High Pressure High Temperature Carbon Dioxide

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Carbon dioxide is widely studied molecular compound because of its importance in life and geological sciences. Despite the simplicity of the molecule, the solid shows several high-pressure polymorphs quenchable at room temperature and its phase diagram isn't still fully characterized [1,2,3]. In particular the structure of the high temperature phases II and IV have not been well established and the claimed molecule pairing in phase II [4] and bent molecular geometry in phase IV [5] have been recently questioned [6].

I present here a FTIR and Raman study of high pressure high temperature CO_2 phases up to 30 GPa performed between 80 and 650 K by using a resistively heated diamond anvils cell and an N₂ flux cryostat. The complete vibrational information gives some constraints on the crystal symmetry, allowing to choose the crystal structures of phases II and IV among those proposed in the literature.

Moreover we have determined the melting curve and the transition lines for high temperature phases, between 300 and 800 K, and found them quite different from published results.

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