Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

trans-(2-Methylthiobenzoato-*O*)-phenylbis(triphenylphosphine)-palladium(II), two conformational isomers

Gert J. Kruger,[a]* Catharine Thompson,[a] Wolfgang H. Meyer,[b] Robert Brüll[b] and Helgard G. Raubenheimer[b]

[a]Department of Chemistry and Biochemistry, Rand Afrikaans University, PO Box 524, Auckland Park, Johannesburg 2006, South Africa, and [b]Department of Chemistry, Stellenbosch University, Private Bag X1, Matieland 7600, South Africa
Correspondence e-mail: gjk@na.rau.ac.za

Received 19 July 1999
Accepted 29 November 1999

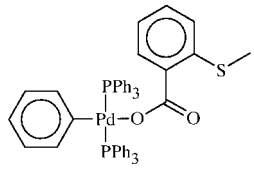
The title compound, *trans*-[Pd(C_6H_5)($C_8H_7O_2S$)($C_{18}H_{15}P$)$_2$], crystallizes in two modifications differing only in the orientation of the 2-methylthiobenzoato ligand. In both cases, this ligand binds to the metal centre *via* one O atom in a monodentate fashion. The only significant difference is a rotation about the C(Ph)—COO bond, with O—C—C—C torsion angles having values of 6.3 (7) and 157.3 (3)° in the two isomeric forms.

Comment

Organometallic catalysts often incorporate hemilabile ligands, *i.e.* ligands that could bind either in a monodentate or a bidentate fashion, so as to facilitate the liberation of one coordination site of the metal centre under the conditions of the catalytic reaction. The title compound is an example of a phenylpalladium compound containing such a hemilabile ligand, namely a methylthioethercarboxylate S—O ligand. Due to their importance in industrial catalytic processes, Pd compounds containing hemilabile P—O ligands have been investigated extensively (Bader & Lindner, 1991). Examples of compounds with hemilabile S—O ligands are, however, quite rare (Britovsek *et al.*, 1996).

We have recently described (Meyer *et al.*, 1998) the synthesis of a series of compounds containing this type of ligand, namely *trans*-[Pd(OOC–C_6H_4–2-S*R*-κO)(C_6H_5){P(C_6H_5)$_3$}$_2$] with R = Me, Et, ^{i}Pr and ^{t}Bu. The crystal structure of one of the compounds in this series, *i.e.* where R = Et, was reported and it was shown that the last two complexes, *i.e.* with R = ^{i}Pr and ^{t}Bu, are hemilabile in solution.

The title compound (with R = Me) forms two distinct polymorphs, co-crystallizing from the same solution and easily distinguishable by their dissimilar crystal shapes. Their habits are monoclinic prismatic for the form we called isomer (I) and spindle-shaped monoclinic prismatic for our isomer (II). We observed the crystals of form (II) to be in the majority in a ratio of about 3:1 between the two forms. The crystal structures of both modifications were determined and are reported and compared in this paper.



(I)/(II)

It was expected that, since the S—O ligands are potentially bidentate, the structures would differ in the way in which the ligands bind to the metal centres. However, they were found to be mono-coordinated in both cases. The molecular configurations are the same in the two forms, *i.e.* a square-planar substitution of the Pd atom by the four ligands, with deviations from the best plane of less than 0.13 Å. The phenyl group and the S—O ligand are *trans* to each other and the S—O ligand bonds through the carboxylate-O rather than the S atom.

The difference between the two modifications lies in the orientation of the S—O ligands. In form (I), the S of the carboxylate ligand is adjacent to the O atom bonded to the Pd atom (O41 in Fig. 1). In form (II), the ligand is rotated around the C(carboxylate)—C(phenyl) bond to bring the S atom in close proximity to the carbonyl O atom (O42 in Fig. 2). The phenyl ligands are oriented perpendicular to the square plane, whereas the S—O ligands tilt at angles of 63.86 (7) and 42.40 (5)° to the molecular plane in forms (I) and (II), respectively. The orientations of the triphenylphosphines are very similar for both forms, as can be seen in the figures and from the torsion angles listed in Tables 1 and 2.

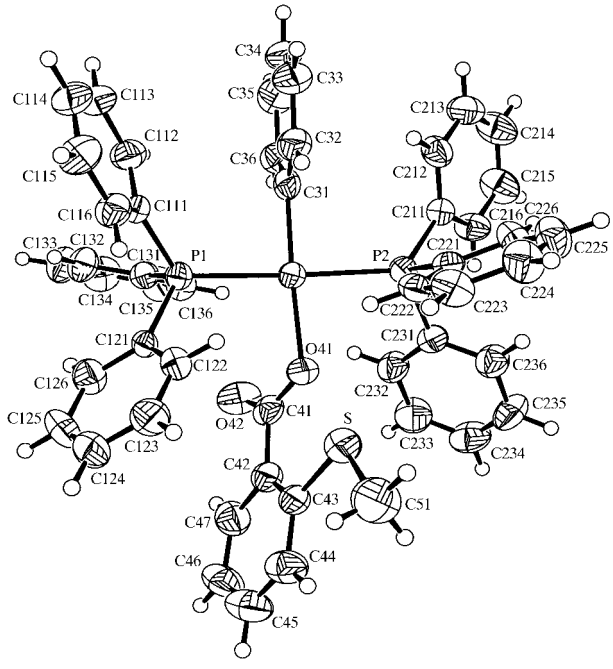


Figure 1
The molecular conformation of form (I) of the title compound, with anisotropic displacement ellipsoids shown at 50% probability level.

No significant intermolecular interactions can be observed in either of the two crystal structures. The packing of the molecules is such that in the case of isomer (I), the phenyl and the sulfur ligands point towards each other, while in the case of isomer (II), the sulfur ligands point towards pockets formed between the triphenylphosphine ligands of neighbouring molecules.

The conformation of modification (I) of the title compound (S oriented towards carboxyl O) is similar to that of its ethyl analogue *trans*-[Pd(OOC–C_6H_4–2-SC_2H_5-κO)(C_6H_5){P(C_6H_5)$_3$}$_2$] (Meyer *et al.*, 1998). The bond lengths and angles (not involving hydrogen) found for the three comparable molecular structures, the latter and forms (I) and (II) of the title compound, agree exceptionally well (all observations are within three standard deviations from the average).

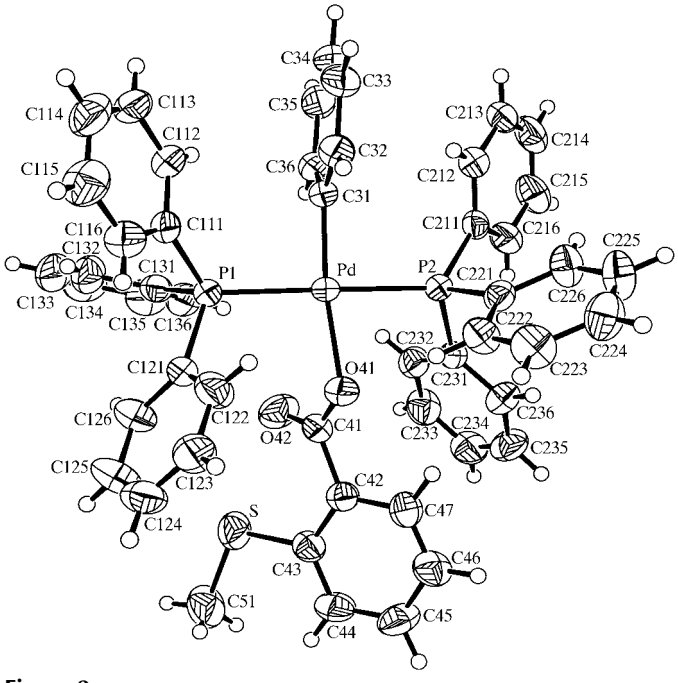


Figure 2
The molecular conformation of form (II) of the title compound, with anisotropic displacement ellipsoids shown at 50% probability level.

Experimental

The title compound was prepared by stirring *trans*-[PdCl(C_6H_5){P(C_6H_5)$_3$}$_2$] with TlOOC–C_6H_4–2-SCH_3 in tetrahydrofuran (THF) with subsequent filtration of TlCl and crystallization from THF/pentane as reported previously (Meyer *et al.*, 1998).

Isomer (I)

Crystal data

[Pd(C_6H_5)($C_8H_7O_2S$)($C_{18}H_{15}P$)$_2$]	D_x = 1.390 Mg m^{-3}
M_r = 875.24	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 43 reflections
a = 18.055 (6) Å	θ = 4.3–12.9°
b = 14.661 (5) Å	μ = 0.61 mm^{-1}
c = 17.598 (6) Å	T = 293 (2) K
β = 116.12 (5)°	Prism, colourless
V = 4182 (2) Å^3	0.25 × 0.13 × 0.10 mm
Z = 4	

Data collection

Philips PW1100 diffractometer	R_{int} = 0.074
ω–2θ scans	θ_{max} = 25°
Absorption correction: by integration (*Xtal*3.6; Hall *et al.*, 1999)	h = −17 → 21
T_{min} = 0.93, T_{max} = 0.95	k = −7 → 17
11 945 measured reflections	l = −20 → 19
7379 independent reflections	3 standard reflections every 50 reflections
4566 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$w = 1/[\sigma^2(F_o^2) + (0.0294P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.093	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.999	$\Delta\rho_{max}$ = 0.51 e Å^{-3}
5827 reflections	$\Delta\rho_{min}$ = −0.46 e Å^{-3}
505 parameters	

Table 1
Selected geometric parameters (Å, °) for (I).

Pd—C31	1.993 (5)	Pd—P1	2.3348 (15)
Pd—O41	2.126 (3)	Pd—P2	2.3494 (15)
C31—Pd—O41	169.92 (19)	C31—Pd—P2	89.87 (14)
C31—Pd—P1	87.55 (14)	O41—Pd—P2	88.29 (10)
O41—Pd—P1	94.52 (10)	P1—Pd—P2	176.99 (5)
O41—C41—C42—C43	6.3 (7)	C31—Pd—P2—C111	29.7 (2)
C31—Pd—P1—C111	−34.7 (2)	Pd—P2—C211—C212	59.6 (5)
Pd—P1—C111—C112	81.9 (4)	Pd—P2—C221—C222	23.7 (4)
Pd—P1—C121—C122	41.0 (4)	Pd—P2—C231—C232	34.6 (4)
Pd—P1—C131—C132	−167.6 (4)		

Isomer (II)

Crystal data

[Pd(C_6H_5)($C_8H_7O_2S$)($C_{18}H_{15}P$)$_2$]	D_x = 1.416 Mg m^{-3}
M_r = 875.24	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 8107 reflections
a = 12.5741 (6) Å	θ = 1.62–28.30°
b = 20.5817 (9) Å	μ = 0.62 mm^{-1}
c = 16.0672 (8) Å	T = 293 (2) K
β = 99.186 (1)°	Spindle, light yellow
V = 4104.8 (3) Å^3	0.35 × 0.20 × 0.18 mm
Z = 4	

Data collection

Siemens SMART CCD diffractometer	10 119 independent reflections
ω scans	8107 reflections with $I > 2\sigma(I)$
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)	R_{int} = 0.024
T_{min} = 0.86, T_{max} = 0.89	θ_{max} = 28.30°
27 445 measured reflections	h = −16 → 16
	k = −23 → 27
	l = −17 → 21

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0331P)^2 + 6.2933P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$(\Delta/\sigma)_{max}$ = 0.002
$wR(F^2)$ = 0.108	$\Delta\rho_{max}$ = 2.13 e Å^{-3}
S = 1.042	$\Delta\rho_{min}$ = −1.31 e Å^{-3}
10 119 reflections	
505 parameters	
H-atom parameters constrained	

In isomer (II), the largest peak and the deepest hole in the residual electron-density function are unusually large, but are in close proximity to the Pd atom (at distances of 0.78 and 0.67 Å, respectively, from the Pd atom directly above and below the molecular plane). As the internal consistency of the data set is excellent, no obvious explanation for the phenomenon could be found.

Table 2
Selected geometric parameters (Å, °) for (II).

Pd—C31	1.982 (3)	Pd—P2	2.3499 (8)
Pd—O41	2.129 (2)	Pd—P1	2.3505 (8)
C31—Pd—O41	170.35 (10)	C31—Pd—P1	90.94 (8)
C31—Pd—P2	89.81 (8)	O41—Pd—P1	94.97 (6)
O41—Pd—P2	84.45 (6)	P2—Pd—P1	178.56 (3)
O41—C41—C42—C43	157.3 (3)	C31—Pd—P2—C111	37.10 (16)
C31—Pd—P1—C111	−38.17 (15)	Pd—P2—C211—C212	55.4 (3)
Pd—P1—C111—C112	64.1 (3)	Pd—P2—C221—C222	32.6 (3)
Pd—P1—C121—C122	56.3 (3)	Pd—P2—C231—C232	54.4 (3)
Pd—P1—C131—C132	−164.0 (3)		

Data collection: *PWPC* (Gomm, 1998) for isomer (I), *SMART* (Siemens, 1996) for isomer (II); cell refinement: *PWPC* for (I), *SAINT* (Siemens, 1996) for (II); data reduction: *Xtal*3.6 (Hall *et al.*, 1999) for (I), *SAINT* for (II); for both isomers, program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL*97.2

We wish to thank the Department of Chemistry of the University of the Witwatersrand for the data collection of isomer (II) on their Siemens diffractometer.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1231). Services for accessing these data are described at the back of the journal.

References

Bader, A. & Lindner, E. (1991). *Coord. Chem. Rev.* **108**, 27–110.
Britovsek, G. J. P., Cavell, K. J. & Keim, W. (1996). *J. Mol. Catal. A Chem.* **110**, 77–87.
Gomm, M. (1998). *PWPC*. Version 1.12/H. Institut für Angewandte Physik, Erlangen, Germany.
Hall, S. R., du Boulay, D. J. & Olthof-Hazekamp, R. (1999). Editors. *Xtal*3.6 *System*. University of Western Australia, Australia.
McArdle, P. (1995). *J. Appl. Cryst.* **28**, 65.
Meyer, W. H., Brüll, R., Raubenheimer, H. G., Thompson, C. & Kruger, G. J. (1998). *J. Organomet. Chem.* **553**, 83–90.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELX*97. University of Göttingen, Germany.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

supporting information

Acta Cryst. (2000). C**56**, 329-331 [doi:10.1107/S0108270199015449]

trans-(2-Methylthiobenzoato-*O*)phenylbis(triphenylphosphine)palladium(II), two conformational isomers

Gert J. Kruger, Catharine Thompson, Wolfgang H. Meyer, Robert Brüll and Helgard G. Raubenheimer

Computing details

Data collection: PWPC (Gomm, 1998) for (I); *SMART* (Siemens, 1996) for (II). Cell refinement: PWPC for (I); *SAINT* (Siemens, 1996) for (II). Data reduction: *Xtal3*.6 (Hall *et al.*, 1999) for (I); *SAINT* for (II). For both compounds, program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

(I) [Trans-(2-methylthiobenzoato)phenylbis(triphenylphosphine)palladium(II)]

Crystal data

$[Pd(C_8H_7O_2S)(C_6H_5)(C_{18}H_{15}P)_2]$
M_r = 875.24
Monoclinic, $P2_1/c$
a = 18.055 (6) Å
b = 14.661 (5) Å
c = 17.598 (6) Å
β = 116.12 (5)°
V = 4182 (2) Å^3
Z = 4
$F(000)$ = 1800
D_x = 1.390 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 43 reflections
θ = 4.3–12.9°
μ = 0.61 mm^{-1}
T = 293 K
Prism, colourless
0.25 × 0.13 × 0.10 mm

Data collection

Philips PW1100 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω–2θ scans
Absorption correction: integration (*Xtal3*.6; Hall et al., 1999)
T_{min} = 0.93, T_{max} = 0.95
11945 measured reflections
7379 independent reflections
4566 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 25°, θ_{min} = 2.3°
h = −17→21
k = −7→17
l = −20→19
3 standard reflections every 50 reflections
intensity decay: 0.0%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.093
S = 1.00
5827 reflections
505 parameters
0 restraints
Primary atom site location: Patterson
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map

H-atom parameters constrained
Calculated $w = 1/[\sigma^2(F_o^2) + (0.0294P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

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 of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness 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 threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement.
The data for isomer (*I*) were measured in two batches, first to a maximum diffraction angle of 23° and then to 25° θ. However, since the average intensity fell below $1.5\sigma(I)$ above 23° θ, only the data below 23° were used in the refinement. The reflections above 23° θ made no significant difference to the structure, as the bond lengths and angles for the two cases, including and excluding the extra data, exhibited no difference greater than 0.003 Å or 0.2°. In addition, the standard uncertainties on the geometrical parameters did not decrease as would be expected for a larger number of observations, but in 20% of cases actually increased.
The H atoms were included in calculated positions at C—H distances of 0.93 Å. The displacement parameters were constrained to be 1.2 times the U_{eq} of the atoms they were bonded to.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pd	0.76568 (2)	0.51880 (3)	0.49523 (3)	0.03648 (13)
P1	0.74305 (8)	0.56173 (8)	0.61106 (9)	0.0358 (3)
P2	0.79202 (8)	0.46874 (9)	0.38264 (9)	0.0377 (3)
S	0.62695 (10)	0.74176 (10)	0.31594 (10)	0.0596 (4)
O41	0.7497 (2)	0.6527 (2)	0.4439 (2)	0.0476 (9)
O42	0.8480 (2)	0.7121 (2)	0.5610 (3)	0.0656 (12)
C111	0.6753 (3)	0.4887 (3)	0.6381 (3)	0.0353 (12)
C112	0.7054 (3)	0.4103 (3)	0.6853 (4)	0.0531 (15)
H112	0.7609	0.3952	0.7051	0.064*
C113	0.6537 (4)	0.3539 (4)	0.7035 (4)	0.0601 (17)
H113	0.6746	0.3010	0.7350	0.072*
C114	0.5719 (4)	0.3757 (4)	0.6753 (4)	0.0654 (18)
H114	0.5374	0.3381	0.6881	0.079*
C115	0.5413 (3)	0.4530 (4)	0.6283 (4)	0.0602 (17)
H115	0.4858	0.4678	0.6091	0.072*
C116	0.5918 (3)	0.5087 (3)	0.6095 (3)	0.0482 (14)
H116	0.5700	0.5607	0.5771	0.058*
C121	0.6908 (3)	0.6719 (3)	0.5956 (3)	0.0335 (12)
C122	0.6278 (3)	0.6896 (3)	0.5173 (3)	0.0447 (14)
H122	0.6156	0.6473	0.4740	0.054*
C123	0.5822 (3)	0.7685 (4)	0.5013 (4)	0.0583 (16)
H123	0.5396	0.7790	0.4478	0.070*
C124	0.5995 (4)	0.8309 (4)	0.5635 (4)	0.0636 (17)
H124	0.5682	0.8839	0.5531	0.076*
C125	0.6626 (4)	0.8158 (4)	0.6409 (4)	0.0634 (18)
H125	0.6748	0.8594	0.6832	0.076*

C126	0.7094 (3)	0.7364 (3)	0.6583 (4)	0.0533 (15)
H126	0.7527	0.7269	0.7117	0.064*
C131	0.8372 (3)	0.5652 (3)	0.7096 (3)	0.0398 (13)
C132	0.8371 (3)	0.5719 (4)	0.7873 (4)	0.0514 (15)
H132	0.7871	0.5749	0.7905	0.062*
C133	0.9097 (4)	0.5745 (4)	0.8608 (4)	0.0639 (17)
H133	0.9082	0.5805	0.9127	0.077*
C134	0.9847 (4)	0.5681 (4)	0.8576 (4)	0.0685 (18)
H134	1.0339	0.5684	0.9071	0.082*
C135	0.9855 (3)	0.5615 (4)	0.7808 (4)	0.0609 (17)
H135	1.0356	0.5577	0.7779	0.073*
C136	0.9128 (3)	0.5604 (3)	0.7072 (3)	0.0468 (14)
H136	0.9146	0.5564	0.6553	0.056*
C211	0.8445 (3)	0.3613 (3)	0.3831 (3)	0.0393 (13)
C212	0.8128 (3)	0.2790 (3)	0.3922 (3)	0.0495 (15)
H212	0.7651	0.2778	0.3998	0.059*
C213	0.8509 (4)	0.1982 (4)	0.3901 (4)	0.0649 (18)
H213	0.8283	0.1432	0.3962	0.078*
C214	0.9211 (4)	0.1974 (4)	0.3791 (4)	0.0700 (19)
H214	0.9461	0.1425	0.3774	0.084*
C215	0.9545 (4)	0.2790 (4)	0.3706 (4)	0.0675 (19)
H215	1.0022	0.2793	0.3628	0.081*
C216	0.9175 (3)	0.3604 (3)	0.3735 (4)	0.0502 (15)
H216	0.9412	0.4152	0.3691	0.060*
C221	0.6934 (3)	0.4583 (3)	0.2885 (3)	0.0365 (13)
C222	0.6271 (3)	0.5099 (3)	0.2853 (3)	0.0432 (13)
H222	0.6330	0.5456	0.3313	0.052*
C223	0.5530 (3)	0.5079 (3)	0.2138 (4)	0.0528 (15)
H223	0.5096	0.5439	0.2116	0.063*
C224	0.5415 (3)	0.4543 (4)	0.1460 (4)	0.0590 (16)
H224	0.4906	0.4526	0.0986	0.071*
C225	0.6065 (4)	0.4027 (4)	0.1488 (4)	0.0613 (17)
H225	0.5998	0.3668	0.1026	0.074*
C226	0.6817 (3)	0.4042 (3)	0.2202 (4)	0.0526 (15)
H226	0.7249	0.3682	0.2220	0.063*
C231	0.8495 (3)	0.5531 (3)	0.3532 (3)	0.0399 (13)
C232	0.9073 (3)	0.6054 (3)	0.4171 (4)	0.0529 (15)
H232	0.9152	0.5981	0.4727	0.064*
C233	0.9538 (4)	0.6693 (4)	0.3979 (4)	0.0690 (19)
H233	0.9935	0.7039	0.4409	0.083*
C234	0.9412 (4)	0.6811 (4)	0.3166 (5)	0.0662 (18)
H234	0.9719	0.7244	0.3041	0.079*
C235	0.8845 (4)	0.6306 (4)	0.2537 (4)	0.0663 (18)
H235	0.8760	0.6395	0.1981	0.080*
C236	0.8383 (3)	0.5648 (4)	0.2722 (4)	0.0552 (15)
H236	0.8000	0.5291	0.2290	0.066*
C31	0.7605 (3)	0.3896 (3)	0.5277 (3)	0.0429 (13)
C32	0.6848 (4)	0.3445 (4)	0.4897 (4)	0.0544 (16)

H32	0.6388	0.3756	0.4510	0.065*
C33	0.6769 (4)	0.2544 (4)	0.5086 (5)	0.073 (2)
H33	0.6256	0.2260	0.4832	0.087*
C34	0.7433 (6)	0.2076 (4)	0.5638 (5)	0.078 (2)
H34	0.7380	0.1467	0.5754	0.094*
C35	0.8188 (5)	0.2504 (4)	0.6028 (4)	0.076 (2)
H35	0.8644	0.2187	0.6415	0.091*
C36	0.8267 (4)	0.3417 (4)	0.5842 (4)	0.0573 (16)
H36	0.8778	0.3702	0.6107	0.069*
C41	0.7902 (4)	0.7192 (4)	0.4915 (4)	0.0441 (14)
C42	0.7580 (3)	0.8137 (3)	0.4550 (4)	0.0452 (14)
C43	0.6867 (3)	0.8315 (3)	0.3811 (4)	0.0451 (14)
C44	0.6634 (4)	0.9223 (4)	0.3579 (4)	0.0594 (17)
H44	0.6172	0.9350	0.3076	0.071*
C45	0.7085 (4)	0.9930 (4)	0.4089 (5)	0.072 (2)
H45	0.6911	1.0527	0.3935	0.086*
C46	0.7791 (4)	0.9766 (4)	0.4826 (5)	0.0687 (18)
H46	0.8098	1.0245	0.5165	0.082*
C47	0.8030 (4)	0.8871 (4)	0.5045 (4)	0.0582 (16)
H47	0.8506	0.8753	0.5538	0.070*
C51	0.5455 (4)	0.7989 (4)	0.2284 (4)	0.082 (2)
H51A	0.5097	0.7543	0.1895	0.099*
H51B	0.5688	0.8367	0.2000	0.099*
H51C	0.5144	0.8360	0.2490	0.099*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd	0.0411 (2)	0.0341 (2)	0.0406 (2)	−0.0005 (2)	0.02392 (19)	−0.0005 (2)
P1	0.0360 (8)	0.0372 (8)	0.0379 (8)	0.0008 (6)	0.0197 (7)	−0.0010 (6)
P2	0.0401 (8)	0.0367 (8)	0.0405 (8)	−0.0036 (6)	0.0217 (7)	−0.0028 (7)
S	0.0770 (11)	0.0498 (9)	0.0500 (10)	−0.0012 (8)	0.0260 (9)	0.0008 (8)
O41	0.063 (3)	0.036 (2)	0.054 (3)	0.0016 (19)	0.035 (2)	0.0046 (19)
O42	0.050 (3)	0.062 (3)	0.072 (3)	−0.001 (2)	0.015 (3)	0.014 (2)
C111	0.040 (3)	0.037 (3)	0.035 (3)	−0.002 (2)	0.022 (3)	−0.001 (2)
C112	0.056 (4)	0.046 (3)	0.065 (4)	−0.003 (3)	0.034 (3)	0.004 (3)
C113	0.082 (5)	0.045 (4)	0.062 (4)	−0.006 (3)	0.039 (4)	0.008 (3)
C114	0.071 (5)	0.061 (4)	0.079 (5)	−0.029 (4)	0.046 (4)	−0.008 (4)
C115	0.036 (3)	0.073 (5)	0.077 (5)	−0.015 (3)	0.030 (3)	−0.001 (4)
C116	0.041 (3)	0.053 (4)	0.054 (4)	−0.005 (3)	0.024 (3)	0.000 (3)
C121	0.034 (3)	0.032 (3)	0.043 (3)	−0.003 (2)	0.026 (3)	−0.004 (3)
C122	0.050 (4)	0.043 (3)	0.043 (4)	0.002 (3)	0.023 (3)	−0.004 (3)
C123	0.058 (4)	0.056 (4)	0.066 (4)	0.013 (3)	0.031 (3)	0.008 (3)
C124	0.081 (5)	0.051 (4)	0.069 (5)	0.022 (3)	0.042 (4)	0.005 (4)
C125	0.074 (5)	0.050 (4)	0.071 (5)	0.002 (3)	0.036 (4)	−0.022 (3)
C126	0.053 (4)	0.056 (4)	0.050 (4)	0.006 (3)	0.022 (3)	−0.002 (3)
C131	0.038 (3)	0.039 (3)	0.047 (4)	0.005 (2)	0.023 (3)	0.003 (3)
C132	0.041 (4)	0.068 (4)	0.049 (4)	−0.003 (3)	0.023 (3)	0.000 (3)

C133	0.067 (5)	0.079 (5)	0.047 (4)	−0.003 (4)	0.026 (4)	0.001 (3)
C134	0.053 (4)	0.078 (5)	0.055 (5)	0.000 (3)	0.005 (4)	0.006 (4)
C135	0.038 (4)	0.072 (4)	0.069 (5)	−0.002 (3)	0.021 (4)	−0.006 (4)
C136	0.043 (4)	0.052 (3)	0.045 (4)	0.007 (3)	0.019 (3)	0.004 (3)
C211	0.043 (3)	0.038 (3)	0.038 (3)	−0.001 (3)	0.019 (3)	0.000 (2)
C212	0.051 (4)	0.048 (4)	0.058 (4)	−0.007 (3)	0.032 (3)	−0.012 (3)
C213	0.083 (5)	0.043 (4)	0.083 (5)	−0.007 (3)	0.050 (4)	−0.003 (3)
C214	0.071 (5)	0.045 (4)	0.096 (6)	0.015 (3)	0.039 (4)	−0.005 (4)
C215	0.052 (4)	0.062 (4)	0.095 (6)	0.012 (3)	0.038 (4)	−0.008 (4)
C216	0.041 (4)	0.044 (3)	0.071 (4)	−0.004 (3)	0.029 (3)	0.000 (3)
C221	0.040 (3)	0.029 (3)	0.042 (3)	−0.002 (2)	0.020 (3)	0.004 (2)
C222	0.047 (3)	0.032 (3)	0.054 (4)	−0.006 (3)	0.026 (3)	−0.005 (3)
C223	0.039 (3)	0.052 (4)	0.060 (4)	−0.001 (3)	0.015 (3)	−0.003 (3)
C224	0.039 (4)	0.072 (4)	0.052 (4)	−0.015 (3)	0.008 (3)	−0.012 (3)
C225	0.055 (4)	0.073 (4)	0.059 (4)	−0.019 (3)	0.028 (4)	−0.023 (3)
C226	0.051 (4)	0.050 (4)	0.063 (4)	−0.007 (3)	0.031 (4)	−0.020 (3)
C231	0.037 (3)	0.041 (3)	0.047 (4)	0.006 (2)	0.023 (3)	0.006 (3)
C232	0.055 (4)	0.058 (4)	0.051 (4)	−0.015 (3)	0.027 (3)	−0.003 (3)
C233	0.064 (5)	0.073 (5)	0.075 (5)	−0.022 (3)	0.034 (4)	−0.009 (4)
C234	0.059 (4)	0.061 (4)	0.090 (6)	−0.011 (3)	0.043 (4)	0.010 (4)
C235	0.073 (5)	0.080 (5)	0.056 (4)	−0.009 (4)	0.038 (4)	0.014 (4)
C236	0.056 (4)	0.060 (4)	0.050 (4)	−0.009 (3)	0.023 (3)	−0.001 (3)
C31	0.049 (4)	0.044 (3)	0.048 (3)	0.009 (3)	0.032 (3)	−0.001 (3)
C32	0.064 (4)	0.048 (4)	0.065 (4)	0.002 (3)	0.042 (4)	0.002 (3)
C33	0.093 (6)	0.057 (4)	0.091 (6)	−0.026 (4)	0.061 (5)	−0.011 (4)
C34	0.136 (7)	0.037 (4)	0.100 (6)	0.002 (5)	0.086 (6)	0.008 (4)
C35	0.100 (6)	0.057 (5)	0.087 (6)	0.032 (4)	0.057 (5)	0.019 (4)
C36	0.062 (4)	0.048 (4)	0.071 (5)	0.011 (3)	0.038 (4)	0.007 (3)
C41	0.044 (4)	0.049 (4)	0.051 (4)	−0.001 (3)	0.031 (3)	0.006 (3)
C42	0.050 (4)	0.043 (3)	0.054 (4)	0.000 (3)	0.033 (3)	0.003 (3)
C43	0.056 (4)	0.038 (3)	0.057 (4)	−0.004 (3)	0.039 (3)	0.001 (3)
C44	0.055 (4)	0.049 (4)	0.084 (5)	0.006 (3)	0.040 (4)	0.009 (4)
C45	0.072 (5)	0.043 (4)	0.107 (6)	0.001 (3)	0.046 (5)	0.004 (4)
C46	0.076 (5)	0.041 (3)	0.095 (6)	−0.013 (4)	0.043 (4)	−0.016 (4)
C47	0.060 (4)	0.055 (4)	0.066 (4)	−0.007 (3)	0.033 (3)	−0.007 (3)
C51	0.084 (5)	0.075 (5)	0.070 (5)	0.004 (4)	0.018 (4)	−0.001 (4)

Geometric parameters (Å, º)

Pd—C31	1.993 (5)	C214—C215	1.377 (7)
Pd—O41	2.126 (3)	C214—H214	0.9300
Pd—P1	2.3348 (15)	C215—C216	1.379 (6)
Pd—P2	2.3494 (15)	C215—H215	0.9300
P1—C131	1.818 (5)	C216—H216	0.9300
P1—C121	1.829 (5)	C221—C226	1.375 (6)
P1—C111	1.839 (5)	C221—C222	1.397 (6)
P2—C221	1.828 (5)	C222—C223	1.376 (7)
P2—C231	1.830 (5)	C222—H222	0.9300

P2—C211	1.837 (5)	C223—C224	1.367 (7)
S—C43	1.767 (5)	C223—H223	0.9300
S—C51	1.801 (6)	C224—C225	1.377 (7)
O41—C41	1.283 (6)	C224—H224	0.9300
O42—C41	1.214 (6)	C225—C226	1.387 (7)
C111—C112	1.382 (6)	C225—H225	0.9300
C111—C116	1.395 (6)	C226—H226	0.9300
C112—C113	1.386 (7)	C231—C236	1.359 (7)
C112—H112	0.9300	C231—C232	1.382 (7)
C113—C114	1.374 (7)	C232—C233	1.396 (7)
C113—H113	0.9300	C232—H232	0.9300
C114—C115	1.368 (7)	C233—C234	1.358 (8)
C114—H114	0.9300	C233—H233	0.9300
C115—C116	1.369 (6)	C234—C235	1.351 (8)
C115—H115	0.9300	C234—H234	0.9300
C116—H116	0.9300	C235—C236	1.405 (7)
C121—C122	1.371 (7)	C235—H235	0.9300
C121—C126	1.378 (6)	C236—H236	0.9300
C122—C123	1.375 (6)	C31—C36	1.365 (7)
C122—H122	0.9300	C31—C32	1.395 (7)
C123—C124	1.353 (7)	C32—C33	1.385 (7)
C123—H123	0.9300	C32—H32	0.9300
C124—C125	1.355 (8)	C33—C34	1.351 (8)
C124—H124	0.9300	C33—H33	0.9300
C125—C126	1.392 (7)	C34—C35	1.378 (9)
C125—H125	0.9300	C34—H34	0.9300
C126—H126	0.9300	C35—C36	1.401 (7)
C131—C132	1.371 (7)	C35—H35	0.9300
C131—C136	1.387 (6)	C36—H36	0.9300
C132—C133	1.378 (7)	C41—C42	1.530 (7)
C132—H132	0.9300	C42—C43	1.394 (7)
C133—C134	1.384 (7)	C42—C47	1.397 (7)
C133—H133	0.9300	C43—C44	1.401 (7)
C134—C135	1.361 (8)	C44—C45	1.378 (8)
C134—H134	0.9300	C44—H44	0.9300
C135—C136	1.379 (7)	C45—C46	1.382 (9)
C135—H135	0.9300	C45—H45	0.9300
C136—H136	0.9300	C46—C47	1.382 (7)
C211—C212	1.374 (6)	C46—H46	0.9300
C211—C216	1.400 (6)	C47—H47	0.9300
C212—C213	1.378 (7)	C51—H51A	0.9600
C212—H212	0.9300	C51—H51B	0.9600
C213—C214	1.365 (7)	C51—H51C	0.9600
C213—H213	0.9300		

C31—Pd—O41	169.92 (19)	C214—C215—H215	119.9
C31—Pd—P1	87.55 (14)	C216—C215—H215	119.9
O41—Pd—P1	94.52 (10)	C215—C216—C211	120.6 (5)

C31—Pd—P2	89.87 (14)	C215—C216—H216	119.7
O41—Pd—P2	88.29 (10)	C211—C216—H216	119.7
P1—Pd—P2	176.99 (5)	C226—C221—C222	118.6 (5)
C131—P1—C121	108.8 (2)	C226—C221—P2	123.6 (4)
C131—P1—C111	102.6 (2)	C222—C221—P2	117.8 (4)
C121—P1—C111	101.2 (2)	C223—C222—C221	119.8 (5)
C131—P1—Pd	113.02 (17)	C223—C222—H222	120.1
C121—P1—Pd	112.64 (16)	C221—C222—H222	120.1
C111—P1—Pd	117.43 (16)	C224—C223—C222	121.5 (5)
C221—P2—C231	104.3 (2)	C224—C223—H223	119.2
C221—P2—C211	103.1 (2)	C222—C223—H223	119.2
C231—P2—C211	103.0 (2)	C223—C224—C225	119.0 (5)
C221—P2—Pd	108.23 (16)	C223—C224—H224	120.5
C231—P2—Pd	112.23 (17)	C225—C224—H224	120.5
C211—P2—Pd	124.03 (17)	C224—C225—C226	120.2 (6)
C43—S—C51	104.1 (3)	C224—C225—H225	119.9
C41—O41—Pd	119.5 (3)	C226—C225—H225	119.9
C112—C111—C116	117.9 (4)	C221—C226—C225	120.8 (5)
C112—C111—P1	120.6 (4)	C221—C226—H226	119.6
C116—C111—P1	121.4 (4)	C225—C226—H226	119.6
C111—C112—C113	120.6 (5)	C236—C231—C232	119.6 (5)
C111—C112—H112	119.7	C236—C231—P2	122.7 (4)
C113—C112—H112	119.7	C232—C231—P2	117.7 (4)
C114—C113—C112	120.3 (6)	C231—C232—C233	119.7 (6)
C114—C113—H113	119.9	C231—C232—H232	120.2
C112—C113—H113	119.9	C233—C232—H232	120.2
C115—C114—C113	119.7 (5)	C234—C233—C232	120.1 (6)
C115—C114—H114	120.1	C234—C233—H233	120.0
C113—C114—H114	120.1	C232—C233—H233	120.0
C114—C115—C116	120.3 (5)	C235—C234—C233	120.6 (6)
C114—C115—H115	119.8	C235—C234—H234	119.7
C116—C115—H115	119.8	C233—C234—H234	119.7
C115—C116—C111	121.2 (5)	C234—C235—C236	120.0 (6)
C115—C116—H116	119.4	C234—C235—H235	120.0
C111—C116—H116	119.4	C236—C235—H235	120.0
C122—C121—C126	118.5 (5)	C231—C236—C235	120.0 (5)
C122—C121—P1	117.6 (4)	C231—C236—H236	120.0
C126—C121—P1	124.0 (4)	C235—C236—H236	120.0
C121—C122—C123	121.5 (5)	C36—C31—C32	117.7 (5)
C121—C122—H122	119.3	C36—C31—Pd	124.1 (4)
C123—C122—H122	119.3	C32—C31—Pd	118.2 (4)
C124—C123—C122	120.0 (6)	C33—C32—C31	121.3 (6)
C124—C123—H123	120.0	C33—C32—H32	119.3
C122—C123—H123	120.0	C31—C32—H32	119.3
C123—C124—C125	119.6 (6)	C34—C33—C32	120.2 (6)
C123—C124—H124	120.2	C34—C33—H33	119.9
C125—C124—H124	120.2	C32—C33—H33	119.9
C124—C125—C126	121.2 (6)	C33—C34—C35	119.8 (6)

C124—C125—H125	119.4	C33—C34—H34	120.1
C126—C125—H125	119.4	C35—C34—H34	120.1
C121—C126—C125	119.2 (5)	C34—C35—C36	119.9 (6)
C121—C126—H126	120.4	C34—C35—H35	120.0
C125—C126—H126	120.4	C36—C35—H35	120.0
C132—C131—C136	117.8 (5)	C31—C36—C35	121.0 (6)
C132—C131—P1	122.9 (4)	C31—C36—H36	119.5
C136—C131—P1	119.3 (4)	C35—C36—H36	119.5
C131—C132—C133	121.3 (5)	O42—C41—O41	125.6 (5)
C131—C132—H132	119.3	O42—C41—C42	120.0 (5)
C133—C132—H132	119.3	O41—C41—C42	114.4 (5)
C132—C133—C134	120.3 (6)	C43—C42—C47	118.8 (5)
C132—C133—H133	119.9	C43—C42—C41	125.8 (5)
C134—C133—H133	119.9	C47—C42—C41	115.3 (5)
C135—C134—C133	118.9 (6)	C42—C43—C44	119.0 (5)
C135—C134—H134	120.6	C42—C43—S	121.0 (4)
C133—C134—H134	120.6	C44—C43—S	120.0 (5)
C134—C135—C136	120.8 (5)	C45—C44—C43	120.6 (6)
C134—C135—H135	119.6	C45—C44—H44	119.7
C136—C135—H135	119.6	C43—C44—H44	119.7
C135—C136—C131	120.9 (5)	C44—C45—C46	121.2 (6)
C135—C136—H136	119.5	C44—C45—H45	119.4
C131—C136—H136	119.5	C46—C45—H45	119.4
C212—C211—C216	117.9 (5)	C45—C46—C47	118.1 (6)
C212—C211—P2	120.9 (4)	C45—C46—H46	120.9
C216—C211—P2	121.2 (4)	C47—C46—H46	120.9
C211—C212—C213	120.9 (5)	C46—C47—C42	122.2 (6)
C211—C212—H212	119.5	C46—C47—H47	118.9
C213—C212—H212	119.5	C42—C47—H47	118.9
C214—C213—C212	121.0 (5)	S—C51—H51A	109.5
C214—C213—H213	119.5	S—C51—H51B	109.5
C212—C213—H213	119.5	H51A—C51—H51B	109.5
C213—C214—C215	119.2 (5)	S—C51—H51C	109.5
C213—C214—H214	120.4	H51A—C51—H51C	109.5
C215—C214—H214	120.4	H51B—C51—H51C	109.5
C214—C215—C216	120.3 (5)		

O41—C41—C42—C43	6.3 (7)	C31—Pd—P2—C111	29.7 (2)
C31—Pd—P1—C111	−34.7 (2)	Pd—P2—C211—C212	59.6 (5)
Pd—P1—C111—C112	81.9 (4)	Pd—P2—C221—C222	23.7 (4)
Pd—P1—C121—C122	41.0 (4)	Pd—P2—C231—C232	34.6 (4)
Pd—P1—C131—C132	−167.6 (4)		

(II) [Trans-(2-methylthiobenzoato)phenylbis(triphenylphosphine)palladium(II)]

Crystal data

$[Pd(C_8H_7O_2S)(C_6H_5)(C_{18}H_{15}P)_2]$	Monoclinic, $P2_1/c$
M_r = 875.24	a = 12.5741 (6) Å

b = 20.5817 (9) Å
c = 16.0672 (8) Å
β = 99.186 (1)°
V = 4104.8 (3) Å^3
Z = 4
F(000) = 1800
D_x = 1.416 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8107 reflections
θ = 1.6–28.3°
μ = 0.62 mm^{-1}
T = 293 K
Spindle, light yellow
0.35 × 0.20 × 0.18 mm

Data collection

Siemens SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: empirical (using intensity measurements) (*SADABS*; Sheldrick, 1996)
T_{min} = 0.86, T_{max} = 0.89

27445 measured reflections
10119 independent reflections
8107 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 28.3°, θ_{min} = 1.6°
h = −16→16
k = −23→27
l = −17→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.108
S = 1.04
10119 reflections
505 parameters
0 restraints
Primary atom site location: Patterson

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
Calculated $w = 1/[\sigma^2(F_o^2) + (0.0331P)^2 + 6.2933P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 2.13 e Å^{-3}
$\Delta\rho_{min}$ = −1.31 e Å^{-3}

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 of F^2 against ALL reflections. The weighted R-factor wR and goodness 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 threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement.

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

	x	y	z	U_{iso}*/U_{eq}
Pd	0.838039 (16)	0.931566 (11)	0.224657 (15)	0.03643 (7)
P1	0.96991 (6)	0.87487 (4)	0.16532 (5)	0.03784 (17)
P2	0.70514 (6)	0.98583 (4)	0.28562 (5)	0.03508 (16)
S	0.67371 (8)	0.67046 (5)	0.15826 (8)	0.0666 (3)
O41	0.70557 (17)	0.87990 (11)	0.15613 (15)	0.0483 (5)
O42	0.7581 (2)	0.78839 (14)	0.22245 (17)	0.0653 (7)
C111	1.0787 (2)	0.92087 (14)	0.1280 (2)	0.0433 (7)
C112	1.1505 (2)	0.95520 (17)	0.1864 (3)	0.0523 (8)
H112	1.1417 (3)	0.95618 (17)	0.2380 (14)	0.063*

C113	1.2365 (3)	0.98799 (18)	0.1612 (3)	0.0620 (10)
H113	1.2797 (12)	1.0095 (6)	0.1975 (10)	0.074*
C114	1.2531 (3)	0.9864 (2)	0.0793 (3)	0.0672 (11)
H114	1.3070 (15)	1.0062 (6)	0.0644 (5)	0.081*
C115	1.1830 (3)	0.9529 (2)	0.0215 (3)	0.0700 (11)
H115	1.1931 (4)	0.9518 (2)	−0.0303 (14)	0.084*
C116	1.0957 (3)	0.92038 (18)	0.0446 (2)	0.0571 (9)
H116	1.0519 (12)	0.8998 (6)	0.0073 (10)	0.068*
C121	0.9083 (2)	0.83028 (15)	0.07225 (19)	0.0404 (6)
C122	0.8474 (3)	0.86501 (19)	0.0083 (3)	0.0633 (10)
H122	0.8371 (4)	0.9069 (11)	0.0150 (3)	0.076*
C123	0.8021 (3)	0.8354 (2)	−0.0664 (3)	0.0641 (10)
H123	0.7656 (10)	0.8588 (6)	−0.1074 (11)	0.077*
C124	0.8135 (3)	0.7703 (2)	−0.0767 (3)	0.0627 (10)
H124	0.7850 (8)	0.7511 (5)	−0.1248 (13)	0.075*
C125	0.8695 (4)	0.7347 (2)	−0.0123 (3)	0.0725 (12)
H125	0.8753 (4)	0.6921 (11)	−0.0182 (3)	0.087*
C126	0.9176 (3)	0.76391 (16)	0.0625 (2)	0.0546 (9)
H126	0.9538 (10)	0.7402 (6)	0.1034 (11)	0.066*
C131	1.0487 (2)	0.81472 (15)	0.2326 (2)	0.0445 (7)
C132	1.1447 (3)	0.79048 (19)	0.2121 (3)	0.0627 (10)
H132	1.1679 (7)	0.8046 (4)	0.1670 (13)	0.075*
C133	1.2037 (3)	0.7444 (2)	0.2624 (3)	0.0760 (13)
H133	1.2637 (17)	0.7297 (4)	0.2491 (5)	0.091*
C134	1.1675 (4)	0.7216 (2)	0.3335 (3)	0.0777 (13)
H134	1.2043 (11)	0.6922 (8)	0.3648 (9)	0.093*
C135	1.0735 (4)	0.7453 (2)	0.3548 (3)	0.0741 (12)
H135	1.0510 (7)	0.7313 (4)	0.4005 (13)	0.089*
C136	1.0136 (3)	0.79158 (18)	0.3042 (2)	0.0569 (9)
H136	0.9531 (16)	0.8061 (4)	0.3179 (4)	0.068*
C211	0.7327 (2)	1.03378 (14)	0.38300 (19)	0.0402 (6)
C212	0.8068 (3)	1.08422 (16)	0.3898 (2)	0.0519 (8)
H212	0.8423 (9)	1.0927 (3)	0.3473 (11)	0.062*
C213	0.8258 (3)	1.12161 (18)	0.4628 (3)	0.0614 (10)
H213	0.8741 (12)	1.1536 (8)	0.4669 (3)	0.074*
C214	0.7714 (3)	1.10992 (19)	0.5283 (3)	0.0649 (11)
H214	0.7846 (5)	1.1340 (6)	0.5753 (12)	0.078*
C215	0.6964 (4)	1.06097 (19)	0.5215 (2)	0.0641 (10)
H215	0.6593 (10)	1.0537 (3)	0.5638 (11)	0.077*
C216	0.6778 (3)	1.02285 (17)	0.4498 (2)	0.0503 (8)
H216	0.6299 (12)	0.9909 (8)	0.4465 (2)	0.060*
C221	0.6278 (2)	1.04205 (15)	0.21161 (19)	0.0391 (6)
C222	0.6096 (3)	1.02714 (17)	0.1263 (2)	0.0496 (8)
H222	0.6384 (8)	0.9902 (9)	0.1073 (5)	0.059*
C223	0.5477 (3)	1.06826 (19)	0.0700 (2)	0.0609 (9)
H223	0.5362 (4)	1.0583 (3)	0.0136 (14)	0.073*
C224	0.5031 (3)	1.1237 (2)	0.0973 (3)	0.0631 (10)
H224	0.4611 (11)	1.1500 (7)	0.0595 (10)	0.076*

C225	0.5217 (3)	1.1395 (2)	0.1809 (3)	0.0650 (10)
H225	0.4926 (8)	1.1766 (9)	0.1992 (5)	0.078*
C226	0.5843 (3)	1.09930 (18)	0.2381 (2)	0.0554 (9)
H226	0.5974 (4)	1.1106 (3)	0.2946 (14)	0.067*
C231	0.6071 (2)	0.92656 (14)	0.31076 (19)	0.0388 (6)
C232	0.6448 (3)	0.87378 (16)	0.3605 (2)	0.0524 (8)
H232	0.7169 (18)	0.8691 (2)	0.3782 (5)	0.063*
C233	0.5742 (3)	0.82818 (18)	0.3837 (3)	0.0634 (10)
H233	0.6000 (7)	0.7947 (8)	0.4180 (9)	0.076*
C234	0.4659 (3)	0.83304 (19)	0.3553 (3)	0.0611 (10)
H234	0.4196 (12)	0.8024 (8)	0.3699 (4)	0.073*
C235	0.4274 (3)	0.8845 (2)	0.3046 (2)	0.0602 (9)
H235	0.3551 (18)	0.8877 (2)	0.2850 (5)	0.072*
C236	0.4970 (3)	0.93151 (18)	0.2829 (2)	0.0501 (8)
H236	0.4703 (7)	0.9661 (9)	0.2499 (8)	0.060*
C31	0.9480 (2)	0.99299 (14)	0.28107 (19)	0.0379 (6)
C32	0.9712 (3)	1.04985 (16)	0.2410 (3)	0.0514 (8)
H32	0.9407 (14)	1.0572 (4)	0.188 (2)	0.062*
C33	1.0430 (3)	1.09599 (19)	0.2836 (3)	0.0670 (11)
H33	1.0584 (8)	1.1338 (19)	0.2563 (14)	0.080*
C34	1.0899 (3)	1.0851 (2)	0.3650 (3)	0.0685 (12)
H34	1.138 (2)	1.1174 (15)	0.3946 (14)	0.082*
C35	1.0690 (3)	1.0291 (2)	0.4054 (3)	0.0616 (10)
H35	1.1036 (15)	1.0214 (4)	0.464 (3)	0.074*
C36	0.9987 (2)	0.98313 (17)	0.3635 (2)	0.0476 (7)
H36	0.9851 (6)	0.9445 (16)	0.3917 (12)	0.057*
C41	0.6922 (2)	0.82099 (15)	0.17526 (19)	0.0404 (6)
C42	0.5848 (2)	0.79218 (15)	0.13719 (19)	0.0416 (6)
C43	0.5663 (3)	0.72614 (15)	0.1253 (2)	0.0459 (7)
C44	0.4657 (3)	0.70409 (18)	0.0889 (2)	0.0569 (9)
H44	0.4541 (4)	0.6591 (11)	0.0783 (4)	0.068*
C45	0.3806 (3)	0.7486 (2)	0.0674 (3)	0.0639 (10)
H45	0.3098 (18)	0.7342 (4)	0.0434 (7)	0.077*
C46	0.4026 (3)	0.81312 (17)	0.0820 (2)	0.0562 (9)
H46	0.3459 (14)	0.8436 (8)	0.0684 (4)	0.067*
C47	0.4981 (3)	0.83456 (17)	0.1138 (2)	0.0489 (8)
H47	0.5092 (4)	0.8808 (11)	0.1215 (3)	0.059*
C51	0.6187 (4)	0.5953 (2)	0.1127 (4)	0.0891 (15)
H511	0.6715	0.5615	0.1246	0.134*
H512	0.5995	0.6004	0.0528	0.134*
H513	0.5558	0.5841	0.1365	0.134*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd	0.02944 (11)	0.03421 (12)	0.04485 (13)	−0.00328 (8)	0.00350 (8)	−0.00943 (9)
P1	0.0321 (3)	0.0350 (4)	0.0456 (4)	0.0008 (3)	0.0038 (3)	−0.0071 (3)
P2	0.0304 (3)	0.0356 (4)	0.0387 (4)	0.0000 (3)	0.0041 (3)	−0.0044 (3)

S	0.0578 (5)	0.0459 (5)	0.0972 (8)	0.0074 (4)	0.0156 (5)	0.0008 (5)
O41	0.0435 (12)	0.0413 (12)	0.0591 (14)	−0.0050 (9)	0.0047 (10)	−0.0053 (10)
O42	0.0518 (14)	0.0721 (17)	0.0649 (16)	0.0012 (13)	−0.0120 (12)	0.0057 (14)
C111	0.0357 (14)	0.0366 (15)	0.0578 (19)	0.0039 (12)	0.0083 (13)	−0.0034 (13)
C112	0.0352 (15)	0.0532 (19)	0.068 (2)	−0.0008 (14)	0.0057 (15)	−0.0069 (17)
C113	0.0346 (16)	0.052 (2)	0.097 (3)	−0.0030 (15)	0.0035 (18)	−0.005 (2)
C114	0.047 (2)	0.059 (2)	0.099 (3)	−0.0002 (17)	0.022 (2)	0.018 (2)
C115	0.068 (3)	0.072 (3)	0.074 (3)	−0.004 (2)	0.024 (2)	0.017 (2)
C116	0.055 (2)	0.054 (2)	0.063 (2)	−0.0045 (16)	0.0097 (17)	−0.0017 (17)
C121	0.0379 (14)	0.0388 (15)	0.0447 (16)	−0.0009 (12)	0.0068 (12)	−0.0079 (13)
C122	0.062 (2)	0.047 (2)	0.072 (3)	0.0131 (17)	−0.0133 (19)	−0.0155 (18)
C123	0.057 (2)	0.070 (3)	0.059 (2)	0.0090 (19)	−0.0120 (18)	−0.0072 (19)
C124	0.067 (2)	0.066 (2)	0.054 (2)	−0.0185 (19)	0.0071 (18)	−0.0174 (19)
C125	0.112 (4)	0.044 (2)	0.059 (2)	−0.016 (2)	0.009 (2)	−0.0141 (18)
C126	0.074 (2)	0.0391 (17)	0.0497 (19)	−0.0079 (16)	0.0060 (17)	−0.0036 (14)
C131	0.0408 (15)	0.0386 (16)	0.0510 (18)	0.0003 (13)	−0.0025 (13)	−0.0066 (13)
C132	0.0492 (19)	0.056 (2)	0.082 (3)	0.0109 (17)	0.0100 (18)	0.004 (2)
C133	0.052 (2)	0.057 (2)	0.116 (4)	0.0151 (19)	0.002 (2)	0.003 (2)
C134	0.068 (3)	0.056 (2)	0.097 (3)	0.007 (2)	−0.022 (2)	0.010 (2)
C135	0.078 (3)	0.072 (3)	0.067 (3)	0.001 (2)	−0.005 (2)	0.015 (2)
C136	0.0533 (19)	0.056 (2)	0.058 (2)	0.0043 (16)	−0.0017 (16)	0.0019 (17)
C211	0.0375 (14)	0.0377 (15)	0.0430 (16)	0.0079 (12)	−0.0010 (12)	−0.0061 (12)
C212	0.0440 (17)	0.0456 (18)	0.066 (2)	0.0013 (14)	0.0075 (16)	−0.0131 (16)
C213	0.0512 (19)	0.0450 (19)	0.083 (3)	0.0060 (15)	−0.0059 (19)	−0.0218 (19)
C214	0.079 (3)	0.053 (2)	0.055 (2)	0.019 (2)	−0.010 (2)	−0.0186 (18)
C215	0.091 (3)	0.057 (2)	0.045 (2)	0.015 (2)	0.0118 (19)	−0.0057 (17)
C216	0.060 (2)	0.0454 (18)	0.0455 (18)	0.0026 (15)	0.0078 (15)	−0.0052 (14)
C221	0.0337 (14)	0.0407 (15)	0.0434 (16)	−0.0002 (12)	0.0079 (12)	0.0021 (13)
C222	0.059 (2)	0.0437 (17)	0.0452 (18)	0.0035 (15)	0.0059 (15)	−0.0009 (14)
C223	0.076 (3)	0.061 (2)	0.0436 (19)	0.0045 (19)	0.0037 (17)	0.0072 (17)
C224	0.063 (2)	0.066 (2)	0.060 (2)	0.0163 (19)	0.0070 (18)	0.0198 (19)
C225	0.074 (3)	0.059 (2)	0.064 (2)	0.029 (2)	0.017 (2)	0.0088 (19)
C226	0.064 (2)	0.056 (2)	0.0475 (19)	0.0170 (17)	0.0128 (16)	0.0006 (16)
C231	0.0355 (14)	0.0404 (15)	0.0417 (15)	−0.0011 (12)	0.0096 (12)	−0.0060 (12)
C232	0.0464 (17)	0.0421 (17)	0.069 (2)	0.0020 (14)	0.0089 (16)	0.0040 (16)
C233	0.070 (2)	0.046 (2)	0.076 (3)	0.0030 (18)	0.019 (2)	0.0129 (18)
C234	0.064 (2)	0.053 (2)	0.072 (2)	−0.0150 (18)	0.029 (2)	−0.0018 (18)
C235	0.0412 (17)	0.076 (3)	0.065 (2)	−0.0127 (17)	0.0147 (16)	−0.004 (2)
C236	0.0387 (16)	0.061 (2)	0.0507 (19)	−0.0015 (15)	0.0072 (14)	0.0024 (16)
C31	0.0312 (13)	0.0343 (14)	0.0474 (16)	−0.0013 (11)	0.0036 (12)	−0.0054 (12)
C32	0.0488 (18)	0.0428 (17)	0.062 (2)	−0.0017 (14)	0.0087 (16)	0.0000 (15)
C33	0.063 (2)	0.0395 (19)	0.103 (3)	−0.0131 (17)	0.029 (2)	−0.007 (2)
C34	0.0417 (18)	0.062 (2)	0.100 (3)	−0.0109 (17)	0.004 (2)	−0.034 (2)
C35	0.0450 (18)	0.066 (2)	0.067 (2)	0.0048 (17)	−0.0094 (17)	−0.0216 (19)
C36	0.0395 (15)	0.0443 (17)	0.0556 (19)	0.0030 (13)	−0.0025 (14)	−0.0053 (15)
C41	0.0422 (15)	0.0390 (15)	0.0402 (16)	−0.0009 (12)	0.0071 (13)	−0.0070 (12)
C42	0.0413 (15)	0.0440 (16)	0.0396 (16)	−0.0047 (13)	0.0074 (12)	−0.0021 (13)
C43	0.0493 (17)	0.0420 (16)	0.0489 (18)	−0.0067 (14)	0.0158 (14)	−0.0033 (14)

C44	0.060 (2)	0.0459 (19)	0.065 (2)	−0.0205 (16)	0.0097 (17)	−0.0041 (16)
C45	0.0451 (18)	0.065 (2)	0.077 (3)	−0.0162 (17)	−0.0019 (18)	0.004 (2)
C46	0.066 (2)	0.0375 (17)	0.064 (2)	−0.0025 (16)	0.0054 (18)	0.0065 (15)
C47	0.0521 (18)	0.0417 (17)	0.0524 (19)	0.0058 (14)	0.0071 (15)	0.0046 (14)
C51	0.086 (3)	0.047 (2)	0.140 (5)	−0.002 (2)	0.036 (3)	−0.011 (3)

Geometric parameters (Å, º)

Pd—C31	1.982 (3)	C214—C215	1.373 (6)
Pd—O41	2.129 (2)	C214—H214	0.8962
Pd—P2	2.3499 (8)	C215—C216	1.384 (5)
Pd—P1	2.3505 (8)	C215—H215	0.8963
P1—C121	1.819 (3)	C216—H216	0.8871
P1—C131	1.828 (3)	C221—C222	1.387 (4)
P1—C111	1.841 (3)	C221—C226	1.394 (4)
P2—C221	1.824 (3)	C222—C223	1.384 (5)
P2—C231	1.825 (3)	C222—H222	0.9163
P2—C211	1.835 (3)	C223—C224	1.373 (5)
S—C43	1.786 (4)	C223—H223	0.9178
S—C51	1.801 (5)	C224—C225	1.366 (6)
O41—C41	1.269 (4)	C224—H224	0.9158
O42—C41	1.229 (4)	C225—C226	1.385 (5)
C111—C112	1.387 (5)	C225—H225	0.9154
C111—C116	1.390 (5)	C226—H226	0.9253
C112—C113	1.389 (5)	C231—C232	1.387 (4)
C112—H112	0.8543	C231—C236	1.388 (4)
C113—C114	1.366 (6)	C232—C233	1.382 (5)
C113—H113	0.8542	C232—H232	0.9110
C114—C115	1.361 (6)	C233—C234	1.369 (6)
C114—H114	0.8575	C233—H233	0.9097
C115—C116	1.386 (5)	C234—C235	1.376 (6)
C115—H115	0.8631	C234—H234	0.9152
C116—H116	0.8585	C235—C236	1.387 (5)
C121—C122	1.379 (5)	C235—H235	0.9157
C121—C126	1.382 (4)	C236—H236	0.9185
C122—C123	1.385 (5)	C31—C32	1.389 (4)
C122—H122	0.8803	C31—C36	1.391 (4)
C123—C124	1.360 (6)	C32—C33	1.410 (5)
C123—H123	0.8830	C32—H32	0.8843
C124—C125	1.368 (6)	C33—C34	1.364 (6)
C124—H124	0.8904	C33—H33	0.9281
C125—C126	1.391 (5)	C34—C35	1.368 (6)
C125—H125	0.8856	C34—H34	0.9741
C126—H126	0.8843	C35—C36	1.393 (5)
C131—C136	1.381 (5)	C35—H35	0.9791
C131—C132	1.393 (5)	C36—H36	0.9432
C132—C133	1.383 (5)	C41—C42	1.512 (4)
C132—H132	0.8743	C42—C43	1.387 (4)

C133—C134	1.377 (7)	C42—C47	1.400 (4)
C133—H133	0.8696	C43—C44	1.383 (5)
C134—C135	1.372 (6)	C44—C45	1.409 (5)
C134—H134	0.8709	C44—H44	0.9491
C135—C136	1.393 (5)	C45—C46	1.370 (5)
C135—H135	0.8775	C45—H45	0.9586
C136—H136	0.8780	C46—C47	1.305 (5)
C211—C216	1.383 (5)	C46—H46	0.9476
C211—C212	1.388 (4)	C47—H47	0.9671
C212—C213	1.392 (5)	C51—H511	0.9600
C212—H212	0.8904	C51—H512	0.9600
C213—C214	1.364 (6)	C51—H513	0.9600
C213—H213	0.8920		

C31—Pd—O41	170.35 (10)	C214—C215—H215	119.9
C31—Pd—P2	89.81 (8)	C216—C215—H215	119.9
O41—Pd—P2	84.45 (6)	C211—C216—C215	121.0 (4)
C31—Pd—P1	90.94 (8)	C211—C216—H216	119.5
O41—Pd—P1	94.97 (6)	C215—C216—H216	119.5
P2—Pd—P1	178.56 (3)	C222—C221—C226	118.5 (3)
C121—P1—C131	105.30 (14)	C222—C221—P2	119.4 (2)
C121—P1—C111	103.46 (15)	C226—C221—P2	122.1 (2)
C131—P1—C111	100.37 (14)	C223—C222—C221	119.8 (3)
C121—P1—Pd	110.39 (10)	C223—C222—H222	120.1
C131—P1—Pd	116.58 (11)	C221—C222—H222	120.1
C111—P1—Pd	119.07 (10)	C224—C223—C222	121.0 (4)
C221—P2—C231	105.06 (14)	C224—C223—H223	119.5
C221—P2—C211	102.88 (14)	C222—C223—H223	119.5
C231—P2—C211	102.29 (14)	C225—C224—C223	119.8 (3)
C221—P2—Pd	111.72 (10)	C225—C224—H224	120.1
C231—P2—Pd	108.98 (10)	C223—C224—H224	120.1
C211—P2—Pd	124.13 (10)	C224—C225—C226	120.0 (4)
C43—S—C51	102.0 (2)	C224—C225—H225	120.0
C41—O41—Pd	118.4 (2)	C226—C225—H225	120.0
C112—C111—C116	118.2 (3)	C225—C226—C221	120.8 (3)
C112—C111—P1	118.6 (3)	C225—C226—H226	119.6
C116—C111—P1	123.2 (3)	C221—C226—H226	119.6
C111—C112—C113	120.2 (4)	C232—C231—C236	118.3 (3)
C111—C112—H112	119.9	C232—C231—P2	118.1 (2)
C113—C112—H112	119.9	C236—C231—P2	123.6 (3)
C114—C113—C112	121.0 (4)	C233—C232—C231	120.8 (3)
C114—C113—H113	119.5	C233—C232—H232	119.6
C112—C113—H113	119.5	C231—C232—H232	119.6
C115—C114—C113	119.2 (4)	C234—C233—C232	120.5 (4)
C115—C114—H114	120.4	C234—C233—H233	119.7
C113—C114—H114	120.4	C232—C233—H233	119.7
C114—C115—C116	121.1 (4)	C233—C234—C235	119.4 (3)
C114—C115—H115	119.4	C233—C234—H234	120.3

C116—C115—H115	119.4	C235—C234—H234	120.3
C115—C116—C111	120.3 (4)	C234—C235—C236	120.6 (3)
C115—C116—H116	119.8	C234—C235—H235	119.7
C111—C116—H116	119.8	C236—C235—H235	119.7
C122—C121—C126	118.3 (3)	C235—C236—C231	120.3 (3)
C122—C121—P1	117.7 (2)	C235—C236—H236	119.9
C126—C121—P1	124.0 (3)	C231—C236—H236	119.9
C121—C122—C123	121.3 (3)	C32—C31—C36	117.8 (3)
C121—C122—H122	119.3	C32—C31—Pd	120.5 (2)
C123—C122—H122	119.3	C36—C31—Pd	121.5 (2)
C124—C123—C122	120.1 (4)	C31—C32—C33	120.5 (4)
C124—C123—H123	119.9	C31—C32—H32	119.7
C122—C123—H123	119.9	C33—C32—H32	119.7
C123—C124—C125	119.2 (4)	C34—C33—C32	120.0 (4)
C123—C124—H124	120.4	C34—C33—H33	120.0
C125—C124—H124	120.4	C32—C33—H33	120.0
C124—C125—C126	121.4 (4)	C33—C34—C35	120.5 (4)
C124—C125—H125	119.3	C33—C34—H34	119.8
C126—C125—H125	119.3	C35—C34—H34	119.8
C121—C126—C125	119.5 (4)	C34—C35—C36	119.9 (4)
C121—C126—H126	120.3	C34—C35—H35	120.1
C125—C126—H126	120.3	C36—C35—H35	120.1
C136—C131—C132	118.5 (3)	C31—C36—C35	121.3 (4)
C136—C131—P1	120.7 (3)	C31—C36—H36	119.3
C132—C131—P1	120.8 (3)	C35—C36—H36	119.3
C133—C132—C131	120.8 (4)	O42—C41—O41	124.7 (3)
C133—C132—H132	119.6	O42—C41—C42	120.4 (3)
C131—C132—H132	119.6	O41—C41—C42	114.9 (3)
C134—C133—C132	120.0 (4)	C43—C42—C47	117.9 (3)
C134—C133—H133	120.0	C43—C42—C41	124.0 (3)
C132—C133—H133	120.0	C47—C42—C41	118.1 (3)
C135—C134—C133	119.9 (4)	C44—C43—C42	120.1 (3)
C135—C134—H134	120.0	C44—C43—S	120.8 (3)
C133—C134—H134	120.0	C42—C43—S	119.1 (2)
C134—C135—C136	120.3 (4)	C43—C44—C45	119.9 (3)
C134—C135—H135	119.9	C43—C44—H44	120.1
C136—C135—H135	119.9	C45—C44—H44	120.1
C131—C136—C135	120.5 (4)	C46—C45—C44	117.6 (3)
C131—C136—H136	119.8	C46—C45—H45	121.2
C135—C136—H136	119.8	C44—C45—H45	121.2
C216—C211—C212	118.2 (3)	C47—C46—C45	122.9 (4)
C216—C211—P2	121.6 (2)	C47—C46—H46	118.5
C212—C211—P2	120.1 (3)	C45—C46—H46	118.5
C211—C212—C213	120.1 (4)	C46—C47—C42	121.5 (3)
C211—C212—H212	119.9	C46—C47—H47	119.2
C213—C212—H212	119.9	C42—C47—H47	119.2
C214—C213—C212	120.9 (4)	S—C51—H511	109.5
C214—C213—H213	119.6	S—C51—H512	109.5

C212—C213—H213	119.6	H511—C51—H512	109.5
C213—C214—C215	119.4 (4)	S—C51—H513	109.5
C213—C214—H214	120.3	H511—C51—H513	109.5
C215—C214—H214	120.3	H512—C51—H513	109.5
C214—C215—C216	120.3 (4)		
O41—C41—C42—C43	157.3 (3)	C31—Pd—P2—C111	37.10 (16)
C31—Pd—P1—C111	−38.17 (15)	Pd—P2—C211—C212	55.4 (3)
Pd—P1—C111—C112	64.1 (3)	Pd—P2—C221—C222	32.6 (3)
Pd—P1—C121—C122	56.3 (3)	Pd—P2—C231—C232	54.4 (3)
Pd—P1—C131—C132	−164.0 (3)		