Abstract Submitted
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**Shock compression of CO2: experiments on Z and first-principles simulations**[1] T.R. MATTSSON, S. ROOT, L. SHULENBURGER, Sandia National Laboratories, Albuquerque, NM 87185, K.R. COCHRANE, Ktech Corp. Albuquerque, NM 87123 — The principal Hugoniot for CO2 is known up to 75 GPa and it displays a plateau in shock pressure interpreted as the result of dissociation [1]. To confidently model the structure of gas-giant planets and the deep carbon cycle of the earth it is important to accurately know the properties of CO2 at even higher pressures. We present results from flyer-plate experiments on Sandia's Z-machine providing data for CO2 between 150 and 600 GPa. We also present Density Functional Theory (DFT) based simulations up to 500 GPa, including a chemical composition analysis. Quantum Monte Carlo (QMC) is applied to assess the accuracy of exchange-correlation functionals. We conclude that the plateau in shock pressure at 50 GPa [1] is consistent with dissociation. Beyond 3.5 g/cm$^3$ density, the shock pressure raises rapidly due to completed dissociation.

[1] W. Nellis, et. al. , J. Chem. Phys. **95**, 5268 (1991).

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