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TITLE: Constraining Cometary Crystal Shapes from IR Spectral Features

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ABSTRACT BODY: A major challenge in deriving the silicate mineralogy of comets is ascertaining how the anisotropic nature of forsterite crystals affects the spectral features' wavelength, relative intensity, and asymmetry. Forsterite features are identified in cometary comae near 10, 11.05-11.2, 16, 19, 23.5, 27.5 and 33 µm [1-10], so accurate models for forsterite's absorption efficiency (Qabs) are a primary requirement to compute IR spectral energy distributions (SEDs, $\lambda F\lambda$ vs. λ) and constrain the silicate mineralogy of comets. Forsterite is an anisotropic crystal, with three crystallographic axes with distinct indices of refraction for the a-, b-, and c-axis. The shape of a forsterite crystal significantly affects its spectral features [13-16]. We need models that account for crystal shape.

The IR absorption efficiencies of forsterite are computed using the discrete dipole approximation (DDA) code DDSCAT [11,12]. Starting from a fiducial crystal shape of a cube, we systematically elongate/reduce one of the crystallographic axes. Also, we elongate/reduce one axis while the lengths of the other two axes are slightly asymmetric (0.8:1.2). The most significant grain shape characteristic that affects the crystalline spectral features is the relative lengths of the crystallographic axes. The second significant grain shape characteristic is breaking the symmetry of all three axes [17].

Synthetic spectral energy distributions using seven crystal shape classes [17] are fit to the observed SED of comet C/1995 O1 (Hale-Bopp). The Hale-Bopp crystalline residual better matches equant, b-platelets, c-platelets, and b-columns spectral shape classes, while a-platelets, a-columns and c-columns worsen the

spectral fits.

Forsterite condensation and partial evaporation experiments demonstrate that environmental temperature and grain shape are connected [18-20]. Thus, grain shape is a potential probe for protoplanetary disk temperatures where the cometary crystalline forsterite formed. The forsterite crystal shapes (equant, b-platelets, c-platelets, b-colums – excluding a- and c-columns) derived from our modeling [17] of comet Hale-Bopp, compared to laboratory synthesis experiments [18], suggests that these crystals are high temperature condensates.

By observing and modeling the crystalline features in comet ISON, we may constrain forsterite crystal shape(s) and link to their formation temperature(s) and environment(s).

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