Supporting Information for the manuscript:

Reaction mechanism between Cu(II)-enolate complex and $O_2$ as a test case for methodology used in DFT computational studies.

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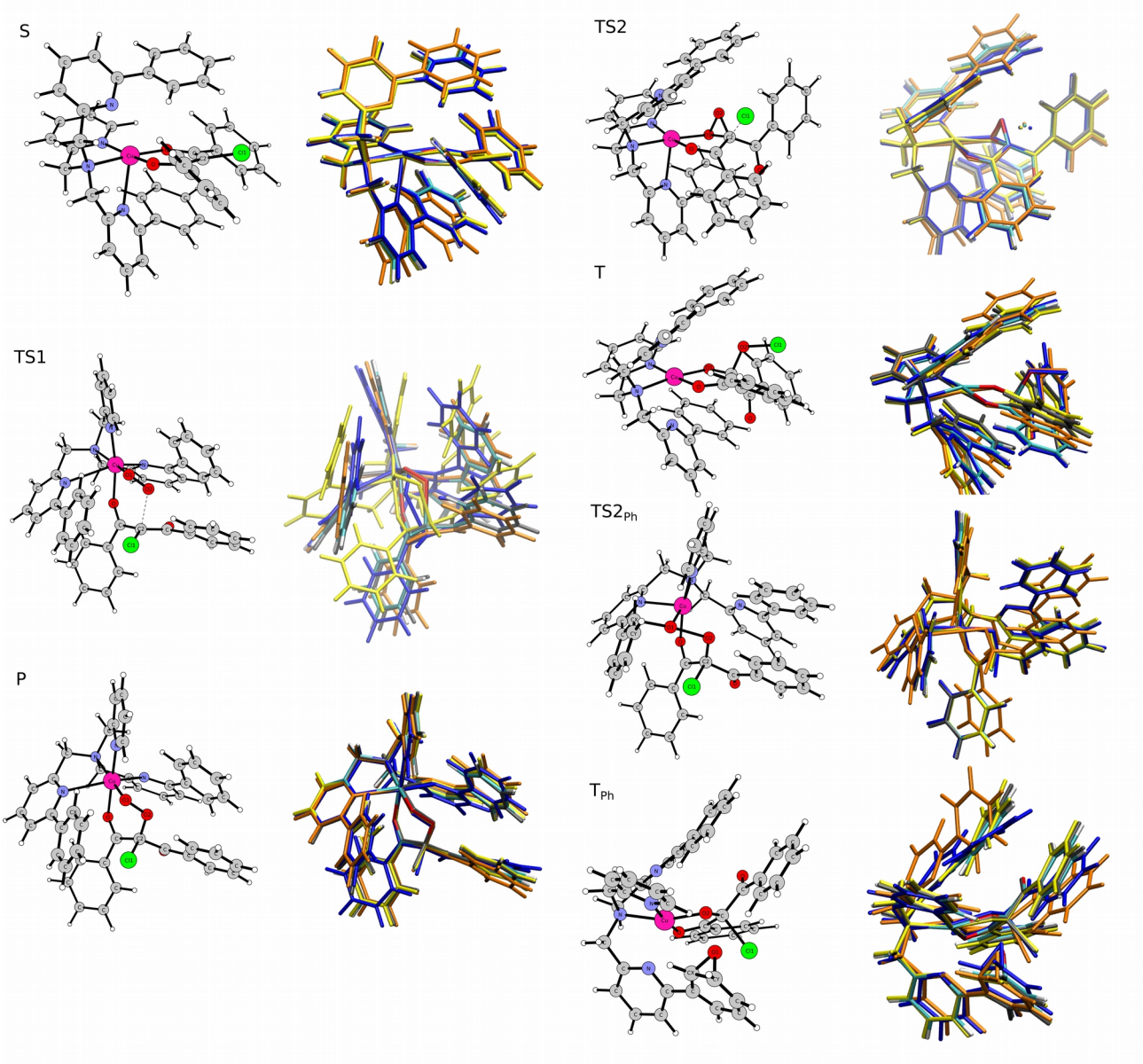


Figure S1 Optimized structures of stationary points for the parent system (**S**). On the left structures optimized at the B3LYP-D2/BS2 level; on the right superimposed structures optimized with the five tested computational methods (color code as in the main text).

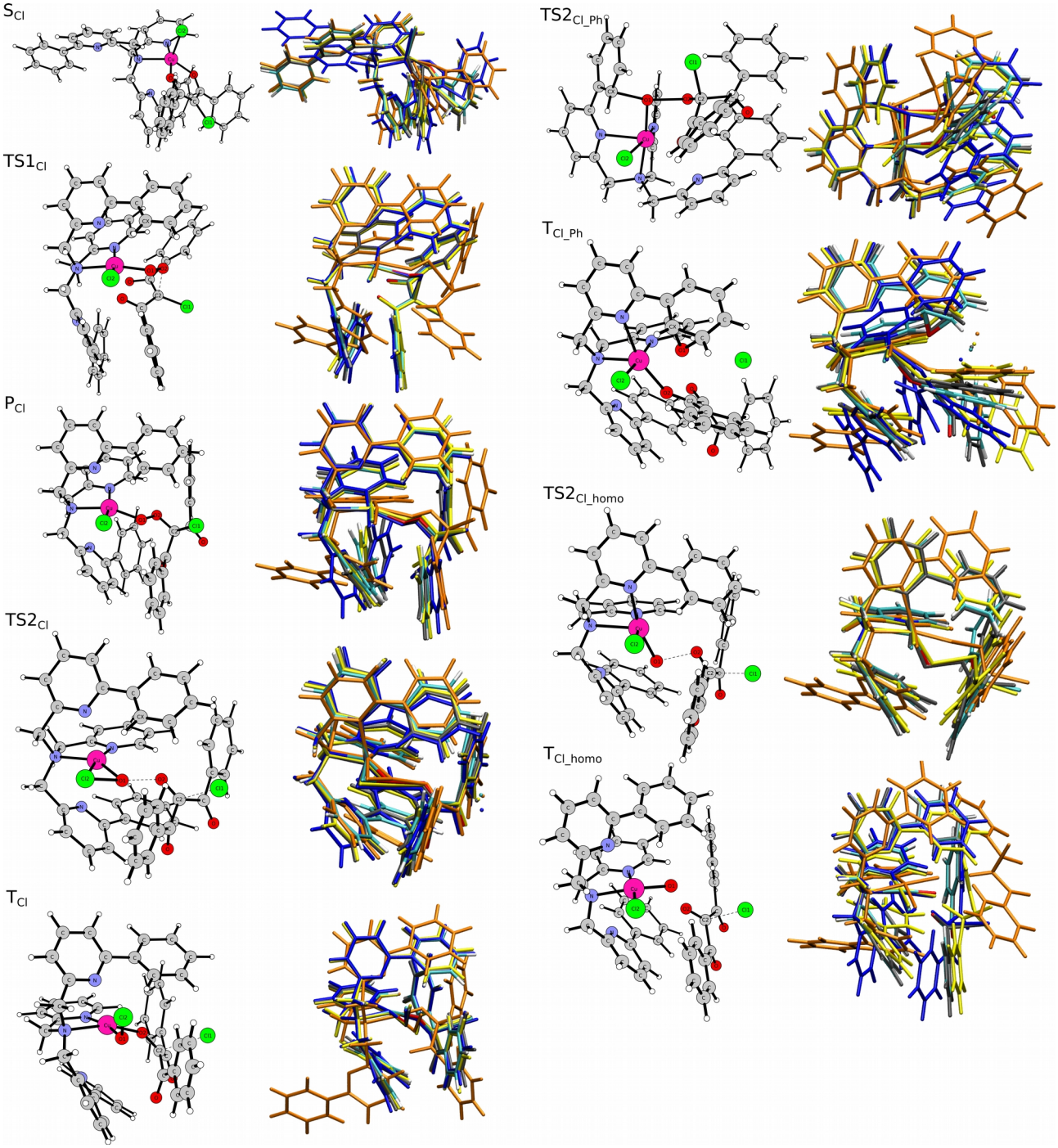


Figure S2 Optimized structures of stationary points for the system with Cl ligand (**$S_{Cl}$**). On the left structures optimized at the B3LYP-D2/BS2 level; on the right superimposed structures optimized with the five tested computational methods (color code as in the main text).

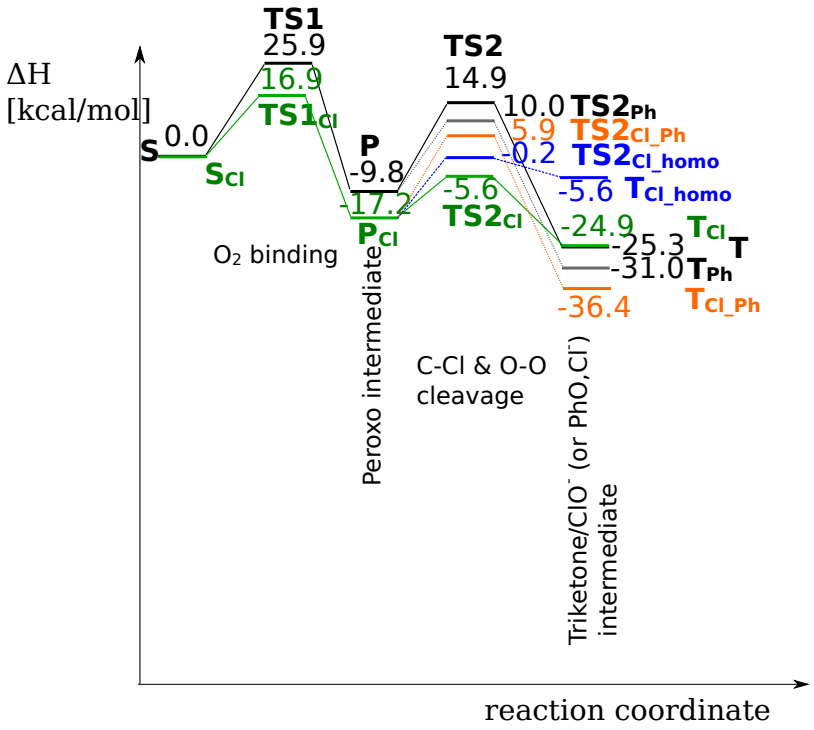


Figure S3. Reaction enthalpy profile computed with the B3LYP-D3/BS3//B3LYP-D2/BS1 model.

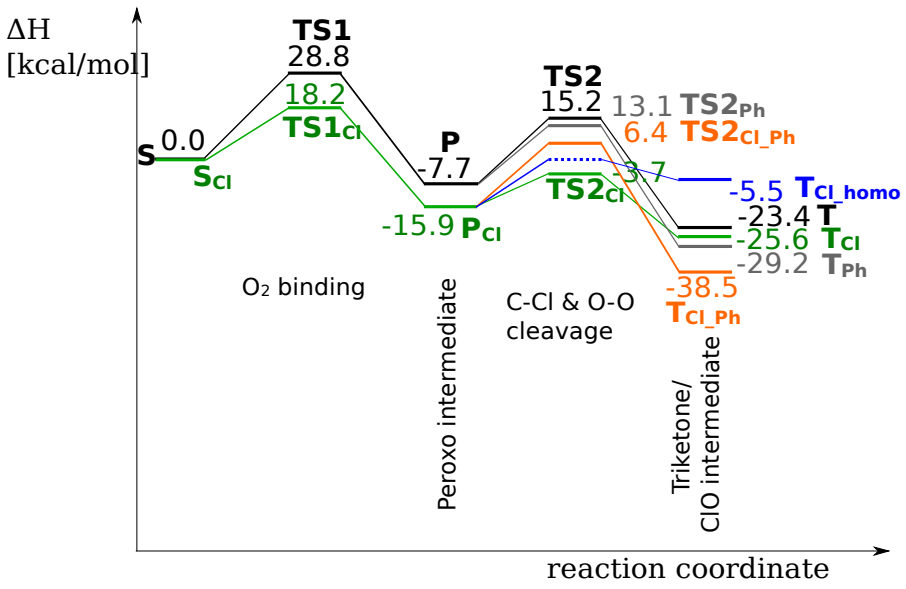


Figure S4. Reaction enthalpy profile computed with the B3LYP-D3/BS3//B3LYP-D2,PCM/BS1 model.

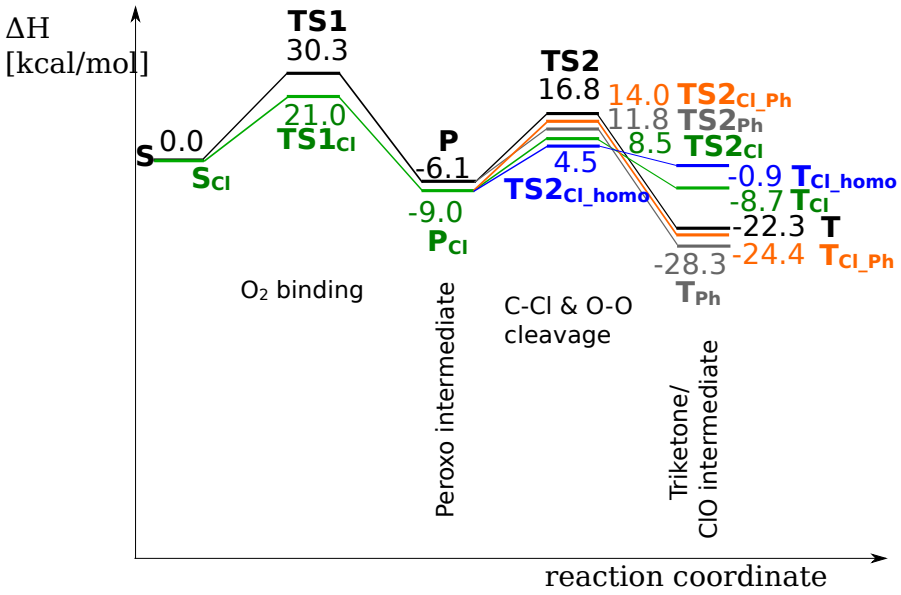


Figure S5. Reaction enthalpy profile computed with the TPSSh-D3/BS3//TPSSh-D2/BS1 model.

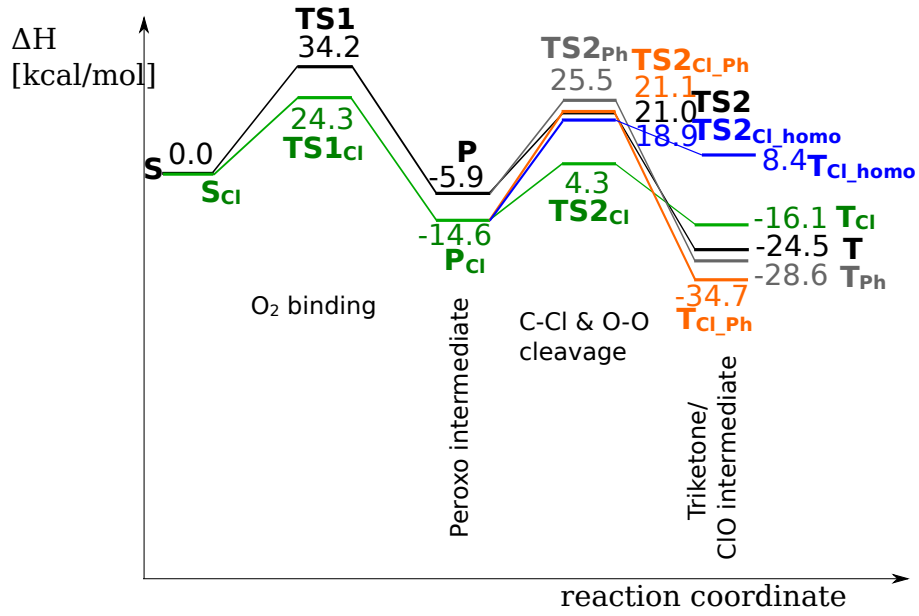


Figure S6. Reaction enthalpy profile computed with the ωB97XD/BS3//ωB97XD/BS1 model.