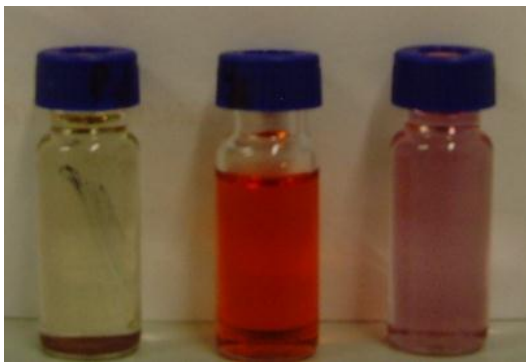


## Supplementary information

**Table 1.** Bond lengths (Å) in compound **3g**

| Bond   | Molecule |          | Bond    | Molecule |         |
|--------|----------|----------|---------|----------|---------|
|        | A        | B        |         | A        | B       |
| Br1-C1 | 1.898(9) | 1.917(8) | C7-C8   | 1.45(1)  | 1.46(1) |
| S1-C7  | 1.68(1)  | 1.668(9) | C8-C9   | 1.37(1)  | 1.38(1) |
| O1-C9  | 1.268(9) | 1.28(1)  | C9-C10  | 1.52(1)  | 1.51(1) |
| O2-C13 | 1.35(1)  | 1.36(1)  | C10-C11 | 1.38(1)  | 1.38(1) |
| O2-C14 | 1.44(1)  | 1.42(1)  | C10-C16 | 1.39(1)  | 1.37(1) |
| N1-C4  | 1.432(9) | 1.42(1)  | C11-C12 | 1.40(1)  | 1.42(1) |
| N1-C7  | 1.34(1)  | 1.350(1) | C12-C13 | 1.39(1)  | 1.37(1) |
| N2-C8  | 1.46(1)  | 1.46(1)  | C13-C15 | 1.35(1)  | 1.37(1) |
| N2-C17 | 1.33(1)  | 1.33(1)  | C15-C16 | 1.39(1)  | 1.39(1) |
| N2-C21 | 1.361(9) | 1.33(1)  | C17-C18 | 1.36(1)  | 1.40(1) |
| N3-C24 | 1.32(1)  | 1.28(1)  | C18-C19 | 1.35(1)  | 1.40(1) |
| N3-C25 | 1.31(1)  | 1.32(1)  | C19-C20 | 1.38(1)  | 1.34(1) |
| C1-C2  | 1.36(1)  | 1.33(1)  | C19-C22 | 1.51(1)  | 1.52(1) |
| C1-C6  | 1.33(1)  | 1.36(1)  | C20-C21 | 1.35(1)  | 1.41(1) |
| C2-C3  | 1.40(1)  | 1.40(1)  | C22-C23 | 1.39(1)  | 1.37(1) |
| C3-C4  | 1.37(1)  | 1.39(1)  | C22-C26 | 1.41(1)  | 1.39(1) |
| C4-C5  | 1.35(1)  | 1.38(1)  | C23-C24 | 1.36(1)  | 1.38(1) |
| C5-C6  | 1.39(1)  | 1.37(1)  | C26-C25 | 1.38(1)  | 1.37(1) |



**Figure 1.** The yellow solution is palladium salt  $\text{Pd}(\text{CH}_3\text{CN})_2\text{Cl}_2$ , the orange solution is the ligand **3d** (in the middle) and the purple violet solution is the complex  $[\text{Pd}^{\text{II}}\text{-3d}]\text{Cl}_2$ , all solution are in DCM (left to right).