Supporting information

Synthesis of Highly-charged C3-Symmetrical Organic Molecule with a Fused Planar Core Structure

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Figure S1. ESI-MS characterization of compound **L(ClO₄)₅Br**. The three MS signals are assigned to be: (i) $m/z = 1139.3$, $[\text{L}(\text{ClO}_4)_4\text{Br}]^+$; (ii) $m/z = 519.2$, $[\text{L}(\text{ClO}_4)_3\text{Br}]^{2+}$; $m/z = 311.2$, $[\text{L}(\text{ClO}_4)_2\text{Br}]^{3+}$.

(a) Side-view

(b) Top-view

Figure S2. A 3D molecular structure of $L(\text{Br})(\text{ClO}_4)_5$. The anions are not shown for clarity (the 3D structure is optimized by ChemDraw MM2 energy minimization; Labels: Blue = N, Grey = C, White = H, and Pink = electron lone-pairs).

ChemDraw MM2 Energy Minimization Parameters and Results:

Software Version: ChemBio3D Ultra 12.0

Pi System: 46 45 18 17 16 19 32 31 30 33 34 1 2 20 3 4
6 5 44 47 48

Stretch: 11.4547

Bend: 64.5938

Stretch-Bend: 2.5239

Torsion: 24.7803

Non-1,4 VDW: -6.0453

1,4 VDW: 33.1485

Charge/Charge: 436.6972

Charge/Dipole: 2.0867

Dipole/Dipole: -4.2836

Total Energy: 564.9562 kcal/mol