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Li_2RuO_3, a valence bond liquid on the honeycomb lattice HARALD JESCHKE, Goethe Universitaet Frankfurt, SIMON A.J. KIMBER, European Synchrotron Radiation Facility Grenoble, I.I. MAZIN, Naval Research Laboratory Washington, JUAN SHEN, Goethe Universitaet Frankfurt, DIMITRI N. ARGYRIOU, European Spallation Source Lund, SERGEY V. STRELTSOV, Ural Federal University Ekaterinburg, ROSER VALENTI, Goethe Universitaet Frankfurt, DANIEL I. KHOMSKII, Universitaet zu Koeln — Li_2RuO_3 has been known to form Ru-Ru dimers at low temperature, but was believed to be homogenous above the transition. We provide new experimental evidence for the melting of the low temperature dimer ordering by comparing x-ray diffraction probing the average crystal structure and the pair distribution function, which provides information about local order. We show that strong dimerization survives well above the ordering temperature $T_s \approx 450$ K and that the high temperature structure is a bond liquid of dynamically disordered dimers with the same 1:2 ratio of short and long bonds. Theoretically, we search for low energy structures of Li_2RuO_3 and find different long range orders of Ru dimer patterns. We can explain not only the low T structure but also the ordering temperature: Due to strong covalency, dimerization leads to a large energy gain but the additional gain through dimer ordering is much smaller and compatible with the experimentally found T_s. Moreover, of the two holes present in Li_2RuO_3 one participates in a strongly covalent bond, which survives at all temperatures, and the other in a weak bond that breaks in the bond-liquid state. This explains why below T_s the effective spin of Ru is 0, and above 1/2, but never 1.

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