ORGANOMETALLICS
Organometallics, 1996, 15(10), 2465-2468, DOI:10.1021/om9600396

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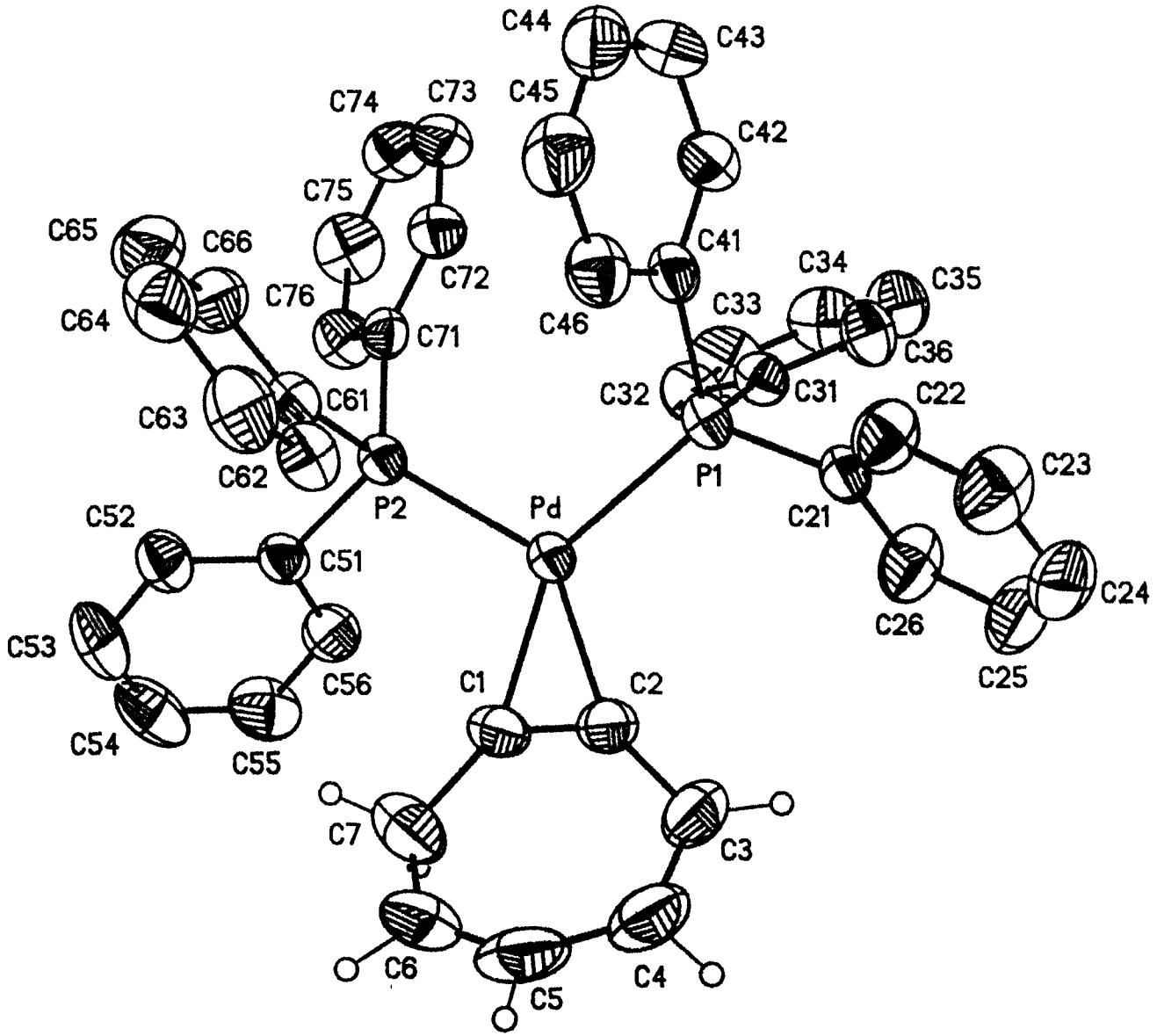

Figure 1. Molecular structure of **4**, with 40% probability ellipsoids, showing the atom numbering scheme.

L2468-2

Supplementary Table 1: Fractional coordinates and equivalent isotropic[a] thermal parameters ($Å^2$) for the non-H atoms of complex 4.

Atom	x	y	z	U
Pd	0.12630(2)	0.09004(2)	0.19200(2)	0.04291(11)
P1	0.24607(8)	0.02319(6)	0.30121(6)	0.0451(3)
P2	0.21141(7)	0.16371(6)	0.11518(6)	0.0448(3)
C1	-0.0255(3)	0.1179(3)	0.1373(3)	0.060(2)
C2	-0.0191(3)	0.0747(2)	0.2016(3)	0.055(2)
C3	-0.0905(4)	0.0506(3)	0.2467(4)	0.081(2)
C4	-0.1759(4)	0.0957(3)	0.2376(4)	0.091(3)
C5	-0.2091(4)	0.1597(4)	0.1830(5)	0.098(3)
C6	-0.1854(4)	0.1858(4)	0.1118(5)	0.099(3)
C7	-0.1096(4)	0.1598(4)	0.0750(4)	0.105(3)
C21	0.1960(3)	-0.0143(2)	0.3870(2)	0.0478(14)
C22	0.2150(4)	0.0189(3)	0.4672(3)	0.068(2)
C23	0.1690(4)	-0.0080(4)	0.5264(3)	0.090(3)
C24	0.1037(4)	-0.0694(3)	0.5073(3)	0.086(2)
C25	0.0826(4)	-0.1043(3)	0.4278(3)	0.088(3)
C26	0.1277(4)	-0.0753(3)	0.3679(3)	0.080(2)
C31	0.3020(3)	-0.0637(2)	0.2670(3)	0.0496(14)
C32	0.3001(3)	-0.0690(3)	0.1813(3)	0.066(2)
C33	0.3444(4)	-0.1329(4)	0.1544(4)	0.089(3)
C34	0.3885(4)	-0.1902(3)	0.2114(4)	0.090(3)
C35	0.3903(4)	-0.1854(3)	0.2962(4)	0.079(2)
C36	0.3473(3)	-0.1226(3)	0.3242(3)	0.065(2)
C41	0.3590(3)	0.0796(2)	0.3624(2)	0.0488(14)
C42	0.4600(3)	0.0529(3)	0.3890(3)	0.070(2)
C43	0.5414(4)	0.1021(4)	0.4285(3)	0.088(2)
C44	0.5227(5)	0.1777(3)	0.4450(3)	0.093(3)
C45	0.4245(5)	0.2042(3)	0.4204(3)	0.086(2)
C46	0.3428(4)	0.1563(3)	0.3793(3)	0.066(2)
C51	0.1274(3)	0.1844(2)	0.0047(2)	0.0490(14)
C52	0.1196(3)	0.2576(3)	-0.0329(3)	0.063(2)
C53	0.0498(4)	0.2700(3)	-0.1149(3)	0.082(2)
C54	-0.0097(4)	0.2103(4)	-0.1599(3)	0.090(2)
C55	-0.0022(4)	0.1379(4)	-0.1239(3)	0.082(2)
C56	0.0670(3)	0.1247(3)	-0.0410(3)	0.065(2)
C61	0.2441(3)	0.2593(2)	0.1649(2)	0.0480(14)
C62	0.1863(3)	0.2874(3)	0.2155(3)	0.062(2)
C63	0.2097(4)	0.3582(3)	0.2573(3)	0.080(2)
C64	0.2908(4)	0.4007(3)	0.2504(4)	0.082(2)
C65	0.3483(4)	0.3751(3)	0.1998(4)	0.084(2)
C66	0.3247(3)	0.3049(3)	0.1567(3)	0.070(2)
C71	0.3339(3)	0.1340(2)	0.0984(3)	0.0479(15)
C72	0.4202(3)	0.1266(3)	0.1708(3)	0.061(2)
C73	0.5144(3)	0.1038(3)	0.1621(3)	0.071(2)
C74	0.5243(4)	0.0882(3)	0.0825(4)	0.078(2)

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Supplementary Table 1 Continued.

C75	0.4385(4)	0.0932(3)	0.0094(4)	0.082(2)
C76	0.3432(3)	0.1163(3)	0.0176(3)	0.065(2)

[a]For anisotropic atoms, the U value is U_{eq}, calculated as $U_{eq} = 1/3\ \Sigma_i\Sigma_j\ U_{ij}\ a_i^*\ a_j^*\ A_{ij}$ where A_{ij} is the dot product of the i^{th} and j^{th} direct space unit cell vectors.

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Supplementary Table 2: Bond Lengths (Å) and Angles (°) for the non-H atoms of complex **4**.

1	2	3	1-2	1-2-3
P1	Pd	P2	2.3049(10)	109.53(4)
P1	Pd	C1		146.31(14)
P2	Pd	C1	2.3131(12)	103.99(14)
P2	Pd	C2		139.74(12)
C1	Pd	C2	2.031(4)	36.0(2)
C2	Pd	P1	2.039(4)	110.30(12)
C21	P1	C31	1.834(4)	102.7(2)
C21	P1	C41		102.8(2)
C21	P1	Pd		114.60(12)
C31	P1	C41	1.838(4)	104.0(2)
C31	P1	Pd		115.91(12)
C41	P1	Pd	1.826(4)	115.05(12)
C51	P2	C61	1.832(3)	104.2(2)
C51	P2	C71		103.4(2)
C51	P2	Pd		111.40(14)
C61	P2	C71	1.827(4)	102.0(2)
C61	P2	Pd		110.75(14)
C71	P2	Pd	1.833(4)	123.18(13)
C2	C1	C7	1.258(6)	134.7(5)
C2	C1	Pd		72.3(2)
C7	C1	Pd	1.458(7)	152.8(4)
C3	C2	Pd	1.438(8)	153.0(3)
C3	C2	C1		134.4(4)
Pd	C2	C1		71.6(3)
C4	C3	C2	1.364(8)	117.4(5)
C5	C4	C3	1.398(9)	128.1(6)
C6	C5	C4	1.360(11)	132.8(6)
C7	C6	C5	1.407(10)	130.0(6)
C1	C7	C6		112.5(5)
C22	C21	C26	1.365(6)	116.8(4)
C22	C21	P1		124.2(3)
C26	C21	P1	1.372(6)	118.7(3)
C23	C22	C21	1.370(8)	121.7(4)
C24	C23	C22	1.354(8)	120.7(5)
C25	C24	C23	1.365(8)	119.6(6)
C26	C25	C24	1.385(8)	119.0(5)
C21	C26	C25		122.1(4)
C32	C31	C36	1.377(6)	119.3(4)
C32	C31	P1		118.2(3)
C36	C31	P1	1.382(6)	122.6(3)
C33	C32	C31	1.387(8)	119.4(4)
C34	C33	C32	1.358(8)	120.6(6)
C35	C34	C33	1.363(10)	120.3(6)
C36	C35	C34	1.369(7)	120.0(5)
C31	C36	C35		120.5(5)

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Supplementary Table 2 continued.

C42	C41	C46	1.382(6)	117.3(4)
C42	C41	P1		125.2(3)
C46	C41	P1	1.381(6)	117.4(3)
C43	C42	C41	1.382(7)	120.8(5)
C44	C43	C42	1.369(9)	120.3(5)
C45	C44	C43	1.346(9)	119.5(5)
C46	C45	C44	1.377(7)	120.9(5)
C41	C46	C45		121.2(5)
C52	C51	C56	1.389(6)	119.4(3)
C52	C51	P2		122.9(3)
C56	C51	P2	1.380(6)	117.6(3)
C53	C52	C51	1.387(6)	119.7(4)
C54	C53	C52	1.370(8)	120.5(5)
C55	C54	C53	1.369(9)	120.4(4)
C56	C55	C54	1.396(6)	119.8(5)
C51	C56	C55		120.2(5)
C62	C61	C66	1.380(7)	117.5(4)
C62	C61	P2		118.1(3)
C66	C61	P2	1.384(6)	124.3(3)
C63	C62	C61	1.384(7)	120.8(5)
C64	C63	C62	1.353(8)	120.5(6)
C65	C64	C63	1.361(9)	120.1(5)
C66	C65	C64	1.384(7)	119.9(5)
C61	C66	C65		121.2(5)
C72	C71	C76	1.382(5)	118.6(4)
C72	C71	P2		118.1(3)
C76	C71	P2	1.381(7)	123.3(3)
C73	C72	C71	1.383(7)	120.6(5)
C74	C73	C72	1.357(9)	120.8(4)
C75	C74	C73	1.382(7)	119.6(5)
C76	C75	C74	1.395(8)	119.8(5)
C71	C76	C75		120.5(4)

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Supplementary Table 3: Anisotropic thermal parameters[a] for the non-H atoms of complex **4**.

Atom	U11	U22	U33	U12	U13	U23
Pd	0.0406(2)	0.0475(2)	0.0389(2)	0.00182(14)	0.00956(11)	0.00705(14)
P1	0.0485(6)	0.0457(6)	0.0381(5)	0.0052(5)	0.0089(4)	0.0039(4)
P2	0.0410(5)	0.0501(6)	0.0419(5)	0.0024(4)	0.0107(4)	0.0080(5)
C1	0.040(2)	0.076(3)	0.062(3)	0.007(2)	0.010(2)	0.008(2)
C2	0.044(2)	0.056(3)	0.063(3)	-0.002(2)	0.015(2)	-0.001(2)
C3	0.069(3)	0.076(3)	0.110(4)	-0.004(3)	0.047(3)	0.017(3)
C4	0.069(3)	0.091(4)	0.130(5)	-0.011(3)	0.057(3)	0.001(4)
C5	0.046(3)	0.098(5)	0.158(6)	-0.001(3)	0.044(4)	-0.018(4)
C6	0.052(3)	0.100(4)	0.137(5)	0.025(3)	0.018(3)	0.019(4)
C7	0.077(4)	0.128(5)	0.101(4)	0.028(4)	0.012(3)	0.040(4)
C21	0.049(2)	0.050(2)	0.042(2)	0.005(2)	0.010(2)	0.009(2)
C22	0.077(3)	0.072(3)	0.059(3)	-0.010(2)	0.029(2)	-0.006(2)
C23	0.108(4)	0.115(5)	0.056(3)	-0.021(4)	0.040(3)	-0.011(3)
C24	0.089(4)	0.114(5)	0.068(3)	-0.008(3)	0.044(3)	0.013(3)
C25	0.099(4)	0.088(4)	0.079(4)	-0.032(3)	0.032(3)	0.009(3)
C26	0.103(4)	0.085(4)	0.052(3)	-0.032(3)	0.027(3)	-0.009(2)
C31	0.050(2)	0.045(2)	0.051(2)	0.003(2)	0.011(2)	-0.003(2)
C32	0.071(3)	0.068(3)	0.057(3)	0.005(2)	0.016(2)	-0.005(2)
C33	0.096(4)	0.102(4)	0.074(3)	0.017(3)	0.032(3)	-0.022(3)
C34	0.082(4)	0.069(3)	0.117(5)	0.016(3)	0.028(3)	-0.026(3)
C35	0.079(3)	0.053(3)	0.102(4)	0.013(2)	0.024(3)	0.005(3)
C36	0.076(3)	0.053(3)	0.066(3)	0.013(2)	0.020(2)	0.005(2)
C41	0.057(2)	0.048(2)	0.038(2)	0.001(2)	0.009(2)	0.005(2)
C42	0.061(3)	0.063(3)	0.073(3)	0.001(2)	0.002(2)	0.011(2)
C43	0.058(3)	0.106(5)	0.078(3)	-0.011(3)	-0.010(3)	0.017(3)
C44	0.103(5)	0.086(4)	0.067(3)	-0.038(4)	-0.007(3)	0.011(3)
C45	0.115(5)	0.059(3)	0.073(3)	-0.021(3)	0.014(3)	-0.009(3)
C46	0.078(3)	0.060(3)	0.056(3)	0.000(2)	0.017(2)	-0.001(2)
C51	0.044(2)	0.061(3)	0.042(2)	0.006(2)	0.014(2)	0.009(2)
C52	0.066(3)	0.069(3)	0.051(2)	0.010(2)	0.016(2)	0.011(2)
C53	0.107(4)	0.085(4)	0.051(3)	0.035(3)	0.020(3)	0.022(3)
C54	0.089(4)	0.123(5)	0.045(3)	0.034(4)	0.001(3)	0.008(3)
C55	0.078(3)	0.108(4)	0.051(3)	-0.002(3)	0.004(2)	-0.009(3)
C56	0.064(3)	0.075(3)	0.053(3)	-0.005(2)	0.011(2)	0.004(2)
C61	0.044(2)	0.049(2)	0.047(2)	0.008(2)	0.008(2)	0.007(2)
C62	0.065(3)	0.059(3)	0.061(3)	0.010(2)	0.017(2)	0.006(2)
C63	0.096(4)	0.072(4)	0.073(3)	0.017(3)	0.026(3)	0.000(3)
C64	0.088(4)	0.051(3)	0.091(4)	0.010(3)	0.007(3)	-0.009(3)
C65	0.066(3)	0.056(3)	0.121(5)	-0.006(3)	0.017(3)	-0.004(3)
C66	0.062(3)	0.055(3)	0.095(4)	0.002(2)	0.026(3)	-0.001(3)
C71	0.047(2)	0.040(2)	0.059(2)	0.003(2)	0.020(2)	0.007(2)
C72	0.048(2)	0.070(3)	0.065(3)	0.001(2)	0.018(2)	0.008(2)
C73	0.050(3)	0.070(3)	0.088(4)	0.007(2)	0.014(2)	0.008(3)
C74	0.063(3)	0.067(3)	0.111(4)	0.011(3)	0.038(3)	-0.007(3)
C75	0.090(4)	0.082(4)	0.085(4)	0.017(3)	0.044(3)	-0.015(3)

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Supplementary Table 3 continued.

C76	0.066(3)	0.065(3)	0.064(3)	0.010(2)	0.022(2)	-0.001(2)

[a] Uij are the mean-square amplitudes of vibration in $Å^2$ from the general temperature factor expression

$\exp[-2\pi^2(h^2a^{*2}U11 + k^2b^{*2}U22 + l^2c^{*2}U33 + 2hka^*b^*U12 + 2hla^*c^*U13 + 2klb^*c^*U23)]$

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Suppelementary Table 4: Fractional coordinates and isotropic thermal parameters ($Å^2$) for the H atoms of complex **4**.

Atom	x	y	z	U
H3	-0.07924	0.00446	0.28171	0.08
H4	-0.21898	0.08149	0.27267	0.08
H5	-0.25772	0.19213	0.19939	0.08
H6	-0.22659	0.22856	0.08212	0.08
H7a	-0.14213	0.12522	0.02785	0.08
H7b	-0.082	0.20372	0.05298	0.08
H22	0.2622	0.06181	0.48226	0.08
H23	0.1845	0.0165	0.58242	0.08
H24	0.07189	-0.08763	0.5493	0.08
H25	0.03696	-0.14825	0.41371	0.08
H26	0.11143	-0.09886	0.31136	0.08
H32	0.26893	-0.02886	0.14048	0.08
H33	0.34414	-0.13686	0.0949	0.08
H34	0.41894	-0.2344	0.19238	0.08
H35	0.42125	-0.22601	0.33645	0.08
H36	0.34891	-0.11945	0.38402	0.08
H42	0.47421	-0.00044	0.37984	0.08
H43	0.61145	0.08324	0.44495	0.08
H44	0.57932	0.21128	0.47365	0.08
H45	0.41129	0.25725	0.43172	0.08
H46	0.27359	0.17678	0.3621	0.08
H52	0.16261	0.29912	-0.00225	0.08
H53	0.04366	0.32075	-0.14054	0.08
H54	-0.05728	0.21969	-0.21684	0.08
H55	-0.04484	0.0965	-0.15546	0.08
H56	0.07254	0.07379	-0.01576	0.08
H62	0.1289	0.25817	0.22216	0.08
H63	0.16935	0.37783	0.29234	0.08
H64	0.30819	0.4492	0.28053	0.08
H65	0.40534	0.40509	0.19368	0.08
H66	0.36433	0.28719	0.12023	0.08
H72	0.41492	0.13763	0.22762	0.08
H73	0.57357	0.09882	0.21312	0.08
H74	0.59059	0.0733	0.0776	0.08
H75	0.44467	0.0812	-0.04696	0.08
H76	0.2837	0.11998	-0.03326	0.08

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Supplementary Table 5: Bond Lengths (Å) and Angles (°) of the H atoms of complex **4**.

1	2	3	1-2	1-2-3
H3	C3	C4	0.960(5)	120.8(6)
H3	C3	C2		121.7(5)
H4	C4	C5	0.960(7)	115.9(6)
H4	C4	C3		116.0(6)
H5	C5	C6	0.960(7)	113.5(6)
H5	C5	C4		113.7(7)
H6	C6	C7	0.960(6)	115.0(7)
H6	C6	C5		115.0(6)
H7a	C7	H7b	0.960(6)	109.5(6)
H7a	C7	C1		108.1(6)
H7a	C7	C6		108.3(5)
H7b	C7	C1	0.960(7)	109.6(5)
H7b	C7	C6		108.7(6)
H22	C22	C23	0.960(5)	119.6(5)
H22	C22	C21		118.7(5)
H23	C23	C24	0.960(5)	119.8(6)
H23	C23	C22		119.5(6)
H24	C24	C25	0.960(6)	120.6(6)
H24	C24	C23		119.9(5)
H25	C25	C26	0.960(5)	120.7(5)
H25	C25	C24		120.3(6)
H26	C26	C21	0.960(5)	118.7(5)
H26	C26	C25		119.1(5)
H32	C32	C33	0.960(4)	120.0(5)
H32	C32	C31		120.7(5)
H33	C33	C34	0.960(6)	119.4(6)
H33	C33	C32		120.0(5)
H34	C34	C35	0.960(6)	119.5(6)
H34	C34	C33		120.2(7)
H35	C35	C36	0.960(5)	119.8(6)
H35	C35	C34		120.2(5)
H36	C36	C31	0.960(5)	119.8(5)
H36	C36	C35		119.7(5)
H42	C42	C43	0.960(5)	119.4(5)
H42	C42	C41		119.8(4)
H43	C43	C44	0.960(5)	119.7(5)
H43	C43	C42		120.0(6)
H44	C44	C45	0.960(6)	120.6(6)
H44	C44	C43		120.0(6)
H45	C45	C46	0.960(6)	119.6(6)
H45	C45	C44		119.5(6)
H46	C46	C41	0.960(5)	119.7(4)
H46	C46	C45		119.2(5)
H52	C52	C53	0.960(4)	120.3(5)
H52	C52	C51		120.0(4)
H53	C53	C54	0.960(6)	119.8(4)

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Supplementary Table 5 continued.

H53	C53	C52		119.7(5)
H54	C54	C55	0.960(5)	120.0(6)
H54	C54	C53		119.6(6)
H55	C55	C56	0.960(5)	120.3(6)
H55	C55	C54		119.9(4)
H56	C56	C51	0.960(5)	120.0(4)
H56	C56	C55		119.8(5)
H62	C62	C63	0.960(5)	118.7(5)
H62	C62	C61		120.5(4)
H63	C63	C64	0.960(6)	118.7(5)
H63	C63	C62		120.7(6)
H64	C64	C65	0.960(5)	119.3(6)
H64	C64	C63		120.6(6)
H65	C65	C66	0.960(6)	119.3(6)
H65	C65	C64		120.9(5)
H66	C66	C61	0.960(6)	118.8(4)
H66	C66	C65		120.0(5)
H72	C72	C73	0.960(5)	119.6(4)
H72	C72	C71		119.8(4)
H73	C73	C74	0.960(4)	119.6(5)
H73	C73	C72		119.5(5)
H74	C74	C75	0.960(6)	120.6(6)
H74	C74	C73		119.8(5)
H75	C75	C76	0.960(6)	120.1(5)
H75	C75	C74		120.0(6)
H76	C76	C71	0.960(4)	119.7(5)
H76	C76	C75		119.8(5)