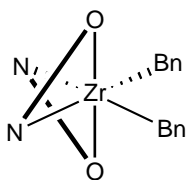


Efficient predetermination of chirality-at-zirconium

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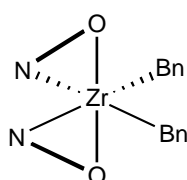


OO1.pdb

Δ-trans,cis,cis

See Scheme 1

See also ZrL2Bn2_Xray.PDB

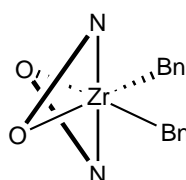


OO2.pdb

Λ-trans,cis,cis

See Scheme 1

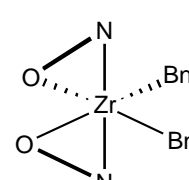
+36 kJ mol⁻¹



NN1.pdb

Δ-cis,trans,cis

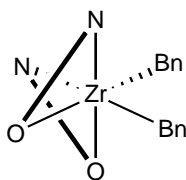
+79.5 kJ mol⁻¹



NN2.pdb

Λ-cis,trans,cis

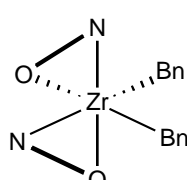
+128.9 kJ mol⁻¹



NO1.pdb

Δ-cis,cis,cis

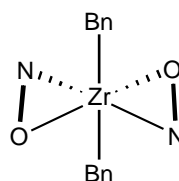
+103.8 kJ mol⁻¹



NO2.pdb

Λ-cis,cis,cis

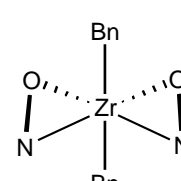
+120.9 kJ mol⁻¹



trans1.pdb

trans,trans,trans

+64.0 kJ mol⁻¹



trans2.pdb

cis,cis,trans

+16.3 kJ mol⁻¹

Associated structure files (.pdb), configuration descriptors, and energies relative to the observed *Δ-trans,cis,cis*-[ZrL₂(CH₂Ph)₂]