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Supplementary data for  
**High pressure co-ordination chemistry of a palladium thioether  
complex: pressure *versus* electrons**

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**Additional graphs showing the structural trends in *cis*-[PdCl<sub>2</sub>([9]aneS<sub>3</sub>)] as a function of pressure:**

**Figure S1: unit cell dimensions and volume**

**Figure S2: the Pd<sup>···</sup>S1 distance**

**Figure S3: the Pd<sup>···</sup>S4' distance**

**Figure S4: torsion angles of the macrocyclic ring**

**Details of literature structural studies on coordination complexes.**

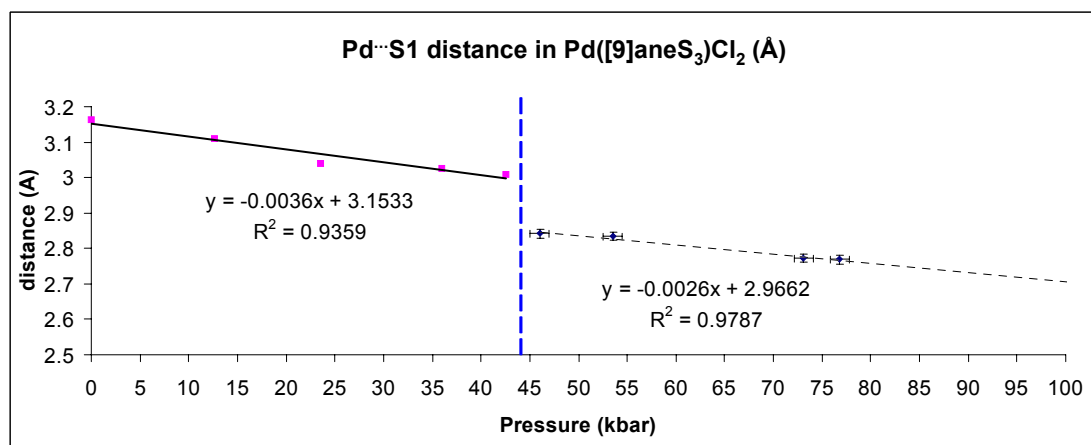
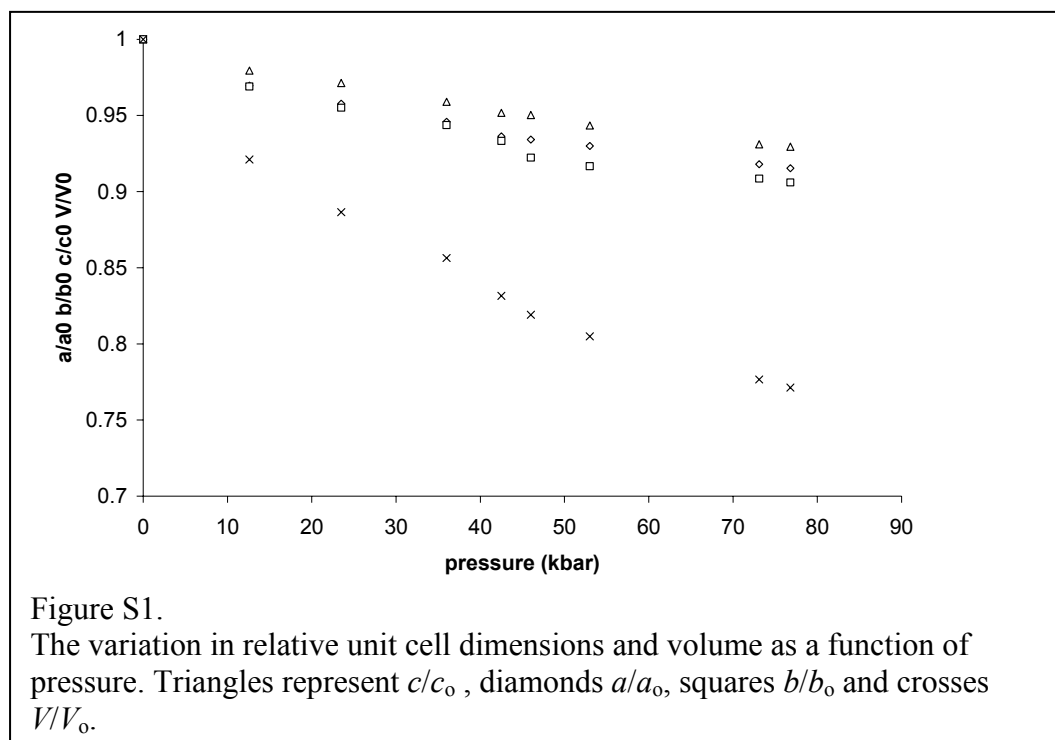


Figure S2.  
The variation in the Pd...S1 distance as a function of pressure. Note the discontinuity and the change in slope at a pressure of 44 kbar (indicated by the blue dashed line).

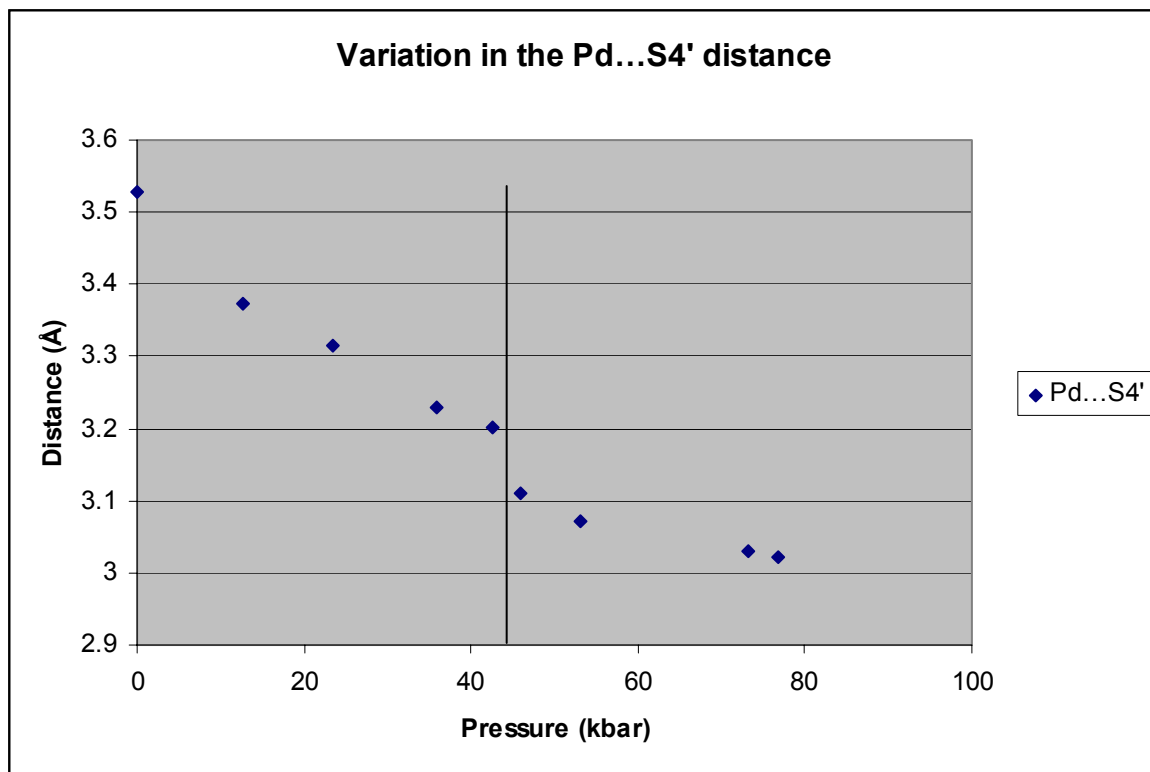


Figure S3.

The variation in the Pd...S4' distance as a function of pressure. Note the discontinuity and the change in slope at 44 kbar (indicated by the vertical line).

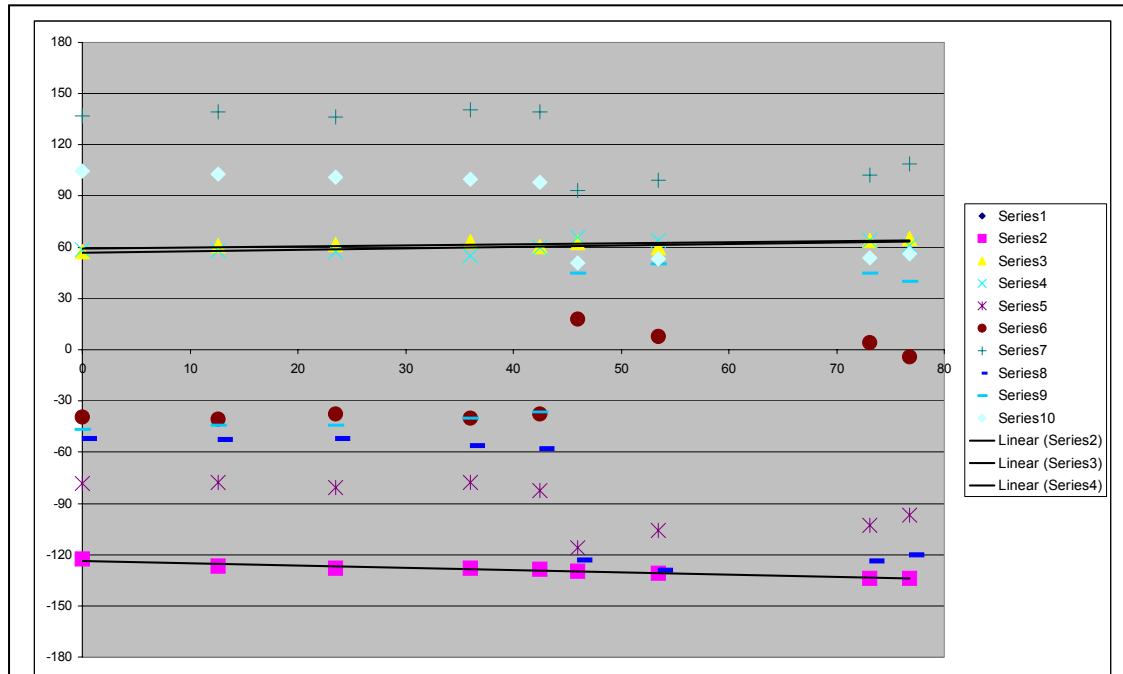


Figure S4.

The variation in the torsion angles of the macrocyclic ring as a function of pressure. The symbols labelled Series2...Series 10 represent the following respective torsion angles: C9S1—C2C3, S1C2—C3S4, C2C3—S4C5, C3S4—C5C6, S4C5—C6S7, C5C6—S7C8, C6S7—C8C9, S7C8—C9S1 and C2S1—C9C8. Note the relative invariance in the first three torsion angles, for which linear fits are plotted, in contrast to the marked changes in the others at 44 kbar.

**Literature on high pressure structural studies on coordination complexes**

(CCDC number and code; chemical name; pressure(s); formula; authors; bibliographic reference)

80952 Ptmglo04

Bis(Dimethylglyoximato-N,N')-Platinum(II)

Pressures 2.39 and 3.14 GPa

C<sub>8</sub> H<sub>14</sub> N<sub>4</sub> O<sub>4</sub> Pt<sub>1</sub>

M.Konno, T.Okamoto, I.Shiratori,

45 142 1989 Acta Crystallogr., Sect. B: Struct. Sci.

125401 Pasgof02

Bis(2,2'-Bi-4,5-Dihydrothiazine-N,N')-Di-Isothiocyanato-Iron(II)

Pressure 0.95 GPa

C<sub>18</sub> H<sub>24</sub> Fe<sub>1</sub> N<sub>6</sub> S<sub>6</sub>

T.Granier, B.Gallois, J.Gaultier, J.-A.Real, J.Zarembowitch

32 5305 1993 Inorg.Chem.

124157 Kekvif02

Bis(1,10-Phenanthroline-N,N')-Di-Isothiocyanato-Iron(II) Low-Spin Polymorph

Pressure about 1.0 GPa

C<sub>26</sub> H<sub>16</sub> Fe<sub>1</sub> N<sub>6</sub> S<sub>2</sub>

T.Granier, B.Gallois, J.Gaultier, J.-A.Real, J.Zarembowitch

32 5305 1993 Inorg.Chem.

162637 Dusbey06 Bis(Bis(Ethylenedithio)Tetrathiafulvalene) Dicyano-silver Alpha' Polymorph

Pressures 5.5, 8 and 11 Kbar

C<sub>10</sub> H<sub>8</sub> S<sub>8</sub> + C<sub>10</sub> H<sub>8</sub> S<sub>8</sub> C<sub>2</sub> Ag<sub>1</sub> N<sub>2</sub> -

P.Guionneau, J.Gaultier, M.Rahal, G.Bravic, J.M.Mellado, D.Chasseau, L.Du Casse, M.Kurmoo, P.Day

5 1639 1995 J.Mater.Chem.

267059 Xecmib03

Bis(N-(2-Pyridylmethylene)-4-Amino-1,1',4',1''-Terphenyl)-Diisothiocyanato-Iron(II) Methanol

Solvate High Spin Polymorph

Pressures 0.16 and 0.40 GPa

C<sub>50</sub> H<sub>36</sub> Fe<sub>1</sub> N<sub>6</sub> S<sub>2</sub> C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>

P.Guionneau, C.Brigouleix, Y.Barrans, A.E.Goeta, J.-F.Letard, J.A.K.Howard, J.Gaultier, D.Chasseau

4 161 2001 C.R.Acad.Sci., Ser.IIc:Chim.

357152 Nibsog01

Catena-(( $\mu$ -2-- $\eta$ -5-,  $\eta$ -5--Cyclopentadienyl)-Potassium)

Pressures 0.028, 0.164, 0.3545, 0.6725, 0.971, 1.2925, 2.1775, 2.8075, 3.856 and 5.1665 GPa

(C<sub>5</sub> H<sub>5</sub> K<sub>1</sub>)<sub>N</sub>

R.E.Dinnebier, S.Van Smaalen, F.Olbrich, S.Carlson

44 964 2005 Inorg.Chem.

329239 Ptmglo06

Bis(Dimethylglyoximato-O,O')-Platinum(II)

Pressure 2.39 GPa

C<sub>8</sub> H<sub>14</sub> N<sub>4</sub> O<sub>4</sub> Pt<sub>1</sub>

I.Shiratori, M.Konno, Y.Taniguchi

29 F123 1989 Synth.Met.

170403 Gamfij10

Catena-(Bis(Bis(Ethylenedithio)Tetrathiafulvalene) ( $\mu$ -2--Isothiocyanato)-Isothiocyanato-Copper)

Kappa Polymorph

Pressure 0.75 MPa

(C<sub>10</sub> H<sub>8</sub> S<sub>8</sub> +)N N(C<sub>10</sub> H<sub>8</sub> S<sub>8</sub>) N(C<sub>2</sub> Cu<sub>1</sub> N<sub>2</sub> S<sub>2</sub> -)

M.Rahal, D.Chasseau, J.Gaultier, L.Ducasse, M.Kurmoo, P.Day

53 159 1997 Acta Crystallogr., Sect. B: Struct. Sci.