Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting information

A Theoretical Exploration of Amine···π Interactions

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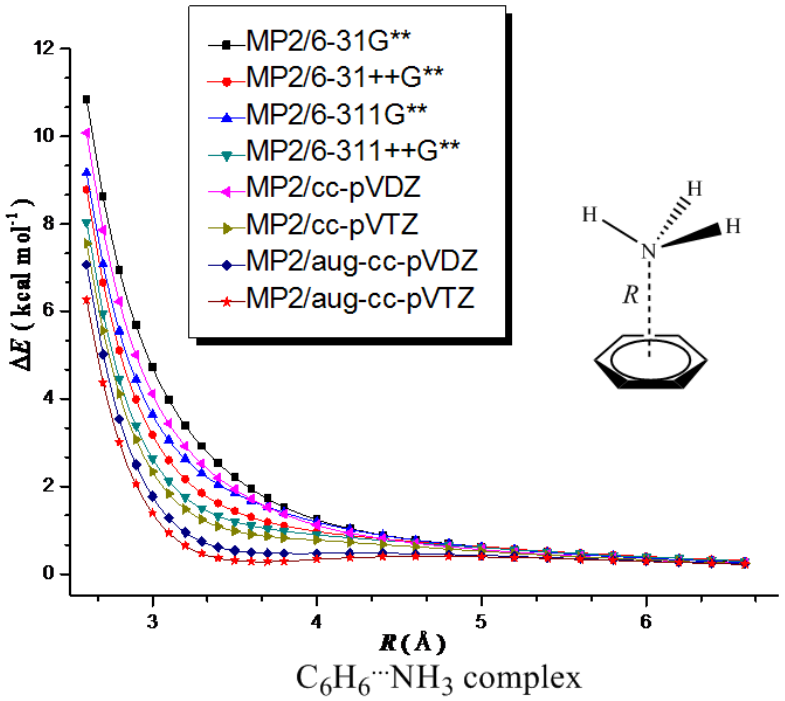

Fig. S1 BSSE corrected MP2 intermolecular interaction potentials of C_6H_6 ···NH_3 complex calculated with eight basis sets.

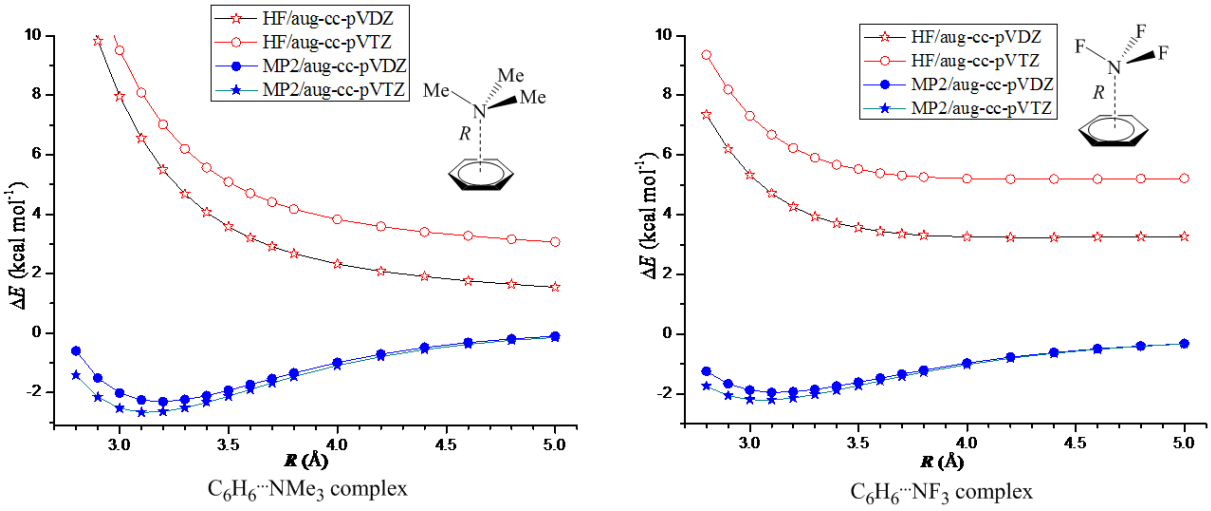

Fig. S2 The comparison of HF and MP2 intermolecular interaction potentials of $C_6H_6\cdots NMe_3$ and $C_6H_6\cdots NF_3$ complex calculated with aug-cc-pVDZ and aug-cc-pVTZ basis sets.

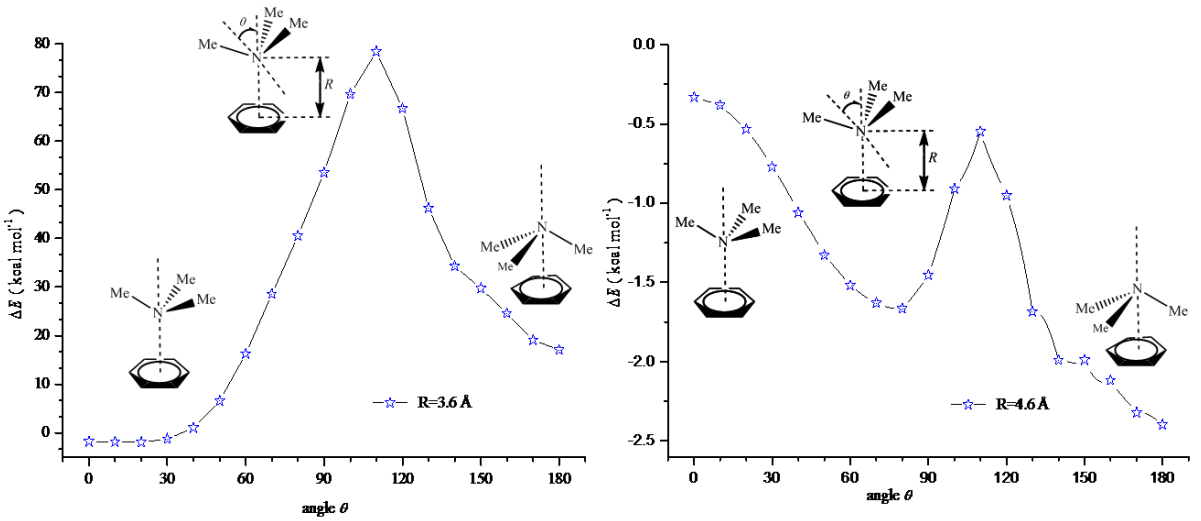

Fig. S3 The orientation dependence of the MP2/aug-cc-pVDZ interaction energy for $C_6H_6\cdots NMe_3$ complex.

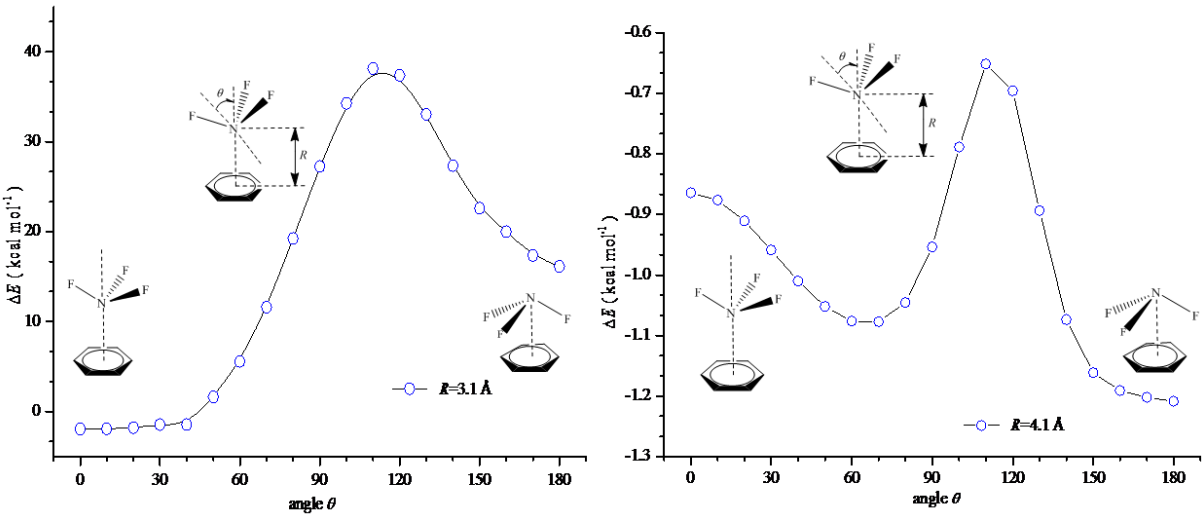

Fig. S4 The orientation dependence of the MP2/aug-cc-pVDZ interaction energy for $C_6H_6\cdots NF_3$ complex.

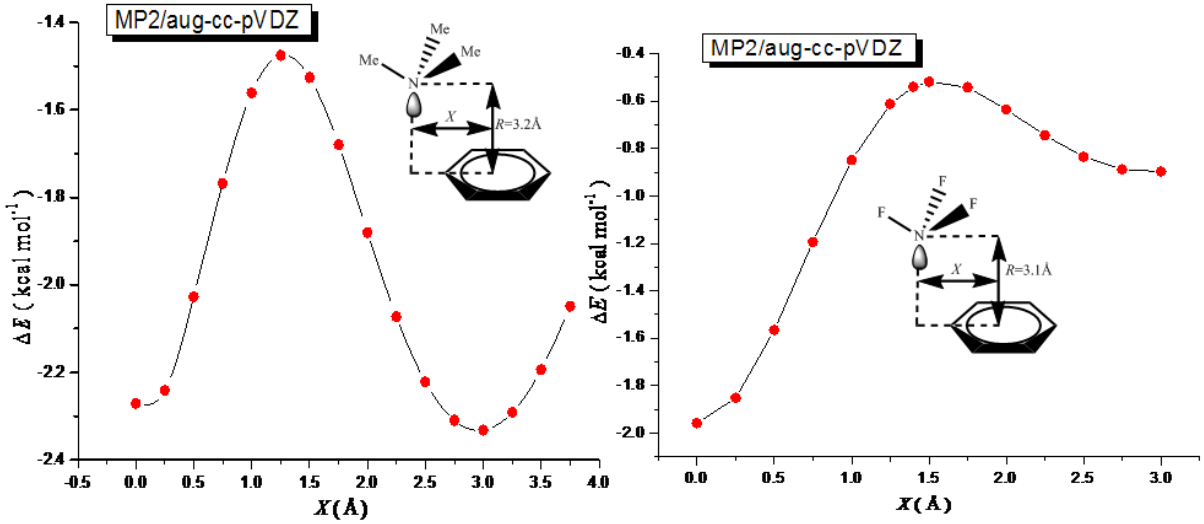

Fig. S5 Calculated interaction energies with changing horizontal displacements (X, Å) of the $C_6H_6\cdots NMe_3$ and $C_6H_6\cdots NF_3$ complexes. The vertical distances are fixed at 3.2 and 3.1 Å, respectively.

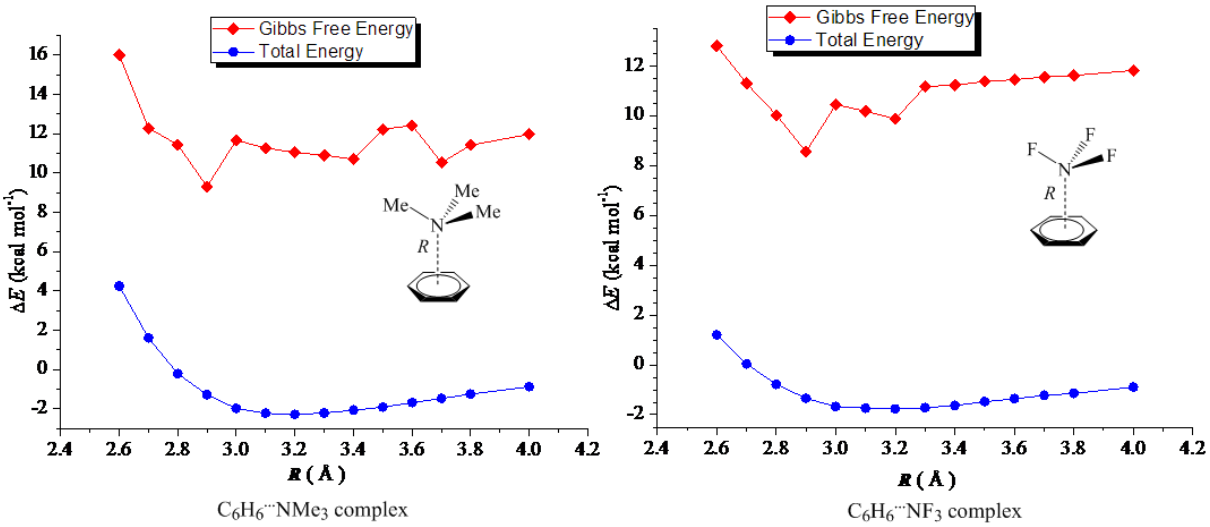

Fig. S6 The comparison of BSSE corrected Gibbs free energy and total energy potentials of $C_6H_6\cdots NMe_3$ and $C_6H_6\cdots NF_3$ complex at the MP2/aug-cc-pVDZ level.

Coordinates and thermodynamic data of the four studied complexes

1. $C_6H_6 \cdots NMe_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.405849
2	6	0	0.000000	1.375132	-0.066055
3	1	0	0.886977	1.892538	0.310304
4	1	0	-0.886977	1.892538	0.310304
5	1	0	0.000000	1.441438	-1.171260
6	6	0	1.190899	-0.687566	-0.066055
7	1	0	1.195498	-1.714414	0.310304
8	1	0	2.082475	-0.178124	0.310304
9	1	0	1.248322	-0.720719	-1.171260
10	6	0	-1.190899	-0.687566	-0.066055
11	1	0	-2.082475	-0.178124	0.310304
12	1	0	-1.195498	-1.714414	0.310304
13	1	0	-1.248322	-0.720719	-1.171260

Sum of electronic and zero-point Energies= -173.810548
Sum of electronic and thermal Energies= -173.804397
Sum of electronic and thermal Enthalpies= -173.803453
Sum of electronic and thermal Free Energies= -173.838803

2. $C_6H_6 \cdots NF_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.399110	-1.599709
2	6	0	1.211659	0.699552	-1.599709
3	6	0	1.211665	-0.699555	-1.599709
4	6	0	0.000000	-1.399103	-1.599709
5	6	0	-1.211665	-0.699555	-1.599709
6	6	0	-1.211659	0.699552	-1.599709
7	1	0	0.000000	2.485480	-1.599709
8	1	0	2.152490	1.242741	-1.599709
9	1	0	2.152489	-1.242740	-1.599709
10	1	0	0.000000	-2.485481	-1.599709
11	1	0	-2.152489	-1.242740	-1.599709
12	1	0	-2.152490	1.242741	-1.599709
13	7	0	0.000000	0.000000	1.500291
14	9	0	0.000000	1.228200	2.099471
15	9	0	-1.063652	-0.614100	2.099471
16	9	0	1.063652	-0.614100	2.099471

Sum of electronic and zero-point Energies= -584.820649
Sum of electronic and thermal Energies= -584.814444
Sum of electronic and thermal Enthalpies= -584.813500
Sum of electronic and thermal Free Energies= -584.851992

3. $C_6F_6\cdots NMe_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.394309	-0.933862
2	6	0	1.207507	0.697154	-0.933862
3	6	0	1.207507	-0.697155	-0.933862
4	6	0	0.000000	-1.394309	-0.933862
5	6	0	-1.207507	-0.697155	-0.933862
6	6	0	-1.207507	0.697154	-0.933862
7	9	0	0.000000	-2.725637	-0.933862
8	9	0	2.360471	-1.362819	-0.933862
9	9	0	2.360471	1.362818	-0.933862
10	9	0	0.000000	2.725637	-0.933862
11	9	0	-2.360471	1.362818	-0.933862
12	9	0	-2.360471	-1.362819	-0.933862
13	7	0	0.000000	0.000000	2.066138
14	6	0	0.000000	1.375132	2.538042
15	1	0	-0.886977	1.892538	2.161683
16	1	0	0.886977	1.892538	2.161683
17	1	0	0.000000	1.441438	3.643247
18	6	0	-1.190899	-0.687566	2.538042
19	1	0	-1.195498	-1.714413	2.161683
20	1	0	-2.082474	-0.178125	2.161683
21	1	0	-1.248322	-0.720719	3.643247
22	6	0	1.190899	-0.687566	2.538042
23	1	0	2.082474	-0.178125	2.161683
24	1	0	1.195498	-1.714413	2.161683
25	1	0	1.248322	-0.720719	3.643247

Sum of electronic and zero-point Energies= -999.616174
Sum of electronic and thermal Energies= -999.602104
Sum of electronic and thermal Enthalpies= -999.601160
Sum of electronic and thermal Free Energies= -999.656440

4. $C_6F_6 \cdots NF_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.394309	-0.980389
2	6	0	1.207507	0.697154	-0.980389
3	6	0	1.207507	-0.697155	-0.980389
4	6	0	0.000000	-1.394309	-0.980389
5	6	0	-1.207507	-0.697155	-0.980389
6	6	0	-1.207507	0.697154	-0.980389
7	9	0	0.000000	-2.725637	-0.980389
8	9	0	2.360471	-1.362819	-0.980389
9	9	0	2.360471	1.362818	-0.980389
10	9	0	0.000000	2.725637	-0.980389
11	9	0	-2.360471	1.362818	-0.980389
12	9	0	-2.360471	-1.362819	-0.980389
13	7	0	0.000000	0.000000	2.119611
14	9	0	0.000000	1.228203	2.718434
15	9	0	-1.063655	-0.614102	2.718434
16	9	0	1.063655	-0.614102	2.718434

Sum of electronic and zero-point Energies= -1179.168161
Sum of electronic and thermal Energies= -1179.156632
Sum of electronic and thermal Enthalpies= -1179.155688
Sum of electronic and thermal Free Energies= -1179.206141