A method for obtaining an iron-containing complex with a spin transition of the formula [Fe(pz)2(BH3CN)2], where pz is pyrazine, comprises obtaining an ethanol solution of Fe(BH3CN)2 by dispersing a twofold excess of 2, 5 % solution of NaBH3CN in ethanol, followed by mixing with a 20 % solution of Fe(OTs)2×6H2O in ethanol, separating the resulting ethanol solution of Fe(BH3CN)2 from the undissolved excess of NaBH3CN by centrifugation. Next, mix the obtained ethanol solution of Fe(BH3CN)2 with a threefold excess of pyrazine (ligand) in ethanol (33 % solution). The resulting mixture is incubated for 60 minutes. Centrifuge the dark red polycrystalline powder [Fe(pz)2(BH3CN)2], followed by washing with ethanol and drying.