

Molecules

Supplement Information

Figure S1. Optimized geometries of diene-lactone **2** and its complexes; (a) diene-lactone **2**, (b) complex of **2** and Ca^{2+} , (c) complex of **2** and K^+ , and (d) complex of **2** and Mg^{2+} .

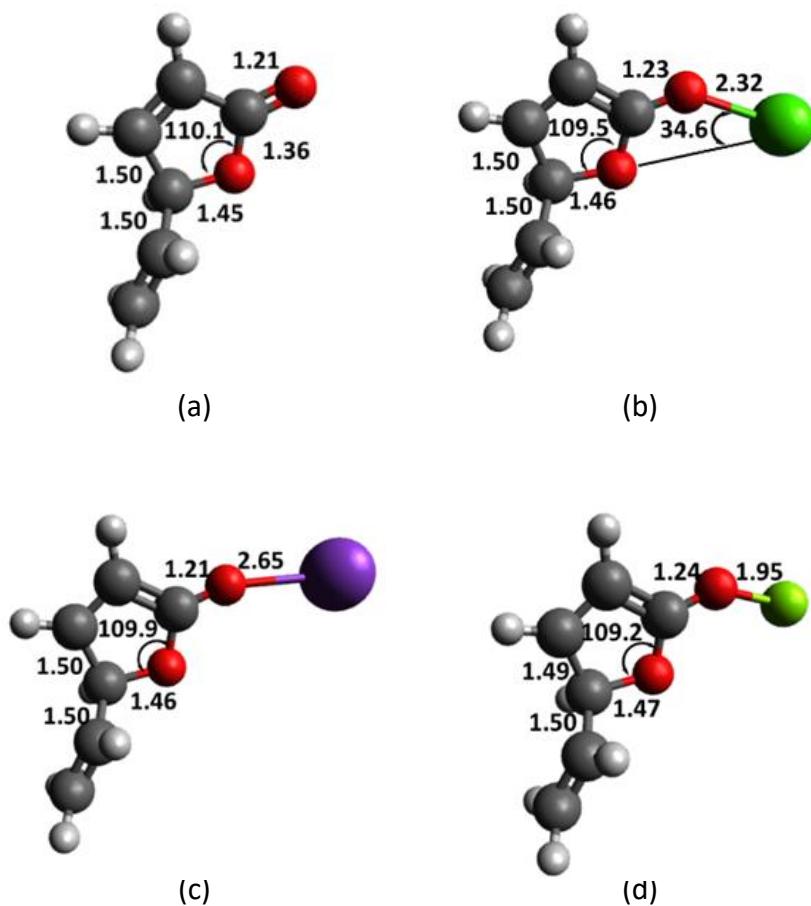


Figure S2. Parameter plots for diene-lactone **2** with B3LYP 6-311+g (2df,2p) and in methanol; (a) cation binding energy vs HOMO stabilization, (b) C₃-O₇ bond distance vs charge transfer, (c) C₃-O₇ bond distance vs charge-to-radius ratio, and (d) C₃ NMR vs C₃ *p*-character.

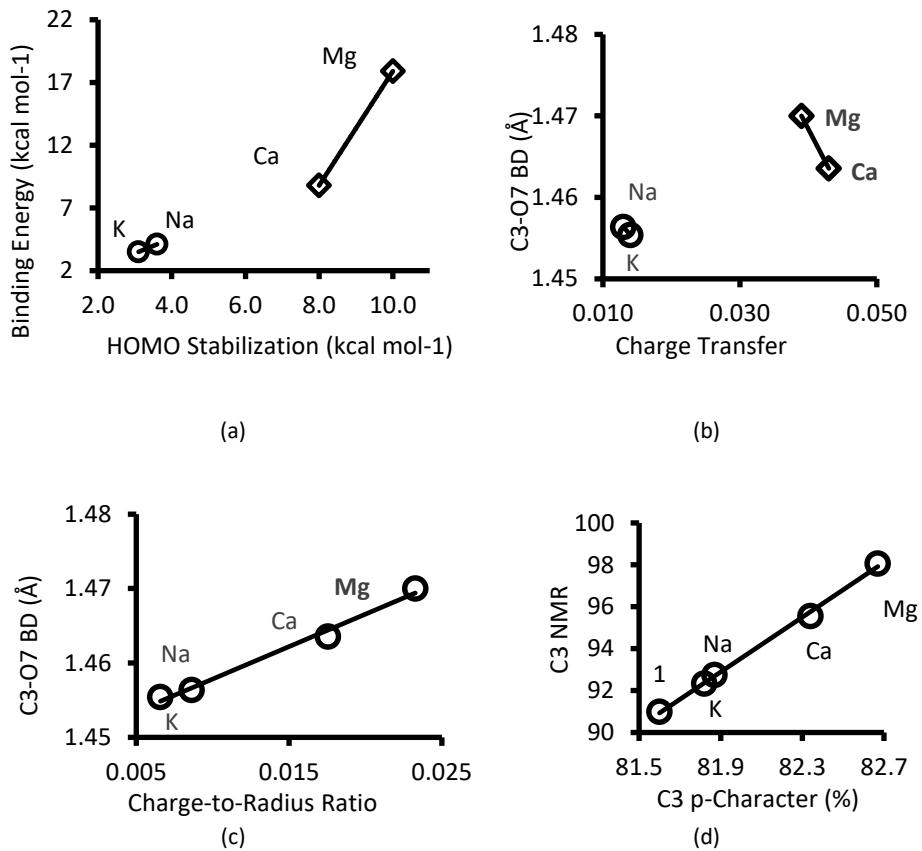


Figure S3. Frontier orbitals of models; (a) HOMO-1 of ene-lactone **2a**, (b) LUMO+1 of **4a**-Ca²⁺ complex, (c) LUMO of **4a**-Ca²⁺ complex, (d) HOMO of diglycolic acid **4**, (e) HOMO-1 of **4**. (g) HOMO of diglycolate **4a**.

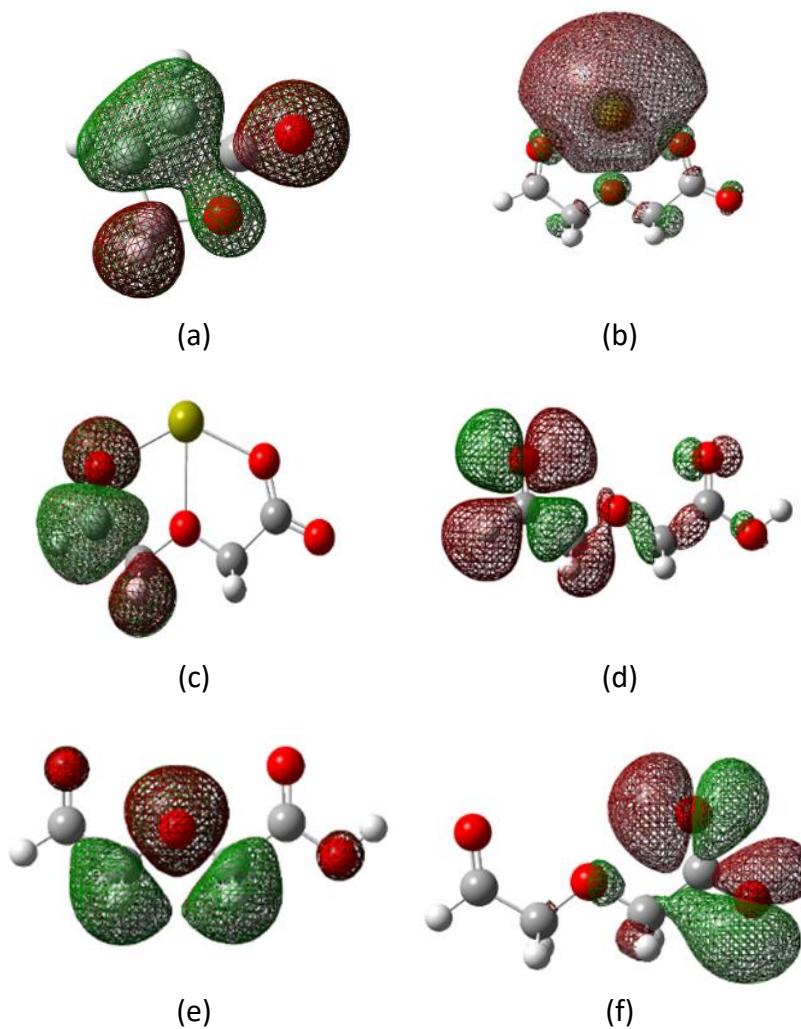
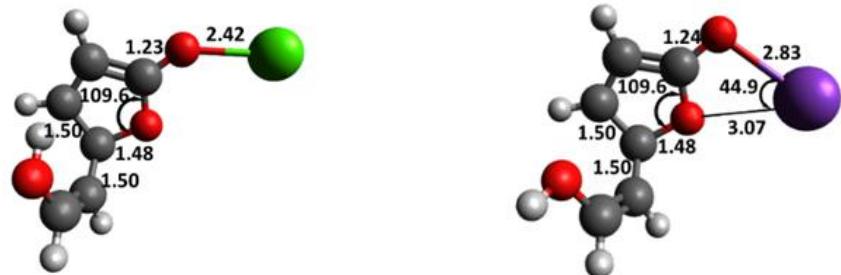
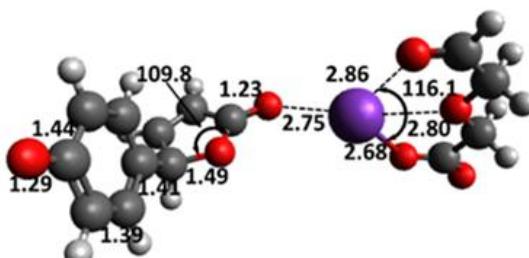


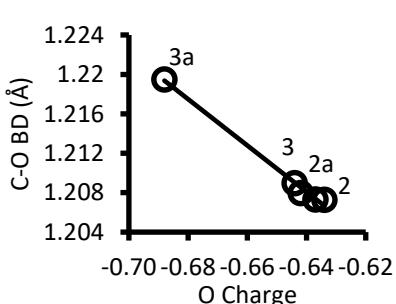
Figure S4. Optimized geometries and parameter plots simple in methanol; (a) complex of enol **3** and Ca^{2+} , (b) complex of enol **3** and K^+ , (c) **5a-4a-K⁺** complex, (d) carbonyl CO bond distance vs carbonyl O charge, (e) HOMO energy vs carbonyl CO bond distance, and (f) C₃-O₇ bond distance vs C₃-O₇ total overlap population.



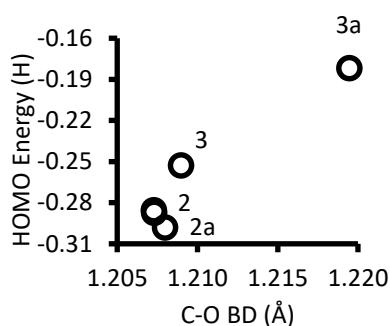
(a)



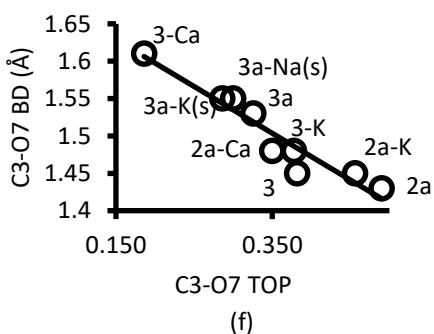
(c)



(d)



(e)



(f)

Figure S5. Structures of intermediates during formation of the acyclic form of **3a**-Ca²⁺.

