Supporting Information

Reversible single-crystal-to-single-crystal photoisomerization of a silver(I) macropolyhedral borane

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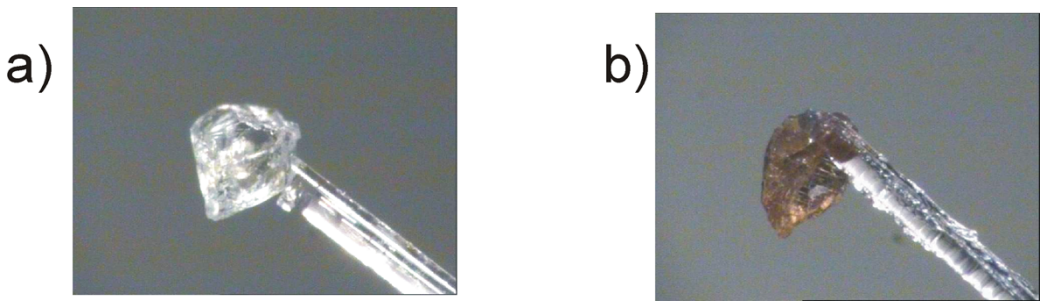

Figure S1. Photo of the single crystal (a) before and (b) after UV irradiation.

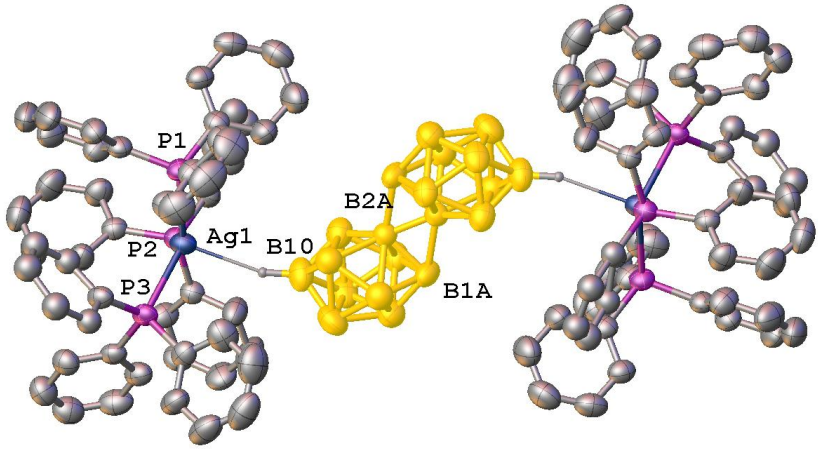

Figure S2. Molecular view of $\{Ag_2(PPh_3)_6[10,10'\text{-}trans\text{-}B_{20}H_{18}]\}$ at 363 K given in representation of atoms with thermal ellipsoids (given at p = 50%). Hydrogen atoms (with an exception of those involved in B – H…Ag bonding) are omitted for clarity. Only major part of disordered complex is given; the minor part is depicted in full text.

Powder X-ray Diffraction Data

Powder patterns were measured on a Bruker D8 Advance Vario diffractometer at RT with LynxEye detector and Ge (111) monochromator, $\lambda(CuK\alpha_1)$ = 1.54060 Å, θ/2θ scan from 4° to 65°, stepsize 0.0191°.

To obtain powder pattern of **1** six single crystals were rubbed to powder after single crystal X-ray diffraction confirmed their composition. Powder X-ray diffraction data (PXRD) of **1** are depicted on Fig. S3. High peaks on the difference curve were assigned to non-uniform distribution of crystallites (the presence of small crystals in a powder).

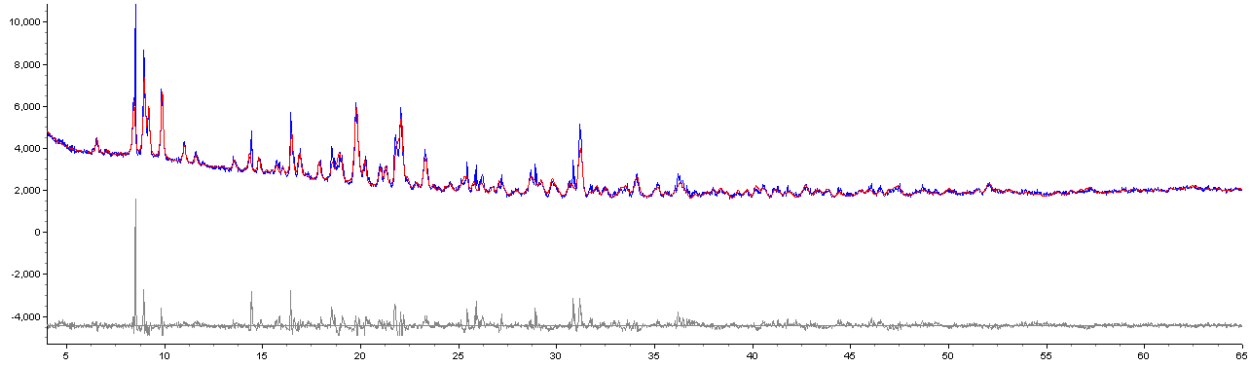

Figure S3. The experimental (blue) and calculated (red) powder patterns for **1** and their difference (gray).

UV irradiation of the powder obtained gave complex **2** (Fig. S4); the PXRD data confirmed full conversion.

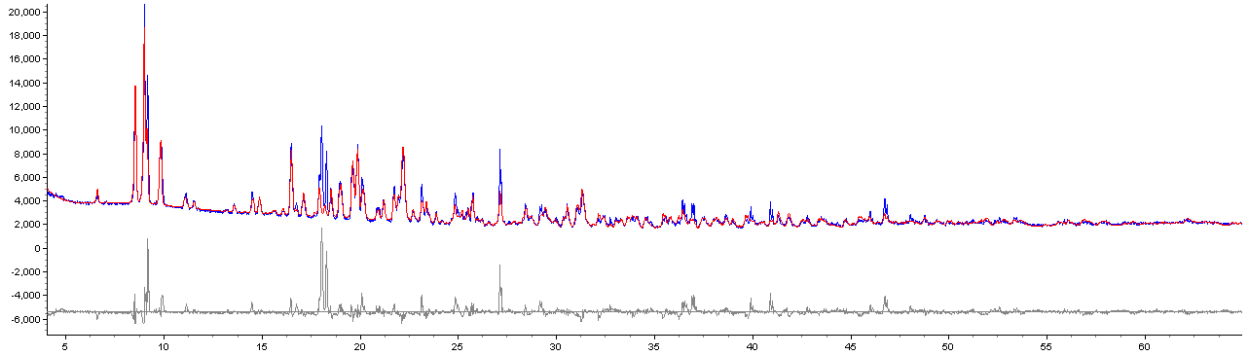

Figure S4. The experimental (blue) and calculated (red) powder patterns for **2** and their difference (gray).

The sample was heated up to 440 K, left at this temperature for 30 min and then cooled. The PXRD confirmed the 100 % reverse conversion to **1** (Fig. S5).

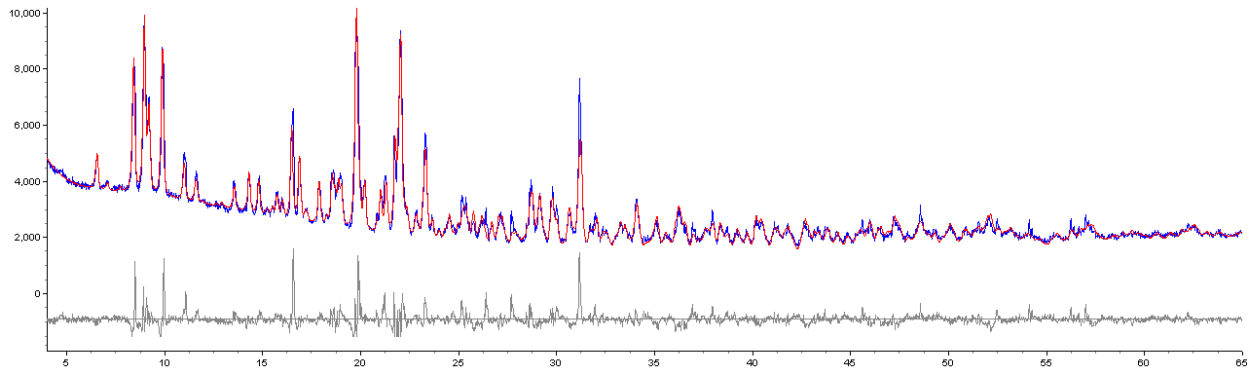

Figure S5. The experimental (blue) and calculated (red) powder patterns for **1** and their difference (gray).

For all the cases crystal data either for **1**, or for **2**, or their mixture were attested to control the rate of conversion. Close unit cells result in the "presence" of about 5 - 8 % of minor component; but taking into account that model mixture of **1** and **2** slightly affected the R_{wp} values and R_{bragg} values remained unchanged, one can conclude that the PXRD samples can successfully be described as one component phases.

Thermogravimetry

TGA was performed using a "Derivatograph-C" (MOM, Hungary) at a heating rate of 10 K/min under an argon atmosphere. DSC measurements were carried out using a "DSC-822e" (Mettler-Toledo) at a heating/cooling rate of ±10 K/min under anargon atmosphere. Six single crystals of **1** were taken from reaction mixture for TGA and DSC analyses, and their composition was approved using the SCXRD. Completeness of solid state reactions after UV irradiation (the direct process) and heating (the reverse process) was controlled using the SCXRD. Although some crystals cracked after irradiation and heating, these retained their single crystalline character.

The TGA analysis showed that compound is stable until 475 K (Fig. S6). The mass loss takes place as a two-step process.

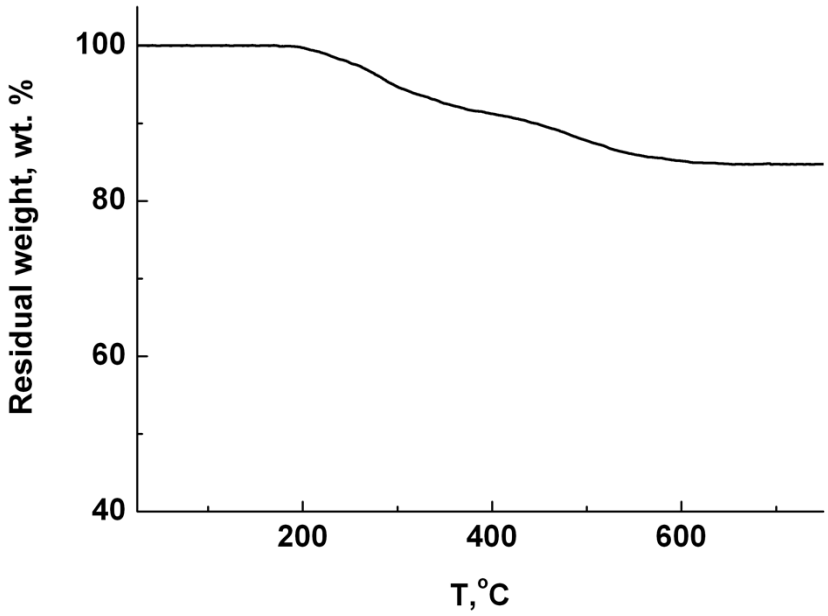

Figure S6. TGA curve of **1** in an argon atmosphere upon heating at a rate 10 K/min.