

The mechanism of Menshutkin reaction in gas and solvent phases from the perspective of reaction electronic flux

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© 2014, Springer-Verlag Berlin Heidelberg. The mechanism of Menshutkin reaction, $\text{NH}_3 + \text{CH}_3\text{Cl} = [\text{CH}_3\text{NH}_3]^+ + \text{Cl}^-$, has been thoroughly studied in both gas and solvent (H_2O and cyclohexane) phase. It has been found that solvents favor the reaction, both thermodynamically and kinetically. The electronic activity that drives the mechanism of the reaction was identified, fully characterized, and associated to specific chemical events, bond forming/breaking processes, by means of the reaction electronic flux. This led to a complete picture of the reaction mechanism that was independently confirmed by natural bond-order analysis and the dual descriptor for chemical reactivity and selectivity along the reaction path.