1.825 (3)	C14—C15	1.381 (5)
P—C13	1.828 (3)	C15—C16	1.362 (6)
P—C19	1.833 (3)	C16—C17	1.370 (6)
N1—C1	1.321 (4)	C17—C18	1.387 (5)
N1—C12	1.360 (4)	C19—C24	1.388 (4)
N2—C10	1.324 (4)	C19—C20	1.389 (5)
N2—C11	1.356 (4)	C20—C21	1.375 (6)
C1—C2	1.383 (5)	C21—C22	1.373 (6)
C2—C3	1.358 (5)	C22—C23	1.373 (6)
C3—C4	1.393 (5)	C23—C24	1.371 (5)
C4—C12	1.402 (4)	C25—C26	1.379 (5)
C4—C5	1.428 (5)	C25—C30	1.386 (5)
C5—C6	1.326 (5)	C26—C27	1.380 (5)
C6—C7	1.438 (5)	C27—C28	1.360 (6)
C7—C8	1.396 (5)	C28—C29	1.364 (6)
C7—C11	1.399 (4)	C29—C30	1.383 (5)
C8—C9	1.347 (6)		
N1—Cu—N2	79.89 (10)	N2—C10—C9	123.4 (3)
N1—Cu—P	123.76 (8)	N2—C11—C7	122.8 (3)
N2—Cu—P	118.59 (8)	N2—C11—C12	117.7 (3)
N1—Cu—Br	102.96 (8)	C7—C11—C12	119.5 (3)
N2—Cu—Br	105.84 (8)	N1—C12—C4	122.5 (3)
P—Cu—Br	118.63 (3)	N1—C12—C11	117.4 (3)
C25—P—C13	103.05 (14)	C4—C12—C11	120.1 (3)

C25—P—C19	103.67 (14)	C18—C13—C14	118.0 (3)
C13—P—C19	103.13 (15)	C18—C13—P	124.4 (3)
C25—P—Cu	114.85 (11)	C14—C13—P	117.6 (3)
C13—P—Cu	114.26 (10)	C15—C14—C13	121.2 (4)
C19—P—Cu	116.23 (11)	C16—C15—C14	119.8 (4)
C1—N1—C12	117.4 (3)	C15—C16—C17	120.2 (4)
C1—N1—Cu	129.6 (2)	C16—C17—C18	119.6 (4)
C12—N1—Cu	112.9 (2)	C13—C18—C17	121.1 (4)
C10—N2—C11	117.4 (3)	C24—C19—C20	117.7 (3)
C10—N2—Cu	130.5 (2)	C24—C19—P	123.7 (3)
C11—N2—Cu	112.1 (2)	C20—C19—P	118.5 (3)
N1—C1—C2	123.4 (3)	C21—C20—C19	121.0 (4)
C3—C2—C1	119.7 (3)	C22—C21—C20	120.3 (4)
C2—C3—C4	119.1 (3)	C21—C22—C23	119.4 (4)
C3—C4—C12	117.9 (3)	C24—C23—C22	120.5 (4)
C3—C4—C5	123.4 (3)	C23—C24—C19	121.0 (4)
C12—C4—C5	118.7 (3)	C26—C25—C30	118.9 (3)
C6—C5—C4	121.4 (3)	C26—C25—P	122.8 (3)
C5—C6—C7	121.5 (3)	C30—C25—P	118.3 (2)
C8—C7—C11	117.1 (3)	C25—C26—C27	119.7 (4)
C8—C7—C6	124.1 (3)	C28—C27—C26	120.9 (4)
C11—C7—C6	118.8 (3)	C27—C28—C29	120.4 (4)
C9—C8—C7	120.3 (3)	C28—C29—C30	119.4 (4)
C8—C9—C10	118.9 (4)	C29—C30—C25	120.7 (3)