Vibrational properties of an OH center in $\beta$-Ga$_2$O$_3$\textsuperscript{1} W. B. FOWLER, P. WEISER, M. STAVOLA, Lehigh University — Theoretical predictions suggest that hydrogen impurities play a crucial role in the electrical conductivity of $\beta$-Ga$_2$O$_3$ by acting as shallow donors and by passivating cation-vacancy acceptor complexes [1,2]. IR spectroscopy of $\beta$-Ga$_2$O$_3$ single crystals treated in an H$_2$ (D$_2$) ambient display a strong vibrational line at 3437 (2546) cm$^{-1}$ originating from an O-H(D) containing defect. This line is thermally stable at 1000°C, which suggests that it may arise from a V$_{Ga}$-H complex. Theoretical calculations using the CRYSTAL06 code [3] with hybridized DFT Hamiltonian and the polarization properties of the O-H vibrational line are used to determine possible microscopic structures for this defect and other possible defects. [1] J. B. Varley et al., Appl. Phys. Lett. 97, 142016 (2010). [2] J. B. Varley et al., J. Phys.: Condens. Matter 23 (2011), 334212. [3] R. Dovesi et al., Crystal06 User’s Manual (University of Torino, Torino, 2006).

\textsuperscript{1}Supported by NSF grant DMR 1160756 and by a Grant-in Aid of Research by Sigma Xi

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Date submitted: 20 Nov 2016

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