

Effects of Solvent on the Relative Stability of Mono and Di-Aluminum Aryloxy Complexes of Bipyridines: Anomalous Behavior of $[(t\text{Bu})_2\text{Al}(\text{OPh})]_2(\mu\text{-4,4-bipy})$

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Supplementary Materials

Table S1. Calculated total energies.

Compound	Energy (Hartrees)
CHCl ₃	-1410.41060535
pyridine	-245.31200369
4,4'-bipy	-489.473944986
bipetha	-567.113876406
bipethe	-565.930166393
AlMe ₂ (OPh)	-622.83285442
[Me ₂ Al(μ-OPh)] ₂	-1245.77424247
AlMe ₂ (OPh)(py)	-868.20463933
Al(^t Bu) ₂ (OPh)	-855.72752456
[(^t Bu) ₂ Al(μ-OPh)] ₂	-1711.55316024
Al(^t Bu) ₂ (OPh)(py)	-1101.10129786
[(^t Bu) ₂ Al(OPh)] ₂ (μ-4,4'-bipy) (1a)	-2201.04687698
[(^t Bu) ₂ Al(OPh)] ₂ (μ-bipetha) (2a)	-2278.69234995
[(^t Bu) ₂ Al(OPh)] ₂ (μ-bipethe) (3a)	-2277.50650599
Al(^t Bu) ₂ (OPh)(4,4'-bipy) (1b)	-1345.26215724
Al(^t Bu) ₂ (OPh)(bipetha) (2b)	-1422.90403996
Al(^t Bu) ₂ (OPh)(bipethe) (3b)	-1421.71957521
4,4'-bipy...CHCl ₃	-1899.89756967
bipetha...CHCl ₃	-1977.53813565
bipethe...CHCl ₃	-1976.35409430
Al(^t Bu) ₂ (OPh)(4,4'-bipy)...CHCl ₃	-2755.68446265
Al(^t Bu) ₂ (OPh)(bipetha)...CHCl ₃	-2833.32755301
Al(^t Bu) ₂ (OPh)(bipethe)...CHCl ₃	-2832.14250987