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-[PdCl₂([9]aneS₃)] as a function of pressure:

Figure S1: unit cell dimensions and volume
Figure S2: the Pd⋯S1 distance
Figure S3: the Pd⋯S4’ distance
Figure S4: torsion angles of the macrocyclic ring

Details of literature structural studies on coordination complexes.
Figure S1.
The variation in relative unit cell dimensions and volume as a function of pressure. Triangles represent $c/c_0$, diamonds $a/a_0$, squares $b/b_0$ and crosses $V/V_0$.

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
C8 H14 N4 O4 Pt1
M.Konno,T.Okamoto,I.Shirotani,

125401 Pasgofo2
Bis(2,2'-Bi-4,5-Dihydrothiazine-N,N')-Di-Isothiocyanato-Iron(II)
Pressure 0.95 GPa
C18 H24 Fe1 N6 S6
T.Granier,B.Gallois,J.Gaultier,J.-A.Real,J.Zarembowitch

124157 Kekvio02
Bis(1,10-Phenanthroline-N,N')-Di-Isothiocyanato-Iron(II) Low-Spin Polymorph
Pressure about 1.0 GPa
C26 H16 Fe1 N6 S2
T.Granier,B.Gallois,J.Gaultier,J.-A.Real,J.Zarembowitch

162637 Dusbey06 Bis(Bis(Ethylenedithio)Tetrathiafulvalene) Dicyano-silver Alpha' Polymorph
Pressures 5.5, 8 and 11 Kbar
C10 H8 S8 + C10 H8 S8 C2 Ag1 N2 -
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
C50 H36 Fe1 N6 S2
P.Guionneau,C.Brigouleix,Y.Barrans,A.E.Goeta,J.-F.Letard,J.A.K.Howard,J.Gaultier,D.Chasseau

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
(C5 H5 K1)N
R.E.Dinnebier,S.Van Smaalen,F.Olbrich,S.Carlson

329239 Ptmglo06
Bis(Dimethylglyoximato-O,O')-Platinum(II)
Pressure 2.39 GPa
C8 H14 N4 O4 Pt1
I.Shirotani,M.Konno,Y.Taniguchi

170403 Gamfij10
Catena-(Bis(Bis(Ethylenedithio)Tetrathiafulvalene) (Mu-2--Isothiocyanato)-Isothiocyanato-Copper) Kappa Polymorph
Pressure 0.75 MPa
(C10 H8 S8 +)N (N(C10 H8 S8)) N(C2 Cu1 N2 S2 -)
M.Rahal,D.Chasseau,J.Gaultier,L.Ducasse,M.Kurmoo,P.Day