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An off axis OH center in ZnO studied by IR spectroscopy PHILIP WEISER, ELLEN FARMER, MICHAEL STAVOLA, W. BEALL FOWLER, Lehigh University — Experiments on H in ZnO have revealed several donor species. Two major H vibrational modes were found at 3326 and 3611 cm⁻¹ and assigned to H donors. The IR line at 3611 cm⁻¹ has been associated with an isolated H donor in a bond-centered configuration. The line at 3326 cm-1 has been suggested to be due to H in an antibonding configuration in the vicinity of another defect (a Ca impurity is one such possibility). The band at 3326 cm⁻¹ has a distinctive dependence on temperature. At low temperature, the 3326 cm⁻¹ band appears to consist of three overlapping components. As the temperature is increased, the relative intensities of the components change and additional sidebands appear. This behavior is reminiscent of our previous findings for an OD-Li center in MgO. In this case, the D atom was found to be displaced off axis and added a hindered-rotation structure to the O-D vibrational band. IR absorption experiments and theory are being used to investigate the possible off-axis motion of the 3326 cm⁻¹ center in ZnO.

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