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Hindered rotation of the 3326 cm⁻¹ OH center in ZnO?¹ PHILIP WEISER, ELLEN FARMER, MICHAEL STAVOLA, W. BEALL FOWLER, Lehigh University — Experiments on H in ZnO have found two OH vibrational lines at 3611 and 3326 cm⁻¹ [1,2]. The IR line at 3611 cm⁻¹ has been assigned to isolated H⁺ in a bond centered configuration. The band at 3326 cm⁻¹ has been assigned to H⁺ in an antibonding configuration in the vicinity of another defect, perhaps Ca [3]. The 3326 cm⁻¹ band has a distinctive dependence on temperature, consisting of several overlapping components whose intensities show thermally activated behavior over the temperature range 4K to 50K. This behavior is reminiscent of previous results for the hindered rotation of an off-axis OD-Li center in MgO [4]. Our results suggest that the off-axis motion of OH centers in oxides might be a common occurrence.

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