(CH3)2O-C6F6 LP away eclipsed dimer MP2/aug-cc-pVDZ
R=4.5 Angstroms
Interaction Energy=-2.10 kcal/mol

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F                  0.00000000    2.71953700   -0.87356400
F                 -2.35518800    1.35976900   -0.87356400
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F                  0.00000000   -2.71953700   -0.87356400
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C                  0.00000000    1.16175600    2.82364700
H                  0.00000000    2.01887900    3.49162000
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C                 -1.16175600   -0.00000000    2.82364700
H                 -2.01887900   -0.00000000    3.49162000
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H                  1.19972200   -0.88948800    2.18557000

(CH3)2O-C6F6 LP away staggered dimer MP2/aug-cc-pVDZ
R=4.5 Angstroms
Interaction Energy=-2.08 kcal/mol

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F                  0.00000000    2.71953700   -0.87356400
F                 -2.35518800    1.35976800   -0.87356400
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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
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C                  1.16175600    0.00000000    2.82364700
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(CHA)2O-C6H5NO2 LP away eclipsed dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.25 kcal/mol

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(CH3)2O-C6H5NO2 LP away staggered dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.12 kcal/mol

(Ch3)2O-C6H5CN LP away eclipsed dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.25 kcal/mol

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(CH3)2O-C6H5CN LP away staggered dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.09 kcal/mol

(CH3)2O-C6H5CF3 LP away eclipsed F towards dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.44 kcal/mol
(CH3)2O-C6H5CF3 LP away staggered F towards dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.32 kcal/mol

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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
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H -0.93111900  0.55319400  2.14270300
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C -1.95269700  -0.72824400  -0.00118600
F -1.27957300  -1.89620000  -0.00118600
F -2.74906700  -0.73979400  1.08106800
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O  3.38194900  -1.48744000  0.00406300
C  2.77031000  -0.96542450  1.16490100
H  3.27764400  -1.39842900  2.02278600
H  2.86237600  0.12540400  1.20213500
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
(CH3)2O-C6H5CF3 LP away staggered F away dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.24 kcal/mol
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C -0.55004200 0.92930100 1.21046000
C -0.98834600 0.39806100 -0.00118900
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H 1.76143000 -1.23438200 -1.19729200
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(CH3)2O-C6H5Br LP away eclipsed dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.63 kcal/mol

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(CH3)2O-C6H5Br LP away staggered dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms

Interaction Energy=-2.46 kcal/mol

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(CH3)2O-C6H5Cl LP away eclipsed dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms

Interaction Energy=-2.54 kcal/mol

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**R=4.6 Angstroms**

**Interaction Energy=-2.39 kcal/mol**

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

**R=4.6 Angstroms**

**Interaction Energy=-2.24 kcal/mol**

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(CH3)2O-C6H5F LP away staggered dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.14 kcal/mol

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(CH3)2O-C6H6 LP away eclipsed dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.27 kcal/mol
(CH₃)₂O-C₆H₆ LP away staggered dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.27 kcal/mol

(CH₃)₂O-C₆H₅CH₃ LP away eclipsed H towards dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.67 kcal/mol
(CH3)2O-C6H5CH3 LP away staggered H towards dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.56 kcal/mol

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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
C   -0.88849800   2.82855800    0.00032800
H   -2.39072300   2.56219800    0.88344200
H   -2.38691200   2.56366400    0.88344200
O   3.22796700    0.32506400   -0.00160900
C   2.44074500    0.16456900   -1.16293200
C   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
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(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
### (CH3)2O-C6H5CH3 (LP away) staggered H away dimer MP2/aug-cc-pVDZ

R = 4.6 Angstroms

Interaction Energy = -2.52 kcal/mol

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

R = 4.6 Angstroms

Interaction Energy = -2.61 kcal/mol

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(CH3)2O-C6H5OCH3 LP away staggered O-LP towards dimer MP2/aug-cc-pVDZ
R=4.6 Angstroms
Interaction Energy=-2.49 kcal/mol

(CH3)2O-C6H5OCH3 LP away eclipsed O-LP away dimer MP2/aug-cc-pVDZ
R=4.9 Angstroms
Interaction Energy=-1.96 kcal/mol
(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  -0.04718800  -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
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H  1.71237700   0.74649000  1.20004400
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(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
(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
(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  1.21000600
C   0.70896300  0.94900100  1.21000600
C   0.73671800  0.97964600  1.21000600
C   1.24371900  0.45113500  0.00682900
H  -1.48848600  3.25301200  0.01099900
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O   -3.06012700 -1.73651100 -0.01667300
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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  1.94649000 -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   -0.38346600  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
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