Formation of *ortho*-Cyano-aminothiophenolate Ligands with Versatile Binding Modes *via* Facile Carbon-Sulfur Bond Cleavage of 2-Aminobenzothiazoles at Mercury(II) Centres

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Supplementary information

1. Synthesis and characterisation data

We have characterised all materials in this communication by IR spectroscopy and elemental analysis. Complexes **1a-d** had only limited solubility in dmso and NMR data were unreliable. For the phosphine derivatives we have evidence to suggest that in solution there is some degree of phosphine mobility and it seems that there is an equilibrium between $HgL(PR_3)$ and $HgL + HgL(PR_3)_2$. Consequently NMR spectra are temperature dependent and also concentration dependent as HgL precipitates. Full details of this will be reported in due course.

$[Hg\{SC_6H_3XN(C{\equiv}N)\}]_n$ (**1a-d**) - A warm solution of 2-aminobenzothiazole (0.20 g, 1.33 mmol) in EtOH (5 cm^3) was added to a warm solution of $Hg(OAc)_2$ (0.21 g, 0.665 mmol) in EtOH (5 cm^3). A yellow precipitate was formed. The mixture was stirred for 2h, and the yellow solid formed was filtered off, washed with EtOH and dried under vacuum to afford **1a** (0.20 g, 86%). **1b-d** were prepared in a similar manner.

1a: IR (KBr) 3064m, 2109vs (CN), 1577m, 1471s, 1433m, 738m, 665m cm^{-1}; Elemental analysis: Found (calc. for $Hg_1S_1N_2C_7H_4$): C 24.17 (24.11); H 1.22 (1.15); N 7.84 (8.03).

1b: IR (KBr) 3062w, 2125vs (CN), 1624s, 1469s, 738m, 675m cm^{-1}; Elemental analysis: Found (calc. for $Hg_1Cl_1S_1N_2C_7H_3$): C 21.84 (21.93); H 0.81 (0.78); N 7.30 (7.31).

1c: IR (KBr) 3062w, 2125vs (CN), 1624s, 1469s, 738m, 675m cm^{-1}. Elemental analysis: Found (calc. for $Hg_1Br_1S_1N_2C_7H_3$): C 19.39 (19.65); H 1.01 (0.70); N 6.38 (6.55).

1d: IR (KBr) 3024w, 2139vs (CN), 1621s, 1479s, 804s, 636m cm^{-1}. Elemental analysis: Found (calc. for $Hg_1S_1N_2C_8H_6$): C 29.67 (29.88); H 2.66 (1.95); N 3.53 (3.87).

$[Hg\{SC_6H_4N(C\equiv N)\}(Ph_2PCH_2CH_2)]_n$ (**2**) - A solution of dppb (0.17 g, θ.43 mmol) in $CHCl_3$ (5 cm^3) was added to **1d** (0.15 g, 0.43 mmol) suspended in $CHCl_3$ (5 cm^3). The mixture was stirred at room temperature for 1h to give a clear solution. This was heated under reflux for 2 h to give a greenish-yellow solid, which was filtered off, washed with $CHCl_3$ and dried under vacuum to afford **2** (0.24 g, 79 %). **2**: IR (KBr) 3055w, 2914w, 2135vs (CN), 1527m, 1481s, 1436s, 729s, 692m, 530vs, 509vs cm^{-1}; Elemental analysis: Found (calc. for $Hg_1S_1N_2P_2C_{35}H_{32}$) C 54.47 (54.22); H 3.92 (4.13); N 3.81 (3.61).

$[Hg\{SC_6H_3BrN(C\equiv N)\}(PPh_3)]_2$ (**3**) - A solution of Ph_3P (0.39 g, 1.52 mmol) in $CHCl_3$ (10 cm^3) was added to **1c** (0.32 g, 0.76 mmol) suspended in $CHCl_3$ (10 cm^3). The mixture was refluxed for 2h. After cooling to room temperature the solution was filtered to remove small amounts of an insoluble solid. The solvent was the left to evaporate slowly to give yellow needles of **3** (0.45 g, 76 %). **3**: IR (KBr) 3072w, 2165vs (CN), 2144vs (CN), 1460vs, 1434vs, 1317s, 1099s, 746s, 690s cm^{-1}; Elemental analysis: Found (calc. for $Hg_1Br_1S_1P_1N_2C_{25}H_{18}$): C 46.50 (46.66); H 2.61 (2.97); N 4.06 (4.12).

$[Hg\{SC_6H_4N(C\equiv N)\}(PPh_3)]_2$ (**4**) - A solution of Ph_3P (0.30 g,−1.14 mmol) in $CHCl_3$ (10 cm^3) was added to **1a** (0.20 g, 0.57 mmol) suspended in $CHCl_3$ (10 cm^3). The mixture was stirred at room temperature for 2 h to give a clear solution. This was heated under reflux for 2 h and then the solvent was left to evaporate at room temperature to give yellow needles of **4** (0.29 g, 83 %). **4**: IR (KBr) 3055w, 2958w, 2140vs (CN), 1568m, 1465s, 1434s, 748s, 690m cm^{-1}; Elemental analysis: Found (calc. for $Hg_1S_1P_1N_2C_{25}H_{19}.CH_2Cl_2$): C 44.06 (44.83); H 2.85 (3.02), N 3.89 (4.02).

2. Crystallographic information for 2

Identification code	z:\i2t1082
Empirical formula	C36 H34 Hg N2 P2 S
Formula weight	789.24
Temperature	200(2) K
Wavelength	0.71073 A
Crystal system, space group	triclinic, P-1
Unit cell dimensions	a = 10.7428(7) A alpha = 72.356(5) deg.
	b = 11.9618(7) A beta = 72.063(5) deg.
	c = 14.0140(9) A gamma = 88.360(5) deg.
Volume	1628.55(18) A^3
Z, Calculated density	2, 1.609 Mg/m^3
Absorption coefficient	4.916 mm^-1
F(000)	780
Crystal size	0.12 x 0.11 x 0.09 mm
Theta range for data collection	3.98 to 29.19 deg.
Limiting indices	-14<=h<=14, -16<=k<=16, -19<=l<=19
Reflections collected / unique	22909 / 8763 [R(int) = 0.0789]
Completeness to theta = 29.19	99.3 %
Max. and min. transmission	0.6660 and 0.5900
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8763 / 0 / 379
Goodness-of-fit on F^2	0.695
Final R indices [I>2sigma(I)]	R1 = 0.0330, wR2 = 0.0517
R indices (all data)	R1 = 0.0852, wR2 = 0.0602
Largest diff. peak and hole	1.780 and -2.638 e.A^-3

Table 3. Bond lengths [A] and angles [deg] for i2t1082.

C(1)-C(2)	1.400(6)
C(1)-C(6)	1.415(7)
C(1)-S	1.768(5)
C(2)-C(3)	1.394(6)
C(2)-N(1)	1.413(6)
C(3)-C(4)	1.399(7)
C(3)-H(1)	0.9500
C(4)-C(5)	1.356(7)
C(4)-H(2)	0.9500
C(5)-C(6)	1.388(6)
C(5)-C(8)	1.525(7)
C(6)-H(3)	0.9500
C(7)-N(2)	1.166(5)
C(7)-N(1)	1.286(6)
C(8)-H(4)	0.9800
C(8)-H(6)	0.9800
C(8)-H(5)	0.9800
C(9)-C(14)	1.371(7)
C(9)-C(10)	1.378(7)
C(9)-P(1)	1.810(5)
C(10)-C(11)	1.379(8)
C(10)-H(7)	0.9500
C(11)-C(12)	1.350(8)

C(11)-H(8)	0.9500
C(12)-C(13)	1.373(8)
C(12)-H(9)	0.9500
C(13)-C(14)	1.377(8)
C(13)-H(10)	0.9500
C(14)-H(11)	0.9500
C(15)-C(16)	1.379(6)
C(15)-C(20)	1.389(6)
C(15)-P(1)	1.812(5)
C(16)-C(17)	1.375(7)
C(16)-H(12)	0.9500
C(17)-C(18)	1.382(7)
C(17)-H(13)	0.9500
C(18)-C(19)	1.374(7)
C(18)-H(14)	0.9500
C(19)-C(20)	1.376(7)
C(19)-H(15)	0.9500
C(20)-H(16)	0.9500
C(21)-C(22)	1.518(6)
C(21)-P(1)	1.831(4)
C(21)-H(17)	0.9900
C(21)-H(18)	0.9900
C(22)-C(22)#1	1.511(8)
C(22)-H(20)	0.9900
C(22)-H(19)	0.9900
C(23)-C(24)	1.402(7)
C(23)-C(28)	1.412(7)
C(23)-P(2)	1.800(5)
C(24)-C(25)	1.372(7)
C(24)-H(21)	0.9500
C(25)-C(26)	1.377(9)
C(25)-H(22)	0.9500
C(26)-C(27)	1.374(9)
C(26)-H(23)	0.9500
C(27)-C(28)	1.383(7)
C(27)-H(24)	0.9500
C(28)-H(25)	0.9500
C(29)-C(30)	1.387(7)
C(29)-C(34)	1.400(7)
C(29)-P(2)	1.816(5)
C(30)-C(31)	1.395(7)
C(30)-H(26)	0.9500
C(31)-C(32)	1.384(9)
C(31)-H(27)	0.9500
C(32)-C(33)	1.372(9)
C(32)-H(28)	0.9500
C(33)-C(34)	1.369(8)
C(33)-H(29)	0.9500
C(34)-H(30)	0.9500
C(35)-C(36)	1.510(6)
C(35)-P(2)	1.830(5)
C(35)-H(32)	0.9900
C(35)-H(31)	0.9900
C(36)-C(36)#2	1.520(9)
C(36)-H(34)	0.9900

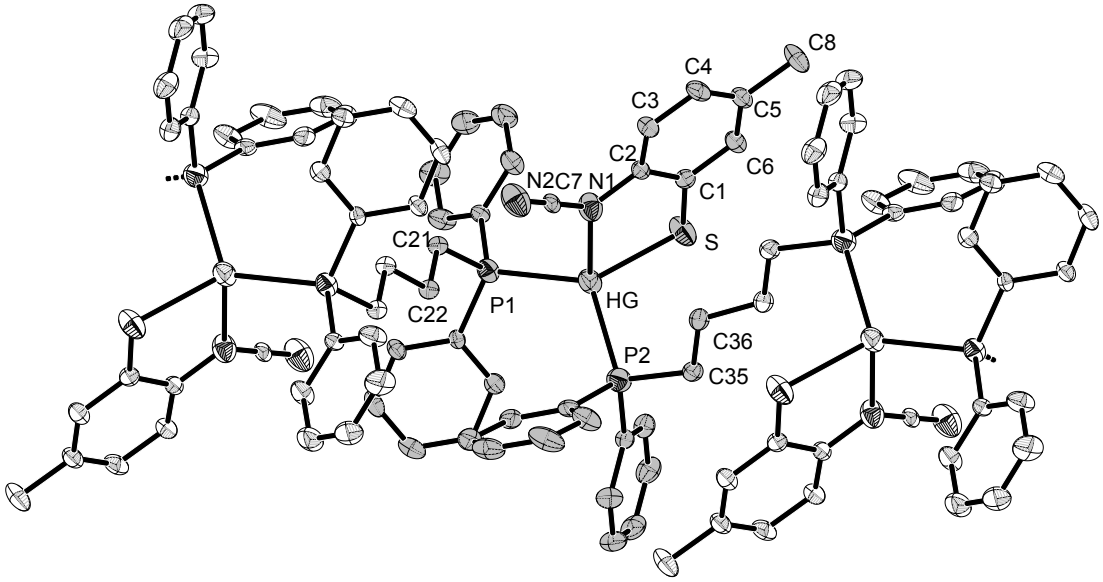
C(36)-H(33)	0.9900
N(1)-Hg#3	2.332(4)
P(1)-Hg	2.4650(12)
P(2)-Hg	2.5522(13)
S-Hg#3	2.4616(13)
Hg-N(1)#3	2.332(4)
Hg-S#3	2.4616(13)

C(2)-C(1)-C(6)	117.7(4)
C(2)-C(1)-S	125.2(4)
C(6)-C(1)-S	117.1(4)
C(3)-C(2)-C(1)	119.5(4)
C(3)-C(2)-N(1)	121.7(4)
C(1)-C(2)-N(1)	118.7(4)
C(2)-C(3)-C(4)	120.5(5)
C(2)-C(3)-H(1)	119.7
C(4)-C(3)-H(1)	119.7
C(5)-C(4)-C(3)	121.3(5)
C(5)-C(4)-H(2)	119.3
C(3)-C(4)-H(2)	119.3
C(4)-C(5)-C(6)	118.4(5)
C(4)-C(5)-C(8)	121.5(5)
C(6)-C(5)-C(8)	120.1(5)
C(5)-C(6)-C(1)	122.5(5)
C(5)-C(6)-H(3)	118.7
C(1)-C(6)-H(3)	118.7
N(2)-C(7)-N(1)	178.8(5)
C(5)-C(8)-H(4)	109.5
C(5)-C(8)-H(6)	109.5
H(4)-C(8)-H(6)	109.5
C(5)-C(8)-H(5)	109.5
H(4)-C(8)-H(5)	109.5
H(6)-C(8)-H(5)	109.5
C(14)-C(9)-C(10)	118.5(5)
C(14)-C(9)-P(1)	118.8(4)
C(10)-C(9)-P(1)	122.6(4)
C(9)-C(10)-C(11)	120.5(6)
C(9)-C(10)-H(7)	119.8
C(11)-C(10)-H(7)	119.8
C(12)-C(11)-C(10)	120.2(6)
C(12)-C(11)-H(8)	119.9
C(10)-C(11)-H(8)	119.9
C(11)-C(12)-C(13)	120.4(6)
C(11)-C(12)-H(9)	119.8
C(13)-C(12)-H(9)	119.8
C(12)-C(13)-C(14)	119.4(6)
C(12)-C(13)-H(10)	120.3
C(14)-C(13)-H(10)	120.3
C(9)-C(14)-C(13)	120.9(5)
C(9)-C(14)-H(11)	119.5
C(13)-C(14)-H(11)	119.5
C(16)-C(15)-C(20)	119.5(4)
C(16)-C(15)-P(1)	119.2(3)
C(20)-C(15)-P(1)	121.1(3)
C(17)-C(16)-C(15)	120.1(5)

C(17)-C(16)-H(12)	119.9
C(15)-C(16)-H(12)	119.9
C(16)-C(17)-C(18)	120.2(5)
C(16)-C(17)-H(13)	119.9
C(18)-C(17)-H(13)	119.9
C(19)-C(18)-C(17)	119.8(5)
C(19)-C(18)-H(14)	120.1
C(17)-C(18)-H(14)	120.1
C(18)-C(19)-C(20)	120.2(5)
C(18)-C(19)-H(15)	119.9
C(20)-C(19)-H(15)	119.9
C(19)-C(20)-C(15)	120.1(4)
C(19)-C(20)-H(16)	120.0
C(15)-C(20)-H(16)	120.0
C(22)-C(21)-P(1)	115.0(3)
C(22)-C(21)-H(17)	108.5
P(1)-C(21)-H(17)	108.5
C(22)-C(21)-H(18)	108.5
P(1)-C(21)-H(18)	108.5
H(17)-C(21)-H(18)	107.5
C(22)#1-C(22)-C(21)	111.5(5)
C(22)#1-C(22)-H(20)	109.3
C(21)-C(22)-H(20)	109.3
C(22)#1-C(22)-H(19)	109.3
C(21)-C(22)-H(19)	109.3
H(20)-C(22)-H(19)	108.0
C(24)-C(23)-C(28)	117.7(5)
C(24)-C(23)-P(2)	123.1(4)
C(28)-C(23)-P(2)	119.1(4)
C(25)-C(24)-C(23)	121.0(6)
C(25)-C(24)-H(21)	119.5
C(23)-C(24)-H(21)	119.5
C(24)-C(25)-C(26)	120.1(6)
C(24)-C(25)-H(22)	119.9
C(26)-C(25)-H(22)	119.9
C(27)-C(26)-C(25)	120.6(6)
C(27)-C(26)-H(23)	119.7
C(25)-C(26)-H(23)	119.7
C(26)-C(27)-C(28)	120.0(6)
C(26)-C(27)-H(24)	120.0
C(28)-C(27)-H(24)	120.0
C(27)-C(28)-C(23)	120.5(6)
C(27)-C(28)-H(25)	119.8
C(23)-C(28)-H(25)	119.8
C(30)-C(29)-C(34)	118.4(5)
C(30)-C(29)-P(2)	118.7(4)
C(34)-C(29)-P(2)	122.9(4)
C(29)-C(30)-C(31)	121.7(5)
C(29)-C(30)-H(26)	119.1
C(31)-C(30)-H(26)	119.1
C(32)-C(31)-C(30)	118.1(6)
C(32)-C(31)-H(27)	121.0
C(30)-C(31)-H(27)	121.0
C(33)-C(32)-C(31)	120.7(6)
C(33)-C(32)-H(28)	119.6

C(31)-C(32)-H(28)	119.6
C(34)-C(33)-C(32)	121.1(6)
C(34)-C(33)-H(29)	119.5
C(32)-C(33)-H(29)	119.5
C(33)-C(34)-C(29)	119.9(6)
C(33)-C(34)-H(30)	120.0
C(29)-C(34)-H(30)	120.0
C(36)-C(35)-P(2)	114.6(3)
C(36)-C(35)-H(32)	108.6
P(2)-C(35)-H(32)	108.6
C(36)-C(35)-H(31)	108.6
P(2)-C(35)-H(31)	108.6
H(32)-C(35)-H(31)	107.6
C(35)-C(36)-C(36)#2	112.2(5)
C(35)-C(36)-H(34)	109.2
C(36)#2-C(36)-H(34)	109.2
C(35)-C(36)-H(33)	109.2
C(36)#2-C(36)-H(33)	109.2
H(34)-C(36)-H(33)	107.9
C(7)-N(1)-C(2)	119.5(4)
C(7)-N(1)-Hg#3	123.5(3)
C(2)-N(1)-Hg#3	116.4(3)
C(9)-P(1)-C(15)	109.2(2)
C(9)-P(1)-C(21)	103.0(2)
C(15)-P(1)-C(21)	105.5(2)
C(9)-P(1)-Hg	113.54(16)
C(15)-P(1)-Hg	113.32(14)
C(21)-P(1)-Hg	111.42(16)
C(23)-P(2)-C(29)	104.7(2)
C(23)-P(2)-C(35)	106.1(2)
C(29)-P(2)-C(35)	109.1(2)
C(23)-P(2)-Hg	112.83(18)
C(29)-P(2)-Hg	115.85(15)
C(35)-P(2)-Hg	107.84(18)
C(1)-S-Hg#3	98.66(17)
N(1)#3-Hg-S#3	80.72(11)
N(1)#3-Hg-P(1)	99.87(10)
S#3-Hg-P(1)	131.83(5)
N(1)#3-Hg-P(2)	109.74(11)
S#3-Hg-P(2)	106.56(4)
P(1)-Hg-P(2)	117.88(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z+1 #2 -x+1,-y+1,-z #3 -x,-y+1,-z


C8
C4
C3
C5
C2
C6
N2C7 N1
C1
S
C21
C22
P1
HG
P2
C36
C35

4. Crystallographic information for 3

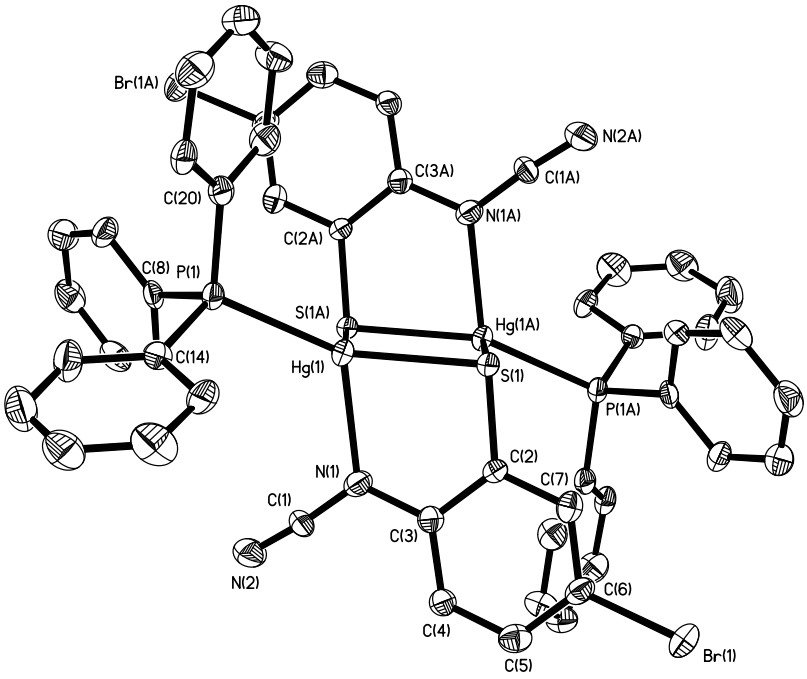
Identification code	str0940	
Chemical formula	$C_{27}H_{20}BrCl_6HgN_2PS$	
Formula weight	928.68	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, P1bar	
Unit cell parameters	a = 9.444(3) Å	α = 86.793(4)°
	b = 12.224(3) Å	β = 79.034(4)°
	c = 13.807(4) Å	γ = 87.326(5)°
Cell volume	1561.4(7) Å^3	
Z	2	
Calculated density	1.975 g/cm^3	
Absorption coefficient μ	6.862 mm^{-1}	
F(000)	888	
Crystal colour and size	yellow, 0.42 × 0.18 × 0.16 mm^3	
Data collection method	Bruker SMART 1K CCD diffractometer	
	ω rotation with narrow frames	
θ range for data collection	2.42 to 28.25°	
Index ranges	h −12 to 12, k −15 to 16, l −17 to 17	
Completeness to θ = 26.00°	96.6 %	
Reflections collected	12571	
Independent reflections	6784 (R_{int} = 0.0489)	
Reflections with $F^2>2\sigma$	5189	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.1607 and 0.4065	
Structure solution	Patterson synthesis	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0426, 0.0000	
Data / restraints / parameters	6784 / 0 / 352	
Final R indices [$F^2>2\sigma$]	R_1 = 0.0449, wR_2 = 0.0945	
R indices (all data)	R_1 = 0.0581, wR_2 = 0.0966	
Goodness-of-fit on F^2	0.942	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	2.471 and −2.651 e Å^{-3}	

Bond lengths [Å] and angles [°] for str0940.

Hg(1)–N(1)	2.266(5)	Hg(1)–P(1)	2.3718(16)
Hg(1)–S(1)	2.4105(16)	Hg(1)–S(1A)	2.8710(17)
Br(1)–C(6)	1.870(6)	P(1)–C(20)	1.779(6)
P(1)–C(14)	1.786(6)	P(1)–C(8)	1.789(7)
S(1)–C(2)	1.757(6)	S(1)–Hg(1A)	2.8710(17)
N(1)–C(1)	1.287(8)	N(1)–C(3)	1.390(8)
N(2)–C(1)	1.154(8)	C(2)–C(7)	1.374(9)
C(2)–C(3)	1.394(8)	C(3)–C(4)	1.391(8)
C(4)–C(5)	1.359(9)	C(5)–C(6)	1.372(9)
C(6)–C(7)	1.377(8)	C(8)–C(13)	1.373(9)
C(8)–C(9)	1.374(9)	C(9)–C(10)	1.352(9)
C(10)–C(11)	1.373(10)	C(11)–C(12)	1.355(10)
C(12)–C(13)	1.371(10)	C(14)–C(15)	1.382(9)
C(14)–C(19)	1.394(9)	C(15)–C(16)	1.376(9)
C(16)–C(17)	1.329(10)	C(17)–C(18)	1.358(11)

C(18)–C(19)	1.381(9)	C(20)–C(25)	1.380(9)
C(20)–C(21)	1.394(8)	C(21)–C(22)	1.367(9)
C(22)–C(23)	1.364(9)	C(23)–C(24)	1.372(9)
C(24)–C(25)	1.366(9)	C(26)–Cl(3)	1.710(9)
C(26)–Cl(1)	1.736(9)	C(26)–Cl(2)	1.748(9)
C(27)–Cl(4)	1.703(8)	C(27)–Cl(6)	1.729(8)
C(27)–Cl(5)	1.735(9)		

N(1)–Hg(1)–P(1)	122.19(13)	N(1)–Hg(1)–S(1)	80.76(14)
P(1)–Hg(1)–S(1)	151.40(6)	N(1)–Hg(1)–S(1A)	86.06(14)
P(1)–Hg(1)–S(1A)	101.62(5)	S(1)–Hg(1)–S(1A)	96.43(5)
C(20)–P(1)–C(14)	108.4(3)	C(20)–P(1)–C(8)	107.0(3)
C(14)–P(1)–C(8)	108.2(3)	C(20)–P(1)–Hg(1)	111.5(2)
C(14)–P(1)–Hg(1)	110.7(2)	C(8)–P(1)–Hg(1)	111.0(2)
C(2)–S(1)–Hg(1)	98.4(2)	C(2)–S(1)–Hg(1A)	99.1(2)
Hg(1)–S(1)–Hg(1A)	83.57(5)	C(1)–N(1)–C(3)	121.8(5)
C(1)–N(1)–Hg(1)	122.1(4)	C(3)–N(1)–Hg(1)	115.7(4)
N(2)–C(1)–N(1)	174.6(7)	C(7)–C(2)–C(3)	119.3(6)
C(7)–C(2)–S(1)	118.1(5)	C(3)–C(2)–S(1)	122.6(5)
N(1)–C(3)–C(4)	122.5(6)	N(1)–C(3)–C(2)	119.2(5)
C(4)–C(3)–C(2)	118.3(6)	C(5)–C(4)–C(3)	121.9(6)
C(4)–C(5)–C(6)	119.4(6)	C(5)–C(6)–C(7)	120.0(6)
C(5)–C(6)–Br(1)	120.2(5)	C(7)–C(6)–Br(1)	119.8(5)
C(2)–C(7)–C(6)	121.0(6)	C(13)–C(8)–C(9)	120.2(6)
C(13)–C(8)–P(1)	120.7(5)	C(9)–C(8)–P(1)	119.1(5)
C(10)–C(9)–C(8)	119.8(6)	C(9)–C(10)–C(11)	120.1(7)
C(12)–C(11)–C(10)	120.5(7)	C(11)–C(12)–C(13)	120.0(7)
C(12)–C(13)–C(8)	119.5(7)	C(15)–C(14)–C(19)	120.5(6)
C(15)–C(14)–P(1)	119.8(5)	C(19)–C(14)–P(1)	119.7(5)
C(16)–C(15)–C(14)	117.8(6)	C(17)–C(16)–C(15)	122.4(7)
C(16)–C(17)–C(18)	120.4(6)	C(17)–C(18)–C(19)	120.4(7)
C(18)–C(19)–C(14)	118.5(7)	C(25)–C(20)–C(21)	119.0(6)
C(25)–C(20)–P(1)	123.7(5)	C(21)–C(20)–P(1)	117.3(5)
C(22)–C(21)–C(20)	120.5(6)	C(23)–C(22)–C(21)	119.9(6)
C(22)–C(23)–C(24)	120.0(7)	C(25)–C(24)–C(23)	121.0(7)
C(24)–C(25)–C(20)	119.5(6)	Cl(3)–C(26)–Cl(1)	109.7(4)
Cl(3)–C(26)–Cl(2)	112.3(5)	Cl(1)–C(26)–Cl(2)	109.0(5)
Cl(4)–C(27)–Cl(6)	111.1(5)	Cl(4)–C(27)–Cl(5)	109.1(5)
Cl(6)–C(27)–Cl(5)	110.4(4)		


Br(1A)
N(2A)
C(3A)
C(1A)
C(20)
N(1A)
C(2A)
C(8)
P(1)
S(1A)
Hg(1A)
C(14)
Hg(1)
S(1)
P(1A)
N(1)
C(2)
C(7)
C(1)
C(3)
N(2)
C(6)
C(4)
C(5)
Br(1)

5. Crystallographic information for 4

Identification code	str0938	
Chemical formula	$C_{25}H_{19}HgN_2PS$	
Formula weight	611.04	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, P1bar	
Unit cell parameters	a = 8.955(3) Å	α = 103.936(5)°
	b = 10.643(4) Å	β = 102.011(5)°
	c = 12.059(4) Å	γ = 101.091(5)°
Cell volume	1054.8(6) Å^3	
Z	2	
Calculated density	1.924 g/cm^3	
Absorption coefficient μ	7.486 mm^{-1}	
F(000)	588	
Crystal colour and size	yellow, 0.12 × 0.07 × 0.04 mm^3	
Data collection method	Bruker SMART 1K CCD diffractometer	
	ω rotation with narrow frames	
θ range for data collection	2.73 to 28.48°	
Index ranges	h −11 to 11, k −13 to 14, l −15 to 15	
Completeness to θ = 26.00°	96.3 %	
Reflections collected	8623	
Independent reflections	4657 (R_{int} = 0.0392)	
Reflections with $F^2>2\sigma$	3744	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.4670 and 0.7539	
Structure solution	Patterson synthesis	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0223, 0.0000	
Data / restraints / parameters	4657 / 0 / 271	
Final R indices [$F^2>2\sigma$]	R_1 = 0.0377, wR_2 = 0.0647	
R indices (all data)	R_1 = 0.0480, wR_2 = 0.0660	
Goodness-of-fit on F^2	0.919	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	1.726 and −1.731 e Å^{-3}	

Bond lengths [Å] and angles [°] for str0938.

Hg(1)–N(1)	2.312(4)	Hg(1)–S(1)	2.3520(15)
Hg(1)–P(1)	2.3731(15)	Hg(1)–N(2A)	2.517(5)
P(1)–C(20)	1.783(5)	P(1)–C(14)	1.788(5)
P(1)–C(8)	1.789(5)	S(1)–C(2)	1.757(6)
N(1)–C(1)	1.287(6)	N(1)–C(3)	1.381(7)
N(2)–C(1)	1.153(6)	N(2)–Hg(1A)	2.517(5)
C(2)–C(7)	1.383(8)	C(2)–C(3)	1.396(7)
C(3)–C(4)	1.380(7)	C(4)–C(5)	1.358(8)
C(5)–C(6)	1.369(9)	C(6)–C(7)	1.353(8)
C(8)–C(9)	1.377(7)	C(8)–C(13)	1.389(7)
C(9)–C(10)	1.363(7)	C(10)–C(11)	1.372(8)
C(11)–C(12)	1.371(8)	C(12)–C(13)	1.363(7)
C(14)–C(19)	1.365(7)	C(14)–C(15)	1.381(7)
C(15)–C(16)	1.361(8)	C(16)–C(17)	1.363(8)
C(17)–C(18)	1.346(8)	C(18)–C(19)	1.374(7)

C(20)–C(21)	1.372(7)	C(20)–C(25)	1.374(7)
C(21)–C(22)	1.356(7)	C(22)–C(23)	1.367(8)
C(23)–C(24)	1.360(8)	C(24)–C(25)	1.362(7)

N(1)–Hg(1)–S(1)	81.76(11)	N(1)–Hg(1)–P(1)	122.04(11)
S(1)–Hg(1)–P(1)	147.76(5)	N(1)–Hg(1)–N(2A)	91.86(14)
S(1)–Hg(1)–N(2A)	109.18(11)	P(1)–Hg(1)–N(2A)	92.66(11)
C(20)–P(1)–C(14)	107.0(2)	C(20)–P(1)–C(8)	107.1(2)
C(14)–P(1)–C(8)	106.2(2)	C(20)–P(1)–Hg(1)	114.73(18)
C(14)–P(1)–Hg(1)	109.15(18)	C(8)–P(1)–Hg(1)	112.18(18)
C(2)–S(1)–Hg(1)	99.64(19)	C(1)–N(1)–C(3)	119.0(4)
C(1)–N(1)–Hg(1)	124.8(4)	C(3)–N(1)–Hg(1)	114.8(3)
C(1)–N(2)–Hg(1A)	121.4(4)	N(2)–C(1)–N(1)	176.2(6)
C(7)–C(2)–C(3)	118.6(5)	C(7)–C(2)–S(1)	117.7(4)
C(3)–C(2)–S(1)	123.6(4)	C(4)–C(3)–N(1)	122.5(5)
C(4)–C(3)–C(2)	118.3(5)	N(1)–C(3)–C(2)	119.1(5)
C(5)–C(4)–C(3)	121.6(6)	C(4)–C(5)–C(6)	120.2(6)
C(7)–C(6)–C(5)	119.3(6)	C(6)–C(7)–C(2)	121.9(6)
C(9)–C(8)–C(13)	119.8(5)	C(9)–C(8)–P(1)	122.0(4)
C(13)–C(8)–P(1)	118.1(4)	C(10)–C(9)–C(8)	120.0(5)
C(9)–C(10)–C(11)	120.1(5)	C(12)–C(11)–C(10)	120.2(5)
C(13)–C(12)–C(11)	120.4(6)	C(12)–C(13)–C(8)	119.5(5)
C(19)–C(14)–C(15)	118.7(5)	C(19)–C(14)–P(1)	120.0(4)
C(15)–C(14)–P(1)	121.3(4)	C(16)–C(15)–C(14)	120.3(5)
C(15)–C(16)–C(17)	120.0(5)	C(18)–C(17)–C(16)	120.4(6)
C(17)–C(18)–C(19)	120.1(5)	C(14)–C(19)–C(18)	120.5(5)
C(21)–C(20)–C(25)	119.4(5)	C(21)–C(20)–P(1)	122.1(4)
C(25)–C(20)–P(1)	118.5(4)	C(22)–C(21)–C(20)	120.2(5)
C(21)–C(22)–C(23)	119.8(6)	C(24)–C(23)–C(22)	120.7(5)
C(23)–C(24)–C(25)	119.5(5)	C(24)–C(25)–C(20)	120.4(5)