Electronic Supplementary Information

Different emissive properties in dithiolate gold(I) complexes as a function of the presence of phenylene spacers†

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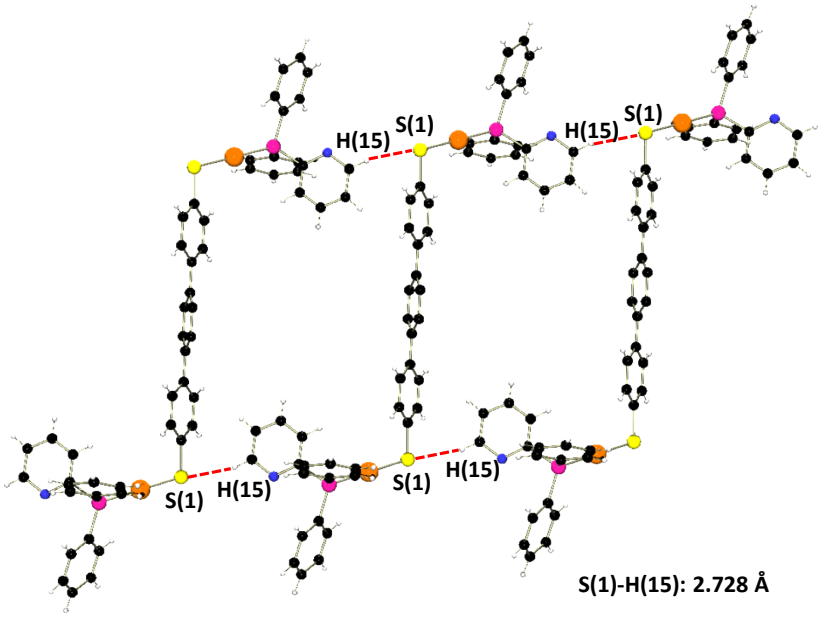

Figure S1. S-(H-C5H4NPh$_2$P) short contacts 2.728 Å of complex **6**

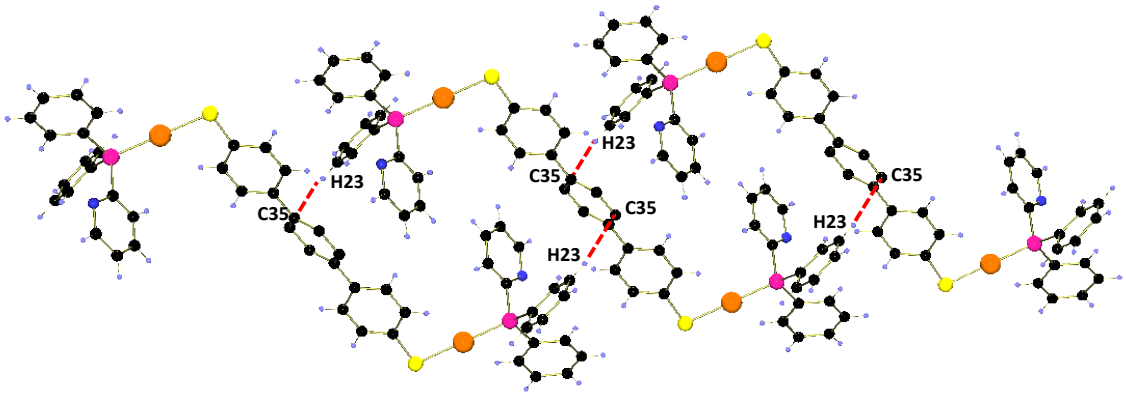

Figure S2. C-(H-C5H4NPh$_2$P) short contacts 2.882 Å of complex **6**

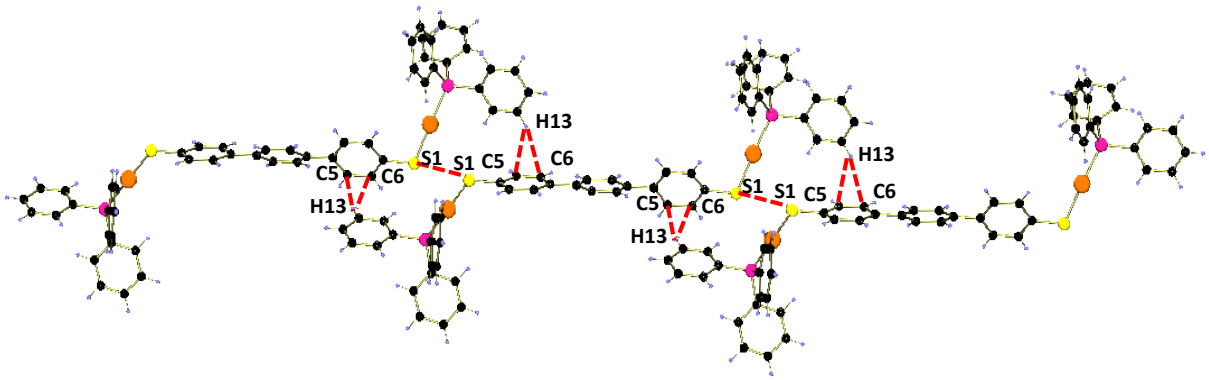

Figure S3. S-S Short contact (3.236 Å) and C-H…π interaction (H-C5:2.866 Å, H-C6:2.863) of complex **2**

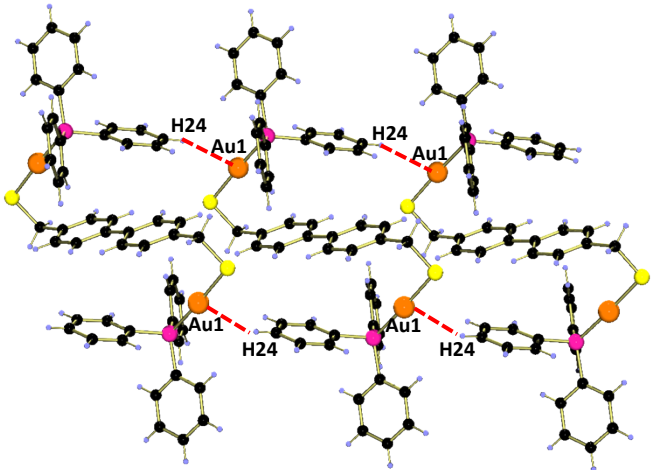

Figure S4. Au-H Short contact (2.850 Å) of complex **4**

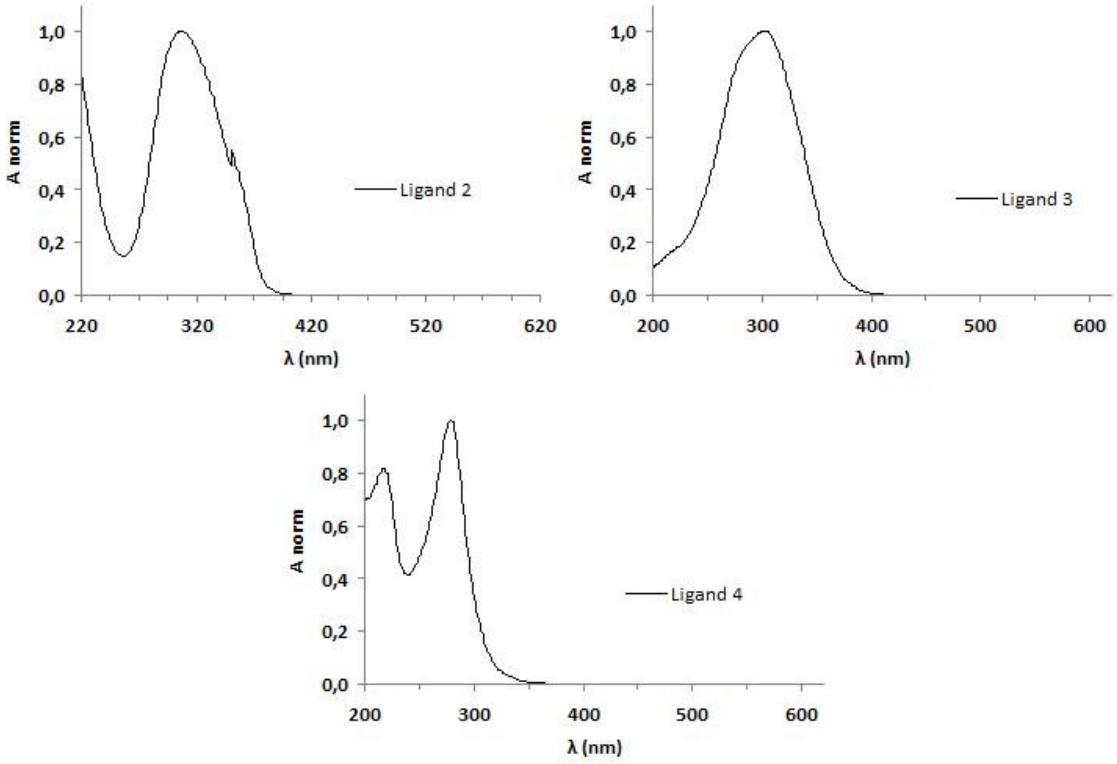

Figure S5. DRUV spectra of **L2**, **L3** and **L4**.

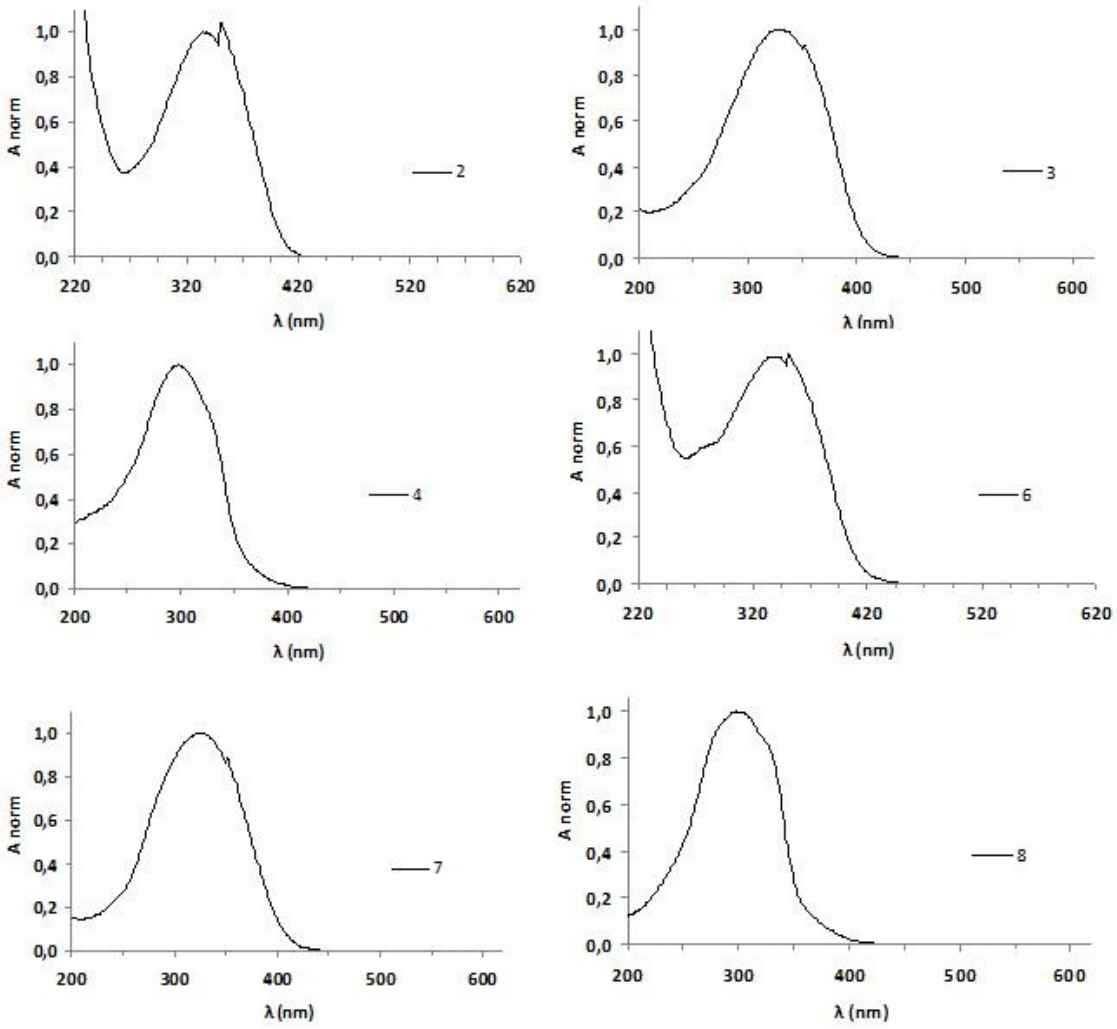

Figure S6. DRUV spectra of complexes **2**-**4**, **6**-**8**.

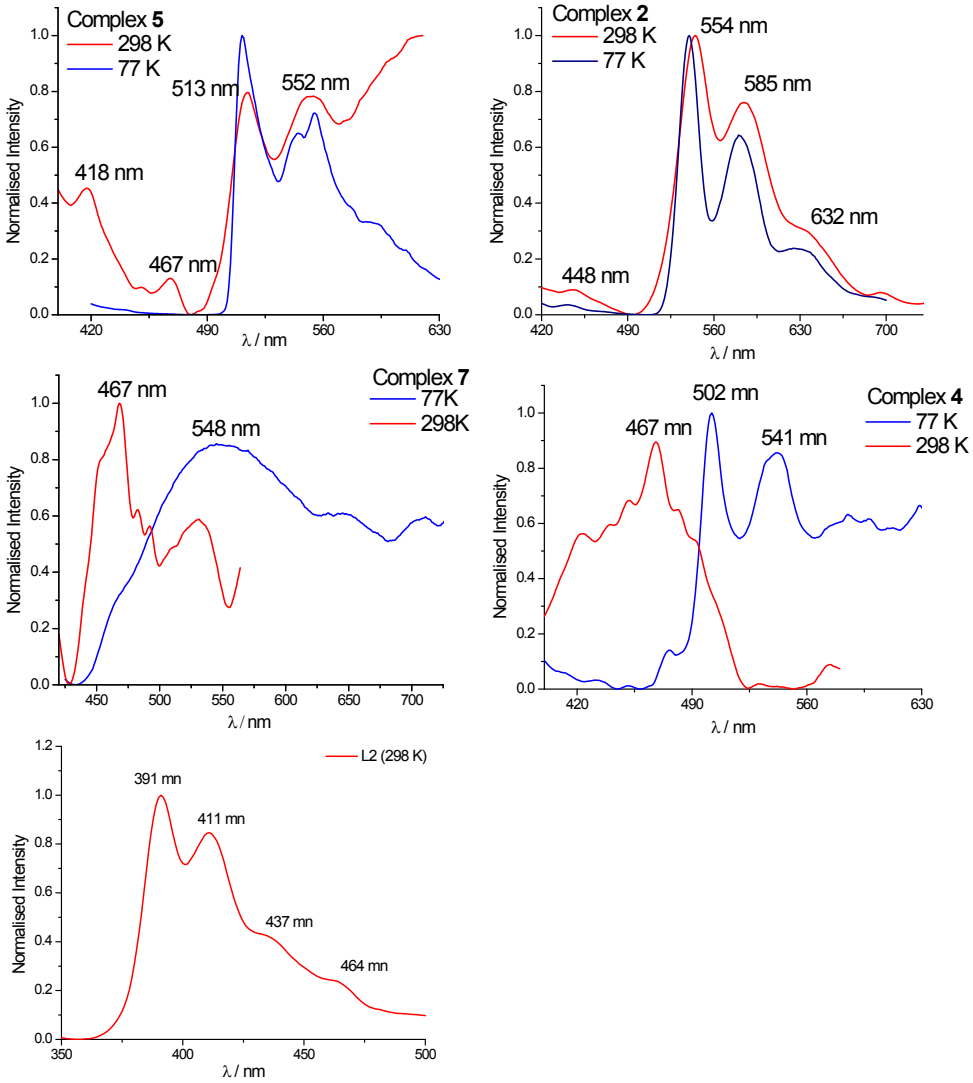

Figure S7. Emission spectra at 298 K (red line) and 77 K (blue line) of complexes **5**, **2**, **7**, **4** and **L2**.

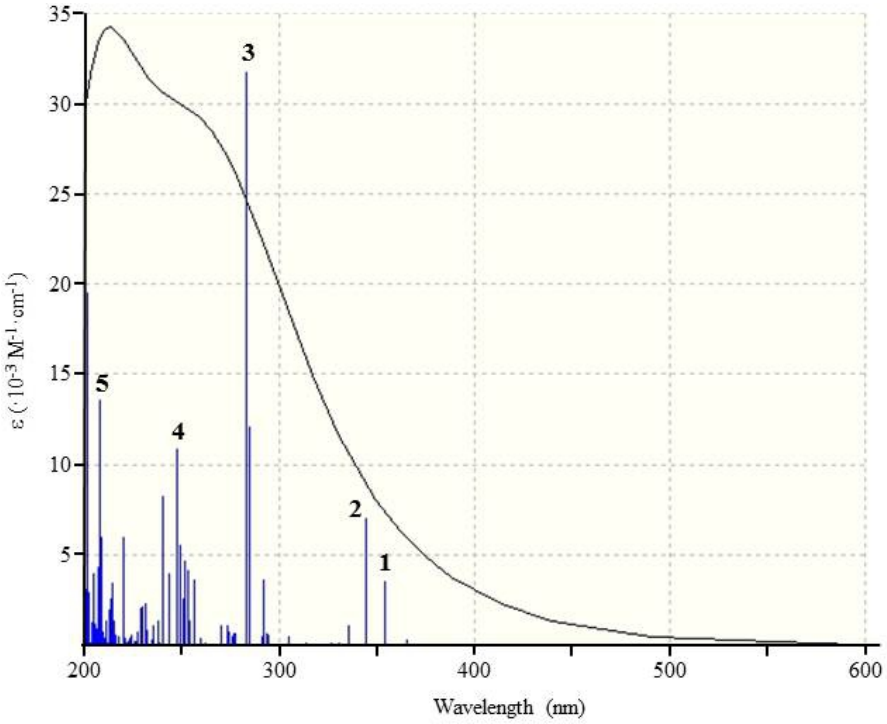

Figure S8. Simulated absorption spectrum for **4** in the gas phase with calculated TD-DFT singlet vertical transitions. 1: S0 → S3 (3.505 eV, f = 0.045), 2: S0 → S5 (3.596 eV, f = 0.090), 3: S0 → S29 (4.383 eV, f = 0.407), 4: S0 → S62 (5.010 eV, f = 0.139), and 5: S0 → S188 (6.162 eV, f = 0.250).

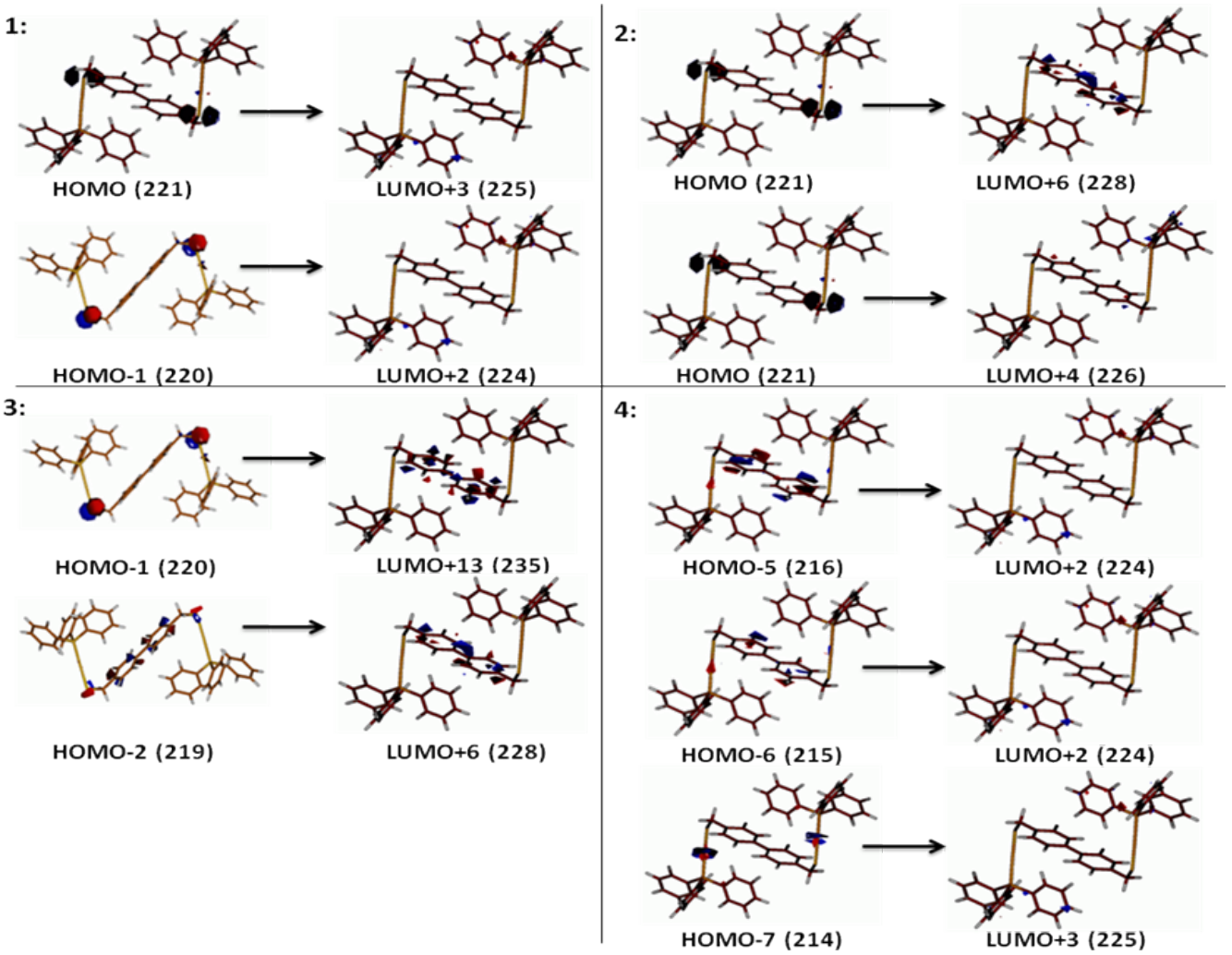

Figure S9. Isosurface drawings of the Kohn-Sham MOs calculated for **4** involved in the principal singlet vertical electronic transitions (see Fig. S8). Contour value = 0.05 e.