

Why does Small Molecule Activation by Al(I) Compounds Occur Only in Aromatic Solvents? Insights from Theory

Shailaja Jain and Kumar Vanka

Email: sm.jain@ncl.res.in

The single site activation of strong σ bonds (such as that of H-H, P-H, and N-H) remains a significant challenge in the main group chemistry, with only a few cases, reported to date. In this regard, recent exciting experiments were done with Al(I) complexes, what is notable is that the reactions of aluminum chemistry have always been carried out in aromatic solvents: benzene, toluene or anisole. The current computational studies with density functional theory (DFT) reveal the interesting reason for this: it is seen that an explicit aromatic solvent molecule acts as a catalyst by converting the Al(I) complex to Al(III) during the process and the efficiency for the H-X (X=H, NHtBu, PPh₂) bond activation in the presence of an explicit benzene solvent molecule has been seen to be orders of magnitude higher than in its absence. The current work, therefore, reveals the chemistry of Al(I) complexes to be richer and more complex than realized to date, and shows it to be dependent on metal-solvent cooperativity, the first known example of its kind in main group chemistry.