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A New Allotropic Modification of the Cubic KOs_2O_6 Pyrochlore. Sergiy Katrych^a, Qinfen F. Gu^b, Zbigniew Bukowski^a, Nikolai D. Zhigadlo^a, Gunter Krauss^b, Janusz Karpinski^a. ^aLaboratory for Solid State Physics, Schafmattstr. 16, ETH Zurich, 8093 Zurich, Switzerland. ^bLaboratory for Crystallography, Wolfgang-Pauli-Str. 10, ETH Zurich, 8093 Zurich, Switzerland.

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A new allotropic triclinic modification of cubic KOs_2O_6 [1, 2], the representative of a new structural type (Pearson symbol $aP18$, $a=5.5668(1)$ Å, $b=6.4519(2)$ Å, $c=7.2356(2)$ Å, $\alpha=65.377(3)^\circ$, $\beta=70.572(3)^\circ$, $\gamma=75.613(2)^\circ$ space group $P-1$, no.2 was synthesized using high pressure (HP) technique. Its structure was determined by single-crystal X-ray diffraction. The structure can be described as two OsO_6 octahedral chains relating to each other through inversion. The novel compound reveals close local structural resemblance to the cubic KOs_2O_6 . Both structures are constructed from the same structural blocks. OsO_6 octahedra building big voids with K atom inside. K has no direct chemical bonding to the rest of the structure.

Quantum chemical calculations were performed on the novel compound and structurally related cubic compound. HP X-ray study showed that cubic KOs_2O_6 phase was stable up to 32.5(2) GPa at room temperature.

The quantum chemical calculations show that at HP the triclinic modification is more stable than the cubic one. A high pressure (32.5(2) GPa) is not sufficient factor for transforming the cubic in to the more dense triclinic prototype. High temperature (at least 900 °C) and a pressure (above 3 GPa) are needed for such possible transformation [3].

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A New Mechanism of the Insulator-Metal Transition in Mott-Hubbard Insulators Induced by Spin Crossover at High Pressures. Igor Lyubutin^a, Sergey Ovchinnikov^{b,c}, Alexander Gavriluk^d, Viktor Struzhkin^e. ^aShubnikov Institute of Crystallography, RAS, 119333, Moscow, Russia. ^bInstitute of Physics, Siberian Division of RAS, 660036, Krasnoyarsk, Russia. ^cSiberian Federal University, 660041, Krasnoyarsk, Russia. ^dInstitute for High Pressure Physics, RAS, 142190, Troitsk, Moscow region, Russia. ^eGeophysical Laboratory, Carnegie Institution of Washington, 5251, Washington DC 20015, USA.

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The insulator-metal transition (IMT) in strongly correlated d -electron systems has been widely discussed since the groundbreaking work by Mott. The commonly accepted mechanisms are the band-width controlled IMT (driven by the broadening of the d -bands), and filling-controlled IMT, induced by the doping of charge carriers into the parent insulator compound. We have discovered and explained a new mechanism of IMT in Mott-Hubbard insulators [1,2]. This mechanism can be initiated by the lattice compression at high pressure and it is driven by a spin transition in $3d^5$ ions from the high-spin (HS) state to the low-spin (LS) state. The HS-LS spin-crossover suppresses the effective Hubbard parameter U_{eff} down to the value enabling the insulator-metal transition according to the Mott mechanism $U_{\text{eff}}/W \approx 1$ (W is a half of the d -bandwidth). We have observed experimentally this type of a Mott-Hubbard IMT in the multiferroic BiFeO_3 [3-5], and similar mechanism must be effective for other $3d^5$ transition-metal compounds such as FeBO_3 , $\text{GdFe}_3(\text{BO}_3)_4$, RFeO_3 ($R = \text{La, Nd, Pr, Lu}$), $\text{Y}_3\text{Fe}_5\text{O}_{12}$, $\alpha\text{-Fe}_2\text{O}_3$, Fe_3O_4 , MnO where the spin crossover was found along with insulator-metal or insulator-semiconductor transitions [5,6]. We call the new IMT mechanism as the “Hubbard energy control” mechanism, to distinguish from the well known “bandwidth control” and “band-filling” mechanisms of the IMT. The classification of possible scenarios of metallization in the other $3d^5$ metal compounds is also performed [1].

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