

*High-pressure studies for understanding mechanical effects on chemical reactions*Boris Zakharov^{1,2}, Anatoly Sidelnikov¹, Stanislav Chizhik¹, Alexander Matvienko^{1,2}, Elena Boldyreva^{1,2}¹Institute Of Solid State Chemistry And Mechanochemistry SB RAS, Novosibirsk, Russian Federation, ²Novosibirsk State University, Novosibirsk, Russia

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Different possibilities of transformation of light or thermal to mechanical motion are widely discussed in recent literature. Solid-state chemical reactions which are mostly accompanied by generation and relaxation of mechanical stresses and strains are strongly related to this topic. Homogeneous and heterogeneous single-crystal to single-crystal chemical reactions are of special interest since they make it possible to follow structural strain by single-crystal X-ray diffraction and optical microscopy. Some of these reactions are accompanied by various photo- and thermomechanical effects, including bending, twisting, curling, jumping of crystals. The structural mechanisms of photo- and thermally induced chemical reactions in crystals are closely related to the anisotropy of mechanical properties, which can be followed particularly well by studying the crystal structure under high pressure or low temperature.

In the title contributions two classes of compounds will be discussed. The first class is Co(III) complexes with general composition $[\text{Co}(\text{NH}_3)_5\text{NO}_2]\text{XY}$ (where X, Y = Cl, Br, I, NO_3) which undergo UV or visible light-induced photoisomerization to give $[\text{Co}(\text{NH}_3)_5\text{ONO}]\text{XY}$ product. This transformation together with reverse reaction on heating accompanied by significant mechanical effects – crystal jumping, cracking, mechanical deformation. The second class represents a series of rare-earth element hydrated oxalates $(\text{REE})_2(\text{C}_2\text{O}_4)_3 \cdot 10\text{H}_2\text{O}$ (REE = Sm, Y) and $\text{SmY}(\text{C}_2\text{O}_4)_3 \cdot 10\text{H}_2\text{O}$ which undergo transformation to single-crystalline dehydrated product $(\text{REE})_2(\text{C}_2\text{O}_4)_3$ with crystal shape change on slight heating. The structures of the two classes of compounds were followed from ambient pressure up to 6–10 GPa in diamond anvil cells. Bulk compressibilities, anisotropic lattice strain on hydrostatic compression and corresponding changes in the atomic coordinates were followed and related to corresponding transformations on heating or irradiation by light including high-pressure in-situ reactions. Moreover a series of phase transitions for $[\text{Co}(\text{NH}_3)_5\text{NO}_2]\text{XY}$ and $[\text{Co}(\text{NH}_3)_5\text{ONO}]\text{XY}$ compounds were detected and discussed not only at high pressures but also at low temperatures allowing to compare relative mechanical properties of compounds with different outer-sphere anions. For $\text{Y}_2(\text{C}_2\text{O}_4)_3 \cdot 10\text{H}_2\text{O}$ the interesting phenomena of high-pressure dehydration giving the same product as heating at ambient pressure has been detected and discussed.

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