Área: FIS

Insights into Dinuclear Pt^{III} Complex Reaction in Solution: A Born-Oppenheimer Metadynamics Approach

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Highlights

Metadynamics uncovers I_d mechanism in Pt(III) halide substitution, closely matching experimental activation free energy.

Resumo/Abstract

This study employs Born-Oppenheimer Molecular Dynamics combined with well-tempered metadynamics[1] to investigate halide substitution reactions of dinuclear Pt(III) complexes and explore its free energy surfaces (FES). Using coordination numbers as collective variables, a dimesional reduced description of the substitution reaction can be given and the prefered mechanism in solution can be attributed. The FES, shown in Figure 1, reveal a dissociative interchange (I_d) mechanism for the chloride substitution. The calculated activation free energy (13.4 kcal/mol), presented in Figure 2, closely matches the experimental value (13.2 kcal/mol)[2], validating the simulation approach. Additionally, reweighting error analysis and block averaging techniques were employed to assess the reliability of the FES, with the resulting average error indicating good convergence.

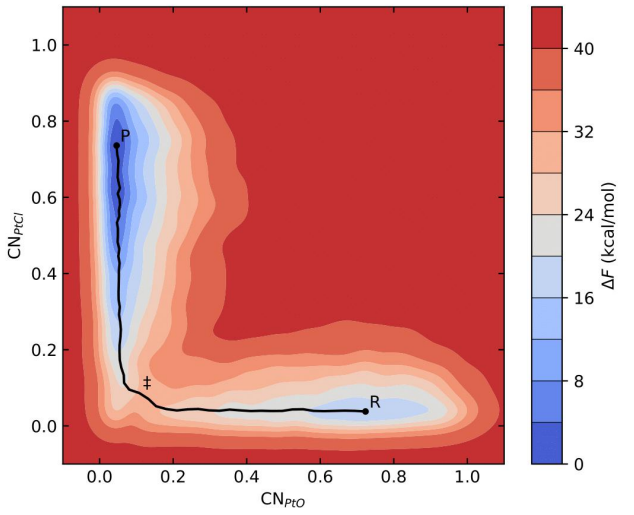

Figure 1. Free Energy landscape.

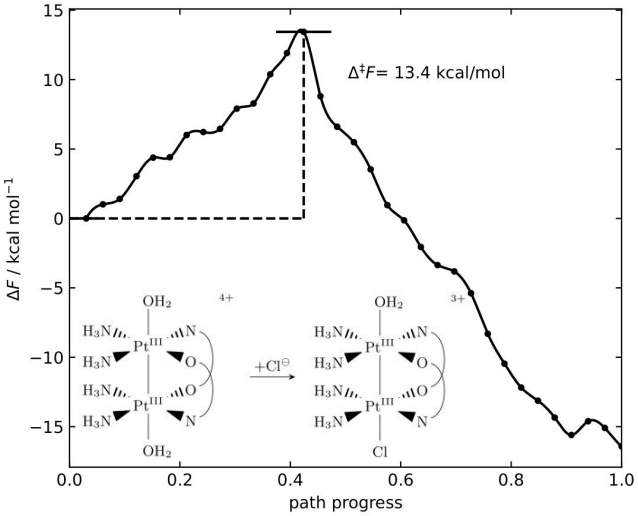

Figure 2. Minimum Free Energy Path.

[1] A. Barducci, et al., Phys. Rev. Lett., 2008, 100, 020603.

[2] N. Saeki, et al., Eur. J. Inorg. Chem., 2001, 8, 2081-2088.

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