Supplementary material (Olofsson-Mårtensson, Kritikos and Noréus) JA991047R

Table of experimental χ_M values of Ba_2PdH_4.

(The experimental susceptibility data are corrected for sampleholder diamagnetism and for core electron diamagnetism using Pascal´s constants.)

T (K)	χ_M ($m^3 \cdot mol^{-1}$)	T (K)	χ_M ($m^3 \cdot mol^{-1}$)
1.189E+1	-5.455E-9	6.421E+1	-2.284E-8
1.215E+1	-7.111E-9	6.740E+1	-2.285E-8
1.276E+1	-5.473E-9	7.093E+1	-2.366E-8
1.338E+1	-6.463E-9	7.448E+1	-2.413E-8
1.410E+1	-7.441E-9	7.828E+1	-2.490E-8
1.480E+1	-3.182E-9	8.230E+1	-2.276E-8
1.559E+1	-1.432E-8	8.653E+1	-2.302E-8
1.636E+1	-8.512E-9	9.001E+1	-2.558E-8
1.720E+1	-1.112E-8	9.453E+1	-2.693E-8
1.805E+1	-7.867E-9	9.936E+1	-2.707E-8
1.904E+1	-8.615E-9	1.045E+2	-1.936E-8
1.982E+1	-1.317E-8	1.097E+2	-1.586E-8
2.084E+1	-5.118E-9	1.153E+2	-2.051E-8
2.192E+1	-1.064E-8	1.213E+2	-2.242E-8
2.297E+1	-1.041E-8	1.273E+2	-2.352E-8
2.401E+1	-1.230E-8	1.339E+2	-1.776E-8
2.513E+1	-1.261E-8	1.408E+2	-1.778E-8
2.629E+1	-1.212E-8	1.465E+2	-1.730E-8
2.772E+1	-1.821E-8	1.529E+2	-1.650E-8
2.924E+1	-1.286E-8	1.618E+2	-1.860E-8
3.073E+1	-1.531E-8	1.702E+2	-1.592E-8
3.208E+1	-1.049E-8	1.788E+2	-1.588E-8
3.383E+1	-1.402E-8	1.881E+2	-1.672E-8
3.542E+1	-1.826E-8	1.976E+2	-1.704E-8
3.736E+1	-1.761E-8	2.077E+2	-2.301E-8
3.939E+1	-2.347E-8	2.183E+2	-2.547E-8
4.131E+1	-1.661E-8	2.294E+2	-2.116E-8
4.358E+1	-2.173E-8	2.411E+2	-2.882E-8
4.568E+1	-1.984E-8	2.512E+2	-2.590E-8
4.806E+1	-1.360E-8	2.637E+2	-2.726E-8
5.058E+1	-2.824E-8	2.774E+2	-2.724E-8
5.314E+1	-2.033E-8	2.915E+2	-2.621E-8
5.522E+1	-1.830E-8	3.064E+2	-2.996E-8
5.812E+1	-2.314E-8	3.221E+2	-3.142E-8
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wR and all goodnesses 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 observed criterion
of F^2^ > 2sigma(F^2^) is used only for calculating _R_factor_obs etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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 '-x, y+1/2, -z'
 '-x, -y, -z'
 'x-1/2, y, -z-1/2'
 '-x-1/2, y-1/2, z-1/2'
 'x, -y-1/2, z'

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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^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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'calc w=1/[\s^2^(Fo^2^)+(0.1282P)^2^+17.0159P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
_refine_ls_hydrogen_treatment    mixed
_refine_ls_extinction_method     SHELXL
_refine_ls_extinction_coef       0.000(3)
_refine_ls_extinction_expression
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry. An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Sr1 Sr2 3.946(2) 5_565 ?
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