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A reactive molecular dynamics study of phenol and phenolic polymers in extreme environments[1] KEITH A. JONES, J. MATTHEW D. LANE, NATHAN W. MOORE, Sandia National Laboratories — Phenolic polymers are key components in composite materials due to their ablative properties, oftentimes exposed to extreme conditions like heating and shock. The chemistry of phenolics under these conditions is not well understood. Phenolic polymers and phenol are studied with two parametrizations of the ReaxFF classical MD potential. We observe that the density of phenol in one parametrization, at six temperatures ranging from 123 K to 423 K, for which experimental density data are available, is in closer agreement with the experimental results. The accuracy of the density of phenol at various temperatures serves as a proxy for the ability of a parametrization to predict the density of a phenolic polymer under shock. Constant temperature pyrolysis of a phenolic polymer, modeled as a collection of linear chains, is then investigated with these two ReaxFF parametrizations at several temperatures ranging from 2000 to 3250 K. The activation energies for water formation, as well as the activation energy associated with the liberation of volatilizable compounds, are extracted and used as a point of comparison with experimental thermogravimetric analysis (TGA) results. The implications for determining the activation energy are discussed.

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