

(CH3)2O-C6F6 LP away eclipsed dimer MP2/aug-cc-pVDZ

R=4.5 Angstroms

Interaction Energy=-2.10 kcal/mol

C	0.00000000	1.38980100	-0.87356400
C	-1.20360300	0.69490100	-0.87356400
C	1.20360300	0.69490100	-0.87356400
C	-1.20360300	-0.69490100	-0.87356400
C	1.20360300	-0.69490100	-0.87356400
C	0.00000000	-1.38980100	-0.87356400
F	0.00000000	2.71953700	-0.87356400
F	-2.35518800	1.35976900	-0.87356400
F	2.35518800	1.35976900	-0.87356400
F	-2.35518800	-1.35976900	-0.87356400
F	2.35518800	-1.35976900	-0.87356400
F	0.00000000	-2.71953700	-0.87356400
O	0.00000000	0.00000000	3.62643600
C	0.00000000	1.16175600	2.82364700
H	0.00000000	2.01887900	3.49162000
H	0.88948800	1.19972200	2.18557000
H	-0.88948800	1.19972200	2.18557000
C	0.00000000	-1.16175600	2.82364700
H	0.00000000	-2.01887900	3.49162000
H	-0.88948800	-1.19972200	2.18557000
H	0.88948800	-1.19972200	2.18557000

(CH3)2O-C6F6 LP away staggered dimer MP2/aug-cc-pVDZ

R=4.5 Angstroms

Interaction Energy=-2.08 kcal/mol

C	0.00000000	1.38980100	-0.87356400
C	-1.20360300	0.69490000	-0.87356400
C	1.20360300	0.69490000	-0.87356400
C	-1.20360300	-0.69490000	-0.87356400
C	1.20360300	-0.69490000	-0.87356400
C	0.00000000	-1.38980100	-0.87356400
F	0.00000000	2.71953700	-0.87356400
F	-2.35518800	1.35976800	-0.87356400
F	2.35518800	1.35976800	-0.87356400
F	-2.35518800	-1.35976800	-0.87356400
F	2.35518800	-1.35976800	-0.87356400
F	0.00000000	-2.71953700	-0.87356400
O	0.00000000	0.00000000	3.62643600
C	-1.16175600	0.00000000	2.82364700
H	-2.01887900	0.00000000	3.49162000
H	-1.19972200	0.88948800	2.18557000
H	-1.19972200	-0.88948800	2.18557000
C	1.16175600	0.00000000	2.82364700
H	2.01887900	0.00000000	3.49162000
H	1.19972200	-0.88948800	2.18557000
H	1.19972200	0.88948800	2.18557000

(CH3)2O-C6H5NO2 LP away eclipsed dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.25 kcal/mol

C	-1.15481600	-2.18413200	0.00000000
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C	-1.15481600	-1.48761400	-1.20800400
C	-1.15481600	-1.48761400	1.20800400
C	-1.15481600	-0.09543300	-1.21907200
C	-1.15481600	-0.09543300	1.21907200
C	-1.15481600	0.57008000	0.00000000
H	-1.15481600	-3.26576400	0.00000000
H	-1.15481600	-2.02763200	-2.14510600
H	-1.15481600	-2.02763200	2.14510600
H	-1.15481600	0.47098200	-2.13807800
H	-1.15481600	0.47098200	2.13807800
N	-1.15481600	2.04105400	0.00000000
O	-1.15481600	2.60970200	-1.09054600
O	-1.15481600	2.60970200	1.09054600
O	3.44518400	-0.80702700	0.00000000
C	2.64239500	-1.96878300	0.00000000
H	3.31036800	-2.82590600	0.00000000
H	2.00431800	-2.00674900	0.88948800
H	2.00431800	-2.00674900	-0.88948800
C	2.64239500	0.35472900	0.00000000
H	3.31036800	1.21185200	0.00000000
H	2.00431800	0.39269500	-0.88948800
H	2.00431800	0.39269500	0.88948800

(CH3)2O-C6H5NO2 LP away staggered dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.12 kcal/mol

C	1.15481600	-2.18413200	0.00000000
C	1.15481600	-1.48761400	1.20800400
C	1.15481600	-1.48761400	-1.20800400
C	1.15481600	-0.09543300	1.21907200
C	1.15481600	-0.09543300	-1.21907200
C	1.15481600	0.57008000	0.00000000
H	1.15481600	-3.26576400	0.00000000
H	1.15481600	-2.02763200	2.14510600
H	1.15481600	-2.02763200	-2.14510600
H	1.15481600	0.47098200	2.13807800
H	1.15481600	0.47098200	-2.13807800
N	1.15481600	2.04105400	0.00000000
O	1.15481600	2.60970200	1.09054600
O	1.15481600	2.60970200	-1.09054600
O	-3.44518400	-0.80702700	0.00000000
C	-2.64239500	-0.80702700	1.16175600
H	-3.31036800	-0.80702700	2.01887900
H	-2.00431800	-1.69651400	1.19972200
H	-2.00431800	0.08246100	1.19972200
C	-2.64239500	-0.80702700	-1.16175600
H	-3.31036800	-0.80702700	-2.01887900
H	-2.00431800	0.08246100	-1.19972200
H	-2.00431800	-1.69651400	-1.19972200

(CH3)2O-C6H5CN LP away eclipsed dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.25 kcal/mol

C	0.23303200	2.30829900	0.00000000
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C	0.56317100	1.69489800	-1.20782300
C	0.56317100	1.69489700	1.20782300
C	1.22237200	0.47009700	-1.21508800
C	1.22237200	0.47009700	1.21508800
C	1.55160800	-0.14162800	0.00000000
H	-0.27965100	3.26086700	0.00000000
H	0.30734800	2.17022000	-2.14516100
H	0.30734700	2.17021900	2.14516100
H	1.48351600	-0.01511100	-2.14577500
H	1.48351600	-0.01511200	2.14577500
C	2.22997200	-1.40203200	0.00000000
N	2.78619800	-2.43550700	0.00000000
O	-3.15827100	-1.09673600	0.00000000
C	-3.00195400	0.30672900	0.00000000
H	-3.99636100	0.74490800	0.00000000
H	-2.45808000	0.64256300	0.88948800
H	-2.45808000	0.64256300	-0.88948800
C	-1.90077500	-1.73927100	0.00000000
H	-2.08275200	-2.81059300	0.00000000
H	-1.32091500	-1.47030000	-0.88948800
H	-1.32091500	-1.47030000	0.88948800

(CH₃)₂O-C₆H₅CN LP away staggered dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.09 kcal/mol

C	-0.40726900	2.28400500	0.00000000
C	-0.68998000	1.64735200	1.20782300
C	-0.68997900	1.64735200	-1.20782300
C	-1.25447800	0.37612200	1.21508800
C	-1.25447800	0.37612200	-1.21508800
C	-1.53641600	-0.25879100	0.00000000
H	0.03176100	3.27268300	0.00000000
H	-0.47090900	2.14069100	2.14516100
H	-0.47090800	2.14069100	-2.14516100
H	-1.47810600	-0.12747900	2.14577500
H	-1.47810600	-0.12747900	-2.14577500
C	-2.11732400	-1.56697400	0.00000000
N	-2.59364200	-2.63962400	0.00000000
O	3.23229400	-0.85427100	0.00000000
C	2.49859100	-0.52846500	1.16175600
H	3.10908000	-0.79955700	2.01887900
H	2.27641700	0.54343500	1.19972200
H	1.55443300	-1.08244700	1.19972200
C	2.49859100	-0.52846400	-1.16175600
H	3.10908100	-0.79955600	-2.01887900
H	1.55443300	-1.08244600	-1.19972200
H	2.27641800	0.54343600	-1.19972200

(CH₃)₂O-C₆H₅CF₃ LP away eclipsed F towards dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.44 kcal/mol

C	-0.94330100	2.50092900	0.00118600
C	-0.45868700	2.00046500	-1.20611000
C	-0.45868700	2.00046500	1.20848200

C	0.50974400	1.00025500	-1.21046300
C	0.50974400	1.00025500	1.21283500
C	0.99014300	0.50675400	0.00118600
H	-1.69380100	3.28012600	0.00118600
H	-0.83170300	2.39053000	-2.14360200
H	-0.83170300	2.39053000	2.14597400
H	0.89459800	0.61049200	-2.14270300
H	0.89459800	0.61049200	2.14507500
C	1.99451900	-0.60436500	0.00118600
F	1.39595800	-1.81223200	0.00118600
F	2.79004700	-0.56595600	-1.08106800
F	2.79004700	-0.56595600	1.08344000
O	-3.28202300	-1.69658100	-0.00406300
C	-3.51339600	-0.30352200	-0.00315000
H	-4.58950200	-0.15238400	-0.00391700
H	-3.08212600	0.16689700	0.88706500
H	-3.08066100	0.16830500	-0.89190900
C	-1.89715700	-1.97279700	-0.00314100
H	-1.78083100	-3.05322100	-0.00390000
H	-1.41160400	-1.55552200	-0.89189900
H	-1.41306900	-1.55693000	0.88707500

(CH₃)₂O-C₆H₅CF₃ LP away staggered F towards dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.32 kcal/mol

C	0.78462200	2.55515800	-0.00118600
C	0.33234400	2.02529000	1.20611000
C	0.33234400	2.02529000	-1.20848200
C	-0.57146300	0.96632200	1.21046300
C	-0.57146300	0.96632200	-1.21283500
C	-1.01997100	0.44366900	-0.00118600
H	1.48478400	3.37988200	-0.00118600
H	0.68016600	2.43797800	2.14360200
H	0.68016600	2.43797800	-2.14597400
H	-0.93111900	0.55319400	2.14270300
H	-0.93111900	0.55319400	-2.14507500
C	-1.95269700	-0.72824400	-0.00118600
F	-1.27957300	-1.89620000	-0.00118600
F	-2.74906700	-0.73979400	1.08106800
F	-2.74906700	-0.73979400	-1.08344000
O	3.38194900	-1.48744000	0.00406300
C	2.77031000	-0.96542500	1.16490100
H	3.27764400	-1.39842900	2.02278600
H	2.86237600	0.12540400	1.20214200
H	1.70749500	-1.22774200	1.20213500
C	2.77233500	-0.96714100	-1.15861000
H	3.28116300	-1.40141000	-2.01496900
H	1.70958600	-1.22951400	-1.19730800
H	2.86446700	0.12363200	-1.19730100

(CH₃)₂O-C₆H₅CF₃ LP away eclipsed F away dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.37 kcal/mol

C	-0.92828700	2.48770900	0.00118900
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C	-0.45340900	1.97799700	1.20848500
C	-0.45340900	1.97799700	-1.20610700
C	0.49567000	0.95940500	1.21283800
C	0.49567000	0.95940500	-1.21046000
C	0.96381000	0.45426000	0.00118900
H	-1.66785200	3.27729100	0.00118900
H	-0.82377300	2.37058100	2.14597700
H	-0.82377300	2.37058100	-2.14359900
H	0.86512300	0.55501400	2.14507800
H	0.86512300	0.55501400	-2.14270000
C	2.02180100	-0.60593300	0.00118900
F	3.25885500	-0.07028700	0.00118900
F	1.94252700	-1.39843300	1.08344300
F	1.94252700	-1.39843300	-1.08106500
O	-3.34704800	-1.66419400	-0.00407100
C	-3.55167300	-0.26695600	-0.00314900
H	-4.62468400	-0.09521600	-0.00390900
H	-3.11145900	0.19510300	0.88706700
H	-3.10997700	0.19649400	-0.89190800
C	-1.96773300	-1.96690900	-0.00315900
H	-1.87214000	-3.04936400	-0.00392500
H	-1.47427400	-1.55901400	-0.89191700
H	-1.47575600	-1.56040400	0.88705700

(CH₃)₂O-C₆H₅CF₃ LP away staggered F away dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.24 kcal/mol

C	0.78363600	2.53699200	-0.00118900
C	0.33886700	2.00080500	-1.20848500
C	0.33886700	2.00080500	1.20610700
C	-0.55004200	0.92930100	-1.21283800
C	-0.55004200	0.92930100	1.21046000
C	-0.98834600	0.39806100	-0.00118900
H	1.47655400	3.36781100	-0.00118900
H	0.68603300	2.41404500	-2.14597700
H	0.68603300	2.41404500	2.14359900
H	-0.89561900	0.50432600	-2.14507800
H	-0.89561900	0.50432600	2.14270000
C	-1.98359500	-0.72124000	-0.00118900
F	-3.24941400	-0.25764600	-0.00118900
F	-1.85886100	-1.50786700	-1.08344300
F	-1.85886100	-1.50786700	1.08106500
O	3.43724300	-1.46888900	0.00407100
C	2.81836900	-0.95547100	1.16490900
H	3.33171400	-1.38133200	2.02279500
H	2.89517200	0.13653900	1.20214300
H	1.75932700	-1.23262500	1.20215000
C	2.82040600	-0.95717300	-1.15860100
H	3.33525300	-1.38428900	-2.01496100
H	1.76143000	-1.23438200	-1.19729200
H	2.89727500	0.13478200	-1.19730000

(CH₃)₂O-C₆H₅Br LP away eclipsed dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.63 kcal/mol

C	-1.01895500	2.48796800	0.00000000
C	-1.01895500	1.78893800	1.20545100
C	-1.01895500	1.78893800	-1.20545100
C	-1.01895500	0.39529300	1.21387200
C	-1.01895500	0.39529300	-1.21387200
C	-1.01895500	-0.28664400	0.00000000
H	-1.01895500	3.56939800	0.00000000
H	-1.01895500	2.32561700	2.14486500
H	-1.01895500	2.32561700	-2.14486500
H	-1.01895500	-0.15521400	2.14419000
H	-1.01895500	-0.15521400	-2.14419000
Br	-1.01895500	-2.16988900	0.00000000
O	3.58104500	1.10066200	0.00000000
C	2.77825600	2.26241900	0.00000000
H	3.44622900	3.11954100	0.00000000
H	2.14017900	2.30038500	-0.88948800
H	2.14017900	2.30038500	0.88948800
C	2.77825600	-0.06109400	0.00000000
H	3.44622800	-0.91821600	0.00000000
H	2.14017900	-0.09906000	0.88948800
H	2.14017900	-0.09906000	-0.88948800

(CH3)2O-C6H5Br LP away staggered dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.46 kcal/mol

C	-1.01895500	-2.48796800	0.00000000
C	-1.01895500	-1.78893800	-1.20545100
C	-1.01895500	-1.78893800	1.20545100
C	-1.01895500	-0.39529300	-1.21387200
C	-1.01895500	-0.39529300	1.21387200
C	-1.01895500	0.28664400	0.00000000
H	-1.01895500	-3.56939800	0.00000000
H	-1.01895500	-2.32561700	-2.14486500
H	-1.01895500	-2.32561700	2.14486500
H	-1.01895500	0.15521400	-2.14419000
H	-1.01895500	0.15521400	2.14419000
Br	-1.01895500	2.16988900	0.00000000
O	3.58104500	-1.10066200	0.00000000
C	2.77825600	-1.10066300	-1.16175600
H	3.44622900	-1.10066300	-2.01887900
H	2.14017900	-1.99015000	-1.19972200
H	2.14017900	-0.21117500	-1.19972200
C	2.77825600	-1.10066300	1.16175600
H	3.44622900	-1.10066300	2.01887900
H	2.14017900	-0.21117500	1.19972200
H	2.14017900	-1.99015000	1.19972200

(CH3)2O-C6H5Cl LP away eclipsed dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.54 kcal/mol

C	1.23730300	-1.99305400	0.00000000
C	1.23730200	-1.29370800	1.20573600
C	1.23730200	-1.29370800	-1.20573600

C	1.23730200	0.09977300	1.21389000
C	1.23730200	0.09977300	-1.21389000
C	1.23730300	0.78056400	0.00000000
H	1.23730300	-3.07449200	0.00000000
H	1.23730100	-1.83014500	2.14538700
H	1.23730100	-1.83014500	-2.14538700
H	1.23730100	0.65454700	2.14171100
H	1.23730100	0.65454700	-2.14171100
Cl	1.23730300	2.51707000	0.00000000
O	-3.36269700	-0.60624400	0.00000000
C	-2.55990800	-1.76800000	0.00000000
H	-3.22788100	-2.62512300	0.00000000
H	-1.92183000	-1.80596400	-0.88948900
H	-1.92183000	-1.80596400	0.88948900
C	-2.55990800	0.55551200	0.00000000
H	-3.22788100	1.41263500	0.00000000
H	-1.92183200	0.59347700	0.88949000
H	-1.92183200	0.59347700	-0.88949000

(CH₃)₂O-C₆H₅Cl LP away staggered dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.39 kcal/mol

C	-1.23730300	-1.99305400	0.00000000
C	-1.23730200	-1.29370900	-1.20573500
C	-1.23730200	-1.29370900	1.20573500
C	-1.23730200	0.09977200	-1.21389000
C	-1.23730200	0.09977200	1.21389000
C	-1.23730300	0.78056400	0.00000000
H	-1.23730300	-3.07449200	0.00000000
H	-1.23730100	-1.83014700	-2.14538500
H	-1.23730100	-1.83014700	2.14538500
H	-1.23730100	0.65454500	-2.14171100
H	-1.23730100	0.65454500	2.14171100
Cl	-1.23730300	2.51707000	0.00000000
O	3.36269700	-0.60624400	0.00000000
C	2.55990900	-0.60624600	-1.16175600
H	3.22788200	-0.60624800	-2.01887800
H	1.92183200	-1.49573400	-1.19972000
H	1.92183200	0.28324200	-1.19972400
C	2.55990900	-0.60624600	1.16175600
H	3.22788200	-0.60624800	2.01887800
H	1.92183200	0.28324200	1.19972400
H	1.92183200	-1.49573400	1.19972000

(CH₃)₂O-C₆H₅F LP away eclipsed dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.24 kcal/mol

C	0.99899500	-1.91902900	0.00000000
C	1.14062100	-1.23545600	1.20660000
C	1.14062100	-1.23545600	-1.20659900
C	1.42337900	0.12931000	1.21548100
C	1.42337900	0.12930900	-1.21548100
C	1.55854600	0.78170900	0.00000000
H	0.77963000	-2.97782300	0.00000000

H	1.03153400	-1.76197300	2.14526100
H	1.03153500	-1.76197400	-2.14526100
H	1.53834700	0.68422000	2.13586400
H	1.53834800	0.68421900	-2.13586400
F	1.83238000	2.10340100	0.00000000
O	-3.22557000	0.36456800	0.00000000
C	-2.67516800	-0.93589500	0.00000000
H	-3.50313900	-1.63967800	0.00000000
H	-2.05806200	-1.10252200	-0.88948800
H	-2.05806300	-1.10252200	0.88948800
C	-2.20378300	1.33929800	0.00000000
H	-2.68397600	2.31411200	0.00000000
H	-1.57127300	1.24702400	0.88948800
H	-1.57127300	1.24702500	-0.88948700

(CH3)2O-C6H5F LP away staggered dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.14 kcal/mol

C	1.05543900	1.88857500	0.00000000
C	1.17674000	1.20110400	-1.20659900
C	1.17674000	1.20110300	1.20660000
C	1.41892000	-0.17144300	-1.21548200
C	1.41892100	-0.17144400	1.21548100
C	1.53469000	-0.82756200	0.00000000
H	0.86755300	2.95340600	0.00000100
H	1.08330800	1.73062500	-2.14526000
H	1.08330900	1.73062300	2.14526200
H	1.51739000	-0.72951700	-2.13586500
H	1.51739100	-0.72951800	2.13586400
F	1.76922700	-2.15679000	-0.00000100
O	-3.23495900	-0.26879800	0.00000000
C	-2.44438200	-0.12930300	-1.16175600
H	-3.10219400	-0.24537100	-2.01887900
H	-1.97057100	0.85752700	-1.19972100
H	-1.66145300	-0.89438600	-1.19972300
C	-2.44438200	-0.12930500	1.16175600
H	-3.10219300	-0.24537400	2.01887900
H	-1.66145300	-0.89438800	1.19972100
H	-1.97057100	0.85752500	1.19972300

(CH3)2O-C6H6 LP away eclipsed dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.27 kcal/mol

C	0.00000000	1.39150000	-1.52843300
C	-1.20507400	0.69575000	-1.52843300
C	1.20507400	0.69575000	-1.52843300
C	-1.20507400	-0.69575000	-1.52843300
C	1.20507400	-0.69575000	-1.52843300
C	0.00000000	-1.39150000	-1.52843300
H	0.00000000	2.47150000	-1.52843300
H	-2.14038200	1.23575000	-1.52843300
H	2.14038200	1.23575000	-1.52843300
H	-2.14038200	-1.23575000	-1.52843300
H	2.14038200	-1.23575000	-1.52843300

H	0.00000000	-2.47150000	-1.52843300
O	0.00000000	0.00000000	3.07156700
C	0.00000000	1.16175600	2.26877800
H	0.00000000	2.01887900	2.93675100
H	0.88948800	1.19972200	1.63070100
H	-0.88948800	1.19972200	1.63070100
C	0.00000000	-1.16175600	2.26877800
H	0.00000000	-2.01887900	2.93675100
H	-0.88948800	-1.19972200	1.63070100
H	0.88948800	-1.19972200	1.63070100

(CH₃)₂O-C₆H₆ LP away staggered dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.27 kcal/mol

C	0.00000000	1.39150000	-1.52843300
C	-1.20507400	0.69575000	-1.52843300
C	1.20507400	0.69575000	-1.52843300
C	-1.20507400	-0.69575000	-1.52843300
C	1.20507400	-0.69575000	-1.52843300
C	0.00000000	-1.39150000	-1.52843300
H	0.00000000	2.47150000	-1.52843300
H	-2.14038200	1.23575000	-1.52843300
H	2.14038200	1.23575000	-1.52843300
H	-2.14038200	-1.23575000	-1.52843300
H	2.14038200	-1.23575000	-1.52843300
H	0.00000000	-2.47150000	-1.52843300
O	0.00000000	0.00000000	3.07156700
C	-1.16175600	0.00000000	2.26877800
H	-2.01887900	0.00000000	2.93675100
H	-1.19972200	0.88948800	1.63070100
H	-1.19972200	-0.88948800	1.63070100
C	1.16175600	0.00000000	2.26877800
H	2.01887900	0.00000000	2.93675100
H	1.19972200	-0.88948800	1.63070100
H	1.19972200	0.88948800	1.63070100

(CH₃)₂O-C₆H₅CH₃ LP away eclipsed H towards dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.67 kcal/mol

C	-0.92668100	-2.00463200	0.00083500
C	-1.09478300	-1.32333000	-1.20334700
C	-1.08975900	-1.32178900	1.20483600
C	-1.42242400	0.03133800	-1.19944400
C	-1.41741700	0.03287400	1.20056600
C	-1.58584000	0.72915200	0.00046100
H	-0.67573300	-3.05712900	0.00098500
H	-0.97535100	-1.84603100	-2.14371500
H	-0.96640400	-1.84328600	2.14536500
H	-1.55629800	0.55401600	-2.13963300
H	-1.54736900	0.55675500	2.14063600
C	-1.90589000	2.19778900	0.00018900
H	-0.99181900	2.79400600	-0.00210000
H	-2.48320800	2.47287100	-0.88158300
H	-2.47952500	2.47400100	0.88400800

O	3.21384500	0.44344000	-0.00136100
C	2.70667200	-0.87448400	-0.00085600
H	3.55742500	-1.55055100	-0.00103500
H	2.09575400	-1.06118600	0.88891500
H	2.09505400	-1.06159700	-0.89006000
C	2.16043700	1.38390800	-0.00116400
H	2.60818800	2.37404300	-0.00156900
H	1.53096800	1.27059900	-0.89037800
H	1.53166800	1.27101000	0.88859800

(CH3)2O-C6H5CH3 LP away staggered H towards dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.56 kcal/mol

C	-0.99970600	-1.96923200	0.00141200
C	-1.14272300	-1.28253600	-1.20294700
C	-1.13752600	-1.28053700	1.20523500
C	-1.42037200	0.08325600	-1.19939600
C	-1.41519200	0.08524900	1.20061400
C	-1.55798100	0.78692400	0.00032800
H	-0.78759500	-3.03023800	0.00183500
H	-1.04262200	-1.80952300	-2.14317900
H	-1.03336600	-1.80596200	2.14590000
H	-1.53499900	0.61024800	-2.13972000
H	-1.52576200	0.61380100	2.14054800
C	-1.82385600	2.26632800	-0.00032600
H	-0.88849800	2.82855800	-0.00281200
H	-2.39072300	2.56219800	-0.88214800
H	-2.38691200	2.56366400	0.88344200
O	3.22796700	0.32506400	-0.00160900
C	2.44074500	0.16456900	-1.16293200
H	3.09494100	0.29722800	-2.02041500
H	1.99264700	-0.83422500	-1.20021200
H	1.63823700	0.90909000	-1.20089600
C	2.44179500	0.16569400	1.16058000
H	3.09676500	0.29918300	2.01734200
H	1.63932100	0.91025100	1.19854800
H	1.99373100	-0.83306400	1.19923200

(CH3)2O-C6H5CH3 LP away eclipsed H away dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.60 kcal/mol

C	-0.89958400	-2.01091500	0.00089000
C	-1.06779400	-1.32925800	1.20485700
C	-1.07277200	-1.33094900	-1.20332600
C	-1.40791500	0.02233000	1.20052400
C	-1.41287600	0.02064400	-1.19948600
C	-1.58776800	0.71570800	0.00039800
H	-0.63213500	-3.05934000	0.00107400
H	-0.93044400	-1.84723800	2.14538900
H	-0.93931000	-1.85025000	-2.14369000
H	-1.53261600	0.54756900	2.14054700
H	-1.54146300	0.54456300	-2.13972200
C	-1.98762400	2.16465200	0.00020700
H	-3.07412100	2.26723400	0.00238100

H	-1.60459900	2.67697600	0.88185500
H	-1.60824900	2.67573600	-0.88373500
O	3.21822600	0.47517600	-0.00135800
C	2.72321000	-0.84736200	-0.00080400
H	3.58015200	-1.51556700	-0.00094400
H	2.11402500	-1.03964300	0.88896800
H	2.11335100	-1.04013500	-0.89000800
C	2.15620400	1.40590600	-0.00121300
H	2.59481900	2.40012100	-0.00165400
H	1.52781600	1.28676800	-0.89043000
H	1.52849000	1.28726000	0.88854600

(CH3)2O-C6H5CH3 LP away staggered H away dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.52 kcal/mol

C	-0.97400800	-1.97594000	0.00161200
C	-1.11660400	-1.28806800	1.20535000
C	-1.12175300	-1.29039600	-1.20283300
C	-1.40604500	0.07527100	1.20056400
C	-1.41117700	0.07295000	-1.19944600
C	-1.55995000	0.77446700	0.00020500
H	-0.74587400	-3.03361600	0.00214700
H	-0.99863800	-1.81049100	2.14605600
H	-1.00780900	-1.81463900	-2.14302200
H	-1.51101300	0.60512000	2.14041000
H	-1.52016500	0.60098100	-2.13985800
C	-1.90545200	2.23732500	-0.00047100
H	-2.98736300	2.38038600	0.00170400
H	-1.50353200	2.73529900	0.88098800
H	-1.50730700	2.73359200	-0.88460200
O	3.23371800	0.35473600	-0.00162900
C	2.44792400	0.18732100	-1.16294200
H	3.10096200	0.32551800	-2.02043300
H	2.00845800	-0.81530500	-1.20011000
H	1.63902400	0.92488800	-1.20100200
C	2.44893500	0.18872600	1.16057000
H	3.10271900	0.32796000	2.01732400
H	1.64006900	0.92633900	1.19844100
H	2.00950200	-0.81385400	1.19933300

(CH3)2O-C6H5OCH3 LP away eclipsed O-LP towards dimer MP2/aug-cc-pVDZ

R=4.6 Angstroms

Interaction Energy=-2.61 kcal/mol

C	-0.01964100	2.26999000	0.00130800
C	-0.34729000	1.65199900	1.20756200
C	-1.00815600	0.42499300	1.20998900
C	-1.33745200	-0.18180400	-0.00034200
C	-1.01189700	0.42863300	-1.20985500
C	-0.35102100	1.65562900	-1.20578000
H	0.49580700	3.22097000	0.00194200
H	-0.08442700	2.12150000	2.14646000
H	-1.26069500	-0.07696300	2.13510100
H	-1.26729700	-0.07053900	-2.13568700
H	-0.09105900	2.12795300	-2.14407000

O	-1.96336200	-1.41100600	-0.00122400
C	-3.38354400	-1.28174000	0.00116600
H	-3.79024600	-2.28909900	0.00028000
H	-3.72185900	-0.74762500	0.89212900
H	-3.72461000	-0.74494900	-0.88713500
O	3.37326400	-1.13371200	-0.00111400
C	3.21616000	0.26966500	-0.00014800
H	4.21032100	0.70840100	0.00012700
H	2.67207400	0.60580400	-0.88939100
H	2.67212100	0.60458400	0.88958400
C	2.11612800	-1.77695100	-0.00152300
H	2.29870600	-2.84817100	-0.00226200
H	1.53614000	-1.50891500	0.88816400
H	1.53609400	-1.50769500	-0.89081100

(CH₃)₂O-C₆H₅OCH₃ LP away staggered O-LP towards dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms

Interaction Energy=-2.49 kcal/mol

C	-0.12333700	2.26672100	0.00266400
C	-0.42242900	1.63368300	1.20853300
C	-1.02654300	0.37776200	1.21019700
C	-1.32774800	-0.24272200	-0.00051100
C	-1.03040300	0.38267600	-1.20964500
C	-0.42627900	1.63858400	-1.20480700
H	0.34812200	3.24025800	0.00388900
H	-0.18130900	2.11414100	2.14772300
H	-1.25590000	-0.13576300	2.13499700
H	-1.26271300	-0.12709000	-2.13578600
H	-0.18815300	2.12285400	-2.14280200
O	-1.89684200	-1.49923800	-0.00215500
C	-3.32144700	-1.43499700	0.00024800
H	-3.68169900	-2.45988500	-0.00125900
H	-3.68382900	-0.91743100	0.89151400
H	-3.68666700	-0.91381800	-0.88774800
O	3.42154000	-0.97840200	-0.00163900
C	2.69783900	-0.63252900	1.16059000
H	3.30007800	-0.92265700	2.01731800
H	2.50746600	0.44542300	1.19994600
H	1.73771200	-1.15839400	1.19792000
C	2.69774700	-0.62954900	-1.16292000
H	3.29991800	-0.91747800	-2.02043700
H	1.73761700	-1.15531600	-1.20152300
H	2.50737100	0.44850100	-1.19949600

(CH₃)₂O-C₆H₅OCH₃ LP away eclipsed O-LP away dimer MP2/aug-cc-pVDZ
R=4.9 Angstroms

Interaction Energy=-1.96 kcal/mol

C	0.88554500	-2.31378800	0.00011000
C	1.07746000	-1.64151100	-1.20634300
C	1.45130100	-0.29892800	-1.20916600
C	1.63451900	0.36706300	0.00097000
C	1.44633000	-0.29831500	1.21067900
C	1.07250200	-1.64090000	1.20700000
H	0.59814600	-3.35659600	-0.00021600

H	0.94152000	-2.16240900	-2.14508800
H	1.61698600	0.23771700	-2.13443700
H	1.60821100	0.23879900	2.13635200
H	0.93270500	-2.16132200	2.14544300
O	2.03508400	1.68700600	0.00145800
C	0.92162000	2.57797400	-0.00105500
H	1.32649000	3.58607100	-0.00047900
H	0.30748700	2.42711100	-0.89191400
H	0.30383100	2.42756200	0.88735000
O	-3.45924900	0.34511300	-0.00103400
C	-2.99866800	-0.98980700	-0.00113400
H	-3.87263600	-1.63558300	-0.00161200
H	-2.39399100	-1.19787700	-0.89042800
H	-2.39468800	-1.19825000	0.88854700
C	-2.37346800	1.24801200	-0.00041900
H	-2.78617400	2.25325800	-0.00037000
H	-1.74905700	1.11270000	0.88928500
H	-1.74836000	1.11307300	-0.88969000

(CH₃)₂O-C₆H₅OCH₃ LP away staggered O-LP away dimer MP2/aug-cc-pVDZ

R=4.7 Angstroms

Interaction Energy=-2.39 kcal/mol

C	-0.86734800	-2.28181200	0.00013300
C	-1.04718800	-1.60601000	1.20647600
C	-1.39667800	-0.25688300	1.20908200
C	-1.56769700	0.41215000	-0.00116100
C	-1.39145700	-0.25668800	-1.21076200
C	-1.04198100	-1.60581500	-1.20686600
H	-0.59886300	-3.32965000	0.00062800
H	-0.92078700	-2.12915500	2.14530500
H	-1.55271800	0.28279800	2.13426500
H	-1.54350300	0.28314300	-2.13652300
H	-0.91153000	-2.12880900	-2.14522500
O	-1.94431600	1.73912500	-0.00186600
C	-0.81491500	2.60980100	0.00064100
H	-1.20148000	3.62505900	-0.00011100
H	-0.20369900	2.44797400	0.89158300
H	-0.19986000	2.44811700	-0.88768100
O	3.33127400	0.24772600	0.00128500
C	2.55487700	0.04532900	-1.16077800
H	3.20177800	0.21309400	-2.01764500
H	2.16114700	-0.97610100	-1.19857500
H	1.71354500	0.74564400	-1.19940000
C	2.55374600	0.04614800	1.16273400
H	3.19981200	0.21451700	2.02011200
H	1.71237700	0.74649000	1.20004400
H	2.15997900	-0.97525600	1.20086800

(CH₃)₂O-C₆H₅N(CH₃)₂ LP away eclipsed N-LP towards dimer MP2/aug-cc-pVDZ

R=4.5 Angstroms

Interaction Energy=-3.14 kcal/mol

C	-0.79438400	2.38895200	0.01442500
C	-0.29766600	1.88671000	-1.18489800
C	-0.32230000	1.85111100	1.20824900

C	0.64692200	0.86537700	-1.19642700
C	0.62216400	0.82959700	1.20883400
C	1.11751200	0.29848000	0.00300800
H	-1.52567900	3.18444100	0.01873100
H	-0.63830800	2.29441800	-2.12736200
H	-0.68239000	2.23071200	2.15521200
H	1.01074800	0.51024600	-2.14783800
H	0.96644200	0.44621700	2.15654800
N	2.02279600	-0.75907500	-0.00340500
C	2.77629200	-0.97506600	-1.22194800
C	2.75112100	-1.01144200	1.22342300
H	3.36660200	-0.09917400	-1.51946100
H	3.45037100	-1.81359600	-1.06920700
H	2.11208000	-1.23501900	-2.04357600
H	3.33491600	-0.14496700	1.55894000
H	2.07022000	-1.29551300	2.02311300
H	3.42845700	-1.84526500	1.05971600
O	-3.13667700	-1.70604700	-0.01775300
C	-3.33599400	-0.30807200	-0.00843300
H	-4.40834400	-0.13225200	-0.00900500
H	-2.89476800	0.14684700	0.88495400
H	-2.89180400	0.15913000	-0.89397700
C	-1.75852200	-2.01400500	-0.01758300
H	-1.66704100	-3.09679100	-0.02490800
H	-1.26278000	-1.60255200	-0.90342700
H	-1.26574400	-1.61483500	0.87550400

(CH₃)₂O-C₆H₅N(CH₃)₂ LP away staggered N-LP towards dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms

Interaction Energy=-2.92 kcal/mol

C	-0.54255200	2.47041700	0.02309700
C	-0.09584400	1.92753700	-1.17818700
C	-0.12310400	1.88632500	1.21484000
C	0.74797700	0.82154000	-1.19368200
C	0.72057900	0.78011900	1.21146000
C	1.16319200	0.20864500	0.00357600
H	-1.19538300	3.33144500	0.03048900
H	-0.39667200	2.36880400	-2.11908500
H	-0.44545400	2.29505400	2.16327700
H	1.07635700	0.43683400	-2.14648700
H	1.02732700	0.36270900	2.15768600
N	1.96446200	-0.92971300	-0.00690100
C	2.69384900	-1.21183000	-1.22659700
C	2.66599400	-1.25394100	1.21865300
H	3.36422800	-0.39465200	-1.52152100
H	3.28569300	-2.11083100	-1.07705400
H	2.00782500	-1.40505600	-2.04870400
H	3.32916200	-0.44766500	1.55672700
H	1.96150200	-1.47508800	2.01778400
H	3.26144300	-2.14749300	1.05176400
O	-3.34093200	-1.44537300	-0.02219400
C	-2.70025700	-0.94679900	-1.17766200
H	-3.22960300	-1.34322200	-2.03992000
H	-2.73230400	0.14774100	-1.20463900

H	-1.65339000	-1.26666800	-1.21671600
C	-2.70501800	-0.97026900	1.14572700
H	-3.23787700	-1.38400900	1.99762300
H	-1.65830700	-1.29090600	1.18260000
H	-2.73722000	0.12350400	1.19467800

(CH3)2O-C6H5N(CH3)2 LP away eclipsed N-LP away dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms

Interaction Energy=-3.00 kcal/mol

C	-0.73553200	2.47798100	0.00981300
C	-0.25746300	1.94975300	1.20554600
C	-0.22984700	1.98024400	-1.18763900
C	0.70896300	0.94900100	1.21000600
C	0.73671800	0.97964600	-1.19529300
C	1.24371900	0.45113500	0.00682900
H	-1.48848600	3.25301200	0.01099900
H	-0.64162000	2.30974400	2.15070800
H	-0.59220100	2.36430800	-2.13193500
H	1.04669200	0.56257300	2.15883800
H	1.09636300	0.61741500	-2.14561600
N	2.24850700	-0.51240300	0.00614700
C	2.42636500	-1.28090800	1.22147400
C	2.45458400	-1.24975200	-1.22393500
H	1.51971500	-1.82182900	1.52073400
H	3.22490900	-2.00072400	1.06324500
H	2.72659100	-0.63514200	2.04407800
H	1.55523800	-1.78260800	-1.55771500
H	2.77351900	-0.58332800	-2.02267600
H	3.24947600	-1.97360000	-1.06571200
O	-3.06012700	-1.73651100	-0.01667300
C	-3.28980200	-0.34318200	-0.01100600
H	-4.36571800	-0.19072000	-0.01363700
H	-2.85998000	0.12333100	0.88196200
H	-2.85447400	0.13147400	-0.89698700
C	-1.67560600	-2.01443200	-0.01366000
H	-1.56059700	-3.09498700	-0.01825000
H	-1.18752700	-1.59439100	-0.89972800
H	-1.19303300	-1.60253400	0.87922000

(CH3)2O-C6H5N(CH3)2 LP away staggered N-LP away dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms

Interaction Energy=-2.76 kcal/mol

C	-0.51699500	2.53259200	0.01374000
C	-0.08710000	1.96281800	1.20868700
C	-0.05619700	1.99464900	-1.18444000
C	0.78852300	0.88171700	1.21167300
C	0.81958200	0.91371000	-1.19356800
C	1.27827300	0.34112400	0.00777300
H	-1.19961100	3.37023300	0.01606700
H	-0.43874700	2.35336400	2.15437200
H	-0.38344600	2.41032700	-2.12816800
H	1.09103300	0.46582200	2.15992900
H	1.14661600	0.52307500	-2.14442200
N	2.19535400	-0.70623500	0.00568400

C	2.30525200	-1.48926600	1.21978400
C	2.33682900	-1.45674100	-1.22556700
H	1.35485700	-1.94967700	1.51800800
H	3.03814100	-2.27561900	1.06051100
H	2.66030900	-0.87342000	2.04349100
H	1.39460800	-1.90873100	-1.56036700
H	2.71282200	-0.81932900	-2.02316500
H	3.06563200	-2.24730200	-1.06839500
O	-3.19969200	-1.46345500	-0.02001900
C	-2.57150300	-0.95129100	-1.17639900
H	-3.08728600	-1.36667700	-2.03795000
H	-2.63545600	0.14172000	-1.20815500
H	-1.51566200	-1.24059700	-1.21207300
C	-2.58030800	-0.96500900	1.14705600
H	-3.10258700	-1.39051500	1.99970900
H	-1.52475400	-1.25476300	1.18731200
H	-2.64454800	0.12755400	1.19123000