

Noncovalent Databases (kcal/mol)

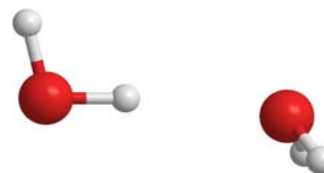
HB6/04		CT7/04		DI6/04		WI7/05		PPS5/05	
Complex	$D_e$	Complex	$D_e$	Complex	$D_e$	Complex	$D_e$	Complex	$D_e$
(NH <sub>3</sub> ) <sub>2</sub>	3.15	C <sub>2</sub> H <sub>4</sub> ...F <sub>2</sub>	1.06	(H <sub>2</sub> S) <sub>2</sub>	1.66	HeNe	0.04	(C <sub>2</sub> H <sub>2</sub> ) <sub>2</sub>	1.34
(HF) <sub>2</sub>	4.57	NH <sub>3</sub> ...F <sub>2</sub>	1.81	(HCl) <sub>2</sub>	2.01	HeAr	0.06	(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub>	1.42
(H <sub>2</sub> O) <sub>2</sub>	4.97	C <sub>2</sub> H <sub>2</sub> ...ClF	3.81	HCl...H <sub>2</sub> S	3.35	Ne <sub>2</sub>	0.08	Sandwich (C <sub>6</sub> H <sub>6</sub> ) <sub>2</sub>	1.81
NH <sub>3</sub> ...H <sub>2</sub> O	6.41	HCN...ClF	4.86	CH <sub>3</sub> Cl...HCl	3.55	NeAr	0.13	T-Shaped (C <sub>6</sub> H <sub>6</sub> ) <sub>2</sub>	2.74
(HCONH <sub>2</sub> ) <sub>2</sub>	14.94	NH <sub>3</sub> ...Cl <sub>2</sub>	4.88	HCN...CH <sub>3</sub> SH	3.59	CH <sub>4</sub> ...Ne	0.22	Parallel-Displaced (C <sub>6</sub> H <sub>6</sub> ) <sub>2</sub>	2.78
(HCOOH) <sub>2</sub>	16.15	H <sub>2</sub> O...ClF	5.36	CH <sub>3</sub> SH...HCl	4.16	C <sub>6</sub> H <sub>6</sub> ...Ne	0.47		
		NH <sub>3</sub> ...ClF	10.62			(CH <sub>4</sub> ) <sub>2</sub>	0.51		
Average	8.37		4.63		3.07		0.22		0.22



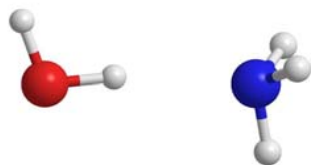
$(\text{NH}_3)_2$



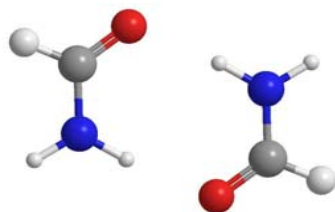
$(\text{HF})_2$



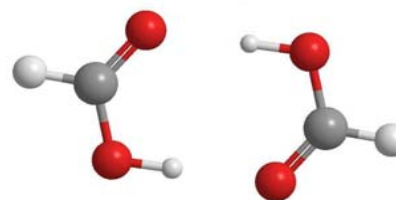
$(\text{H}_2\text{O})_2$



$\text{NH}_3 \cdots \text{H}_2\text{O}$

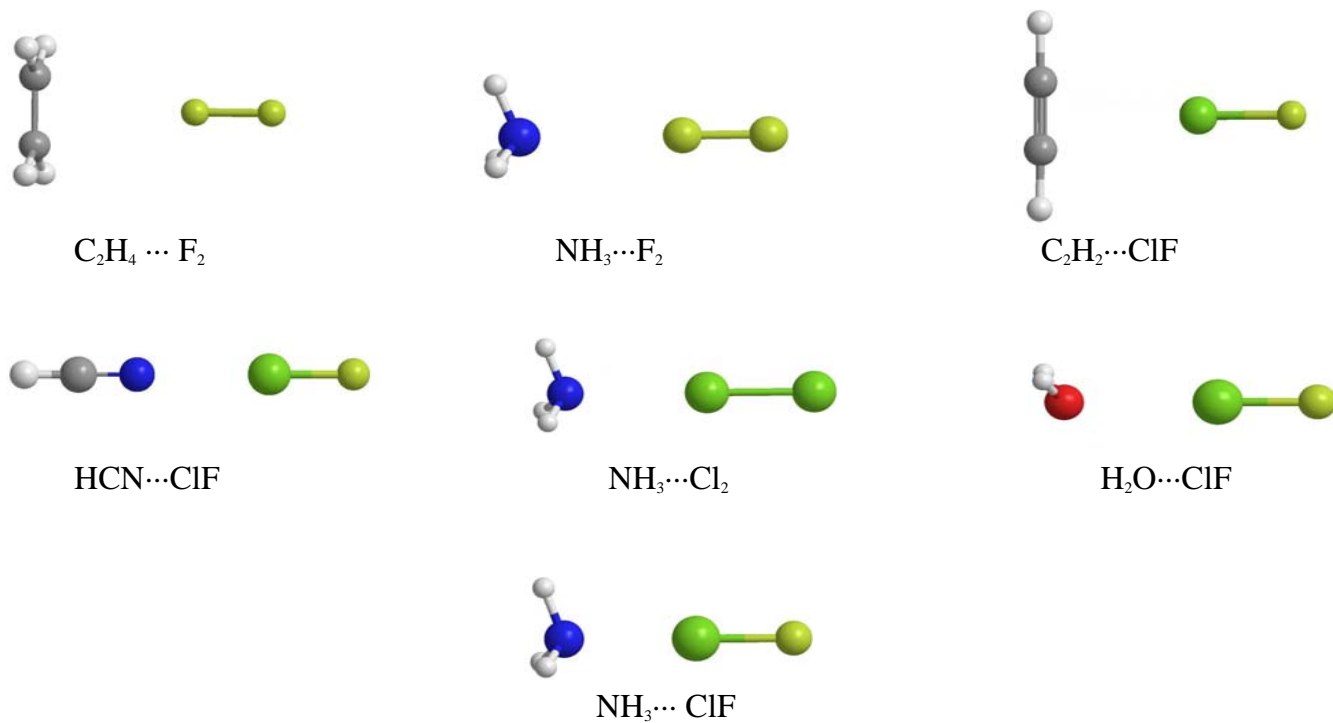


$(\text{HCONH}_2)_2$

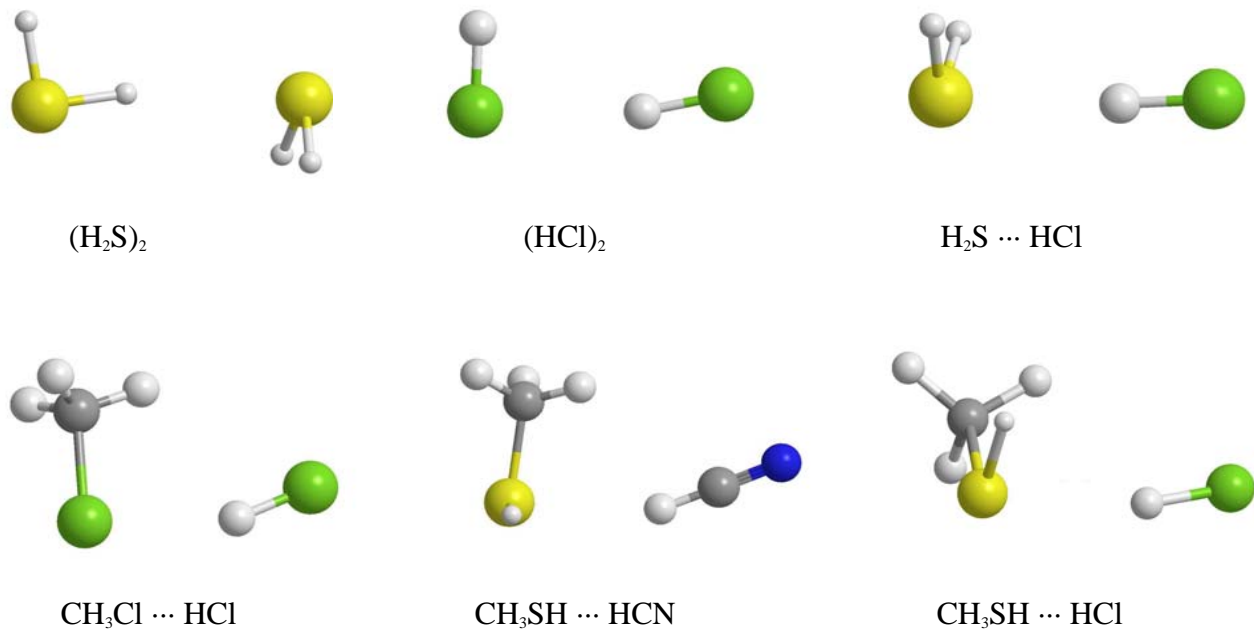


$(\text{HCOOH})_2$

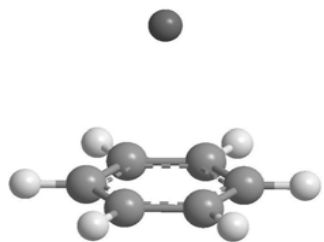
**Figure 1. Geometries of the dimers in the HB6/04 database**



**Figure 2. Geometries of the complexes in the CT7/04 database**



**Figure 3. Geometries of the dimers in the DI6/04 database**



$\text{C}_6\text{H}_6 \cdots \text{Ne}$

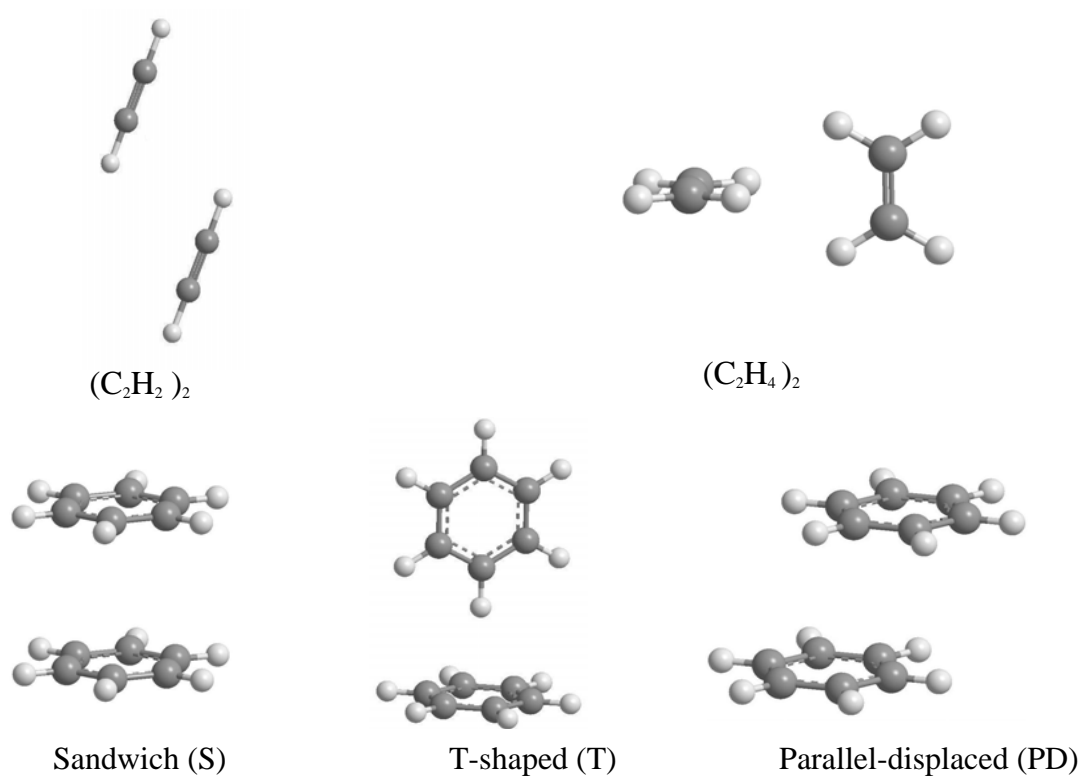


$\text{CH}_4 \cdots \text{Ne}$



$(\text{CH}_4)_2$

**Figure 4. Geometries of selected dimers in the WI7/05 database**



**Figure 5. Geometries of the dimers in the PPS/05 database**