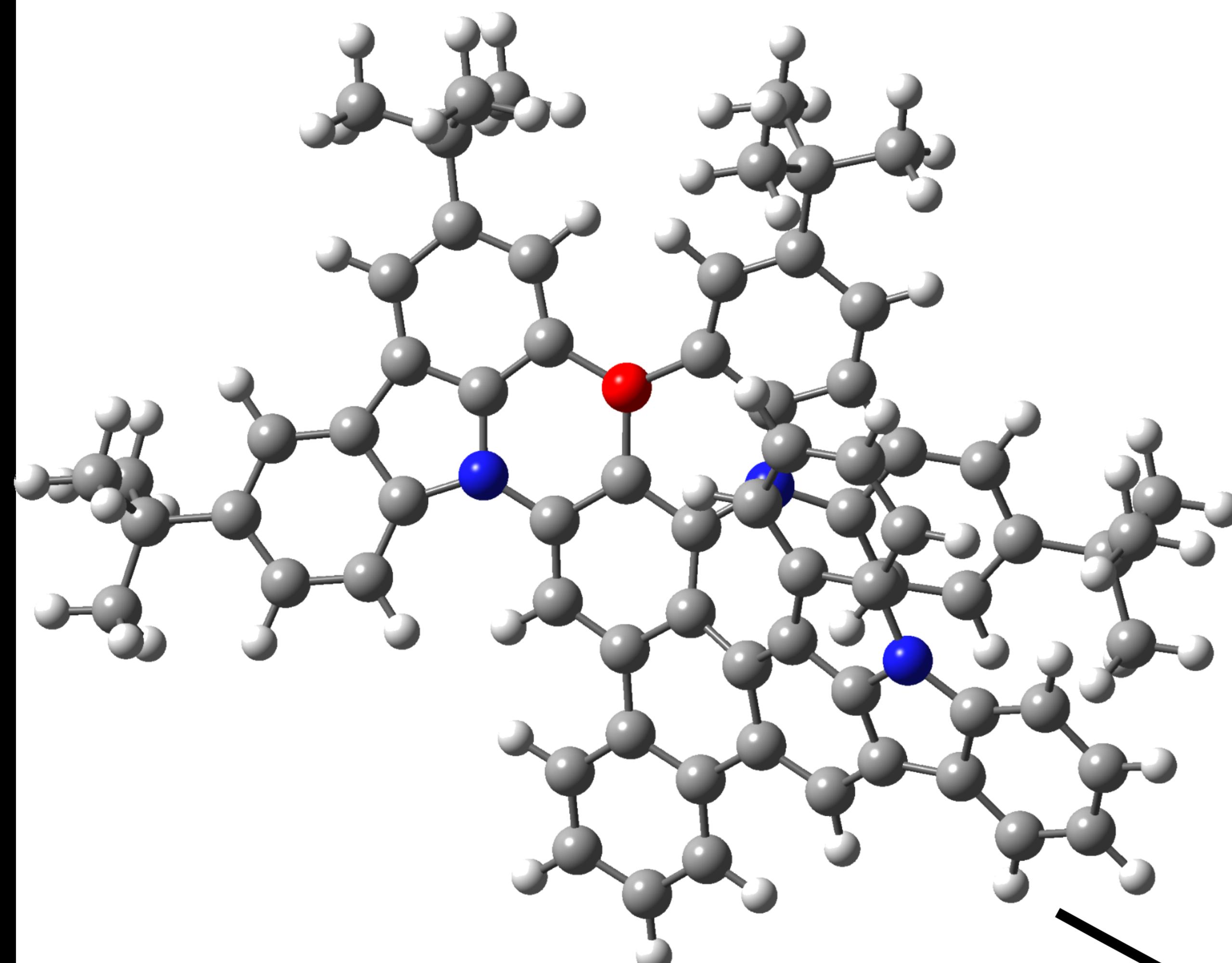


Figure S9. HOMO and LUMO distributions, HOMO–LUMO energy level gap, and oscillator strength of BN-DBC.

(P)-BN-TP-ICz

Energy

S_1



S_0

$E^{S1}(S_0)$

)

$E^{S0}(S_0)$

)

$E^{S1}(S_1)$

E_{em}

$E^{S0}(S_1)$

λ_{S1}

$$E^{S0}(S_0) = 0 \text{ eV}$$

$$E^{S1}(S_0) = 2.56 \text{ eV}$$

$$E^{S0}(S_1) = 0.12 \text{ eV}$$

$$E^{S1}(S_1) = 2.46 \text{ eV}$$

$$\lambda = \lambda_{S0} + \lambda_{S1} = 0.22 \text{ eV}$$

λ_{S0}

Geometry

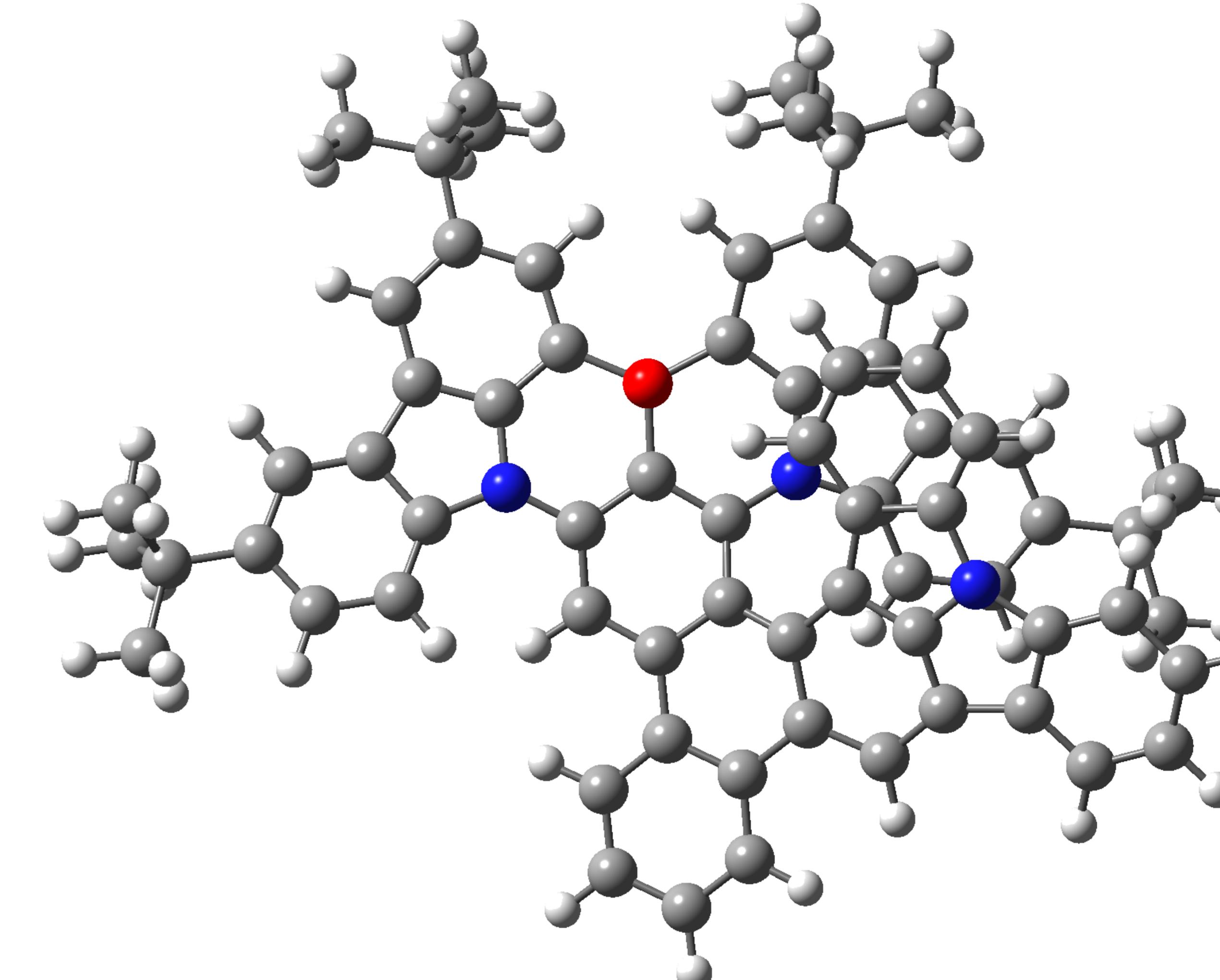


Figure S22. Optimized S_0 and S_1 structures, single point energy, and reorganization energy (λ) of *(P)*-BN-TP-ICz.