

Properties

HOMO-LUMO Gap: not accessible eV

HOMO : not accessible eV

LUMO : not accessible eV

Dipole moment = 22.64 D

Hyperpolarizability zzz component (aligned z with molecular dipole) = 723.71 E-30 esu

Bond length alteration parameter = 4.332 Å

Bond length alteration was based on the following input:

index-list: [9, 12, 13, 14, 18, 17]

first index: None, last index: None