Supplementary information

Long-lived and Oxygen-Responsive Photoluminescence in the Solid State of Copper(I) Complexes Bearing Fluorinated Diphosphine and Bipyridine Ligands

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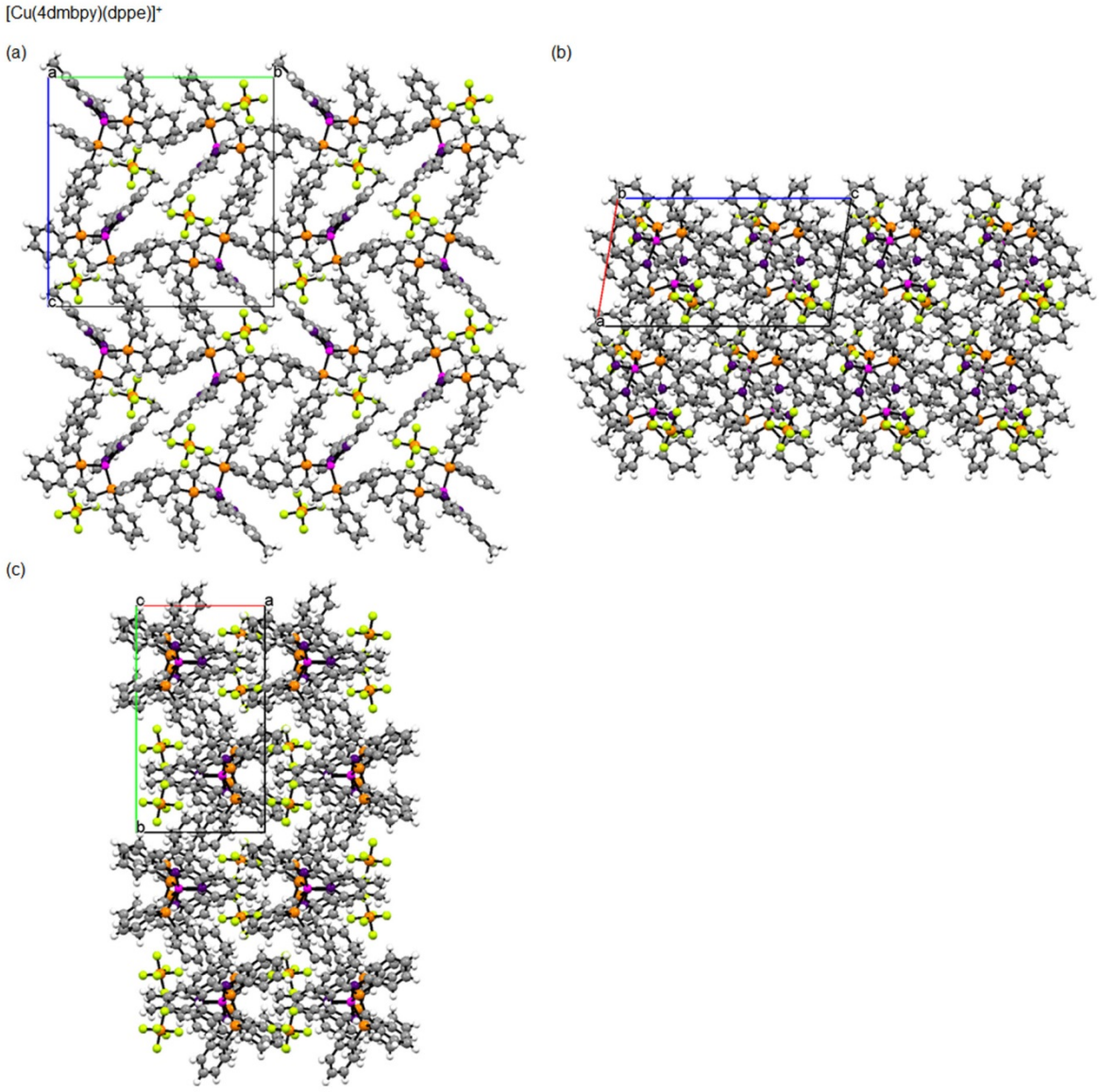

Fig. S1. Crystal structure of **2**·PF_6 viewed along a-axis (a), b-axis (b), and c-axis (c).

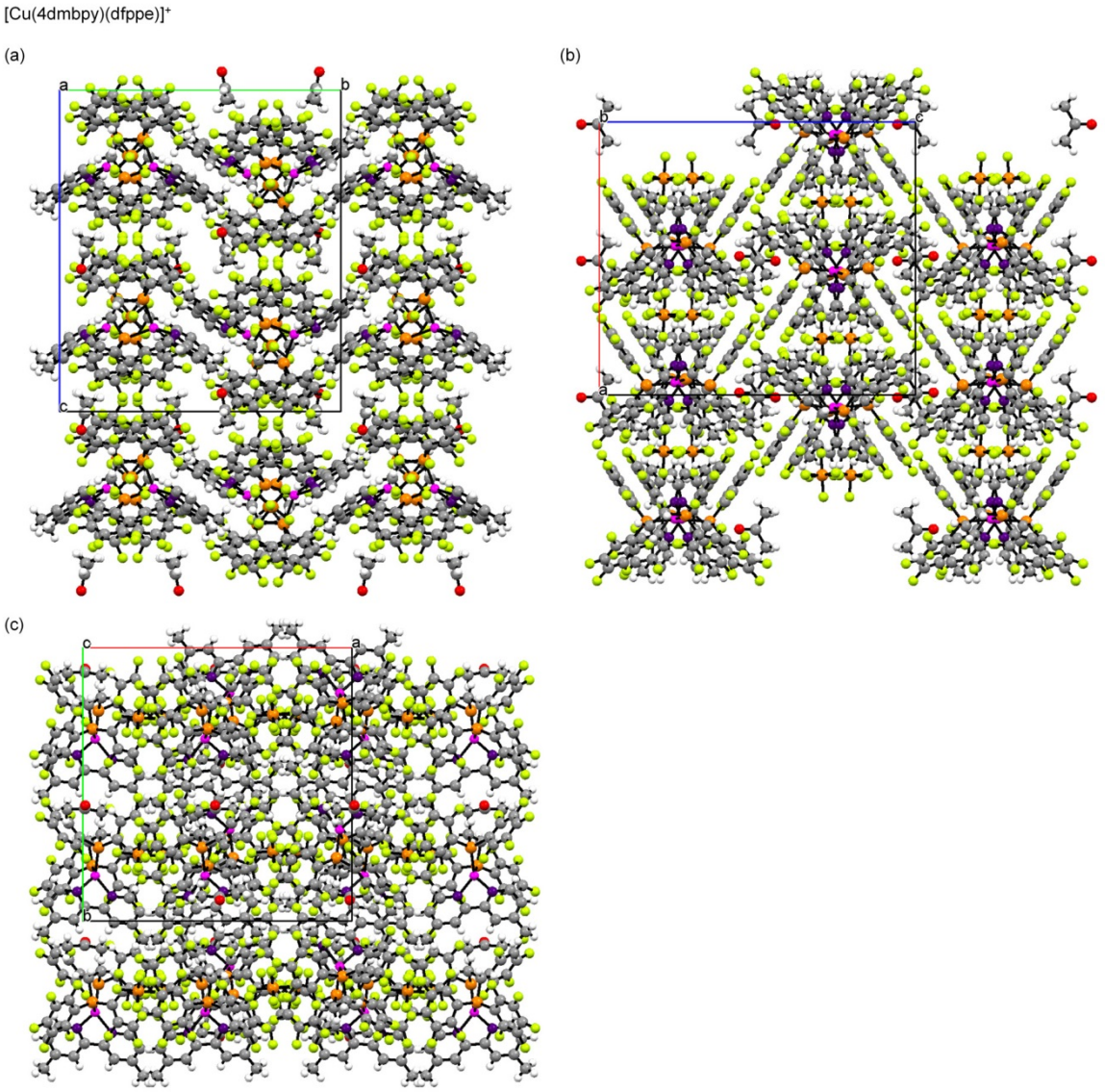

Fig. S2. Crystal structure of **4**·PF_6 viewed along a-axis (a), b-axis (b), and c-axis (c).

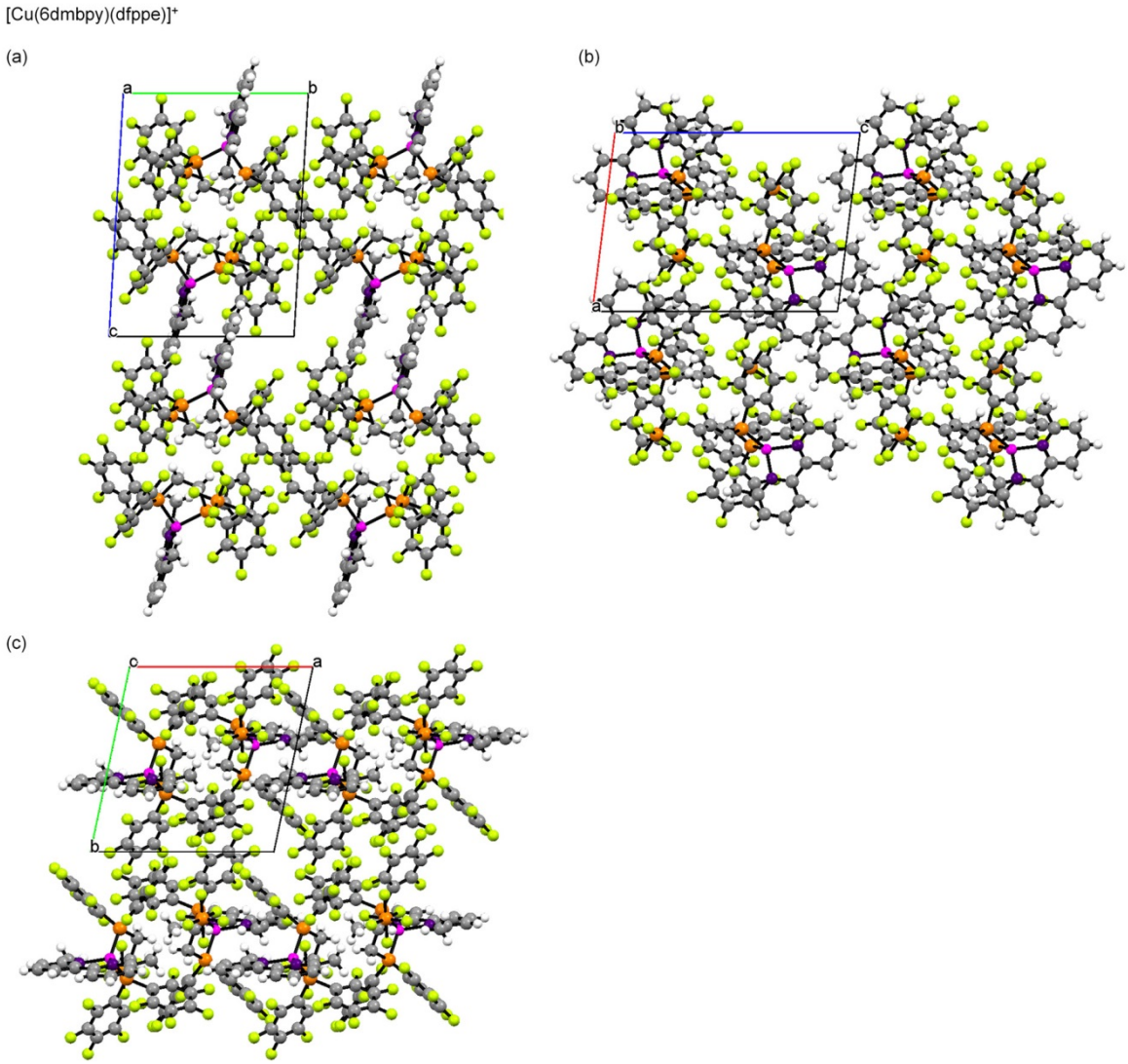

Fig. S3. Crystal structure of **5**·PF_6 viewed along a-axis (a), b-axis (b), and c-axis (c).

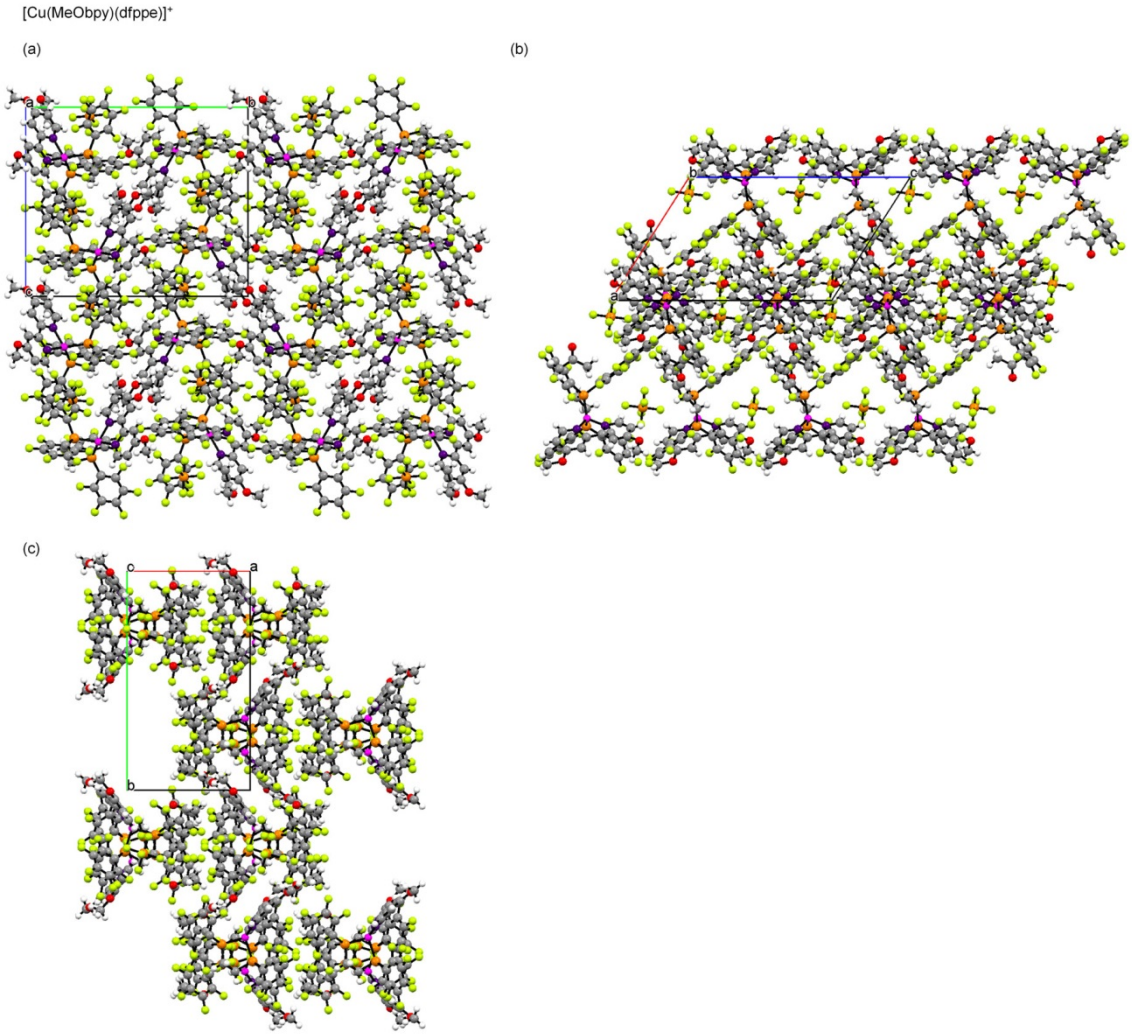

Fig. S4. Crystal structure of **6**·PF_6 viewed along a-axis (a), b-axis (b), and c-axis (c).

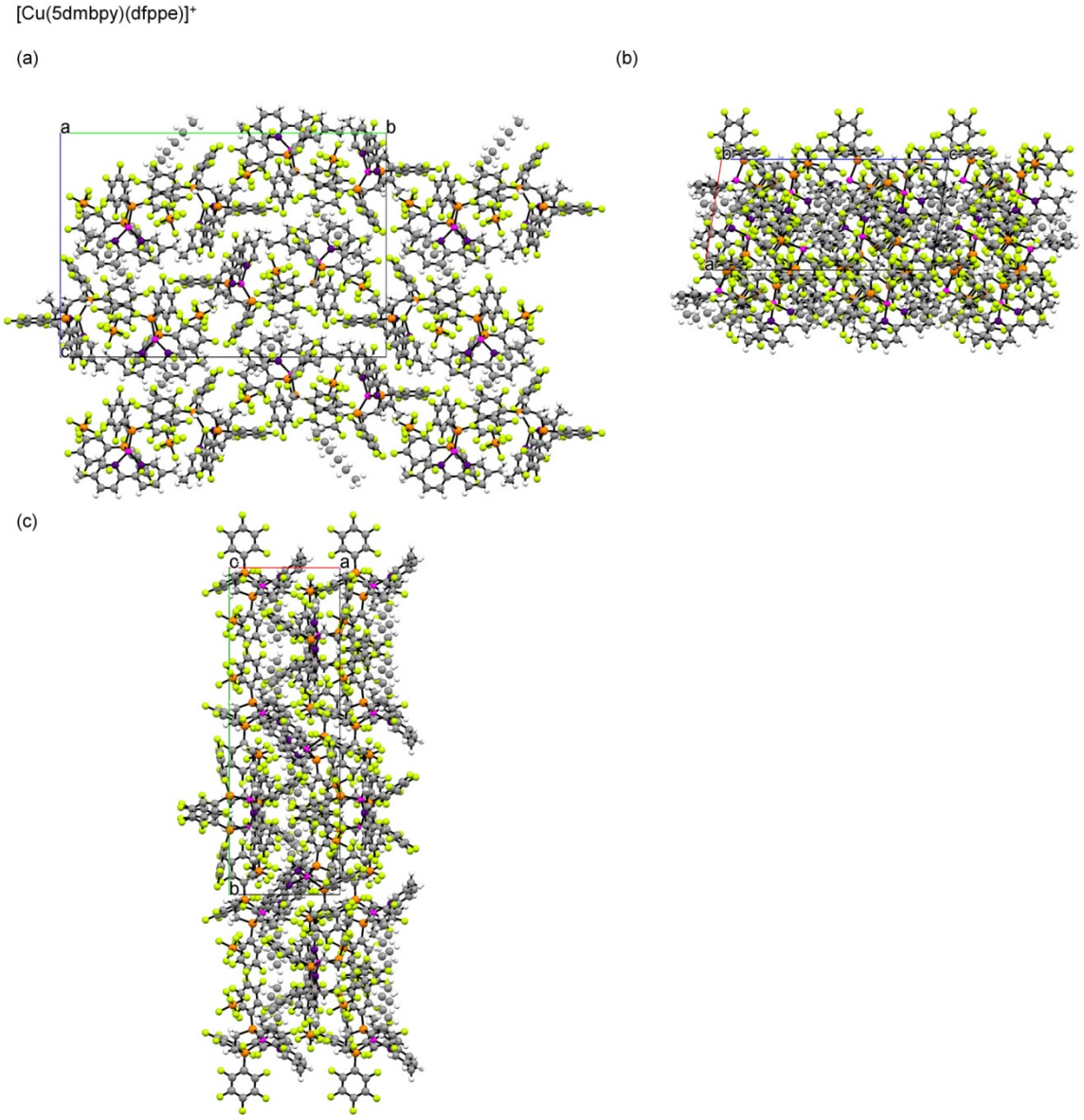

Fig. S5. Crystal structure of **7**·PF_6 viewed along a-axis (a), b-axis (b), and c-axis (c).

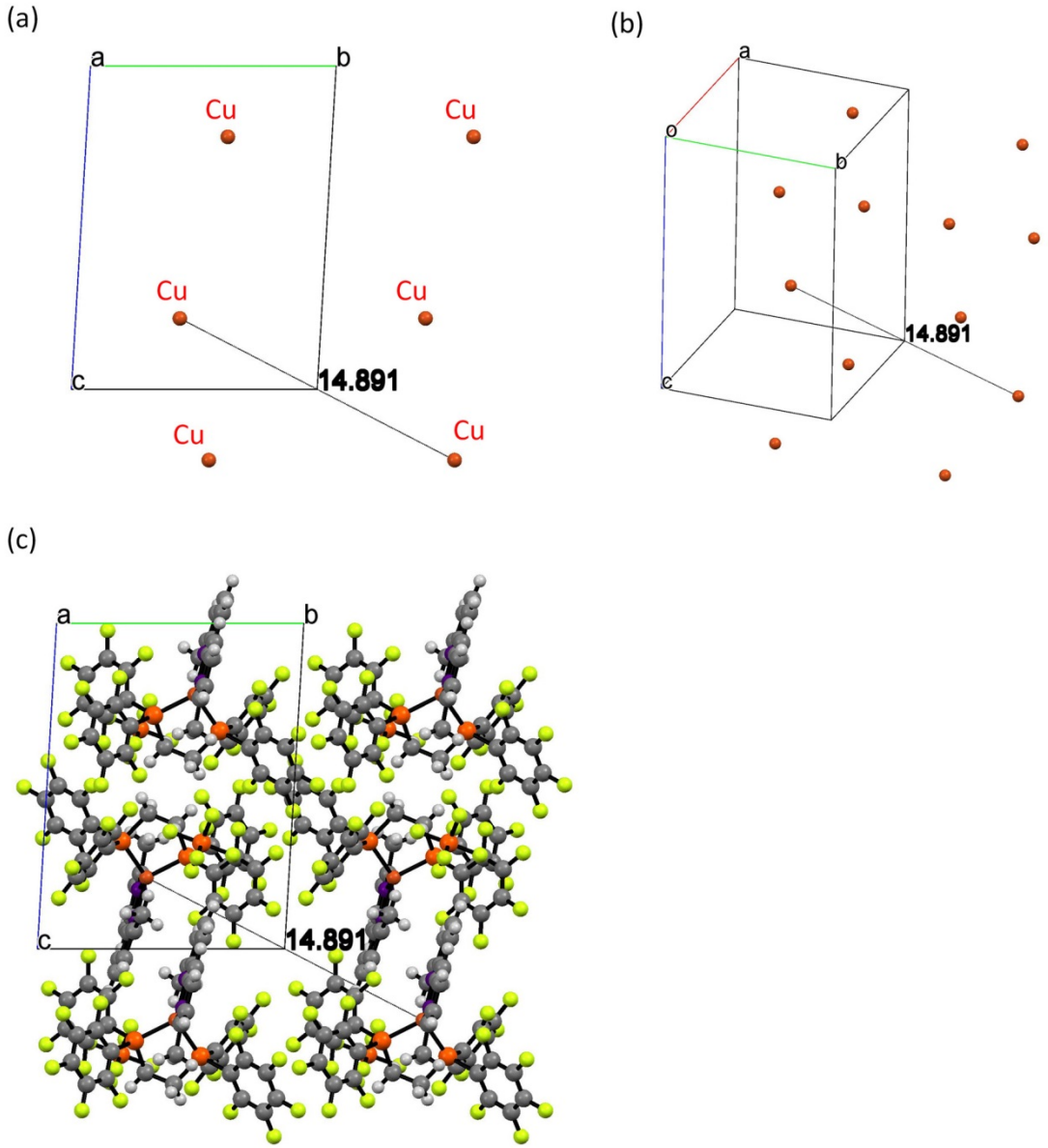

Fig. S6. Copper centers and unit cell of the crystal structure of **5**·PF_6 viewed along a-axis (a) and viewed obliquely (b). The distance (14.891 Å) between two copper center is included in the figure. (c) the crystal structure of **5**·PF_6 viewed along a-axis.

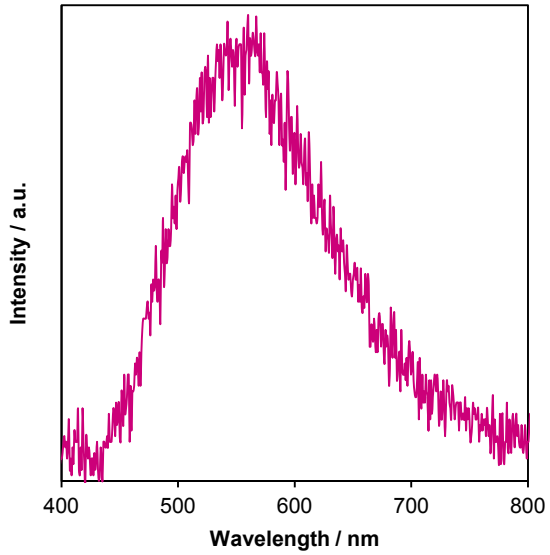

Fig. S7. Emission spectra of **5**·PF_6 in CH_2Cl_2 degassed by argon bubbling at room temperature. Excitation light is 370 nm.

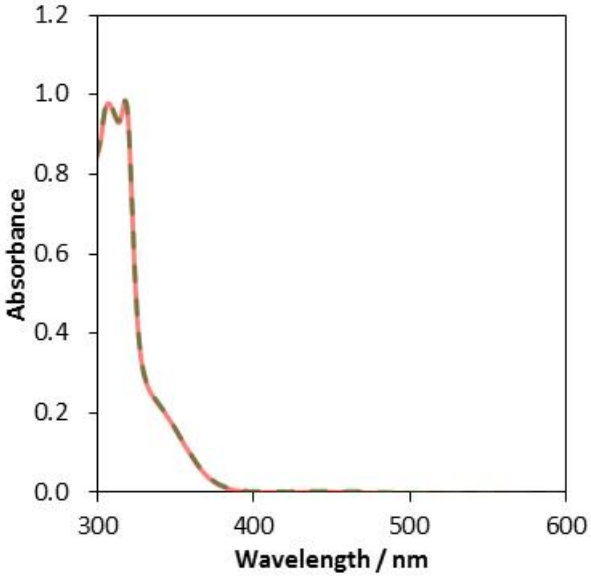

Fig. S8. Changes in the absorption spectra of **5**·PF_6 in degassed dichloromethane at room temperature before (red, solid line) and after (green, dashed line) taken photophysical measurements.

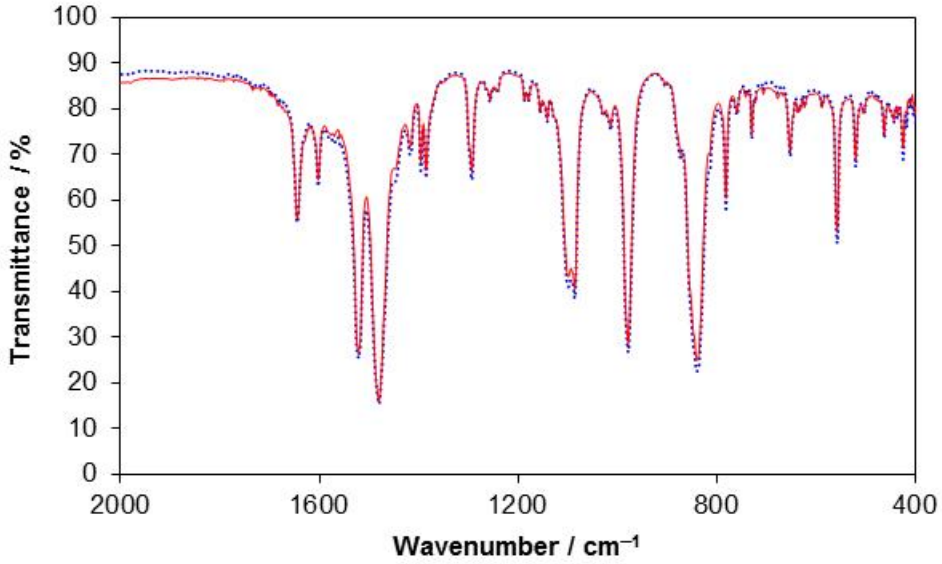

Fig. S9. IR spectra in KBr pellet of **5**·PF_6 upon 10 times repeated operations of exposing the sample to the vacuum and the air (blue dotted line) and before the operations (red solid line).

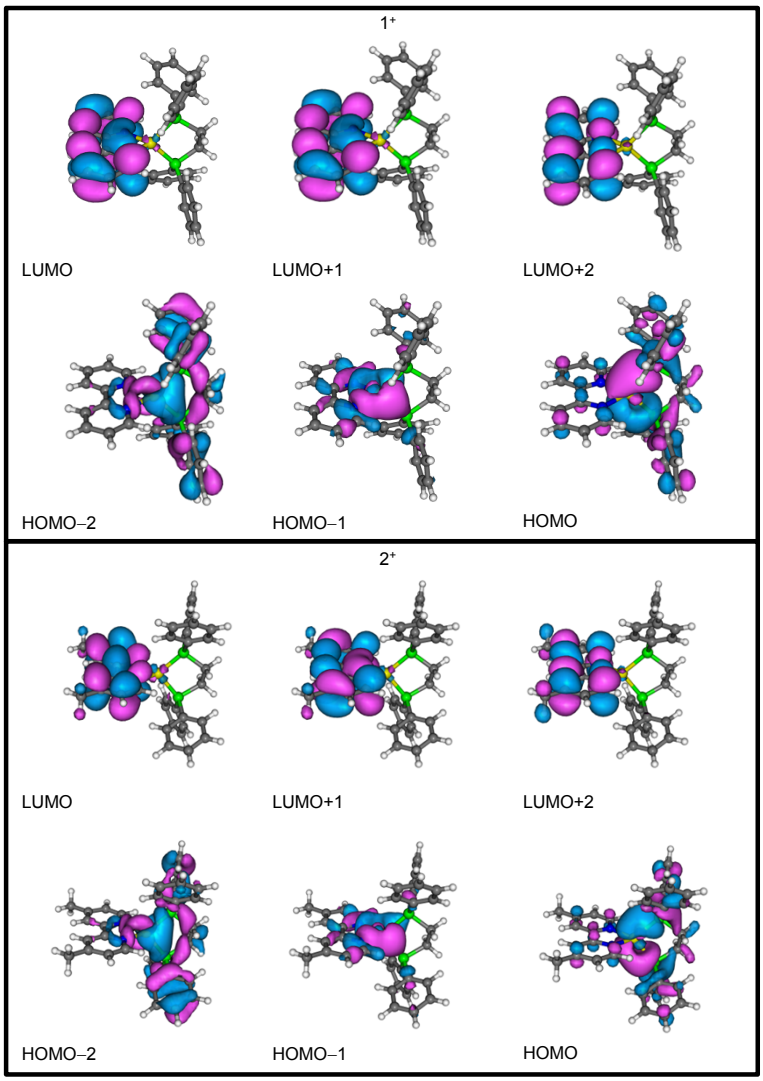

Fig. S10. Kohn-Sham orbitals of $\mathbf{1}^+$ and $\mathbf{2}^+$. Orbitals calculated based on the optimized structure in the S_0 (singlet ground) states (contour value 0.02).

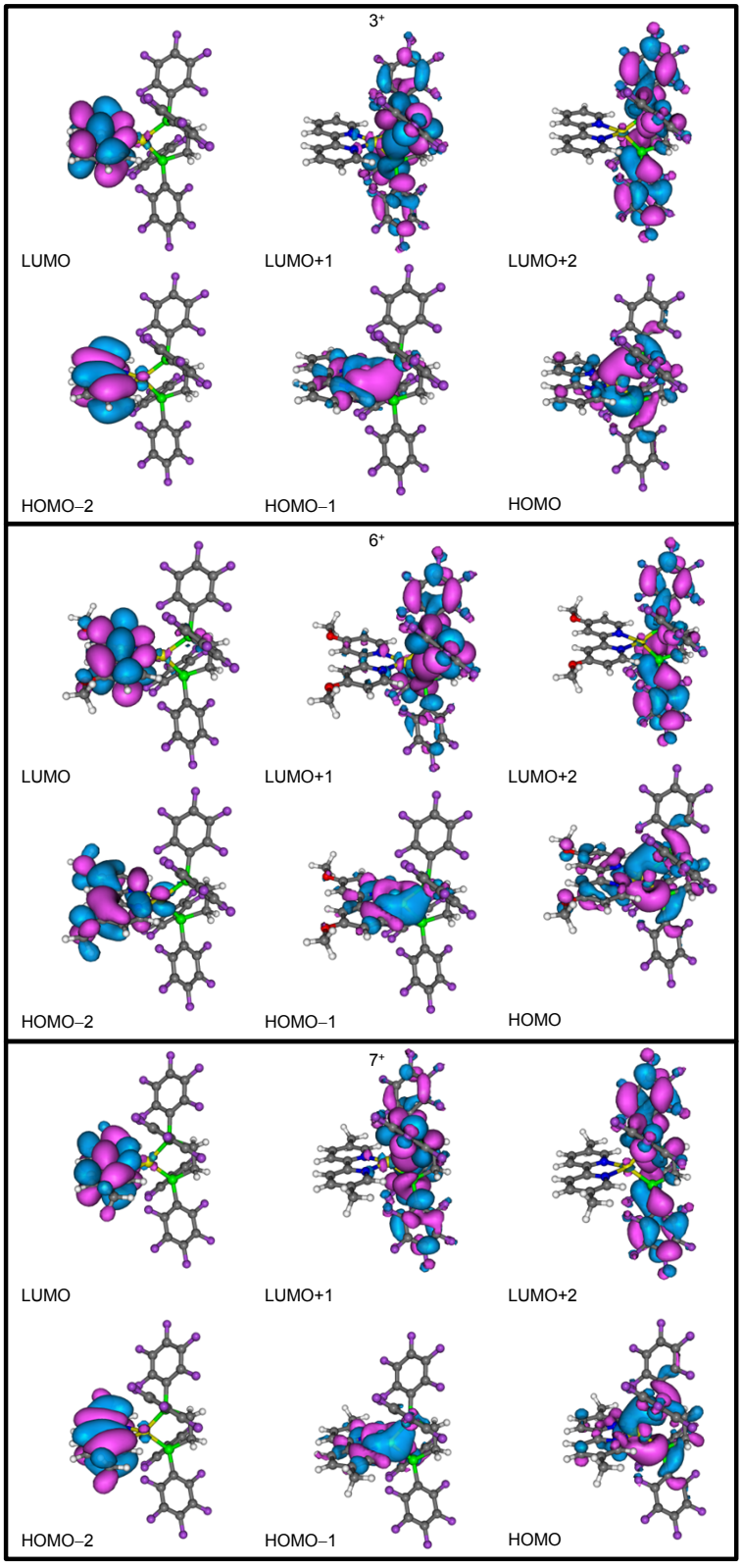

Fig. S11. Kohn-Sham orbitals of **3**$^{+}$, **6**$^{+}$ and **7**$^{+}$. Orbitals calculated based on the optimized structure in the S_0 (singlet ground) states (contour value 0.02).

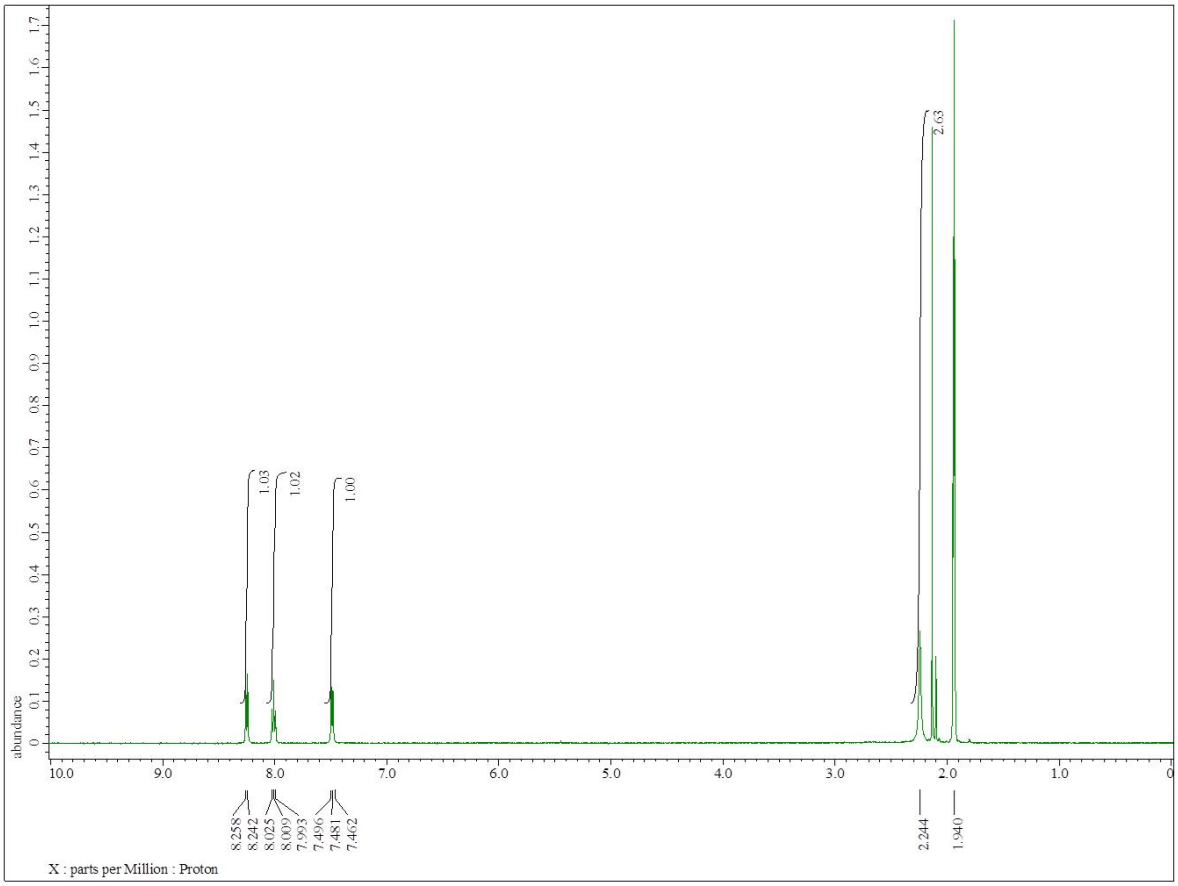

Fig. S12. ^{1}H NMR spectrum of the red solid in CD_3CN at room temperature.