Molecular and Supramolecular Structures of Triiodides and Polyiodobismuthates of Phenylenediammonium and Its N,N-dimethyl Derivative

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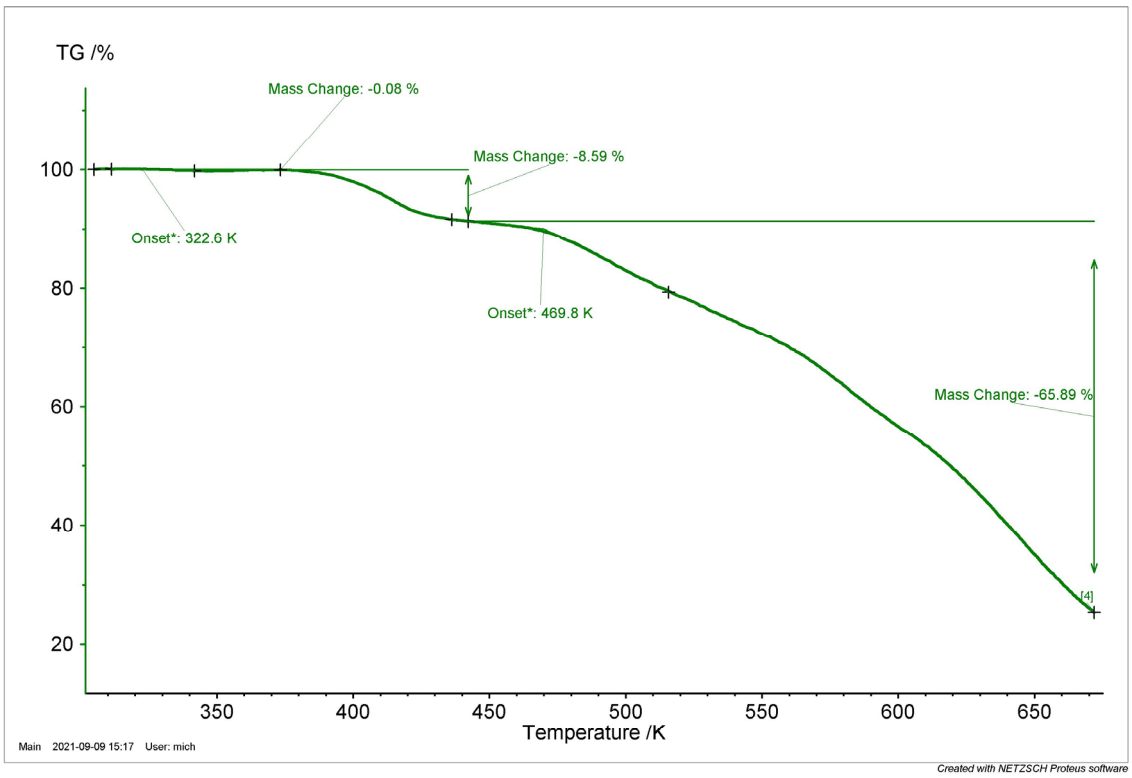

Figure S1. Thermal analysis data for **1**. Compound **1** decomposes in two steps. Near 310 K it loses 27.41 %, which corresponds to one I_2 molecule (calc. 24,5 %). At the second stage, near 380 K, it loses another 28.90 %, which can be attributed to one I_2 molecule and one water molecule (calc. 28.0 % in total).

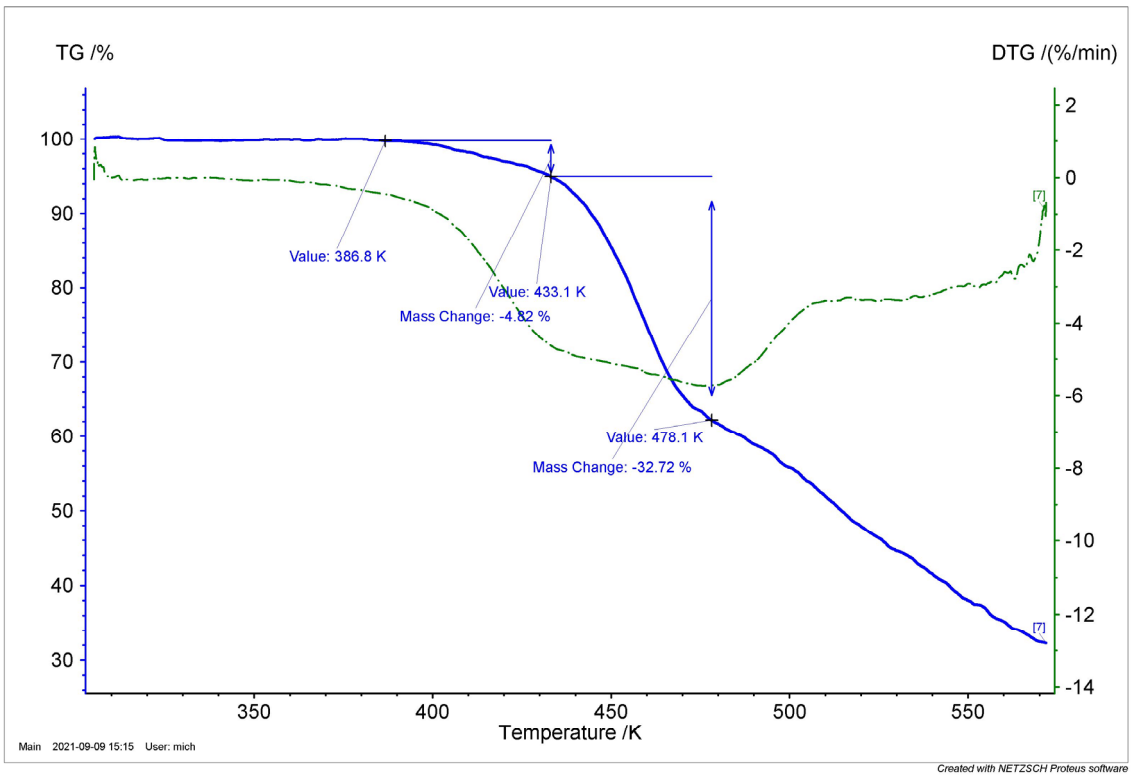

Figure S2. Thermal analysis data for **2**. Compound **2** begins to decompose at 387 K. There are no clearly defined stages of decomposition on the graph, but the total value of the mass loss to the inflection point at 478 K is 37,55 %, which is attributed to a I_2 molecule (calc. 39,3 %).

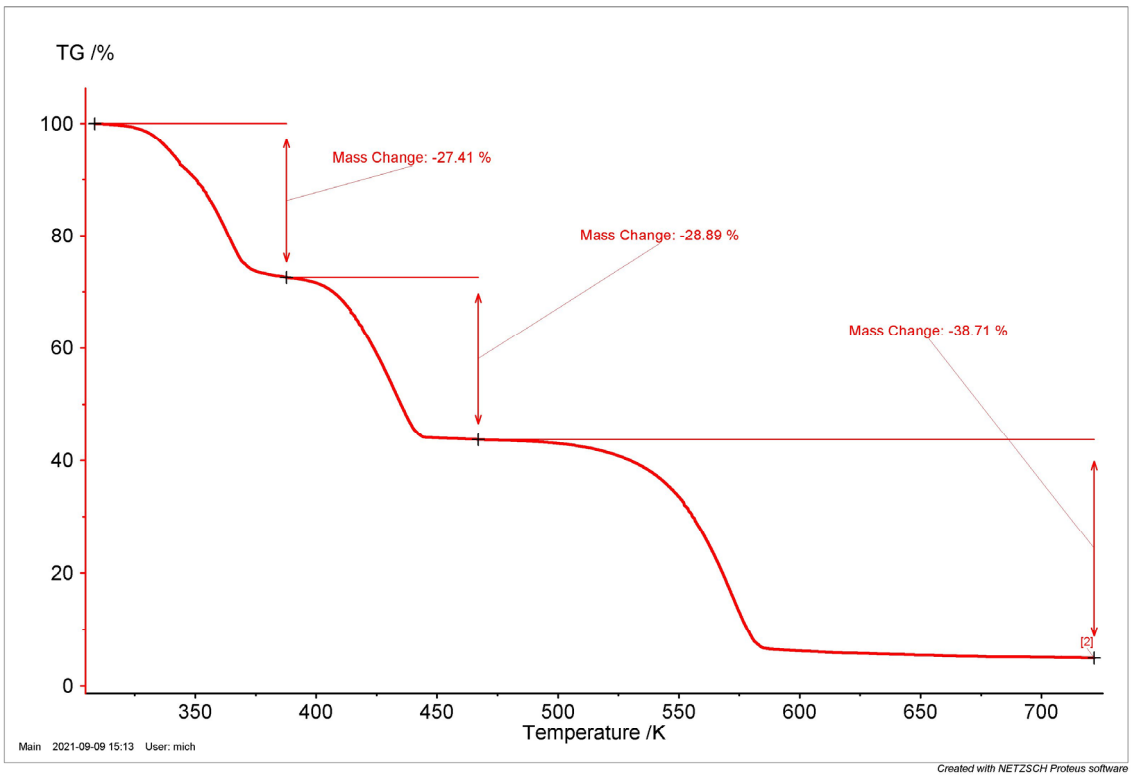

Figure S3. Thermal analysis data for **4**. Compound **4** is stable up to 373 K, then it loses 8.67 % of its mass, which may correspond to the removal of part of I2 and water molecules, so that ½ I_2 and all H_2O (calc. 9.9 % in total) are released.

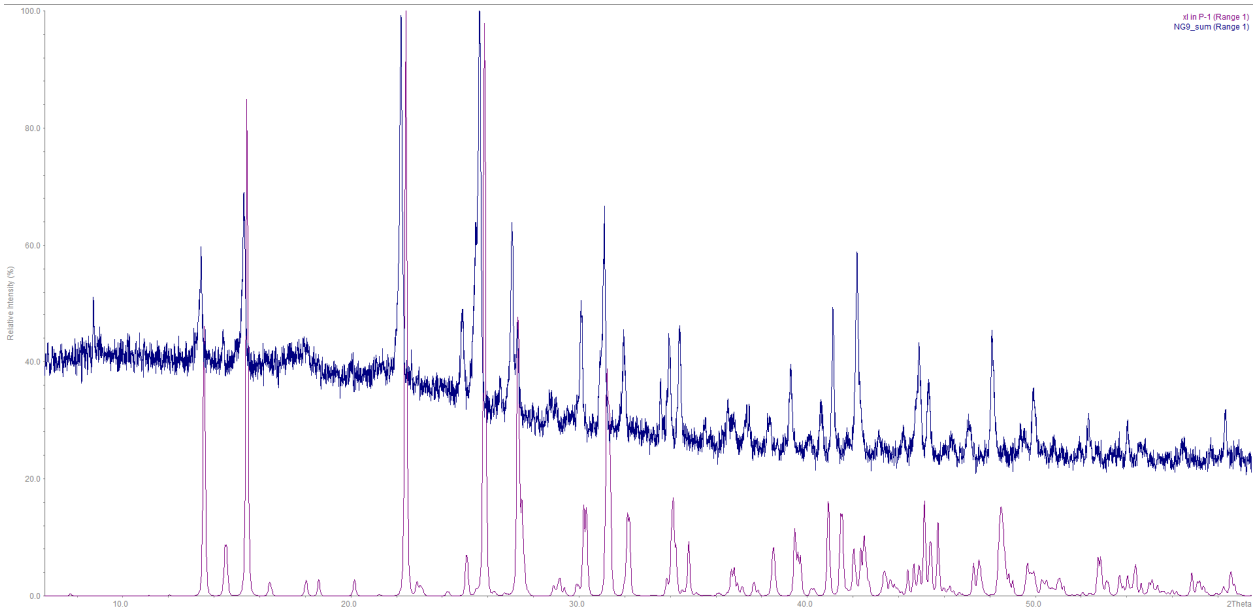

Figure S4. X-ray powder diffraction pattern for **1**. Experimental profile (measured at room temperature), blue; calculated from the crystal data (measured at 100 K), magenta.

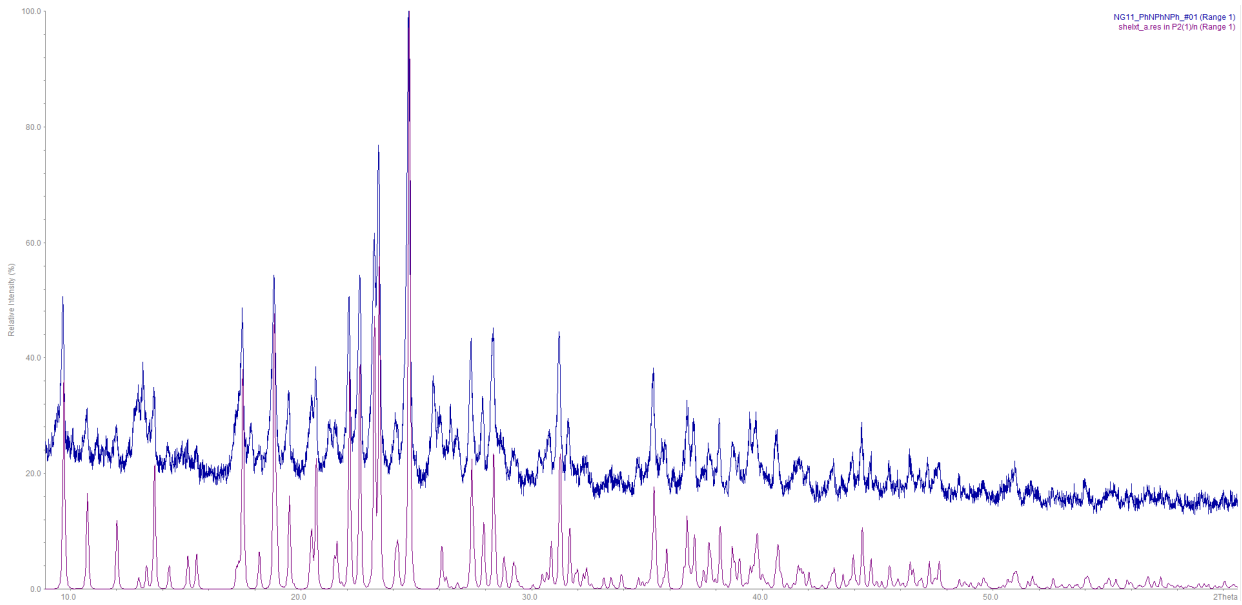

Figure S5. X-ray powder diffraction pattern for **2**. Experimental profile, blue; calculated from the crystal data, magenta.

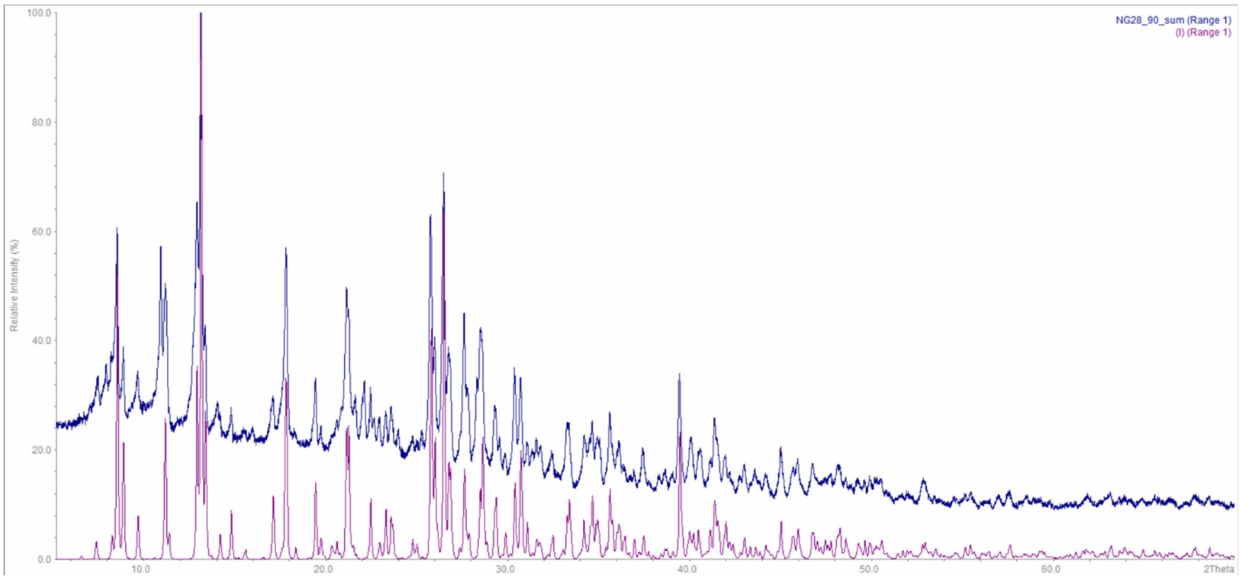

Figure S6. X-ray powder diffraction pattern for **4**. Experimental profile, blue; calculated from the crystal data, magenta.