Supporting Information for

Effects of aromatic trifluoromethylation, fluorination, and methylation on intermolecular π-π interactions

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Contents

1. Calculated dipole moment (DM) and quadrupole moments (QM) for all the monomers studied in this manuscript,

Table **S1**. Calculated dipole moments (DM/Debye) and quadrupole moments (QM/Debye-Ang) of all monomers at MP2/aug-cc-pvDZ level and at B97D/TZV (for monomers marked with *) level of theory.

Monomer	DM	QM					
Number		XX	YY	ZZ	XY	XZ	YZ
1	0.0001	-32.0081	-32.0092	-41.3387	0.0001	0.0000	0.0000
2	3.1863	-54.3734	-50.8280	-61.3873	-0.0002	0.2007	-0.0001
3	3.0118	-87.8965	-69.5629	-81.3755	0.0002	0.4149	0.0001
4	0.0892	-105.7704	-105.7329	-101.2924	0.0004	0.5021	-0.0205
5	4.9271	-76.9317	-69.0169	-81.3077	0.0019	-0.2300	0.0009
6	0.0010	-93.7695	-69.6635	-81.3861	-0.0006	0.3522	0.0000
7	1.8593	-41.4455	-34.2156	-44.5103	0.0000	0.0004	0.0000
8	1.8530	-49.5600	-39.4757	-47.7248	0.0000	0.0000	0.0004
9	-0.0031	-50.7290	-50.7299	-49.8380	-0.0003	0.0010	0.0012
10	0.4041	-38.7008	-38.9146	-47.5183	-0.0028	-0.0107	0.0002
11	0.3815	-44.9313	-45.8889	-53.7101	-0.0013	-0.0322	0.0000
12	0.6679	-45.9882	-45.5986	-53.7930	0.0000	0.0001	0.0001
13	2.3484	-29.3337	-36.6620	-39.1958	-0.0391	-0.0033	0.0002
14	0.6220	-65.6795	-48.1314	-59.2594	0.0001	0.0044	-0.0001
15	0.4892	-48.0029	-31.5963	-42.4240	0.0013	-0.0008	0.0020
16	2.8657	-45.1652	-36.2623	-45.3581	0.0007	-0.0650	0.0001
17	0.7462	-35.2595	-31.5934	-41.7208	0.0000	0.0017	0.0000
18*	0.001	-51.0403	-67.3744	-73.6603	-2.8646	0.0000	0.0000
19*	0.2423	-134.0090	-103.0536	-115.3822	18.1786	0.0004	0.0000
20*	0.0001	-76.2625	-78.0652	-80.5175	15.5510	0.0000	0.0000
21*	0.0704	-60.4151	-81.1817	-86.1831	0.3875	-0.0006	-0.0003

2. Correlation between calculated dimerization energies by MP2 and DFT-D methods

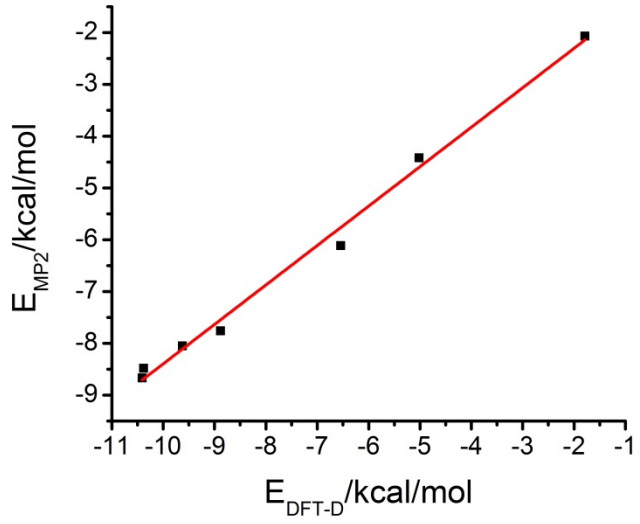
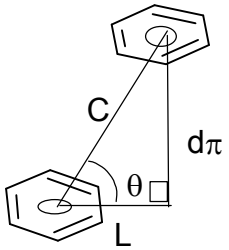


Figure S1. Correlation between calculated dimerization energies by MP2 and DFT-D methods

3. Calculation of horizontal displacement distances and intermolecular displacement degrees of dimers



L= horizontal displacement

C= centroid distance

dπ= π–π distance between rings

θ= intermolecular displacement in degrees

Figure S2. Diagram for calculation of horizontal displacement distances and intermolecular displacement degrees of dimers

To calculate the intermolecular orientation parameters, the following approach was used: First, the dimer geometry was optimized in Gaussian 09 at the MP2/6-31g* level of theory. After calculations were converged, the coordinates were exported into *.pdb form using the utility in Gaussview. These pdb files were then analyzed using Mercury 3.1.1 crystallographic software. Centroids were calculated for each of the rings, and the distance was measured in Angstroms. For the π–π distance measurements, one of the rings was chosen to be a plane, and the average distance between this plane and the opposing ring was measured by recording the distance from each aromatic ring atom of the other molecule to the plane, and then averaging the results to account for tilting. Once C and dπ were found, θ(the displacement angle between the rings) was calculated by taking the arcsine of the ratio

between dπ and C. With this angle calculated, it was then possible to arrive at L (horizontal displacement) by taking the cosine of θ and multiplying it by C.

Table **S2** Geometry parameters of optimized dimers

Dimer	Monomer pair	d_{center}/Å	$d_{\pi-\pi}$/Å	θ/deg	d_{disp}/Å
A	1,1	4.281	4.281	90	0
B	1,2	4.954	N/A	156.46	1.979
C	1,3	3.921	3.606	66.88	1.540
D	1,4	3.817	3.601	70.63	1.266
E	5,5	3.839	3.665	72.68	1.143
F	6,6	3.764	3.626	74.44	1.010
G	2,2	3.94	3.646	67.73	1.493
H	3,3	3.778	3.665	75.95	0.917
I	1,7	4.055	3.767	68.28	1.501
J	1,8	3.967	3.473	61.10	1.917
K	1,9	3.894	3.894	90.00	0
L	10,10	4.698	3.905	56.22	2.612
M	11,11	4.076	3.668	64.15	1.778
N	12,12	4.65	N/A	116.97	2.109
O	7,7	3.929	3.758	73.03	1.147
W	13,13	3.905	3.645	68.97	1.401
X	14,14	3.769	3.575	71.54	1.194
Y	15,15	3.834	3.537	67.30	1.480
Z	16,16	3.738	3.520	70.34	1.258

d_{center}/Å **centroid distance**
$d_{\pi-\pi}$/Å **π–π distance between rings**
θ/deg **displacement angle**
d_{disp}/Å **displacement distance**

3. Coordinates and energies of optimized geometries of monomers and dimers

Output file coordinates and energies of the monomers (All energies obtained at MP2/aug-cc-pvDZ level of theory) Frequency calculations performed on all monomers at MP@/6-31g(d) and revealed no imaginary frequencies). BSSE correction was applied to MP2 calculations for dimers

Monomer energies at MP2/aug-cc-pvDZ level

Monomer 1
benzene

C	-1.36500	0.29800	-0.00000
C	-0.42500	1.33100	0.00000
C	0.94000	1.03300	-0.00000
C	1.36500	-0.29800	0.00000
C	0.42500	-1.33100	-0.00000
C	-0.94000	-1.03300	0.00000
H	-2.42700	0.52900	0.00000
H	-0.75500	2.36600	-0.00000
H	1.67200	1.83700	0.00000
H	2.42700	-0.52900	-0.00000
H	0.75500	-2.36600	0.00000
H	-1.67200	-1.83700	0.00000

E(H)= -231.53931789

Monomer 2
trifluoromethylbenzene

C	2.13300	-1.21000	0.00100
C	2.83100	-0.00000	0.01700
C	2.13300	1.21000	0.00100
C	0.73800	1.21500	-0.02500
C	0.04800	0.00000	-0.04300
C	0.73800	-1.21500	-0.02500
H	2.67500	-2.15200	0.00900
H	3.91800	-0.00000	0.03700
H	2.67500	2.15200	0.00900
H	0.18900	2.15200	-0.04400
H	0.18900	-2.15200	-0.04400
C	-1.44700	0.00000	-0.00100
F	-1.91200	-0.00100	1.27200
F	-1.97100	1.09100	-0.60900
F	-1.97100	-1.09100	-0.61000

E(H)= -567.93340877

Monomer 3
13CF3benzene

C	1.20000	0.30200	0.03800
C	1.21000	1.69900	0.03700
C	-0.00000	2.39300	-0.00000
C	-1.21000	1.69900	-0.03700
C	-1.20000	0.30200	-0.03800
C	-0.00000	-0.40700	-0.00000
H	2.15300	2.23600	0.07200
H	-0.00000	3.48000	0.00000
H	-2.15300	2.23600	-0.07200
H	0.00000	-1.49200	-0.00000
C	-2.50100	-0.44200	-0.00100
F	-2.94600	-0.59400	1.26800
F	-3.46900	0.21200	-0.68500
F	-2.38900	-1.67900	-0.53600
C	2.50100	-0.44200	0.00100
F	3.46900	0.21200	0.68500
F	2.38900	-1.67900	0.53500

```
F          2.94600       -0.59400       -1.26800
E(H)= -904.32501113

Monomer 4
135CF3benzene
C         -0.74200       -1.17200       -0.04400
C         -1.39900        0.05900       -0.06900
C         -0.64100        1.23000       -0.04400
C          0.75200        1.18400        0.00700
C          1.38600       -0.05800        0.03200
C          0.65000       -1.24300        0.00700
H         -2.48200        0.10400       -0.12000
H          1.33300        2.10000        0.02400
H          1.15300       -2.20500        0.02400
C          2.88500       -0.12100        0.00200
F          3.34700       -0.13700       -1.26800
F          3.44000        0.94700        0.61800
F          3.34900       -1.23400        0.61200
C         -1.54800       -2.43700       -0.00000
F         -2.72800       -2.29700       -0.64200
F         -0.88700       -3.46700       -0.57400
F         -1.82200       -2.79500        1.27500
C         -1.33800        2.55800       -0.00000
F         -1.58500        2.93600        1.27400
F         -0.59200        3.53000       -0.57100
F         -2.52500        2.51800       -0.64500
E(H)= -1240.71444280

Monomer 5
12CF3benzene
C          0.70400        0.49600       -0.02400
C         -0.70400        0.49600        0.02400
C         -1.38900        1.71400        0.02600
C         -0.69500        2.92400        0.01500
C          0.69700        2.92300       -0.01500
C          1.39000        1.71400       -0.02600
H         -2.47300        1.71200        0.05400
H          2.47400        1.71100       -0.05400
H         -1.24600        3.86100        0.02200
H          1.24800        3.86000       -0.02200
C         -1.53000       -0.76600       -0.00500
C          1.52900       -0.76600        0.00500
F          2.80900       -0.52200       -0.37000
F          1.58200       -1.29900        1.24500
F          1.05200       -1.71100       -0.83200
F         -1.05300       -1.71000        0.83200
F         -2.80900       -0.52100        0.37000
F         -1.58300       -1.29900       -1.24500
E(H)= -904.31869607

Monomer 6
14CF3Benzene
C         -0.69600        1.21500       -0.01700
C          0.69600        1.21500        0.01600
C          1.38600        0.00000        0.03900
C          0.69600       -1.21500        0.01600
C         -0.69600       -1.21500       -0.01700
C         -1.38600        0.00000       -0.03900
H         -1.24400        2.15200       -0.03500
H          1.24400        2.15200        0.03500
H          1.24400       -2.15200        0.03500
H         -1.24400       -2.15200       -0.03500
C         -2.88400        0.00000       -0.00400
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C          2.88400       -0.00000        0.00400
F         -3.40100        1.09200       -0.61200
F         -3.34800       -0.00300        1.26800
F         -3.40000       -1.09000       -0.61700
F          3.40100        1.09200        0.61400
F          3.40000       -1.09100        0.61500
F          3.34800       -0.00100       -1.26800
E(H)= -904.32524224

Monomer 7
fluorobenzene
C         -1.83600       -0.00000        0.00000
C         -1.13600       -1.20900       -0.00100
C          0.26000       -1.21800        0.00000
C          0.92800        0.00000        0.00000
C          0.26000        1.21800        0.00100
C         -1.13600        1.20900       -0.00100
H         -2.92200        0.00000       -0.00000
H         -1.67700       -2.15300        0.00000
H          0.83000       -2.14300        0.00000
H          0.83000        2.14300        0.00000
H         -1.67700        2.15300        0.00000
F          2.28700       -0.00000       -0.00000
E(H)= -330.59843400

Monomer 8
13difluorobenzene
C          1.21500        1.08500       -0.00100
C          1.18500       -0.30500        0.00000
C          0.00000       -1.03100       -0.00000
C         -1.18500       -0.30500        0.00000
C         -1.21500        1.08500       -0.00100
C         -0.00000        1.77300        0.00100
H          2.16900        1.60200        0.00000
H         -2.16900        1.60200        0.00000
H          0.00000        2.85900        0.00000
H          0.00000       -2.11500        0.00100
F         -2.35600       -0.98700        0.00000
F          2.35600       -0.98700        0.00000
E(H)= -429.65625714

Monomer 9
135trifluorobenzene
C         -1.11600        0.86500        0.00100
C          0.18500        1.35400        0.00000
C          1.30700        0.53400        0.00100
C          1.08000       -0.83800       -0.00000
C         -0.19100       -1.39800        0.00000
C         -1.26600       -0.51700        0.00000
H         -1.97200        1.52900       -0.00100
H          2.31000        0.94300        0.00000
H         -0.33800       -2.47200       -0.00100
F         -2.51800       -1.02900       -0.00000
F          0.36900        2.69500       -0.00100
F          2.15000       -1.66700       -0.00000
E(H)= -528.71272569

Monomer 10
toluene
C          0.19700       -1.20300       -0.00800
C         -1.19900       -1.20700        0.00200
C         -1.90300       -0.00000        0.00900
C         -1.20000        1.20600        0.00200
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```
C          0.19600        1.20300       -0.00800
C          0.91400        0.00100       -0.01700
H          0.73800       -2.14800       -0.01900
H         -1.73800       -2.15200        0.00300
H         -2.99000       -0.00100        0.01500
H         -1.73900        2.15100        0.00300
H          0.73600        2.14800       -0.01900
C          2.42100        0.00000        0.01200
H          2.82400       -0.87300       -0.50900
H          2.82400        0.89700       -0.46700
H          2.79700       -0.02400        1.04100
E(H)= -270.73175114

Monomer 11
Metaxylene
C         -0.00000        1.82400        0.00000
C         -1.20900        1.12800        0.01600
C         -1.22300       -0.27200        0.01700
C          0.00000       -0.95100       -0.00000
C          1.22400       -0.27100       -0.01700
C          1.20900        1.12800       -0.01600
H          2.15000        1.67600       -0.03100
H         -2.15000        1.67600        0.03100
H          0.00000       -2.04200       -0.00000
C          2.52500       -1.03100        0.01100
C         -2.52500       -1.03100       -0.01100
H         -0.00000        2.91200       -0.00000
H          3.31400       -0.47800       -0.50800
H          2.86300       -1.20100        1.03900
H          2.42200       -2.00700       -0.47100
H         -2.86900       -1.19000       -1.03900
H         -3.31100       -0.48400        0.52000
H         -2.41900       -2.01300        0.45900
E(H)= -309.92399641

Monomer 12
Orthoxylene
C          0.47800        0.70500        0.00000
C          0.47800       -0.70500       -0.00000
C         -0.74500       -1.38600       -0.00000
C         -1.95900       -0.69700       -0.00000
C         -1.95900        0.69700        0.00000
C         -0.74500        1.38600       -0.00000
H         -0.74500       -2.47500       -0.00000
H         -0.74500        2.47500        0.00000
H         -2.89700       -1.24700       -0.00000
H         -2.89700        1.24700        0.00000
C          1.77500       -1.47100        0.00000
C          1.77500        1.47100       -0.00000
H          2.38100        1.23500        0.88100
H          2.38100        1.23400       -0.88100
H          1.58700        2.54800       -0.00000
H          1.58800       -2.54800       -0.00000
H          2.38100       -1.23500        0.88100
H          2.38200       -1.23400       -0.88100
E(H)= -309.92529036


Monomer 13
Pyridine
C         -1.14900       -0.71500       -0.00000
C         -1.19400        0.68000       -0.00000
C          0.00800        1.38800       -0.00000
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```
C          1.20100        0.66700        0.00000
C          1.14100       -0.72700        0.00000
H         -2.15000        1.19600        0.00000
H          2.16300        1.17200        0.00100
H          2.05500       -1.32000       -0.00100
H         -2.06900       -1.29700        0.00200
N         -0.00800       -1.42700       -0.00000
H          0.01400        2.47500       -0.00000
E(H)= -247.56368800

Monomer 14
4CF3pyridine
C          0.75700       -1.20300       -0.02300
C          2.15000       -1.14600        0.00200
C          2.15000        1.14600        0.00200
C          0.75700        1.20300       -0.02300
C          0.05200        0.00000       -0.03800
H          0.23900       -2.15700       -0.04100
H          2.73700       -2.06200        0.01000
H          2.73700        2.06200        0.01000
H          0.23900        2.15700       -0.04100
C         -1.44600       -0.00000       -0.00100
F         -1.90500       -0.00000        1.27200
F         -1.96100        1.09100       -0.61100
F         -1.96100       -1.09100       -0.61200
N          2.85400       -0.00000        0.01600
E(H)= -583.95520434

Monomer 15
fluoropyridine
C         -1.15700       -1.14500        0.00000
C          0.23700       -1.20700       -0.00000
C          0.92200       -0.00000       -0.00000
C          0.23700        1.20700       -0.00000
C         -1.15600        1.14500       -0.00000
H          0.77200       -2.15000        0.00100
H          0.77300        2.15000        0.00000
H         -1.74000        2.06300        0.00200
H         -1.74100       -2.06300       -0.00000
N         -1.86200        0.00000        0.00000
F          2.27400       -0.00000        0.00000
E(H)= -346.62295284

Monomer 16
4methylpyridine
C          1.22000        1.14200        0.00300
C         -0.17400        1.19100       -0.00800
C         -0.90700        0.00000       -0.01600
C         -0.17400       -1.19000       -0.00800
C          1.22000       -1.14200        0.00300
H         -0.68100        2.15300       -0.01700
H         -0.68100       -2.15300       -0.01700
H          1.80300       -2.06200        0.00400
H          1.80300        2.06200        0.00400
N          1.93100       -0.00000        0.00800
C         -2.41100        0.00000        0.01000
H         -2.78300       -0.00200        1.04000
H         -2.81300        0.88700       -0.48800
H         -2.81300       -0.88600       -0.49000
E(H)= -286.75702298

Monomer 17
Thiophene
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```
C          0.00000        1.23500       -0.00300
C          1.27200        0.71200       -0.00100
C          1.27500       -0.70800        0.00100
C          0.00400       -1.23600        0.00300
S         -1.19100       -0.00100       -0.00000
H         -0.29800        2.27500        0.01400
H          2.16600        1.32700        0.00100
H          2.17100       -1.32000       -0.00300
H         -0.28900       -2.27800       -0.00600
E(H)= -552.01791301
```

Bipyridine monomers: Energy calculated at B97D/TZV level of theory

Monomer 18
Bipyridine

```
C          0.74500       -0.00800       -0.00000
C          1.46200       -1.22200       -0.00000
C          2.86000       -1.18600        0.00000
C          3.51600        0.05500        0.00000
C          2.73300        1.21800       -0.00000
N          1.37700        1.20500       -0.00000
H          0.91400       -2.15700       -0.00000
H          4.60000        0.12300        0.00100
H          3.19500        2.20200       -0.00100
C         -0.74500        0.00800       -0.00000
C         -1.46200        1.22200       -0.00000
N         -1.37700       -1.20500       -0.00000
C         -2.86000        1.18600        0.00000
H         -0.91400        2.15700       -0.00000
C         -2.73300       -1.21800       -0.00000
C         -3.51600       -0.05500        0.00000
H         -3.19500       -2.20200       -0.00100
H         -4.60000       -0.12300        0.00100
H         -3.43100        2.11200        0.00100
H          3.43100       -2.11200        0.00100
E(H)= -495.02261525
```

Monomer 19
4CF3bipyridine

```
C          0.65100        0.35900       -0.02900
C          1.86700       -0.35100       -0.02900
C          3.06200        0.37400       -0.03700
C          3.03300        1.77600       -0.03200
C          1.77900        2.40200       -0.03200
N          0.60700        1.72400       -0.03000
H          1.85600       -1.43400       -0.03300
H          3.94800        2.35800       -0.03700
H          1.70200        3.48500       -0.03400
C         -0.65100       -0.35900       -0.02900
C         -1.86700        0.35100       -0.02900
N         -0.60700       -1.72400       -0.03000
C         -3.06200       -0.37400       -0.03700
H         -1.85600        1.43400       -0.03300
C         -1.77900       -2.40200       -0.03200
C         -3.03300       -1.77600       -0.03200
H         -1.70200       -3.48500       -0.03400
H         -3.94700       -2.35800       -0.03700
C         -4.37200        0.36700        0.01500
C          4.37200       -0.36700        0.01500
F         -5.45100       -0.40600       -0.44700
F         -4.69700        0.75900        1.33100
F         -4.35400        1.54200       -0.75400
F          4.35500       -1.54100       -0.75500
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F          4.69600       -0.76000        1.33100
F          5.45100        0.40600       -0.44500
E(H)= -1168.90040263

Monomer 20
4,4'-fluorobipyridine
C         -0.72300       -0.17900        0.00000
C         -1.70700        0.83000       -0.00000
C         -3.03300        0.42100       -0.00000
C         -3.39600       -0.92400        0.00000
C         -2.34600       -1.85400        0.00000
N         -1.03600       -1.50900        0.00000
H         -1.42600        1.87600       -0.00000
H         -4.43700       -1.22800        0.00000
H         -2.55800       -2.92000        0.00000
C          0.72300        0.17900        0.00000
C          1.70700       -0.83000       -0.00000
N          1.03600        1.50900        0.00000
C          3.03300       -0.42100       -0.00000
H          1.42600       -1.87600       -0.00000
C          2.34600        1.85400        0.00000
C          3.39600        0.92400        0.00000
H          2.55800        2.92000        0.00000
H          4.43700        1.22800        0.00000
F          4.04200       -1.39400       -0.00000
F         -4.04200        1.39400       -0.00000
E(H)= -693.45334889

Monomer 21
4,4'CH3bipyridine
C         -0.71600        0.20600       -0.00100
C         -1.74700       -0.75400       -0.00900
C         -3.08800       -0.34500       -0.00700
C         -3.35100        1.03900       -0.00500
C         -2.27600        1.93600        0.00100
N         -0.97600        1.54900        0.00400
H         -1.48200       -1.80600       -0.01700
H         -4.37300        1.41000       -0.01100
H         -2.44800        3.01000        0.00200
C          0.71600       -0.20600       -0.00100
C          1.74700        0.75400       -0.00900
N          0.97600       -1.54900        0.00400
C          3.08800        0.34500       -0.00700
H          1.48200        1.80600       -0.01700
C          2.27600       -1.93600        0.00100
C          3.35100       -1.03900       -0.00500
H          2.44800       -3.01000        0.00200
H          4.37300       -1.41000       -0.01100
C          4.21600        1.35500        0.01000
H          3.87100        2.33700       -0.33500
H          4.61100        1.47800        1.02900
H          5.04900        1.03100       -0.62800
C         -4.21600       -1.35500        0.01000
H         -3.87200       -2.33600       -0.33700
H         -4.61000       -1.48000        1.03000
H         -5.05000       -1.03000       -0.62600
E(H)= -573.60632696

Dimer Output Geometries and energies at MP2/aug-cc-pvDZ//MP2/6-31g(d)
Dimer 1,1
Benzene dimer
C         -2.13900       -1.25800       -0.60800
C         -2.13800       -0.10300       -1.39400
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C         -2.13900        1.15500       -0.78700
C         -2.14200        1.25800        0.60600
C         -2.14300        0.10300        1.39200
C         -2.14200       -1.15500        0.78500
H         -2.13700       -2.23700       -1.08100
H         -2.13500       -0.18300       -2.47800
H         -2.13700        2.05400       -1.39800
H         -2.14100        2.23700        1.07900
H         -2.14300        0.18300        2.47600
H         -2.14100       -2.05400        1.39600
C          2.14200       -1.25800       -0.60600
C          2.14300       -0.10300       -1.39200
C          2.14200        1.15500       -0.78500
C          2.13900        1.25800        0.60800
C          2.13800        0.10300        1.39400
C          2.13900       -1.15500        0.78700
H          2.14100       -2.23700       -1.07900
H          2.14300       -0.18300       -2.47600
H          2.14100        2.05400       -1.39600
H          2.13700        2.23700        1.08100
H          2.13500        0.18300        2.47800
H          2.13700       -2.05400        1.39800
E(corrected)= -463.08193418

Dimer 1,2
Benzene and trifluoromethylbenzene
C          2.94400        2.11600        0.18300
C          1.77700        2.84400       -0.05800
C          0.57700        2.17600       -0.31500
C          0.53700        0.78300       -0.33100
C          1.71100        0.06400       -0.09100
C          2.91600        0.72100        0.17100
H          3.87900        2.63400        0.38000
H          1.80300        3.93100       -0.04900
H         -0.33400        2.73800       -0.50300
H         -0.39400        0.26100       -0.53400
H          3.82000        0.14900        0.35300
C         -3.23000        1.30900        0.42400
C         -3.34900        0.88100       -0.90000
C         -3.10200       -0.45500       -1.22800
C         -2.73500       -1.36200       -0.23100
C         -2.61400       -0.93300        1.09400
C         -2.86200        0.40200        1.42100
H         -3.42700        2.34800        0.68100
H         -3.63900        1.58600       -1.67600
H         -3.19600       -0.78800       -2.25800
H         -2.53800       -2.40000       -0.48600
H         -2.32200       -1.63900        1.86800
H         -2.76600        0.73500        2.45200
C          1.64800       -1.43000       -0.04700
F          1.18900       -1.87800        1.14800
F          0.81700       -1.92700       -0.99400
F          2.86200       -2.00100       -0.23900
E(corrected)= -799.47976590

Dimer 1,3
Benzene and 13CF3benzene
C         -0.24200        1.52100        0.45500
C          0.56200        0.97500        1.45900
C          0.27600       -0.29800        1.95000
C         -0.79600       -1.02600        1.43700
C         -1.58900       -0.46700        0.43200
C         -1.31800        0.80600       -0.07000
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H          1.39500        1.54600        1.85800
H          0.89800       -0.72700        2.73000
H         -1.02300       -2.01700        1.81900
H         -1.94600        1.24000       -0.84200
C          3.12900       -0.29000       -0.76200
C          3.75000       -1.04600        0.23600
C          3.27900       -2.32600        0.53800
C          2.18700       -2.85000       -0.15800
C          1.56600       -2.09400       -1.15600
C          2.03700       -0.81500       -1.45700
H          3.49600        0.70500       -1.00000
H          4.60500       -0.64000        0.77300
H          3.76600       -2.91700        1.31000
H          1.82300       -3.84800        0.07300
H          0.71500       -2.50200       -1.69600
H          1.55400       -0.22600       -2.23300
C         -2.69900       -1.27600       -0.16500
F         -2.24800       -2.06800       -1.16900
F         -3.27400       -2.09100        0.75000
F         -3.67300       -0.49500       -0.68400
C          0.10300        2.85900       -0.12100
F          0.67700        3.67000        0.79800
F          0.97900        2.74500       -1.14900
F         -0.98800        3.49800       -0.60200
E(corrected)= -1135.87407383

Dimer 1,4
Benzene and 135CF3benzene
C          0.05300       -1.18600       -0.93100
C          0.68100        0.02500       -1.21400
C          0.01700        1.21300       -0.91200
C         -1.25700        1.20300       -0.34500
C         -1.86600       -0.02200       -0.07500
C         -1.22100       -1.22300       -0.36500
H          1.67700        0.04300       -1.64200
H         -1.76500        2.13500       -0.11400
H         -1.70200       -2.17300       -0.14900
C          2.51800       -1.28800        1.89400
C          3.28400       -0.17200        1.55000
C          2.79300        1.11300        1.78900
C          1.53400        1.28300        2.36900
C          0.76600        0.16700        2.71200
C          1.25800       -1.11800        2.47400
H          2.90200       -2.28900        1.71200
H          4.26600       -0.30500        1.10200
H          3.39100        1.98200        1.52400
H          1.15400        2.28400        2.55900
H         -0.21300        0.29800        3.16600
H          0.66300       -1.98800        2.74500
C         -3.19600       -0.04800        0.61700
F         -3.04500       -0.06400        1.96300
F         -3.94000        1.03900        0.31200
F         -3.91300       -1.14400        0.28300
C          0.71200       -2.48200       -1.30100
F          2.04500       -2.34500       -1.46800
F          0.51100       -3.42600       -0.35300
F          0.20800       -2.97000       -2.45800
C          0.63800        2.53200       -1.26500
F          0.13900        3.00800       -2.42900
F          0.38900        3.46500       -0.31700
F          1.97800        2.44100       -1.40900
E(corrected)= -1472.26612880
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Dimer 1,17
Benzene and thiophene

C	-3.07700	-0.32100	-0.85000
C	-2.87000	1.00800	-0.47500
C	-2.04700	1.30600	0.61400
C	-1.43100	0.27600	1.32700
C	-1.63900	-1.05300	0.95300
C	-2.46200	-1.35200	-0.13500
H	-3.71800	-0.55300	-1.69700
H	-3.35000	1.81100	-1.03000
H	-1.88400	2.34100	0.90600
H	-0.78200	0.50800	2.16800
H	-1.15600	-1.85500	1.50600
H	-2.62500	-2.38700	-0.42600
C	1.44800	-0.17800	-1.22300
C	1.60400	1.16100	-0.95300
C	2.41500	1.39400	0.18800
C	2.85600	0.22500	0.76700
S	2.28500	-1.15300	-0.08400
H	0.86800	-0.63900	-2.01200
H	1.14700	1.94300	-1.55100
H	2.66800	2.37700	0.57200
H	3.49100	0.10600	1.63500

E(corrected)= -783.56201434

Dimer 2,17
Trifluoromethylbenzene and thiophene

C	-1.72300	1.41800	-0.77900
C	-0.98800	2.59500	-0.64600
C	-0.11100	2.75800	0.42900
C	0.02900	1.74200	1.37700
C	-0.70200	0.56100	1.25300
C	-1.57800	0.40800	0.17600
H	-2.41400	1.28800	-1.60800
H	-1.10200	3.38800	-1.38200
H	0.46100	3.67700	0.52900
H	0.71200	1.86700	2.21300
H	-0.59800	-0.23200	1.98700
C	1.80600	-0.72600	-1.13900
C	2.52000	0.44300	-1.26200
C	3.48400	0.60200	-0.23100
C	3.48000	-0.44900	0.65800
S	2.30700	-1.63000	0.23300
H	1.00500	-1.09300	-1.76600
H	2.35400	1.15700	-2.06200
H	4.15600	1.45000	-0.14400
H	4.11100	-0.59500	1.52500
C	-2.31200	-0.88200	-0.00600
F	-3.52100	-0.69900	-0.58900
F	-2.52300	-1.52100	1.16800
F	-1.62400	-1.74200	-0.80200

E(corrected)= -1119.95868674

Dimer 3,17
13CF3benzene and thiophene

C	-1.20900	-1.60400	1.48500
C	0.00000	-1.83200	2.14100
C	1.20900	-1.60400	1.48500
C	1.19900	-1.14000	0.16700
C	0.00000	-0.91100	-0.50600
C	-1.19900	-1.14000	0.16700
H	-2.15400	-1.77300	1.99400
H	0.00000	-2.18800	3.16800

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H          2.15400       -1.77300        1.99400
H          0.00000       -0.54000       -1.52400
C         -1.23600        2.62100        0.28300
C         -0.71000        2.29400        1.51200
C          0.71000        2.29400        1.51200
C          1.23500        2.62100        0.28300
S         -0.00000        2.92900       -0.86900
H         -2.27700        2.69600       -0.00100
H         -1.32400        2.06400        2.37700
H          1.32400        2.06400        2.37700
H          2.27700        2.69700       -0.00200
C         -2.50800       -0.95000       -0.53500
F         -3.04800       -2.13900       -0.89700
F         -2.38800       -0.20700       -1.65700
F         -3.41500       -0.33700        0.26400
C          2.50800       -0.95000       -0.53500
F          3.04800       -2.13900       -0.89800
F          2.38800       -0.20700       -1.65700
F          3.41500       -0.33700        0.26400
E(corrected)= -1456.35307420

Dimer 4,17
135CF3Benzene and thiophene
C         -1.28200       -1.21900       -0.32500
C         -0.02700       -1.20100       -0.93500
C          0.60400        0.00100       -1.25100
C         -0.03900        1.19900       -0.93900
C         -1.29400        1.20800       -0.33000
C         -1.90600       -0.00800       -0.02700
H         -1.76600       -2.16100       -0.08600
H          1.58400        0.00500       -1.71400
H         -1.78500        2.14700       -0.09300
C          2.07800       -1.22200        2.05100
C          3.17200       -0.76500        1.35100
C          3.23300        0.65200        1.30600
C          2.18500        1.24500        1.97300
S          1.13000        0.07600        2.65600
H          1.78800       -2.24600        2.24700
H          3.89900       -1.42700        0.89100
H          4.01400        1.21700        0.80700
H          1.98500        2.30100        2.10200
C         -3.21600       -0.01400        0.70300
F         -3.95300       -1.10400        0.39500
F         -3.95600        1.07800        0.40800
F         -3.02900       -0.02200        2.04200
C          0.58000        2.51100       -1.31900
F         -0.01300        3.02500       -2.42200
F          0.43800        3.42600       -0.33200
F          1.89800        2.39700       -1.58600
C          0.60200       -2.50900       -1.31200
F          0.46700       -3.42300       -0.32400
F          1.92000       -2.38400       -1.57900
F          0.01400       -3.02900       -2.41400
E(corrected)= -1792.74393339

2,2
CF3benzene CF3Benzene dimer
C          0.21800        1.70700       -1.36500
C          1.23800        0.75800       -1.28700
C          2.04500        0.71400       -0.14900
C          1.85200        1.61500        0.90200
C          0.83200        2.56100        0.81300
C          0.01600        2.60900       -0.32000
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H          1.39600        0.04800       -2.09300
H          2.48800        1.56800        1.78200
H         -0.78300        3.34400       -0.38400
C         -1.85100       -1.61600       -0.90100
C         -0.83100       -2.56100       -0.81100
C         -0.01500       -2.60800        0.32200
C         -0.21800       -1.70500        1.36700
C         -1.23900       -0.75700        1.28800
C         -2.04500       -0.71400        0.14900
H         -2.48600       -1.56900       -1.78200
H         -0.67200       -3.26300       -1.62600
H          0.78400       -3.34300        0.38700
H          0.42100       -1.73700        2.24500
H         -1.39700       -0.04700        2.09300
C          3.17900       -0.25700       -0.06200
F          4.36900        0.33600       -0.32800
F          3.28400       -0.79400        1.18000
F          3.04700       -1.28600       -0.93200
H          0.67400        3.26300        1.62900
H         -0.42200        1.73900       -2.24300
C         -3.17900        0.25700        0.06100
F         -4.36900       -0.33700        0.32700
F         -3.04800        1.28600        0.93000
F         -3.28400        0.79200       -1.18200
E(corrected)= -1135.87755433

3,3
13CF3benzene 13CF3benzene
C         -0.79600        0.07400        1.96000
C         -0.46700       -1.21100        1.52700
C         -1.23900       -1.81600        0.53300
C         -2.33500       -1.15800       -0.02600
C         -2.64900        0.12500        0.42000
C         -1.88500        0.74900        1.40900
H         -2.14000        1.74900        1.74500
C          2.40300        1.12600       -0.02100
C          2.50500       -0.16600       -0.53700
C          1.57700       -0.64500       -1.46300
C          0.53400        0.18400       -1.87900
C          0.41200        1.47600       -1.36800
C          1.35300        1.94000       -0.44600
H          3.14000        1.49800        0.68400
H          1.67600       -1.65000       -1.86300
H         -0.18800       -0.17900       -2.60500
H         -0.39900        2.12200       -1.69200
C          1.20300        3.30600        0.15200
F          2.40200        3.86300        0.43700
F          0.54500        4.15000       -0.67300
F          0.50400        3.26100        1.31500
H          0.38800       -1.73300        1.94500
H         -2.93200       -1.63700       -0.79700
C         -3.76100        0.88100       -0.23900
C         -0.93200       -3.21200        0.08700
F          0.35700       -3.54800        0.32200
F         -1.70600       -4.12100        0.72100
F         -1.15100       -3.36500       -1.24300
F         -3.30000        1.61300       -1.28600
F         -4.71600        0.05700       -0.72600
F         -4.35800        1.74400        0.61200
H         -0.19700        0.55500        2.72900
C          3.58500       -1.07100       -0.02800
F          4.70600       -0.38500        0.29100
F          3.92600       -2.01300       -0.93500
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F          3.18900       -1.72300        1.09400
E(corrected)=-1808.66284740

Dimer 5,5
12CF3benzene 12CF3benzene
C          0.64400       -1.67300        1.92500
C          0.19900       -0.37400        2.15900
C          0.88600        0.70500        1.60400
C          2.00400        0.50000        0.79100
C          2.46500       -0.81300        0.56800
C          1.76600       -1.88800        1.12600
H          0.11300       -2.52000        2.35000
H         -0.67800       -0.19600        2.77600
H          0.53900        1.71700        1.78400
H          2.11800       -2.89800        0.94800
C         -2.06200       -0.57500       -0.77500
C         -2.33800        0.78700       -0.54600
C         -1.51300        1.76000       -1.11900
C         -0.40200        1.39500       -1.87900
C         -0.11300        0.04800       -2.08200
C         -0.93800       -0.92900       -1.52700
H         -1.73400        2.80800       -0.95300
H         -0.72100       -1.97900       -1.69500
C          3.63200       -1.13500       -0.32800
C          2.70900        1.72000        0.25700
F          4.06900       -2.40200       -0.13000
F          3.29500       -1.04300       -1.63700
F          4.68700       -0.32200       -0.11900
F          3.04600        1.58700       -1.04600
F          1.91900        2.81900        0.34000
F          3.83500        1.99600        0.94800
H          0.23300        2.16500       -2.31000
H          0.75800       -0.24600       -2.66200
C         -3.53400        1.26600        0.23500
C         -2.89200       -1.69200       -0.19500
F         -2.62900       -2.86900       -0.81200
F         -2.63700       -1.88300        1.12100
F         -4.21600       -1.46800       -0.32700
F         -3.71400        0.56200        1.37600
F         -3.39200        2.56400        0.60100
F         -4.67400        1.18600       -0.48300
E(corrected)=-1808.65091036

Dimer 6,6
14CF3benzene 14CF3benzene
C          1.12700        1.34700        1.39900
C          2.24000        0.99100        0.63400
C          2.56600       -0.35100        0.42400
C          1.77700       -1.34700        0.99600
C          0.66300       -0.99000        1.76000
C          0.33900        0.35200        1.97200
H          0.88400        2.39400        1.55600
H          3.43200       -0.61600       -0.17500
H          2.01700       -2.39400        0.83800
H         -0.53100        0.61800        2.56500
C         -1.12700        1.34700       -1.39900
C         -0.33900        0.35200       -1.97200
C         -0.66300       -0.99000       -1.76000
C         -1.77800       -1.34600       -0.99600
C         -2.56600       -0.35100       -0.42400
C         -2.24000        0.99100       -0.63400
H         -0.88400        2.39400       -1.55600
H          0.53100        0.61800       -2.56500
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H         -2.01700       -2.39400       -0.83700
H         -3.43200       -0.61500        0.17500
C          3.03300        2.06200       -0.04800
C         -0.14200       -2.06300        2.42600
F          3.06600        3.20400        0.67600
F          2.49600        2.37800       -1.25500
F          4.31100        1.68300       -0.27300
F          0.39300       -2.41700        3.61800
F         -1.41500       -1.66600        2.66400
F         -0.20300       -3.18500        1.67100
C         -3.03300        2.06300        0.04800
C          0.14200       -2.06300       -2.42600
F         -3.06600        3.20400       -0.67600
F         -2.49600        2.37800        1.25500
F         -4.31100        1.68400        0.27300
F          1.41500       -1.66700       -2.66400
F          0.20300       -3.18500       -1.67100
F         -0.39300       -2.41700       -3.61800
E(corrected)= -1808.66429722

Dimer 7,7
Fluorobenzene fluorobenzene
C          1.72100       -1.09500        0.00300
C          1.82800       -0.43500        1.22100
C          2.05600        0.94200        1.21100
C          2.17400        1.63100        0.00200
C          2.06600        0.94000       -1.20700
C          1.83900       -0.43800       -1.21500
H          1.72900       -0.99600        2.14500
H          2.14000        1.47700        2.15400
H          2.34600        2.70400        0.00200
H          2.15900        1.47200       -2.15000
H          1.74800       -1.00100       -2.13900
C         -2.17400       -1.63100       -0.00200
C         -2.06600       -0.94000        1.20700
C         -1.83900        0.43800        1.21500
C         -1.72100        1.09500       -0.00300
C         -1.82800        0.43500       -1.22100
C         -2.05600       -0.94200       -1.21100
H         -2.34600       -2.70400       -0.00200
H         -2.15900       -1.47200        2.15000
H         -1.74800        1.00100        2.13900
H         -1.72900        0.99600       -2.14500
H         -2.14000       -1.47700       -2.15400
F          1.49800       -2.43600        0.00300
F         -1.49800        2.43600       -0.00300


Dimer 1,7
Benzene fluorobenzene dimer
C         -1.65400        0.51700       -1.21800
C         -1.37400        1.12400       -0.00000
C         -1.65500        0.51800        1.21800
C         -2.24000       -0.74900        1.20900
C         -2.53300       -1.38500        0.00000
C         -2.23900       -0.75000       -1.20900
H         -1.41300        1.03400       -2.14200
H         -1.41500        1.03500        2.14100
H         -2.46800       -1.23900        2.15300
H         -2.99000       -2.37100        0.00000
H         -2.46600       -1.24100       -2.15200
C          2.30500        0.33100       -1.20900
C          2.50800        1.00000        0.00000
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C          2.30400        0.33200        1.20900
C          1.89700       -1.00400        1.21000
C          1.69200       -1.67200        0.00100
C          1.89700       -1.00500       -1.20900
H          2.46400        0.85100       -2.15100
H          2.82100        2.04100       -0.00000
H          2.46200        0.85300        2.15100
H          1.73600       -1.52400        2.15200
H          1.37100       -2.71100        0.00100
H          1.73800       -1.52500       -2.15000
F         -0.81100        2.36100       -0.00100
E(corrected)= -562.14352484

1,8
13diflurobenzene benzene
C          1.01800        0.00000       -1.12200
C          1.40600       -1.18300       -0.50800
C          2.16600       -1.21600        0.65500
C          2.54000       -0.00100        1.23300
C          2.16700        1.21400        0.65600
C          1.40800        1.18300       -0.50800
H          0.41100        0.00100       -2.02000
H          2.44500       -2.17000        1.09000
H          3.13600       -0.00100        2.14200
H          2.44700        2.16800        1.09000
C         -2.75300        0.00200       -0.92100
C         -2.46300       -1.20900       -0.28700
C         -1.88300       -1.21000        0.98300
C         -1.59400       -0.00100        1.62000
C         -1.88200        1.20900        0.98500
C         -2.46200        1.21100       -0.28500
H         -3.20700        0.00300       -1.91000
H         -2.68700       -2.15000       -0.78300
H         -1.65600       -2.15300        1.47600
H         -1.13900       -0.00200        2.60800
H         -1.65400        2.15100        1.48000
H         -2.68500        2.15400       -0.77900
F          1.03100       -2.35600       -1.07800
F          1.03400        2.35700       -1.07700
E(corrected)= -661.20356564

Dimer 1,9
135trifluorobenzene and benzene
C         -1.51800        0.80500        1.16000
C         -1.51100       -0.58200        1.23800
C         -1.51800       -1.40700        0.12000
C         -1.51700       -0.78100       -1.12000
C         -1.52300        0.60000       -1.27500
C         -1.51600        1.36100       -0.11300
H         -1.50700        1.42300        2.05000
H         -1.50800       -2.48700        0.21100
H         -1.51700        1.06100       -2.25600
C          2.37900        0.79800        1.14400
C          2.38000       -0.59400        1.26100
C          2.37800       -1.39100        0.11400
C          2.37500       -0.79600       -1.15000
C          2.37400        0.59600       -1.26600
C          2.37500        1.39300       -0.12000
H          2.38200        1.41900        2.03700
H          2.38400       -1.05700        2.24500
H          2.38200       -2.47400        0.20500
H          2.37500       -1.41700       -2.04300
H          2.37300        1.05900       -2.25100
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H          2.37500        2.47700       -0.21100
F         -1.50000       -1.15900        2.46300
F         -1.51000        2.71000       -0.22600
F         -1.51100       -1.55400       -2.23200
E(corrected)=-760.25876491

10,10
Toluene and toluene
C         -1.69600       -1.03800       -1.30000
C         -1.17700        0.24700       -1.13300
C         -1.74800        1.13900       -0.21700
C         -2.85600        0.71400        0.52700
C         -3.37900       -0.57100        0.36600
C         -2.80200       -1.45000       -0.55200
H         -0.30200        0.55300       -1.70500
H         -3.30900        1.39400        1.24700
H         -3.20700       -2.45200       -0.68000
C          2.00500       -1.41000       -0.16600
C          2.85200       -0.81400       -1.10100
C          3.25400        0.51400       -0.93700
C          2.80900        1.23400        0.17400
C          1.96200        0.63100        1.10500
C          1.54800       -0.69800        0.95000
H          1.69700       -2.44600       -0.30000
H          3.20000       -1.38600       -1.95900
H          3.91700        0.97900       -1.66200
H          3.12500        2.26500        0.31700
H          1.62100        1.19800        1.97000
C         -1.20400        2.53700       -0.07100
H         -4.23700       -0.88300        0.95600
H         -1.23500       -1.71800       -2.01200
C          0.58500       -1.32500        1.92300
H          0.75700       -2.40300        2.00800
H          0.69000       -0.88600        2.92000
H         -0.44900       -1.17500        1.59500
H         -0.11700        2.54400       -0.18500
H         -1.62600        3.20600       -0.82900
H         -1.44800        2.95400        0.91100
E(corrected)=-541.47242908

12,12
Orthoxylene orthoxylene dimer
C          3.37900        0.10600       -1.21200
C          3.10400       -1.23100       -0.92200
C          2.28000       -1.54400        0.16100
C          1.71800       -0.54400        0.96100
C          1.99800        0.80700        0.67000
C          2.82800        1.11100       -0.41500
H          4.02200        0.36500       -2.05000
H          3.53100       -2.02500       -1.53000
H          2.06700       -2.58800        0.38900
H          3.04500        2.15400       -0.63900
C         -1.66200       -0.64400       -0.74300
C         -2.76800       -0.26500        0.04600
C         -3.06800        1.09500        0.19000
C         -2.29600        2.07700       -0.43400
C         -1.20100        1.70000       -1.21100
C         -0.89000        0.34700       -1.35900
H         -3.92200        1.38800        0.79800
H         -0.02600        0.05500       -1.95200
C          1.39900        1.90800        1.50300
C          0.81000       -0.90500        2.10600
H         -2.54900        3.12700       -0.31200
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H          -0.58700        2.45400       -1.69800
C          -3.61700       -1.30700        0.72600
C          -1.31700       -2.09800       -0.92900
H           1.74100        2.88600        1.15300
H           1.67800        1.81100        2.55900
H           0.30500        1.89200        1.44800
H           1.17800       -0.50200        3.05600
H          -0.19800       -0.50200        1.95000
H           0.73100       -1.99100        2.21000
H          -1.12700       -2.59200        0.03000
H          -2.13200       -2.64400       -1.41700
H          -0.41900       -2.20400       -1.54300
H          -4.42800       -0.83800        1.28900
H          -3.02800       -1.91300        1.42400
H          -4.06500       -1.99600        0.00100
E(corrected)= -619.86141357

12,12
Metaxylene and metaxylene
C          -2.54900       -0.05800       -1.43800
C          -2.29000        1.17300       -0.83300
C          -1.76800        1.22900        0.46500
C          -1.52000        0.02800        1.13700
C          -1.77600       -1.21500        0.55000
C          -2.29400       -1.24500       -0.75100
H          -2.50700       -2.20200       -1.22400
C           1.51900        0.03000       -1.13700
C           1.76600        1.23200       -0.46500
C           2.28800        1.17600        0.83300
C           2.54900       -0.05400        1.43800
C           2.29600       -1.24200        0.75100
C           1.77800       -1.21300       -0.55000
H           1.10400        0.06200       -2.14500
H           2.49200        2.10000        1.37100
H           2.95700       -0.08700        2.44700
H           2.51100       -2.19900        1.22400
C           1.46900       -2.48500       -1.29500
H          -2.49600        2.09700       -1.37200
H          -1.10500        0.06100        2.14500
C          -1.46400       -2.48700        1.29500
C          -1.51100        2.54800        1.14700
H          -2.95600       -0.09100       -2.44700
C           1.50600        2.55000       -1.14700
H          -1.94500       -3.34900        0.82400
H          -0.38500       -2.66900        1.31900
H          -1.81200       -2.43100        2.33200
H          -2.28600        2.77000        1.88800
H          -1.49700        3.36900        0.42400
H          -0.54800        2.53500        1.66600
H           1.95200       -3.34600       -0.82400
H           1.81400       -2.42900       -2.33200
H           0.38900       -2.67100       -1.31700
H           2.28100        2.77200       -1.88900
H           0.54300        2.53600       -1.66600
H           1.49200        3.37100       -0.42400
E(corrected)= -619.86004409

14,14
Pyridine pyridine
C          -1.55700        1.13500        0.91400
C          -1.28200       -0.11700        1.46500
C          -1.68000       -1.25700        0.76800
C          -2.33900       -1.09100       -0.44900
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C         -2.56700        0.20300       -0.91800
H         -0.76100       -0.19400        2.41600
H         -2.67100       -1.94800       -1.03000
C          2.34000        1.09000        0.45100
C          2.56700       -0.20500        0.91700
C          1.55600       -1.13400       -0.91600
C          1.28200        0.11900       -1.46500
C          1.68100        1.25800       -0.76700
H          2.67300        1.94600        1.03200
H          3.07800       -0.37000        1.86500
H          1.25700       -2.04200       -1.43600
H          0.76100        0.19800       -2.41500
H         -3.07800        0.36700       -1.86500
H         -1.25900        2.04400        1.43400
N         -2.18800        1.31400       -0.26000
N          2.18700       -1.31500        0.25800
H         -1.47700       -2.24900        1.16300
H          1.47900        2.25000       -1.16000
E(corrected)=-495.13506947

Dimer 14,14
4CF3pyridine 4CF3pyridine
C          0.23900        1.61300       -1.32600
C          1.29800        0.70500       -1.28800
C          2.09100        0.67300       -0.14300
C          1.80700        1.54600        0.90800
C          0.72800        2.41500        0.76600
H          1.49200        0.03800       -2.12200
H          2.40600        1.54400        1.81500
C         -1.80600       -1.54700       -0.90700
C         -0.72600       -2.41500       -0.76200
C         -0.24000       -1.61000        1.32900
C         -1.30000       -0.70300        1.28900
C         -2.09100       -0.67300        0.14300
H         -2.40400       -1.54700       -1.81400
H         -0.46900       -3.11300       -1.55800
H          0.40700       -1.66200        2.20300
H         -1.49500       -0.03500        2.12200
C          3.27700       -0.23800       -0.04400
F          4.43200        0.44600       -0.22900
F          3.35300       -0.81300        1.17900
F          3.24200       -1.22500       -0.96300
H          0.47200        3.11200        1.56200
H         -0.40800        1.66600       -2.19900
C         -3.27700        0.23700        0.04200
F         -4.43200       -0.44800        0.22500
F         -3.24400        1.22400        0.96100
F         -3.35100        0.81200       -1.18100
N         -0.05700        2.46300       -0.32700
N          0.05800       -2.46100        0.33100
E(corrected)=-1167.91961475


Dimer 15,15
4fluoropyridine 4fluoropyridine
C         -1.04100       -1.12300       -1.29300
C         -1.42100        0.21800       -1.26300
C         -2.17600        0.63600       -0.17700
C         -2.53300       -0.25400        0.82600
C         -2.09600       -1.57200        0.69000
H         -1.13900        0.91600       -2.04400
H         -3.12600        0.07200        1.67400
C          2.53200        0.25700       -0.82600
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C          2.09400        1.57500       -0.68600
C          1.04100        1.12000        1.29500
C          1.42200       -0.22100        1.26200
C          2.17700       -0.63600        0.17400
H          3.12600       -0.06600       -1.67500
H          2.34900        2.31500       -1.44300
H          0.44800        1.49600        2.12700
H          1.14100       -0.92100        2.04200
H         -2.35100       -2.31000        1.44800
H         -0.44800       -1.50200       -2.12300
N         -1.36100       -2.02200       -0.34300
N          1.36000        2.02100        0.34800
F         -2.57200        1.92500       -0.09400
F          2.57300       -1.92500        0.08800
```

E(corrected)= -693.25337795

Dimer 16,16
Methylpyridine methylpyridine

```
C         -1.07200       -1.31200       -1.28300
C         -1.42400        0.03600       -1.29200
C         -2.05900        0.59400       -0.17800
C         -2.31300       -0.26700        0.89400
C         -1.92600       -1.60500        0.81400
H         -1.19700        0.64900       -2.16200
H         -2.81000        0.10000        1.79000
C          2.31300        0.26700       -0.89400
C          1.92600        1.60500       -0.81300
C          1.07200        1.31100        1.28400
C          1.42400       -0.03700        1.29200
C          2.05900       -0.59400        0.17700
H          2.81000       -0.09900       -1.79000
H          2.12100        2.28500       -1.64200
H          0.57600        1.75500        2.14600
H          1.19700       -0.65000        2.16100
H         -2.12100       -2.28400        1.64300
H         -0.57600       -1.75600       -2.14500
N         -1.30600       -2.14400       -0.25100
N          1.30600        2.14300        0.25200
C          2.40100       -2.05700        0.12700
H          2.87700       -2.38000        1.05700
H          1.49200       -2.65200       -0.00900
H          3.08300       -2.27400       -0.70000
C         -2.40100        2.05700       -0.12800
H         -1.49100        2.65200        0.00700
H         -2.87700        2.38000       -1.05900
H         -3.08300        2.27500        0.69800
```

E(corrected)= -573.52676339

All of the following dimers were optimized and energy extracted from B97D/TZV

Dimer 18,18
Bipyridine bipyridine

```
C          0.74500       -1.83800        0.00800
C          1.46200       -1.81200        1.22100
C          2.85900       -1.83200        1.18600
C          3.51400       -1.87200       -0.05400
C          2.73100       -1.88800       -1.21700
N          1.37700       -1.87300       -1.20500
H          0.91200       -1.77600        2.15500
H          4.59800       -1.88600       -0.12200
H          3.19400       -1.91300       -2.20100
C         -0.74300       -1.83800       -0.00700
C         -1.45900       -1.81300       -1.22100
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```
N          -1.37400       -1.87400        1.20500
C          -2.85600       -1.83500       -1.18500
H          -0.91000       -1.77700       -2.15500
C          -2.72900       -1.89000        1.21700
C          -3.51100       -1.87500        0.05400
H          -3.19100       -1.91500        2.20100
H          -4.59600       -1.88900        0.12200
H          -3.42700       -1.81600       -2.11100
H           3.42900       -1.81300        2.11100
C           0.74300        1.83800        0.00700
C           1.45900        1.81300        1.22100
C           2.85700        1.83500        1.18500
C           3.51100        1.87400       -0.05400
C           2.72800        1.89000       -1.21700
N           1.37400        1.87400       -1.20500
H           0.91000        1.77700        2.15500
H           4.59600        1.88900       -0.12300
H           3.19100        1.91500       -2.20100
C          -0.74500        1.83800       -0.00700
C          -1.46200        1.81200       -1.22100
N          -1.37700        1.87300        1.20500
C          -2.85900        1.83200       -1.18500
H          -0.91300        1.77600       -2.15500
C          -2.73100        1.88800        1.21700
C          -3.51400        1.87200        0.05400
H          -3.19400        1.91300        2.20100
H          -4.59800        1.88500        0.12200
H          -3.42900        1.81300       -2.11100
H           3.42700        1.81600        2.11100
E(H)=-990.05448715

Dimer 19,19
4CF3bipyridine 4CF3bipyridine
C           0.74300        0.03000       -1.74000
C           1.50000       -1.14500       -1.58500
C           2.89200       -1.04100       -1.54700
C           3.50400        0.21300       -1.67200
C           2.67500        1.33100       -1.83200
N           1.32400        1.26000       -1.86000
H           0.99600       -2.09800       -1.48900
H           4.58200        0.32100       -1.63900
H           3.10300        2.32400       -1.93000
C          -0.74000       -0.02100       -1.74000
C          -1.49600        1.15400       -1.58200
N          -1.32100       -1.25100       -1.86300
C          -2.88800        1.05000       -1.54500
H          -0.99200        2.10600       -1.48400
C          -2.67200       -1.32100       -1.83500
C          -3.50100       -0.20300       -1.67200
H          -3.10100       -2.31300       -1.93600
H          -4.57900       -0.31100       -1.64000
C           0.43800        0.59500        1.42200
C           1.83800        0.46100        1.50000
C           2.61300        1.62100        1.46500
C           1.99700        2.87800        1.37000
C           0.60100        2.91800        1.30000
N          -0.17500        1.80800        1.32700
H           2.28400       -0.52300        1.57200
H           2.58400        3.79000        1.34000
H           0.07400        3.86400        1.22000
C          -0.44100       -0.60200        1.41900
C          -1.84100       -0.46900        1.49900
N           0.17300       -1.81500        1.31700
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```
C         -2.61500       -1.62900        1.45800
H         -2.28700        0.51400        1.57600
C         -0.60300       -2.92500        1.28500
C         -1.99900       -2.88600        1.35600
H         -0.07600       -3.87100        1.19900
H         -2.58600       -3.79700        1.32100
C         -3.70900        2.28500       -1.28700
C          3.71200       -2.27700       -1.29200
C          4.11200        1.55600        1.56800
C         -4.11400       -1.56500        1.56200
F         -5.03800        2.15400       -1.71700
F         -3.76100        2.59600        0.08800
F         -3.18300        3.42100       -1.92600
F          3.19700       -3.40500       -1.95500
F          3.74200       -2.60700        0.07900
F          5.04700       -2.13900       -1.70000
F          4.62600        0.26700        1.38800
F          4.57400        2.01000        2.81800
F          4.73800        2.37900        0.60200
F         -4.57700       -2.02900        2.80800
F         -4.74000       -2.38100        0.58900
F         -4.62900       -0.27500        1.39100
E(H)= -2337.82734451



Dimer 20,20
4fluorobipyridine 4fluorobipyridine
C          0.72200       -1.80300       -0.17800
C          1.70600       -1.77300        0.83000
C          3.03100       -1.78600        0.42200
C          3.39400       -1.82500       -0.92200
C          2.34400       -1.84900       -1.85200
N          1.03500       -1.83900       -1.50800
H          1.42400       -1.74000        1.87500
H          4.43400       -1.83500       -1.22600
H          2.55500       -1.87600       -2.91800
C         -0.72100       -1.80400        0.17900
C         -1.70500       -1.77400       -0.82900
N         -1.03300       -1.83800        1.50800
C         -3.03000       -1.78700       -0.42100
H         -1.42300       -1.74200       -1.87400
C         -2.34300       -1.84800        1.85300
C         -3.39300       -1.82500        0.92300
H         -2.55400       -1.87500        2.91800
H         -4.43300       -1.83500        1.22600
C          0.72100        1.80400       -0.17900
C          1.70500        1.77400        0.82900
C          3.03000        1.78700        0.42100
C          3.39300        1.82500       -0.92300
C          2.34300        1.84800       -1.85300
N          1.03300        1.83800       -1.50800
H          1.42300        1.74200        1.87400
H          4.43300        1.83600       -1.22700
H          2.55400        1.87600       -2.91800
C         -0.72200        1.80400        0.17900
C         -1.70600        1.77300       -0.83000
N         -1.03500        1.83900        1.50800
C         -3.03100        1.78600       -0.42200
H         -1.42400        1.74000       -1.87400
C         -2.34400        1.84900        1.85200
C         -3.39400        1.82500        0.92300
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H         -2.55500        1.87700        2.91800
H         -4.43400        1.83500        1.22600
F         -4.03900       -1.75300       -1.39200
F          4.04000       -1.75100        1.39200
F          4.03900        1.75300        1.39100
F         -4.04000        1.75100       -1.39200
E(H)=-1386.91893556

Dimer 21,21
4methylbipyridine 4methylbipyridine
C         -1.98800       -1.29000        0.04300
C         -2.96200       -0.85300       -0.87600
C         -4.26400       -0.57500       -0.44100
C         -4.54800       -0.74700        0.92800
C         -3.53400       -1.20000        1.77900
N         -2.27300       -1.47300        1.36600
H         -2.68000       -0.73000       -1.91600
H         -5.54100       -0.54000        1.32100
H         -3.72700       -1.35300        2.83900
C         -0.59000       -1.55500       -0.39500
C          0.39600       -1.94100        0.52800
N         -0.31600       -1.38900       -1.72600
C          1.70900       -2.18000        0.09200
H          0.12700       -2.03400        1.57400
C          0.95500       -1.61300       -2.13500
C          1.98500       -2.01200       -1.27500
H          1.14500       -1.45700       -3.19400
H          2.99000       -2.16600       -1.66000
C          0.59100        1.55300        0.40000
C         -0.40100        1.94200       -0.51700
C         -1.71000        2.18000       -0.07300
C         -1.97900        2.00800        1.29500
C         -0.94400        1.60600        2.14800
N          0.32500        1.38300        1.73100
H         -0.13700        2.03900       -1.56400
H         -2.98100        2.16100        1.68700
H         -1.12800        1.44700        3.20800
C          1.98600        1.29000       -0.04700
C          2.96700        0.85400        0.86500
N          2.26300        1.47500       -1.37200
C          4.26600        0.57600        0.42200
H          2.69200        0.73100        1.90700
C          3.52200        1.20200       -1.79300
C          4.54200        0.74900       -0.94900
H          3.70800        1.35600       -2.85500
H          5.53300        0.54300       -1.34800
C          2.78000       -2.61700        1.06700
H          2.69000       -2.07200        2.01500
H          2.68800       -3.69000        1.29100
H          3.78100       -2.44100        0.65700
C         -5.33300       -0.11100       -1.40800
H         -4.89600        0.17100       -2.37300
H         -6.06800       -0.90900       -1.59000
H         -5.88200        0.75200       -1.00800
C         -2.78700        2.62100       -1.04000
H         -2.69800        3.69500       -1.25800
H         -2.70100        2.08200       -1.99100
H         -3.78600        2.44000       -0.62600
C          5.34200        0.11200        1.38200
H          6.07600        0.91100        1.56200
H          4.91000       -0.17300        2.34800
H          5.89000       -0.74800        0.97600
E(H)=-1147.23068817
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5. complete list of reference 57.

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