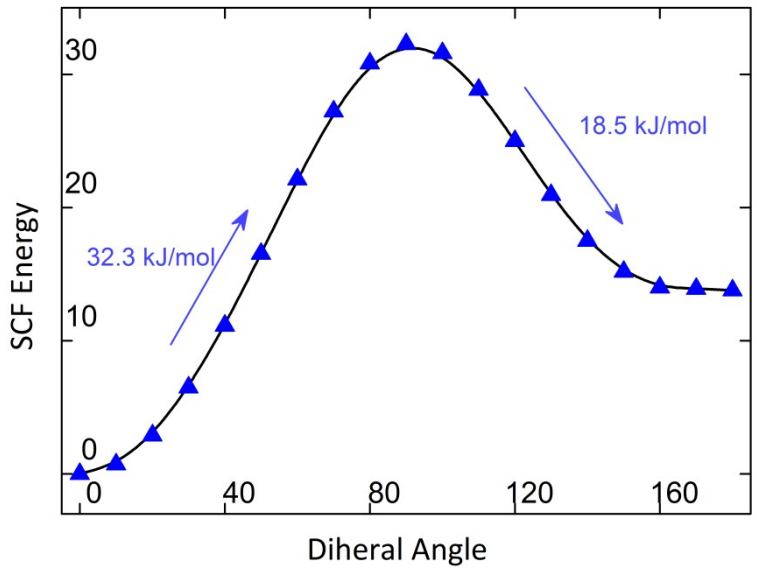

Figure S1 Energy profiles by relaxed scan of the N2C2C1N3 dihedral of L.

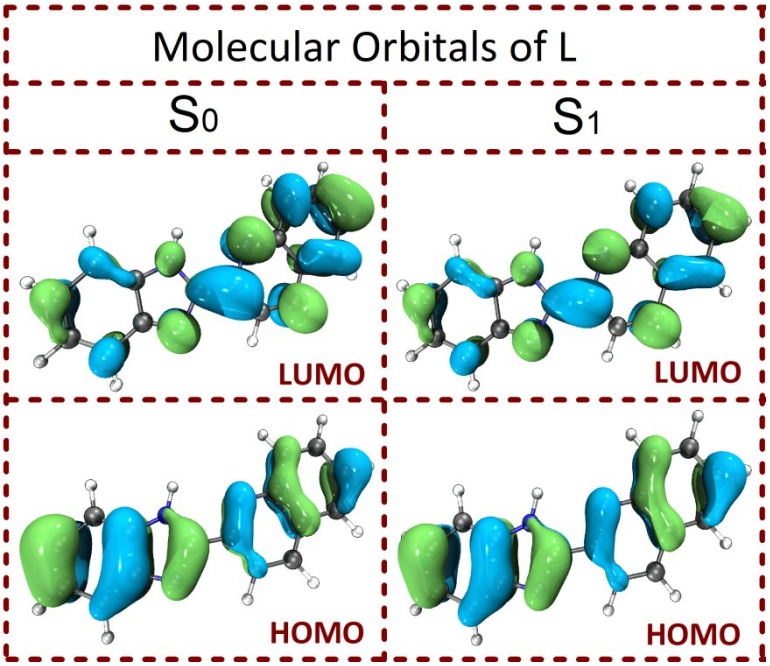

Figure S2 Molecular orbitals involved in the excitation and emission processes of L.

As is known, Hg^{2+} mainly exhibits two coordination models when interacting with a Lewis base. On one hand, by coordinating with three electron donors, a triangle is usually formed. On the other, by coordinating with four electron donors, a tetrahedral is usually formed. Density functional study is performed to check the chances of availability of the two organometallics. As is shown in Figure S3, the Hg^{2+} trends to form three coordination bonds with electron donors other than four. A tetra-coordinated starting geometry used for geometry optimization eventually leads to a tri-coordinated optimized geometry (Figure S4).

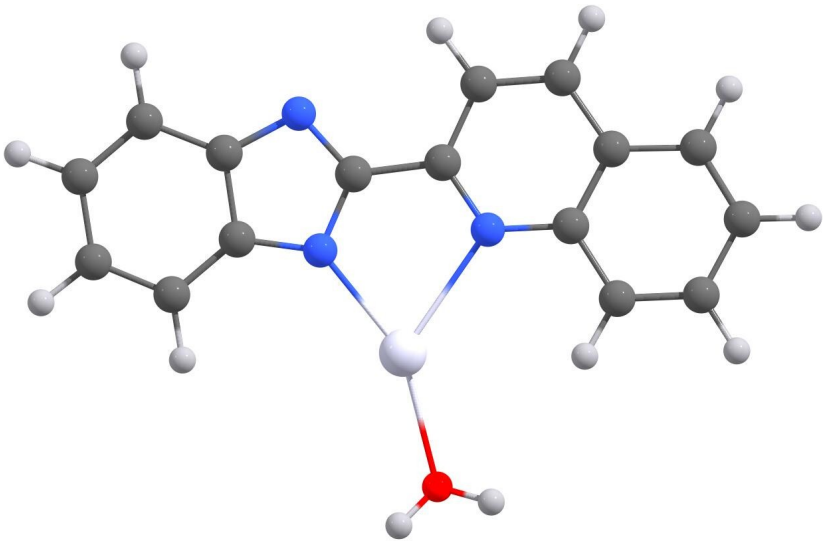

Figure S3 Optimized tri-coordinated structure.

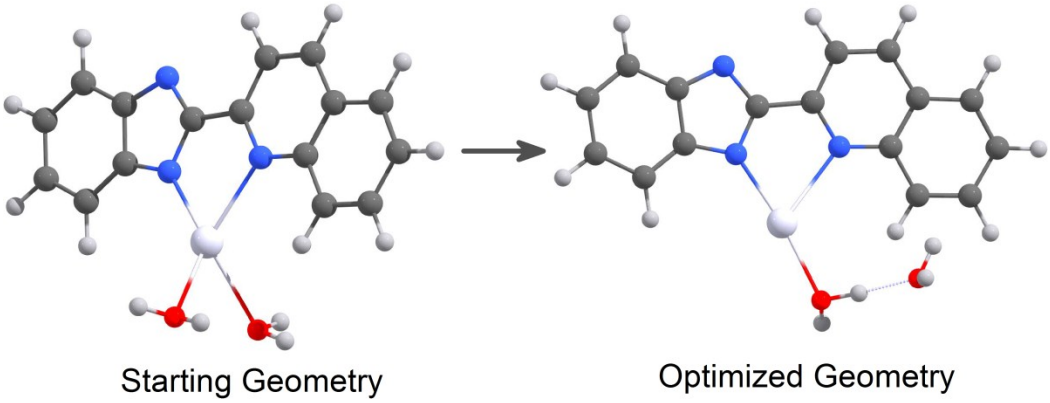

Figure S4 Starting geometry and optimized geometry for tetra-coordinated Hg-L.

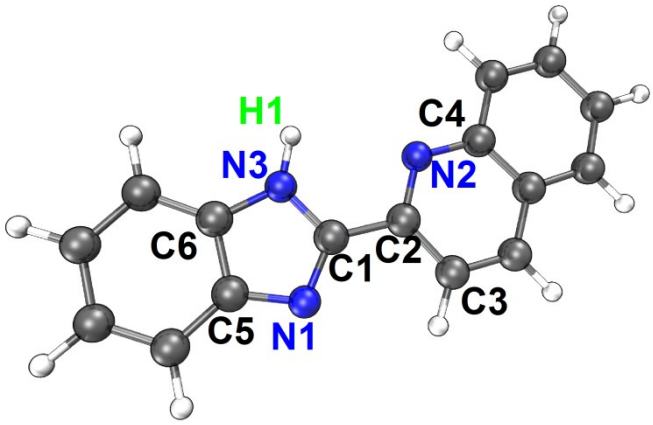

Figure S5 Optimized ground state structure of probe L.

Table S1 Structural information of probe L in S_0 state.

Structural information	Value
Bond	Bond Length (Å)
C1-C2	1.466
C1-N3	1.366
C1-N1	1.319
C2-N2	1.320
C5-C6	1.415
C2-C3	1.418
Angle	Angle Value (°)
C2-C1-N3	121.6
C1-C2-N2	116.5
C2-C1-N1	125.8
C1-C2-C3	120.1
Dihedral Angle	Dihedral Angle Value (°)
N2-C2-C1-N3	0.0