

ELUCIDATION OF PROTON-ASSISTED FLUXIONALITY IN TRANSITION-METAL OXIDE CLUSTERS

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The phenomenon of fluxionality in the reactions of transition-metal oxide clusters provides many opportunities in various industrial and catalytic processes. We present an electronic structure investigation of the fluxionality pathways when anionic W_3O_6 and Mo_3O_6 clusters react with three small molecules - water, ammonia and hydrogen sulfide. The presentation features a detailed understanding of (a) how the fluxionality pathway occurs and (b) the various factors that affect the fluxionality pathway - such as the metal, different spin-states and the nature of the non-metal in the reacting small molecule.