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N,*N*,*N*-Tris(diphenylphosphorylmethyl)amine

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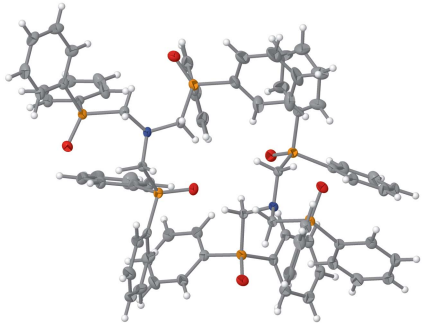
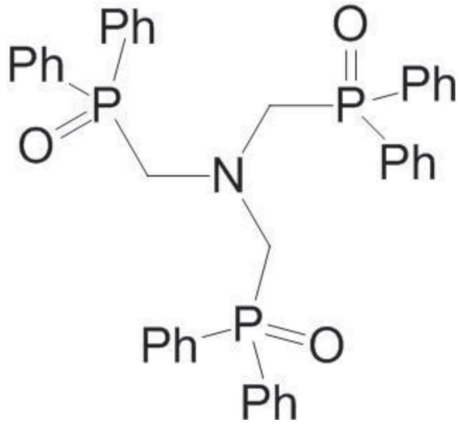
The structure of *N*,*N*,*N*-tris(diphenylphosphorylmethyl)amine, $C_{39}H_{36}NO_3P_3$, at 103 K has monoclinic ($P2_1/c$) symmetry. Two molecules, each with pseudo-threefold rotation symmetry, crystallize in the asymmetric unit of the monoclinic unit cell. The compound acts as ligand for the stabilization of metal ions with flexible coordination enabling three- or fourfold coordination.

3D view



Chemical scheme



Structure description

Phosphine oxides act as ligands for stabilizing oxophilic metal ions *via* complex formation. Many complexes of phosphine oxides stabilizing lanthanide and actinide ions have been described (some recent examples are: Baulin *et al.*, 2015; Bowden *et al.*, 2015; Dong *et al.*, 2015; Hasegawa *et al.*, 2015; Hirai *et al.*, 2015, 2016; Tolpygin *et al.*, 2015; Yanagisawa *et al.*, 2015). Tripodal ligands form a pocket in which the metal can be embedded *via* spherical coordination and therefore create a shielded pocket contributing to an even greater stabilization of the complexes (see: Cecconi *et al.*, 2000, 2001*a*,*b*; Fu *et al.*, 2011; Li *et al.*, 2010; Somov & Chausov, 2014, 2015; Somov *et al.*, 2015, 2016).

In the crystal structure of *N*,*N*,*N*-tris(diphenylphosphorylmethyl)amine, the two molecules in the asymmetric unit show a comparable arrangement (r.m.s. deviation = 0.5340 Å), even if there are no hydrogen-bond bridges or other external influences (Figs. 1 and 2). Both molecules exhibit a polar pocket with a tripodal arrangement of the $N(CH_2PR_2O)_3$ group; the P and O atoms of this group show a nearly planar arrangement (mean deviation for the selected atoms from this plane for molecule 1 = 0.065 Å and for molecule 2 = 0.074 Å). The molecules are oriented such that the O atoms point always in the direction of a P atom of a neighbouring arm, establishing an average intramolecular P—O distance of 4.46 (5) Å. The reason of this arrangement is probably found in a dipole–dipole interaction between the partially negative O atom and the partial positive P atom. This arrangement leads, for both molecules, to the formation of a hydrophobic

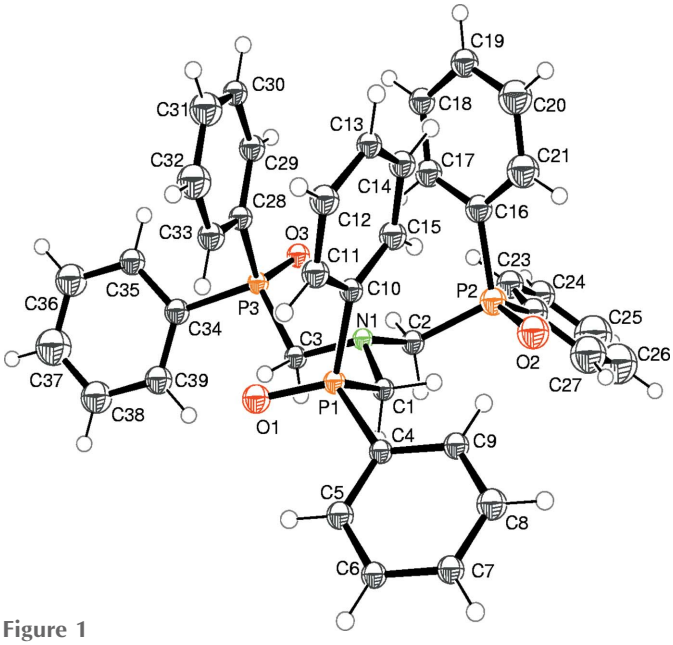


Figure 1
View of the molecular structure of one of the molecules of *N*,*N*,*N*-tris(diphenylphosphorylmethyl)amine in the asymmetric unit, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

outer sphere of the molecules formed by the phenyl rings sitting at the outside and shielding the polar pocket.

There are no remarkable supramolecular features present in the structures.

For *N*,*N*,*N*-tris(diphenylphosphorylmethyl)amine, coordination with a Be atom has been shown in the complex aqua-

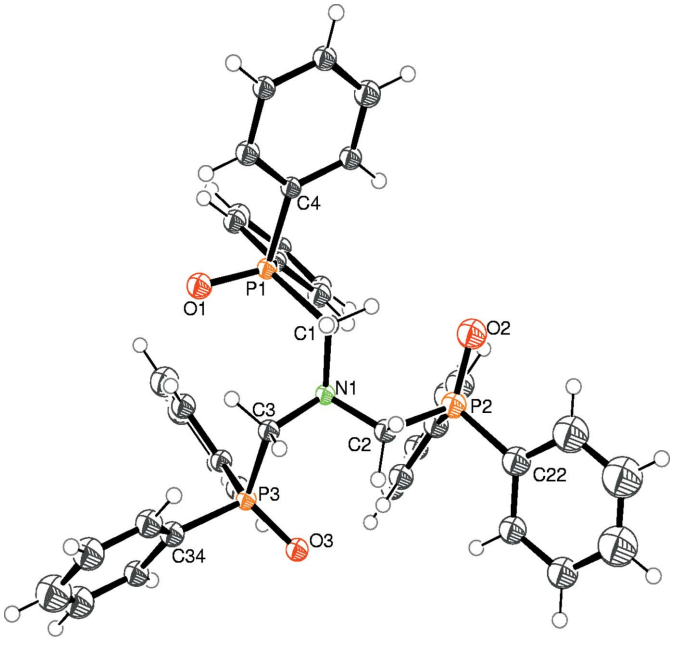


Figure 2
View along the pseudo-threefold rotation axis of one of the *N*,*N*,*N*-tris(diphenylphosphorylmethyl)amine molecules present in the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{39}H_{36}NO_3P_3$
M_r	659.60
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	103
a, b, c (Å)	10.9219 (10), 25.078 (2), 24.870 (2)
β (°)	95.515 (1)
V (Å^3)	6780.3 (10)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.22
Crystal size (mm)	0.10 × 0.07 × 0.05
Data collection	
Diffractometer	Bruker APEXII Quazar
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.953, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	122037, 16105, 11728
R_{int}	0.061
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.109, 1.01
No. of reflections	16105
No. of parameters	843
H-atom treatment	Only H-atom displacement parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.40

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS2013* (Sheldrick, 2008), *SHELXL2017* (Sheldrick, 2015), *XPMA* (Zsolnai, 1996), *ORTEP-3 for Windows* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

[*N*,*N*,*N*-tris(diphenylphosphorylmethyl)amine-κ^3O,O',O'']beryllium(II) diperchlorate (Cecconi *et al.*, 2000). The structure of the ligand itself has not been reported. There exist bidentate ligands incorporating the $RN(CH_2PR'_2O)_2$ moiety (Elsegood *et al.*, 2013; Enthaler & Nagel, 2014; Hursthouse *et al.*, 2003; Musina *et al.*, 2015; Priya *et al.*, 2003; Yang *et al.*, 2010).

Synthesis and crystallization

To a solution of 3.09 g (15.3 mmol) diphenylphospine oxide dissolved in 20 ml dry tetrahydrofuran (THF) in a Schlenk tube, 9.7 ml of a 1.6 *M* solution of methyllithium in Et_2O were added. This solution was then added to a solution of 0.83 g (5.1 mmol) of tris(chloromethyl)amine in 20 ml dry THF (Figs. 3). The solvent was removed under vacuum, and the residue was extracted with Et_2O. *N*,*N*,*N*-Tris(diphenylphospho-

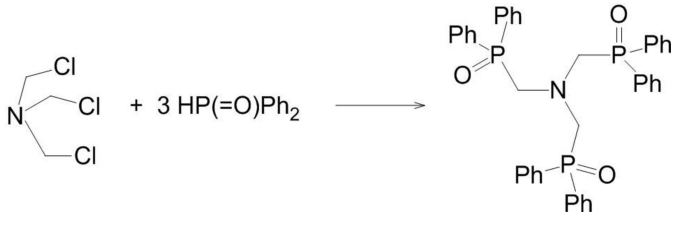


Figure 3
The preparation of the title compound.

rylmethyl)amine was obtained as a crystalline product (yield 80%, 2.5 g).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms attached to C atoms were fixed geometrically with fixed bond lengths and refined isotropically using a riding model.

Funding information

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full crystallographic data

IUCrData (2017). **2**, x171479 [https://doi.org/10.1107/S2414314617014791]

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Crystal data

$C_{39}H_{36}NO_3P_3$
M_r = 659.60
Monoclinic, $P2_1/c$
a = 10.9219 (10) Å
b = 25.078 (2) Å
c = 24.870 (2) Å
β = 95.515 (1)°
V = 6780.3 (10) Å^3
Z = 8
$F(000)$ = 2768
D_x = 1.292 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9834 reflections
θ = 2.3–27.7°
μ = 0.22 mm^{-1}
T = 103 K
Plates, colourless
0.10 × 0.07 × 0.05 mm

Data collection

Bruker APEXII Quazar diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 66 pixels mm^{-1}
combined ω– and phi–scan
Absorption correction: multi-scan (sadabs)
T_{min} = 0.953, T_{max} = 0.99
122037 measured reflections
16105 independent reflections
11728 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 28.3°, θ_{min} = 1.2°
h = −14→14
k = −33→32
l = −33→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.109
S = 1.01
16105 reflections
843 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
Only H-atom displacement parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 5.4914P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.79011 (5)	0.62151 (2)	−0.12042 (2)	0.01831 (11)
P2	0.63329 (5)	0.62870 (2)	0.05351 (2)	0.02301 (12)
P3	0.55451 (5)	0.76785 (2)	−0.07543 (2)	0.01861 (11)
P4	0.36014 (5)	0.88739 (2)	0.12751 (2)	0.01853 (11)
P5	0.10685 (5)	0.86584 (2)	−0.04030 (2)	0.01839 (11)
P6	0.10461 (5)	0.73715 (2)	0.09964 (2)	0.02016 (11)
O1	0.80469 (13)	0.66437 (6)	−0.16077 (5)	0.0241 (3)
O2	0.70905 (15)	0.57987 (6)	0.04848 (6)	0.0312 (4)
O3	0.49328 (13)	0.77722 (6)	−0.02502 (5)	0.0229 (3)
O4	0.39175 (13)	0.84659 (6)	0.17029 (5)	0.0239 (3)
O5	0.17959 (13)	0.91595 (6)	−0.04209 (5)	0.0246 (3)
O6	0.02638 (14)	0.71782 (6)	0.05104 (5)	0.0260 (3)
N1	0.68834 (15)	0.68040 (6)	−0.03998 (6)	0.0171 (3)
N2	0.21699 (15)	0.82391 (6)	0.05487 (6)	0.0171 (3)
C1	0.78999 (18)	0.64463 (8)	−0.05105 (7)	0.0194 (4)
H1A	0.787769	0.613050	−0.027280	0.026 (2)*
H1B	0.868570	0.663403	−0.040909	0.026 (2)*
C2	0.68655 (19)	0.68687 (8)	0.01902 (7)	0.0197 (4)
H2A	0.632804	0.717442	0.025816	0.026 (2)*
H2B	0.770738	0.695709	0.034858	0.026 (2)*
C3	0.70148 (18)	0.73311 (8)	−0.06518 (7)	0.0184 (4)
H3A	0.735306	0.728487	−0.100420	0.026 (2)*
H3B	0.760333	0.754978	−0.041800	0.026 (2)*
C4	0.91934 (18)	0.57623 (8)	−0.11559 (8)	0.0211 (4)
C5	1.01796 (19)	0.58845 (9)	−0.14473 (8)	0.0251 (5)
H5	1.015273	0.619544	−0.166628	0.033 (3)*
C6	1.1202 (2)	0.55553 (10)	−0.14201 (9)	0.0312 (5)
H6	1.187678	0.564235	−0.161806	0.033 (3)*
C7	1.1242 (2)	0.50998 (9)	−0.11049 (9)	0.0311 (5)
H7	1.194005	0.487245	−0.109067	0.033 (3)*
C8	1.0270 (2)	0.49743 (9)	−0.08104 (10)	0.0321 (5)
H8	1.030393	0.466257	−0.059245	0.033 (3)*
C9	0.9242 (2)	0.53038 (9)	−0.08331 (9)	0.0283 (5)
H9	0.857545	0.521813	−0.063005	0.033 (3)*
C10	0.65566 (18)	0.58094 (8)	−0.13825 (8)	0.0199 (4)
C11	0.6439 (2)	0.55947 (9)	−0.19059 (8)	0.0258 (5)
H11	0.705613	0.566100	−0.214195	0.035 (3)*
C12	0.5426 (2)	0.52867 (9)	−0.20789 (9)	0.0283 (5)
H12	0.535000	0.514231	−0.243369	0.035 (3)*
C13	0.4526 (2)	0.51881 (9)	−0.17379 (9)	0.0290 (5)
H13	0.383796	0.497161	−0.185533	0.035 (3)*
C14	0.4630 (2)	0.54062 (10)	−0.12242 (9)	0.0348 (6)
H14	0.400514	0.534297	−0.099138	0.035 (3)*
C15	0.5643 (2)	0.57171 (10)	−0.10467 (8)	0.0301 (5)
H15	0.570594	0.586631	−0.069396	0.035 (3)*

C16	0.4747 (2)	0.61749 (9)	0.02914 (8)	0.0241 (4)
C17	0.3925 (2)	0.65785 (9)	0.01293 (9)	0.0283 (5)
H17	0.419529	0.693869	0.013479	0.041 (3)*
C18	0.2703 (2)	0.64576 (10)	−0.00418 (9)	0.0336 (5)
H18	0.213709	0.673588	−0.014308	0.041 (3)*
C19	0.2315 (2)	0.59315 (10)	−0.00640 (9)	0.0364 (6)
H19	0.148133	0.585013	−0.017915	0.041 (3)*
C20	0.3136 (2)	0.55230 (10)	0.00808 (9)	0.0364 (6)
H20	0.287273	0.516219	0.005390	0.041 (3)*
C21	0.4344 (2)	0.56429 (9)	0.02652 (9)	0.0313 (5)
H21	0.490186	0.536378	0.037416	0.041 (3)*
C22	0.6376 (2)	0.65232 (9)	0.12251 (8)	0.0283 (5)
C23	0.5647 (2)	0.69389 (11)	0.13777 (9)	0.0368 (6)
H23	0.508542	0.710689	0.111517	0.055 (4)*
C24	0.5729 (2)	0.71128 (12)	0.19125 (10)	0.0438 (7)
H24	0.522829	0.739803	0.201511	0.055 (4)*
C25	0.6549 (3)	0.68649 (12)	0.22928 (9)	0.0485 (8)
H25	0.660756	0.698053	0.265810	0.055 (4)*
C26	0.7274 (3)	0.64563 (11)	0.21475 (10)	0.0475 (7)
H26	0.782704	0.628805	0.241299	0.055 (4)*
C27	0.7208 (3)	0.62830 (10)	0.16103 (9)	0.0395 (6)
H27	0.772765	0.600377	0.150942	0.055 (4)*
C28	0.46179 (19)	0.72860 (8)	−0.12457 (8)	0.0211 (4)
C29	0.3384 (2)	0.72150 (9)	−0.11850 (9)	0.0319 (5)
H29	0.304592	0.735614	−0.087718	0.040 (3)*
C30	0.2635 (2)	0.69362 (11)	−0.15750 (11)	0.0404 (6)
H30	0.178619	0.688800	−0.153447	0.040 (3)*
C31	0.3138 (2)	0.67300 (10)	−0.20219 (9)	0.0360 (6)
H31	0.263019	0.654055	−0.228861	0.040 (3)*
C32	0.4365 (2)	0.67979 (9)	−0.20817 (8)	0.0315 (5)
H32	0.470200	0.665176	−0.238751	0.040 (3)*
C33	0.5112 (2)	0.70773 (9)	−0.16998 (8)	0.0258 (5)
H33	0.595789	0.712751	−0.174543	0.040 (3)*
C34	0.58512 (19)	0.82821 (8)	−0.11178 (7)	0.0210 (4)
C35	0.4843 (2)	0.85512 (9)	−0.13775 (9)	0.0309 (5)
H35	0.403638	0.841453	−0.135993	0.039 (3)*
C36	0.5013 (2)	0.90163 (9)	−0.16603 (10)	0.0353 (6)
H36	0.432198	0.919675	−0.183636	0.039 (3)*
C37	0.6176 (2)	0.92196 (9)	−0.16885 (9)	0.0335 (6)
H37	0.628548	0.953830	−0.188483	0.039 (3)*
C38	0.7184 (2)	0.89605 (9)	−0.14316 (8)	0.0326 (5)
H38	0.798653	0.910183	−0.144882	0.039 (3)*
C39	0.7021 (2)	0.84904 (9)	−0.11468 (8)	0.0274 (5)
H39	0.771554	0.831168	−0.097151	0.039 (3)*
C40	0.32483 (18)	0.85967 (8)	0.06036 (7)	0.0189 (4)
H40A	0.310170	0.889394	0.034340	0.025 (2)*
H40B	0.397426	0.839629	0.050418	0.025 (2)*
C41	0.18464 (18)	0.81164 (8)	−0.00284 (7)	0.0181 (4)

H41A	0.130935	0.779761	−0.005717	0.025 (2)*
H41B	0.260751	0.802781	−0.019579	0.025 (2)*
C42	0.24160 (18)	0.77409 (8)	0.08536 (7)	0.0193 (4)
H42A	0.289777	0.782709	0.120031	0.025 (2)*
H42B	0.293073	0.750740	0.064638	0.025 (2)*
C43	0.48673 (18)	0.93204 (8)	0.11987 (7)	0.0195 (4)
C44	0.59703 (19)	0.92280 (9)	0.15184 (8)	0.0258 (5)
H44	0.603601	0.893774	0.176488	0.035 (3)*
C45	0.6969 (2)	0.95618 (10)	0.14745 (8)	0.0300 (5)
H45	0.771901	0.949974	0.169195	0.035 (3)*
C46	0.6877 (2)	0.99845 (9)	0.11155 (9)	0.0285 (5)
H46	0.756433	1.021128	0.108623	0.035 (3)*
C47	0.5783 (2)	1.00775 (9)	0.07983 (8)	0.0271 (5)
H47	0.572156	1.036811	0.055209	0.035 (3)*
C48	0.47797 (19)	0.97482 (8)	0.08394 (8)	0.0240 (4)
H48	0.403050	0.981379	0.062260	0.035 (3)*
C49	0.23395 (18)	0.92915 (8)	0.14350 (8)	0.0195 (4)
C50	0.2382 (2)	0.94835 (9)	0.19651 (8)	0.0247 (5)
H50	0.305917	0.939453	0.221783	0.035 (3)*
C51	0.1448 (2)	0.98013 (9)	0.21241 (8)	0.0295 (5)
H51	0.149771	0.993869	0.248153	0.035 (3)*
C52	0.0439 (2)	0.99198 (9)	0.17623 (9)	0.0291 (5)
H52	−0.021173	1.013189	0.187383	0.035 (3)*
C53	0.0381 (2)	0.97288 (9)	0.12388 (9)	0.0296 (5)
H53	−0.031125	0.981043	0.099129	0.035 (3)*
C54	0.13244 (19)	0.94193 (9)	0.10734 (8)	0.0260 (5)
H54	0.128111	0.929316	0.071191	0.035 (3)*
C55	−0.03716 (18)	0.87709 (8)	−0.01214 (7)	0.0197 (4)
C56	−0.0857 (2)	0.92877 (9)	−0.01684 (8)	0.0248 (5)
H56	−0.040249	0.956237	−0.032152	0.028 (3)*
C57	−0.1992 (2)	0.94012 (9)	0.00061 (8)	0.0294 (5)
H57	−0.231478	0.975273	−0.002645	0.028 (3)*
C58	−0.2659 (2)	0.90017 (9)	0.02284 (8)	0.0284 (5)
H58	−0.344789	0.907747	0.034003	0.028 (3)*
C59	−0.2178 (2)	0.84918 (9)	0.02886 (8)	0.0260 (5)
H59	−0.263277	0.822098	0.044762	0.028 (3)*
C60	−0.10332 (19)	0.83740 (8)	0.01176 (7)	0.0219 (4)
H60	−0.070263	0.802475	0.016323	0.028 (3)*
C61	0.06819 (18)	0.83747 (8)	−0.10663 (7)	0.0196 (4)
C62	0.0980 (2)	0.86625 (9)	−0.15147 (8)	0.0271 (5)
H62	0.140942	0.899094	−0.146598	0.034 (3)*
C63	0.0650 (2)	0.84708 (10)	−0.20344 (9)	0.0351 (6)
H63	0.084768	0.867037	−0.233905	0.034 (3)*
C64	0.0037 (2)	0.79910 (10)	−0.21069 (8)	0.0313 (5)
H64	−0.018171	0.786077	−0.246189	0.034 (3)*
C65	−0.0261 (2)	0.76992 (9)	−0.16672 (8)	0.0272 (5)
H65	−0.068475	0.736963	−0.171922	0.034 (3)*
C66	0.00615 (19)	0.78899 (9)	−0.11479 (8)	0.0237 (4)

H66	−0.014204	0.768850	−0.084548	0.034 (3)*
C67	0.01997 (19)	0.77783 (8)	0.14301 (7)	0.0196 (4)
C68	0.0756 (2)	0.81575 (9)	0.17843 (8)	0.0240 (4)
H68	0.161390	0.822314	0.179234	0.038 (3)*
C69	0.0053 (2)	0.84393 (9)	0.21253 (8)	0.0284 (5)
H69	0.043558	0.869783	0.236511	0.038 (3)*
C70	−0.1194 (2)	0.83469 (9)	0.21189 (8)	0.0285 (5)
H70	−0.166562	0.853679	0.235735	0.038 (3)*
C71	−0.1752 (2)	0.79776 (10)	0.17645 (9)	0.0324 (5)
H71	−0.261315	0.791824	0.175472	0.038 (3)*
C72	−0.1065 (2)	0.76929 (9)	0.14229 (8)	0.0278 (5)
H72	−0.145666	0.743775	0.118193	0.038 (3)*
C73	0.1731 (2)	0.68403 (8)	0.14147 (8)	0.0247 (5)
C74	0.2498 (2)	0.69481 (10)	0.18835 (10)	0.0356 (6)
H74	0.261482	0.730590	0.200281	0.076 (5)*
C75	0.3089 (2)	0.65381 (11)	0.21757 (11)	0.0431 (6)
H75	0.360825	0.661260	0.249550	0.076 (5)*
C76	0.2917 (3)	0.60195 (12)	0.19984 (11)	0.0559 (8)
H76	0.333542	0.573719	0.219339	0.076 (5)*
C77	0.2156 (4)	0.59091 (12)	0.15480 (12)	0.0760 (12)
H77	0.202907	0.554957	0.143585	0.076 (5)*
C78	0.1562 (3)	0.63188 (10)	0.12494 (10)	0.0547 (9)
H78	0.104030	0.623900	0.093173	0.076 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0175 (3)	0.0196 (3)	0.0183 (2)	−0.0006 (2)	0.00430 (19)	−0.00088 (19)
P2	0.0280 (3)	0.0239 (3)	0.0174 (2)	−0.0019 (2)	0.0036 (2)	−0.0001 (2)
P3	0.0182 (3)	0.0195 (3)	0.0180 (2)	−0.0006 (2)	0.00107 (19)	−0.00319 (19)
P4	0.0155 (2)	0.0242 (3)	0.0155 (2)	−0.0027 (2)	−0.00039 (18)	0.00124 (19)
P5	0.0182 (3)	0.0198 (3)	0.0168 (2)	−0.0024 (2)	−0.00013 (19)	0.00007 (19)
P6	0.0229 (3)	0.0189 (3)	0.0187 (2)	−0.0019 (2)	0.00194 (19)	−0.00013 (19)
O1	0.0273 (8)	0.0235 (8)	0.0221 (7)	−0.0012 (6)	0.0060 (6)	0.0025 (6)
O2	0.0385 (10)	0.0269 (9)	0.0285 (8)	0.0035 (7)	0.0053 (7)	0.0053 (6)
O3	0.0225 (8)	0.0254 (8)	0.0215 (7)	−0.0004 (6)	0.0048 (6)	−0.0044 (6)
O4	0.0224 (8)	0.0291 (8)	0.0195 (7)	−0.0030 (6)	−0.0015 (6)	0.0045 (6)
O5	0.0245 (8)	0.0237 (8)	0.0248 (7)	−0.0065 (6)	−0.0009 (6)	0.0013 (6)
O6	0.0300 (8)	0.0248 (8)	0.0225 (7)	−0.0066 (7)	−0.0002 (6)	−0.0036 (6)
N1	0.0168 (8)	0.0192 (9)	0.0156 (7)	0.0009 (7)	0.0035 (6)	−0.0024 (6)
N2	0.0168 (8)	0.0188 (9)	0.0154 (7)	−0.0015 (7)	0.0006 (6)	0.0011 (6)
C1	0.0172 (10)	0.0211 (11)	0.0199 (9)	0.0000 (8)	0.0014 (7)	−0.0025 (7)
C2	0.0218 (10)	0.0213 (11)	0.0159 (9)	−0.0022 (8)	0.0014 (7)	−0.0028 (7)
C3	0.0195 (10)	0.0180 (10)	0.0178 (9)	−0.0020 (8)	0.0022 (7)	−0.0016 (7)
C4	0.0178 (10)	0.0231 (11)	0.0225 (9)	−0.0016 (8)	0.0017 (8)	−0.0048 (8)
C5	0.0238 (11)	0.0310 (12)	0.0209 (9)	0.0005 (9)	0.0043 (8)	−0.0022 (8)
C6	0.0202 (11)	0.0451 (15)	0.0293 (11)	0.0014 (10)	0.0070 (9)	−0.0067 (10)
C7	0.0228 (12)	0.0323 (13)	0.0374 (12)	0.0075 (10)	−0.0018 (9)	−0.0119 (10)

C8	0.0294 (13)	0.0235 (12)	0.0421 (13)	0.0027 (10)	−0.0041 (10)	0.0023 (10)
C9	0.0212 (11)	0.0266 (12)	0.0378 (12)	−0.0025 (9)	0.0061 (9)	0.0019 (9)
C10	0.0184 (10)	0.0193 (10)	0.0218 (9)	0.0026 (8)	0.0007 (8)	0.0004 (8)
C11	0.0244 (11)	0.0290 (12)	0.0247 (10)	−0.0001 (9)	0.0052 (8)	−0.0036 (8)
C12	0.0272 (12)	0.0284 (12)	0.0284 (11)	0.0019 (10)	−0.0019 (9)	−0.0061 (9)
C13	0.0206 (11)	0.0298 (13)	0.0348 (11)	−0.0039 (9)	−0.0066 (9)	0.0013 (9)
C14	0.0234 (12)	0.0531 (16)	0.0280 (11)	−0.0104 (11)	0.0035 (9)	0.0023 (10)
C15	0.0259 (12)	0.0447 (14)	0.0199 (10)	−0.0071 (10)	0.0028 (8)	−0.0028 (9)
C16	0.0286 (12)	0.0272 (12)	0.0180 (9)	−0.0051 (9)	0.0093 (8)	−0.0046 (8)
C17	0.0289 (12)	0.0259 (12)	0.0313 (11)	−0.0054 (10)	0.0083 (9)	−0.0084 (9)
C18	0.0273 (13)	0.0355 (14)	0.0395 (13)	−0.0061 (10)	0.0108 (10)	−0.0101 (10)
C19	0.0295 (13)	0.0449 (16)	0.0365 (12)	−0.0140 (11)	0.0124 (10)	−0.0120 (11)
C20	0.0432 (15)	0.0324 (14)	0.0364 (12)	−0.0189 (12)	0.0183 (11)	−0.0091 (10)
C21	0.0404 (14)	0.0274 (13)	0.0279 (11)	−0.0077 (11)	0.0121 (10)	−0.0006 (9)
C22	0.0354 (13)	0.0314 (13)	0.0186 (9)	−0.0094 (10)	0.0047 (9)	0.0002 (8)
C23	0.0328 (13)	0.0521 (16)	0.0259 (11)	−0.0039 (12)	0.0040 (9)	−0.0096 (11)
C24	0.0404 (15)	0.0606 (18)	0.0323 (12)	−0.0130 (13)	0.0127 (11)	−0.0173 (12)
C25	0.066 (2)	0.0595 (19)	0.0205 (11)	−0.0260 (16)	0.0075 (12)	−0.0062 (11)
C26	0.069 (2)	0.0476 (17)	0.0244 (11)	−0.0149 (15)	−0.0053 (12)	0.0054 (11)
C27	0.0555 (17)	0.0350 (14)	0.0269 (11)	−0.0068 (12)	−0.0019 (11)	0.0044 (10)
C28	0.0214 (10)	0.0193 (11)	0.0219 (9)	−0.0004 (8)	−0.0014 (8)	−0.0018 (8)
C29	0.0261 (12)	0.0335 (13)	0.0359 (12)	−0.0011 (10)	0.0022 (9)	−0.0101 (10)
C30	0.0222 (12)	0.0453 (16)	0.0521 (15)	−0.0059 (11)	−0.0043 (11)	−0.0124 (12)
C31	0.0386 (14)	0.0305 (13)	0.0352 (12)	−0.0013 (11)	−0.0155 (10)	−0.0088 (10)
C32	0.0416 (14)	0.0292 (13)	0.0217 (10)	0.0060 (11)	−0.0070 (9)	−0.0048 (9)
C33	0.0271 (12)	0.0296 (12)	0.0199 (9)	0.0029 (9)	−0.0015 (8)	−0.0025 (8)
C34	0.0256 (11)	0.0190 (10)	0.0182 (9)	0.0025 (8)	0.0016 (8)	−0.0051 (7)
C35	0.0271 (12)	0.0268 (12)	0.0387 (12)	0.0041 (10)	0.0028 (10)	−0.0001 (10)
C36	0.0423 (15)	0.0238 (12)	0.0390 (13)	0.0112 (11)	−0.0005 (11)	0.0012 (10)
C37	0.0548 (16)	0.0200 (12)	0.0255 (11)	−0.0012 (11)	0.0035 (10)	−0.0010 (9)
C38	0.0409 (14)	0.0311 (13)	0.0250 (10)	−0.0116 (11)	−0.0008 (10)	0.0000 (9)
C39	0.0308 (12)	0.0292 (12)	0.0211 (9)	−0.0048 (10)	−0.0027 (8)	0.0015 (8)
C40	0.0157 (10)	0.0233 (11)	0.0179 (8)	−0.0017 (8)	0.0025 (7)	0.0002 (7)
C41	0.0188 (10)	0.0193 (10)	0.0162 (8)	0.0005 (8)	0.0018 (7)	−0.0008 (7)
C42	0.0198 (10)	0.0203 (10)	0.0181 (9)	0.0021 (8)	0.0026 (7)	0.0010 (7)
C43	0.0159 (10)	0.0252 (11)	0.0179 (9)	−0.0027 (8)	0.0033 (7)	−0.0029 (8)
C44	0.0213 (11)	0.0354 (13)	0.0204 (9)	−0.0044 (9)	0.0001 (8)	0.0011 (9)
C45	0.0203 (11)	0.0436 (14)	0.0259 (10)	−0.0064 (10)	0.0002 (8)	−0.0039 (10)
C46	0.0246 (12)	0.0306 (13)	0.0314 (11)	−0.0107 (10)	0.0085 (9)	−0.0090 (9)
C47	0.0321 (12)	0.0228 (12)	0.0279 (10)	−0.0021 (9)	0.0100 (9)	0.0000 (8)
C48	0.0218 (11)	0.0270 (12)	0.0232 (10)	−0.0006 (9)	0.0021 (8)	−0.0019 (8)
C49	0.0167 (10)	0.0202 (10)	0.0218 (9)	−0.0045 (8)	0.0036 (7)	0.0004 (8)
C50	0.0243 (11)	0.0278 (12)	0.0215 (9)	−0.0044 (9)	−0.0014 (8)	−0.0009 (8)
C51	0.0339 (13)	0.0328 (13)	0.0223 (10)	−0.0016 (10)	0.0053 (9)	−0.0047 (9)
C52	0.0254 (12)	0.0294 (13)	0.0340 (11)	0.0011 (10)	0.0108 (9)	0.0004 (9)
C53	0.0208 (11)	0.0375 (14)	0.0304 (11)	0.0033 (10)	0.0012 (9)	0.0045 (10)
C54	0.0218 (11)	0.0359 (13)	0.0201 (9)	−0.0003 (9)	0.0011 (8)	−0.0012 (9)
C55	0.0186 (10)	0.0251 (11)	0.0146 (8)	−0.0001 (8)	−0.0021 (7)	−0.0030 (7)

C56	0.0278 (12)	0.0243 (11)	0.0214 (9)	−0.0004 (9)	−0.0019 (8)	0.0009 (8)
C57	0.0304 (12)	0.0309 (13)	0.0259 (10)	0.0099 (10)	−0.0016 (9)	−0.0019 (9)
C58	0.0228 (11)	0.0373 (14)	0.0249 (10)	0.0052 (10)	0.0011 (8)	−0.0083 (9)
C59	0.0246 (11)	0.0302 (12)	0.0231 (10)	−0.0019 (9)	0.0020 (8)	−0.0040 (9)
C60	0.0243 (11)	0.0224 (11)	0.0189 (9)	−0.0010 (9)	0.0006 (8)	−0.0032 (8)
C61	0.0162 (10)	0.0235 (11)	0.0188 (9)	0.0002 (8)	−0.0001 (7)	−0.0019 (8)
C62	0.0324 (13)	0.0260 (12)	0.0236 (10)	−0.0066 (10)	0.0056 (9)	0.0006 (8)
C63	0.0444 (15)	0.0407 (14)	0.0205 (10)	−0.0044 (12)	0.0056 (9)	0.0032 (9)
C64	0.0349 (13)	0.0386 (14)	0.0202 (10)	0.0001 (11)	0.0011 (9)	−0.0078 (9)
C65	0.0226 (11)	0.0292 (12)	0.0295 (11)	−0.0044 (9)	0.0011 (9)	−0.0063 (9)
C66	0.0215 (11)	0.0271 (12)	0.0229 (10)	−0.0030 (9)	0.0037 (8)	0.0019 (8)
C67	0.0217 (10)	0.0198 (10)	0.0172 (9)	−0.0012 (8)	0.0021 (7)	0.0042 (7)
C68	0.0223 (11)	0.0280 (12)	0.0219 (9)	−0.0025 (9)	0.0031 (8)	−0.0016 (8)
C69	0.0337 (13)	0.0280 (12)	0.0242 (10)	−0.0018 (10)	0.0054 (9)	−0.0043 (9)
C70	0.0280 (12)	0.0358 (13)	0.0231 (10)	0.0065 (10)	0.0099 (9)	0.0013 (9)
C71	0.0207 (12)	0.0467 (15)	0.0304 (11)	−0.0047 (10)	0.0057 (9)	0.0029 (10)
C72	0.0244 (11)	0.0347 (13)	0.0240 (10)	−0.0058 (10)	0.0018 (8)	−0.0017 (9)
C73	0.0292 (12)	0.0218 (11)	0.0240 (10)	0.0034 (9)	0.0083 (8)	0.0039 (8)
C74	0.0347 (14)	0.0287 (13)	0.0416 (13)	−0.0033 (11)	−0.0054 (11)	0.0102 (10)
C75	0.0382 (15)	0.0423 (16)	0.0478 (15)	0.0036 (12)	−0.0004 (12)	0.0169 (12)
C76	0.084 (2)	0.0392 (17)	0.0452 (16)	0.0284 (16)	0.0095 (15)	0.0129 (12)
C77	0.157 (4)	0.0220 (15)	0.0446 (17)	0.0199 (19)	−0.013 (2)	−0.0017 (12)
C78	0.103 (3)	0.0271 (14)	0.0306 (13)	0.0006 (15)	−0.0106 (14)	−0.0010 (10)

Geometric parameters (Å, º)

P1—O1	1.4893 (15)	C24—C25	1.386 (4)
P1—C10	1.806 (2)	C25—C26	1.364 (4)
P1—C4	1.806 (2)	C26—C27	1.400 (3)
P1—C1	1.8203 (19)	C28—C29	1.382 (3)
P2—O2	1.4900 (17)	C28—C33	1.399 (3)
P2—C16	1.802 (2)	C29—C30	1.395 (3)
P2—C22	1.812 (2)	C30—C31	1.386 (4)
P2—C2	1.816 (2)	C31—C32	1.373 (4)
P3—O3	1.4950 (14)	C32—C33	1.382 (3)
P3—C28	1.8027 (19)	C34—C39	1.389 (3)
P3—C34	1.811 (2)	C34—C35	1.396 (3)
P3—C3	1.823 (2)	C35—C36	1.384 (3)
P4—O4	1.4923 (14)	C36—C37	1.377 (4)
P4—C43	1.804 (2)	C37—C38	1.381 (3)
P4—C49	1.805 (2)	C38—C39	1.395 (3)
P4—C40	1.8159 (19)	C43—C48	1.394 (3)
P5—O5	1.4897 (15)	C43—C44	1.397 (3)
P5—C55	1.804 (2)	C44—C45	1.387 (3)
P5—C61	1.8089 (19)	C45—C46	1.383 (3)
P5—C41	1.8124 (19)	C46—C47	1.388 (3)
P6—O6	1.4926 (14)	C47—C48	1.383 (3)
P6—C67	1.803 (2)	C49—C54	1.396 (3)

P6—C73	1.807 (2)	C49—C50	1.400 (3)
P6—C42	1.824 (2)	C50—C51	1.382 (3)
N1—C1	1.474 (2)	C51—C52	1.387 (3)
N1—C3	1.476 (2)	C52—C53	1.383 (3)
N1—C2	1.478 (2)	C53—C54	1.384 (3)
N2—C42	1.473 (2)	C55—C60	1.396 (3)
N2—C40	1.476 (2)	C55—C56	1.401 (3)
N2—C41	1.477 (2)	C56—C57	1.382 (3)
C4—C5	1.389 (3)	C57—C58	1.384 (3)
C4—C9	1.401 (3)	C58—C59	1.385 (3)
C5—C6	1.385 (3)	C59—C60	1.390 (3)
C6—C7	1.384 (3)	C61—C62	1.393 (3)
C7—C8	1.383 (3)	C61—C66	1.397 (3)
C8—C9	1.390 (3)	C62—C63	1.394 (3)
C10—C15	1.381 (3)	C63—C64	1.380 (3)
C10—C11	1.403 (3)	C64—C65	1.380 (3)
C11—C12	1.383 (3)	C65—C66	1.390 (3)
C12—C13	1.381 (3)	C67—C68	1.395 (3)
C13—C14	1.384 (3)	C67—C72	1.396 (3)
C14—C15	1.390 (3)	C68—C69	1.390 (3)
C16—C17	1.387 (3)	C69—C70	1.381 (3)
C16—C21	1.404 (3)	C70—C71	1.380 (3)
C17—C18	1.395 (3)	C71—C72	1.385 (3)
C18—C19	1.385 (3)	C73—C78	1.378 (3)
C19—C20	1.386 (4)	C73—C74	1.395 (3)
C20—C21	1.388 (3)	C74—C75	1.383 (3)
C22—C23	1.387 (3)	C75—C76	1.380 (4)
C22—C27	1.393 (3)	C76—C77	1.358 (4)
C23—C24	1.395 (3)	C77—C78	1.391 (4)

O1—P1—C10	112.22 (9)	C22—C23—C24	120.7 (2)
O1—P1—C4	111.41 (9)	C25—C24—C23	119.3 (3)
C10—P1—C4	105.90 (9)	C26—C25—C24	120.6 (2)
O1—P1—C1	114.74 (9)	C25—C26—C27	120.5 (3)
C10—P1—C1	109.72 (9)	C22—C27—C26	119.5 (3)
C4—P1—C1	102.06 (9)	C29—C28—C33	119.72 (19)
O2—P2—C16	111.55 (10)	C29—C28—P3	119.11 (16)
O2—P2—C22	112.59 (10)	C33—C28—P3	121.09 (16)
C16—P2—C22	107.84 (10)	C28—C29—C30	120.1 (2)
O2—P2—C2	114.51 (10)	C31—C30—C29	119.6 (2)
C16—P2—C2	107.93 (10)	C32—C31—C30	120.4 (2)
C22—P2—C2	101.79 (9)	C31—C32—C33	120.4 (2)
O3—P3—C28	112.76 (9)	C32—C33—C28	119.7 (2)
O3—P3—C34	113.96 (9)	C39—C34—C35	118.9 (2)
C28—P3—C34	103.69 (9)	C39—C34—P3	123.74 (16)
O3—P3—C3	114.64 (8)	C35—C34—P3	117.38 (17)
C28—P3—C3	105.29 (9)	C36—C35—C34	120.3 (2)
C34—P3—C3	105.48 (9)	C37—C36—C35	120.5 (2)

O4—P4—C43	111.94 (9)	C36—C37—C38	120.0 (2)
O4—P4—C49	111.71 (9)	C37—C38—C39	119.8 (2)
C43—P4—C49	105.80 (9)	C34—C39—C38	120.5 (2)
O4—P4—C40	114.03 (9)	N2—C40—P4	114.49 (13)
C43—P4—C40	103.76 (9)	N2—C41—P5	113.55 (13)
C49—P4—C40	108.99 (9)	N2—C42—P6	114.76 (13)
O5—P5—C55	111.53 (9)	C48—C43—C44	119.66 (19)
O5—P5—C61	112.51 (9)	C48—C43—P4	122.65 (15)
C55—P5—C61	106.24 (9)	C44—C43—P4	117.69 (16)
O5—P5—C41	115.03 (9)	C45—C44—C43	119.8 (2)
C55—P5—C41	107.51 (9)	C46—C45—C44	120.3 (2)
C61—P5—C41	103.33 (9)	C45—C46—C47	120.1 (2)
O6—P6—C67	112.44 (9)	C48—C47—C46	120.2 (2)
O6—P6—C73	113.57 (9)	C47—C48—C43	120.06 (19)
C67—P6—C73	106.28 (9)	C54—C49—C50	118.68 (19)
O6—P6—C42	115.07 (9)	C54—C49—P4	124.56 (15)
C67—P6—C42	107.85 (9)	C50—C49—P4	116.74 (15)
C73—P6—C42	100.65 (10)	C51—C50—C49	120.61 (19)
C1—N1—C3	111.10 (15)	C50—C51—C52	120.0 (2)
C1—N1—C2	109.53 (15)	C53—C52—C51	119.9 (2)
C3—N1—C2	109.53 (14)	C52—C53—C54	120.4 (2)
C42—N2—C40	111.31 (14)	C53—C54—C49	120.36 (19)
C42—N2—C41	109.76 (15)	C60—C55—C56	119.20 (19)
C40—N2—C41	109.30 (15)	C60—C55—P5	124.05 (16)
N1—C1—P1	116.12 (12)	C56—C55—P5	116.71 (16)
N1—C2—P2	114.58 (13)	C57—C56—C55	120.5 (2)
N1—C3—P3	111.54 (13)	C56—C57—C58	119.9 (2)
C5—C4—C9	119.4 (2)	C57—C58—C59	120.2 (2)
C5—C4—P1	117.83 (16)	C58—C59—C60	120.4 (2)
C9—C4—P1	122.74 (16)	C59—C60—C55	119.7 (2)
C6—C5—C4	120.3 (2)	C62—C61—C66	118.81 (18)
C7—C6—C5	120.1 (2)	C62—C61—P5	118.32 (15)
C8—C7—C6	120.3 (2)	C66—C61—P5	122.83 (15)
C7—C8—C9	120.1 (2)	C61—C62—C63	120.3 (2)
C8—C9—C4	119.8 (2)	C64—C63—C62	120.0 (2)
C15—C10—C11	119.31 (19)	C63—C64—C65	120.46 (19)
C15—C10—P1	124.32 (15)	C64—C65—C66	119.7 (2)
C11—C10—P1	116.33 (16)	C65—C66—C61	120.68 (19)
C12—C11—C10	120.1 (2)	C68—C67—C72	118.86 (19)
C13—C12—C11	120.3 (2)	C68—C67—P6	123.12 (16)
C12—C13—C14	119.7 (2)	C72—C67—P6	117.97 (15)
C13—C14—C15	120.5 (2)	C69—C68—C67	120.0 (2)
C10—C15—C14	120.1 (2)	C70—C69—C68	120.6 (2)
C17—C16—C21	119.3 (2)	C71—C70—C69	119.7 (2)
C17—C16—P2	123.95 (17)	C70—C71—C72	120.4 (2)
C21—C16—P2	116.76 (18)	C71—C72—C67	120.5 (2)
C16—C17—C18	120.2 (2)	C78—C73—C74	119.0 (2)
C19—C18—C17	120.0 (2)	C78—C73—P6	119.46 (17)

C18—C19—C20	120.4 (2)	C74—C73—P6	121.34 (17)
C19—C20—C21	119.8 (2)	C75—C74—C73	120.5 (2)
C20—C21—C16	120.3 (2)	C76—C75—C74	119.4 (3)
C23—C22—C27	119.4 (2)	C77—C76—C75	120.6 (3)
C23—C22—P2	122.79 (17)	C76—C77—C78	120.5 (3)
C27—C22—P2	117.78 (19)	C73—C78—C77	120.0 (3)