Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

For

The relative position of π-π interacting rings notably changes the nature of the substituent effect

Enrique M. Cabaleiro-Lago[a] , Jesús Rodríguez-Otero[b] and Saulo A. Vázquez[b]

[a.] *Facultade de Ciencias (Dpto. de Química Física), Universidade de Santiago de Compostela, Campus de Lugo. Avda. Alfonso X El Sabio s/n 27002 Lugo, Galicia (Spain).*
[b.] *CIQUS and Facultade de Química (Dpto. de Química Física), Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Galicia (Spain).*

Table S1. Interaction energies and their components (kcal mol^{-1}) as obtained at the SAPT2+(3) δMP_2/aug-cc-pVTZ level for the optimised structures of parallel-displaced substituted benzene dimers.

			$R_2<0$						$R_2>0$		
	E_{dis}	E_{rep}	E_{ele}	E_{ind}	E_{tot}		E_{dis}	E_{rep}	E_{ele}	E_{ind}	E_{tot}
NH_2b*	-7.57	7.40	-3.58	-0.79	-4.54	**NH_2b***	-6.86	5.84	-1.05	-0.41	-2.49
NH_2	-7.79	6.28	-0.75	-0.50	-2.76	**NH_2**	-6.99	6.03	-1.33	-0.45	-2.74
OH	-7.48	6.21	-1.36	-0.52	-3.14	**OH**	-6.85	5.91	-1.37	-0.42	-2.72
CH_3	-6.59	5.73	-2.13	-0.56	-3.55	**CH_3**	-6.94	5.95	-1.27	-0.45	-2.71
Bz	-6.63	5.77	-1.37	-0.46	-2.68	**Bz**	-6.63	5.77	-1.37	-0.46	-2.68
F	-7.09	5.86	-1.44	-0.38	-3.06	**F**	-6.74	5.81	-1.57	-0.41	-2.91
CN	-8.48	7.19	-2.49	-0.51	-4.29	**CN**	-7.17	6.16	-2.07	-0.50	-3.57
NO_2	-9.38	7.71	-3.05	-0.46	-5.19	**NO_2**	-7.26	6.19	-2.15	-0.48	-3.70

* In NH_2b the hydrogen atoms of the amino group point towards the other phenyl ring.

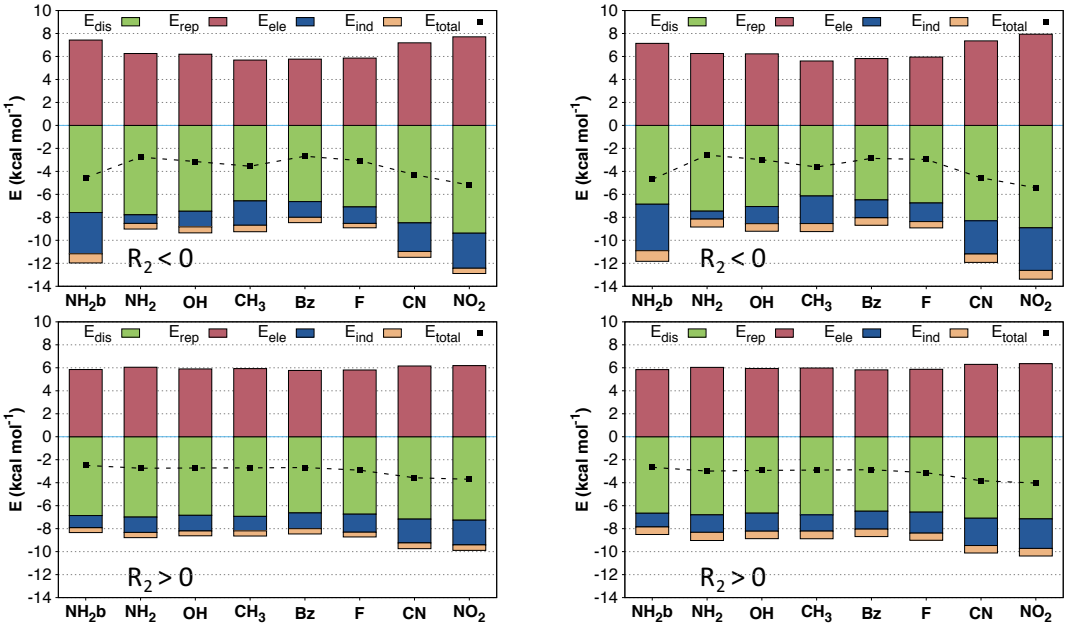

Figure S1. Contributions to the total interaction energy obtained for parallel-displaced substituted benzene dimers. Left: SAPT2+(3) δMP_2/aug-cc-pVTZ. Right: F-SAPT0/jun-cc-pVDZ.

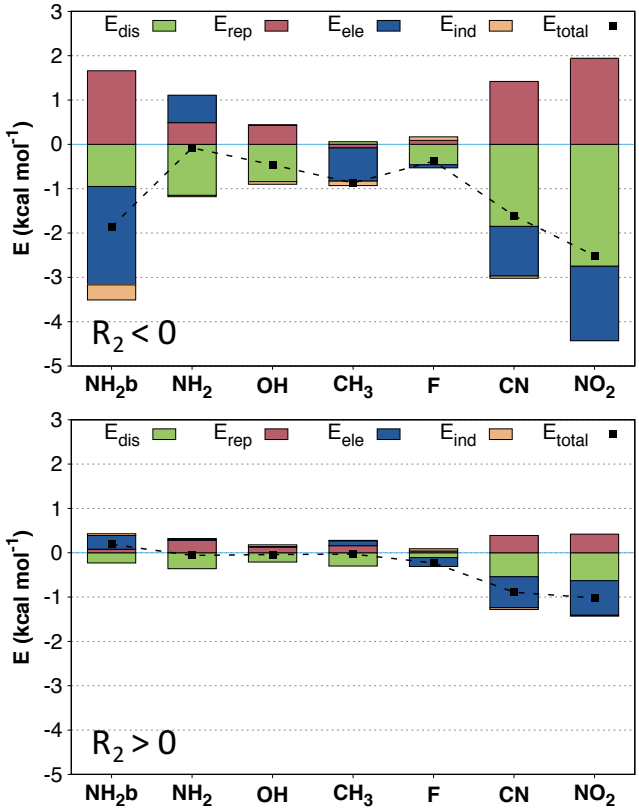

Figure S2. Energy changes relative to benzene dimer and its contributions as obtained for the optimised parallel-displaced dimer geometries at the SAPT2+(3) δMP_2/aug-cc-pVTZ level.

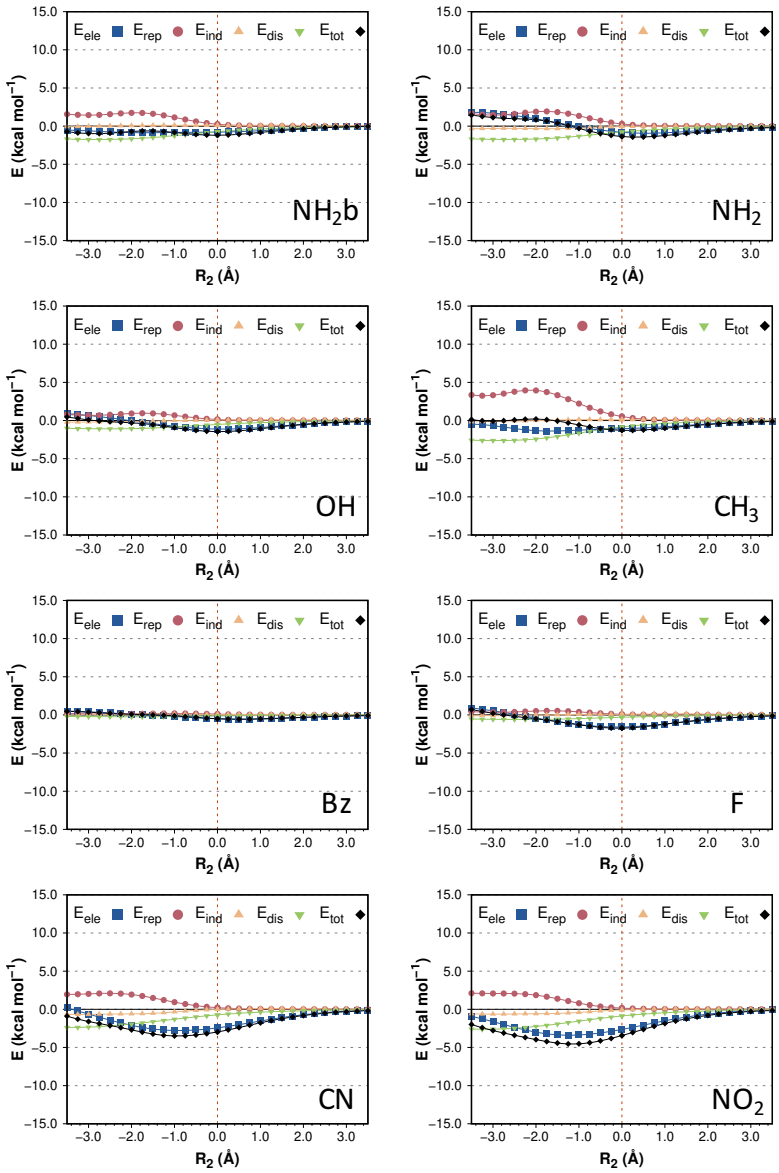

Figure S3. Contributions to the interaction energy from the substituent in parallel-displaced substituted benzene dimers at the F-SAPT0/jun-cc-pVDZ level.

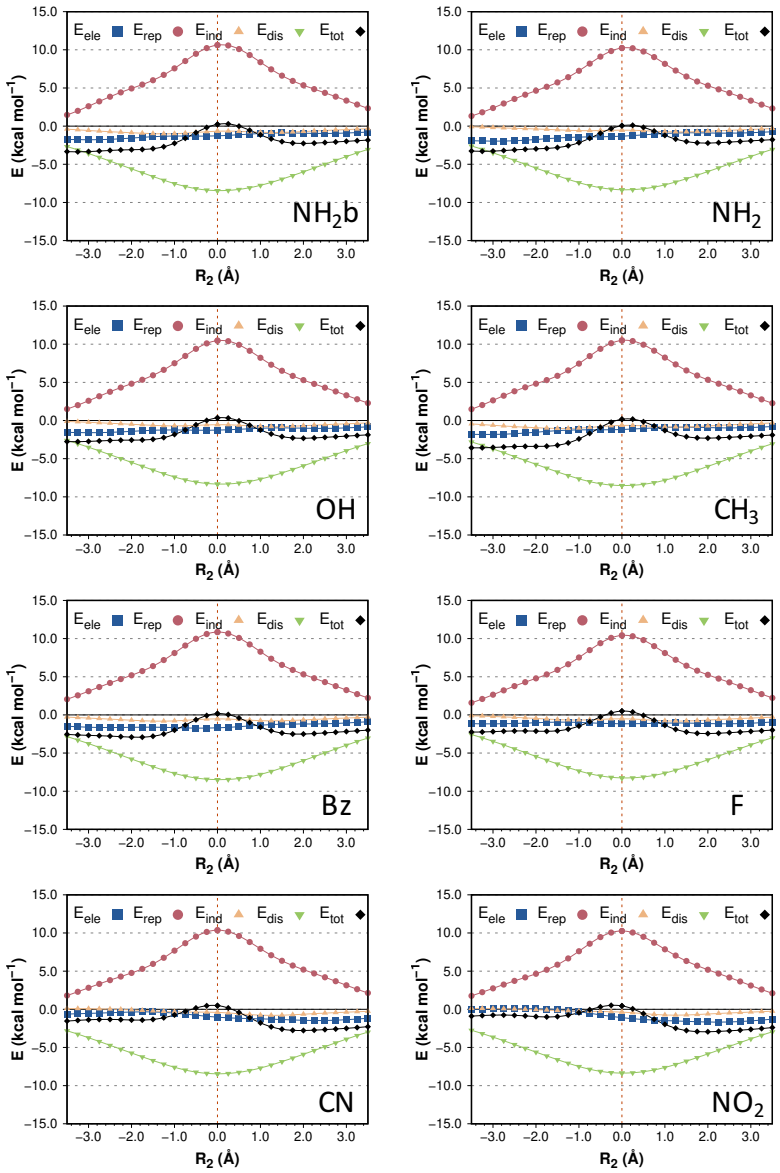

Figure S4. Contributions to the interaction energy from the phenyl group in parallel-displaced substituted benzene dimers at the F-SAPT0/jun-cc-pVDZ level.

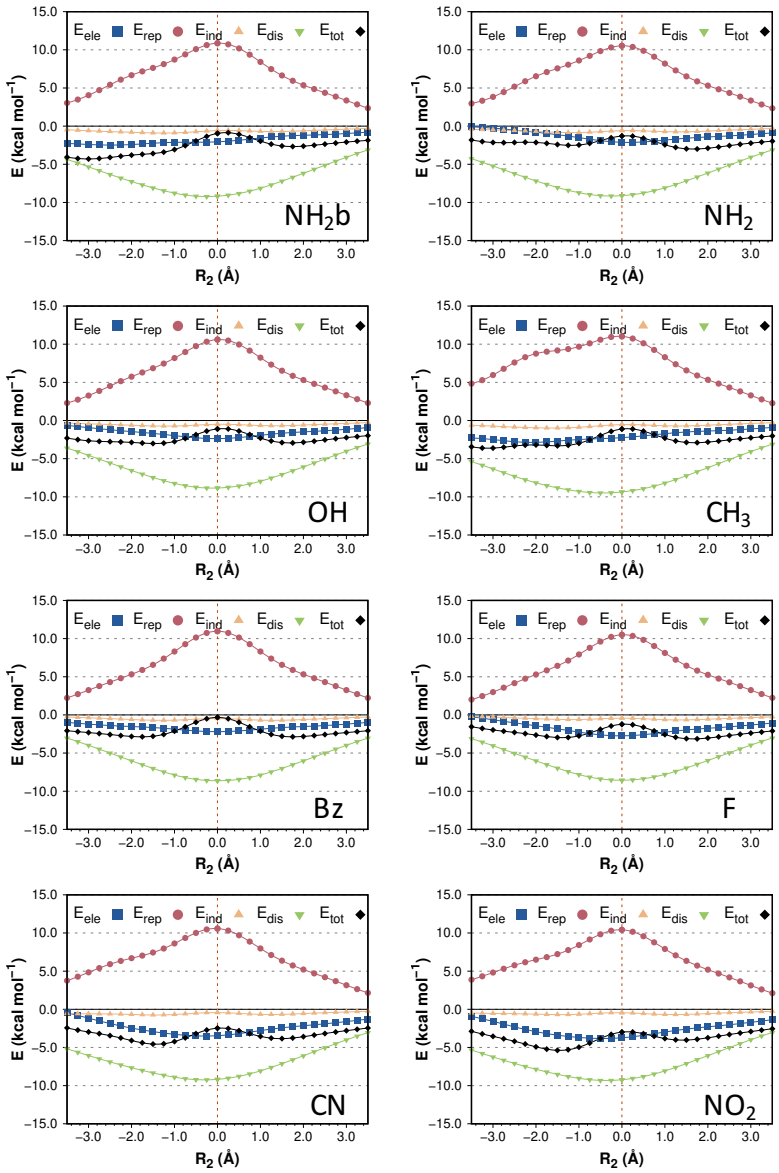

Figure S5. Total contributions to the interaction energy in parallel-displaced substituted benzene dimers at the F-SAPT0/jun-cc-pVDZ level.

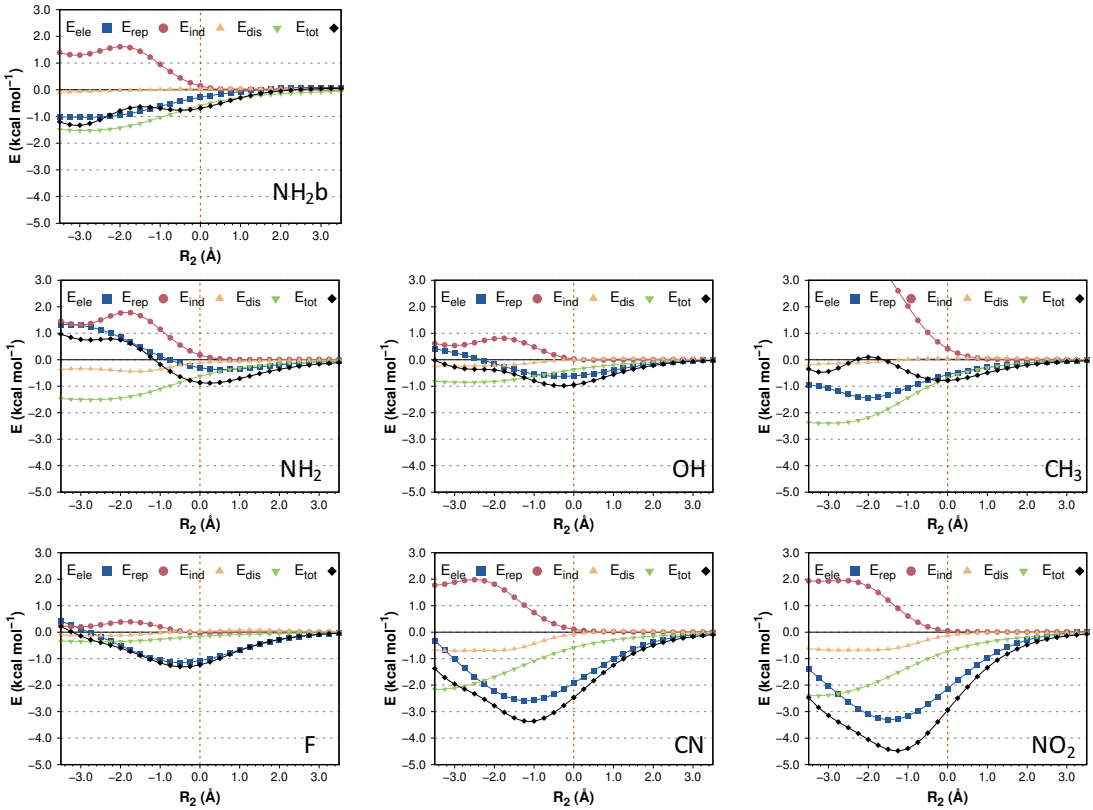

Figure S6. Substituent contributions to energy changes (relative to the benzene dimer) on the components of the interaction energy in parallel-displaced dimers keeping R_1 = 3.5 Å. F-SAPT0/jun-cc-pVDZ.

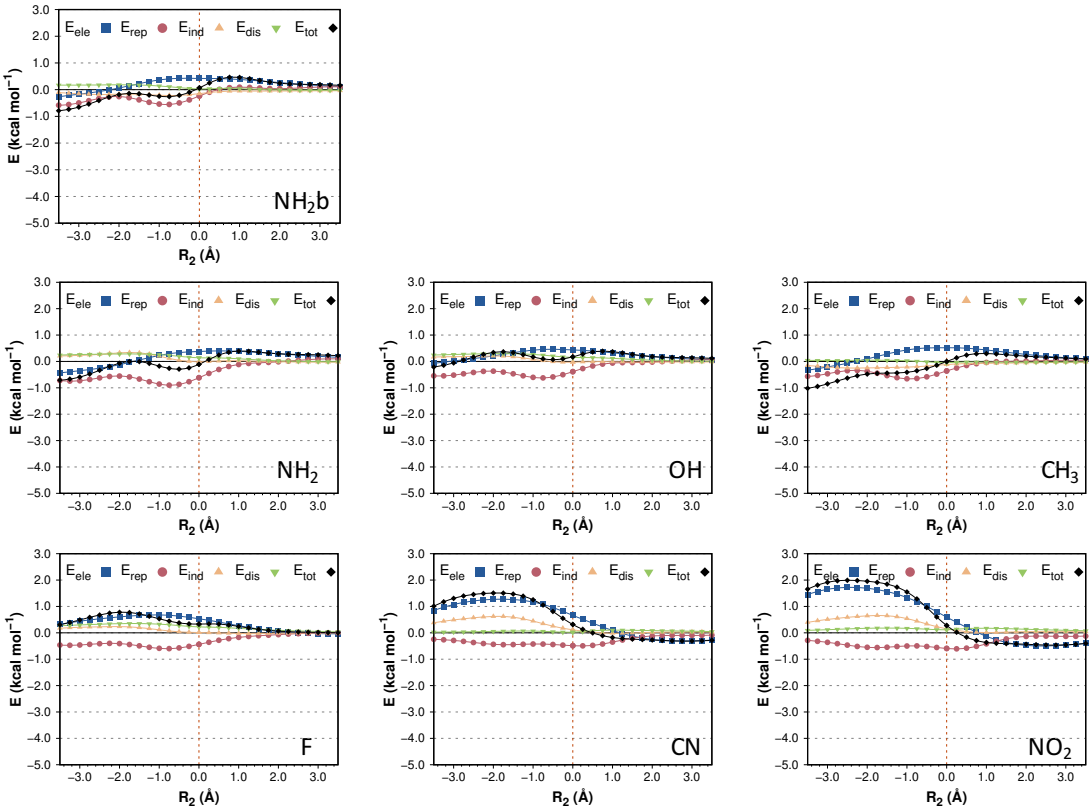

Figure S7. Phenyl ring contributions to energy changes (relative to the benzene dimer) on the components of the interaction energy in parallel-displaced dimers keeping R_1 = 3.5 Å. F-SAPT0/jun-cc-pVDZ.

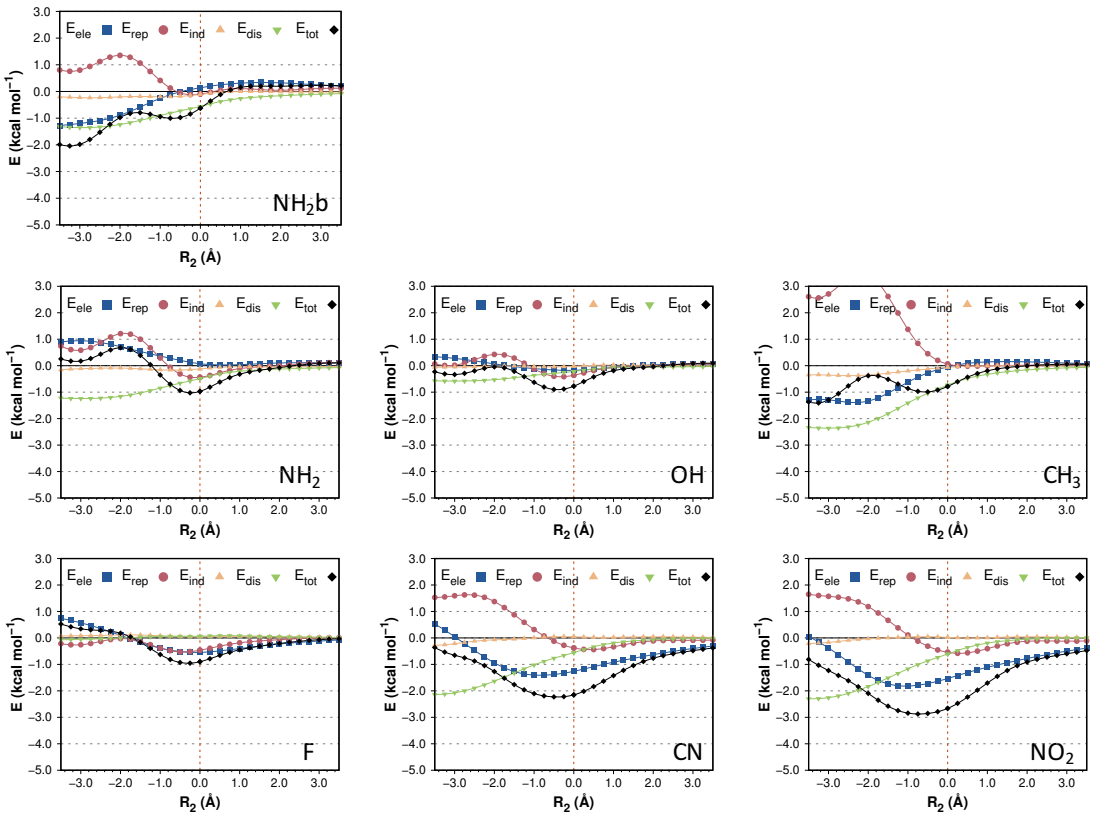

Figure S8. Energy changes on the components of the interaction energy in parallel-displaced dimers relative to the benzene dimer keeping R_1 = 3.5 Å. F-SAPT0/jun-cc-pVDZ.

Table S2. Interaction energies and their components (kcal mol^{-1}) as obtained at the SAPT2+(3) δMP_2/aug-cc-pVTZ level for the optimised structures of T-shaped substituted benzene dimers.

			$R_2<0$						$R_2>0$		
	E_{dis}	E_{rep}	E_{ele}	E_{ind}	E_{tot}		E_{dis}	E_{rep}	E_{ele}	E_{ind}	E_{tot}
NH_2	-4.88	4.08	-1.82	-0.50	-3.13	**NH_2**	-4.53	3.65	-1.43	-0.40	-2.71
OHb*	-4.95	4.36	-2.28	-0.63	-3.49	**OHb***	-4.53	3.71	-1.58	-0.45	-2.86
OH	-4.55	3.72	-1.57	-0.44	-2.84	**OH**	-4.59	3.84	-1.76	-0.45	-2.95
CH_3	-4.94	4.05	-1.70	-0.45	-3.04	**CH_3**	-4.58	3.73	-1.52	-0.41	-2.78
Bz	-4.46	3.69	-1.58	-0.42	-2.77	**Bz**	-4.46	3.69	-1.58	-0.42	-2.77
F	-4.59	3.87	-1.86	-0.51	-3.09	**F**	-4.59	3.92	-1.95	-0.50	-3.12
CN	-5.14	4.56	-2.46	-0.71	-3.76	**CN**	-4.81	4.24	-2.41	-0.66	-3.63
NO_2	-5.55	4.70	-2.32	-0.72	-3.88	**NO_2**	-5.03	4.45	-2.60	-0.69	-3.87

* In OHb the hydrogen atoms of the amino group point towards the other phenyl ring.

Table S3. Interaction energies (kcal mol^{-1}) as obtained at the F-SAPT0/jun-cc-pVDZ level for the optimised structures of T-shaped substituted benzene dimers.

			$R_2<0$						$R_2>0$		
	E_{dis}	E_{rep}	E_{ele}	E_{ind}	E_{tot}		E_{dis}	E_{rep}	E_{ele}	E_{ind}	E_{tot}
NH_2	-4.31	3.86	-2.00	-0.55	-2.99	**NH_2**	-4.00	3.47	-1.64	-0.48	-2.66
OHb*	-4.36	4.16	-2.55	-0.67	-3.43	**OHb***	-4.00	3.54	-1.82	-0.52	-2.81
OH	-4.02	3.55	-1.73	-0.50	-2.69	**OH**	-4.06	3.66	-2.03	-0.52	-2.95
CH_3	-4.39	3.83	-1.87	-0.51	-2.94	**CH_3**	-4.06	3.54	-1.70	-0.48	-2.70
H	-3.94	3.51	-1.77	-0.48	-2.68	**H**	-3.94	3.51	-1.77	-0.48	-2.68
F	-4.05	3.71	-2.11	-0.56	-3.01	**F**	-4.07	3.75	-2.25	-0.57	-3.13
CN	-4.62	4.39	-2.82	-0.78	-3.83	**CN**	-4.31	4.10	-2.74	-0.70	-3.65
NO_2	-4.90	4.55	-2.73	-0.87	-3.95	**NO_2**	-4.49	4.31	-3.03	-0.77	-3.98

* In OHb the hydrogen atoms of the amino group point towards the other phenyl ring.

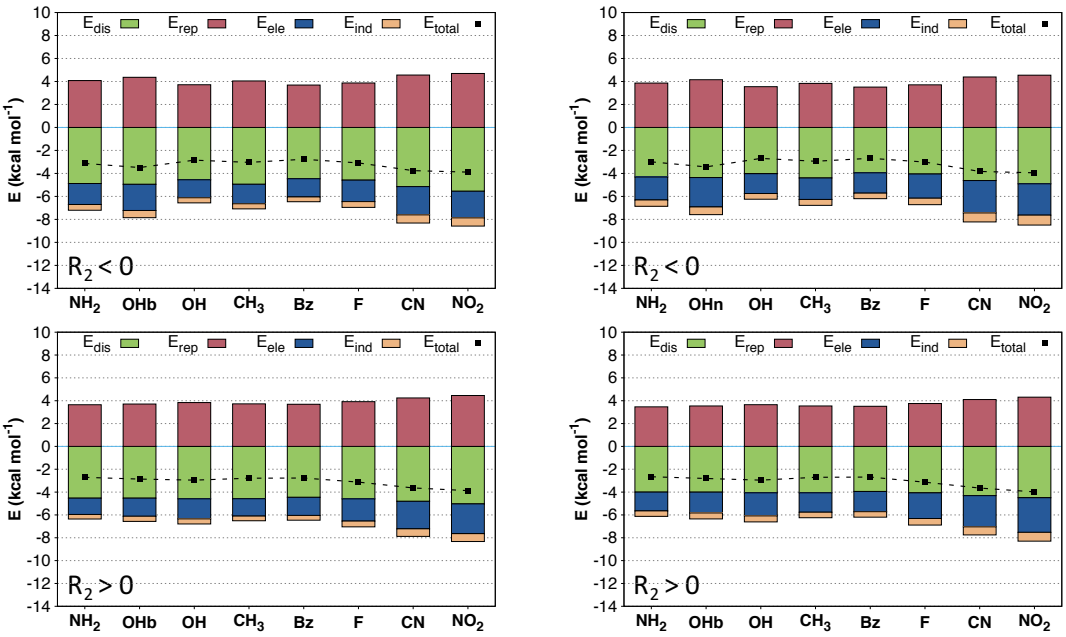

Figure S9. Contributions to the total interaction energy obtained for T-shaped substituted benzene dimers. Left: SAPT2+(3) δMP_2/aug-cc-pVTZ. Right: F-SAPT0/jun-cc-pVDZ.

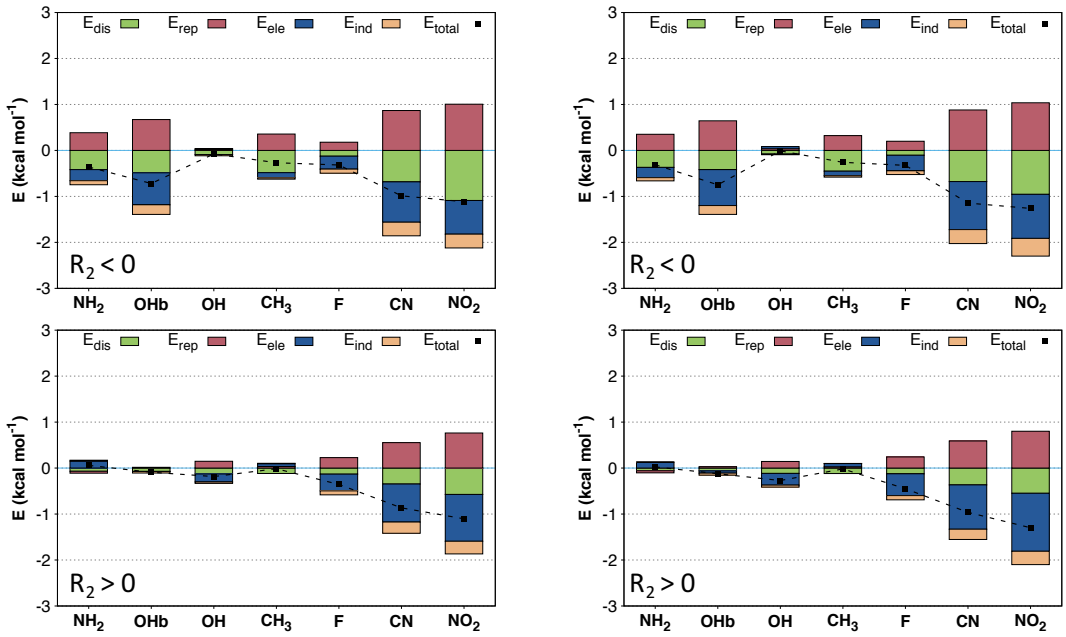

Figure S10. Energy changes relative to benzene dimer and its contributions as obtained for the optimised T-shaped dimer geometries. Left: SAPT2+(3) δMP_2/aug-cc-pVTZ. Right: F-SAPT0/jun-cc-pVDZ.

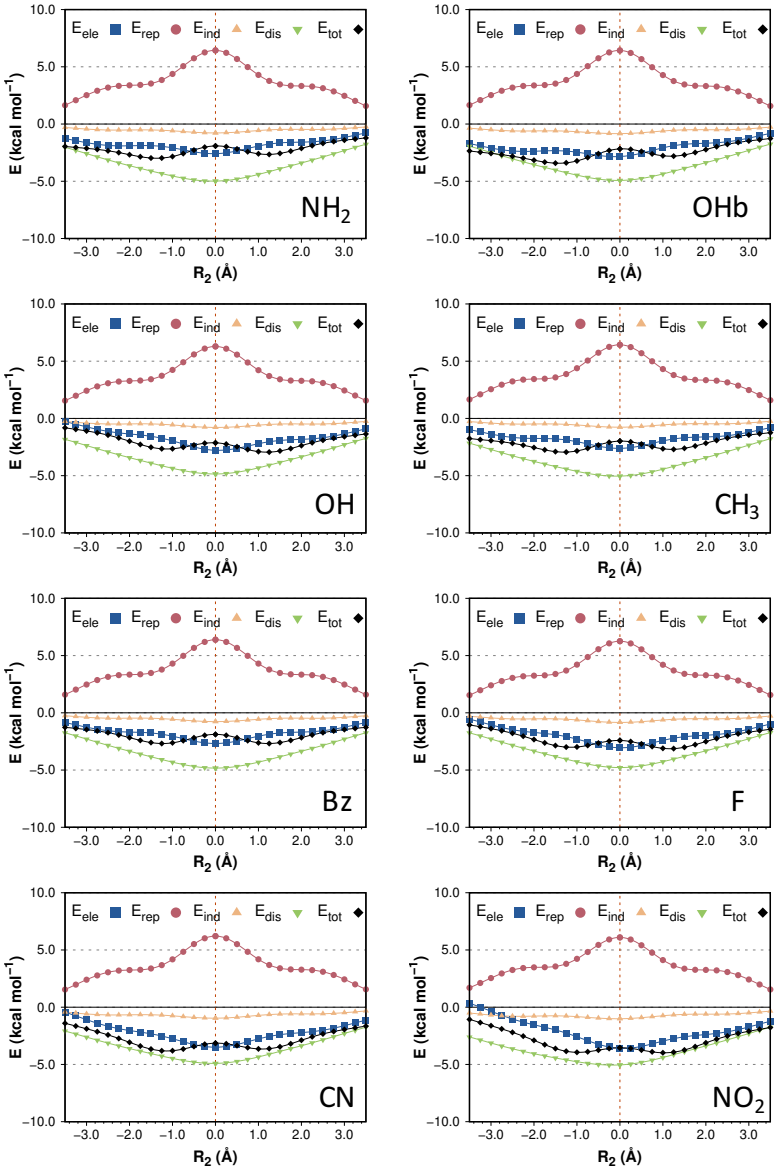

Figure S11. Total contributions to the interaction energy in T-shaped substituted benzene dimers at the F-SAPT0/jun-cc-pVDZ level.

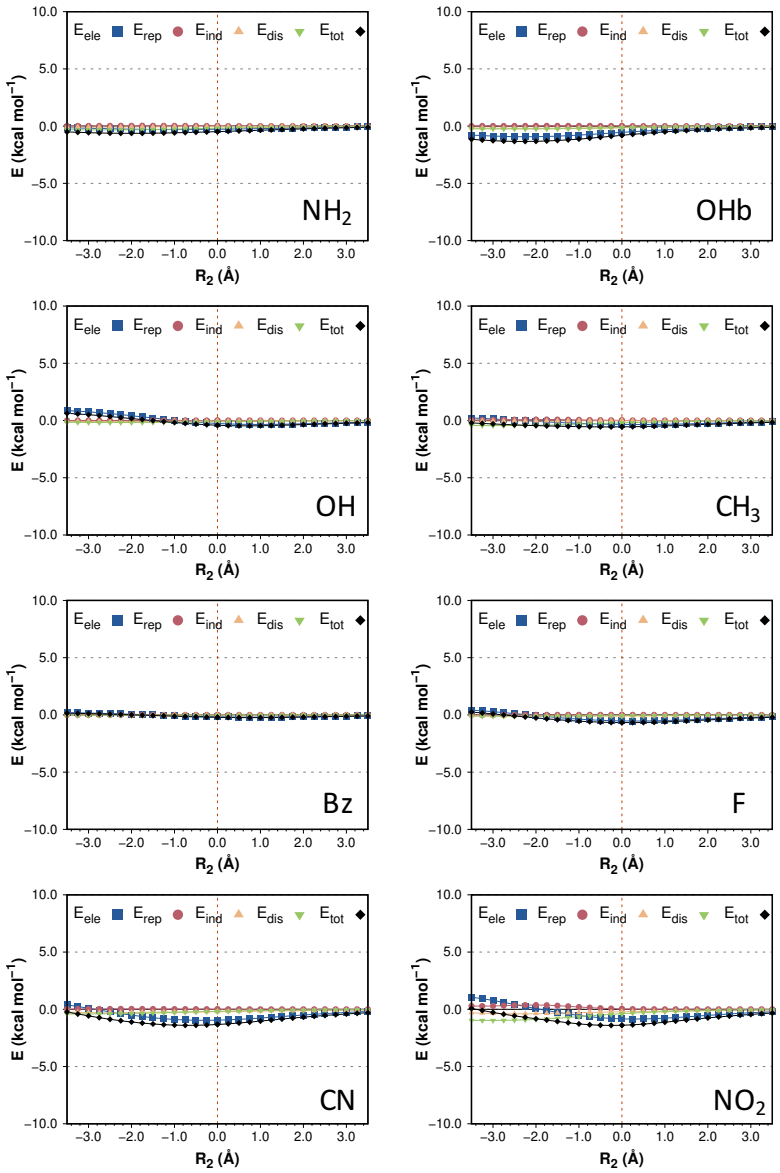

Figure S12. Contributions to the interaction energy from the substituent in T-shaped substituted benzene dimers at the F-SAPT0/jun-cc-pVDZ level.

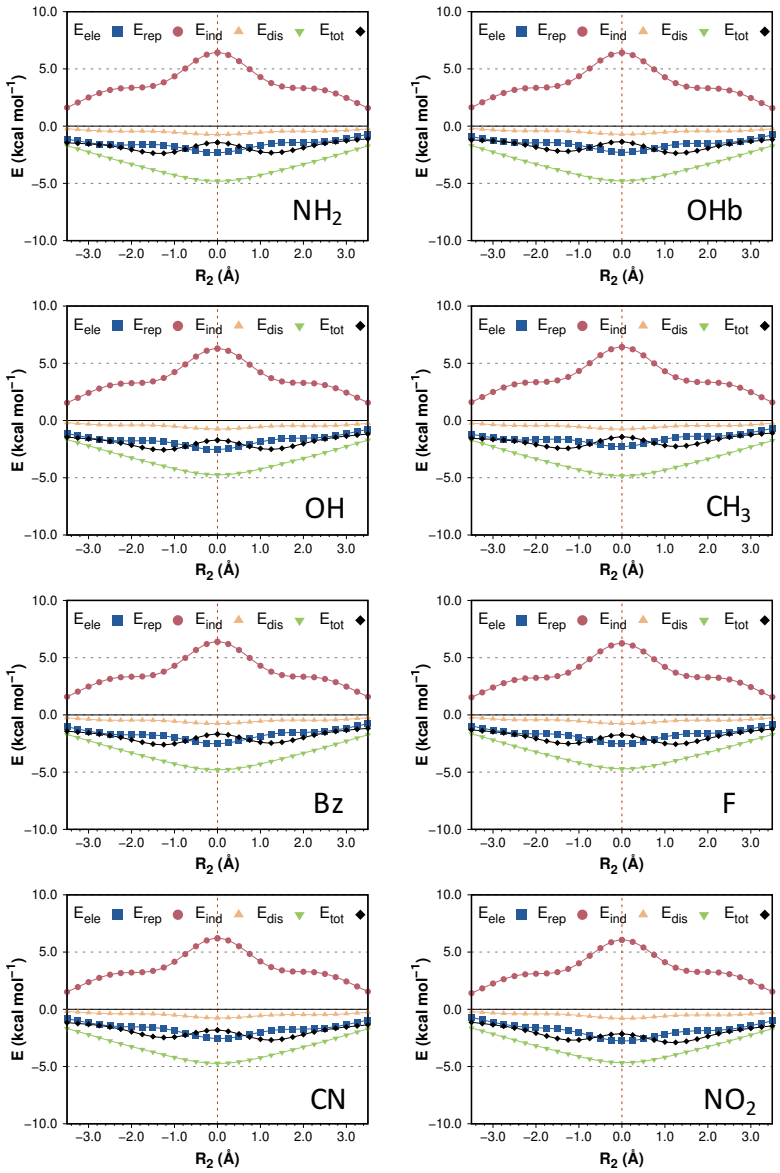

Figure S13. Contributions to the interaction energy from the phenyl group in T-shaped substituted benzene dimers at the F-SAPT0/jun-cc-pVDZ level.

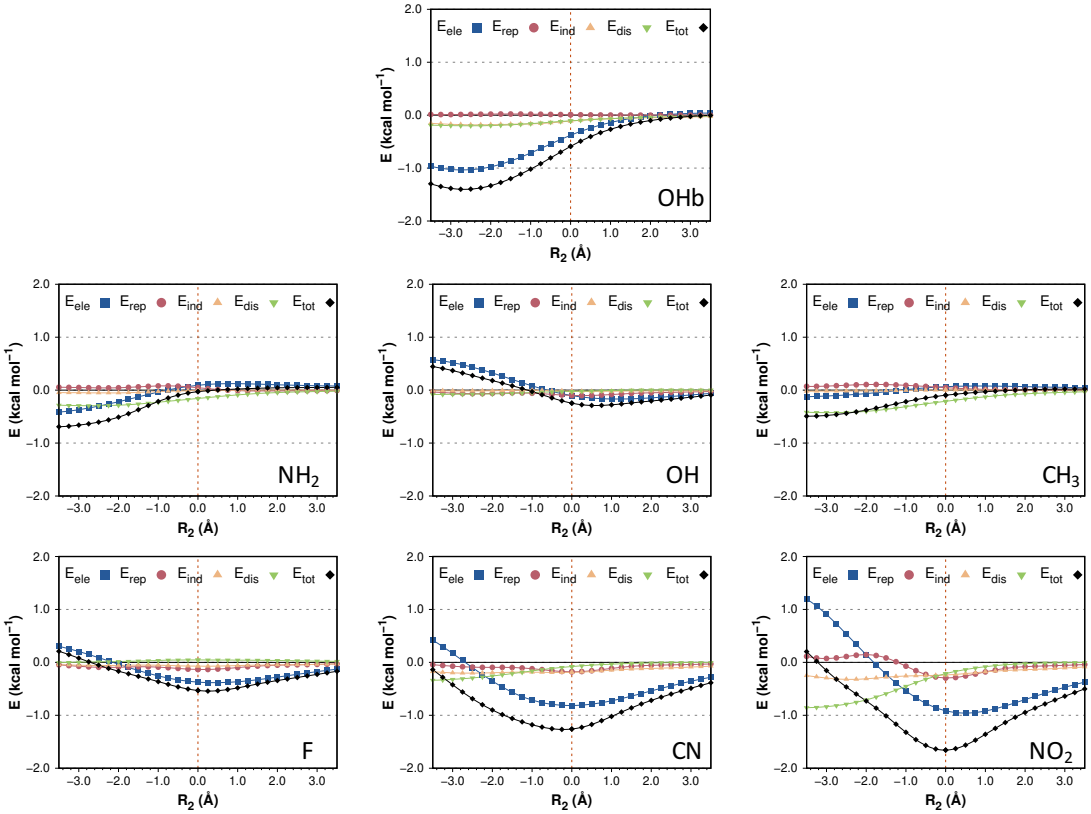

Figure S14. Total differences relative to the benzene dimer for the T-shaped complexes at the F-SAPT0/jun-cc-pVDZ level. In OHb the hydrogen atom of the hydroxyl group points towards the benzene molecule.

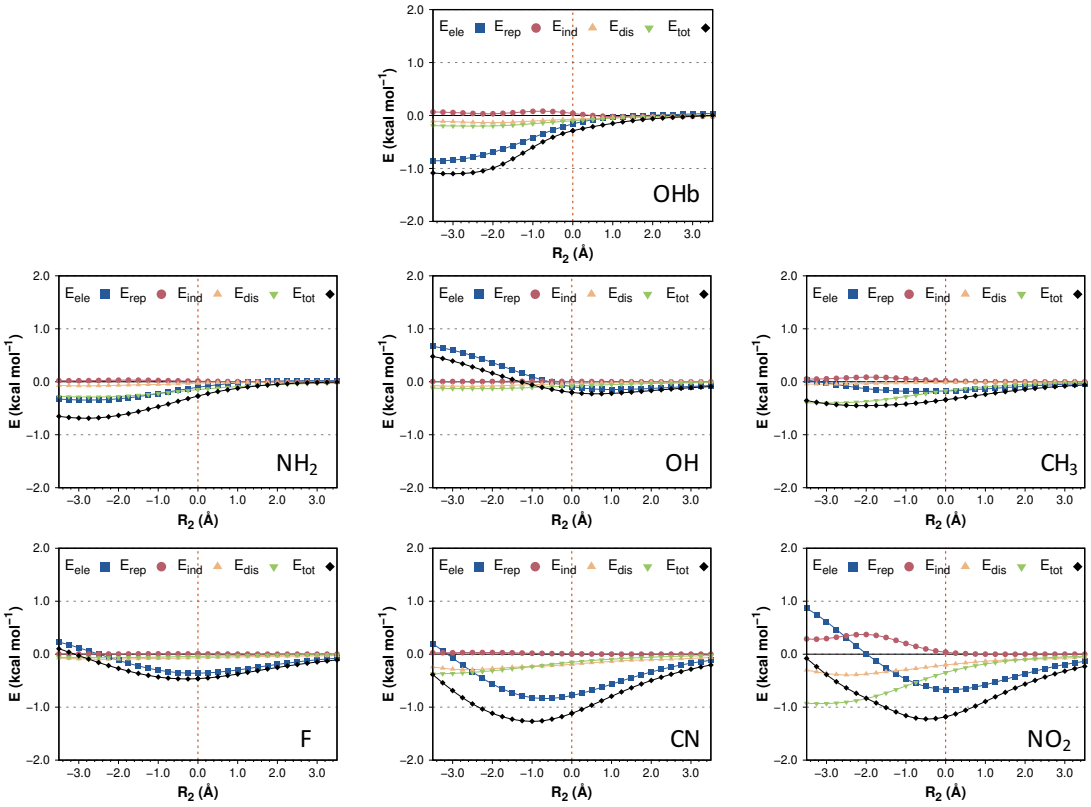

Figure S15. Energy changes relative to benzene dimer for the T-shaped complexes associated to the substituent at the F-SAPT0/jun-cc-pVDZ level. In OHb the hydrogen atom of the hydroxyl group points towards the benzene molecule.

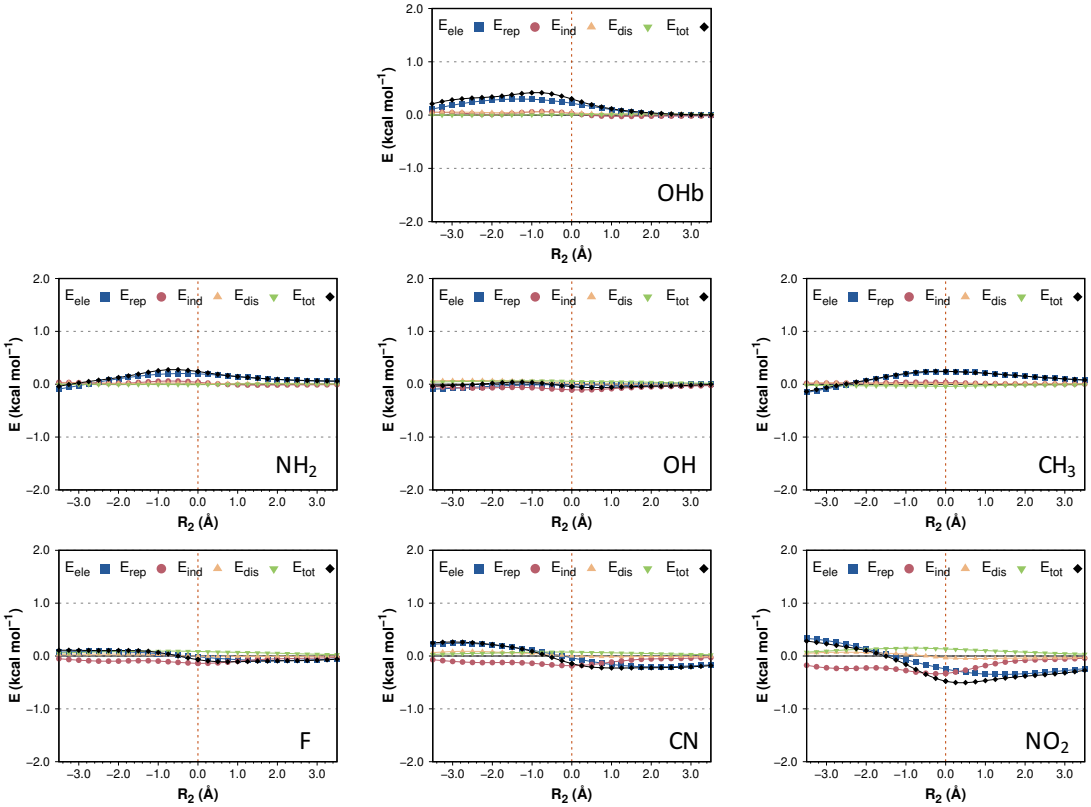

Figure S16. Energy changes relative to benzene dimer for the T-shaped complexes associated to the phenyl group at the F-SAPT0/jun-cc-pVDZ level. In OHb the hydrogen atom of the hydroxyl group points towards the benzene molecule.

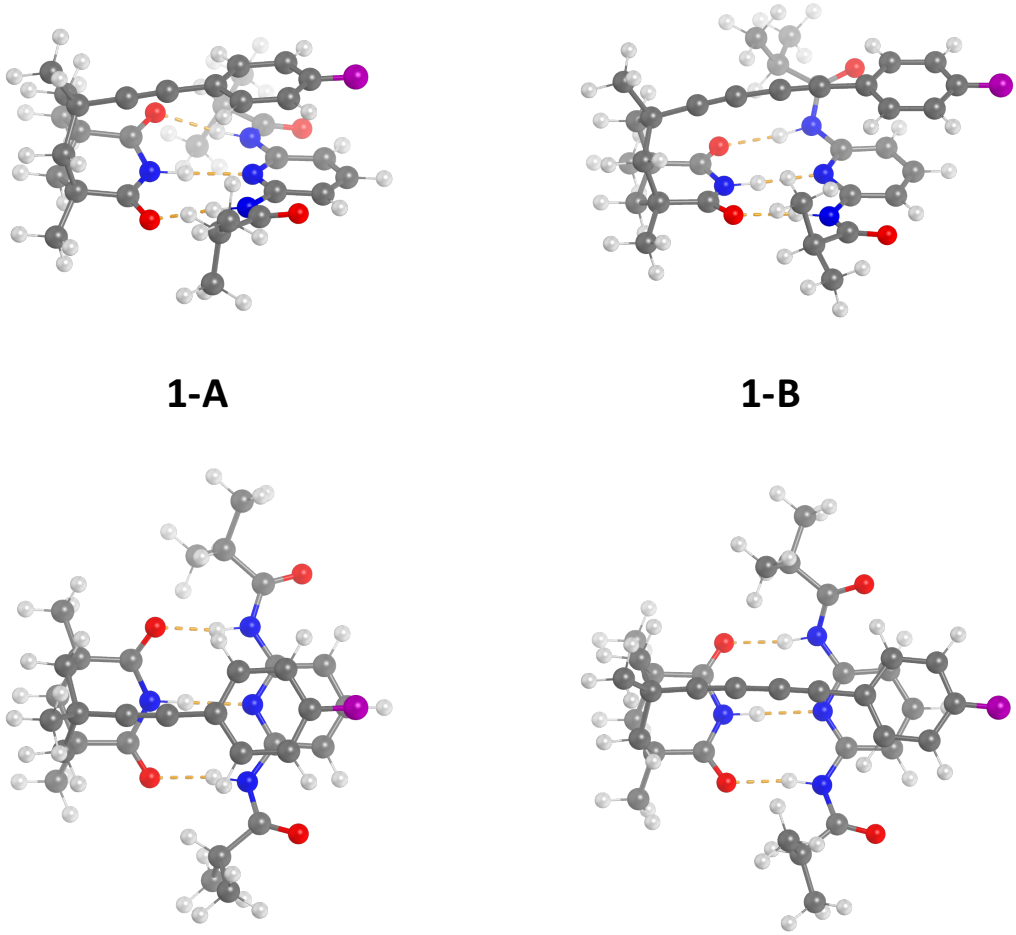

Figure S17. Optimised structures of dimers **1-A** and **1-B** at the PBE0-D3BJ/def2-TZVP level. The fluorinated derivative is shown to highlight the position of the substituent.

Table S4. Interaction energies and their components (kcal mol^{-1}) as obtained at the F-SAPT0/jun-cc-pVDZ level for the optimised structures for complexes **1-A** and **1-B**.

			1-A						1-B		
	E_{dis}	E_{rep}	E_{ele}	E_{ind}	E_{tot}		E_{dis}	E_{rep}	E_{ele}	E_{ind}	E_{tot}
NH_2b*	-28.53	48.78	-40.53	-13.00	-33.28	**NH_2b***	-29.52	46.88	-38.86	-12.63	-34.14
NH_2	-28.53	49.27	-39.77	-13.14	-32.16	**NH_2**	-29.82	47.35	-39.23	-12.61	-34.31
OH	-27.74	48.85	-40.34	-13.10	-32.33	**OH**	-29.89	47.66	-39.60	-12.70	-34.53
CH_3	-28.12	48.14	-39.29	-12.84	-32.11	**CH_3**	-29.52	46.89	-38.69	-12.52	-33.84
H	-26.37	46.72	-38.24	-12.64	-30.53	**H**	-29.07	46.84	-38.76	-12.52	-33.51
F	-27.25	48.48	-39.13	-12.94	-30.85	**F**	-29.51	47.44	-39.62	-12.66	-34.35
CN	-28.92	49.81	-39.92	-13.13	-32.16	**CN**	-30.25	47.82	-40.10	-12.67	-35.20

* In NH_2b the hydrogen atoms of the amino group point towards the other phenyl ring.

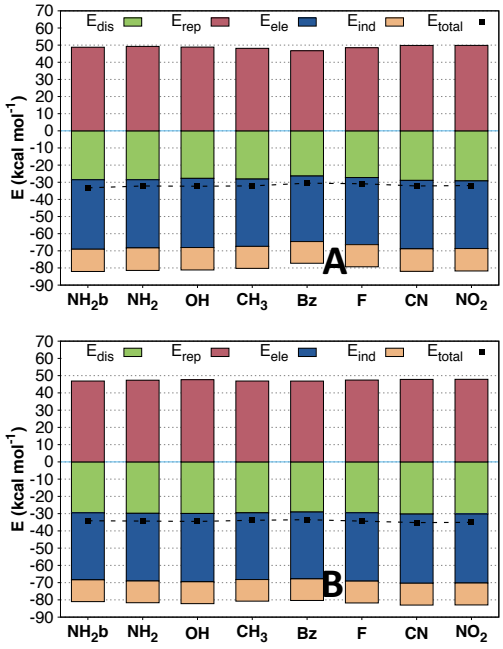

Figure S18. Contributions to the total interaction energy obtained for **1-A** and **1-B** dimers at the F-SAPT0/jun-cc-pVDZ level.

Table S5. Energy differences (kcal mol^{-1}) obtained for **1-A** and **1-B** dimers relative to unsubstituted dimers as obtained with F-SAPT0/jun-cc-pVDZ.

			1-A						1-B		
	E_{dis}	E_{rep}	E_{ele}	E_{ind}	E_{tot}		E_{dis}	E_{rep}	E_{ele}	E_{ind}	E_{tot}
NH_2b*	-2.16	2.06	-2.29	-0.36	-2.75	**NH_2b***	-0.45	0.04	-0.10	-0.11	-0.63
NH_2	-2.16	2.55	-1.53	-0.50	-1.63	**NH_2**	-0.75	0.51	-0.47	-0.09	-0.80
OH	-1.37	2.13	-2.10	-0.46	-1.80	**OH**	-0.82	0.82	-0.84	-0.18	-1.02
CH_3	-1.75	1.42	-1.05	-0.20	-1.58	**CH_3**	-0.45	0.05	0.07	0.00	-0.33
F	-0.88	1.76	-0.89	-0.30	-0.32	**F**	-0.44	0.60	-0.86	-0.14	-0.84
CN	-2.55	3.09	-1.68	-0.49	-1.63	**CN**	-1.18	0.98	-1.34	-0.15	-1.69
NO_2	-2.84	3.13	-1.22	-0.45	-1.38	**NO_2**	-1.13	1.04	-1.26	-0.20	-1.54

* In NH_2b the hydrogen atoms of the amino group point towards the other phenyl ring.

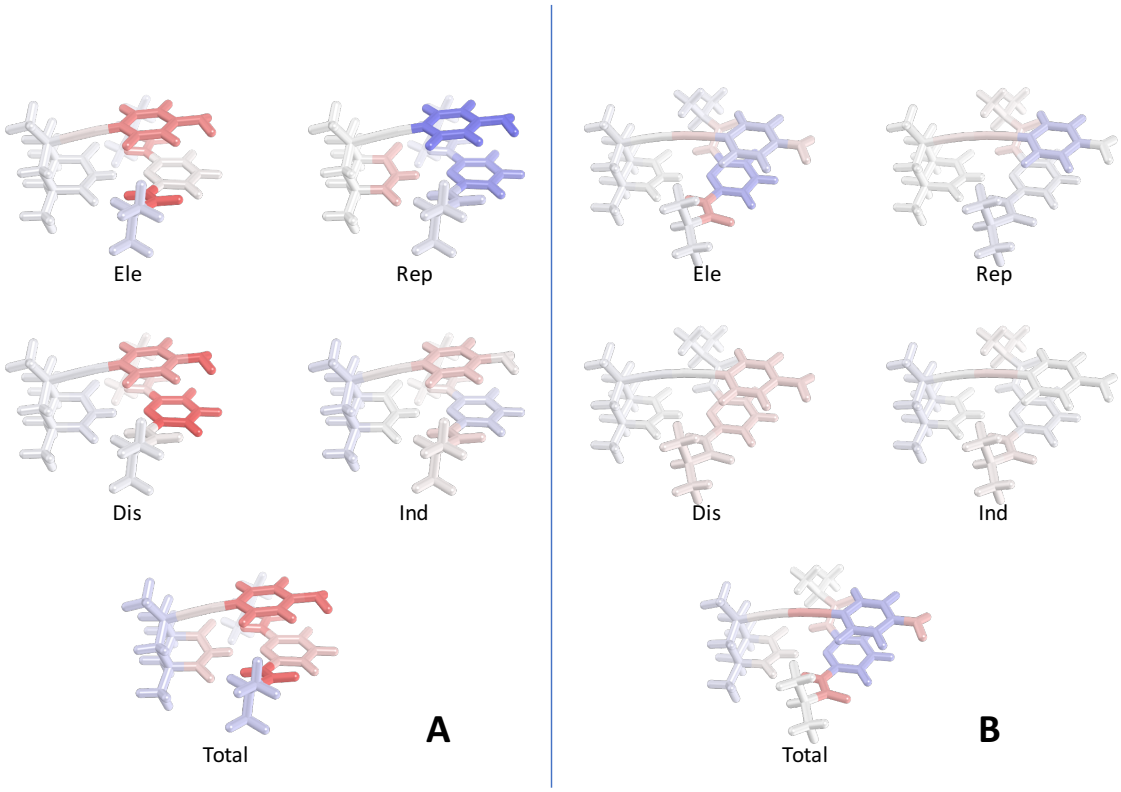

Figure S19. Energy changes relative to unsubstituted complexes at the F-SAPT0/jun-cc-pVDZ level. Substituent = NH_2b. The colour scale runs from -3.0 kcal mol^{-1} (red) to +3.0 kcal mol^{-1} (blue).

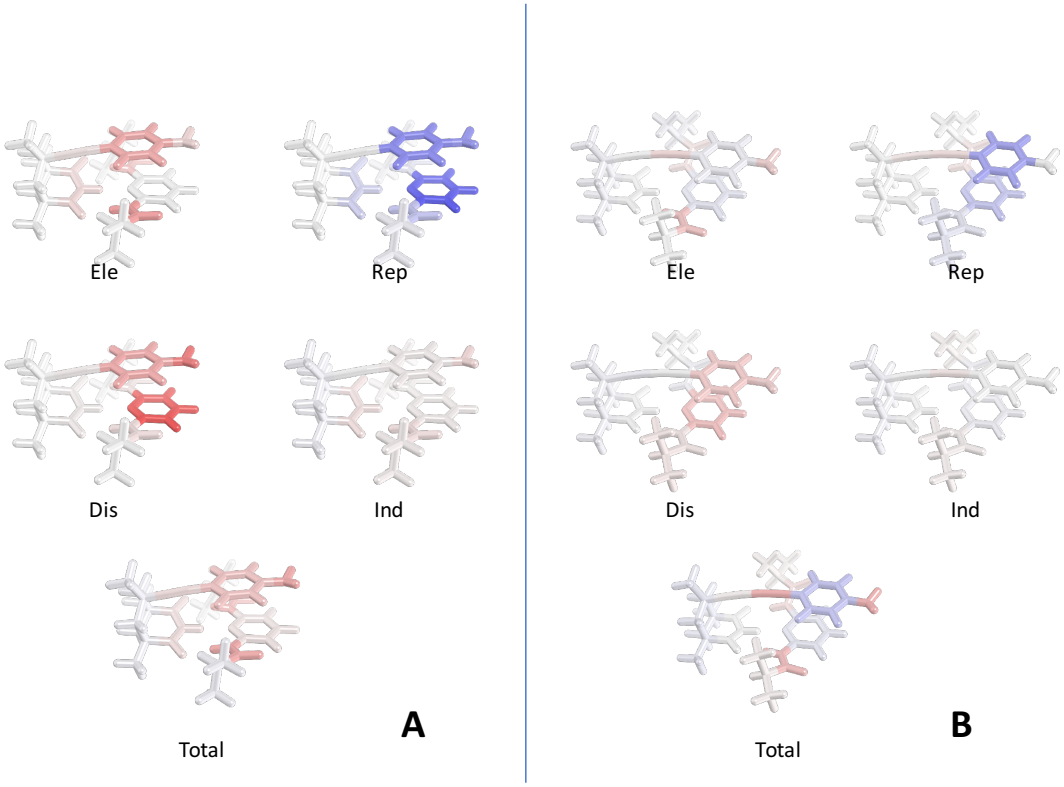

Figure S20. Energy changes relative to unsubstituted complexes at the F-SAPT0/jun-cc-pVDZ level. Substituent = NH_2. The colour scale runs -3.0 kcal mol^{-1} (red) to +3.0 kcal mol^{-1} (blue).

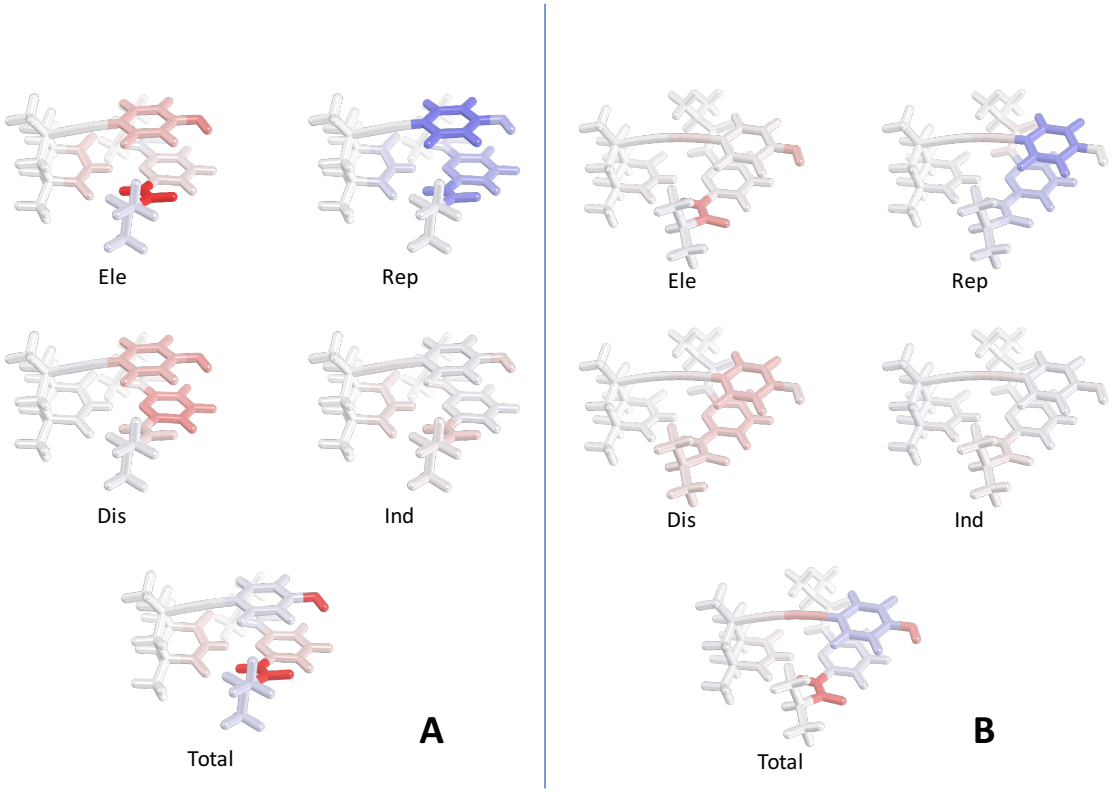

Figure S21. Energy changes relative to unsubstituted complexes at the F-SAPT0/jun-cc-pVDZ level. Substituent = OH. The colour scale runs from -3.0 kcal mol^{-1} (red) to +3.0 kcal mol^{-1} (blue).

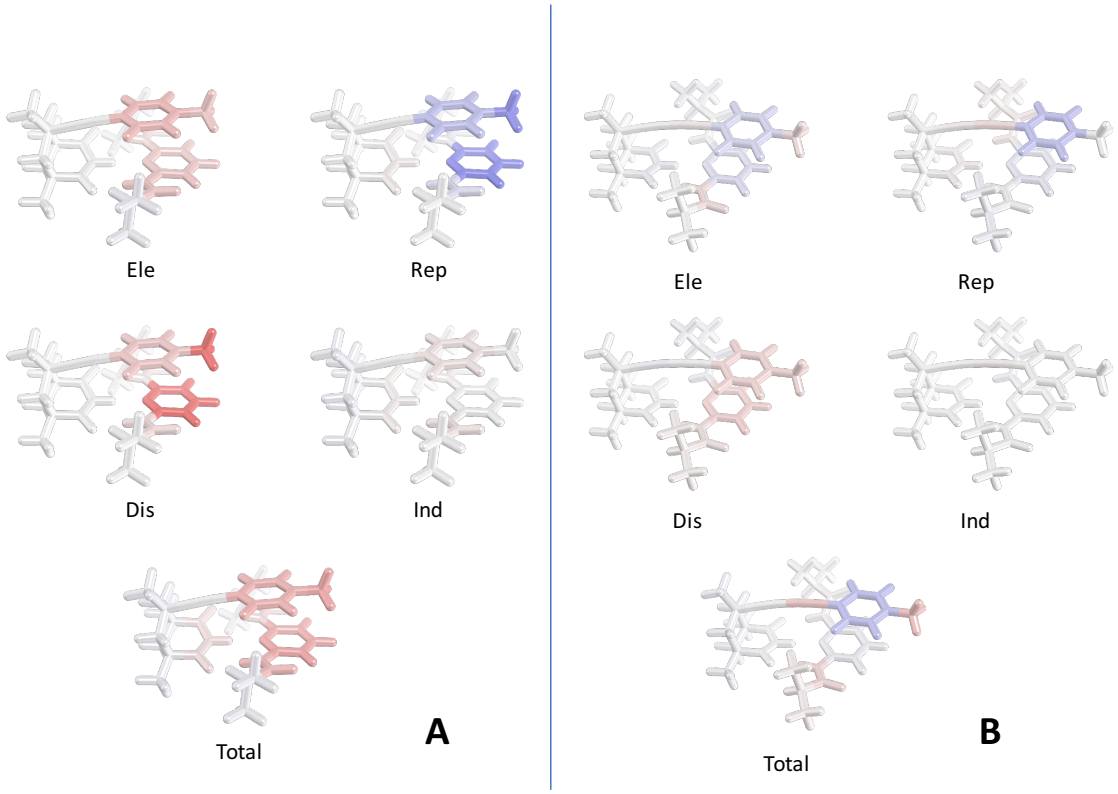

Figure S22. Energy changes relative to unsubstituted complexes at the F-SAPT0/jun-cc-pVDZ level. Substituent = CH_3. The colour scale runs from -3.0 kcal mol^{-1} (red) to +3.0 kcal mol^{-1} (blue).

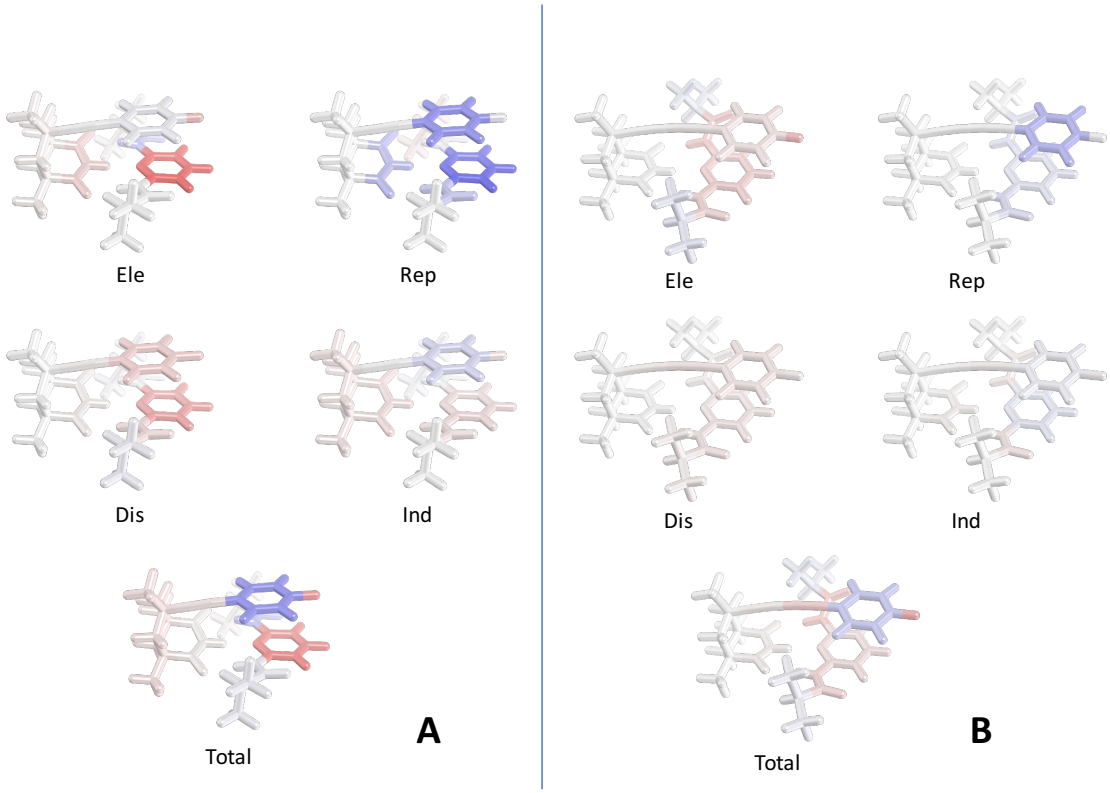

Figure S23. Energy changes relative to unsubstituted complexes at the F-SAPT0/jun-cc-pVDZ level. Substituent = F. The colour scale runs from -3.0 kcal mol^{-1} (red) to +3.0 kcal mol^{-1} (blue).

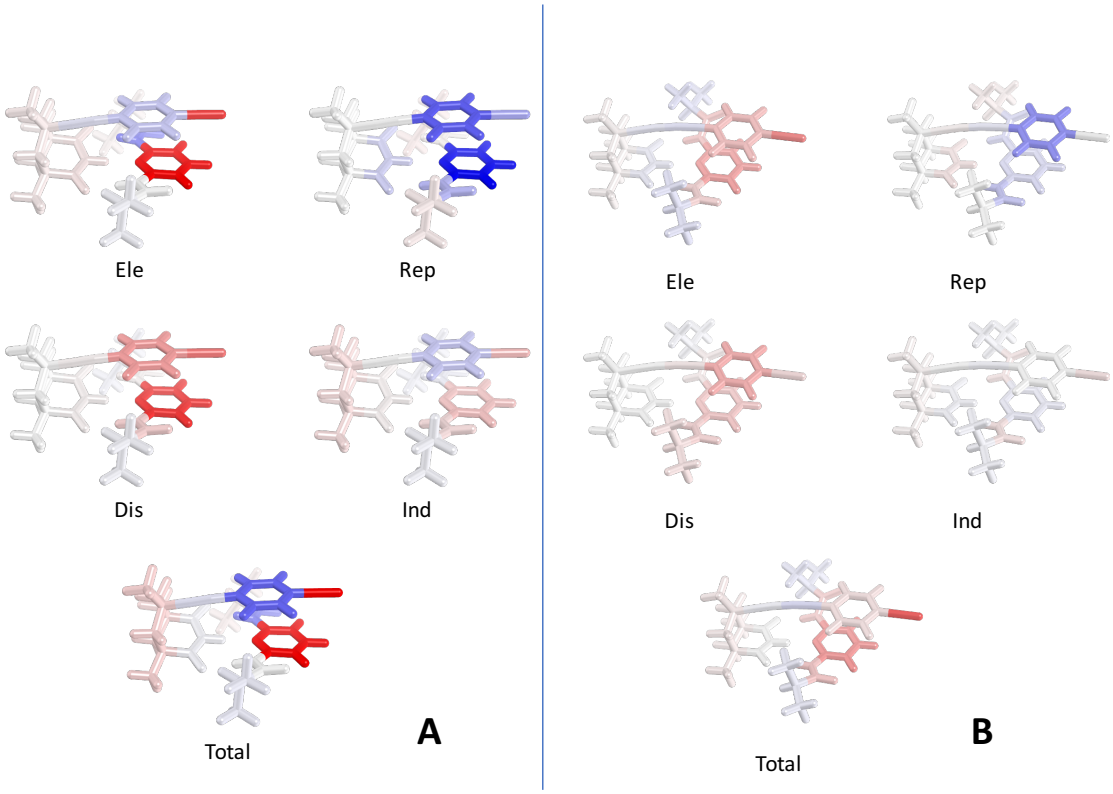

Figure S24. Energy changes relative to unsubstituted complexes at the F-SAPT0/jun-cc-pVDZ level. Substituent = CN. The colour scale runs from -3.0 kcal mol^{-1} (red) to +3.0 kcal mol^{-1} (blue).

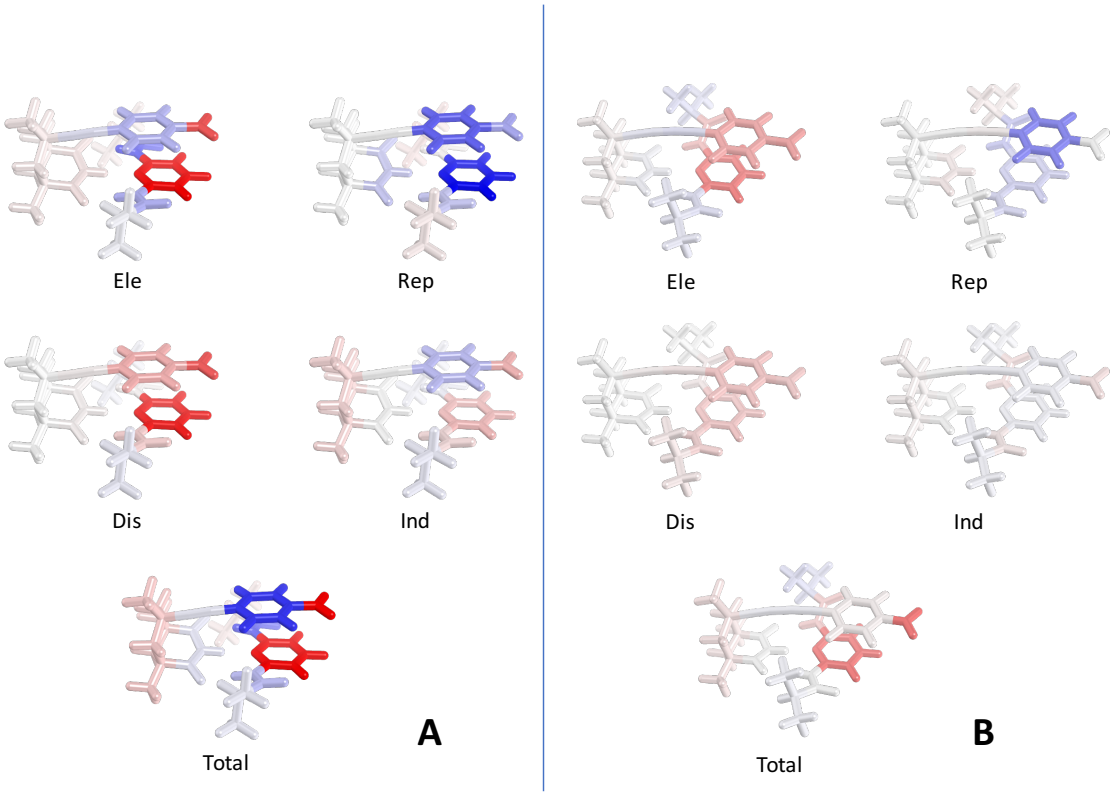

Figure S25. Energy changes relative to unsubstituted complexes at the F-SAPT0/jun-cc-pVDZ level. Substituent = NO_2. The colour scale runs from -3.0 kcal mol^{-1} (red) to +3.0 kcal mol^{-1} (blue).

Table S6. Optimised geometry (Å) and interaction energy (kcal mol^{-1}) for dimers **1-A** and **1-B** at the PBE0-D3BJ/def2-TZVP level. Only the substituent is optimised while keeping the rest of the molecule frozen at the optimised geometry obtained for the unsubstituted dimer.

	R_{centr}	R_1	R_2	ΔE_{int}	ΔE_{com}		R_{centr}	R_1	R_2	ΔE_{int}	ΔE_{com}
NH_2b*	3.70	3.34	-1.59	-29.72	-26.03	**NH_2b***	3.70	3.53	1.09	-30.79	-26.10
NH_2	3.70	3.34	-1.59	-28.73	-25.02	**OHb**	3.70	3.53	1.09	-30.84	-26.14
OH	3.70	3.34	-1.59	-28.89	-25.34	**OH**	3.70	3.53	1.09	-30.81	-26.29
CH_3	3.70	3.34	-1.59	-28.92	-25.28	**CH_3**	3.70	3.53	1.09	-30.52	-25.90
Bz	3.70	3.34	-1.59	-27.63	-24.20	**Bz**	3.70	3.53	1.09	-30.24	-25.84
F	3.70	3.34	-1.59	-27.76	-23.99	**F**	3.70	3.53	1.09	-30.67	-25.90
CN	3.70	3.34	-1.59	-28.21	-24.60	**CN**	3.70	3.53	1.09	-30.94	-26.39
NO_2	3.70	3.34	-1.59	-27.90	-24.05	**NO_2**	3.70	3.53	1.09	-30.73	-25.94

* In NH_2b the hydrogen atoms of the amino group point towards the other phenyl ring.

Table S7. Interaction energies and their components (kcal mol^{-1}) as obtained at the F-SAPT0 level for the optimised structures of **1-A** and **1-B** dimers. Only the substituent is optimised while keeping the rest of the molecule frozen at the optimised geometry obtained for the unsubstituted dimer.

			R_2<0						R_2>0		
	E_{dis}	E_{rep}	E_{ele}	E_{ind}	E_{tot}		E_{dis}	E_{rep}	E_{ele}	E_{ind}	E_{tot}
NH_2b	-27.20	46.90	-39.30	-12.92	-32.53	**NH_2b**	-29.29	46.77	-38.95	-12.66	-34.13
NH_2	-27.10	46.66	-38.35	-12.77	-31.56	**NH_2**	-29.24	46.67	-39.02	-12.62	-34.22
OH	-26.67	46.51	-38.81	-12.75	-31.72	**OH**	-29.11	46.70	-39.14	-12.59	-34.14
CH_3	-27.48	47.04	-38.72	-12.75	-31.91	**CH_3**	-29.34	46.82	-38.76	-12.56	-33.84
Bz	-26.37	46.72	-38.24	-12.64	-30.53	**Bz**	-29.07	46.84	-38.76	-12.52	-33.51
F	-26.24	46.28	-37.91	-12.56	-30.42	**F**	-28.96	46.69	-39.14	-12.54	-33.95
CN	-27.32	46.68	-38.00	-12.60	-31.24	**CN**	-29.24	46.73	-39.29	-12.52	-34.32
NO_2	-27.52	46.61	-37.43	-12.55	-30.89	**NO_2**	-29.24	46.74	-39.12	-12.50	-34.12

* In NH_2b the hydrogen atoms of the amino group point towards the other phenyl ring.

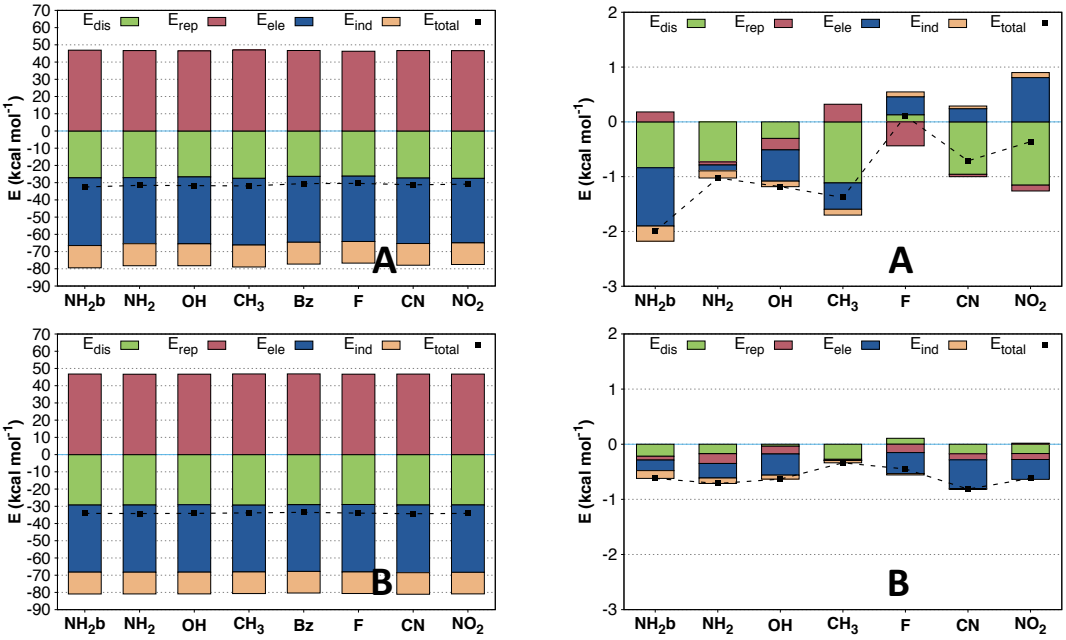

Figure S26. Contributions to the total interaction energy (left) and differences relative to the unsubstituted dimer (right) obtained for **1-A** and **1-B** complexes. Only the substituent while keeping the rest of the molecule frozen at the optimised geometry obtained for the unsubstituted dimer.

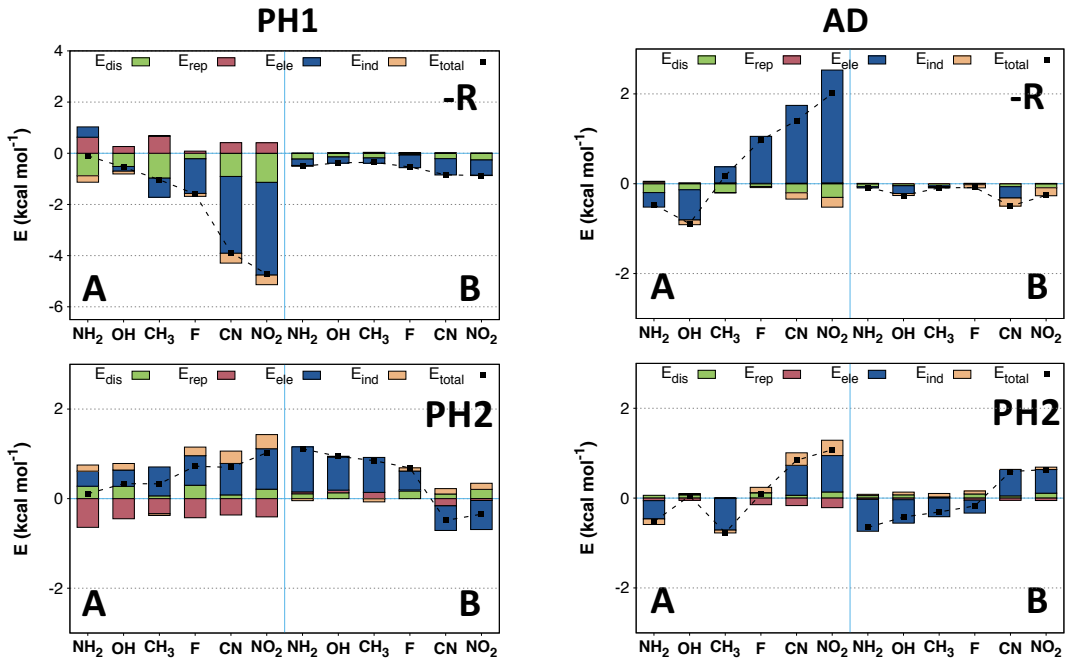

Figure S27. Contributions to the energy differences from interactions of the PH1 group (left) and AD1+AD1+IP1+IP2 (right) relative to the unsubstituted dimer optimizing only the substituent while keeping the rest of the molecule frozen at the optimized geometry obtained for the unsubstituted dimer.

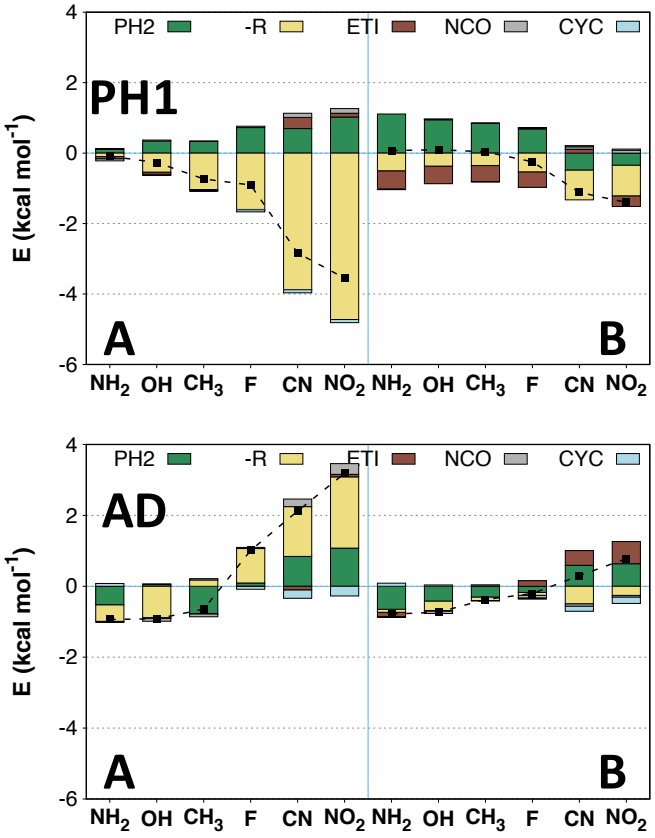

Figure S28. Contributions to the energy differences from interactions of the PH1 group (top) and AD1+AD1+IP1+IP2 (bottom) with the fragments defined in molecules **A** and **B** relative to the unsubstituted dimer optimising only the substituent while keeping the rest of the molecule frozen at the optimised geometry obtained for the unsubstituted dimer.

Energy contributions (kcal mol^{-1}) and its components for each pair of fragments as defined in Figure 8 at the F-SAPT0/jun-cc-pVDZ level in complexes 1-A.

1A

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	PH2	1.212	5.563	-0.099	-0.290	-6.419	-0.033
PH1	ET1	-0.266	0.035	0.112	-0.009	-0.409	-0.536
PH1	NCO	-17.015	12.804	-2.964	-1.828	-3.853	-12.856
PH1	CYC	-2.286	0.152	-0.212	0.054	-0.417	-2.709
PH1	R	-0.429	0.115	-0.011	-0.003	-0.173	-0.502
AD1	PH2	-1.311	3.161	0.059	-0.536	-2.809	-1.435
AD1	ET1	-1.517	0.018	-0.157	-0.072	-0.245	-1.975
AD1	NCO	-10.224	9.794	-1.031	-1.990	-2.555	-6.005
AD1	CYC	2.069	0.053	0.196	-0.142	-0.249	1.927
AD1	R	0.391	0.001	0.012	-0.006	-0.027	0.372
AD2	PH2	-1.354	0.396	0.090	-0.096	-0.988	-1.951
AD2	ET1	-0.528	0.004	-0.080	-0.020	-0.092	-0.715
AD2	NCO	-10.480	9.696	-1.026	-1.994	-2.583	-6.386
AD2	CYC	2.065	0.053	0.168	-0.137	-0.233	1.916
AD2	R	0.377	-0.000	0.015	-0.000	-0.010	0.382
IP1	PH2	-0.843	0.462	-0.057	0.209	-1.125	-1.356
IP1	ET1	0.511	0.010	-0.092	0.023	-0.174	0.279
IP1	NCO	0.837	2.092	-0.736	0.136	-1.424	0.905
IP1	CYC	-0.137	0.012	0.141	0.024	-0.356	-0.315
IP1	R	-0.019	0.000	0.013	0.002	-0.007	-0.012
IP2	PH2	-0.234	0.003	0.011	0.079	-0.217	-0.357
IP2	ET1	0.152	0.001	-0.042	0.008	-0.041	0.079
IP2	NCO	0.908	2.250	-0.680	0.147	-1.515	1.110
IP2	CYC	-0.076	0.040	0.127	0.022	-0.443	-0.330
IP2	R	-0.041	0.000	0.015	0.001	-0.002	-0.028

1A-NH_2b

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	PH2	1.511	6.349	-0.321	-0.329	-6.999	0.211
PH1	ET1	-0.571	0.026	0.078	-0.009	-0.394	-0.871
PH1	NCO	-16.488	11.628	-2.623	-1.757	-3.659	-12.899
PH1	CYC	-2.273	0.139	-0.086	0.055	-0.404	-2.568
PH1	R	-1.049	1.443	0.050	-0.031	-1.456	-1.044
AD1	PH2	-2.216	3.309	-0.006	-0.521	-2.775	-2.209
AD1	ET1	-1.277	0.011	-0.159	-0.058	-0.202	-1.685
AD1	NCO	-10.511	9.941	-1.131	-2.052	-2.562	-6.316
AD1	CYC	2.096	0.055	0.226	-0.142	-0.239	1.996
AD1	R	-0.249	0.047	-0.037	-0.039	-0.153	-0.430
AD2	PH2	-2.035	0.859	0.045	-0.144	-1.357	-2.632
AD2	ET1	-0.577	0.004	-0.098	-0.024	-0.105	-0.800
AD2	NCO	-10.647	9.616	-1.096	-2.012	-2.546	-6.685
AD2	CYC	2.107	0.054	0.198	-0.139	-0.227	1.992
AD2	R	0.134	0.017	-0.018	-0.005	-0.083	0.045
IP1	PH2	-0.718	0.338	-0.070	0.206	-1.011	-1.255
IP1	ET1	0.467	0.005	-0.094	0.018	-0.141	0.255
IP1	NCO	0.830	2.333	-0.784	0.131	-1.465	1.045
IP1	CYC	-0.136	0.012	0.147	0.023	-0.339	-0.293
IP1	R	0.174	0.001	0.008	0.013	-0.034	0.161
IP2	PH2	-0.237	0.013	-0.020	0.098	-0.317	-0.464
IP2	ET1	0.204	0.001	-0.052	0.009	-0.050	0.112
IP2	NCO	0.925	2.552	-0.776	0.145	-1.589	1.257
IP2	CYC	-0.096	0.028	0.143	0.022	-0.404	-0.306
IP2	R	0.099	0.000	0.014	0.006	-0.018	0.102

1A-NH_2

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	**PH2**	1.370	6.408	0.017	-0.290	-7.057	0.449
PH1	**ET1**	-0.484	0.037	0.141	-0.011	-0.435	-0.753
PH1	**NCO**	-17.028	12.644	-2.914	-1.841	-3.835	-12.973
PH1	**CYC**	-2.334	0.150	-0.224	0.056	-0.419	-2.771
PH1	**R**	-0.275	1.107	-0.251	-0.034	-1.278	-0.730
AD1	**PH2**	-1.909	3.401	0.011	-0.554	-2.875	-1.927
AD1	**ET1**	-1.518	0.019	-0.171	-0.071	-0.250	-1.991
AD1	**NCO**	-10.422	10.045	-1.062	-2.072	-2.591	-6.101
AD1	**CYC**	2.096	0.054	0.213	-0.147	-0.253	1.964
AD1	**R**	0.232	0.034	0.035	-0.032	-0.131	0.138
AD2	**PH2**	-1.866	0.526	0.047	-0.111	-1.121	-2.525
AD2	**ET1**	-0.528	0.004	-0.087	-0.021	-0.099	-0.730
AD2	**NCO**	-10.547	9.775	-1.048	-2.027	-2.589	-6.436
AD2	**CYC**	2.108	0.054	0.185	-0.139	-0.231	1.976
AD2	**R**	0.281	0.008	0.045	-0.002	-0.064	0.267
IP1	**PH2**	-0.758	0.377	-0.072	0.203	-1.023	-1.273
IP1	**ET1**	0.553	0.011	-0.102	0.023	-0.173	0.313
IP1	**NCO**	0.803	2.246	-0.784	0.135	-1.460	0.940
IP1	**CYC**	-0.133	0.013	0.153	0.025	-0.367	-0.309
IP1	**R**	-0.112	0.000	-0.001	0.011	-0.031	-0.133
IP2	**PH2**	-0.182	0.005	-0.012	0.081	-0.243	-0.350
IP2	**ET1**	0.180	0.001	-0.045	0.009	-0.043	0.101
IP2	**NCO**	0.906	2.320	-0.726	0.146	-1.528	1.118
IP2	**CYC**	-0.074	0.031	0.138	0.022	-0.418	-0.299
IP2	**R**	-0.128	0.000	0.012	0.004	-0.014	-0.126

1A-OH

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	**PH2**	1.465	5.975	0.057	-0.270	-6.718	0.509
PH1	**ET1**	-0.417	0.031	0.091	-0.009	-0.404	-0.709
PH1	**NCO**	-16.933	12.553	-2.888	-1.836	-3.815	-12.920
PH1	**CYC**	-2.294	0.150	-0.222	0.054	-0.414	-2.727
PH1	**R**	-0.831	0.697	-0.153	-0.011	-0.885	-1.183
AD1	**PH2**	-1.699	4.034	0.038	-0.636	-3.065	-1.328
AD1	**ET1**	-1.384	0.015	-0.170	-0.064	-0.223	-1.827
AD1	**NCO**	-10.488	9.860	-1.130	-2.033	-2.554	-6.346
AD1	**CYC**	2.041	0.054	0.222	-0.141	-0.244	1.933
AD1	**R**	-1.276	0.034	-0.079	-0.034	-0.123	-1.478
AD2	**PH2**	-1.738	0.416	0.082	-0.100	-1.016	-2.356
AD2	**ET1**	-0.529	0.004	-0.086	-0.020	-0.096	-0.728
AD2	**NCO**	-10.619	9.943	-1.042	-2.059	-2.612	-6.389
AD2	**CYC**	2.087	0.054	0.170	-0.139	-0.234	1.938
AD2	**R**	1.045	0.004	0.027	-0.001	-0.042	1.032
IP1	**PH2**	-0.931	0.416	-0.055	0.224	-1.096	-1.441
IP1	**ET1**	0.494	0.006	-0.094	0.021	-0.151	0.276
IP1	**NCO**	0.824	2.201	-0.765	0.130	-1.412	0.978
IP1	**CYC**	-0.120	0.012	0.137	0.023	-0.339	-0.288
IP1	**R**	0.323	0.000	-0.024	0.009	-0.028	0.281
IP2	**PH2**	-0.202	0.003	-0.001	0.078	-0.219	-0.341
IP2	**ET1**	0.173	0.001	-0.044	0.008	-0.043	0.095
IP2	**NCO**	0.900	2.343	-0.699	0.150	-1.547	1.147
IP2	**CYC**	-0.082	0.041	0.133	0.023	-0.446	-0.331
IP2	**R**	-0.146	-0.000	0.025	0.002	-0.009	-0.128

1A-CH_3

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	**PH2**	1.652	5.797	-0.149	-0.303	-6.692	0.304
PH1	**ET1**	-0.330	0.030	0.103	-0.009	-0.400	-0.606
PH1	**NCO**	-16.961	12.635	-2.927	-1.830	-3.824	-12.907
PH1	**CYC**	-2.287	0.150	-0.181	0.054	-0.414	-2.677
PH1	**R**	-1.281	1.097	0.027	-0.030	-1.324	-1.511
AD1	**PH2**	-1.887	3.386	0.025	-0.547	-2.902	-1.925
AD1	**ET1**	-1.465	0.015	-0.157	-0.068	-0.234	-1.909
AD1	**NCO**	-10.260	9.759	-1.061	-1.996	-2.547	-6.105
AD1	**CYC**	2.077	0.053	0.207	-0.141	-0.245	1.951
AD1	**R**	0.484	0.024	0.011	-0.049	-0.158	0.312
AD2	**PH2**	-1.846	0.441	0.071	-0.096	-1.038	-2.469
AD2	**ET1**	-0.520	0.004	-0.084	-0.020	-0.093	-0.713
AD2	**NCO**	-10.524	9.740	-1.054	-2.017	-2.588	-6.443
AD2	**CYC**	2.077	0.053	0.177	-0.138	-0.233	1.935
AD2	**R**	0.627	0.004	0.020	0.009	-0.058	0.601
IP1	**PH2**	-0.828	0.463	-0.073	0.212	-1.141	-1.367
IP1	**ET1**	0.502	0.009	-0.094	0.022	-0.166	0.273
IP1	**NCO**	0.842	2.112	-0.750	0.135	-1.422	0.916
IP1	**CYC**	-0.137	0.012	0.145	0.024	-0.349	-0.305
IP1	**R**	0.028	0.000	0.019	0.015	-0.035	0.028
IP2	**PH2**	-0.193	0.004	-0.008	0.080	-0.225	-0.342
IP2	**ET1**	0.161	0.001	-0.044	0.008	-0.041	0.085
IP2	**NCO**	0.904	2.305	-0.704	0.148	-1.531	1.123
IP2	**CYC**	-0.078	0.040	0.132	0.022	-0.443	-0.327
IP2	**R**	-0.045	0.000	0.026	0.003	-0.013	-0.029

1A-F

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	**PH2**	1.551	6.407	0.075	-0.272	-6.827	0.932
PH1	**ET1**	-0.247	0.040	0.104	-0.014	-0.446	-0.562
PH1	**NCO**	-17.190	13.219	-3.086	-1.890	-3.933	-12.881
PH1	**CYC**	-2.294	0.157	-0.299	0.054	-0.427	-2.808
PH1	**R**	-2.047	0.278	-0.132	-0.006	-0.447	-2.354
AD1	**PH2**	-1.280	3.433	0.137	-0.573	-2.922	-1.204
AD1	**ET1**	-1.601	0.025	-0.180	-0.079	-0.276	-2.111
AD1	**NCO**	-10.356	9.957	-1.058	-2.053	-2.590	-6.100
AD1	**CYC**	2.015	0.053	0.183	-0.146	-0.258	1.846
AD1	**R**	0.626	0.011	-0.037	-0.012	-0.061	0.528
AD2	**PH2**	-1.445	0.337	0.127	-0.083	-0.947	-2.011
AD2	**ET1**	-0.521	0.005	-0.081	-0.018	-0.092	-0.707
AD2	**NCO**	-10.442	9.841	-1.021	-2.021	-2.608	-6.251
AD2	**CYC**	2.038	0.054	0.152	-0.137	-0.234	1.873
AD2	**R**	1.025	0.001	0.009	-0.001	-0.023	1.012
IP1	**PH2**	-0.985	0.390	-0.056	0.207	-1.031	-1.475
IP1	**ET1**	0.558	0.013	-0.090	0.026	-0.186	0.322
IP1	**NCO**	0.798	2.141	-0.730	0.137	-1.434	0.913
IP1	**CYC**	-0.120	0.014	0.130	0.025	-0.372	-0.324
IP1	**R**	0.124	0.000	0.015	0.004	-0.015	0.128
IP2	**PH2**	-0.269	0.002	0.017	0.073	-0.197	-0.375
IP2	**ET1**	0.145	0.001	-0.038	0.009	-0.039	0.078
IP2	**NCO**	0.891	2.063	-0.627	0.147	-1.459	1.016
IP2	**CYC**	-0.059	0.034	0.114	0.022	-0.426	-0.315
IP2	**R**	-0.048	-0.000	0.033	0.001	-0.005	-0.019

1A-CN

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	**PH2**	1.538	6.983	0.165	-0.245	-7.324	1.117
PH1	**ET1**	0.026	0.035	0.120	-0.014	-0.425	-0.259
PH1	**NCO**	-17.215	13.434	-3.149	-1.904	-3.974	-12.807
PH1	**CYC**	-2.244	0.159	-0.381	0.051	-0.427	-2.842
PH1	**R**	-4.078	0.963	-0.420	-0.059	-1.381	-4.974
AD1	**PH2**	-0.920	3.664	0.219	-0.665	-3.049	-0.751
AD1	**ET1**	-1.537	0.028	-0.170	-0.075	-0.272	-2.025
AD1	**NCO**	-10.381	9.963	-1.061	-2.042	-2.596	-6.117
AD1	**CYC**	1.915	0.053	0.160	-0.142	-0.260	1.725
AD1	**R**	0.344	0.014	-0.134	-0.032	-0.138	0.054
AD2	**PH2**	-1.134	0.368	0.172	-0.093	-1.000	-1.688
AD2	**ET1**	-0.585	0.004	-0.071	-0.016	-0.088	-0.757
AD2	**NCO**	-10.254	9.627	-0.962	-1.956	-2.586	-6.131
AD2	**CYC**	1.987	0.053	0.126	-0.134	-0.234	1.798
AD2	**R**	1.623	0.002	-0.024	0.019	-0.062	1.559
IP1	**PH2**	-1.155	0.364	-0.034	0.224	-1.010	-1.612
IP1	**ET1**	0.536	0.013	-0.072	0.025	-0.181	0.322
IP1	**NCO**	0.781	2.079	-0.672	0.135	-1.395	0.928
IP1	**CYC**	-0.099	0.014	0.109	0.024	-0.369	-0.321
IP1	**R**	0.357	0.000	-0.001	0.012	-0.033	0.335
IP2	**PH2**	-0.360	0.002	0.032	0.076	-0.206	-0.455
IP2	**ET1**	0.121	0.001	-0.035	0.008	-0.037	0.058
IP2	**NCO**	0.888	1.953	-0.561	0.146	-1.427	0.999
IP2	**CYC**	-0.057	0.034	0.098	0.021	-0.428	-0.331
IP2	**R**	-0.018	-0.000	0.047	0.002	-0.014	0.017

1A-NO_2

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	**PH2**	1.726	7.111	0.228	-0.251	-7.264	1.550
PH1	**ET1**	-0.116	0.041	0.069	-0.016	-0.461	-0.483
PH1	**NCO**	-17.257	13.551	-3.177	-1.916	-3.996	-12.795
PH1	**CYC**	-2.234	0.162	-0.393	0.050	-0.431	-2.847
PH1	**R**	-4.831	0.940	-0.453	-0.018	-1.688	-6.049
AD1	**PH2**	-0.947	3.519	0.245	-0.607	-2.973	-0.763
AD1	**ET1**	-1.432	0.030	-0.161	-0.087	-0.284	-1.935
AD1	**NCO**	-10.365	9.939	-1.042	-2.037	-2.597	-6.102
AD1	**CYC**	1.919	0.053	0.146	-0.143	-0.261	1.714
AD1	**R**	1.028	0.018	-0.159	-0.070	-0.201	0.615
AD2	**PH2**	-1.030	0.340	0.189	-0.080	-0.964	-1.546
AD2	**ET1**	-0.488	0.006	-0.064	-0.020	-0.092	-0.659
AD2	**NCO**	-10.249	9.678	-0.948	-1.962	-2.598	-6.079
AD2	**CYC**	1.979	0.053	0.116	-0.134	-0.235	1.780
AD2	**R**	1.932	0.007	-0.046	0.016	-0.083	1.826
IP1	**PH2**	-1.145	0.341	-0.038	0.210	-0.975	-1.606
IP1	**ET1**	0.505	0.013	-0.063	0.030	-0.185	0.300
IP1	**NCO**	0.780	2.096	-0.654	0.136	-1.402	0.956
IP1	**CYC**	-0.103	0.014	0.104	0.025	-0.371	-0.331
IP1	**R**	0.355	0.000	0.009	0.015	-0.044	0.335
IP2	**PH2**	-0.390	0.002	0.038	0.071	-0.196	-0.474
IP2	**ET1**	0.108	0.001	-0.030	0.010	-0.038	0.050
IP2	**NCO**	0.887	1.898	-0.538	0.147	-1.415	0.979
IP2	**CYC**	-0.057	0.036	0.094	0.021	-0.432	-0.338
IP2	**R**	-0.035	-0.000	0.044	-0.000	-0.021	-0.012

Energy contribution (kcal mol^{-1}) and its components for each pair of fragments as defined in Figure 8 at the F-SAPT0/jun-cc-pVDZ level in complexes 1-B.

1B

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	**PH2**	-0.131	6.007	-0.357	-0.092	-6.764	-1.336
PH1	**ET1**	0.126	0.068	0.100	-0.027	-0.483	-0.215
PH1	**ET2**	0.338	2.433	0.220	-0.201	-2.033	0.757
PH1	**NCO**	-16.218	11.346	-2.536	-1.706	-3.619	-12.733
PH1	**CYC**	-2.225	0.135	-0.226	0.056	-0.413	-2.673
PH1	**R**	-0.537	0.006	0.040	-0.002	-0.059	-0.552
AD1	**PH2**	0.017	0.261	0.118	-0.073	-1.001	-0.677
AD1	**ET1**	-0.756	0.001	-0.080	-0.032	-0.132	-0.999
AD1	**ET2**	-1.197	0.081	-0.077	-0.060	-0.367	-1.620
AD1	**NCO**	-10.132	8.865	-0.984	-1.819	-2.406	-6.476
AD1	**CYC**	2.096	0.050	0.179	-0.132	-0.220	1.973
AD1	**R**	0.123	0.000	-0.008	0.000	-0.006	0.110
AD2	**PH2**	-1.284	1.025	0.037	-0.499	-1.232	-1.953
AD2	**ET1**	-1.113	0.010	-0.129	-0.077	-0.230	-1.538
AD2	**ET2**	-0.581	0.251	-0.017	-0.133	-0.582	-1.062
AD2	**NCO**	-10.537	10.302	-1.100	-2.089	-2.618	-6.042
AD2	**CYC**	1.990	0.054	0.199	-0.141	-0.254	1.849
AD2	**R**	-0.046	0.000	-0.018	-0.001	-0.005	-0.069
IP1	**PH2**	-0.476	0.209	-0.017	0.044	-0.616	-0.856
IP1	**ET1**	0.134	0.005	-0.081	0.016	-0.163	-0.088
IP1	**ET2**	0.116	0.098	-0.079	0.044	-0.292	-0.113
IP1	**NCO**	0.991	2.404	-0.817	0.140	-1.546	1.173
IP1	**CYC**	-0.106	0.012	0.161	0.020	-0.339	-0.252
IP1	**R**	0.045	0.000	0.004	0.000	-0.003	0.047
IP2	**PH2**	-0.157	0.016	-0.003	0.128	-0.353	-0.370
IP2	**ET1**	-0.094	0.693	-0.130	-0.003	-0.676	-0.210
IP2	**ET2**	-0.047	0.290	-0.016	0.066	-0.570	-0.276
IP2	**NCO**	0.895	2.164	-0.659	0.149	-1.507	1.043
IP2	**CYC**	-0.067	0.055	0.153	0.023	-0.581	-0.417
IP2	**R**	0.070	0.000	0.002	0.001	-0.002	0.071

1B-NH_2b

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	PH2	0.902	6.484	-0.413	-0.098	-6.896	-0.020
PH1	ET1	-0.034	0.059	0.089	-0.021	-0.464	-0.372
PH1	ET2	0.110	2.139	0.207	-0.196	-1.987	0.272
PH1	NCO	-16.240	11.262	-2.482	-1.686	-3.604	-12.750
PH1	CYC	-2.242	0.134	-0.171	0.056	-0.409	-2.631
PH1	R	-0.388	0.014	0.067	-0.010	-0.302	-0.619
AD1	PH2	-0.371	0.350	0.134	-0.104	-1.108	-1.099
AD1	ET1	-0.706	0.001	-0.080	-0.034	-0.134	-0.952
AD1	ET2	-1.267	0.091	-0.126	-0.078	-0.389	-1.768
AD1	NCO	-10.152	8.906	-1.006	-1.825	-2.414	-6.491
AD1	CYC	2.133	0.050	0.196	-0.133	-0.220	2.025
AD1	R	-0.228	0.001	-0.027	-0.003	-0.035	-0.292
AD2	PH2	-1.334	0.811	0.084	-0.407	-1.164	-2.011
AD2	ET1	-1.085	0.007	-0.130	-0.071	-0.214	-1.493
AD2	ET2	-0.764	0.231	-0.085	-0.139	-0.558	-1.315
AD2	NCO	-10.525	10.272	-1.107	-2.079	-2.608	-6.047
AD2	CYC	2.053	0.054	0.213	-0.141	-0.248	1.931
AD2	R	-0.187	0.001	-0.030	-0.003	-0.025	-0.245
IP1	PH2	-0.596	0.292	-0.036	0.050	-0.693	-0.984
IP1	ET1	0.150	0.006	-0.083	0.015	-0.174	-0.086
IP1	ET2	0.196	0.132	-0.111	0.045	-0.334	-0.072
IP1	NCO	0.986	2.439	-0.843	0.139	-1.557	1.163
IP1	CYC	-0.111	0.012	0.172	0.020	-0.340	-0.247
IP1	R	0.120	0.000	-0.004	0.002	-0.017	0.102
IP2	PH2	-0.290	0.020	-0.008	0.112	-0.362	-0.528
IP2	ET1	-0.011	0.559	-0.140	0.001	-0.623	-0.213
IP2	ET2	0.089	0.337	-0.051	0.063	-0.595	-0.157
IP2	NCO	0.904	2.176	-0.676	0.148	-1.507	1.044
IP2	CYC	-0.076	0.039	0.167	0.023	-0.533	-0.380
IP2	R	0.105	0.000	0.001	0.002	-0.011	0.098

1B-NH_2

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	PH2	0.790	6.891	-0.404	-0.098	-7.099	0.081
PH1	ET1	-0.018	0.060	0.094	-0.021	-0.469	-0.355
PH1	ET2	0.056	2.134	0.263	-0.191	-2.002	0.260
PH1	NCO	-16.227	11.239	-2.481	-1.685	-3.599	-12.754
PH1	CYC	-2.242	0.134	-0.216	0.057	-0.409	-2.678
PH1	R	-0.839	0.012	0.015	-0.012	-0.328	-1.153
AD1	PH2	-0.594	0.337	0.114	-0.095	-1.085	-1.323
AD1	ET1	-0.715	0.001	-0.080	-0.035	-0.134	-0.963
AD1	ET2	-1.222	0.086	-0.116	-0.078	-0.382	-1.712
AD1	NCO	-10.155	8.907	-0.991	-1.826	-2.414	-6.478
AD1	CYC	2.135	0.050	0.191	-0.134	-0.221	2.022
AD1	R	0.211	0.001	0.007	-0.001	-0.034	0.183
AD2	PH2	-1.351	0.918	0.071	-0.433	-1.223	-2.018
AD2	ET1	-1.081	0.007	-0.127	-0.073	-0.216	-1.490
AD2	ET2	-0.786	0.236	-0.081	-0.142	-0.568	-1.341
AD2	NCO	-10.514	10.212	-1.092	-2.069	-2.602	-6.064
AD2	CYC	2.050	0.054	0.210	-0.141	-0.249	1.924
AD2	R	-0.079	0.000	-0.007	-0.004	-0.027	-0.116
IP1	PH2	-0.495	0.231	-0.032	0.048	-0.639	-0.888
IP1	ET1	0.150	0.007	-0.085	0.016	-0.178	-0.090
IP1	ET2	0.192	0.128	-0.105	0.046	-0.330	-0.070
IP1	NCO	0.985	2.487	-0.850	0.139	-1.572	1.189
IP1	CYC	-0.112	0.012	0.174	0.020	-0.344	-0.249
IP1	R	-0.014	0.000	-0.004	0.002	-0.016	-0.032
IP2	PH2	-0.284	0.021	-0.008	0.116	-0.370	-0.525
IP2	ET1	-0.021	0.572	-0.139	0.001	-0.628	-0.215
IP2	ET2	0.098	0.331	-0.049	0.064	-0.594	-0.150
IP2	NCO	0.901	2.237	-0.691	0.148	-1.527	1.068
IP2	CYC	-0.077	0.042	0.170	0.023	-0.545	-0.388
IP2	R	0.030	0.000	-0.005	0.002	-0.011	0.016

1B-OH

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	**PH2**	0.444	6.732	-0.336	-0.095	-7.007	-0.262
PH1	**ET1**	0.025	0.063	0.087	-0.026	-0.480	-0.331
PH1	**ET2**	0.111	2.247	0.211	-0.196	-2.041	0.333
PH1	**NCO**	-16.228	11.317	-2.508	-1.703	-3.618	-12.740
PH1	**CYC**	-2.232	0.135	-0.210	0.056	-0.412	-2.663
PH1	**R**	-0.816	0.008	0.060	-0.008	-0.226	-0.982
AD1	**PH2**	-0.084	0.519	0.143	-0.138	-1.252	-0.812
AD1	**ET1**	-0.719	0.001	-0.083	-0.037	-0.136	-0.974
AD1	**ET2**	-1.258	0.091	-0.117	-0.084	-0.398	-1.766
AD1	**NCO**	-10.178	8.892	-1.019	-1.826	-2.407	-6.539
AD1	**CYC**	2.106	0.050	0.195	-0.133	-0.220	1.999
AD1	**R**	-0.673	0.001	-0.045	-0.003	-0.029	-0.749
AD2	**PH2**	-1.611	0.875	0.059	-0.424	-1.154	-2.256
AD2	**ET1**	-1.092	0.009	-0.129	-0.078	-0.224	-1.515
AD2	**ET2**	-0.627	0.235	-0.053	-0.147	-0.575	-1.166
AD2	**NCO**	-10.556	10.360	-1.108	-2.102	-2.625	-6.032
AD2	**CYC**	2.008	0.054	0.202	-0.142	-0.252	1.871
AD2	**R**	0.328	0.000	-0.013	-0.002	-0.018	0.295
IP1	**PH2**	-0.635	0.328	-0.030	0.055	-0.731	-1.014
IP1	**ET1**	0.141	0.007	-0.086	0.017	-0.179	-0.100
IP1	**ET2**	0.188	0.132	-0.099	0.048	-0.338	-0.068
IP1	**NCO**	1.004	2.411	-0.850	0.140	-1.554	1.151
IP1	**CYC**	-0.107	0.012	0.167	0.020	-0.345	-0.252
IP1	**R**	0.213	0.000	-0.030	0.002	-0.013	0.172
IP2	**PH2**	-0.196	0.013	-0.007	0.112	-0.327	-0.404
IP2	**ET1**	-0.072	0.672	-0.131	-0.001	-0.668	-0.201
IP2	**ET2**	0.038	0.298	-0.029	0.068	-0.583	-0.209
IP2	**NCO**	0.902	2.147	-0.656	0.150	-1.503	1.041
IP2	**CYC**	-0.069	0.049	0.156	0.023	-0.566	-0.407
IP2	**R**	0.044	0.000	0.013	0.002	-0.007	0.050

1B-CH_3

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	**PH2**	0.624	6.464	-0.424	-0.103	-6.950	-0.390
PH1	**ET1**	0.033	0.061	0.092	-0.024	-0.472	-0.310
PH1	**ET2**	0.135	2.181	0.236	-0.193	-2.005	0.355
PH1	**NCO**	-16.212	11.300	-2.521	-1.696	-3.611	-12.741
PH1	**CYC**	-2.228	0.135	-0.211	0.056	-0.410	-2.659
PH1	**R**	-0.773	0.008	0.082	-0.006	-0.260	-0.949
AD1	**PH2**	-0.226	0.320	0.137	-0.078	-1.075	-0.922
AD1	**ET1**	-0.710	0.001	-0.078	-0.034	-0.132	-0.953
AD1	**ET2**	-1.184	0.083	-0.103	-0.076	-0.379	-1.659
AD1	**NCO**	-10.111	8.837	-0.986	-1.813	-2.403	-6.476
AD1	**CYC**	2.111	0.050	0.184	-0.132	-0.220	1.992
AD1	**R**	0.092	0.000	-0.016	-0.002	-0.030	0.043
AD2	**PH2**	-1.234	0.923	0.082	-0.448	-1.200	-1.878
AD2	**ET1**	-1.080	0.008	-0.127	-0.076	-0.220	-1.495
AD2	**ET2**	-0.637	0.232	-0.054	-0.144	-0.568	-1.171
AD2	**NCO**	-10.522	10.275	-1.099	-2.083	-2.611	-6.040
AD2	**CYC**	2.016	0.054	0.203	-0.141	-0.250	1.882
AD2	**R**	-0.106	0.001	-0.030	-0.002	-0.020	-0.158
IP1	**PH2**	-0.594	0.265	-0.024	0.045	-0.669	-0.977
IP1	**ET1**	0.139	0.005	-0.079	0.016	-0.167	-0.086
IP1	**ET2**	0.168	0.113	-0.094	0.046	-0.315	-0.082
IP1	**NCO**	0.989	2.410	-0.826	0.139	-1.548	1.164
IP1	**CYC**	-0.109	0.012	0.165	0.020	-0.338	-0.249
IP1	**R**	0.093	0.000	0.004	0.002	-0.013	0.086
IP2	**PH2**	-0.300	0.017	-0.001	0.120	-0.350	-0.514
IP2	**ET1**	-0.054	0.620	-0.131	-0.000	-0.648	-0.213
IP2	**ET2**	0.045	0.308	-0.033	0.066	-0.584	-0.198
IP2	**NCO**	0.902	2.157	-0.665	0.149	-1.504	1.038
IP2	**CYC**	-0.071	0.046	0.158	0.023	-0.556	-0.400
IP2	**R**	0.118	0.000	0.004	0.002	-0.007	0.116

1B-F

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	**PH2**	0.211	6.322	-0.271	-0.087	-6.763	-0.589
PH1	**ET1**	0.096	0.069	0.084	-0.029	-0.494	-0.275
PH1	**ET2**	0.128	2.372	0.183	-0.194	-2.088	0.401
PH1	**NCO**	-16.151	11.252	-2.498	-1.704	-3.610	-12.710
PH1	**CYC**	-2.216	0.135	-0.220	0.056	-0.414	-2.659
PH1	**R**	-1.069	0.004	0.068	-0.006	-0.134	-1.136
AD1	**PH2**	-0.148	0.371	0.140	-0.088	-1.091	-0.816
AD1	**ET1**	-0.751	0.001	-0.084	-0.038	-0.139	-1.011
AD1	**ET2**	-1.139	0.090	-0.087	-0.084	-0.395	-1.614
AD1	**NCO**	-10.183	8.937	-1.011	-1.836	-2.413	-6.505
AD1	**CYC**	2.083	0.051	0.181	-0.133	-0.221	1.961
AD1	**R**	0.043	0.000	-0.039	-0.000	-0.015	-0.012
AD2	**PH2**	-1.548	1.205	0.044	-0.507	-1.283	-2.089
AD2	**ET1**	-1.074	0.009	-0.131	-0.082	-0.230	-1.507
AD2	**ET2**	-0.607	0.246	-0.036	-0.156	-0.594	-1.147
AD2	**NCO**	-10.599	10.367	-1.138	-2.106	-2.625	-6.101
AD2	**CYC**	1.976	0.054	0.203	-0.141	-0.254	1.839
AD2	**R**	-0.252	0.001	-0.058	-0.003	-0.013	-0.325
IP1	**PH2**	-0.507	0.211	-0.026	0.045	-0.620	-0.896
IP1	**ET1**	0.133	0.009	-0.084	0.019	-0.186	-0.109
IP1	**ET2**	0.142	0.127	-0.074	0.049	-0.332	-0.089
IP1	**NCO**	0.999	2.402	-0.814	0.141	-1.551	1.177
IP1	**CYC**	-0.105	0.012	0.156	0.020	-0.348	-0.264
IP1	**R**	0.162	0.000	-0.001	0.001	-0.007	0.155
IP2	**PH2**	-0.195	0.016	-0.004	0.127	-0.344	-0.400
IP2	**ET1**	-0.096	0.675	-0.125	0.000	-0.669	-0.215
IP2	**ET2**	0.007	0.286	-0.013	0.071	-0.579	-0.227
IP2	**NCO**	0.905	2.157	-0.661	0.150	-1.508	1.042
IP2	**CYC**	-0.065	0.055	0.147	0.023	-0.581	-0.421
IP2	**R**	0.198	0.000	0.001	0.001	-0.005	0.195

1B-CN

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	**PH2**	-0.829	6.389	-0.239	-0.063	-7.020	-1.762
PH1	**ET1**	0.274	0.072	0.084	-0.031	-0.492	-0.093
PH1	**ET2**	0.346	2.531	0.167	-0.197	-2.064	0.782
PH1	**NCO**	-16.014	11.123	-2.459	-1.692	-3.596	-12.638
PH1	**CYC**	-2.173	0.134	-0.239	0.055	-0.413	-2.636
PH1	**R**	-1.209	0.013	0.051	-0.014	-0.302	-1.461
AD1	**PH2**	0.222	0.634	0.128	-0.179	-1.299	-0.494
AD1	**ET1**	-0.812	0.002	-0.086	-0.043	-0.145	-1.084
AD1	**ET2**	-1.032	0.103	-0.039	-0.086	-0.412	-1.466
AD1	**NCO**	-10.193	8.967	-1.021	-1.829	-2.413	-6.488
AD1	**CYC**	2.029	0.051	0.173	-0.131	-0.221	1.901
AD1	**R**	-0.391	0.001	-0.091	-0.006	-0.037	-0.524
AD2	**PH2**	-1.370	1.376	0.010	-0.536	-1.370	-1.889
AD2	**ET1**	-1.031	0.009	-0.121	-0.080	-0.223	-1.446
AD2	**ET2**	-0.439	0.217	0.025	-0.144	-0.569	-0.911
AD2	**NCO**	-10.614	10.336	-1.148	-2.091	-2.617	-6.133
AD2	**CYC**	1.931	0.054	0.193	-0.139	-0.251	1.788
AD2	**R**	-0.599	0.001	-0.109	-0.007	-0.027	-0.741
IP1	**PH2**	-0.482	0.215	-0.029	0.063	-0.653	-0.885
IP1	**ET1**	0.115	0.017	-0.084	0.020	-0.213	-0.145
IP1	**ET2**	0.053	0.155	-0.031	0.050	-0.361	-0.134
IP1	**NCO**	1.014	2.341	-0.776	0.142	-1.539	1.182
IP1	**CYC**	-0.100	0.012	0.141	0.020	-0.359	-0.286
IP1	**R**	0.328	0.000	-0.018	0.004	-0.016	0.298
IP2	**PH2**	-0.108	0.019	-0.012	0.132	-0.370	-0.339
IP2	**ET1**	-0.102	0.589	-0.104	0.004	-0.632	-0.246
IP2	**ET2**	-0.108	0.273	0.021	0.070	-0.553	-0.297
IP2	**NCO**	0.922	2.133	-0.651	0.151	-1.506	1.049
IP2	**CYC**	-0.062	0.052	0.129	0.022	-0.568	-0.426
IP2	**R**	0.340	0.000	-0.008	0.004	-0.011	0.325

1B-NO_2

Frag1	Frag2	Elst	Exch	IndAB	IndBA	Disp	Total
PH1	**PH2**	-0.893	6.498	-0.204	-0.082	-6.893	-1.573
PH1	**ET1**	0.234	0.069	0.076	-0.032	-0.499	-0.151
PH1	**ET2**	0.137	2.396	0.152	-0.185	-2.095	0.404
PH1	**NCO**	-16.043	11.224	-2.492	-1.707	-3.614	-12.631
PH1	**CYC**	-2.167	0.135	-0.241	0.055	-0.415	-2.633
PH1	**R**	-1.217	0.011	0.027	-0.011	-0.359	-1.548
AD1	**PH2**	0.403	0.534	0.151	-0.119	-1.234	-0.265
AD1	**ET1**	-0.754	0.002	-0.080	-0.045	-0.143	-1.020
AD1	**ET2**	-0.951	0.096	-0.048	-0.099	-0.413	-1.415
AD1	**NCO**	-10.147	8.873	-1.005	-1.815	-2.402	-6.495
AD1	**CYC**	2.026	0.050	0.165	-0.130	-0.221	1.890
AD1	**R**	-0.212	0.001	-0.094	-0.008	-0.051	-0.364
AD2	**PH2**	-1.749	1.466	-0.008	-0.550	-1.354	-2.195
AD2	**ET1**	-0.999	0.010	-0.120	-0.088	-0.230	-1.428
AD2	**ET2**	-0.324	0.218	0.021	-0.167	-0.586	-0.838
AD2	**NCO**	-10.645	10.436	-1.163	-2.112	-2.634	-6.118
AD2	**CYC**	1.908	0.055	0.190	-0.139	-0.254	1.759
AD2	**R**	-0.379	0.001	-0.108	-0.003	-0.034	-0.524
IP1	**PH2**	-0.547	0.246	-0.029	0.051	-0.665	-0.943
IP1	**ET1**	0.107	0.011	-0.076	0.021	-0.196	-0.132
IP1	**ET2**	0.083	0.139	-0.035	0.052	-0.350	-0.112
IP1	**NCO**	1.014	2.309	-0.764	0.142	-1.527	1.172
IP1	**CYC**	-0.101	0.012	0.135	0.020	-0.349	-0.283
IP1	**R**	0.319	0.000	-0.012	0.003	-0.022	0.289
IP2	**PH2**	-0.068	0.015	-0.008	0.134	-0.334	-0.261
IP2	**ET1**	-0.143	0.677	-0.096	0.003	-0.669	-0.228
IP2	**ET2**	-0.085	0.254	0.023	0.075	-0.559	-0.293
IP2	**NCO**	0.917	2.079	-0.630	0.152	-1.492	1.025
IP2	**CYC**	-0.058	0.060	0.122	0.022	-0.589	-0.443
IP2	**R**	0.316	0.000	-0.005	0.002	-0.013	0.301

Cartesian coordinates (Å) for the optimised structures of the benzene derivatives dimers at the PBE0-D3BJ/def2-TZVP level. The phenyl ring structure C_6H_5- is kept unchanged.

Benzene

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38754149
C	1.20164618	0.00000000	2.08131223
C	2.40329236	0.00000000	1.38754149
C	2.40329236	0.00000000	0.00000000
C	1.20164618	0.00000000	-0.69377075
H	-0.93885752	0.00000000	-0.54204964
H	-0.93885752	0.00000000	1.92959113
H	1.20164618	0.00000000	3.16541152
H	3.34214987	0.00000000	1.92959113
H	3.34214987	0.00000000	-0.54204964
H	1.20164618	0.00000000	-1.77787002

-NH_2

N	1.20164547	-0.05649700	-2.08331275
H	0.36670422	0.29197806	-2.52496937
H	2.03659382	0.29196098	-2.52496849

-OH

O	1.14467709	0.00000000	-2.04973617
H	2.03836351	0.00000000	-2.40318837

-CH3

C	1.19337523	0.00000000	-2.19568060
H	2.20674803	0.00000000	-2.59934931
H	0.67584952	0.87979275	-2.58762844
H	0.67584952	-0.87979275	-2.58762844

-F

F	1.20164618	0.00000000	-2.02794859

-CN

C	1.20164618	0.00000000	-2.12146186
N	1.20164618	0.00000000	-3.27306689

-NO_2

N	1.20164618	0.00000000	-2.15465090
O	2.27717462	0.00000000	-2.71308914
O	0.12611774	0.00000000	-2.71308914

Cartesian coordinates (Å) for the optimised structures of the **1A** dimers at the PBE0-D3BJ/def2-TZVP level.

1A

C	-0.48570933	-2.51159962	-0.88216375
C	-0.31337069	-3.89283317	-0.92794132
C	0.97814966	-4.37302246	-0.84453120
C	2.05063723	-3.51334262	-0.70235967
C	1.77349526	-2.14995457	-0.65991411
N	0.53577172	-1.65825617	-0.76847347
H	-1.17176625	-4.53823993	-1.01504914
H	1.15360873	-5.44235357	-0.88252816
H	3.06932977	-3.85646207	-0.62611157
N	-1.73198176	-1.91063392	-0.96350219
H	-1.73047170	-0.90363010	-1.10894514
N	2.75483810	-1.18782591	-0.46570389
H	2.41775317	-0.25372743	-0.24308563
C	-2.95496805	-2.48865863	-0.75836275
O	-3.12360056	-3.66788813	-0.52290157
C	4.11561385	-1.34689376	-0.49479631
O	4.67565086	-2.40190068	-0.70771357
C	-4.11331303	-1.51105865	-0.88019198
H	-3.77215909	-0.52986971	-0.53639442
C	4.87795885	-0.04783229	-0.28153176
H	4.31326973	0.56913349	0.42343678
C	6.26017125	-0.32854802	0.27773007
H	6.80737766	0.60679552	0.41562612
H	6.82550689	-0.96822481	-0.40134855
H	6.20408424	-0.83907812	1.24102448
C	4.95194257	0.70444586	-1.61015829
H	5.49391522	1.64402754	-1.48060788
H	3.95756994	0.93825387	-1.99586004
H	5.47909818	0.10714938	-2.35830401
C	-5.28380732	-1.97125964	-0.03119055
H	-6.11886923	-1.27422789	-0.13115337
H	-5.01310280	-2.03244203	1.02519011
H	-5.61562632	-2.96265076	-0.34233930
C	-4.49975764	-1.38528054	-2.35324558
H	-5.33858070	-0.69435045	-2.46410411
H	-4.80335846	-2.35662435	-2.75163239
H	-3.66997774	-1.00709626	-2.95287639
C	-1.18795153	3.41393030	1.45274488
C	-2.07756124	3.59327070	0.20861954
C	-1.43430423	3.22757147	-1.14001114
C	-0.12013724	3.97842269	-1.28684604
C	0.83861294	3.58219735	-0.17457631
C	0.22038281	3.97229098	1.17795444
H	-3.00372813	3.02847181	0.33925029
H	-2.35038250	4.65248405	0.14157566
H	0.32621063	3.77256181	-2.26514362
H	-0.30739130	5.05593296	-1.23938234
H	0.89070549	3.67836815	1.98894761
H	0.15916570	5.06647210	1.18546315
C	-1.81099258	4.18157926	2.62353742
H	-2.80945828	3.79966440	2.84326938
H	-1.20084136	4.07042648	3.52142094
H	-1.88826413	5.24468206	2.38105312
C	2.18391542	4.27726981	-0.32942357
H	2.64700869	4.02702401	-1.28653929
H	2.04455874	5.35989614	-0.28874386
H	2.86882050	3.97935853	0.46398706
C	-2.39999487	3.57539869	-2.26371021
H	-2.61954082	4.64518764	-2.24080959
H	-1.97057718	3.33418796	-3.23847567
H	-3.33241576	3.02098955	-2.16068785
C	-1.09150234	2.00412851	1.82477576
C	-0.96311879	0.84291469	2.11966401
C	1.06480385	2.08059501	-0.23426978
O	2.05791845	1.55297984	0.22498693
N	0.11140314	1.31841435	-0.86070397
C	-1.15361820	1.73647100	-1.18846878
O	-1.99700489	0.92556895	-1.51348751
H	0.25933150	0.29109795	-0.83775987
C	-0.73470700	-0.53956382	2.35760204
C	0.57109530	-1.00252661	2.54305003
C	0.81369076	-2.35640733	2.68879361
C	-0.23756961	-3.26133297	2.65014646
C	-1.53867190	-2.80842894	2.48181410
C	-1.78933559	-1.45555554	2.34108068
H	1.38763653	-0.29065867	2.54247409
H	1.83073478	-2.70976186	2.81090219
H	-2.35799144	-3.51475623	2.42813940
H	-2.80038904	-1.09533112	2.19327016
H	-0.04215904	-4.32324344	2.73851634

1A-NH_2b

C	-0.53446684	-2.52212678	-0.96050480
C	-0.35992933	-3.90200874	-1.04458700
C	0.92961039	-4.38440098	-0.94761679
C	1.99662181	-3.52919764	-0.75049629
C	1.71829191	-2.16519018	-0.68254112
N	0.48355541	-1.67019740	-0.81250729
H	-1.21530621	-4.54429439	-1.17337697
H	1.10834334	-5.45166402	-1.02219675
H	3.01368496	-3.87267810	-0.65701981
N	-1.78364201	-1.92726615	-1.03519693
H	-1.79116004	-0.91368986	-1.13052889
N	2.69595597	-1.21057489	-0.45008156
H	2.35887870	-0.26225786	-0.29573882
C	-2.99675608	-2.51846204	-0.80600572
O	-3.14789666	-3.70309909	-0.58269720
C	4.04658202	-1.39709530	-0.30627069
O	4.60084663	-2.47358962	-0.39252089
C	-4.16720974	-1.55183267	-0.88238439
H	-3.82827362	-0.57368785	-0.52932343
C	4.81283671	-0.10560485	-0.06706883
H	4.19373386	0.54995114	0.55165795
C	6.12390106	-0.38944545	0.64178942
H	6.67161949	0.54155900	0.80444806
H	6.74467392	-1.06134280	0.04753988
H	5.95866568	-0.86461375	1.61062783
C	5.03847974	0.59218875	-1.40831165
H	5.58988987	1.52315150	-1.25862650
H	4.09397833	0.83507434	-1.89864972
H	5.62164012	-0.04541087	-2.07762699
C	-5.31205852	-2.03950141	-0.01392027
H	-6.15514218	-1.34815865	-0.08006563
H	-5.01428986	-2.11687758	1.03408045
H	-5.64345205	-3.02781831	-0.33522116
C	-4.58940699	-1.40283310	-2.34346452
H	-5.43631232	-0.71737850	-2.42139775
H	-4.89412524	-2.36912595	-2.75326937
H	-3.77714056	-1.00619174	-2.95516525
C	-1.09984183	3.47095067	1.47170760
C	-2.07564872	3.62765286	0.29060200
C	-1.53034909	3.23586711	-1.09369926
C	-0.23080009	3.98401134	-1.34728975
C	0.80489049	3.60666981	-0.29934829
C	0.28479142	4.02302979	1.08621291
H	-2.98922199	3.06541181	0.49823641
H	-2.35451825	4.68529193	0.22126675
H	0.14487820	3.76168917	-2.35140323
H	-0.41561569	5.06211267	-1.30439881
H	1.01121608	3.74271982	1.85251099
H	0.22562600	5.11743483	1.07711839
C	-1.63783280	4.26230973	2.66815387
H	-2.61731192	3.88436473	2.96639039

H	-0.96488603	4.16687154	3.52194735
H	-1.73380158	5.32125793	2.41337878
C	2.13541631	4.29786030	-0.56264628
H	2.52902512	4.03084097	-1.54597847
H	1.99850457	5.38110149	-0.53086346
H	2.87548443	4.01359758	0.18493740
C	-2.57398421	3.56516569	-2.15159197
H	-2.79062417	4.63559976	-2.13205269
H	-2.21603824	3.30570108	-3.15029588
H	-3.49708876	3.01473416	-1.97181263
C	-0.97413884	2.06593743	1.85186779
C	-0.82036550	0.90107083	2.12325903
C	1.02758107	2.10422250	-0.35038661
O	2.05116404	1.58316083	0.04444933
N	0.03585110	1.33267700	-0.90152621
C	-1.25033357	1.74426259	-1.14191187
O	-2.11042725	0.92758086	-1.40344313
H	0.18736573	0.30843389	-0.87223529
C	-0.57679277	-0.48230343	2.31648724
C	0.72673985	-0.95093394	2.51147972
C	0.99070200	-2.30100960	2.58568702
C	-0.04105815	-3.23658912	2.45974021
C	-1.35031260	-2.77092717	2.30239791
C	-1.61042070	-1.42006634	2.23367726
H	1.53899838	-0.23664134	2.57406116
H	2.01133389	-2.64566351	2.71292058
H	-2.16117649	-3.48232016	2.19230457
H	-2.62664023	-1.07397631	2.08562312
N	0.21999956	-4.58757949	2.52791813
H	-0.47327364	-5.17644385	2.09514169
H	1.15839172	-4.85425645	2.27734591

1A-NH_2

C	-0.51981163	-2.50106044	-0.85990952
C	-0.36005987	-3.88380113	-0.85884451
C	0.92458262	-4.37358435	-0.73973790
C	2.00268954	-3.51910800	-0.61355721
C	1.73839701	-2.15247916	-0.62234256
N	0.50774522	-1.65216256	-0.76460209
H	-1.22359322	-4.52370805	-0.93212577
H	1.08899844	-5.44494123	-0.73364044
H	3.01691982	-3.86787377	-0.50943305
N	-1.76124600	-1.89344383	-0.96825411
H	-1.75082498	-0.88918167	-1.13321030
N	2.72697461	-1.19392942	-0.44683117
H	2.39541419	-0.24915279	-0.26338282
C	-2.98812931	-2.45370665	-0.74284786
O	-3.16839942	-3.62449910	-0.47274926
C	4.08487389	-1.36975102	-0.42170941
O	4.63969568	-2.43986183	-0.56490391
C	-4.13837480	-1.46953940	-0.88900415
H	-3.78932831	-0.48377206	-0.56760213
C	4.85605821	-0.07032618	-0.24362243
H	4.28571317	0.57576313	0.42999468
C	6.22684828	-0.34196504	0.34698053
H	6.77865815	0.59370528	0.46276354
H	6.79859096	-1.00780600	-0.30093164
H	6.15154032	-0.81997415	1.32554736
C	4.95700668	0.63474749	-1.59613534
H	5.50676478	1.57288907	-1.49111439
H	3.97080729	0.86499705	-2.00395940
H	5.48868735	0.00695771	-2.31569702
C	-5.31372861	-1.89942500	-0.03090766
H	-6.14263327	-1.19785068	-0.14907133
H	-5.04489888	-1.93638530	1.02710397
H	-5.65370751	-2.89528758	-0.31820286
C	-4.52236245	-1.37410020	-2.36490717
H	-5.35516232	-0.67872504	-2.49244852
H	-4.83374264	-2.35160511	-2.74184858
H	-3.68875381	-1.01655968	-2.97181070
C	-1.19050669	3.40229593	1.44932380
C	-2.09227816	3.58418016	0.21430671
C	-1.45920016	3.23312597	-1.14327330
C	-0.15034876	3.99158076	-1.29644544
C	0.81962098	3.59213761	-0.19529546
C	0.21094855	3.97271857	1.16419800
H	-3.01261607	3.01079626	0.34913854
H	-2.37481321	4.64152745	0.15645601
H	0.28826958	3.79489009	-2.28019706
H	-0.34242607	5.06779676	-1.23924639
H	0.89006045	3.67931104	1.96805446
H	0.14349190	5.06666125	1.17637288
C	-1.80788080	4.16170986	2.62836853
H	-2.80096637	3.77044825	2.85622876
H	-1.18827974	4.05034685	3.51977230
H	-1.89635687	5.22571219	2.39252939
C	2.16041231	4.29412523	-0.35785538
H	2.61649702	4.05153148	-1.32034140
H	2.01644590	5.37587284	-0.30964944
H	2.85333973	3.99479640	0.42803848
C	-2.43667674	3.58511557	-2.25541718
H	-2.66035248	4.65381436	-2.22244948
H	-2.01555896	3.35275144	-3.23599667
H	-3.36588466	3.02619116	-2.14774017
C	-1.07420529	1.99098376	1.81076207
C	-0.91891374	0.82911739	2.09464987
C	1.05189770	2.09180179	-0.26749061
O	2.05360789	1.56639243	0.17550909
N	0.09715723	1.32888289	-0.89113256
C	-1.17141685	1.74419137	-1.20616220
O	-2.01323520	0.93282239	-1.53509944
H	0.24501852	0.30179616	-0.86620546
C	-0.66115317	-0.54553464	2.32946261
C	0.64779887	-0.99063710	2.54236668
C	0.92679623	-2.33176593	2.68845146
C	-0.09606024	-3.28416709	2.62302184
C	-1.40883103	-2.84152517	2.42657394
C	-1.68280523	-1.49871845	2.28830300
H	1.45263257	-0.26568255	2.56690429
H	1.95204936	-2.65719621	2.82848017
H	-2.21217116	-3.56505484	2.34486771
H	-2.70311425	-1.17324543	2.12333109
N	0.18765620	-4.62487734	2.69448409
H	1.06970714	-4.89173889	3.09419459
H	-0.57349031	-5.24843091	2.89695761

1A-OH

C	-0.49829374	-2.51836257	-0.87521843
C	-0.32419286	-3.89944650	-0.90191987
C	0.96520101	-4.37907257	-0.78235374
C	2.03293925	-3.51630317	-0.63306033
C	1.75573542	-2.15196008	-0.62185932
N	0.51968101	-1.66170219	-0.75711826
H	-1.17959589	-4.54664713	-1.00373265
H	1.14232443	-5.44844475	-0.79710849
H	3.04940851	-3.85806131	-0.52834958
N	-1.74612658	-1.92222551	-0.98475035
H	-1.74628952	-0.91556321	-1.13711317
N	2.73641656	-1.18924600	-0.43271288
H	2.40093619	-0.25055192	-0.22661331
C	-2.96486029	-2.49819190	-0.75830802
O	-3.12639282	-3.66957330	-0.47559326
C	4.09747358	-1.35125180	-0.45715714
O	4.65576417	-2.40934567	-0.65810161
C	-4.13003896	-1.53515812	-0.91891864
H	-3.79792710	-0.54012292	-0.60858911
C	4.86234386	-0.05180039	-0.25650294
H	4.29835180	0.57370480	0.44128602
C	6.24333861	-0.32996530	0.30705725
H	6.79261141	0.60550707	0.43555457
H	6.80781952	-0.97818147	-0.36458164
H	6.18502182	-0.83013176	1.27562924

C	4.93928874	0.68631866	-1.59289929
H	5.48268685	1.62630471	-1.47263486
H	3.94579667	0.91804220	-1.98197907
H	5.46629467	0.08024439	-2.33407995
C	-5.30177027	-1.97378441	-0.06027751
H	-6.14098711	-1.28667452	-0.18927262
H	-5.03707440	-1.99430427	0.99930658
H	-5.62551146	-2.97786354	-0.33746080
C	-4.50959082	-1.46318716	-2.39746772
H	-5.35122856	-0.78095278	-2.53653662
H	-4.80595046	-2.44924359	-2.76396635
H	-3.67850029	-1.10204728	-3.00586781
C	-1.14716234	3.43909973	1.48244018
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C	-1.45726083	3.22790483	-1.10391912
C	-0.14654093	3.97696275	-1.28763248
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C	0.25329290	3.99576272	1.16742726
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H	-2.34438538	4.66195650	0.18677772
H	0.27665280	3.76313625	-2.27451304
H	-0.33225814	5.05488944	-1.24425618
H	0.94328434	3.71066715	1.96495651
H	0.19240725	5.09003665	1.16367908
C	-1.74284871	4.21937285	2.65880943
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H	-1.11160031	4.11747908	3.54313246
H	-1.82706972	5.28016840	2.40806612
C	2.18086889	4.27768783	-0.38994781
H	2.62006692	4.01551843	-1.35513859
H	2.04584856	5.36116039	-0.35786722
H	2.88361167	3.98616219	0.39011061
C	-2.45000703	3.57066182	-2.20544654
H	-2.66626277	4.64113590	-2.18424677
H	-2.04601814	3.32166959	-3.18908709
H	-3.38107118	3.01963762	-2.07540791
C	-1.03857100	2.03202814	1.86109319
C	-0.90225193	0.86845929	2.14480628
C	1.05807916	2.08624698	-0.24364929
O	2.05731424	1.56092634	0.20426856
N	0.09449726	1.32057742	-0.85070769
C	-1.17637262	1.73664233	-1.15482536
O	-2.02369404	0.92418838	-1.46736962
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C	-0.68762883	-0.51809814	2.35868523
C	0.60182283	-1.00922864	2.59151359
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C	-0.22146087	-3.25981811	2.56730070
C	-1.51363764	-2.78612219	2.36369032
C	-1.74160703	-1.42880971	2.26309941
H	1.42715208	-0.31074478	2.65803745
H	1.83540245	-2.75026635	2.85127107
H	-2.33511454	-3.48403241	2.24082107
H	-2.74478332	-1.06154960	2.08312445
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H	-0.73305205	-5.08060648	2.42278679

1A-CH_3

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C	-0.30985762	-3.89869863	-0.92237981
C	0.98160140	-4.37695212	-0.82952290
C	2.05148467	-3.51518935	-0.68164764
C	1.77224010	-2.15157820	-0.64765324
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H	-1.16665086	-4.54548701	-1.01447715
H	1.15875872	-5.44619690	-0.86322351
H	3.07023317	-3.85626889	-0.59740382
N	-1.73228873	-1.92037622	-0.96739198
H	-1.73378812	-0.91221703	-1.10591319
N	2.75182697	-1.18829550	-0.45309068
H	2.41352094	-0.25223007	-0.24009511
C	-2.95262339	-2.50213387	-0.75694783
O	-3.11619861	-3.68186673	-0.51917638
C	4.11289569	-1.34847501	-0.46670147
O	4.67438014	-2.40608258	-0.66267572
C	-4.11480848	-1.52917216	-0.87615383
H	-3.77626841	-0.54668667	-0.53381900
C	4.87396157	-0.04782509	-0.25956617
H	4.30532156	0.57439276	0.43750124
C	6.25325751	-0.32372471	0.30912269
H	6.79915333	0.61297116	0.44297142
H	6.82271234	-0.96807264	-0.36207481
H	6.19227732	-0.82709104	1.27588428
C	4.95467958	0.69431077	-1.59352167
H	5.49579481	1.63494521	-1.46815541
H	3.96230857	0.92508644	-1.98603220
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C	-5.28117065	-1.99310687	-0.02352423
H	-6.11890582	-1.29900335	-0.12149173
H	-5.00703649	-2.05239012	1.03208501
H	-5.61059646	-2.98584319	-0.33299728
C	-4.50551999	-1.40535305	-2.34823421
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H	-4.80714257	-2.37774068	-2.74563166
H	-3.67839904	-1.02487176	-2.95014676
C	-1.17352116	3.43305477	1.46225113
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C	-0.13016311	3.97496494	-1.29085881
C	0.83818095	3.58508775	-0.18484213
C	0.23319487	3.98676397	1.17020826
H	-2.99929303	3.03969346	0.36847410
H	-2.34758169	4.66189267	0.15123695
H	0.30701516	3.76239797	-2.27189184
H	-0.31607036	5.05290870	-1.24849616
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H	0.17460970	5.08115269	1.16972014
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H	-1.16726567	4.10584167	3.52545721
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C	2.18300401	4.27710150	-0.35743340
H	2.63737811	4.01826773	-1.31646854
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H	2.87448440	3.98489554	0.43239503
C	-2.41886352	3.56744311	-2.24451586
H	-2.63672783	4.63768571	-2.22735107
H	-1.99859077	3.31859736	-3.22137254
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C	-1.07509028	2.02548687	1.84145340
C	-0.94539829	0.86335854	2.13291438
C	1.06252160	2.08287543	-0.23717360
O	2.05957384	1.55719627	0.21577579
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C	0.81506839	-2.35478498	2.65173738
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H	1.40328814	-0.29396297	2.54702275
H	1.83369193	-2.71135018	2.76131114
H	-2.35011470	-3.49224617	2.36482473
H	-2.78629345	-1.07672693	2.18369299
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H	1.04308320	-4.98846115	2.36924081

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H	1.12011765	-5.43184248	-0.65117125
H	3.05204130	-3.85318614	-0.49036304
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H	2.43362706	-0.23614213	-0.25854151
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O	-3.14357618	-3.59852711	-0.42419745
C	4.12125572	-1.34293905	-0.52463107
O	4.67077807	-2.40624384	-0.72106941
C	-4.10795723	-1.45652684	-0.91687102
H	-3.76697004	-0.46385968	-0.60733532
C	4.89182602	-0.04059678	-0.36776831
H	4.35277076	0.59124849	0.34453911
C	6.29349063	-0.31022405	0.14635613
H	6.84522148	0.62741179	0.24479365
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C	4.91672828	0.68361268	-1.71379429
H	5.46246792	1.62565093	-1.62415744
H	3.90895968	0.90893875	-2.06876159
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C	-5.30389159	-1.87035294	-0.07966405
H	-6.13000258	-1.17224153	-0.23221043
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H	-5.63613956	-2.87199825	-0.35539965
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C	-2.09069180	3.56274822	0.19390253
C	-1.41712545	3.23244559	-1.14940135
C	-0.10575853	3.99499751	-1.25288632
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C	0.18435201	3.94105187	1.21705550
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H	-2.37301147	4.62035106	0.14374100
H	0.36185913	3.81305526	-2.22599318
H	-0.30156994	5.06995460	-1.18655396
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H	0.11399305	5.03434601	1.24412159
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H	-2.87767280	3.71562741	2.81581382
H	-1.28549586	3.98660279	3.53162185
H	-1.95889176	5.17557606	2.39807993
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H	2.66086153	4.06111089	-1.19487729
H	2.02788619	5.37039900	-0.18492729
H	2.84661393	3.98178000	0.55869909
C	-2.36234950	3.59796348	-2.28469320
H	-2.58953667	4.66559570	-2.24366506
H	-1.91179695	3.38025050	-3.25542656
H	-3.29293735	3.03567708	-2.21243316
C	-1.12181207	1.95211960	1.80552866
C	-0.98385340	0.79177008	2.09982383
C	1.07074000	2.08388730	-0.21445191
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N	0.13263679	1.32708711	-0.86973820
C	-1.12566030	1.74493442	-1.22155289
O	-1.95641225	0.93563870	-1.58193810
H	0.28179816	0.29926707	-0.85443057
C	-0.73808266	-0.58513575	2.34950816
C	0.57303028	-1.02989815	2.54346080
C	0.84327369	-2.37526117	2.70759195
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C	-1.77760721	-1.51847182	2.33943703
H	1.38160449	-0.30946026	2.53668372
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C	0.93867627	-4.36540421	-0.66883440
C	2.02152693	-3.51202006	-0.57292160
C	1.76327961	-2.14501915	-0.60859911
N	0.53206769	-1.64298852	-0.74432277
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N	-1.73766706	-1.87451539	-0.94492459
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H	2.42989797	-0.24646313	-0.24379670
C	-2.96848915	-2.41771159	-0.69467107
O	-3.14803836	-3.56515241	-0.34046883
C	4.11445784	-1.35451018	-0.52843257
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C	-4.11611515	-1.44753451	-0.92557928
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C	4.88809991	-0.05430482	-0.36937401
H	4.35523740	0.57395279	0.35099555
C	6.29308896	-0.32928708	0.13270749
H	6.84755244	0.60663586	0.23185129
H	6.82665614	-0.98060431	-0.56083173
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C	4.90418011	0.67793954	-1.71122555
H	5.45113812	1.61908404	-1.61978553
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H	-5.64370780	-2.84163728	-0.31145444
C	-4.46286610	-1.43877640	-2.41403259
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H	-4.76604540	-2.43664328	-2.74061269
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C	-1.23805034	3.36209725	1.45254586
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C	0.83359892	3.57509661	-0.11081345
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H	-2.37811100	4.61226131	0.13703556
H	0.38239149	3.81072924	-2.21089679
H	-0.28795727	5.06697857	-1.17557647
H	0.82211556	3.63302823	2.05528617
H	0.10241748	5.02896738	1.25555906
C	-1.90320956	4.10273289	2.61830395
H	-2.90500463	3.71003504	2.80044412
H	-1.31964851	3.98151546	3.53236256
H	-1.98126844	5.16886348	2.39089622
C	2.18010406	4.27765934	-0.21142112
H	2.67244845	4.04760468	-1.15889011
H	2.03543596	5.35880638	-0.15424615
H	2.84228555	3.96689576	0.59619226
C	-2.34298424	3.60500464	-2.29403567
H	-2.56762855	4.67301201	-2.24978092

H	-1.88512286	3.39068365	-3.26200238
H	-3.27567171	3.04494883	-2.23243571
C	-1.13724428	1.94939352	1.81174872
C	-0.99721531	0.79198969	2.11583497
C	1.06644175	2.07546638	-0.19180532
O	2.04642973	1.54140203	0.28825122
N	0.13271822	1.32147997	-0.85697680
C	-1.11780797	1.74412281	-1.23043655
O	-1.94407194	0.93861127	-1.60889922
H	0.28072737	0.29265671	-0.84588371
C	-0.73645994	-0.58183062	2.36104436
C	0.58283578	-1.00720512	2.54727407
C	0.86864186	-2.34874253	2.68797479
C	-0.16364703	-3.28622097	2.64269078
C	-1.48501907	-2.86950090	2.47976234
C	-1.76661949	-1.52575915	2.34751465
H	1.37984352	-0.27439453	2.54446371
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H	-2.27751830	-3.60355184	2.41853594
H	-2.78750299	-1.19664636	2.20045423
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N	0.39247194	-5.79809280	2.79208276

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C	-0.50180809	-2.48689308	-0.80072283
C	-0.34862218	-3.87011698	-0.74906632
C	0.93650193	-4.36204571	-0.62637150
C	2.02043777	-3.50850902	-0.54465495
C	1.76253219	-2.14242699	-0.59570928
N	0.53102947	-1.64167979	-0.73483081
H	-1.21443439	-4.51059392	-0.78919332
H	1.09569915	-5.43299927	-0.57535433
H	3.03273962	-3.86220706	-0.43724773
N	-1.73780686	-1.87183912	-0.93341542
H	-1.71738840	-0.88166470	-1.16728790
N	2.75552462	-1.18282145	-0.45576275
H	2.43252855	-0.24408882	-0.23436484
C	-2.97278502	-2.41439057	-0.69980932
O	-3.15780033	-3.56261914	-0.35273497
C	4.11312527	-1.34995628	-0.55304856
O	4.65344000	-2.41028656	-0.78289346
C	-4.11611670	-1.44135980	-0.93979528
H	-3.77546047	-0.43812135	-0.66542592
C	4.88895536	-0.05084633	-0.39561063
H	4.36532468	0.57302777	0.33531802
C	6.29993439	-0.32948129	0.08740231
H	6.85627766	0.60548374	0.18508314
H	6.82418420	-0.97707742	-0.61663891
H	6.29742007	-0.83133278	1.05675350
C	4.88876564	0.68931111	-1.73318834
H	5.43693024	1.62988240	-1.64296055
H	3.87466491	0.91911688	-2.06709909
H	5.37392088	0.08503291	-2.50369362
C	-5.31987588	-1.82131488	-0.09784061
H	-6.14371492	-1.12883586	-0.28429847
H	-5.08803585	-1.79747920	0.96929343
H	-5.65102205	-2.83252484	-0.33740967
C	-4.45105155	-1.43215283	-2.43092289
H	-5.27700084	-0.74458550	-2.62620060
H	-4.75330353	-2.42957744	-2.75962633
H	-3.59729356	-1.11277393	-3.03116619
C	-1.24209078	3.35966548	1.45317506
C	-2.09271533	3.55423906	0.18382375
C	-1.40266671	3.23127660	-1.15312670
C	-0.08815282	3.99110509	-1.23709366
C	0.83505062	3.57396549	-0.10274610
C	0.17022889	3.93396782	1.23580595
H	-3.01599344	2.97631567	0.27028885
H	-2.37679315	4.61124610	0.13505744
H	0.39151899	3.80988885	-2.20434885
H	-0.28198501	5.06643644	-1.17148501
H	0.81616037	3.63154798	2.06326478
H	0.09791273	5.02699458	1.26155858
C	-1.91142621	4.09877696	2.61762882
H	-2.91362732	3.70553448	2.79620576
H	-1.33063795	3.97730333	3.53339529
H	-1.98917925	5.16494741	2.39056202
C	2.18208700	4.27621499	-0.19775499
H	2.67778629	4.04688490	-1.14363479
H	2.03748654	5.35733981	-0.14004691
H	2.84114390	3.96444768	0.61200798
C	-2.33399937	3.60576298	-2.29686675
H	-2.55849109	4.67379968	-2.25269708
H	-1.87293304	3.39192034	-3.26339601
H	-3.26701689	3.04590126	-2.23876678
C	-1.14308885	1.94687713	1.81247810
C	-1.00501172	0.78990503	2.11902107
C	1.06748708	2.07422015	-0.18254629
O	2.04467684	1.53981649	0.30273097
N	0.13620165	1.32070170	-0.85172234
C	-1.11264785	1.74390522	-1.23043421
O	-1.93759736	0.93876336	-1.61236678
H	0.28369179	0.29162098	-0.84093875
C	-0.74431977	-0.58330260	2.36761597
C	0.57622659	-1.00522550	2.55744961
C	0.86456912	-2.34669996	2.70228257
C	-0.17544494	-3.25911203	2.65777640
C	-1.49397771	-2.87123424	2.49225732
C	-1.77551325	-1.52706619	2.35442977
H	1.37190480	-0.27118470	2.55377744
H	1.87872805	-2.70044971	2.82389796
H	-2.27037228	-3.62100514	2.43535230
H	-2.79588255	-1.19853583	2.20368371
N	0.13468360	-4.68592736	2.75772243
O	1.30087671	-4.99865125	2.87430830
O	-0.79108302	-5.46614288	2.71135780

Cartesian coordinates (Å) for the optimised structures of the **1B** dimers at the PBE0-D3BJ/def2-TZVP level.

1B

C	2.00585732	-0.85303113	-1.40760740
C	3.34916701	-0.64772164	-1.71255460
C	3.76708446	0.65501438	-1.89653398
C	2.88343781	1.70710494	-1.76048377
C	1.56300786	1.39838211	-1.45525426
N	1.12152075	0.14572525	-1.31902551
H	4.01911014	-1.48909861	-1.77200849
H	4.80621846	0.85389128	-2.13185345
H	3.18861861	2.73628679	-1.85453585
N	1.48100230	-2.10782917	-1.13081291
H	0.49295565	-2.12527510	-0.88927342
N	0.60483495	2.38740545	-1.26052281
H	-0.36714525	2.08994319	-1.30666726
C	2.16483530	-3.27674429	-0.91758375
O	3.35626734	-3.41748869	-1.10197064
C	0.82769304	3.64615720	-0.77152464
O	1.93066460	4.10708631	-0.55367815
C	1.29286694	-4.38981860	-0.35940901
H	0.29162770	-4.29154081	-0.78801727
C	-0.44714125	4.41221648	-0.45908591
H	-1.23125145	4.07039379	-1.14021933
C	-0.87625524	4.07225874	0.96835418
H	-1.79316771	4.60967941	1.22199206
H	-0.10141378	4.36824684	1.67990398
H	-1.06289564	3.00391105	1.09192760
C	-0.22846032	5.90370701	-0.63657502
H	-1.13899664	6.45103037	-0.38199779
H	0.04182628	6.14781616	-1.66595665
H	0.57979423	6.24964366	0.00925110
C	1.17717178	-4.19807111	1.15336863
H	0.55128370	-4.98217185	1.58524072
H	0.73025766	-3.23421635	1.40507190
H	2.16410754	-4.25842080	1.62015374
C	1.87007468	-5.74841353	-0.70937756
H	1.24799492	-6.54144522	-0.28809573
H	2.88105931	-5.84875188	-0.31203198
H	1.92516720	-5.89183715	-1.79022361
C	-3.69783311	-0.22423706	1.76745458
C	-3.90451523	-1.66865502	1.27124910
C	-3.65393371	-1.89956475	-0.22789083
C	-4.51953521	-0.93617099	-1.02450173
C	-4.13803990	0.50106052	-0.70716230
C	-4.35925610	0.76871716	0.79206164
H	-3.28150159	-2.34648028	1.85925363
H	-4.94949038	-1.94171219	1.45666205
H	-4.41278035	-1.12672766	-2.09733001
H	-5.57232124	-1.09960943	-0.77275511
H	-4.04133766	1.78558030	1.03497271
H	-5.44155526	0.72051365	0.95575001
C	-4.34717350	-0.07027016	3.14810099
H	-3.89659530	-0.76125003	3.86239461
H	-4.21013181	0.94477148	3.52468661
H	-5.41814892	-0.27914261	3.08511931
C	-4.97029434	1.48610980	-1.51477157
H	-4.83652766	1.32533379	-2.58657767
H	-6.02824231	1.35397993	-1.27717260
H	-4.68369590	2.51332034	-1.29116951
C	-3.97641357	-3.34692458	-0.56970482
H	-5.02183562	-3.55635980	-0.33209827
H	-3.82096190	-3.54253823	-1.63288384
H	-3.34228451	-4.02989737	-0.00509842
C	-2.27043244	0.04338938	1.90586534
C	-1.07611072	0.20281052	2.01180354
C	-2.67401878	0.70537805	-1.05012548
O	-2.21987538	1.79523997	-1.33203909
N	-1.85939459	-0.39777538	-1.03809423
C	-2.19245050	-1.63877761	-0.55417750
O	-1.33439750	-2.48545591	-0.41653388
H	-0.84682446	-0.21987370	-1.17210820
C	0.27367731	0.34192426	2.02637487
C	1.47934818	0.43512073	1.95336930
C	2.88373737	0.51557786	1.80716754
C	3.50678562	1.75043269	1.59873595
C	4.87700117	1.80853915	1.42285024
C	5.63701807	0.64733927	1.44512930
C	5.02307652	-0.58215601	1.64321749
C	3.65521607	-0.65240664	1.82502636
H	2.90800532	2.65082158	1.54296179
H	5.35081691	2.76778396	1.25122540
H	5.61002009	-1.49278511	1.64178212
H	3.16624341	-1.60845512	1.96553743
H	6.70993952	0.69904958	1.29971156

1B-NH_2b

C	-1.77758791	0.90364820	-1.47195643
C	-3.11652046	0.74325048	-1.82010734
C	-3.57020207	-0.54480145	-2.02046684
C	-2.72741228	-1.62576456	-1.85654267
C	-1.40806616	-1.36071529	-1.50697458
N	-0.92968136	-0.12307930	-1.35844559
H	-3.75544965	1.60681244	-1.89851850
H	-4.60676023	-0.70940333	-2.29215214
H	-3.06261727	-2.64450175	-1.96026542
N	-1.22159137	2.14087782	-1.17763315
H	-0.23809119	2.12822163	-0.91687222
N	-0.49073295	-2.37895275	-1.27557719
H	0.49027611	-2.10813619	-1.26693177
C	-1.87481994	3.32779991	-0.97128314
O	-3.05810120	3.50510706	-1.17858091
C	-0.77177363	-3.63661677	-0.81399930
O	-1.89601031	-4.07423449	-0.66831189
C	-0.98104805	4.41175448	-0.39064514
H	0.02221231	4.29037975	-0.80841315
C	0.46506079	-4.43292982	-0.43218300
H	1.28960177	-4.11883933	-1.07812638
C	0.83522372	-4.08793713	1.01067302
H	1.72440189	-4.64638188	1.31281887
H	0.02021757	-4.35568295	1.68781615
H	1.04459299	-3.02374166	1.13286342
C	0.21595085	-5.91993675	-0.60535186
H	1.09945613	-6.48742442	-0.30395808
H	-0.01358741	-6.16813549	-1.64360828
H	-0.62958044	-6.23858928	0.00589289
C	-0.88762632	4.20303003	1.12140808
H	-0.24401269	4.96481155	1.56694537
H	-0.47189004	3.22448729	1.36964471
H	-1.87730223	4.28845761	1.57853103
C	-1.51688897	5.78873601	-0.73421337
H	-0.87779509	6.56042088	-0.29897360
H	-2.52897535	5.91373203	-0.34666677
H	-1.55630746	5.94336113	-1.81420860
C	3.88961646	0.16433971	1.80551573
C	4.13742010	1.59080261	1.27710348
C	3.89597728	1.79503403	-0.22744434
C	4.73457208	0.78913505	-1.00002464
C	4.31054195	-0.62845014	-0.65040852
C	4.52555008	-0.86786853	0.85430956
H	3.53184442	2.29827717	1.84817403
H	5.18915890	1.84011293	1.45844811
H	4.63526196	0.95827992	-2.07719104
H	5.79122299	0.92744027	-0.74932340
H	4.17950097	-1.86966968	1.12016614
H	5.60899856	-0.84565813	1.01682291
C	4.53210368	0.02423388	3.19040964
H	4.09855136	0.74329180	3.88735102

H	4.36530190	-0.97768654	3.58952394
H	5.60890641	0.20161822	3.12715790
C	5.11275325	-1.65560170	-1.43588079
H	4.98368862	-1.51472502	-2.51110861
H	6.17421131	-1.54973621	-1.20070820
H	4.79561235	-2.66849288	-1.18937148
C	4.26206391	3.22415621	-0.60100164
H	5.31282627	3.40748899	-0.36533849
H	4.11453822	3.40039227	-1.66871221
H	3.64752841	3.93822853	-0.05346025
C	2.45437639	-0.06013691	1.93868689
C	1.25334637	-0.18193065	2.02358062
C	2.84102669	-0.79719944	-0.99043674
O	2.35353685	-1.88051339	-1.24051285
N	2.06234725	0.33121577	-1.01896418
C	2.42868619	1.57063569	-0.55574745
O	1.59547760	2.44542671	-0.44206867
H	1.04640896	0.18142368	-1.15900412
C	-0.09943071	-0.27914445	2.01372582
C	-1.30681519	-0.33432816	1.90884480
C	-2.70396318	-0.36886746	1.72777001
C	-3.37615677	-1.57708361	1.50672690
C	-4.73425205	-1.59471217	1.28257125
C	-5.47163836	-0.40670488	1.25981822
C	-4.80287367	0.80206334	1.48045605
C	-3.44655281	0.81925554	1.70884077
H	-2.81642758	-2.50378377	1.47863877
H	-5.23342362	-2.54020200	1.09919983
H	-5.35455733	1.73534145	1.45026261
H	-2.93732512	1.76355547	1.85728237
N	-6.83369585	-0.42807776	1.06330052
H	-7.25719163	0.42953799	0.75260367
H	-7.21287775	-1.25027977	0.62578181

1B-NH_2

C	-1.75918944	0.94835542	-1.47396620
C	-3.10237682	0.80679073	-1.81243076
C	-3.57734119	-0.47465964	-2.00685872
C	-2.74736851	-1.56678640	-1.85061560
C	-1.42143932	-1.32049606	-1.51309811
N	-0.92431265	-0.08992680	-1.36669952
H	-3.73103594	1.67842117	-1.88393214
H	-4.61995420	-0.62420176	-2.26300950
H	-3.09824635	-2.58067593	-1.94987267
N	-1.18485004	2.17800968	-1.18018109
H	-0.19971386	2.15180080	-0.92731849
N	-0.51604160	-2.35214601	-1.29041729
H	0.46835774	-2.09437508	-1.28839637
C	-1.82271105	3.36933956	-0.95302372
O	-3.00672174	3.56151456	-1.14200139
C	-0.80936313	-3.60614516	-0.82746503
O	-1.93759419	-4.02977118	-0.67086431
C	-0.91072969	4.43790401	-0.37191954
H	0.08863775	4.30592741	-0.79551086
C	0.42021502	-4.41980681	-0.45824646
H	1.24497508	-4.11179768	-1.10667343
C	0.80242139	-4.08895204	0.98469893
H	1.68694141	-4.65937610	1.27814361
H	-0.01183556	-4.35210067	1.66456947
H	1.02424928	-3.02795775	1.11269989
C	0.15194048	-5.90253888	-0.63959422
H	1.02970076	-6.48291832	-0.34596655
H	-0.08542551	-6.14123215	-1.67833099
H	-0.69473727	-6.21442921	-0.02644067
C	-0.81310079	4.21837282	1.13834386
H	-0.15722699	4.96846997	1.58591375
H	-0.40968109	3.23257611	1.37813103
H	-1.79954952	4.31383221	1.60041659
C	-1.43014786	5.82392822	-0.70436103
H	-0.77982366	6.58461083	-0.26631932
H	-2.43927797	5.95890020	-0.31249056
H	-1.47123841	5.98625128	-1.78319202
C	3.87619063	0.11972023	1.81712737
C	4.14944793	1.54372427	1.29498731
C	3.92368698	1.75585443	-0.21087786
C	4.75346252	0.73987321	-0.97970048
C	4.30531751	-0.67223945	-0.63820209
C	4.50373325	-0.91928900	0.86759736
H	3.54981224	2.25859641	1.86312478
H	5.20324489	1.77678391	1.48578278
H	4.66560805	0.91385602	-2.05709569
H	5.80997776	0.86150716	-0.71987999
H	4.14012637	-1.91642959	1.12750119
H	5.58601528	-0.91434442	1.03912764
C	4.50679138	-0.03387165	3.20615485
H	4.07906908	0.68962642	3.90210762
H	4.32230569	-1.03432822	3.60113699
H	5.58651867	0.12769451	3.15088594
C	5.09903422	-1.70888237	-1.41973609
H	4.98127520	-1.56312723	-2.49560058
H	6.15987761	-1.61939256	-1.17515259
H	4.76483538	-2.71766944	-1.17899325
C	4.31408727	3.18037817	-0.57715551
H	5.36557493	3.34729845	-0.33265496
H	4.17767913	3.36187964	-1.64545623
H	3.70591394	3.90200713	-0.03243265
C	2.43707613	-0.08488823	1.94083271
C	1.23464231	-0.19480021	2.02216290
C	2.83644410	-0.81793685	-0.99154672
O	2.33609448	-1.89260495	-1.25301691
N	2.07372207	0.32131125	-1.01836048
C	2.45584264	1.55431926	-0.55109609
O	1.63563739	2.44183477	-0.44225559
H	1.05638631	0.18673165	-1.16527425
C	-0.11880797	-0.28308507	2.00895530
C	-1.32593483	-0.33451740	1.89970644
C	-2.72171040	-0.37113882	1.70758460
C	-3.39036906	-1.58345613	1.49786966
C	-4.74548877	-1.60628364	1.25755846
C	-5.48377628	-0.41961907	1.20876523
C	-4.81902695	0.79303195	1.41879761
C	-3.46521825	0.81547836	1.66314493
H	-2.82954785	-2.50975958	1.49090204
H	-5.23995745	-2.55432869	1.07466570
H	-5.36967075	1.72566266	1.36067641
H	-2.95942620	1.76281788	1.80405999
N	-6.82396164	-0.43968765	0.89374055
H	-7.30946973	-1.30678278	1.04794989
H	-7.35803688	0.37403776	1.14661065

1B-OH

C	-1.79329100	0.84838409	-1.48216244
C	-3.12775678	0.65021719	-1.82699575
C	-3.54758296	-0.65040174	-2.02254946
C	-2.67389397	-1.70653638	-1.85755759
C	-1.36103396	-1.40440152	-1.51486182
N	-0.91640012	-0.15383314	-1.37019404
H	-3.79132484	1.49506026	-1.90479938
H	-4.58024825	-0.84492408	-2.28861088
H	-2.98256440	-2.73419206	-1.95696865
N	-1.27129746	2.10172066	-1.18997859
H	-0.28228737	2.11889834	-0.95101344
N	-0.41653723	-2.39895905	-1.28640497
H	0.55894865	-2.10958492	-1.30486080
C	-1.96126103	3.25869029	-0.93991853
O	-3.15857171	3.39127388	-1.09504251
C	-0.66562170	-3.64659708	-0.78055868
O	-1.77894258	-4.09132994	-0.58361482
C	-1.08866883	4.37024688	-0.37957119
H	-0.09066669	4.27908934	-0.81684278
C	0.59212723	-4.41971591	-0.42058374
H	1.39831025	-4.09631217	-1.08475179

C	0.98436660	-4.06092625	1.01286945
H	1.88857214	-4.60272475	1.30050119
H	0.18698779	-4.33835699	1.70673724
H	1.17790605	-2.99256914	1.12500221
C	0.36330013	-5.91168715	-0.58064559
H	1.26040015	-6.46374814	-0.29100340
H	0.12035674	-6.16984526	-1.61343609
H	-0.46680593	-6.23900752	0.04690895
C	-0.95991797	4.16687785	1.13051315
H	-0.32784275	4.94594474	1.56242004
H	-0.51364399	3.19992304	1.37137671
H	-1.94230164	4.22761816	1.60692208
C	-1.67332243	5.72977233	-0.71373618
H	-1.05222047	6.52143837	-0.28849860
H	-2.68243488	5.82213144	-0.30968351
H	-1.73467550	5.88326686	-1.79290363
C	3.85822156	0.23075299	1.80455356
C	4.07890634	1.66585717	1.28745628
C	3.85265246	1.87405446	-0.21898927
C	4.72460991	0.89267047	-0.98620211
C	4.32980586	-0.53683963	-0.65109640
C	4.52859934	-0.78116546	0.85516249
H	3.45002237	2.35572366	1.85487461
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H	4.63563809	1.06615749	-2.06357108
H	5.77432708	1.05421754	-0.72076067
H	4.20141365	-1.79216230	1.10991739
H	5.60884303	-0.73626929	1.03313807
C	4.48790258	0.09700710	3.19620195
H	4.03043889	0.80186459	3.89233670
H	4.33998345	-0.91087410	3.58762135
H	5.56086617	0.29943824	3.14558615
C	5.16744646	-1.53953232	-1.43099801
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H	6.22265605	-1.40953162	-1.18040649
H	4.87161419	-2.56131891	-1.19496505
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H	5.23360336	3.51942692	-0.32808749
H	4.05297796	3.49323693	-1.64716880
H	3.55263653	4.00985594	-0.03506860
C	2.42730643	-0.02674901	1.92408892
C	1.22939489	-0.17468850	2.00725722
C	2.86963980	-0.73830274	-1.01189085
O	2.41270652	-1.83027713	-1.28085170
N	2.06254798	0.37023779	-1.03454184
C	2.39542999	1.61732282	-0.56718637
O	1.54116823	2.47298630	-0.46370528
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C	-1.32724026	-0.36877105	1.88806562
C	-2.72511486	-0.41084060	1.69769938
C	-3.39120752	-1.62426524	1.48367294
C	-4.74879339	-1.64721344	1.24834046
C	-5.46752422	-0.45663488	1.21181432
C	-4.81936359	0.75678706	1.42052060
C	-3.46202891	0.77789885	1.66154927
H	-2.82770946	-2.54888856	1.46853717
H	-5.26526236	-2.58138739	1.06668466
H	-5.37296134	1.68898559	1.36764029
H	-2.95375012	1.72327269	1.80336852
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H	-7.16574153	0.35422808	0.94513314

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C	-3.56957124	-0.49955645	-2.01083650
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C	-1.41166912	-1.33617984	-1.51244313
N	-0.92175399	-0.10344400	-1.36033037
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H	-3.08026854	-2.60354235	-1.96121652
N	-1.19142807	2.16263820	-1.17360949
H	-0.20886549	2.13885985	-0.91099595
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H	0.48243735	-2.10576073	-1.30338694
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O	-3.01118548	3.54881150	-1.18260202
C	-0.79074805	-3.61634196	-0.82119615
O	-1.91781212	-4.03596386	-0.64795093
C	-0.92613100	4.43254639	-0.39046321
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H	1.25988394	-4.12364942	-1.12333547
C	0.83977291	-4.10281320	0.97300683
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H	1.04978656	-6.49554508	-0.36236856
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C	4.51054118	-0.93353328	0.84474281
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H	5.20180351	1.75717487	1.49350794
H	4.66188838	0.93547701	-2.05818835
H	5.80850344	0.87277509	-0.72357268
H	4.15059265	-1.93502008	1.09276369
H	5.59268913	-0.92690591	1.01648736
C	4.51214476	-0.07621488	3.19426283
H	4.08296570	0.63755625	3.89926269
H	4.33169763	-1.08204702	3.57720519
H	5.59110071	0.08970110	3.13947676
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H	5.35289887	3.35229232	-0.30608730
H	4.16328887	3.37628709	-1.61705950
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C	-1.32018895	-0.34599756	1.90989681
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H	-5.27299220	-2.48729193	1.07360784
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C	-6.96503146	-0.35786372	1.02459186
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H	-7.51212697	-0.26166011	1.96769604

1B-F

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H	-3.73284099	1.65242258	-1.90593823
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O	-3.04017643	3.51819756	-1.07814962
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H	1.75931277	-4.64878059	1.25694608
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H	-0.66050007	-6.19298887	0.00819825
C	-0.81721173	4.20194611	1.15153146
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H	-0.39881456	3.21954151	1.37973726
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H	-0.84181906	6.57578767	-0.23893297
H	-2.49190171	5.92488978	-0.26528002
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C	3.83462863	0.12615373	1.81539028
C	4.11378902	1.55357313	1.30589798
C	3.91621502	1.77309297	-0.20293174
C	4.76285798	0.76305340	-0.96132799
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C	4.48106146	-0.90721492	0.87228600
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H	4.69465332	0.94245238	-2.03921578
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H	4.11460678	-1.90650205	1.11968270
H	5.55944719	-0.90123203	1.06603389
C	4.43953772	-0.03367307	3.21543066
H	3.99823478	0.68534395	3.90746869
H	4.25098723	-1.03671119	3.60171886
H	5.51944307	0.13089428	3.17935089
C	5.12622262	-1.68249098	-1.40636211
H	5.02948977	-1.53185742	-2.48358791
H	6.18158716	-1.59037591	-1.14022254
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C	4.30923070	3.20052062	-0.55443651
H	5.35549946	3.36914122	-0.28973912
H	4.19218063	3.38710155	-1.62410308
H	3.68913263	3.91778942	-0.01747588
C	2.39443039	-0.08244541	1.91779025
C	1.19280273	-0.19792575	1.99443546
C	2.85212379	-0.80132606	-1.01767260
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N	2.08378185	0.33437243	-1.04161704
C	2.45527931	1.56855845	-0.56856492
O	1.63008363	2.45265060	-0.47041783
H	1.06865851	0.19612157	-1.19822145
C	-0.16084310	-0.29170654	1.97527171
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C	-2.76669315	-0.38721824	1.68171905
C	-3.42219660	-1.60470508	1.46736096
C	-4.78529788	-1.63310056	1.24506502
C	-5.48292296	-0.44011413	1.23094374
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H	-5.44592784	1.69349002	1.38887867
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N	-0.79557326	-0.07403489	-1.38676993
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H	-4.47665683	-0.57114040	-2.36356893
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N	-1.04278432	2.19615787	-1.18735571
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N	-0.40926985	-2.34344781	-1.32199852
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C	-1.68956301	3.35671072	-0.84741273
O	-2.89078175	3.51598298	-0.92059638
C	-0.72820735	-3.56644048	-0.79574983
O	-1.86507977	-3.93588289	-0.57727473
C	-0.76150868	4.42560291	-0.29497685
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H	1.30414347	-4.13867767	-1.10734723
C	0.89875461	-4.07925102	0.99162909
H	1.77075544	-4.67276302	1.27616812
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H	1.15481055	-3.02390784	1.10311377
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H	1.02667591	-6.49391550	-0.31306105
H	-0.09682219	-6.13203411	-1.63237921
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H	0.09443104	4.91920454	1.62997958
H	-0.15763033	3.18610166	1.39813738
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H	-2.30972239	5.91742400	-0.12141445
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C	4.25101946	1.52440168	1.27363057
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C	4.89934660	0.67541469	-0.97351672
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H	4.84091951	0.83447977	-2.05510742
H	5.95119833	0.78310668	-0.69010805
H	4.18874904	-1.93906461	1.15670195
H	5.65174145	-0.96148009	1.09140490

C	4.53659861	-0.03023978	3.21690257
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H	4.32830360	-1.02179010	3.62210465
H	5.61927394	0.11412783	3.18265178
C	5.21566291	-1.78569772	-1.36767064
H	5.12711327	-1.65514067	-2.44815578
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H	4.85956021	-2.78525927	-1.12000579
C	4.49496458	3.12964490	-0.61712638
H	5.54286383	3.28119654	-0.34875165
H	4.38869399	3.29772375	-1.69091017
H	3.88701569	3.87040408	-0.09849773
C	2.49997977	-0.07051485	1.91202521
C	1.29766187	-0.17253040	1.99351377
C	2.95755349	-0.85157319	-1.00805740
O	2.44580731	-1.92011251	-1.27183808
N	2.21124441	0.29841379	-1.05376597
C	2.60704147	1.53648878	-0.61153935
O	1.80011433	2.43968846	-0.53976551
H	1.19430541	0.17765669	-1.21112490
C	-0.05638037	-0.25298585	1.97195696
C	-1.26175212	-0.29960341	1.86454542
C	-2.65891300	-0.32727592	1.65539743
C	-3.31950688	-1.54239961	1.44148215
C	-4.67370492	-1.55579081	1.18467676
C	-5.38580938	-0.35670744	1.13124578
C	-4.73276789	0.85881805	1.34042279
C	-3.38033548	0.87169348	1.60270931
H	-2.75887777	-2.46806217	1.43790760
H	-5.18372770	-2.49312723	1.00284696
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C	-3.18410674	-0.44821111	-2.16514080
C	-2.36162126	-1.54353382	-1.98786433
C	-1.04868935	-1.30296969	-1.60137407
N	-0.55518805	-0.07534292	-1.42535459
H	-3.34036138	1.70324713	-2.02363417
H	-4.21401207	-0.59334135	-2.47084767
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H	0.83294104	-2.10782968	-1.37581661
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H	-0.45489246	6.58182414	-0.23322463
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C	4.68739464	-0.08109103	3.27689297
H	4.24166729	0.64717372	3.95624489
H	4.47520138	-1.07997839	3.66152678
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H	5.39502004	-1.60730819	-2.40151423
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H	5.73999629	3.29647524	-0.21567401
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C	1.47105669	-0.19923504	1.99441831
C	3.19255165	-0.83945419	-0.99266306
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C	-3.14848381	-1.50857367	1.32489318
C	-4.49917202	-1.49986024	1.04381466
C	-5.17079452	-0.28936292	1.02091770
C	-4.53472979	0.91535716	1.26957329
C	-3.18547339	0.90389870	1.55237112
H	-2.59759817	-2.43989260	1.30483993
H	-5.03332908	-2.41364625	0.82443212
H	-5.09348975	1.83916376	1.21889729
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N	-6.59993786	-0.28002218	0.70084549
O	-7.17311238	0.78801855	0.72324050
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