

Volume 77 (2021)

Supporting information for article:

One- and two-dimensional Pb^{II} compounds resulting from PbBr2 and Pb(SCN)2 with pyrimidine-2-thione

VĂnia Denise Schwade and Bárbara Tirloni



Figure S1 (a) The coordination polyhedron of the Pb^{II} centre in (I) [Symmetry codes: (i) x, y, -z+3/2; (ii) x, -y+1/2, -z+1; (iii) -x+1, -y, -z+1; (iv) -x+1, -y, z+1/2; (v) -x+1, y+1/2, -z+3/2.]. (b) The coordination polyhedron of the Pb^{II} centre in (IIa) [Symmetry code: (i) x-1, y, z.]. (c) The coordination polyhedron of the Pb^{II} centre in (IIb) [Symmetry codes: (i) -x+3/2, y-1/2, -z+3/2; (ii) -x+3/2, y+1/2, -z+3/2; (iii) x, y-1, z; (iv) x, y+1, z].



Figure S2 TG-DSC curves of (I) in N₂ atmosphere.



Figure S3 View of compound (IIb) in the *ab* plane.



Figure S4 View of compound (IIb) in the *ac* plane.



Figure S5 FT-IR spectrum of (I).



Figure S6 FT-IR spectrum of (IIa).



Figure S7 Diffuse reflectance spectra of (I) and (IIa).



Figure S8 Comparative for the precipitated solid from reaction of PbBr₂ and HSpym in DMF (14 ml). The red and blue dashed lines represent the presence of (IIa) and (IIb), respectively, in the experimental PXRD pattern of the precipitate.



Figure S9 FT-IR spectrum of the white solid obtained by transformation of (II) in solution.



Figure S10 PXRD diffractogram of the white solid obtained by transformation of (II) in solution. Bruker D8 Advance diffractometer (Cu- $K\alpha$ radiation), slit of 0.2°, 0.2 s per step and a step size of 0.01°.



Figure S11Appearance of compound (II) (yellow) and compound $\{[Pb(Spym)Br] \cdot DMF\}n$ (white).