

Supporting information

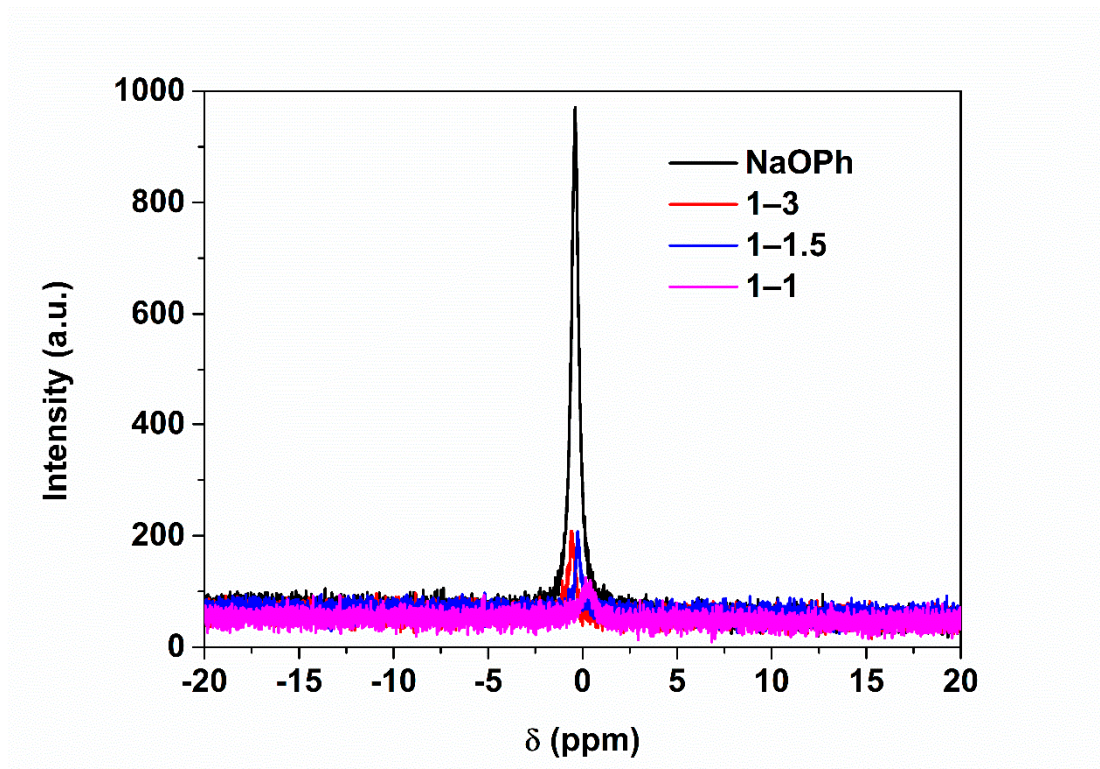


Figure S1. Liquid ^{23}Na NMR characterizations on the reaction of $\text{YCl}_3\text{-}n\text{NaOPh}$ ($n=1, 1.5, 3$) with increase of the molar ratio of NaOPh.

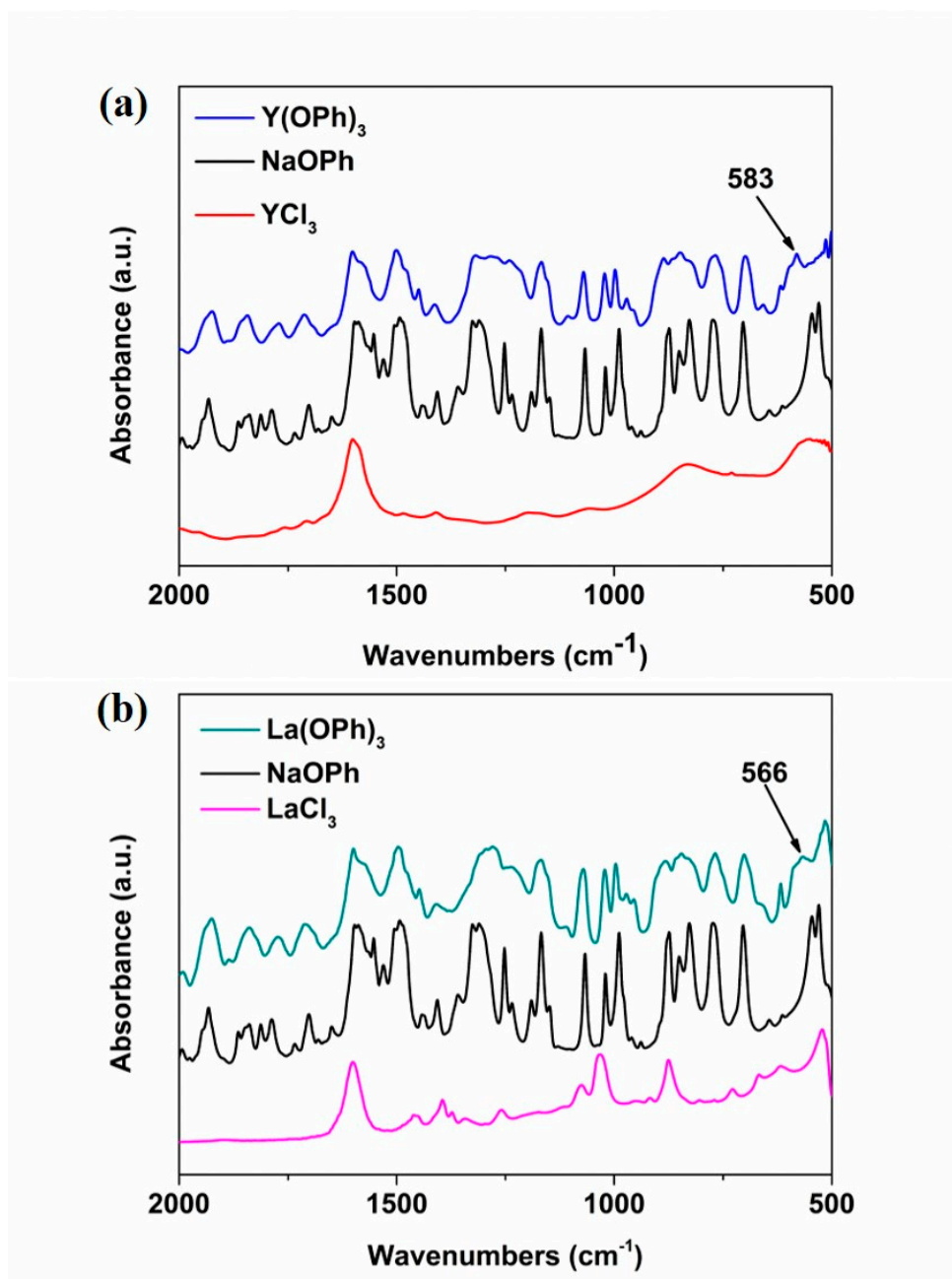


Figure S2. FT-IR spectra of (a) yttrium phenoxide and (b) lanthanum phenoxides compared with sodium phenoxide and their chlorides.

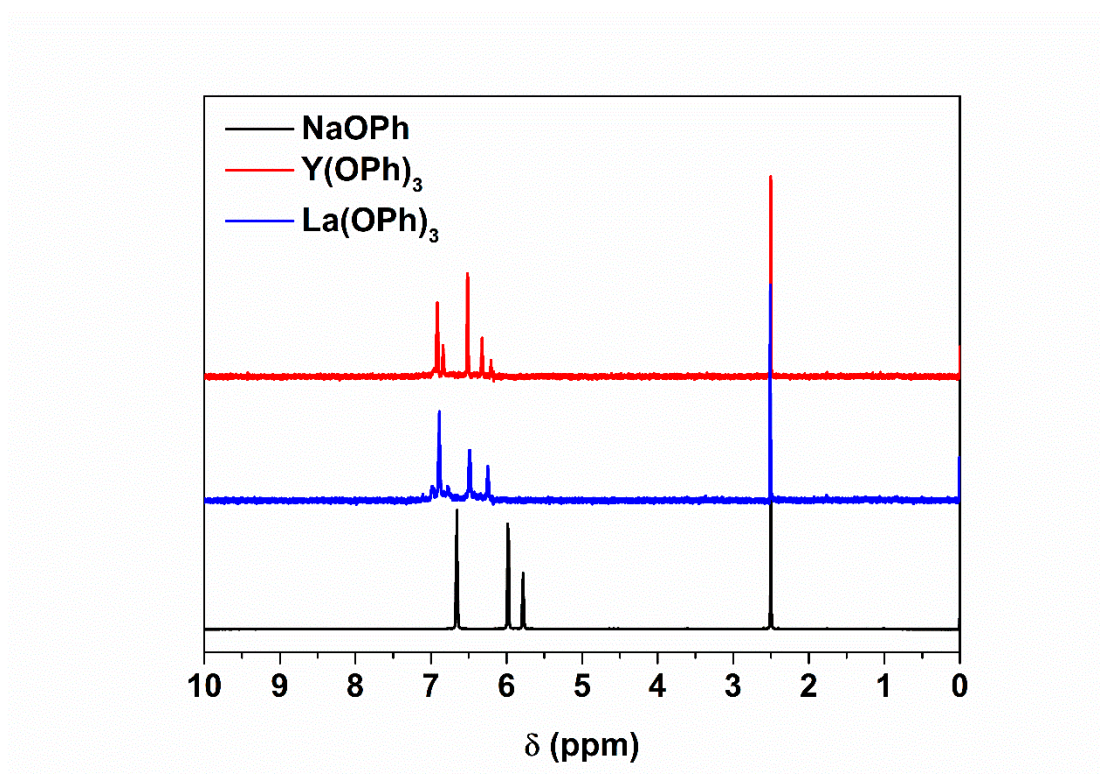


Figure S3. ^1H NMR spectra of Y(OPh)_3 and La(OPh)_3 after removing solvent compared with NaOPh , respectively.

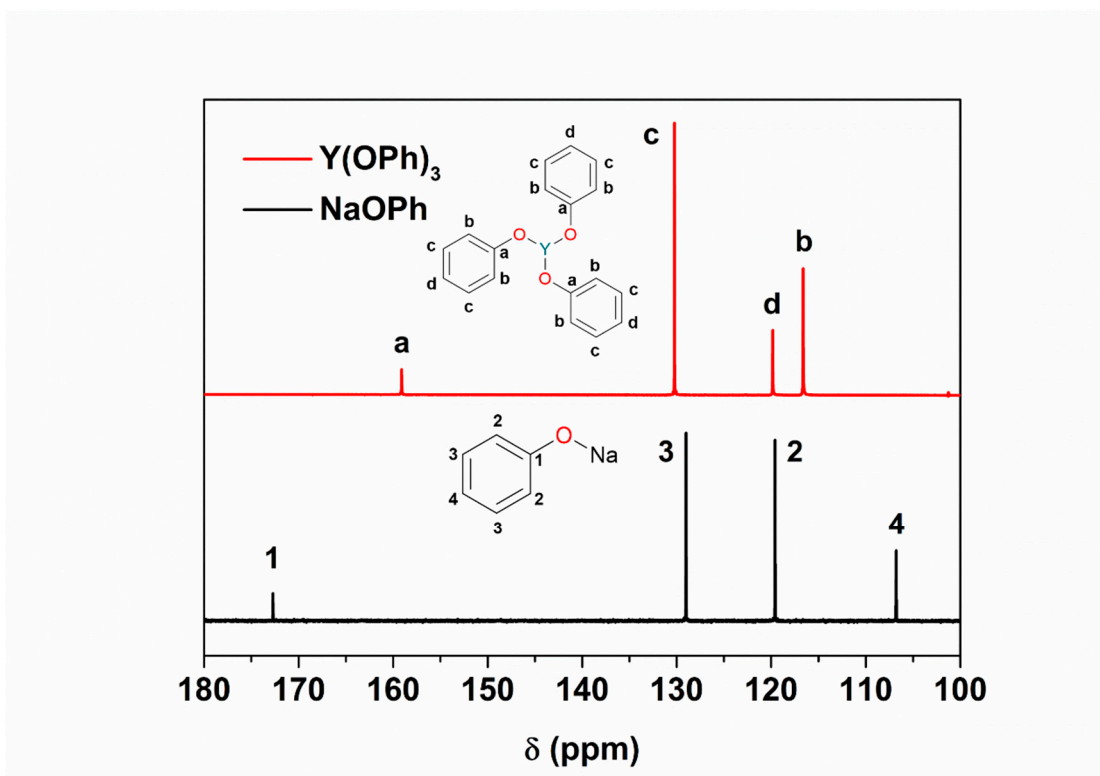


Figure S4. ^{13}C NMR of Y(OPh)_3 compared with NaOPh .

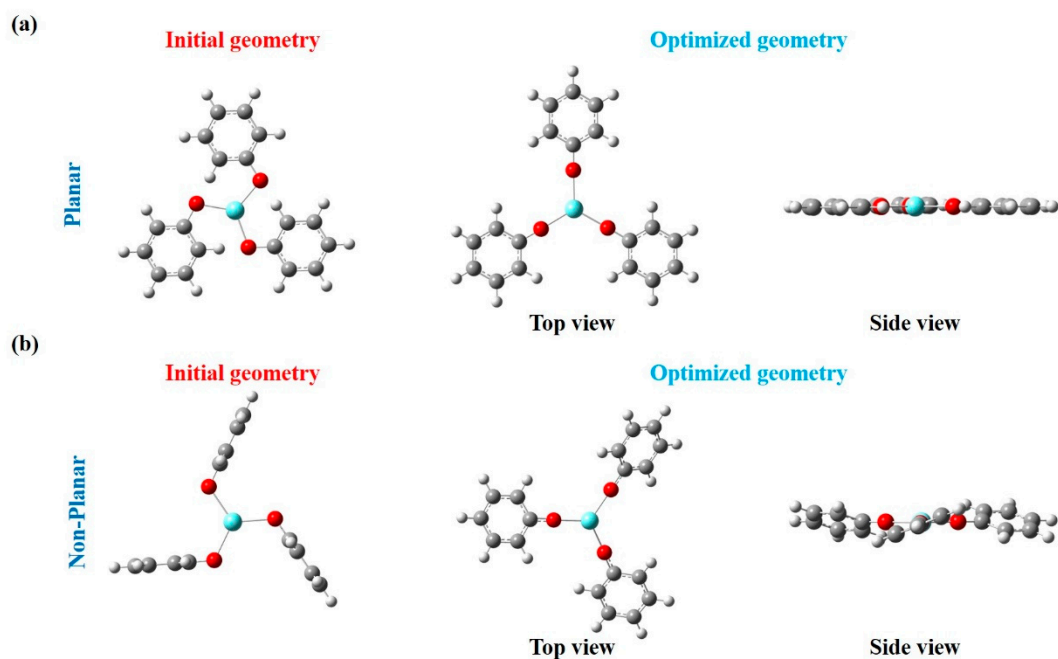


Figure S5. (a, b) Initial geometries (Parallel and Vertical) and optimized geometries (top view and side view) of yttrium phenoxide. (black: C; red: O; white: H; greenish-blue: Y.)

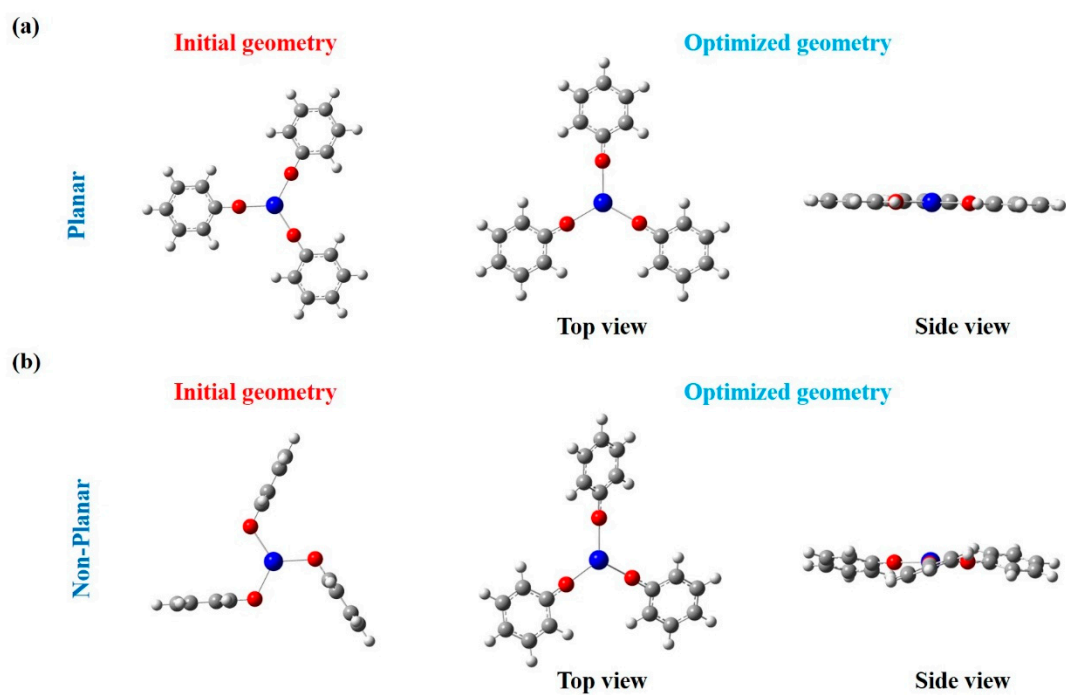


Figure S6. (a, b) Initial geometries (Parallel and Vertical) and optimized geometries (top view and side view) of lanthanum phenoxide. (black: C; red: O; white: H; blue: La.)

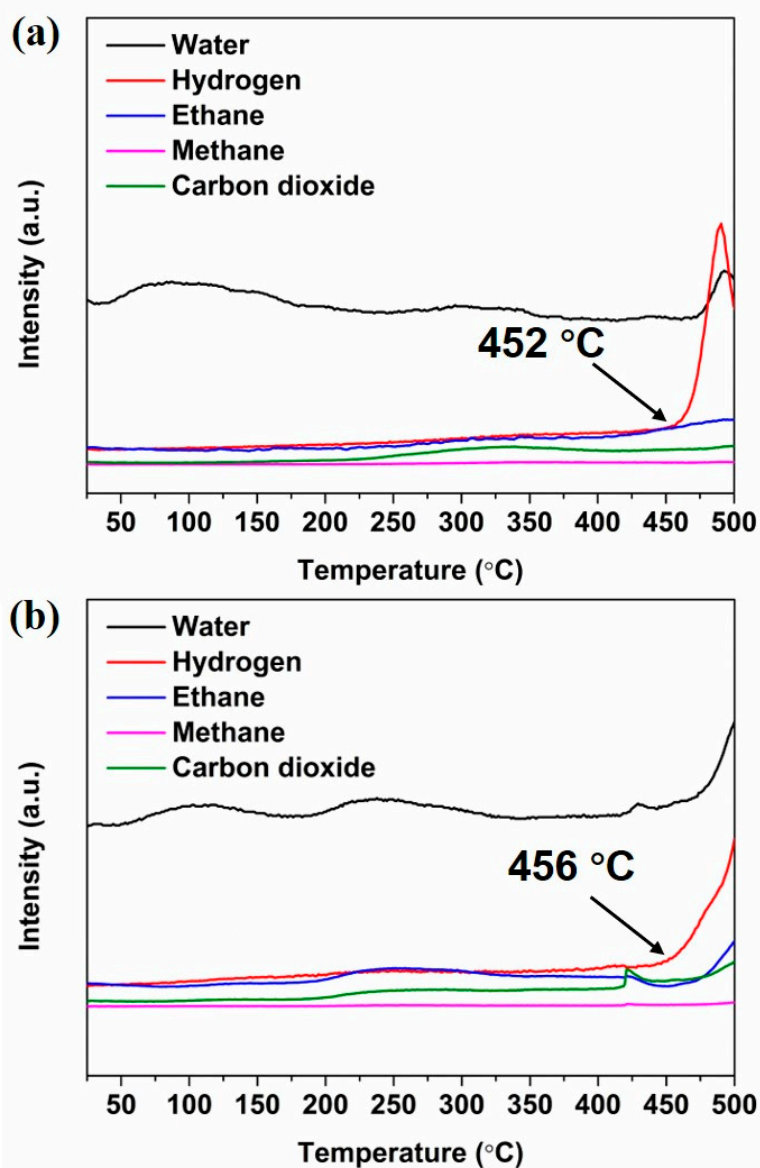


Figure S7. TPD-MS results of (a) yttrium phenoxide and (b) lanthanum phenoxide from 25 to 500 °C at a heating rate of 2 °C/min under Ar flow.

Table S1. The single point energies of two optimized structures of Y(OPh)₃.

Structure	Non-planar	Planar
Energy/kJ mol ⁻¹	-2518479.4650	-2518479.0016
Charge of Y	2.152	2.151
Charge of O	-0.898	-0.899
HOMO/eV	-6.0469	-6.0551
LUMO/eV	-2.4735	-2.4637

Table S2. The single point energies of two optimized structures of La(OPh)₃.

Structure	Non-planar	Planar
Energy/kJ mol ⁻¹	-2500734.6118	-2500734.5769
Charge of La	2.277	2.276
Charge of O	-0.927	-0.928
HOMO/eV	-5.9111	-5.9103
LUMO/eV	-2.5070	-2.4985

Table S3. Comparison of Y(III) and La(III) phenoxides between the present study and previous research.

	Y(III) and La(III) phenoxides in the present study	Y(III) and La(III) phenoxides in the previous study
Organic anion	Unsubstituted phenoxide group	Substituted phenoxide groups
Synthetic process	The synthetic process was characterized by quasi in situ ^1H NMR and UV-Vis spectra	The final products were well characterized.
Neutral ligand	Neutral ligands (ethanol) have been completely removed	Neutral ligands generally remain in the system and can stable the molecular structure