Mono-alkylated bisphosphines as dopants for ESI-MS analysis of catalytic reactions

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Figure SI1. MS/MS of $[RhCl(PPh_3)(\mathbf{4}^+)_2]^+$. Loss of PPh₃ (586 m/z) and loss of $\mathbf{4}^+$ (generating two charged fragments, $\mathbf{4}^+$ at 517 *m*/z and $[RhCl(PPh_3)(\mathbf{4}^+)]^+$ at 917 *m*/z) are competitive; while $\mathbf{4}^+$ is a better ligand, it experiences Coloumbic repulsion from the other charged ligand and is therefore eliminated more easily).



Figure SI2. Positive-ion ESI-MS of RhCl(PPh₃)₃ + $\mathbf{4}^{+}$ BF₄⁻ in H₂-saturated chlorobenzene at a cone voltage of 10 V.



Figure SI3. MS/MS of $[RhCl(PPh_3)(\mathbf{4}^+)(C_4H_8)]^+$. Only a small proportion of the product ions involve loss of C_4H_8 ; the predominant fragmentation pathway is loss of PPh₃ then $\mathbf{4}^+$.



Figure SI4. Variation in total ion current (TIC) with cone voltage for the positive-ion ESI-MS of RhCl(PPh₃)₃ + $\mathbf{4}^+$ BF₄⁻ in chlorobenzene. Note the linear response of TIC with voltage. Data were collected for 20 s at each value of cone voltage up to 43 V.



Figure SI5. MS/MS of $[Rh_2Cl_2(PPh_3)_3(\mathbf{4}^*)]^*$. Neither loss of PPh₃ or loss of $\mathbf{4}^*$ is observed; instead, the dimer cleaves in two symmetrically.

Electronic Supplementary Information for Dalton Transactions This journal is © The Royal Society of Chemistry 2009 X-ray Structure Report for [Ph₂P(CH₂)₄PPh₂CH₂Ph]⁺ [PF₆]⁻ (4⁺ PF₆⁻)

The compound crystallizes as colourless block-like crystals. There are four molecules of the phosphine cation and associated PF_6 anion in the unit cell of the primitive, acentric, orthorhombic space group $P2_12_12_1$. This is a chiral space group. The correct enantiomorph of the space group was determined by comparison of intesities of Friedel pairs of reflections. This resulted in an absolute structure parameter of 0.2 (Flack parameter). This vale is indicative of racemic twinning. A racemic twin law was applied to the refined structure.

CRYSTAL SUMMARY

Crystal data for $C_{35}H_{35}F_6P_3$; $M_r = 662.54$; orthorhombic; space group $P2_12_12_1$; a = 10.1738(4) Å; b = 15.8803(7) Å; c = 19.7059(8) Å; $a = 90^{\circ}$; $\beta = 90^{\circ}$; $\gamma = 90^{\circ}$; V = 3183.7(2) Å³; Z = 4; T = 100(2) K; λ (Mo-K α) = 0.71073 Å; μ (Mo-K α) = 0.247 mm⁻¹; $d_{calc} = 1.382g.cm^{-3}$; 24326 reflections collected; 6483 unique ($R_{int} = 0.0470$); giving $R_1 = 0.0426$, w $R_2 = 0.0937$ for 5506 data with [I>2 σ (I)] and $R_1 = 0.0546$, w $R_2 = 0.1004$ for all 6483 data. Residual electron density (e⁻.Å⁻³) max/min: 0.407/-0.303.

An arbitrary sphere of data were collected on a colourless block-like crystal, having approximate dimensions of $0.20 \times 0.18 \times 0.15$ mm, on a Bruker APEX-II diffractometer using a combination of ω -and φ -scans of 0.3° . Data were corrected for absorption and polarization effects and analyzed for space group determination. The structure was solved by direct methods and expanded routinely. The model was refined by full-matrix least-squares analysis of F² against all reflections. All non-hydrogen atoms were refined with anisotropic thermal displacement parameters. Unless otherwise noted, hydrogen atoms were included in calculated positions. Thermal parameters for the hydrogens were tied to the isotropic thermal parameter of the atom to which they are bonded (1.2 ×).

Electronic Supplementary Information for Dalton Transactions This journal is © The Royal Society of Chemistry 2009 **Table 1. Crystal data and structure refinement**

Empirical formula	C35 H35 F6 P3
Formula weight	662.54
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P212121
Unit cell dimensions	$a = 10.1738(4) \text{ Å} \qquad \alpha = 90^{\circ}$
	$b = 15.8803(7) \text{ Å} \qquad \beta = 90^{\circ}$
	$c = 19.7059(8) \text{ Å} \qquad \gamma = 90^{\circ}$
Volume	$3183.7(2) \text{ Å}^3$
Ζ	4
Density (calculated)	1.382 g.cm ⁻³
Absorption coefficient (μ)	0.247 mm ⁻¹
F(000)	1376
Crystal size	$0.20 \times 0.18 \times 0.15 \text{ mm}^3$
ω range for data collection	1.65 to 26.46°
Index ranges	$-12 \le h \le 12, -17 \le k \le 19, -24 \le l \le 24$
Reflections collected	24326
Independent reflections	$6483 [R_{int} = 0.0470]$
Completeness to $\theta = 26.46^{\circ}$	99.4 %
Absorption correction	numerical
Max. and min. transmission	1.0000 and 0.8915
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6483 / 0 / 398
Goodness-of-fit on F^2	1.032
Final R indices $[I \ge 2\sigma(I)]$	$R_1 = 0.0426$, $wR_2 = 0.0937$
R indices (all data)	$R_1 = 0.0546$, $wR_2 = 0.1004$
Absolute structure parameter	0.20(8)
Largest diff. peak and hole	0.407 and -0.303 e ⁻ .Å ⁻³

Table 2.	Atomic coordinates an	d equivalent isotrop	ic displacement parameters ((Å ²).
U(eq) is d	efined as one third of	the trace of the ortho	ogonalized U _{ij} tensor.	

	Х	У	Z	U(eq)
P(1)	0.43911(6)	-0.07444(4)	0.39599(4)	0.020(1)
P(2)	0.66646(7)	0.20173(5)	0.63754(4)	0.026(1)
C(1)	0.4454(3)	0.02584(17)	0.43879(13)	0.022(1)
C(2)	0.5707(3)	0.03763(19)	0.48077(14)	0.026(1)
C(3)	0.5564(3)	0.10887(18)	0.53208(14)	0.025(1)
C(4)	0.6895(3)	0.13399(19)	0.56284(14)	0.028(1)
C(11)	0.3929(3)	-0.15446(18)	0.45708(14)	0.025(1)
C(12)	0.2707(3)	-0.13429(17)	0.49698(13)	0.023(1)
C(13)	0.2820(3)	-0.09898(19)	0.56205(14)	0.027(1)
C(14)	0.1726(3)	-0.0832(2)	0.60072(15)	0.032(1)
C(15)	0.0482(3)	-0.1022(2)	0.57601(16)	0.034(1)
C(16)	0.0354(3)	-0.13650(18)	0.51111(16)	0.030(1)
C(17)	0.1460(3)	-0.15234(18)	0.47206(14)	0.027(1)
C(21)	0.5979(2)	-0.10213(17)	0.36331(14)	0.022(1)
C(22)	0.6514(3)	-0.05444(17)	0.31082(14)	0.025(1)
C(23)	0.7763(3)	-0.07162(19)	0.28731(15)	0.029(1)
C(24)	0.8481(3)	-0.13674(18)	0.31585(14)	0.028(1)
C(25)	0.7961(3)	-0.18406(19)	0.36758(15)	0.029(1)
C(26)	0.6703(3)	-0.16720(18)	0.39145(15)	0.027(1)
C(31)	0.3230(3)	-0.06791(17)	0.32780(13)	0.022(1)
C(32)	0.2263(3)	-0.00573(19)	0.32792(15)	0.028(1)
C(33)	0.1358(3)	-0.00202(19)	0.27488(15)	0.029(1)
C(34)	0.1414(3)	-0.05962(19)	0.22335(14)	0.029(1)
C(35)	0.2363(3)	-0.1208(2)	0.22326(16)	0.035(1)
C(36)	0.3289(3)	-0.12475(18)	0.27529(14)	0.030(1)
C(41)	0.5902(3)	0.29445(18)	0.59840(15)	0.026(1)
C(42)	0.4751(3)	0.3245(2)	0.62749(16)	0.033(1)
C(43)	0.4120(3)	0.3950(2)	0.60161(17)	0.038(1)
C(44)	0.4617(3)	0.4359(2)	0.54664(19)	0.041(1)
C(45)	0.5777(3)	0.4062(2)	0.51604(16)	0.036(1)
C(46)	0.6406(3)	0.33610(19)	0.54203(14)	0.028(1)
C(51)	0.8318(3)	0.24425(17)	0.65345(14)	0.024(1)

C(52)	0.9404(3)	0.23186(18)	0.61195(15)	0.028(1)
C(53)	1.0627(3)	0.26680(18)	0.62861(15)	0.029(1)
C(54)	1.0765(3)	0.31335(18)	0.68701(15)	0.029(1)
C(55)	0.9689(3)	0.32657(19)	0.72902(14)	0.028(1)
C(56)	0.8482(3)	0.29167(18)	0.71258(14)	0.029(1)
P(3)	0.82858(7)	0.12914(5)	0.14822(4)	0.025(1)
F(1)	0.92418(17)	0.04997(11)	0.14040(9)	0.041(1)
F(2)	0.73054(18)	0.20635(12)	0.15520(10)	0.047(1)
F(3)	0.8681(2)	0.13496(15)	0.22559(10)	0.066(1)
F(4)	0.7859(2)	0.12172(15)	0.07099(9)	0.060(1)
F(5)	0.71247(18)	0.06754(13)	0.16917(11)	0.056(1)
F(6)	0.94375(19)	0.18987(13)	0.12776(15)	0.078(1)
H(1A)	0.4399	0.0714	0.4046	0.027
H(1B)	0.3682	0.0309	0.4691	0.027
H(2A)	0.5909	-0.0154	0.5051	0.031
H(2B)	0.6451	0.0501	0.4500	0.031
H(3A)	0.4963	0.0909	0.5689	0.030
H(3B)	0.5168	0.1584	0.5095	0.030
H(4A)	0.7422	0.1643	0.5284	0.033
H(4B)	0.7383	0.0827	0.5762	0.033
H(11A)	0.3792	-0.2083	0.4327	0.030
H(11B)	0.4666	-0.1627	0.4892	0.030
H(13A)	0.3666	-0.0859	0.5795	0.033
H(14A)	0.1820	-0.0591	0.6446	0.039
H(15A)	-0.0275	-0.0921	0.6031	0.041
H(16A)	-0.0494	-0.1490	0.4936	0.036
H(17A)	0.1366	-0.1757	0.4279	0.032
H(22A)	0.6018	-0.0100	0.2912	0.030
H(23A)	0.8129	-0.0389	0.2517	0.035
H(24A)	0.9340	-0.1487	0.2995	0.033
H(25A)	0.8461	-0.2284	0.3871	0.035
H(26A)	0.6340	-0.2003	0.4270	0.033
H(32A)	0.2221	0.0339	0.3640	0.033
H(33A)	0.0703	0.0406	0.2745	0.035
H(34A)	0.0792	-0.0572	0.1875	0.034
H(35A)	0.2391	-0.1609	0.1875	0.042
H(36A)	0.3957	-0.1665	0.2745	0.035

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0 4390	0 2964	0.6657	0.040
0.4370	0.2704	0.0057	0.040
0.3336	0.4148	0.6224	0.046
0.4183	0.4842	0.5291	0.049
0.6129	0.4343	0.4775	0.043
0.7189	0.3162	0.5212	0.034
0.9318	0.1993	0.5718	0.034
1.1360	0.2583	0.5996	0.034
1.1597	0.3365	0.6986	0.035
0.9780	0.3595	0.7690	0.034
0.7754	0.3001	0.7420	0.035
	0.4390 0.3336 0.4183 0.6129 0.7189 0.9318 1.1360 1.1597 0.9780 0.7754	0.43900.29640.33360.41480.41830.48420.61290.43430.71890.31620.93180.19931.13600.25831.15970.33650.97800.35950.77540.3001	0.43900.29640.66570.33360.41480.62240.41830.48420.52910.61290.43430.47750.71890.31620.52120.93180.19930.57181.13600.25830.59961.15970.33650.69860.97800.35950.76900.77540.30010.7420

Table 3. Anisotropic displacement parameters $(\text{\AA})^2$ for agojsm3. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h² a^{*2} U₁₁ + ... + 2 h k a^{*} b^{*} U₁₂]

	U_{11}	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
P(1)	0.0185(3)	0.0203(4)	0.0213(3)	0.0000(3)	-0.0007(3)	0.0002(3)
P(2)	0.0271(4)	0.0289(4)	0.0230(4)	-0.0012(3)	-0.0013(3)	-0.0043(3)
C(1)	0.0225(13)	0.0210(15)	0.0227(14)	0.0010(12)	-0.0001(11)	-0.0023(11)
C(2)	0.0259(14)	0.0235(15)	0.0275(15)	-0.0021(12)	-0.0040(12)	-0.0023(12)
C(3)	0.0275(14)	0.0226(16)	0.0248(14)	-0.0028(12)	-0.0021(12)	-0.0017(12)
C(4)	0.0324(16)	0.0226(16)	0.0286(15)	-0.0021(13)	-0.0052(12)	0.0004(12)
C(11)	0.0266(15)	0.0217(16)	0.0260(15)	0.0022(13)	-0.0007(12)	0.0006(11)
C(12)	0.0222(13)	0.0220(16)	0.0234(15)	0.0058(13)	0.0001(11)	-0.0017(11)
C(13)	0.0189(13)	0.0343(18)	0.0292(16)	0.0025(13)	-0.0037(11)	-0.0045(12)
C(14)	0.0320(15)	0.0414(19)	0.0235(15)	0.0009(14)	0.0050(13)	-0.0022(14)
C(15)	0.0250(15)	0.042(2)	0.0358(17)	0.0067(15)	0.0078(13)	0.0004(13)
C(16)	0.0211(14)	0.0273(17)	0.0413(17)	0.0072(15)	-0.0032(12)	-0.0044(12)
C(17)	0.0268(15)	0.0249(16)	0.0290(15)	0.0008(12)	-0.0022(12)	-0.0042(12)
C(21)	0.0184(12)	0.0243(15)	0.0234(14)	-0.0052(12)	-0.0008(11)	0.0003(10)
C(22)	0.0278(14)	0.0196(15)	0.0279(14)	0.0019(12)	-0.0024(12)	0.0039(12)
C(23)	0.0292(14)	0.0282(17)	0.0302(16)	0.0031(14)	0.0065(12)	-0.0025(13)
C(24)	0.0224(14)	0.0285(17)	0.0319(15)	-0.0049(13)	0.0013(12)	0.0008(12)
C(25)	0.0234(14)	0.0298(17)	0.0349(17)	0.0016(14)	-0.0040(12)	0.0064(11)
C(26)	0.0252(14)	0.0273(16)	0.0295(15)	0.0054(13)	-0.0002(13)	0.0010(12)
C(31)	0.0219(13)	0.0222(15)	0.0206(13)	0.0011(12)	-0.0016(11)	-0.0026(11)
C(32)	0.0254(14)	0.0267(17)	0.0311(16)	-0.0090(13)	-0.0028(12)	0.0061(12)
C(33)	0.0221(14)	0.0309(16)	0.0345(17)	-0.0017(14)	-0.0058(12)	0.0080(12)
C(34)	0.0216(14)	0.0376(19)	0.0268(15)	-0.0001(13)	-0.0031(11)	-0.0008(12)
C(35)	0.0358(17)	0.0336(19)	0.0364(17)	-0.0119(15)	-0.0086(14)	0.0065(14)
C(36)	0.0276(14)	0.0278(17)	0.0333(16)	-0.0041(14)	-0.0061(13)	0.0090(13)
C(41)	0.0288(15)	0.0211(15)	0.0290(16)	-0.0048(13)	-0.0056(12)	-0.0053(12)
C(42)	0.0289(15)	0.039(2)	0.0324(17)	-0.0053(14)	0.0003(12)	-0.0054(13)
C(43)	0.0261(15)	0.040(2)	0.049(2)	-0.0116(17)	0.0017(15)	0.0028(13)
C(44)	0.0306(17)	0.0260(18)	0.066(2)	-0.0025(17)	-0.0163(16)	0.0013(13)
C(45)	0.0376(17)	0.0295(18)	0.0404(18)	0.0034(15)	-0.0087(14)	-0.0090(14)
C(46)	0.0276(15)	0.0285(17)	0.0292(15)	-0.0063(13)	-0.0021(12)	-0.0024(13)
C(51)	0.0251(14)	0.0213(15)	0.0269(15)	0.0019(12)	-0.0065(12)	-0.0047(12)

C(52)	0.0279(14)	0.0313(17)	0.0259(15)	0.0000(13)	-0.0038(13)	0.0025(12)
C(53)	0.0257(14)	0.0289(17)	0.0315(16)	0.0032(13)	-0.0002(12)	0.0021(12)
C(54)	0.0296(15)	0.0273(17)	0.0309(16)	0.0051(14)	-0.0082(13)	-0.0030(13)
C(55)	0.0358(17)	0.0287(17)	0.0199(14)	-0.0028(13)	-0.0051(12)	-0.0009(13)
C(56)	0.0328(16)	0.0290(17)	0.0256(15)	0.0011(13)	0.0005(12)	-0.0021(13)
P(3)	0.0211(3)	0.0281(4)	0.0273(4)	0.0017(3)	0.0012(3)	0.0047(3)
F(1)	0.0370(9)	0.0386(11)	0.0470(11)	0.0071(9)	0.0047(9)	0.0155(8)
F(2)	0.0410(10)	0.0407(12)	0.0604(13)	0.0013(10)	0.0081(10)	0.0214(9)
F(3)	0.0737(15)	0.0814(17)	0.0416(12)	-0.0196(12)	-0.0205(11)	0.0295(13)
F(4)	0.0697(14)	0.0835(17)	0.0267(10)	-0.0036(11)	-0.0049(9)	0.0382(12)
F(5)	0.0286(10)	0.0552(13)	0.0847(16)	0.0323(12)	-0.0052(10)	-0.0042(9)
F(6)	0.0300(11)	0.0471(13)	0.156(3)	0.0421(15)	0.0092(13)	-0.0025(9)

Table 4. Bond lengths [Å].

atom-atom	distance	atom-atom	distance	
P(1)-C(31)	1.792(3)	P(1)-C(21)	1.794(3)	P(1)-
C(1)	1.803(3)	P(1)-C(11)	1.813(3)	P(2)-
C(41)	1.834(3)	P(2)-C(4)	1.838(3)	P(2)-
C(51)	1.840(3)	C(1)-C(2)	1.531(4)	C(2)-
C(3)	1.524(4)	C(3)-C(4)	1.536(4)	C(11)-
C(12)	1.506(4)	C(12)-C(17)	1.390(4)	C(12)-
C(13)	1.404(4)	C(13)-C(14)	1.372(4)	C(14)-
C(15)	1.389(4)	C(15)-C(16)	1.396(4)	C(16)-
C(17)	1.387(4)	C(21)-C(26)	1.384(4)	C(21)-
C(22)	1.393(4)	C(22)-C(23)	1.380(4)	C(23)-
C(24)	1.386(4)	C(24)-C(25)	1.373(4)	C(25)-
C(26)	1.390(4)	C(31)-C(36)	1.374(4)	C(31)-
C(32)	1.394(4)	C(32)-C(33)	1.394(4)	C(33)-
C(34)	1.368(4)	C(34)-C(35)	1.370(4)	C(35)-
C(36)	1.393(4)	C(41)-C(42)	1.389(4)	C(41)-
C(46)	1.391(4)	C(42)-C(43)	1.387(4)	C(43)-
C(44)	1.361(5)	C(44)-C(45)	1.408(5)	C(45)-
C(46)	1.382(4)	C(51)-C(52)	1.389(4)	C(51)-
C(56)	1.397(4)	C(52)-C(53)	1.401(4)	C(53)-
C(54)	1.375(4)	C(54)-C(55)	1.389(4)	C(55)-
C(56)	1.386(4)	P(3)-F(6)	1.570(2)	P(3)-
F(3)	1.579(2)	P(3)-F(2)	1.5866(18)	P(3)-
F(4)	1.5871(19)	P(3)-F(5)	1.5883(19)	P(3)-
F(1)	1.5969(18)	C(1)-H(1A)	0.9900	C(1)-
H(1B)	0.9900	C(2)-H(2A)	0.9900	C(2)-
H(2B)	0.9900	C(3)-H(3A)	0.9900	C(3)-
H(3B)	0.9900	C(4)-H(4A)	0.9900	C(4)-
H(4B)	0.9900	C(11)-H(11A)	0.9900	C(11)-
H(11B)	0.9900	C(13)-H(13A)	0.9500	C(14)-
H(14A)	0.9500	C(15)-H(15A)	0.9500	C(16)-
H(16A)	0.9500	C(17)-H(17A)	0.9500	C(22)-
H(22A)	0.9500	C(23)-H(23A)	0.9500	C(24)-
H(24A)	0.9500	C(25)-H(25A)	0.9500	C(26)-
H(26A)	0.9500	C(32)-H(32A)	0.9500	C(33)-
H(33A)	0.9500	C(34)-H(34A)	0.9500	C(35)-
H(35A)	0.9500	C(36)-H(36A)	0.9500	C(42)-
H(42A)	0.9500	C(43)-H(43A)	0.9500	C(44)-
H(44A)	0.9500	C(45)-H(45A)	0.9500	C(46)-
H(46A)	0.9500	C(52)-H(52A)	0.9500	C(53)-
H(53A)	0.9500	C(54)-H(54A)	0.9500	C(55)-
H(55A)	0.9500	C(56)-H(56A)	0.9500	

Table 5.Bond angles [°].

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	atom-atom-atom	angle	atom-atom-atom	angle	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(31)-P(1)-C(21)	109 80(12)	C(31)-P(1)-C(1)	108 86(13)	C(21)-
$\begin{array}{cccccc} P(1) & 107.47(13) & C(1)-P(1)-C(11) & 108.53(13) & C(4)-\\ P(2)-C(51) & 103.58(13) & C(4)-P(2)-C(51) & 99.43(13) & C(4)-\\ P(2)-C(51) & 103.58(13) & C(2)-C(1)-P(1) & 112.99(19) & C(3)-\\ C(2)-C(1) & 111.7(2) & C(2)-C(3)-C(4) & 111.7(2) & C(3)-\\ C(4)-P(2) & 110.84(19) & C(12)-C(11)-P(1) & 114.3(2) & C(17)-\\ C(12)-C(13) & 118.7(2) & C(17)-C(12)-C(11) & 121.7(2) & C(13)-\\ C(12)-C(11) & 119.6(2) & C(14)-C(13)-C(12) & 120.9(3) & C(13)-\\ C(14)-C(15) & 120.3(3) & C(14)-C(15)-C(16) & 119.4(3) & C(17)-\\ C(16)-C(15) & 120.3(3) & C(14)-C(15)-C(16) & 119.4(3) & C(17)-\\ C(16)-C(15) & 120.2(3) & C(16)-C(17)-C(12) & 120.5(3) & C(26)-\\ C(21)-C(22) & 119.7(2) & C(26)-C(22)-C(21) & 120.1(3) & C(22)-\\ C(23)-C(24) & 119.8(3) & C(25)-C(24)-C(23) & 120.4(3) & C(24)-\\ C(25)-C(26) & 120.1(3) & C(21)-C(26)-C(25) & 119.9(3) & C(36)-\\ C(31)-C(32) & 119.8(2) & C(33)-C(34)-C(35) & 119.9(3) & C(34)-\\ C(33)-C(32) & 119.8(2) & C(33)-C(34)-C(35) & 119.9(3) & C(34)-\\ C(35)-C(36) & 120.5(3) & C(31)-C(36)-C(35) & 119.7(3) & C(42)-\\ C(41)-P(2) & 124.2(2) & C(43)-C(44)-P(2) & 117.3(2) & C(46)-\\ C(41)-C(46) & 118.5(3) & C(42)-C(41) & 120.1(3) & C(42)-\\ C(41)-C(46) & 118.5(3) & C(42)-C(41) & 120.1(3) & C(44)-\\ C(43)-C(42) & 120.4(3) & C(43)-C(44)-C(45) & 119.5(3) & C(46)-\\ C(41)-C(46) & 118.2(3) & C(52)-C(53) & 120.8(3) & C(54)-\\ C(53)-C(54) & 119.9(3) & C(55)-C(56)-C(51) & 121.1(3) & F(6)-\\ P(3)-F(3) & 91.25(15) & F(6)-P(3)-F(4) & 88.54(13) & F(6)-\\ P(3)-F(3) & 91.25(15) & F(6)-P(3)-F(4) & 88.54(13) & F(6)-\\ P(3)-F(3) & 91.25(15) & F(6)-P(3)-F(4) & 88.54(13) & F(6)-\\ P(3)-F(1) & 90.24(11) & F(3)-P(3)-F(1) & 90.90(11) & F(3)-\\ P(3)-F(1) & 90.24(11) & F(3)-P(3)-F(1) & 80.90(11) & F(6)-\\ P(3)-F(1) & 90.24(11) & F(3)-P(3)-F(1) & 80.90(11) & F(6)-\\ P(3)-F(1) & 178.55(15) & F(2)-P(3)-F(4) & 88.54(13) & F(2)-\\ P(3)-F(1) & 178.55(15) & F(2)-P(3)-F(4) & 88.54(13) & F(2)-\\ P(3)-F(4) & 178.55(15) & F(2)-P(3)-F(4) & 88.54(13) & F(2)-\\ P(3)-F(1) & 178.57(15) & F(2)-P(3)-F(4) & 80.50(11) & F(6)-\\ P(3)-F(1) & 179.47(11) & F(3)-P(3)-F(1) & 80.90(11) & F(6)$	P(1)-C(1)	110.62(12)	C(31)-P(1)-C(11)	111.57(13)	C(21)-
$\begin{array}{ccccccc} P(2)-C(1) & 100.77(13) & C(41)-P(2)-C(51) & 99.43(13) & C(4)-\\ P(2)-C(51) & 103.58(13) & C(2)-C(1)-P(1) & 112.99(19) & C(3)-\\ C(2)-C(1) & 111.7(2) & C(2)-C(3)-C(4) & 111.7(2) & C(3)-\\ C(4)-P(2) & 110.84(19) & C(12)-C(11)-P(1) & 114.3(2) & C(17)-\\ C(12)-C(13) & 118.7(2) & C(17)-C(12)-C(11) & 121.7(2) & C(13)-\\ C(14)-C(15) & 120.3(3) & C(14)-C(15)-C(16) & 119.4(3) & C(17)-\\ C(16)-C(15) & 120.3(3) & C(14)-C(15)-C(16) & 119.4(3) & C(17)-\\ C(16)-C(15) & 120.2(3) & C(16)-C(17)-C(12) & 120.5(3) & C(26)-\\ C(21)-C(22) & 119.7(2) & C(26)-C(21)-P(1) & 121.2(2) & C(22)-\\ C(23)-C(24) & 119.8(3) & C(23)-C(24)-C(23) & 120.4(3) & C(24)-\\ C(25)-C(26) & 120.1(3) & C(21)-C(26)-C(25) & 119.9(3) & C(36)-\\ C(31)-C(32) & 119.8(2) & C(36)-C(31)-P(1) & 119.9(2) & C(32)-\\ C(31)-C(32) & 119.8(2) & C(36)-C(31)-P(1) & 119.9(2) & C(32)-\\ C(31)-C(32) & 119.8(2) & C(36)-C(35) & 119.7(3) & C(44)-\\ C(35)-C(36) & 120.5(3) & C(31)-C(36)-C(35) & 119.7(3) & C(44)-\\ C(35)-C(36) & 120.5(3) & C(31)-C(36)-C(35) & 119.7(3) & C(42)-\\ C(41)-P(2) & 124.2(2) & C(43)-C(44)-P(4) & 119.5(3) & C(44)-\\ C(43)-C(42) & 120.4(3) & C(43)-C(44)-C(45) & 119.5(3) & C(46)-\\ C(41)-P(2) & 124.2(2) & C(43)-C(41) & 121.1(3) & C(44)-\\ C(43)-C(44) & 120.0(3) & C(45)-C(45) & 120.5(3) & C(52)-\\ C(51)-C(56) & 118.2(3) & C(52)-C(53) & 120.8(3) & C(54)-\\ C(53)-C(52) & 120.0(3) & C(53)-C(54)-C(55) & 120.0(3) & C(55)-\\ C(51)-P(2) & 116.7(2) & C(51)-C(52)-C(53) & 120.8(3) & C(54)-\\ C(53)-C(54) & 119.9(3) & C(55)-C(56)-C(51) & 121.1(3) & F(6)-\\ P(3)-F(3) & 91.25(15) & F(6)-P(3)-F(4) & 82.20(11) & F(6)-\\ P(3)-F(3) & 91.25(15) & F(6)-P(3)-F(4) & 90.20(14) & F(3)-\\ P(3)-F(4) & 178.55(15) & F(2)-P(3)-F(1) & 90.88(11) & F(5)-\\ P(3)-F(1) & 90.4(11) & F(3)-P(3)-F(1) & 90.88(11) & F(6)-\\ P(3)-F(3) & 90.9(11) & F(4)-P(3)-F(1) & 90.88(11) & F(6)-\\ P(3)-F(1) & 90.0 & H(1A)-C(1)-H(1B) & 109.0 & P(1)-\\ C(1)-H(1B) & 109.0 & H(1A)-C(1)-H(1B) & 109.0 & P(1)-\\ C(1)-H(1B) & 109.0 & H(1A)-C(1)-H(1B) & 109.3 & C(4)-\\ C(3)-H(2A) & 109.3 & C(1)-C(2)-H(2B) & 109.3 & C(4)-\\ C(3)-H(2B) & 107.9 & C$	P(1)-C(11)	107.47(13)	C(1)-P(1)-C(11)	108.53(13)	C(41)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	P(2)-C(4)	100 77(13)	C(41)-P(2)-C(51)	99 43(13)	C(4)-
$\begin{array}{ccccc} (2)-C(1) & 111.7(2) & C(2)-C(3)-C(4) & 111.7(2) & C(3)-C(4)-P(2) & 110.84(19) & C(12)-C(11)-P(1) & 114.3(2) & C(17)-C(12)-C(13) & 118.7(2) & C(17)-C(12)-C(11) & 121.7(2) & C(3)-C(12)-C(11) & 121.7(2) & C(3)-C(12)-C(11) & 121.7(2) & C(13)-C(12)-C(11) & 121.7(2) & C(13)-C(12)-C(11) & 120.9(3) & C(13)-C(12)-C(15) & 120.3(3) & C(14)-C(15)-C(16) & 119.4(3) & C(17)-C(12)-C(15) & 120.2(3) & C(16)-C(17)-C(12) & 120.2(3) & C(22)-C(21)-P(1) & 121.2(2) & C(22)-C(21)-P(1) & 121.2(2) & C(22)-C(21)-P(1) & 121.2(2) & C(22)-C(21)-P(1) & 121.2(2) & C(22)-C(23)-C(24) & 119.8(3) & C(25)-C(26) & 120.1(3) & C(21)-C(26)-C(25) & 119.9(3) & C(36)-C(35)-C(32) & 119.8(3) & C(34)-C(33)-C(31)-P(1) & 119.9(2) & C(32)-C(31)-P(1) & 120.3(2) & C(33)-C(32)-C(31) & 119.6(3) & C(34)-C(33)-C(32) & 120.1(3) & C(33)-C(34)-C(35) & 120.3(3) & C(34)-C(35)-C(36) & 120.5(3) & C(34)-C(35) & 119.7(3) & C(42)-C(41)-P(2) & 117.3(2) & C(46)-C(41)-P(2) & 117.3(2) & C(46)-C(41)-P(2) & 117.3(2) & C(46)-C(41)-P(2) & 124.2(2) & C(43)-C(44)-C(45) & 119.5(3) & C(42)-C(41)-P(2) & 125.1(2) & C(56)-C(51)-P(2) & 125.1(2) & C(56)-C(55)-C(54) & 119.9(3) & C(55)-C(56)-C(51) & 121.1(3) & F(6)-P(3)-F(3) & 90.9(11) & F(3)-P(3)-F(4) & 93.2(11) & F(6)-P(3)-F(4) & 90.20(14) & F(3)-P(3)-F(4) & 90.20(14) & F(3)-P(3)-F(4) & 90.20(14) & F(3)-P(3)-F(5) & 89.19(11) & F(4)-P(3)-F(1) & 90.99(11) & F(2)-P(3)-F(1) & 90.99(11) & F(3)-P(3)-F(1) & 90.99(11) & F(3)-P(3)-F(1) & 90.99(11) & F(3)-P(3)-F(1) & 90.99(11) & F(3)-P(3)-F$	P(2)-C(51)	103 58(13)	C(2)-C(1)-P(1)	112,99(19)	C(3)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(2) - C(1)	1117(2)	C(2)-C(3)-C(4)	1117(2)	C(3)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(4)-P(2)	110.84(19)	C(12)-C(11)-P(1)	114.7(2) 114.3(2)	C(17)-
$\begin{array}{ccccc} C(12)-C(11) & 119.6(2) & C(14)-C(13)-C(12) & 120.9(3) & C(13)-C(14)-C(15) & 120.3(3) & C(14)-C(15)-C(16) & 119.4(3) & C(17)-C(16)-C(15) & 120.2(3) & C(16)-C(17)-C(12) & 120.5(3) & C(26)-C(21)-P(1) & 119.0(2) & C(23)-C(21)-P(1) & 121.2(2) & C(22)-C(21)-P(1) & 119.0(2) & C(23)-C(22)-C(21) & 120.1(3) & C(22)-C(23)-C(24) & 119.8(3) & C(25)-C(24)-C(23) & 120.4(3) & C(24)-C(25)-C(26) & 120.1(3) & C(21)-C(26)-C(25) & 119.9(3) & C(36)-C(31)-P(1) & 119.9(2) & C(32)-C(31)-P(1) & 119.8(2) & C(36)-C(31)-P(1) & 119.9(2) & C(32)-C(31)-P(1) & 120.3(2) & C(33)-C(32)-C(31) & 119.6(3) & C(34)-C(35)-C(36) & 120.5(3) & C(31)-C(36)-C(35) & 119.7(3) & C(42)-C(41)-P(2) & 117.3(2) & C(46)-C(41)-P(2) & 117.3(2) & C(46)-C(41)-P(2) & 117.3(2) & C(46)-C(41)-P(2) & 117.3(2) & C(46)-C(41)-P(2) & 122.4(2) & C(43)-C(42)-C(41) & 121.1(3) & C(44)-C(45) & 119.5(3) & C(42)-C(44) & 120.0(3) & C(45)-C(46)-C(41) & 120.5(3) & C(52)-C(51)-P(2) & 116.7(2) & C(51)-C(52)-C(53) & 120.8(3) & C(54)-C(55)-C(54) & 119.9(3) & C(53)-C(54)-C(55) & 120.0(3) & C(55)-C(55) & 120.0(3) & C(56)-C(51)-P(2) & 116.7(2) & C(51)-C(52)-C(51) & 121.1(3) & F(6)-C(55)-C(54) & 119.9(3) & C(55)-C(55) & 120.0(3) & C(56)-C(51) & 121.1(3) & F(6)-P(3)-F(4) & 90.29(11) & F(3)-P(3)-F(4) & 90.29(11) & F(3)-P(3)-F(4) & 90.29(11) & F(3)-P(3)-F(5) & 90.01(13) & F(6)-P(3)-F(4) & 90.29(11) & F(6)-P(3)-F(4) & 90.29(11) & F(6)-P(3)-F(5) & 90.01(13) & F(6)-P(3)-F(4) & 90.99(11) & F(2)-P(3)-F(1) & 90.99(11) & F(2)-P(3)-F(1) & 89.61(10) & C(2)-C(1)+H(1B) & 109.0 & P(1)-C(1)+H(1A) & 109.0$	C(12)- $C(13)$	118 7(2)	C(12) - C(12) - C(11)	121.7(2)	C(13)-
$\begin{array}{ccccc} C(14)-C(15) & 120.3(3) & C(14)-C(15)-C(16) & 119.4(3) & C(17)-C(16)-C(15) & 120.2(3) & C(16)-C(17)-C(12) & 120.5(3) & C(26)-C(21)-C(22) & 119.7(2) & C(26)-C(21)-P(1) & 121.2(2) & C(22)-C(21) & 120.1(3) & C(22)-C(21) & 120.1(3) & C(22)-C(22)-C(21) & 120.1(3) & C(22)-C(22)-C(24) & 119.8(3) & C(25)-C(24)-C(23) & 120.4(3) & C(24)-C(25)-C(26) & 120.1(3) & C(21)-C(26)-C(25) & 119.9(3) & C(36)-C(31)-C(32) & 119.8(2) & C(36)-C(31)-P(1) & 119.9(2) & C(32)-C(31)-P(1) & 120.3(2) & C(33)-C(32)-C(31) & 119.6(3) & C(34)-C(35)-C(36) & 120.5(3) & C(31)-C(35) & 120.3(3) & C(34)-C(35)-C(36) & 120.5(3) & C(31)-C(35) & 120.3(3) & C(34)-C(35)-C(36) & 120.5(3) & C(31)-C(35) & 120.3(3) & C(42)-C(41)-P(2) & 117.3(2) & C(46)-C(41)-P(2) & 117.3(2) & C(46)-C(41)-C(46) & 118.5(3) & C(42)-C(41)-P(2) & 117.3(2) & C(46)-C(41)-C(46) & 118.5(3) & C(42)-C(41) & 121.1(3) & C(44)-C(45) & 119.5(3) & C(45)-C(44)-C(45) & 119.5(3) & C(45)-C(45)-C(44) & 120.0(3) & C(53)-C(54)-C(15) & 120.8(3) & C(55)-C(56) & 118.2(3) & C(52)-C(51)-P(2) & 125.1(2) & C(56)-C(51)-P(2) & 125.1(2) & C(56)-C(51)-P(2) & 125.1(2) & C(56)-C(51)-P(2) & 125.1(2) & C(56)-C(51)-P(2) & 125.1(3) & F(6)-C(51)-P(2) & 125.1(3) & F(6)-C(51)-P(2) & 125.1(3) & F(6)-C(51)-P(2) & 125.1(3) & F(6)-C(51)-P(2) & 120.8(3) & C(54)-C(55) & 120.0(3) & C(56)-C(51)-P(2) & 120.8(3) & C(54)-C(55)-C(54) & 119.9(3) & C(55)-C(56)-C(51) & 121.1(3) & F(6)-C(51)-F(2) & 90.96(11) & F(3)-P(3)-F(5) & 80.90(11) & F(3)-P(3)-F(1) & 89.90(11) & F(3)-P(3)-F(5) & 80.90(11) & F(3)-P(3)-F(5) & 80.90(11) & F(3)-P(3)-F(5) & 80.90(11) & F(3)-P(3)-F(1) & 89.90(11) & F(2)-P(3)-F(1) & 89.90(11) & F(2)-P(3)-F(1) & 89.90(11) & F(2)-P(3)-F(1) & 89.90(11) & F(2)-P(3)-F(1) & 89.90(11) & F(3)-P(3)-F(1) & 89$	C(12)- $C(11)$	119.6(2)	C(14)-C(12)-C(12)	120.9(3)	C(13)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C(12) \cdot C(11)$ C(14) - C(15)	120.3(3)	C(14)-C(15)-C(16)	1194(3)	C(17)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(16)-C(15)	120.3(3) 120.2(3)	C(16)-C(17)-C(12)	120 5(3)	C(26)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(21)- $C(22)$	120.2(3) 119 7(2)	C(26)-C(21)-P(1)	120.3(3) 121.2(2)	C(22)-
$\begin{array}{ccccc} C(23)-C(24) & 119.8(3) & C(25)-C(24)-C(23) & 120.4(3) & C(24)-C(25)-C(26) & 120.1(3) & C(21)-C(26)-C(25) & 119.9(3) & C(36)-C(31)-P(1) & 120.3(2) & C(36)-C(31)-P(1) & 119.9(2) & C(32)-C(31)-P(1) & 120.3(2) & C(33)-C(32)-C(31) & 119.6(3) & C(34)-C(35)-C(36) & 120.5(3) & C(31)-C(36)-C(35) & 120.3(3) & C(34)-C(35)-C(36) & 120.5(3) & C(31)-C(36)-C(35) & 119.7(3) & C(42)-C(41)-C(46) & 118.5(3) & C(42)-C(41)-P(2) & 117.3(2) & C(46)-C(41)-P(2) & 124.2(2) & C(43)-C(44)-C(45) & 119.5(3) & C(46)-C(41)-P(2) & 124.2(2) & C(43)-C(44)-C(45) & 119.5(3) & C(46)-C(41)-P(2) & 124.2(2) & C(43)-C(44)-C(45) & 119.5(3) & C(46)-C(41)-P(2) & 126.3(3) & C(52)-C(51)-P(2) & 126.3(3) & C(52)-C(51)-P(2) & 125.1(2) & C(56)-C(51)-P(2) & 116.7(2) & C(51)-C(52)-C(53) & 120.8(3) & C(54)-C(55)-C(54) & 119.9(3) & C(55)-C(56)-C(51) & 121.1(3) & F(6)-P(3)-F(2) & 91.79(11) & F(6)-P(3)-F(4) & 90.20(14) & F(3)-P(3)-F(2) & 91.79(11) & F(6)-P(3)-F(4) & 90.20(14) & F(3)-P(3)-F(2) & 91.79(11) & F(6)-P(3)-F(4) & 90.20(14) & F(3)-P(3)-F(5) & 89.19(11) & F(4)-P(3)-F(5) & 90.01(13) & F(6)-P(3)-F(1) & 90.24(11) & F(3)-P(3)-F(1) & 90.89(11) & F(2)-P(3)-F(1) & 90.89(11) & F(2)-P(3)-F(1) & 90.24(11) & F(3)-P(3)-F(1) & 90.89(11) & F(2)-P(3)-F(1) & 90.89(11)$	C(21) - P(1)	119.0(2)	C(23)-C(22)-C(21)	1201(2)	C(22)-
$\begin{array}{ccccc} C(25) - C(26) & (12) - C(26) - C(25) & (12) - C(26) - C(25) & (13) - C(25) & (13) - C(25) & (13) - C(32) & (13) - C(32) - C(31) - C(13) & (12) - C(26) - C(25) & (13) - 9(1) & (12) - 9(2) & (12) - 2(3) - C(3) & (13) - C(3) - C(3) - C(3) & (13) - C(3) - C(3) - C(3) - C(3) - C(3) & (13) - C(3) - C(3) - C(3) & (13) - C(3) - C(3) - C(3) & (13) - C(3) & (12) - C(3) - C(4) - C(4) - C(46) & (18) - (53) & (12) - C(43) - C(42) - C(41) - P(2) & (17) - 3(2) & C(46) - C(41) - P(2) & (12) - 2(3) & (12) - C(43) - C(42) - C(41) & (12) - 1(3) & C(44) - C(43) - C(42) & (12) - 0(3) & C(43) - C(44) - C(45) & (119) - 5(3) & C(46) - C(44) - C(42) & (12) - 0(3) & C(53) - C(44) - C(45) & (12) - 0(3) & C(56) - C(51) - P(2) & (15) - P(2) & (15) - P(2) & (12) - 0(3) & C(55) - C(54) & (12) - 0(3) & C(55) - C(54) & (12) - 0(3) & C(55) - C(56) - C(51) & (12) - 0(3) & C(56) - C(55) - C(54) & (13) - 9(3) - F(2) & 90 - 96(11) & F(3) - P(3) - F(3) & 91 - 25(15) & F(6) - P(3) - F(4) & 88 - 20(11) & F(6) - P(3) - F(3) & 91 - 25(15) & F(6) - P(3) - F(4) & 88 - 20(11) & F(6) - P(3) - F(4) & 88 - 20(11) & F(6) - P(3) - F(5) & 90 - 01(13) & F(6) - P(3) - F(5) & 91 - 91 - 91 - 178 - 55(15) & F(2) - P(3) - F(5) & 90 - 01(13) & F(6) - P(3) - F(5) & 91 - 91 - 178 - 178 - 178 - 178 - 178 - 178 - 178 - 178 - 178 - 17$	C(23)-C(24)	119.8(3)	C(25) - C(24) - C(23)	120.1(3) 120.4(3)	C(24)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(25) - C(26)	1201(3)	C(21)-C(26)-C(25)	119 9(3)	C(36)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(31)-C(32)	119 8(2)	C(36)-C(31)-P(1)	119.9(3) 119.9(2)	C(32)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(31)-P(1)	120.3(2)	C(33)-C(32)-C(31)	119.6(3)	C(32)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(33)-C(32)	120.3(2) 120.1(3)	C(33)-C(34)-C(35)	1203(3)	C(34)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(35) - C(36)	120.1(3) 120.5(3)	C(31)-C(36)-C(35)	119 7(3)	C(42)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(41)- $C(46)$	120.5(3) 118 5(3)	C(42)-C(41)-P(2)	117.7(3) 117.3(2)	C(46)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(41)-P(2)	1242(2)	C(43)-C(42)-C(41)	121 1(3)	C(44)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(43)-C(42)	1204(3)	C(43)-C(44)-C(45)	119 5(3)	C(46)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(45)- $C(44)$	120.1(3) 120.0(3)	C(45)-C(46)-C(41)	120.5(3)	C(52)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(51)- $C(56)$	120.0(3) 118 2(3)	C(52)-C(51)-P(2)	120.3(5) 125.1(2)	C(56)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(51)- $P(2)$	116.2(3) 116.7(2)	C(51) - C(52) - C(53)	120.1(2) 120.8(3)	C(50)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C(51) \Gamma(2)$ C(53) - C(52)	120.0(3)	C(53)- $C(54)$ - $C(55)$	120.0(3) 120.0(3)	C(54)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(55) - C(54)	120.0(3) 119 9(3)	C(55) - C(56) - C(51)	120.0(3) 121 1(3)	E(6)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	P(3)-F(3)	91 25(15)	F(6)-P(3)-F(2)	90.96(11)	F(3)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	P(3)-F(2)	91.29(13)	F(6)-P(3)-F(4)	90.20(14)	F(3)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	P(3)-F(4)	178 55(15)	F(2)-P(3)-F(4)	88 20(11)	F(6)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	P(3)-F(5)	170.35(13) 179.75(14)	F(3)-P(3)-F(5)	88 54(13)	$F(2)_{-}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	P(3)-F(5)	89 19(11)	F(4)-P(3)-F(5)	90.01(13)	F(6)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	P(3)-F(1)	90.24(11)	F(3)-P(3)-F(1)	89.09(11)	$F(2)_{-}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	P(3)-F(1)	$178\ 49(11)$	F(4)-P(3)-F(1)	90.89(11)	F(5)-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	P(3)-F(1)	89 61(10)	C(2)-C(1)-H(1A)	109.0	$P(1)_{-}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C(1)-H(1\Delta)$	109.01(10)	C(2) - C(1) - H(1R)	109.0	$P(1)_{-}$
C(1) H(H2) 107.0 107.0 $C(3)$ $C(2)$ -H(2A) 109.3 $C(1)$ -C(2)-H(2A) 109.3 $C(3)$ - $C(2)$ -H(2B) 109.3 $C(1)$ -C(2)-H(2B) 109.3 H(2A)- $C(2)$ -H(2B) 107.9 $C(2)$ -C(3)-H(3A) 109.3 $C(4)$ - $C(3)$ -H(3A) 109.3 $C(2)$ -C(3)-H(3B) 109.3 $C(4)$ - $C(3)$ -H(3B) 109.3 $H(3A)$ -C(3)-H(3B) 107.9 $C(3)$ - $C(4)$ -H(4A) 109.5 $P(2)$ -C(4)-H(4A) 109.5 $C(3)$ -	C(1)-H(1R)	109.0	H(1A)-C(1)-H(1B)	107.8	C(3)-
C(2) - H(2R) 109.3 $C(1) - C(2) - H(2R)$ 109.3 $C(3) - H(2R)$ $C(2) - H(2B)$ 109.3 $C(1) - C(2) - H(2B)$ 109.3 $H(2A) - C(2) - H(2B)$ $C(2) - H(2B)$ 107.9 $C(2) - C(3) - H(3A)$ 109.3 $C(4) - C(3) - H(3B)$ $C(3) - H(3B)$ 109.3 $H(3A) - C(3) - H(3B)$ 109.3 $C(4) - C(3) - H(3B)$ $C(4) - H(4A)$ 109.5 $P(2) - C(4) - H(4A)$ 109.5 $C(3) - C(3) - H(3B)$	C(2) - H(2A)	109.0	C(1)-C(2)-H(2A)	109.3	C(3)
C(2)-H(2B) 109.3 $C(1)$ - $C(2)$ -H(2D) 109.3 $H(2A)$ - $C(2)$ -H(2B) 107.9 $C(2)$ - $C(3)$ -H(3A) 109.3 $C(4)$ - $C(3)$ -H(3A) 109.3 $C(2)$ - $C(3)$ -H(3B) 109.3 $C(4)$ - $C(3)$ -H(3B) 109.3 $H(3A)$ - $C(3)$ -H(3B) 107.9 $C(3)$ - $C(4)$ -H(4A) 109.5 $P(2)$ - $C(4)$ -H(4A) 109.5 $C(3)$ -	C(2) - H(2R)	109.3	C(1)-C(2)-H(2R)	109.3	$H(2\Delta)_{-}$
C(2) - C(3) - H(2B) 107.5 $C(4) - C(4) - C(3) - H(3B)$ 109.3 $C(4) - C(4) - C(3) - H(3B)$ $C(3) - H(3B)$ 109.3 $H(3A) - C(3) - H(3B)$ 107.9 $C(3) - C(4) - H(4A)$ $C(4) - H(4A)$ 109.5 $P(2) - C(4) - H(4A)$ 109.5 $C(3) - C(3) -$	C(2) - H(2R)	107.9	$C(2) - C(3) - H(3\Delta)$	109.3	$C(4)_{-}$
C(3) $H(3H)$ 107.5 $C(2)$ - $C(3)$ - $H(3B)$ 107.5 $C(4)$ - $C(3)$ - $H(3B)$ 109.5 $H(3A)$ - $C(3)$ - $H(3B)$ 107.9 $C(3)$ - $C(4)$ - $H(4A)$ 109.5 $P(2)$ - $C(4)$ - $H(4A)$ 109.5 $C(3)$ -	C(2) H(2D) C(3)-H(3A)	109.3	C(2) = C(3) - H(3R)	109.3	$C(4)_{-}$
C(4)-H(4A) 109.5 $P(2)-C(4)-H(4A)$ 109.5 $C(3)-$	C(3)-H(3R)	109.3	H(3A)-C(3)-H(3B)	107.9	$C(3)_{-}$
	C(4)-H(4A)	109.5	P(2)-C(4)-H(4A)	109.5	C(3)

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C(4)-H(4B)	109.5	P(2)-C(4)-H(4B)	109.5	H(4A)-
C(4)-H(4B)	108.1	C(12)-C(11)-H(11A)	108.7	P(1)-
C(11)-H(11A)	108.7	C(12)-C(11)-H(11B)	108.7	P(1)-
С(11)-Н(11В)	108.7	H(11A)-C(11)-H(11B)	107.6	C(14)-
С(13)-Н(13А)	119.6	C(12)-C(13)-H(13A)	119.6	C(13)-
C(14)-H(14A)	119.8	C(15)-C(14)-H(14A)	119.8	C(14)-
C(15)-H(15A)	120.3	C(16)-C(15)-H(15A)	120.3	C(17)-
C(16)-H(16A)	119.9	C(15)-C(16)-H(16A)	119.9	C(16)-
C(17)-H(17A)	119.8	C(12)-C(17)-H(17A)	119.8	C(23)-
C(22)-H(22A)	119.9	C(21)-C(22)-H(22A)	119.9	C(22)-
C(23)-H(23A)	120.1	C(24)-C(23)-H(23A)	120.1	C(25)-
C(24)-H(24A)	119.8	C(23)-C(24)-H(24A)	119.8	C(24)-
C(25)-H(25A)	120.0	C(26)-C(25)-H(25A)	120.0	C(21)-
C(26)-H(26A)	120.1	C(25)-C(26)-H(26A)	120.1	C(33)-
C(32)-H(32A)	120.2	C(31)-C(32)-H(32A)	120.2	C(34)-
C(33)-H(33A)	120.0	C(32)-C(33)-H(33A)	120.0	C(33)-
C(34)-H(34A)	119.8	C(35)-C(34)-H(34A)	119.8	C(34)-
C(35)-H(35A)	119.8	C(36)-C(35)-H(35A)	119.8	C(31)-
C(36)-H(36A)	120.1	C(35)-C(36)-H(36A)	120.1	C(43)-
C(42)-H(42A)	119.5	C(41)-C(42)-H(42A)	119.5	C(44)-
C(43)-H(43A)	119.8	C(42)-C(43)-H(43A)	119.8	C(43)-
C(44)-H(44A)	120.3	C(45)-C(44)-H(44A)	120.3	C(46)-
C(45)-H(45A)	120.0	C(44)-C(45)-H(45A)	120.0	C(45)-
C(46)-H(46A)	119.7	C(41)-C(46)-H(46A)	119.7	C(51)-
C(52)-H(52A)	119.6	C(53)-C(52)-H(52A)	119.6	C(54)-
C(53)-H(53A)	120.0	C(52)-C(53)-H(53A)	120.0	C(53)-
C(54)-H(54A)	120.0	C(55)-C(54)-H(54A)	120.0	C(56)-
C(55)-H(55A)	120.0	C(54)-C(55)-H(55A)	120.0	C(55)-
C(56)-H(56A)	119.5	C(51)-C(56)-H(56A)	119.5	

Table 6. Torsion angles [°].

atom-atom-atom-atom	angle	atom-atom-atom-atom	angle	
C(31)-P(1)-C(1)-C(2)	-160.38(19)	C(21)-P(1)-C(1)-C(2)	-39.7(2)	C(11)-
P(1)-C(1)-C(2)	78.0(2)	P(1)-C(1)-C(2)-C(3)	-163.0(2)	C(1)-
C(2)-C(3)-C(4)	-167.2(2)	C(2)-C(3)-C(4)-P(2)	-167.0(2)	C(41)-
P(2)-C(4)-C(3)	-64.4(2)	C(51)-P(2)-C(4)-C(3)	-167.0(2)	C(31)-
P(1)-C(11)-C(12)	-68.1(2)	C(21)-P(1)-C(11)-C(12)	171.52(19)	C(1)-
P(1)-C(11)-C(12)	51.9(2)	P(1)-C(11)-C(12)-C(17)	84.8(3)	P(1)-
C(11)-C(12)-C(13)	-97.4(3)	C(17)-C(12)-C(13)-C(14)	0.6(4)	C(11)-
C(12)-C(13)-C(14)	-177.3(3)	C(12)-C(13)-C(14)-C(15)	0.2(5)	C(13)-
C(14)-C(15)-C(16)	-0.9(5)	C(14)-C(15)-C(16)-C(17)	0.8(5)	C(15)-
C(16)-C(17)-C(12)	-0.1(4)	C(13)-C(12)-C(17)-C(16)	-0.6(4)	C(11)-
C(12)-C(17)-C(16)	177.2(3)	C(31)-P(1)-C(21)-C(26)	-130.1(2)	C(1)-
P(1)-C(21)-C(26)	109.7(2)	C(11)-P(1)-C(21)-C(26)	-8.6(3)	C(31)-
P(1)-C(21)-C(22)	53.0(3)	C(1)-P(1)-C(21)-C(22)	-67.2(2)	C(11)-
P(1)-C(21)-C(22)	174.5(2)	C(26)-C(21)-C(22)-C(23)	-0.5(4)	P(1)-
C(21)-C(22)-C(23)	176.5(2)	C(21)-C(22)-C(23)-C(24)	0.3(4)	C(22)-
C(23)-C(24)-C(25)	-0.3(4)	C(23)-C(24)-C(25)-C(26)	0.4(4)	C(22)-
C(21)-C(26)-C(25)	0.6(4)	P(1)-C(21)-C(26)-C(25)	-176.3(2)	C(24)-
C(25)-C(26)-C(21)	-0.5(4)	C(21)-P(1)-C(31)-C(36)	38.5(3)	C(1)-
P(1)-C(31)-C(36)	159.7(2)	C(11)-P(1)-C(31)-C(36)	-80.6(2)	C(21)-
P(1)-C(31)-C(32)	-141.9(2)	C(1)-P(1)-C(31)-C(32)	-20.7(3)	C(11)-
P(1)-C(31)-C(32)	99.1(2)	C(36)-C(31)-C(32)-C(33)	0.3(4)	P(1)-
C(31)-C(32)-C(33)	-179.3(2)	C(31)-C(32)-C(33)-C(34)	0.6(4)	C(32)-
C(33)-C(34)-C(35)	-0.5(4)	C(33)-C(34)-C(35)-C(36)	-0.5(5)	C(32)-
C(31)-C(36)-C(35)	-1.3(4)	P(1)-C(31)-C(36)-C(35)	178.3(2)	C(34)-
C(35)-C(36)-C(31)	1.4(5)	C(4)-P(2)-C(41)-C(42)	129.4(2)	C(51)-
P(2)-C(41)-C(42)	-124.7(2)	C(4)-P(2)-C(41)-C(46)	-50.8(3)	C(51)-
P(2)-C(41)-C(46)	55.1(3)	C(46)-C(41)-C(42)-C(43)	-0.6(4)	P(2)-
C(41)-C(42)-C(43)	179.2(2)	C(41)-C(42)-C(43)-C(44)	0.3(5)	C(42)-
C(43)-C(44)-C(45)	0.1(5)	C(43)-C(44)-C(45)-C(46)	-0.3(5)	C(44)-
C(45)-C(46)-C(41)	0.0(4)	C(42)-C(41)-C(46)-C(45)	0.5(4)	P(2)-
C(41)-C(46)-C(45)	-179.3(2)	C(41)-P(2)-C(51)-C(52)	-97.7(3)	C(4)-
P(2)-C(51)-C(52)	5.9(3)	C(41)-P(2)-C(51)-C(56)	83.2(2)	C(4)-
P(2)-C(51)-C(56)	-173.3(2)	C(56)-C(51)-C(52)-C(53)	-0.7(4)	P(2)-
C(51)-C(52)-C(53)	-179.8(2)	C(51)-C(52)-C(53)-C(54)	0.6(4)	C(52)-
C(53)-C(54)-C(55)	-0.8(4)	C(53)-C(54)-C(55)-C(56)	1.0(4)	C(54)-
C(55)-C(56)-C(51)	-1.1(4)	C(52)-C(51)-C(56)-C(55)	1.0(4)	P(2)-
C(51)-C(56)-C(55)	-179.8(2)			