

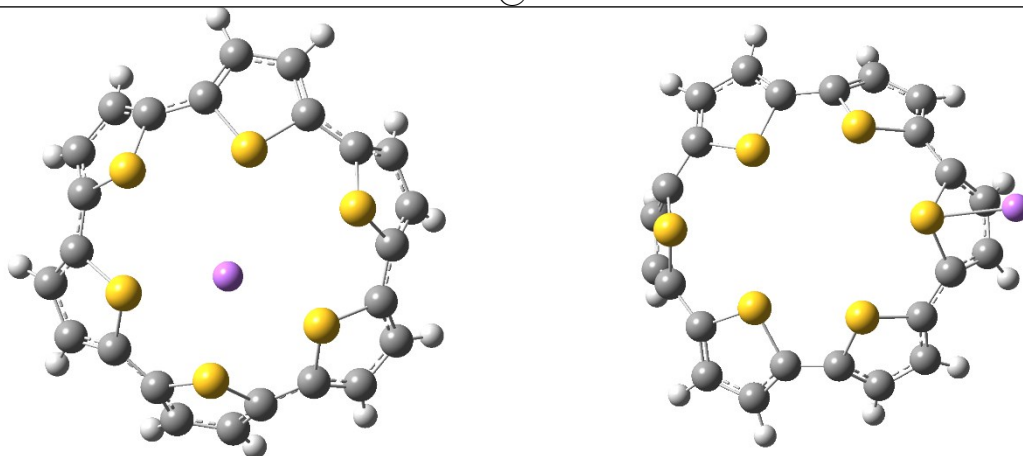
**Remarkable static and dynamic NLO response of alkalis and superalkalis doped
macrocyclic [hexa-]thiophene complexes; a DFT approach**

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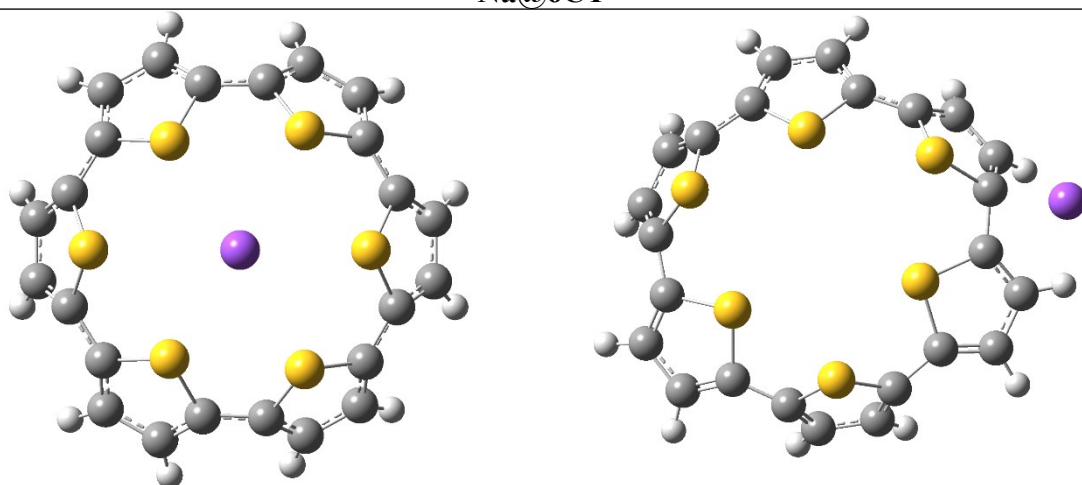
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Li@6CT



Na@6CT



K@6CT

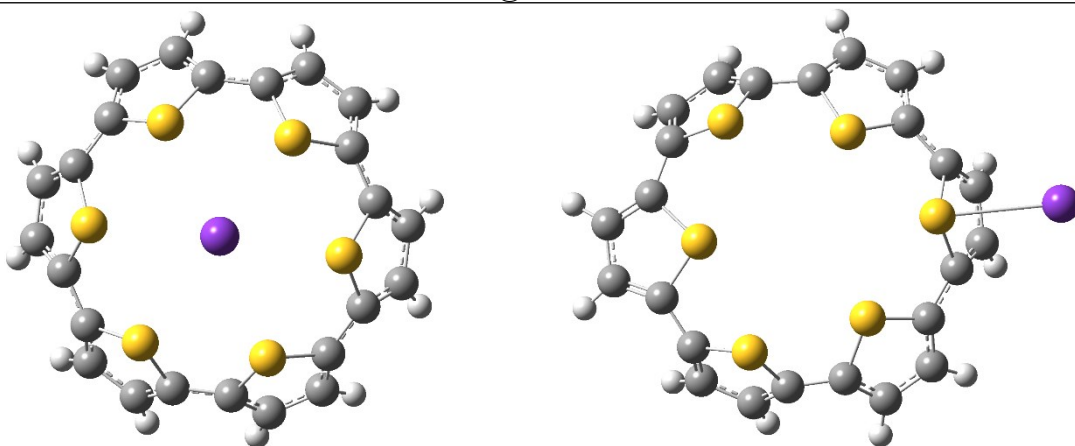


Figure. S1. The possible optimized geometries of AA@6CT complexes.

$\text{Li}_3\text{O}@6\text{CT}$

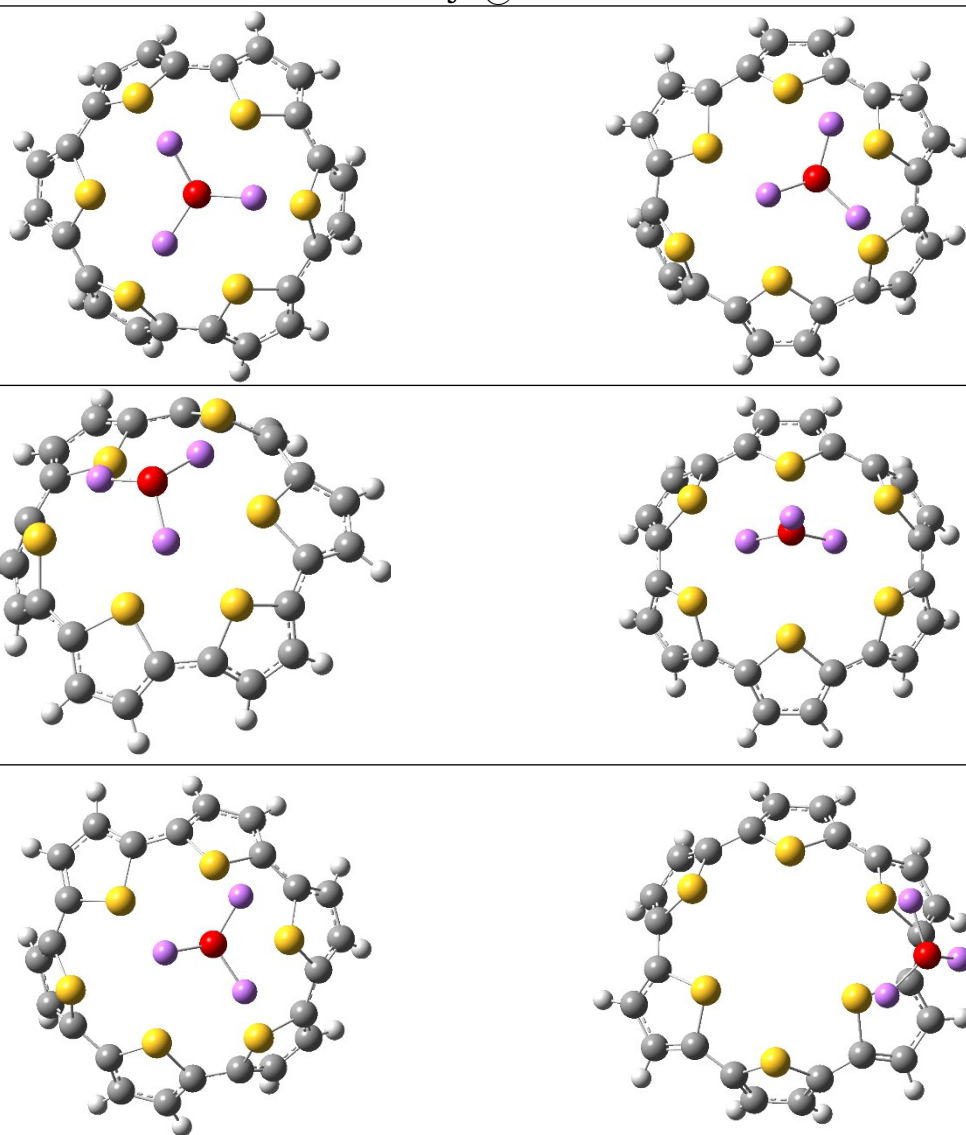


Figure. S2. The possible optimized geometries of $\text{Li}_3\text{O}@6\text{CT}$ complexes.

$\text{Na}_3\text{O}@6\text{CT}$

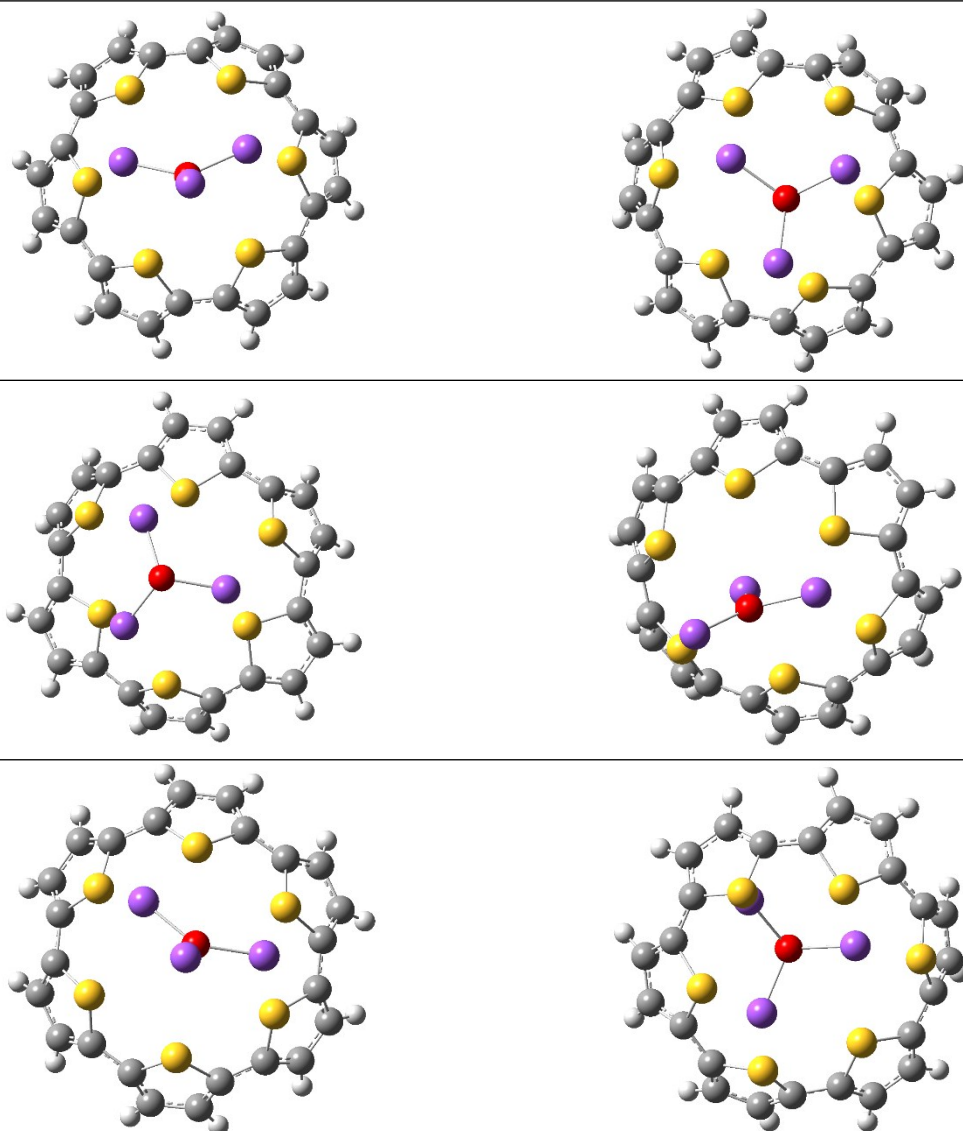


Figure. S3. The possible optimized geometries of $\text{Na}_3\text{O}@6\text{CT}$ complexes.

$K_3O@6CT$

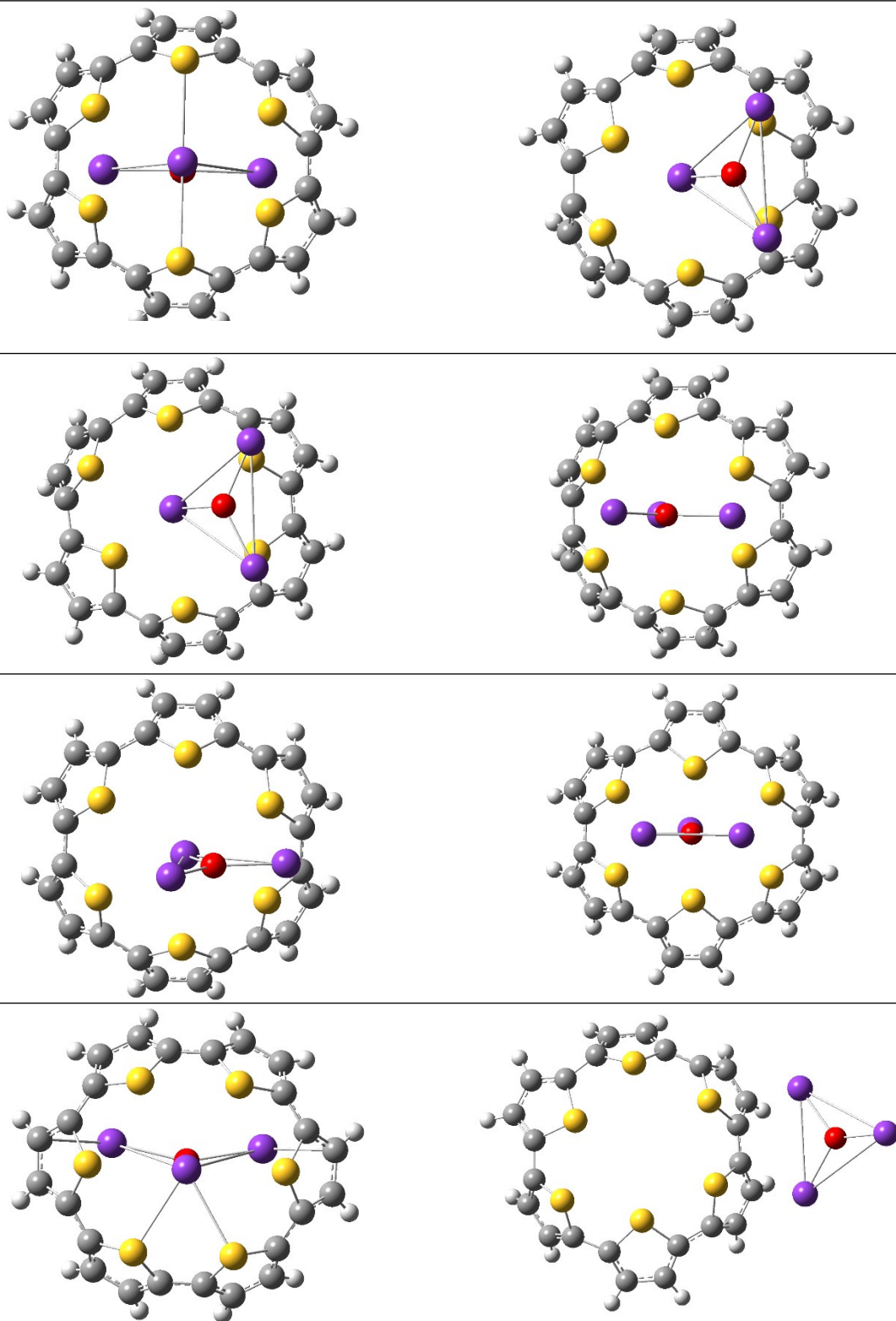


Figure. S2. The possible optimized geometries of $K_3O@6CT$ complexes.