

## ***Supporting Information***

# STACKING INTERACTIONS OF RESONANCE-ASSISTED HYDROGEN-BRIDGED RINGS. A SYSTEMATIC STUDY OF CRYSTAL STRUCTURES AND QUANTUM CHEMICAL CALCULATIONS

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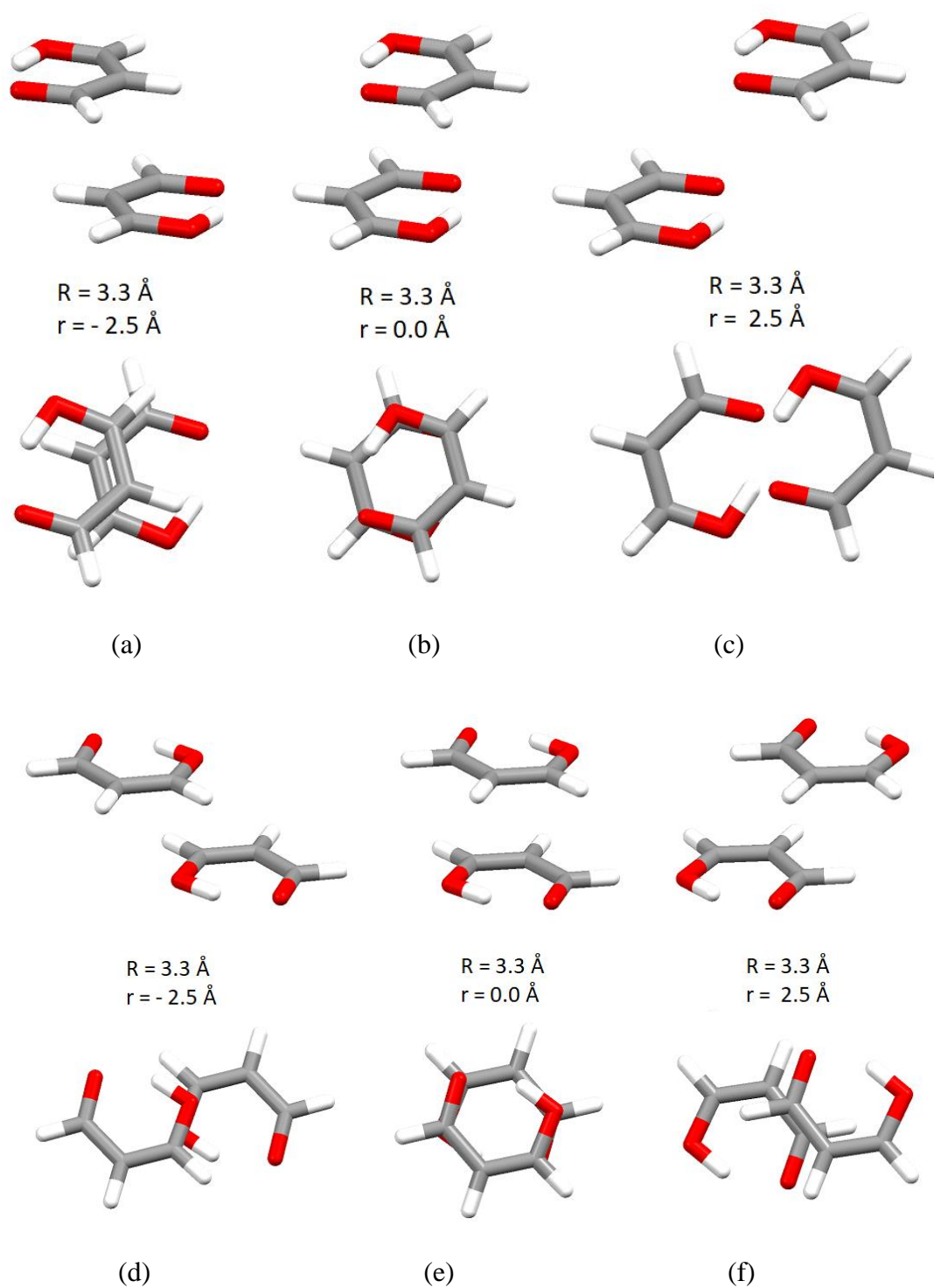
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## **Evaluation of Quantum Chemical Methods for Calculating Stacking Interaction Energies between RAHB Rings**

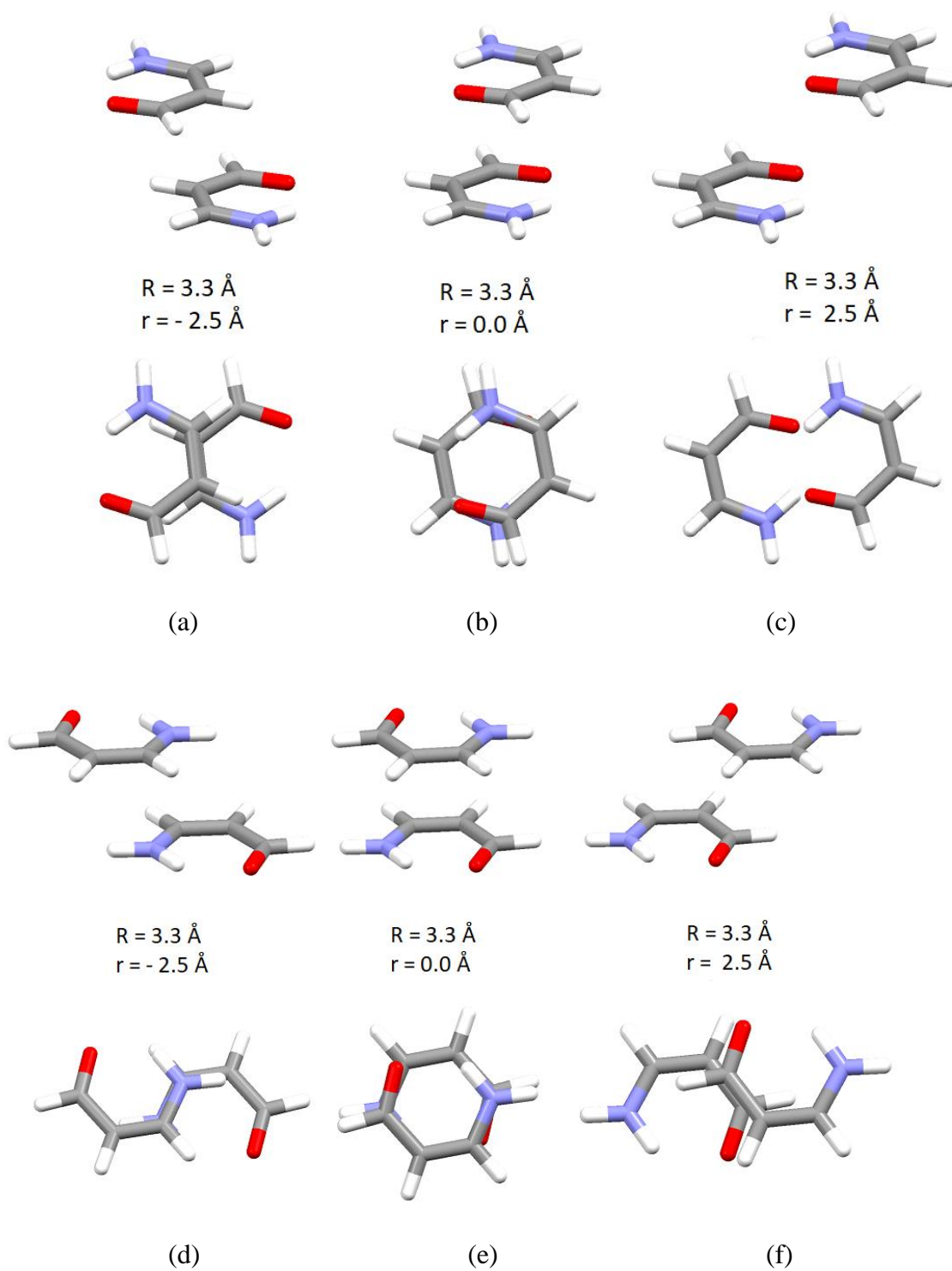
The criterion for reliability of methods for calculating potential energy curves is based on agreement with CCSD(T)/CBS method. Extrapolation to complete basis set (CBS) is performed by method of Mackie and Di Labio<sup>1</sup>.

MP2/aug-cc-pVDZ method is used for potential energy curves calculation, since it is in accord with CCSD(T)/CBS at certain critical points. Geometries corresponding to the selected critical points are shown in Figures S1-S3.

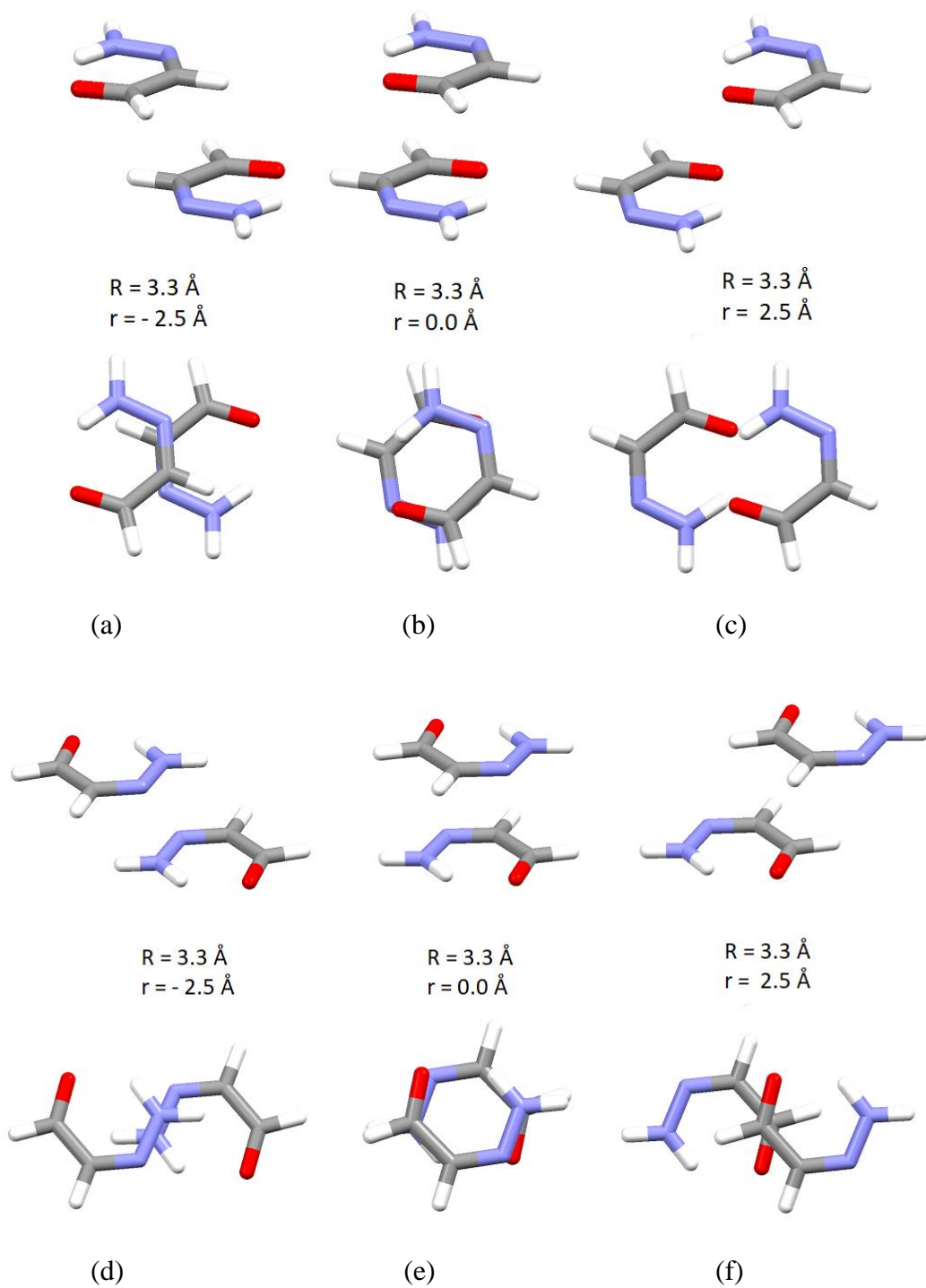
Potential energy curves were calculated in  $\Omega$ -C direction (Figures S1a-c, S2a-c and S3a-c) and in the orthogonal direction in the molecular plane (Figures S1d-f, S2d-f and S3d-f). Critical points, that were used for methods testing, along  $\Omega$ -C direction, correspond to orientation 1 (offset value of -2.5 Å, Figures S1a, S2a and S3a), orientation 2 (sandwich geometry, Figures S1b, S2b and S3b) and orientation 3 (offset value of 2.5 Å, Figures S1c, S1c and S2c). The corresponding geometries of the selected critical points along the direction orthogonal to  $\Omega$ -C are orientation 4 (offset value of -2.5 Å, Figures S1d, S2d and S3d), orientation 3 (sandwich geometry, Figures S1e, S2e and S3e) and orientation 5 (offset value of 2.5 Å, Figures S1f, S2f and S3f). All distances between the ring planes were set to 3.3 Å. The monomers were in antiparallel position. Different methods were tested, including MP2 and some DFT functionals, with D3 correction of Grimme. The basis set effect was also tested. The results are shown in Tables S1-S15.



**Figure S1.** Geometries used for evaluation of methods for calculating interaction energies of  $\text{H}_4\text{C}_3\text{O}_2$  dimer, corresponding to: (a) orientation 1; (b) and (e) orientation 2; (c) orientation 3; (d) orientation 4; (f) orientation 5



**Figure S2.** Geometries used for evaluation of methods for calculating interaction energies of  $\text{H}_5\text{C}_3\text{NO}$  dimer, corresponding to: (a) orientation 1; (b) and (e) orientation 2; (c) orientation 3; (d) orientation 4; (f) orientation 5



**Figure S3.** Geometries used for evaluation of methods for calculating interaction energies of  $\text{H}_4\text{C}_2\text{N}_2\text{O}$  dimer, corresponding to: (a) orientation 1; (b) and (e) orientation 2; (c) orientation 3; (d) orientation 4; (f) orientation 5

**Table S1.** Interaction energies (in kcal/mol) of H<sub>4</sub>C<sub>3</sub>O<sub>2</sub> dimer of orientation 1

orientation 1	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-0.33	-1.67	-2.02	-0.88
TPSS-D3	-2.04	-2.11	-2.25	-2.24
BLYP-D3	-1.93	-2.12	-2.11	-2.11
BP86-D3	-2.15	-2.33	-2.41	-2.36
PBE1PBE-D3	-2.00	-2.14	-2.29	-2.29
M05-D3	-1.78	-1.86	-2.19	-2.21
M06-D3	-1.92	-2.08	-2.49	-2.50
M052X-D3	-1.80	-2.17	-2.34	-2.30
M06HF-D3	-2.17	-2.28	-2.93	-2.88
<b>CCSD(T)/CBS</b>	<b>-2.19</b>			

**Table S2.** Interaction energies (in kcal/mol) of H<sub>4</sub>C<sub>3</sub>O<sub>2</sub> dimer of orientation 2

orientation 2	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-1.48	-3.25	-3.76	-2.59
TPSS-D3	-3.37	-3.59	-3.69	-3.74
BLYP-D3	-3.72	-3.95	-3.96	-3.99
BP86-D3	-3.48	-3.91	-3.95	-3.93
PBE1PBE-D3	-3.47	-3.78	-3.88	-3.95
M05-D3	-3.95	-3.99	-4.46	-4.63
M06-D3	-3.74	-4.08	-4.29	-4.48
M052X-D3	-3.63	-4.31	-4.28	-4.37
M06HF-D3	-3.89	-4.30	-4.66	-4.83
<b>CCSD(T)/CBS</b>	<b>-4.31</b>			

**Table S3.** Interaction energies (in kcal/mol) of H<sub>4</sub>C<sub>3</sub>O<sub>2</sub> dimer of orientation 3

orientation 3	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-0.73	-1.19	-1.56	-1.17
TPSS-D3	-1.82	-1.72	-1.89	-1.88
BLYP-D3	-1.67	-1.49	-1.62	-1.60
BP86-D3	-1.15	-1.16	-1.24	-1.19
PBE1PBE-D3	-1.61	-1.65	-1.78	-1.78
M05-D3	-1.53	-1.79	-2.01	-2.02
M06-D3	-1.67	-1.82	-1.75	-1.85
M052X-D3	-1.34	-1.72	-1.74	-1.77
M06HF-D3	-1.22	-1.38	-1.45	-1.60
<b>CCSD(T)/CBS</b>	<b>-1.67</b>			



**Table S4.** Interaction energies (in kcal/mol) of H<sub>4</sub>C<sub>3</sub>O<sub>2</sub> dimer of orientation 4

orientation 4	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-0.83	-1.64	-2.06	-1.61
TPSS-D3	-2.10	-2.20	-2.35	-2.38
BLYP-D3	-2.05	-2.10	-2.21	-2.23
BP86-D3	-1.60	-1.81	-1.88	-1.86
PBE1PBE-D3	-2.02	-2.24	-2.38	-2.42
M05-D3	-2.12	-2.41	-2.72	-2.78
M06-D3	-2.04	-2.46	-2.57	-2.75
M052X-D3	-1.90	-2.44	-2.49	-2.56
M06HF-D3	-1.84	-2.32	-2.50	-2.72
<b>CCSD(T)/CBS</b>	<b>-2.33</b>			

**Table S5.** Interaction energies (in kcal/mol) of H<sub>4</sub>C<sub>3</sub>O<sub>2</sub> dimer of orientation 5

orientation 5	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-0.83	-2.14	-2.46	-1.43
TPSS-D3	-2.36	-2.47	-2.59	-2.55
BLYP-D3	-2.36	-2.50	-2.51	-2.47
BP86-D3	-2.35	-2.56	-2.64	-2.56
PBE1PBE-D3	-2.37	-2.54	-2.67	-2.62
M05-D3	-2.33	-2.48	-2.81	-2.79
M06-D3	-2.35	-2.65	-2.90	-2.94
M052X-D3	-2.30	-2.72	-2.87	-2.78
M06HF-D3	-2.64	-2.80	-3.31	-3.23
<b>CCSD(T)/CBS</b>	<b>-2.79</b>			

**Table S6.** Interaction energies (in kcal/mol) of H<sub>5</sub>C<sub>3</sub>NO dimer of orientation 1

orientation 1	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-0.14	-1.76	-2.25	-0.83
TPSS-D3	-2.22	-2.35	-2.54	-2.53
BLYP-D3	-2.12	-2.39	-2.39	-2.38
BP86-D3	-2.43	-2.71	-2.86	-2.80
PBE1PBE-D3	-2.08	-2.29	-2.50	-2.50
M05-D3	-1.89	-2.01	-2.42	-2.42
M06-D3	-2.22	-2.51	-3.15	-3.09
M052X-D3	-1.86	-2.31	-2.58	-2.58
M06HF-D3	-2.14	-2.38	-3.14	-3.18
<b>CCSD(T)/CBS</b>	<b>-2.32</b>			

**Table S7.** Interaction energies (in kcal/mol) of H<sub>5</sub>C<sub>3</sub>NO dimer of orientation 2

orientation 2	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-0.47	-2.40	-3.02	-1.42
TPSS-D3	-2.92	-3.16	-3.30	-3.22
BLYP-D3	-3.22	-3.50	-3.48	-3.39
BP86-D3	-3.21	-3.66	-3.77	-3.61
PBE1PBE-D3	-2.79	-3.14	-3.30	-3.23
M05-D3	-3.25	-3.36	-3.85	-3.85
M06-D3	-3.38	-3.87	-4.28	-4.32
M052X-D3	-2.73	-3.39	-3.55	-3.54
M06HF-D3	-2.62	-3.06	-3.57	-3.78
<b>CCSD(T)/CBS</b>	<b>-3.50</b>			

**Table S8.** Interaction energies (in kcal/mol) of H<sub>5</sub>C<sub>3</sub>NO dimer of orientation 3

orientation 3	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-0.70	-1.06	-1.46	-0.81
TPSS-D3	-2.07	-1.85	-1.99	-1.83
BLYP-D3	-1.91	-1.58	-1.69	-1.53
BP86-D3	-1.40	-1.32	-1.41	-1.19
PBE1PBE-D3	-1.71	-1.66	-1.79	-1.62
M05-D3	-1.68	-1.85	-2.06	-1.92
M06-D3	-1.49	-1.62	-1.57	-1.51
M052X-D3	-1.33	-1.51	-1.63	-1.48
M06HF-D3	-0.78	-0.82	-1.00	-0.94
<b>CCSD(T)/CBS</b>	<b>-1.52</b>			

**Table S9.** Interaction energies (in kcal/mol) of H<sub>5</sub>C<sub>3</sub>NO dimer of orientation 4

orientation 4	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-2.25	-3.38	-3.80	-2.84
TPSS-D3	-4.23	-4.28	-4.33	-4.43
BLYP-D3	-4.13	-4.21	-4.09	-4.18
BP86-D3	-4.06	-4.26	-4.27	-4.32
PBE1PBE-D3	-4.17	-4.33	-4.42	-4.50
M05-D3	-4.11	-4.26	-4.54	-4.66
M06-D3	-4.30	-4.63	-5.06	-5.14
M052X-D3	-4.05	-4.46	-4.65	-4.73
M06HF-D3	-4.26	-4.55	-5.09	-5.26
<b>CCSD(T)/CBS</b>	<b>-4.02</b>			

**Table S10.** Interaction energies (in kcal/mol) of H<sub>5</sub>C<sub>3</sub>NO dimer of orientation 5

orientation 5	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-0.06	-1.45	-1.95	-0.89
TPSS-D3	-1.57	-1.74	-1.96	-1.90
BLYP-D3	-1.61	-1.78	-1.90	-1.84
BP86-D3	-1.50	-1.80	-1.99	-1.87
PBE1PBE-D3	-1.48	-1.73	-1.95	-1.90
M05-D3	-1.66	-1.88	-2.34	-2.31
M06-D3	-1.80	-2.18	-2.51	-2.53
M052X-D3	-1.39	-1.89	-2.12	-2.08
M06HF-D3	-1.50	-1.73	-2.32	-2.30
<b>CCSD(T)/CBS</b>	<b>-2.19</b>			

**Table S11.** Interaction energies (in kcal/mol) of H<sub>4</sub>C<sub>2</sub>N<sub>2</sub>O dimer of orientation 1

orientation 1	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-0.33	-1.66	-2.15	-1.14
TPSS-D3	-1.27	-1.38	-1.50	-1.44
BLYP-D3	-1.38	-1.54	-1.50	-1.45
BP86-D3	-1.28	-1.52	-1.58	-1.48
PBE1PBE-D3	-1.12	-1.33	-1.48	-1.44
M05-D3	-1.34	-1.42	-1.85	-1.81
M06-D3	-1.27	-1.39	-1.92	-1.89
M052X-D3	-0.91	-1.33	-1.57	-1.54
M06HF-D3	-1.09	-1.15	-1.84	-1.91
<b>CCSD(T)/CBS</b>	<b>-1.93</b>			



**Table S12.** Interaction energies (in kcal/mol) of H<sub>4</sub>C<sub>2</sub>N<sub>2</sub>O dimer of orientation 2

orientation 2	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	0.62	-0.90	-1.30	0.30
TPSS-D3	-1.11	-1.09	-1.03	-0.82
BLYP-D3	-1.63	-1.52	-1.27	-1.07
BP86-D3	-1.42	-1.57	-1.45	-1.19
PBE1PBE-D3	-0.90	-1.01	-0.98	-0.80
M05-D3	-1.32	-1.21	-1.43	-1.32
M06-D3	-1.59	-1.68	-1.93	-1.91
M052X-D3	-0.78	-1.07	-1.17	-1.04
M06HF-D3	-0.72	-0.78	-1.19	-1.35
<b>CCSD(T)/CBS</b>	<b>-1.62</b>			

**Table S13.** Interaction energies (in kcal/mol) of H<sub>4</sub>C<sub>2</sub>N<sub>2</sub>O dimer of orientation 3

orientation 3	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-0.36	-0.72	-1.00	-0.40
TPSS-D3	-1.73	-1.52	-1.56	-1.46
BLYP-D3	-1.60	-1.29	-1.28	-1.17
BP86-D3	-1.11	-1.02	-1.01	-0.86
PBE1PBE-D3	-1.36	-1.31	-1.35	-1.25
M05-D3	-1.28	-1.43	-1.52	-1.46
M06-D3	-0.99	-1.14	-1.02	-1.04
M052X-D3	-0.97	-1.11	-1.16	-1.07
M06HF-D3	-0.46	-0.50	-0.60	-0.64
<b>CCSD(T)/CBS</b>	<b>-1.08</b>			

**Table S14.** Interaction energies (in kcal/mol) of H<sub>4</sub>C<sub>2</sub>N<sub>2</sub>O dimer of orientation 4

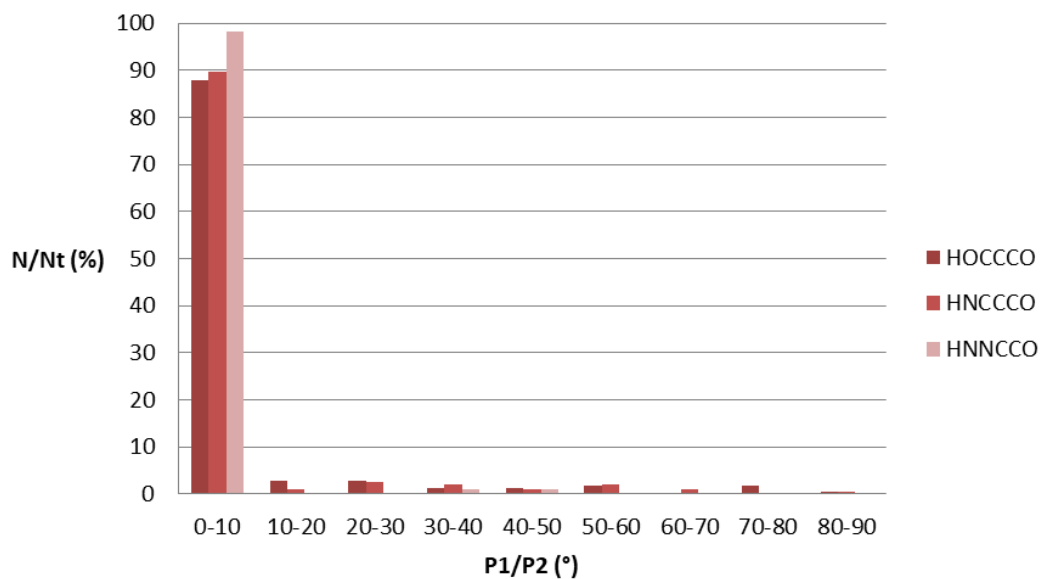
orientation 4	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-0.80	-1.60	-1.84	-0.92
TPSS-D3	-2.38	-2.28	-2.21	-2.15
BLYP-D3	-2.36	-2.20	-1.97	-1.90
BP86-D3	-2.10	-2.12	-2.02	-1.93
PBE1PBE-D3	-2.17	-2.20	-2.18	-2.12
M05-D3	-2.12	-2.15	-2.27	-2.25
M06-D3	-2.20	-2.32	-2.54	-2.60
M052X-D3	-1.92	-2.14	-2.25	-2.20
M06HF-D3	-1.98	-2.15	-2.54	-2.60
<b>CCSD(T)/CBS</b>	<b>-1.90</b>			

**Table S15.** Interaction energies (in kcal/mol) of H<sub>4</sub>C<sub>2</sub>N<sub>2</sub>O dimer of orientation 5

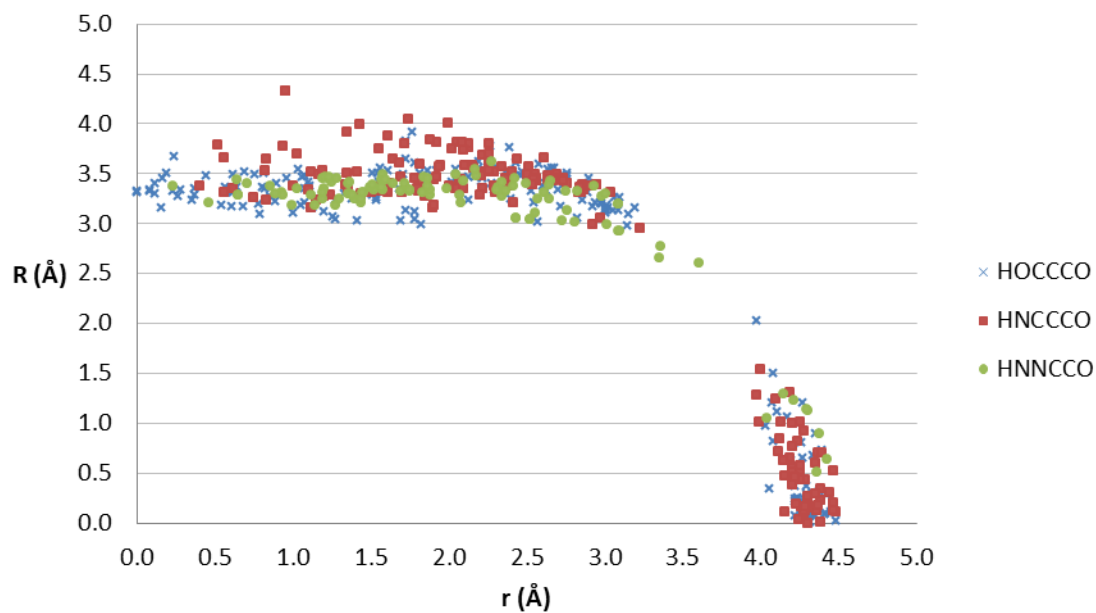
orientation 5	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-31++G**
MP2	-0.46	-1.72	-2.10	-1.00
TPSS-D3	-1.82	-1.85	-1.98	-1.84
BLYP-D3	-1.88	-1.89	-1.89	-1.77
BP86-D3	-1.75	-1.88	-1.97	-1.79
PBE1PBE-D3	-1.75	-1.90	-2.04	-1.90
M05-D3	-1.84	-1.95	-2.28	-2.21
M06-D3	-1.81	-2.07	-2.32	-2.30
M052X-D3	-1.66	-2.08	-2.25	-2.10
M06HF-D3	-1.76	-2.02	-2.48	-2.34
<b>CCSD(T)/CBS</b>	<b>-2.30</b>			

### The relevance of model systems for interaction energy calculations

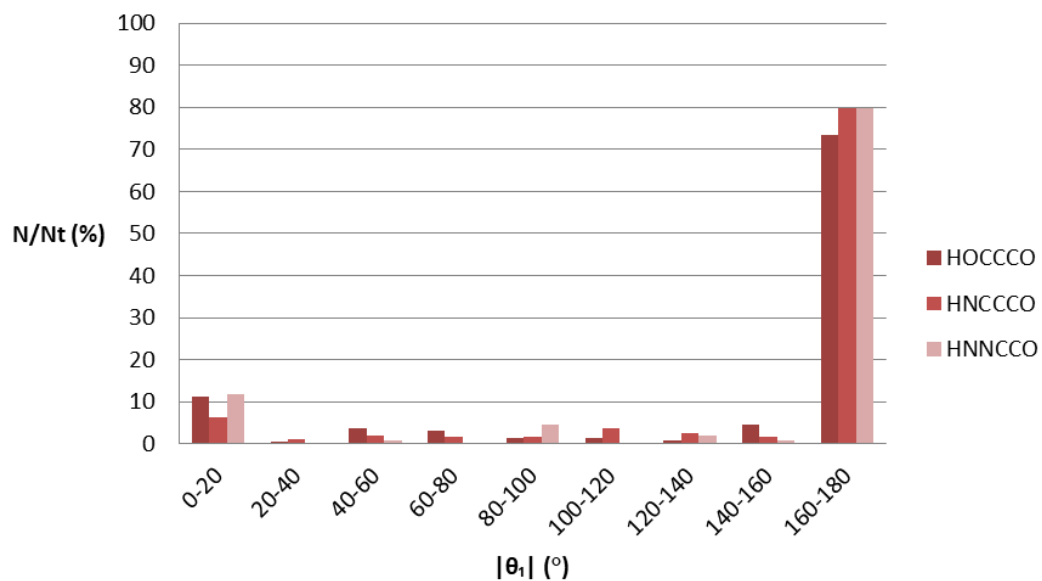
Three molecules are chosen for quantum chemical calculations of interaction energies between H<sub>4</sub>C<sub>3</sub>O<sub>2</sub>, H<sub>5</sub>C<sub>3</sub>NO and H<sub>4</sub>C<sub>2</sub>N<sub>2</sub>O (Figure 6) due to relatively high abundance of their derivatives in crystal structures (Table 1). Trends concerning mutual orientations of interacting rings in crystal structures of derivatives of the three selected molecules (HOCCCO, HNCCCO and HNNCCO, as HDZYXA sequence for derivatives of H<sub>4</sub>C<sub>3</sub>O<sub>2</sub>, H<sub>5</sub>C<sub>3</sub>NO and H<sub>4</sub>C<sub>2</sub>N<sub>2</sub>O, respectively) are the same as overall trends (Figures 3-5), since rings are predominantly parallel (Figure S4), distances between ring planes are mostly typical for stacking (Figure S5) and rings are preferentially in *anti* orientation (Figure S6).



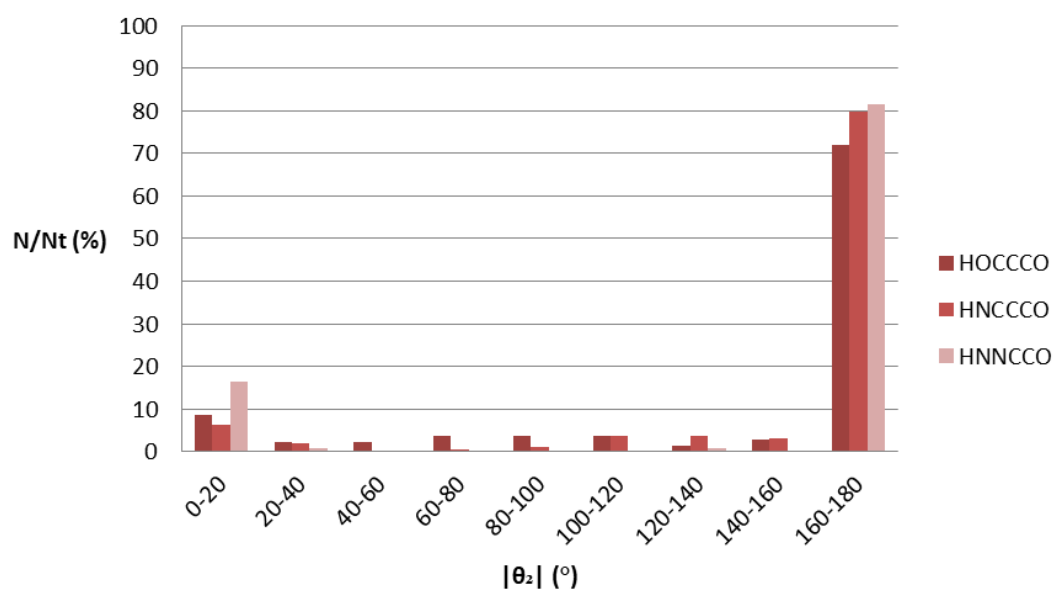
**Figure S4.** Distribution of dihedral angles between ring planes. Frequencies of occurrence of a particular range of angles are given in the form of percentage of the total number (Nt) of structures in every group of rings.



**Figure S5.** Dependence of distances between planes of interacting rings on offset values, given for three groups of rings separately



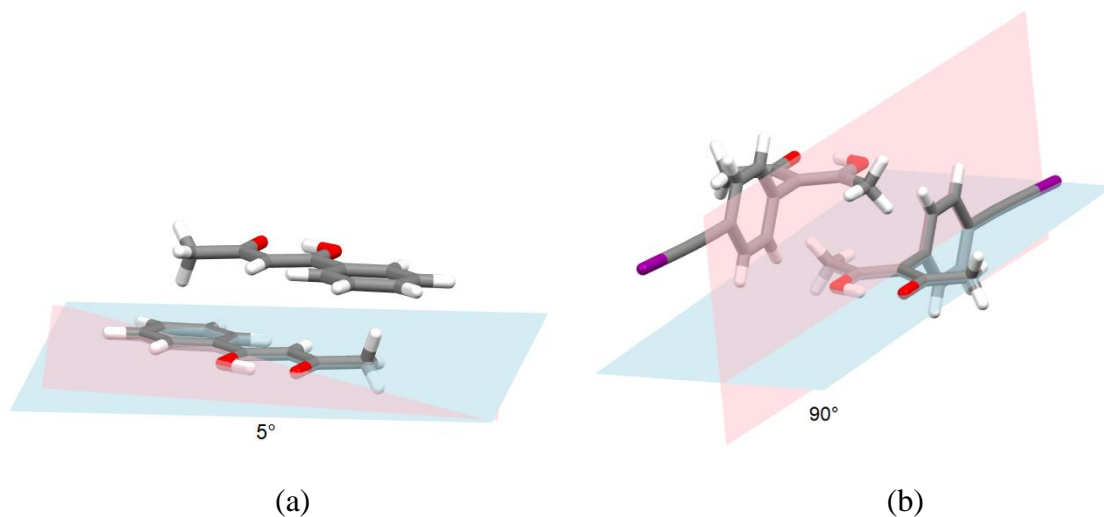
(a)



(b)

**Figure S6.** Distributions of absolute values of torsion angles a)  $H_1\Omega_1\Omega_2H_2$  ( $\theta_1$ ) and b)  $A_1\Omega_1\Omega_2A_2$  ( $\theta_2$ ) (Figure 3). Frequencies of occurrence of a particular range of torsion angles are given in the form of percentage of the total number (Nt) of structures in every group of rings.

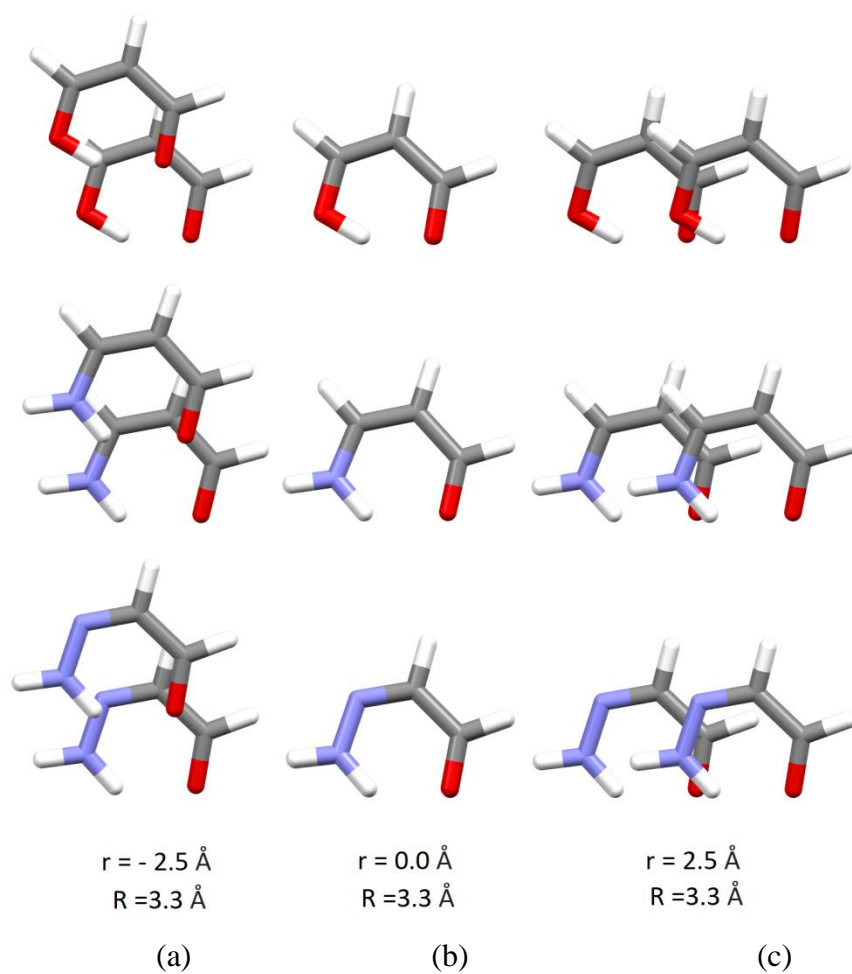
## Substituents on RAHB rings



**Figure S7.** Some examples of phenyl substituted RAHB structures found in CSD; (a) fragment of crystal structure CINWEE-RAHB (blue) and phenyl ring (red) within the same molecule are almost in the same plane; (b) fragment of crystal structure BZOYAC02-RAHB (blue) and phenyl ring (red) do not belong to the same plane

## Parallel orientation of dimers

Interaction energies were calculated also for several parallel orientations: the sandwich geometries and the geometries with horizontal displacements of 2.5 Å along  $\Omega$ -C and the orthogonal direction and fixed distances between ring planes of 3.3 Å (Figure S8) in order to compare the interaction energies of parallel and antiparallel orientations of the same horizontal displacements and distances between ring planes. The obtained interaction energies at MP2/aug-cc-pVDZ level are given in Table S16.



**Figure S8.** Dimer geometries used for calculations of interaction energies of parallel stacking RAHB/RAHB interactions; (a) along  $\Omega$ -C direction; (b) sandwich orientation (c) orthogonal to  $\Omega$ -C direction



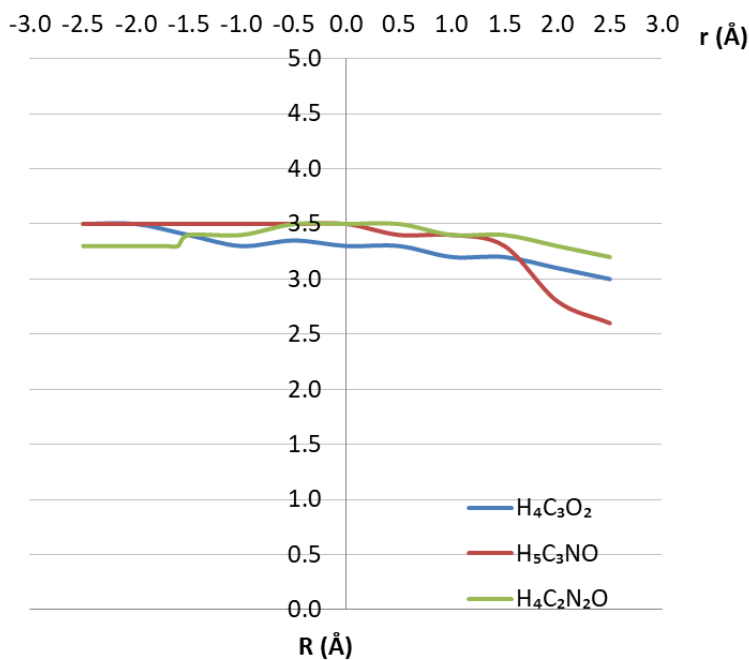
**Table S16.** Interaction energies of several model systems of parallel and antiparallel orientations with horizontal displacements of 2.5 Å along  $\Omega$ -C and the orthogonal direction and fixed distances between ring planes of 3.3 Å in all model systems; orientations 1-5 are given in Figures S1-S3.

Model system	Interaction energies (kcal/mol) at MP2/aug-cc-pVDZ		
$\Omega$ -C direction	Parallel	Antiparallel (orientation 1)	Antiparallel (orientation 3)
H <sub>4</sub> C <sub>3</sub> O <sub>2</sub>	-1.34	-2.02	-1.56
H <sub>5</sub> C <sub>3</sub> NO	-0.75	-2.25	-1.46
H <sub>4</sub> C <sub>2</sub> N <sub>2</sub> O	-1.56	-2.15	-1.00
Sandwich		Antiparallel (orientation 2)	
H <sub>4</sub> C <sub>3</sub> O <sub>2</sub>	0.64	-3.76	
H <sub>5</sub> C <sub>3</sub> NO	1.72	-3.02	
H <sub>4</sub> C <sub>2</sub> N <sub>2</sub> O	-0.12	-1.30	
Orthogonal to $\Omega$ -C direction		Antiparallel (orientation 4)	Antiparallel (orientation 5)
H <sub>4</sub> C <sub>3</sub> O <sub>2</sub>	-1.53	-2.06	-2.46
H <sub>5</sub> C <sub>3</sub> NO	-1.99	-3.80	-1.95
H <sub>4</sub> C <sub>2</sub> N <sub>2</sub> O	-2.39	-1.84	-2.10

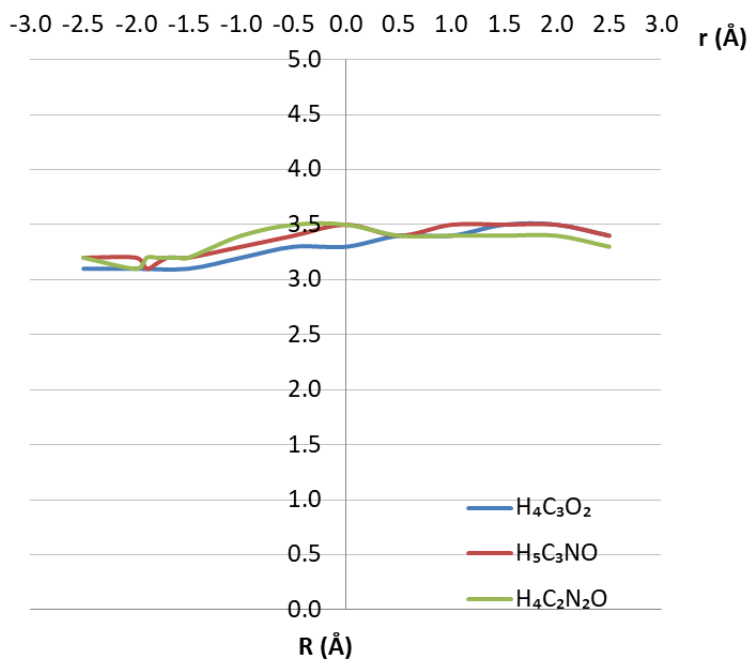
Sandwich geometries are disfavored due to electrostatic reasons (Figure 11), but displaced geometries are not, since the overlap of regions of electrostatic potentials of opposite sign can occur. The interactions are mostly weaker than the corresponding antiparallel interactions (Tables S1-S15).

## Dependences of optimal distances of parallel ring planes on horizontal displacements

Dependences of optimal distances between the two molecular planes in the dimer on offset values are given in Figure S9. Optimal distances between the ring planes, obtained by ab initio calculations (Figure S9) are in accordance with the data from crystal structures (Figure 4), since the distances between ring planes are mostly between 3.0 and 4.0 Å, in the range of offset values between 0.0 and 2.5 Å, while calculated optimal distances, in the same range of offset values, are mostly between 3.0 and 3.5 Å.



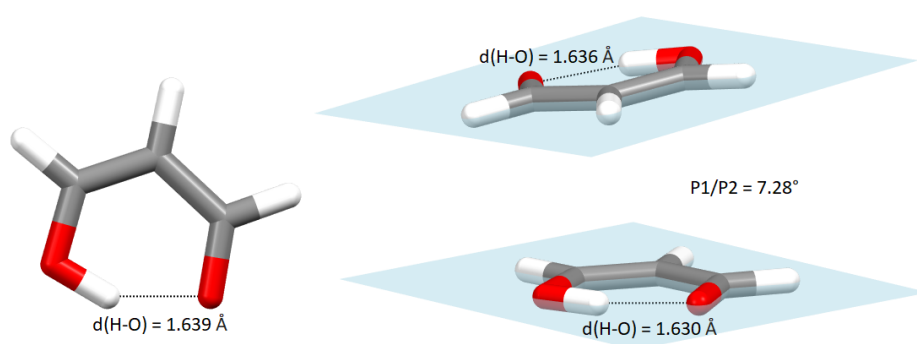
(a)



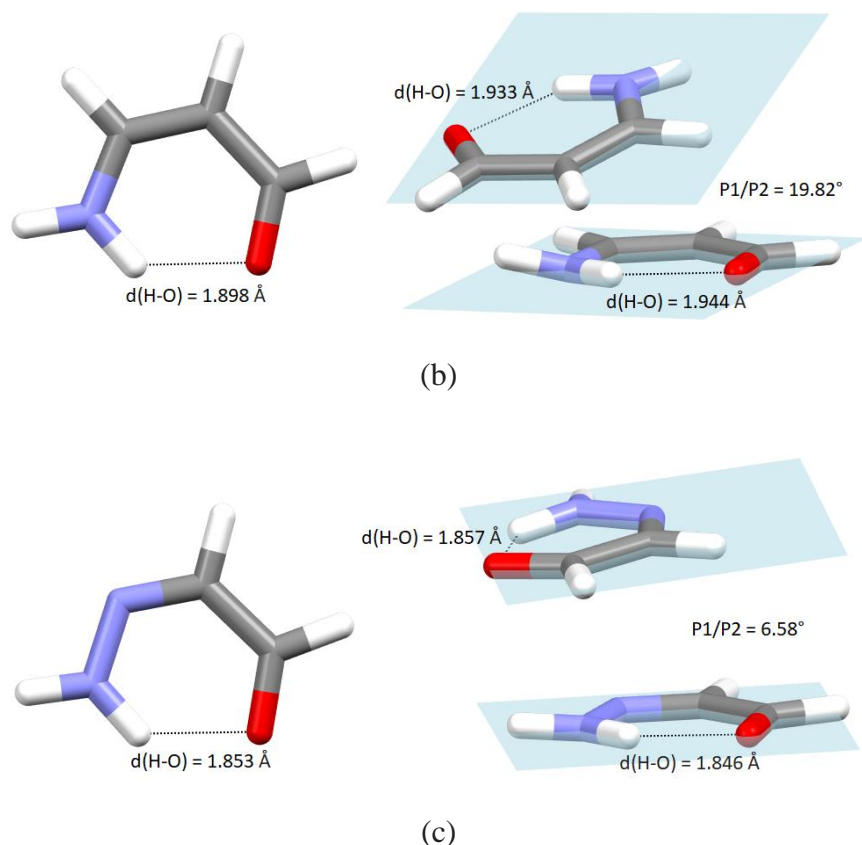
(b)

**Figure S9.** Calculated dependences of distances between the ring planes on offset values of the two ring centers for three selected homodimers a) along  $\Omega$ -C direction; b) along the direction orthogonal to  $\Omega$ -C

### Optimized dimer structures



(a)



**Figure S10.** Optimized monomers (left), with H-O bond distance and optimized dimers (right) with H-O bond distances and angles between the ring planes; (a) malonaldehyde ( $C_3H_4O_2$ ); (b)  $C_3H_5NO$ ; (c)  $C_2H_4N_2O$

The calculations of potential energy curves (Figure 9) were single point, i. e. the coordinates of optimized monomers were unchanged during interaction energy calculations. However, if we optimize dimer geometries (at the same level that we used for optimizing monomers, MP2/cc-pVTZ), using geometries of the potential curves minima as starting geometries, we observe changes in intramolecular hydrogen bond distances. Stacked arrangement is preserved in  $C_3H_4O_2$  dimer, where H-O distances in dimer geometry (1.630 Å and 1.636 Å) are slightly decreased comparing with H-O distance in the monomer (1.639 Å) (Figure S10a). There is a disruption of the stacking arrangement in  $C_3H_5NO$  dimer, with the increase of the H-O distance (1.944 Å and

1.933 Å) comparing with the monomer (1.898 Å) (Figure S10b). The geometry of optimized C<sub>2</sub>H<sub>4</sub>N<sub>2</sub>O dimer is also stacking geometry, where H-O distance is slightly decreased in one of the molecules (1.846 Å) comparing with the monomer (1.853 Å), while it is slightly increased in the other (1.857 Å). The Figure S10c shows that there is the overlap of the shorter H-O bond area with the edge of the other RAHB ring, while the longer H-O bond area does not overlap with RAHB ring in the optimized structure.

## References

1. Mackie, I. D.; DiLabio, G. A. Approximations to Complete Basis Set-Extrapolated, Highly Correlated Non-Covalent Interaction Energies. *J. Chem. Phys.* 2011, 135 (13), 134318. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010**, 132 (15), 154104.