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TAUC DIAGRAM AND Z-SCAN STUDIES FOR NONLINEAR OPTICAL MATERIALS

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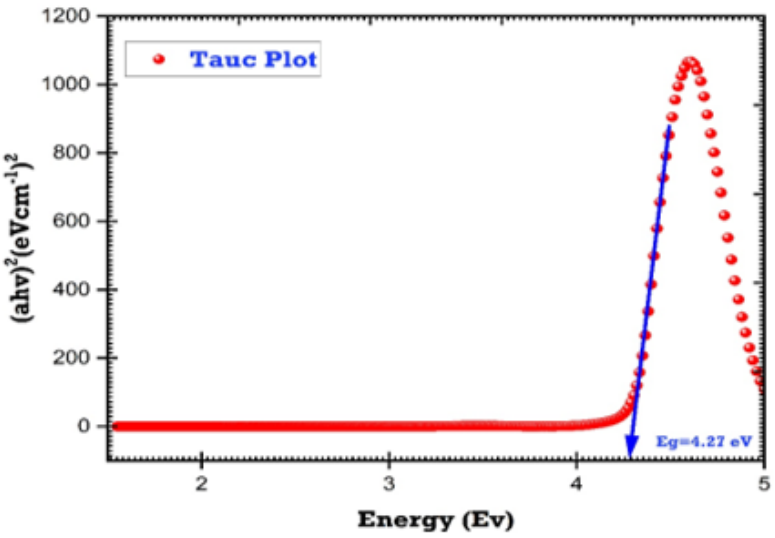
TAUC DIAGRAM

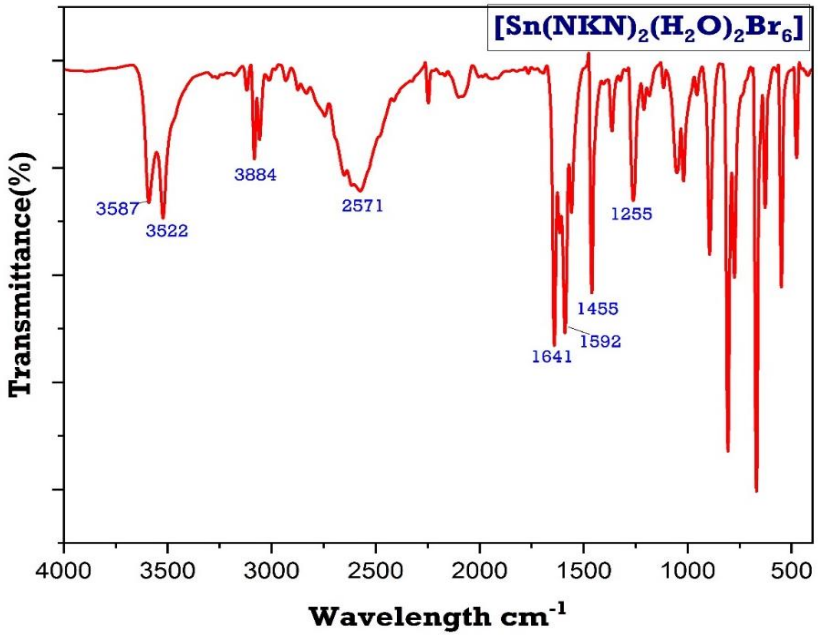
The UV-DRS analysis of $Br_6\,Sn\,(C_6\,H_5N_2)_2\,(H_2O)_2$ is presented in Fig. 2. The UV-Vis reflectance spectrum shows a sharp absorption edge at 422 nm, which corresponds to the optical transition in the material. The strong absorption in the UV region indicates the presence of π-π* electronic transitions, which are characteristic of the conjugated system present in $Br_6\,Sn\,(C_6\,H_5N_2)_2\,(H_2O)_2$.



Compound	Mr	Compared	C %	H %	N %	O %
Br_6 $Sn(C_6$ $H_5N_2)_2$ $(H_2O)_2$	1034.12 gr/mole	Theoretical	41.77	6.57	5.41	21.66
		Practical	41.39	6.42	5.29	21.46

To determine the optical band gap, the Kubelka-Munk function was applied, and the Tauc plot was constructed by plotting $(F(R)h\upsilon)^2$ *versus* $h\upsilon$. The extrapolation of the linear portion of the curve gives a direct band gap energy of 4.27 eV, suggesting that 3AP18C6 exhibits a semiconducting nature. This band gap value indicates potential applications in optoelectronic and nonlinear optical devices, where a moderate band gap is desirable for efficient photon absorption and charge transport.

FT-IR spectroscopy.



The provided image shows the FT-IR transmittance spectrum of the compound $[Sn(NKN)(H_2O)_2Br_3]$, plotted as transmittance (%) against wavenumber (cm^{-1}) over a range from 4000 cm^{-1} to 500 cm^{-1}. FT-IR spectroscopy is a powerful technique used to identify the functional groups and chemical bonds within a material by measuring the absorption of infrared light at specific wavenumbers. The

transmittance spectrum indicates the percentage of infrared light transmitted through the sample, with dips (lower transmittance values) corresponding to absorption bands where molecular vibrations occur.The spectrum exhibits several sharp and broad peaks, indicating the presence of various vibrational modes associated with the compound's molecular structure. Notable peaks are labeled at specific wavenumbers: 3567, 3562, 3884, 2571, 1255, 1641, 1582, and 1455 cm^{-1}.

3567 cm^{-1} and 3562 cm^{-1}: These high-wavenumber peaks likely correspond to O-H stretching vibrations from the water molecules (H_2O) coordinated in the compound. The slight splitting may indicate hydrogen bonding or different coordination environments of the water ligands. 3884 cm^{-1}: This unusually high wavenumber could be an artifact or mislabeling, as typical O-H or N-H stretches are below 3700 cm^{-1}. It might require verification against the raw data or could indicate an overtone or combination band. 2571 cm^{-1}: This peak may be associated with N-H stretching, possibly from the "NKN" moiety (if it represents a nitrogen-containing ligand), though this is lower than typical N-H stretches (around 3300–3500 cm^{-1}), suggesting possible hydrogen bonding or coordination effects.

Z-scan studies. The nonlinear absorption, nonlinear refractive index, and third-order nonlinear susceptibility were determined by standard equations . The NLO properties of the cocrystal were experimentally determined by the Z-scan technique. Here, the open and closed aperture Z-scan curves are used fornonlinear absorption and nonlinear refractive index measurements. The transmittance intensity variations corresponding to the z values, and the closed and open aperture z-scan curves are represented.

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