

Electronic Supplementary Information

What Accounts for the Color Purity of Tetradentate Pt Complexes ? A Computational Analysis

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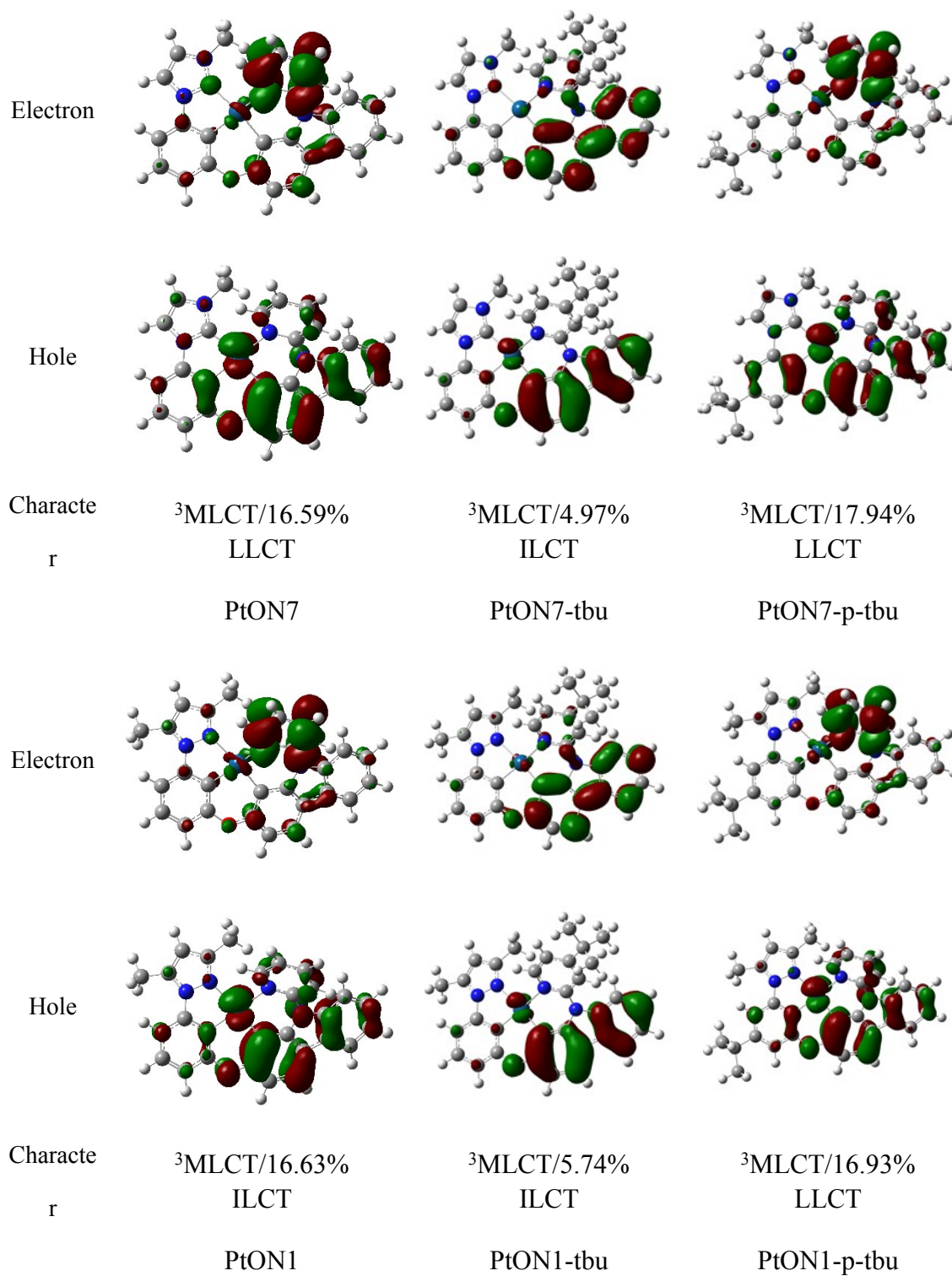


Figure S1 NTO pairs computed at the optimized geometries of T_1 of all the studied complexes.

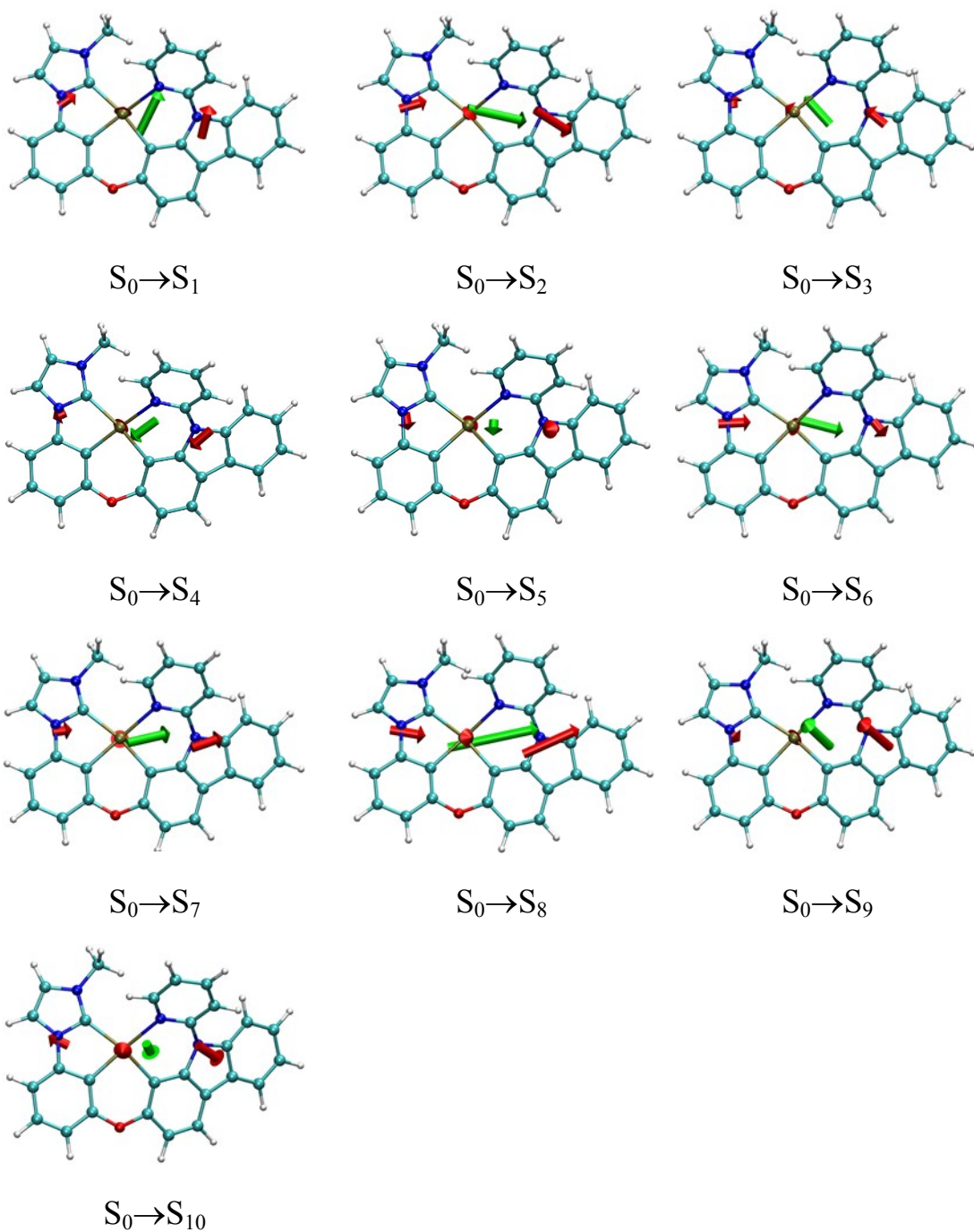


Figure S2. The contribution of different ligands for the transition dipole moment $\mu(S_0 \rightarrow S_l)$ vector and whole compound vector of PtON7 compound. The vector of the ligands and Pt atom are marked by the red, the whole compound vector is marked by the green.

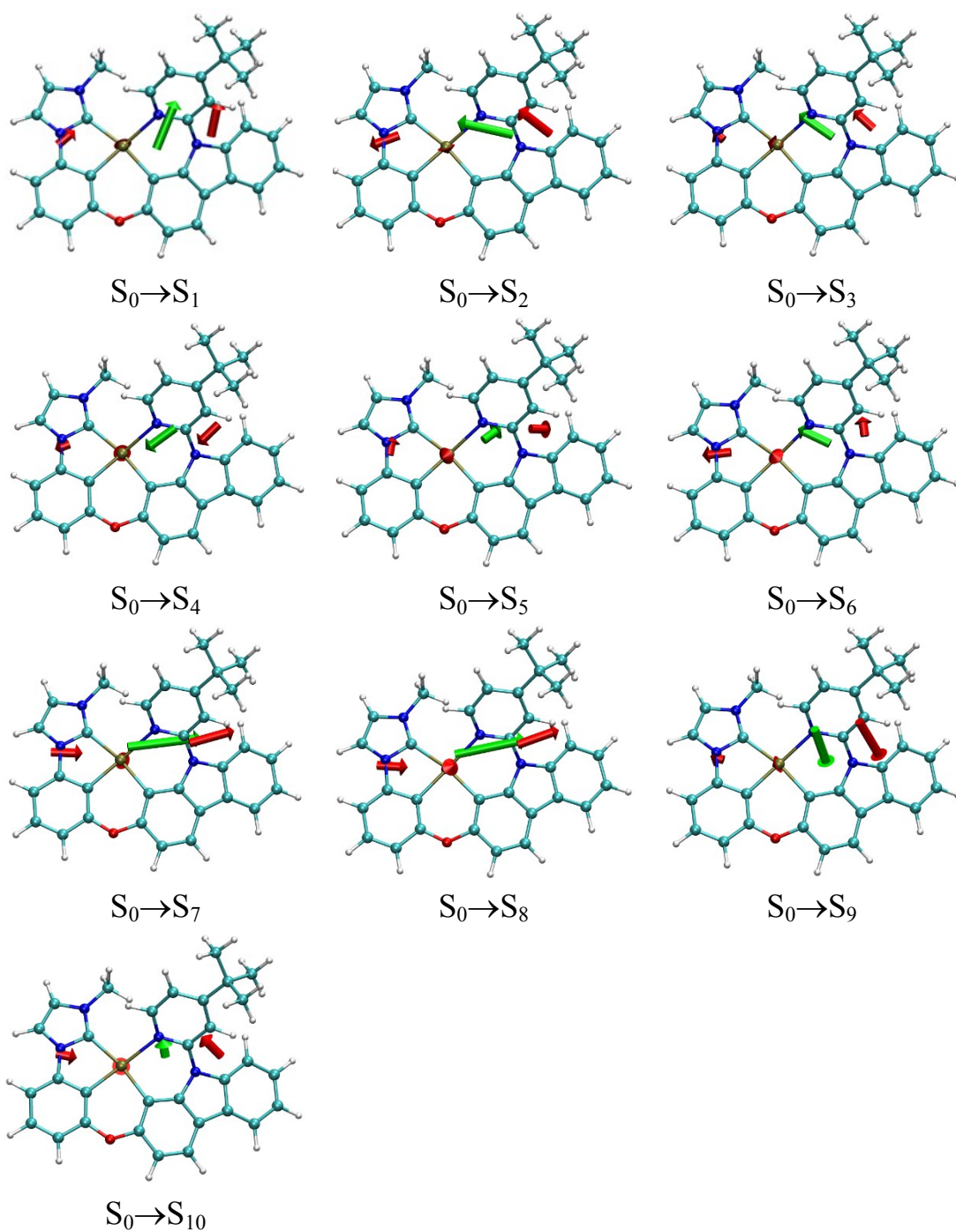


Figure S3. The contribution of different ligands for the transition dipole moment $\mu(S_0 \rightarrow S_l)$ vector and whole compound vector of PtON7-tbu compound. The vector of the ligands and Pt atom are marked by the red, the whole compound vector is marked by the green.

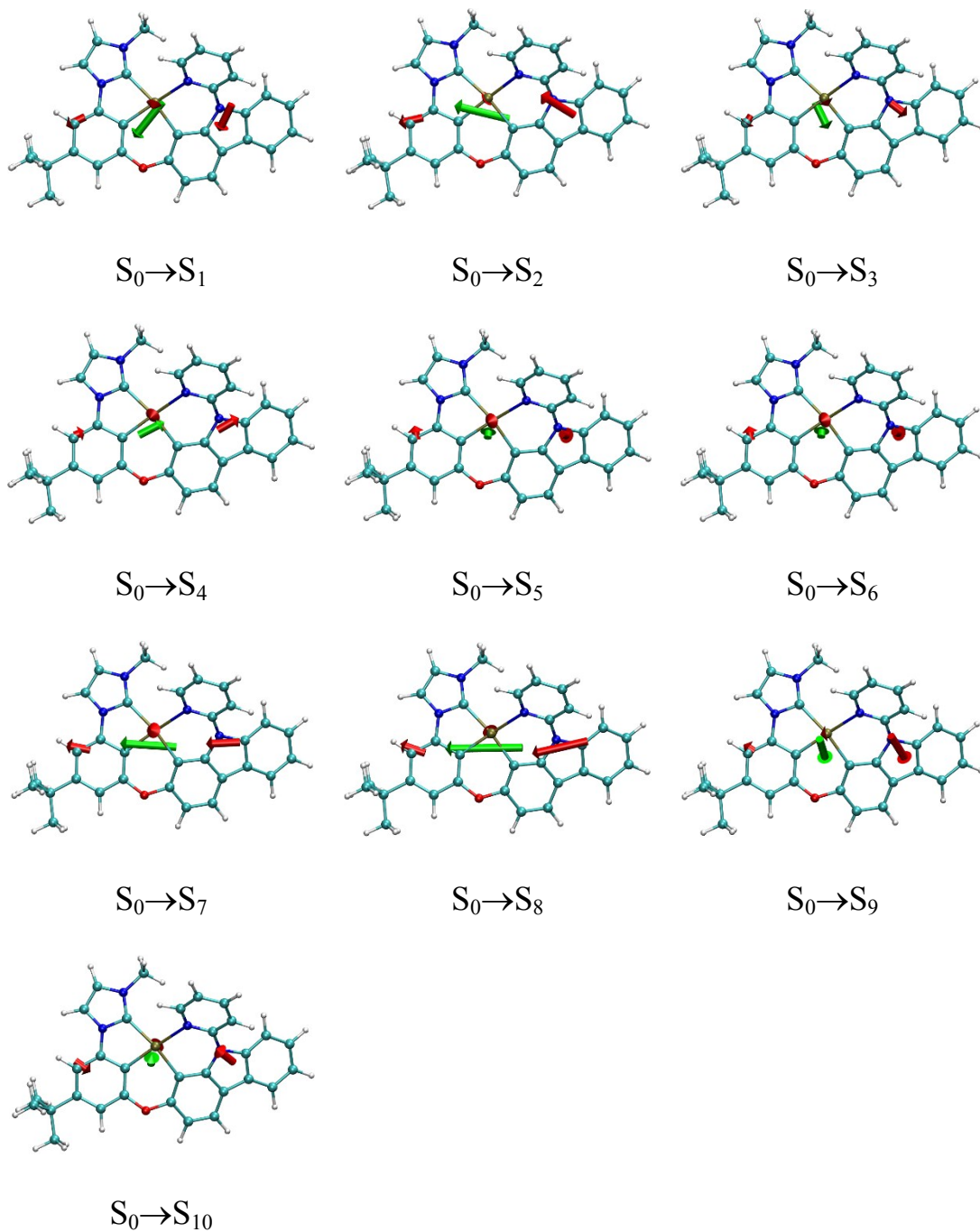


Figure S4. The contribution of different ligands for the transition dipole moment $\mu(S_0 \rightarrow S_l)$ vector and whole compound vector of PtON7-p-tbu compound. The vector of the ligands and Pt atom are marked by the red, the whole compound vector is marked by the green.

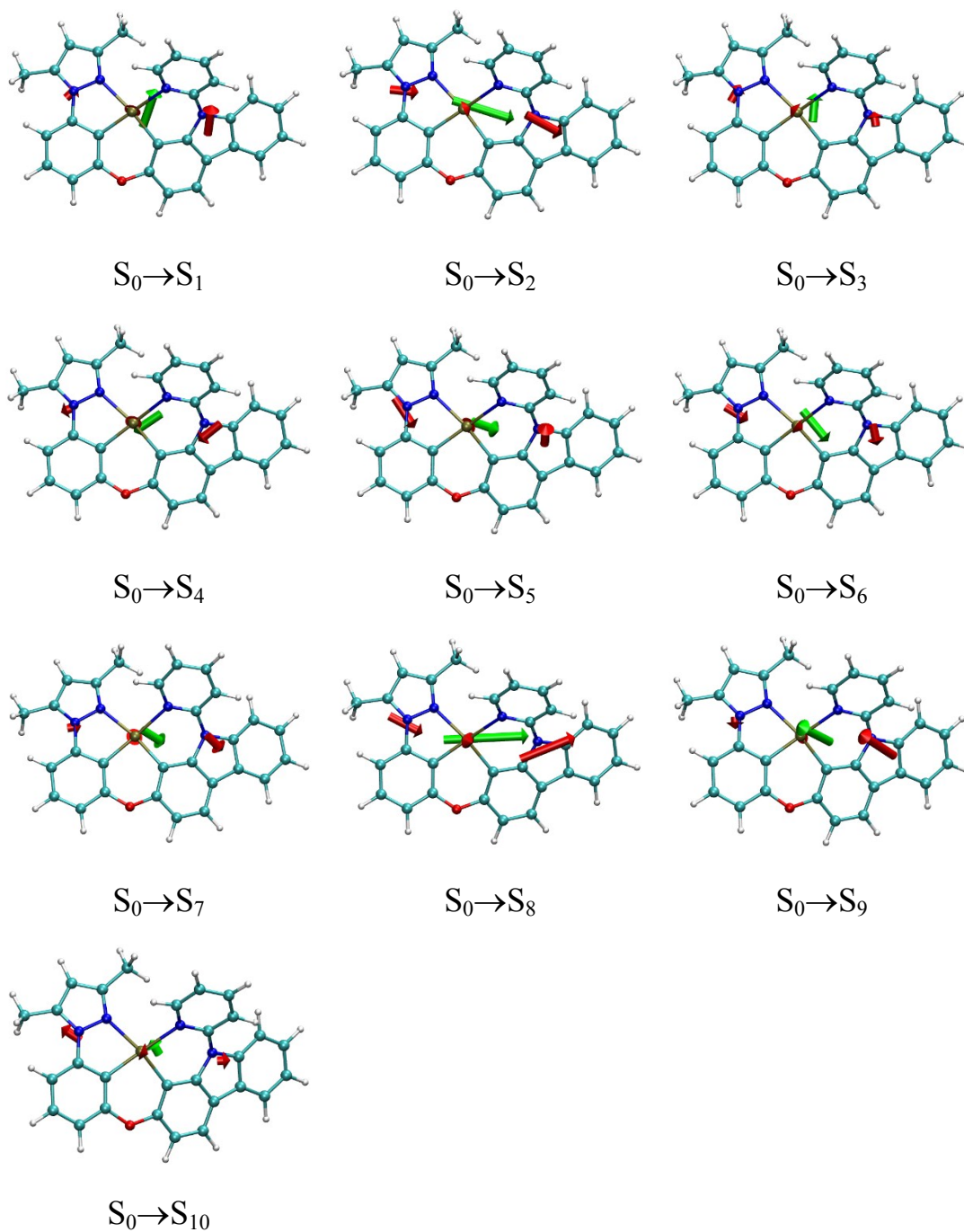


Figure S5. The contribution of different ligands for the transition dipole moment $\mu(S_0 \rightarrow S_l)$ vector and whole compound vector of PtON1 compound. The vector of the ligands and Pt atom are marked by the red, the whole compound vector is marked by the green.

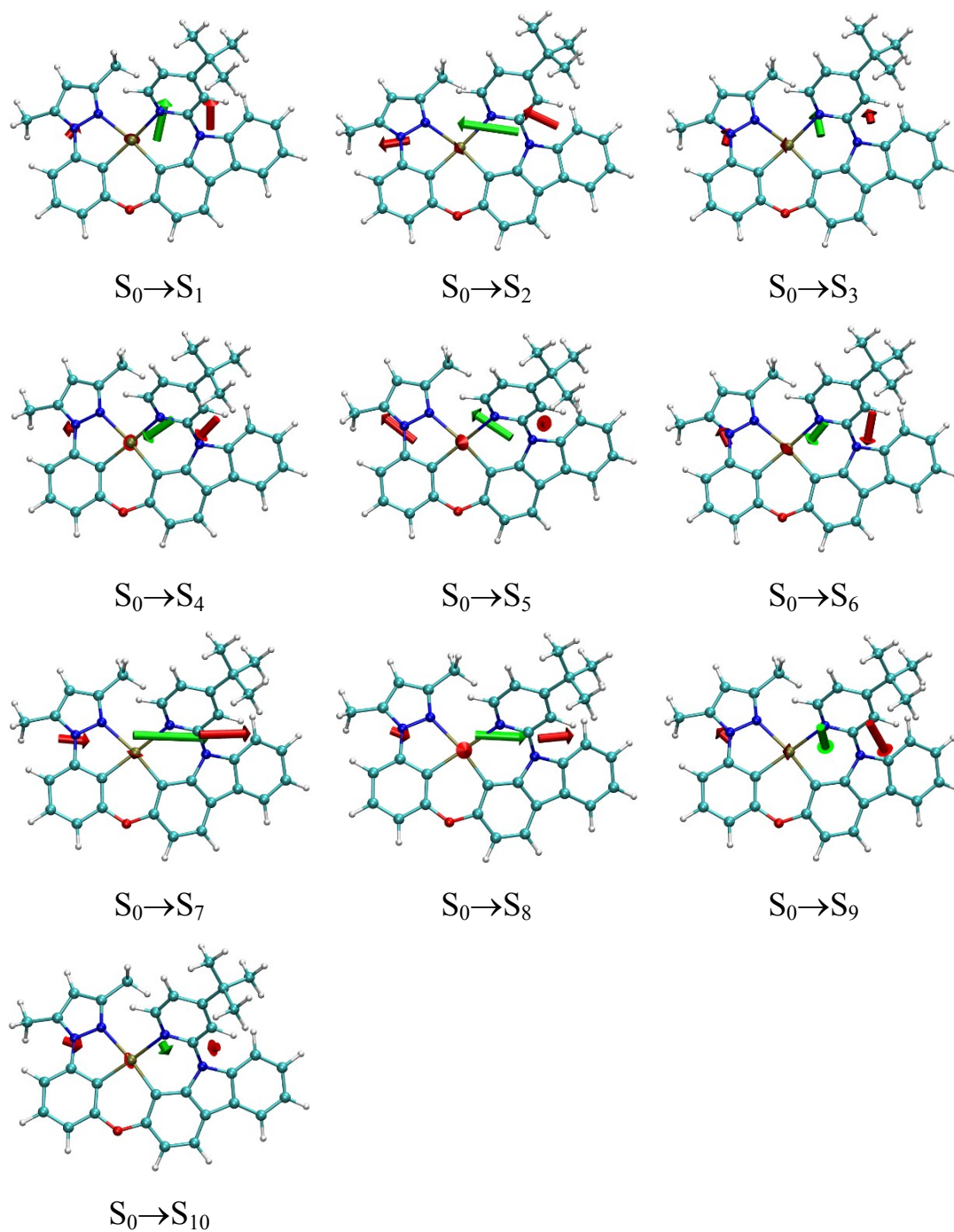


Figure S6. The contribution of different ligands for the transition dipole moment $\mu(S_0 \rightarrow S_i)$ vector and whole compound vector of PtON1-tbu compound. The vector of the ligands and Pt atom are marked by the red, the whole compound vector is marked by the green.

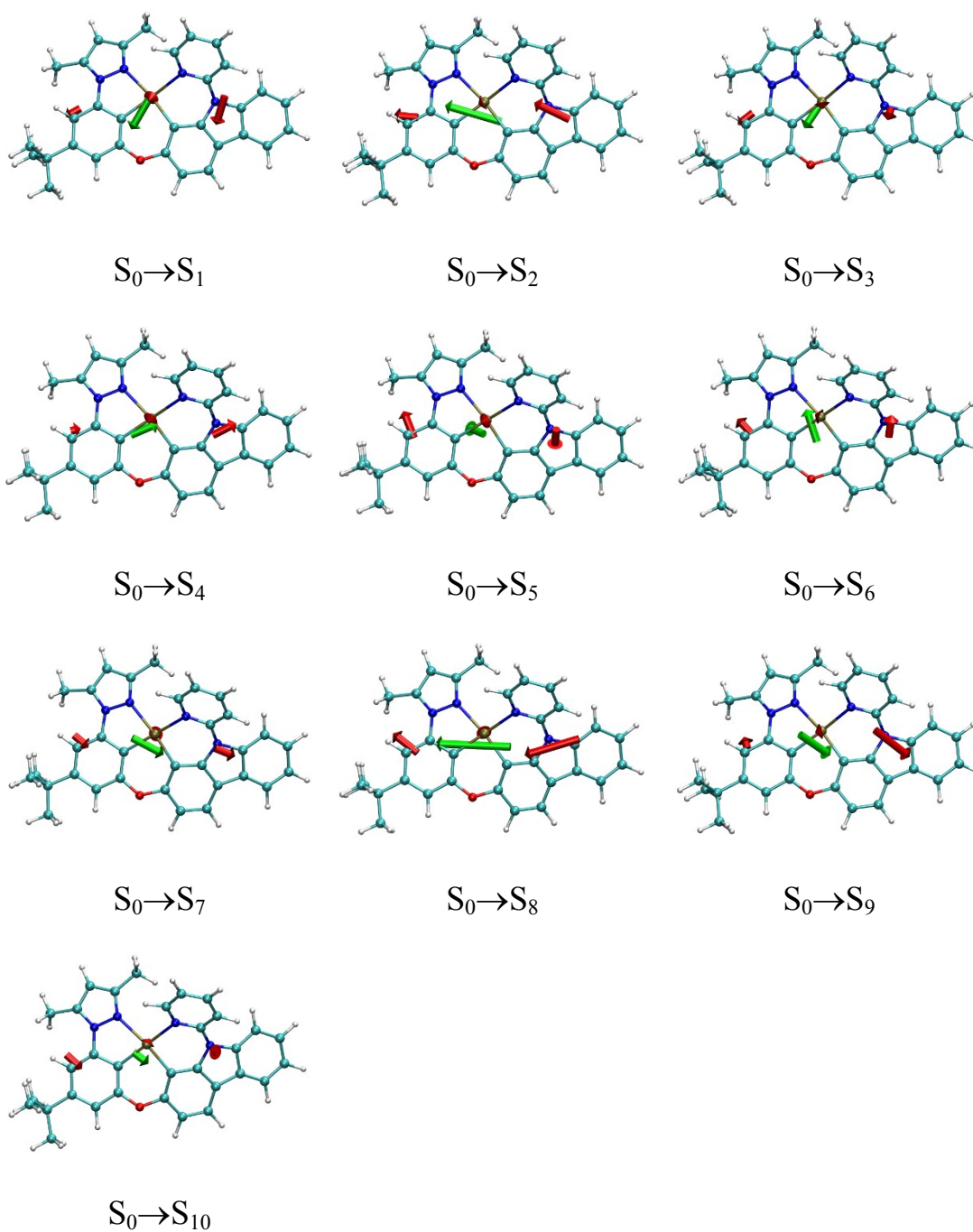


Figure S7. The contribution of different ligands for the transition dipole moment $\mu(S_0 \rightarrow S_l)$ vector and whole compound vector of PtON1-p-tbu compound. The vector of the ligands and Pt atom are marked by the red, the whole compound vector is marked by the green.

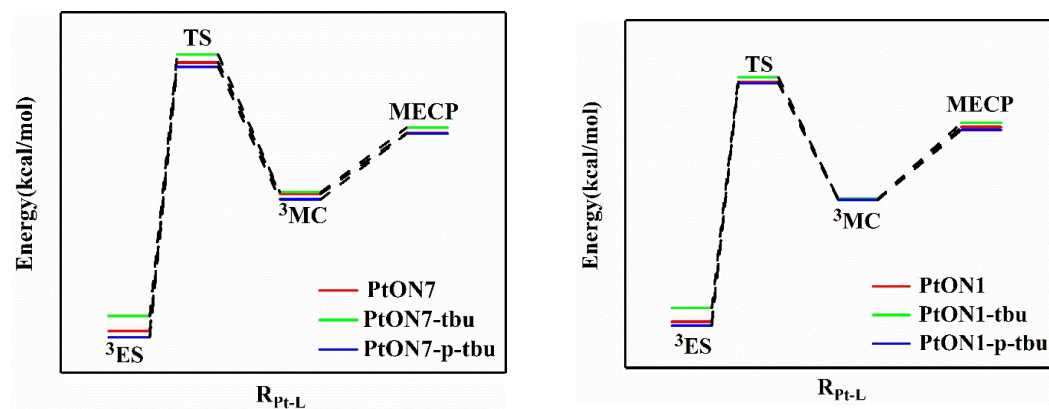


Figure S8. Relative energetic profiles of the thermal deactivation process.

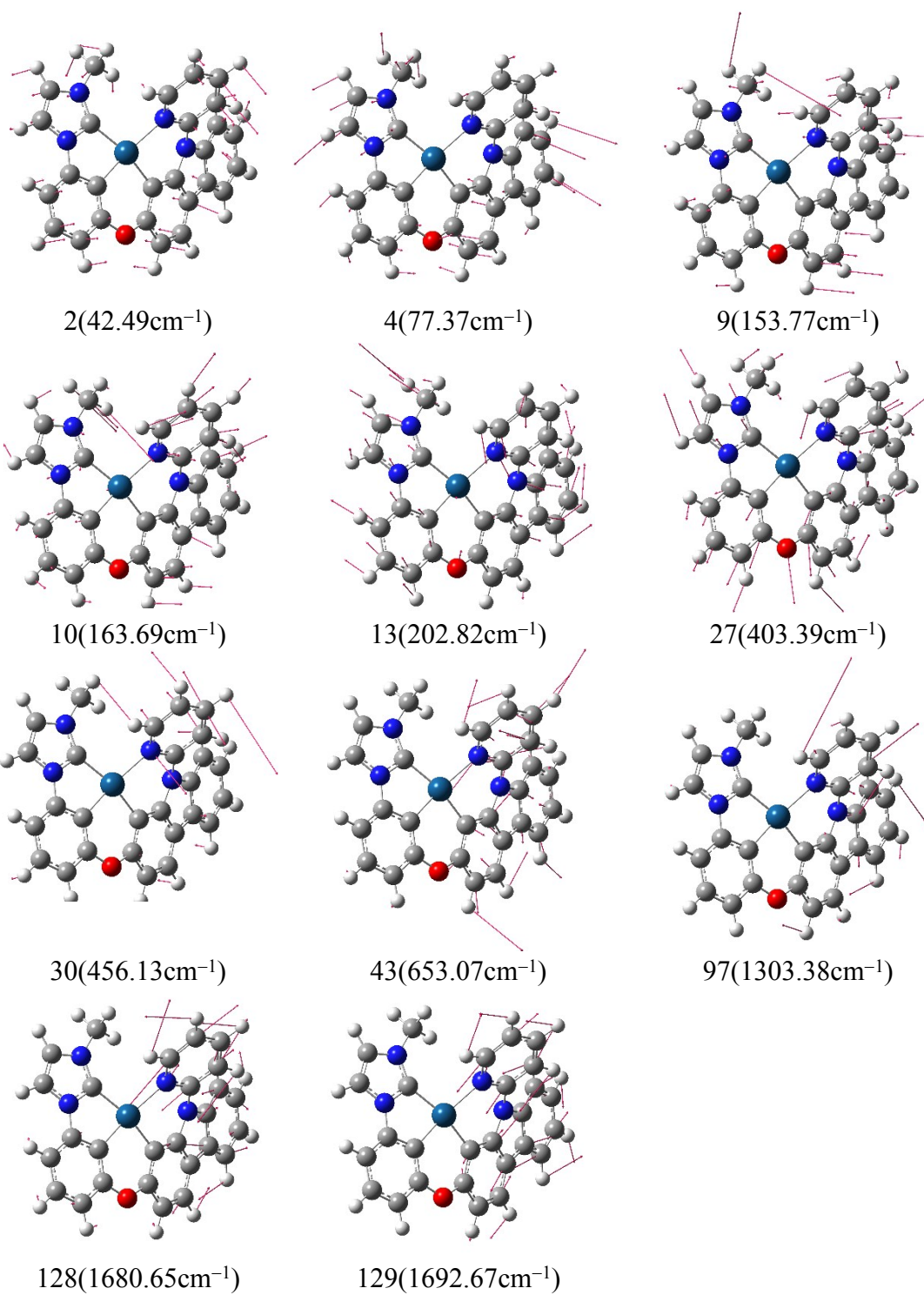


Figure S9. The displacement vectors of the vibration normal modes of compound PtON7 in the emission spectra.

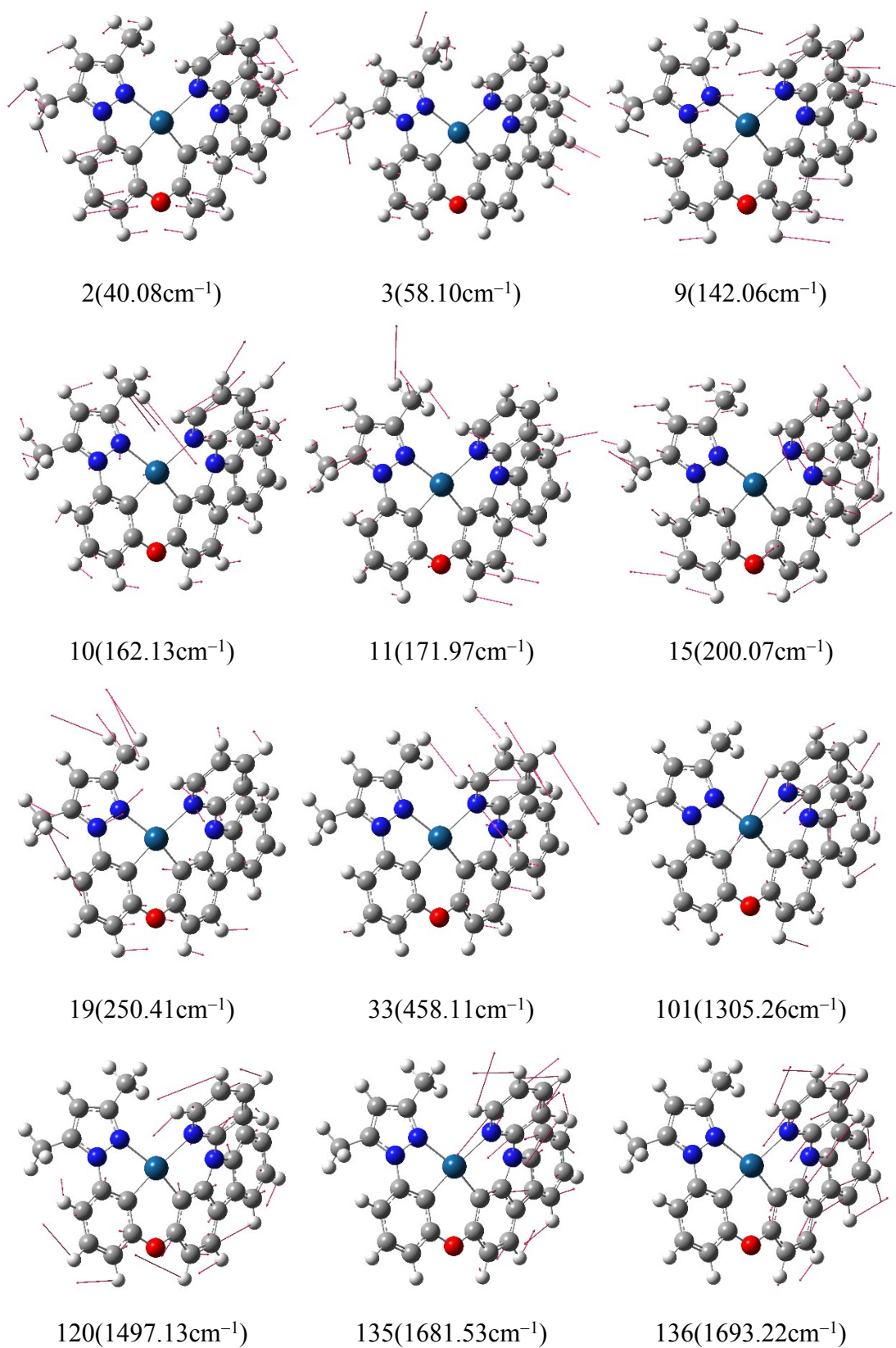


Figure S10. The displacement vectors of the vibration normal modes of compound PtON1 in the emission spectra.