Supporting Information

for

On the Nature of σ-σ, σ-π, and π-π Stacking in Extended Systems

Enrique M. Cabaleiro-Lago,*[a] Jesús Rodríguez-Otero [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. Ionization potentials and HOMO energies in a.u. for the molecules considered in this study. A shift parameter is applied in SAPT(DFT) calculations corresponding to IP+E(HOMO). PBE0/cc-pVTZ.

	IP	E_{HOMO}		IP	E_{HOMO}
C_6H_6	0.34234	-0.26638	C_6H_{12}	0.37627	-0.30455
$C_{10}H_8$	0.29418	-0.23097	$C_{10}H_{18}$	0.34577	-0.28577
$C_{14}H_{10}$	0.26447	-0.20924	$C_{14}H_{24}$	0.32885	-0.27595
$C_{18}H_{12}$	0.24444	-0.19498	$C_{18}H_{30}$	0.31813	-0.27025
$C_{22}H_{14}$	0.23010	-0.18495	$C_{22}H_{36}$	0.31048	-0.26625
$C_{26}H_{16}$	0.21938	-0.17758	$C_{26}H_{42}$	0.30482	-0.26356
$C_{16}H_{10}$	0.26687	-0.21269	$C_{16}H_{26}$	0.32168	-0.27009
$C_{20}H_{12}$	0.24767	-0.19801	$C_{20}H_{32}$	0.31225	-0.26438
$C_{24}H_{12}$	0.26447	-0.21710	$C_{24}H_{36}$	0.30343	-0.25793

Table S2. Distances (Å) at the minimum for each of the dimers studied. TPSS-D3BJ/def2-TZVP. C_n as in Figure 1.

	cross	glike	slip	stack
		π-π		
C_6	3.921	3.579	3.579	3.926
C_{10}	3.580	3.476	3.511	3.841
C_{14}	3.433	3.435	3.479	3.805
C_{18}	3.368	3.416	3.462	3.783
C_{22}	3.373	3.404	3.450	3.773
C_{26}	3.345	3.396	3.439	3.741
C_{16}	3.518	3.422	3.409	3.771
C_{20}	3.398	3.384	3.384	3.748
C_{24}	3.496	3.386	3.386	3.714
		σ-π		
C_6	4.226	4.020	4.022	4.226
C_{10}	4.100	3.982	4.006	4.180
C_{14}	4.016	3.957	3.993	4.154
C_{18}	3.998	3.972	4.014	4.167
C_{22}	3.962	3.939	3.982	4.132
C_{26}	3.930	3.935	3.978	4.125
C_{16}	4.101	3.965	3.957	4.150
C_{20}	4.074	3.946	3.947	4.139
C_{24}	4.088	3.939	3.940	4.128
		σ-σ		
C_6	4.847	4.603	4.604	4.611
C_{10}	4.686	4.575	4.607	4.571
C_{14}	4.602	4.583	4.582	4.562
C_{18}	4.641	4.542	4.670	4.579
C_{22}	4.549	4.575	4.579	4.552
C_{26}	4.517	4.573	4.578	4.549
C_{16}	4.719	4.575	4.561	4.549
C_{20}	4.675	4.562	4.561	4.545
C_{24}	4.717	4.559	4.558	4.532

Table S3. Interaction energies (kcal mol^{-1}) at the minimum for each of the dimers studied as obtained at the TPSS-D3BJ/def2-TZVPP level. C_n as in Figure 1.

	cross	glike	slip	stack
		π-π		
C_6	-2.04	-2.81	-2.81	-2.04
C_{10}	-6.03	-6.27	-5.96	-4.64
C_{14}	-10.22	-9.94	-9.26	-7.38
C_{18}	-12.16	-13.66	-12.63	-10.15
C_{22}	-12.87	-17.39	-16.05	-12.93
C_{26}	-13.37	-21.13	-19.53	-16.05
C_{16}	-11.67	-12.10	-12.45	-9.30
C_{20}	-17.47	-16.68	-16.68	-12.44
C_{24}	-20.14	-21.06	-21.06	-16.20
		σ-π		
C_6	-3.20	-3.25	-3.25	-3.20
C_{10}	-6.12	-6.40	-6.10	-6.06
C_{14}	-8.34	-9.70	-9.00	-9.04
C_{18}	-9.38	-12.74	-11.96	-11.86
C_{22}	-10.09	-16.35	-14.87	-15.04
C_{26}	-10.56	-19.67	-17.80	-18.07
C_{16}	-10.91	-11.40	-11.71	-10.82
C_{20}	-14.50	-15.10	-15.10	-14.09
C_{24}	-18.05	-19.04	-19.04	-17.57
		σ-σ		
C_6	-2.29	-2.43	-2.42	-2.71
C_{10}	-4.60	-4.78	-4.54	-5.15
C_{14}	-6.40	-7.21	-6.76	-7.67
C_{18}	-7.02	-9.76	-8.79	-10.06
C_{22}	-7.88	-12.18	-11.20	-12.78
C_{26}	-8.28	-14.68	-13.43	-15.35
C_{16}	-8.13	-8.51	-8.80	-9.29
C_{20}	-11.01	-11.28	-11.28	-12.10
C_{24}	-13.49	-14.31	-14.31	-15.27

Table S4. Interaction energies (kcal mol^{-1}) at the minimum for each of the dimers studied as obtained at the MP2.X level. C_n as in Figure 1.

	cross	glike	slip	stack
		π-π		
C_6	-1.91	-3.03	-3.03	-1.90
C_{10}	-6.38	-6.87	-6.48	-4.53
C_{14}	-10.70	-10.77	-10.08	-7.27
C_{18}	-12.42	-14.67	-13.73	-10.09
C_{22}	-13.27	-18.54	-17.40	-12.93
C_{26}	-13.85	-22.29	-21.10	-15.80
C_{16}	-12.07	-12.81	-13.06	-9.06
C_{20}	-17.77	-17.04	-17.05	-11.70
C_{24}	-19.99	-20.82	-20.84	-15.09
		σ-π		
C_6	-3.25	-3.44	-3.44	-3.24
C_{10}	-6.27	-6.81	-6.43	-6.23
C_{14}	-8.21	-10.29	-9.45	-9.29
C_{18}	-9.05	-13.36	-12.57	-12.14
C_{22}	-9.84	-17.27	-15.63	-15.53
C_{26}	-10.46	-20.76	-18.74	-18.66
C_{16}	-11.01	-11.76	-12.11	-10.91
C_{20}	-14.46	-15.24	-15.24	-13.97
C_{24}	-17.81	-18.89	-18.89	-17.20
		σ-σ		
C_6	-1.85	-2.05	-2.05	-2.50
C_{10}	-3.80	-4.02	-3.88	-4.70
C_{14}	-5.21	-6.07	-5.80	-6.90
C_{18}	-5.49	-8.12	-7.43	-8.82
C_{22}	-6.39	-10.25	-9.61	-11.33
C_{26}	-6.80	-12.33	-11.53	-13.56
C_{16}	-6.58	-7.01	-7.23	-8.02
C_{20}	-8.91	-9.20	-9.21	-10.39
C_{24}	-10.68	-11.32	-11.31	-12.63

Table S5. Interaction energies (kcal mol^{-1}) at the minimum for each of the dimers studies as obtained with SAPT(DFT). C_n as in Figure 1.

	cross	glike	slip	stack
		π-π		
C_6	-1.72	-2.76	-2.76	-1.69
C_{10}	-5.93	-6.41	-6.02	-4.17
C_{14}	-10.06	-10.27	-9.46	-6.81
C_{18}	-12.02	-14.19	-12.97	-9.50
C_{22}	-12.85	-18.15	-16.52	-12.09
C_{26}	-13.50	-22.15	-20.12	-12.38
C_{16}	-11.51	-12.36	-12.78	-8.62
C_{20}	-17.38	-16.75	-16.75	-11.34
C_{24}	-19.84	-21.06	-21.06	-14.97
		σ-π		
C_6	-3.18	-3.26	-3.26	-3.18
C_{10}	-6.07	-6.44	-6.13	-6.07
C_{14}	-8.03	-9.72	-9.03	-9.03
C_{18}	-8.98	-12.72	-11.99	-11.83
C_{22}	-9.65	-16.28	-14.88	-14.96
C_{26}				
C_{16}	-10.79	-11.32	-11.61	-10.77
C_{20}	-14.21	-14.77	-14.77	-13.85
C_{24}	-17.69	-18.50	-18.49	-17.23
		σ-σ		
C_6	-1.98	-2.12	-2.12	-2.57
C_{10}	-4.01	-4.23	-4.00	-4.83
C_{14}	-5.56	-6.32	-5.94	-7.07
C_{18}	-5.99	-8.56	-7.70	-9.12
C_{22}	-6.80	-10.57	-9.75	-11.54
C_{26}				
C_{16}	-7.04	-7.45	-7.70	-8.46
C_{20}	-9.56	-9.79	-9.79	-10.91
C_{24}	-11.62	-12.28	-12.28	-13.53

Table S6. Interaction energies (kcal mol^{-1}) for the most stable structures. C_n as in Figure 1.

	TPSS-D3BJ	MP2.X	SAPT(DFT)
		π-π	
C_6	-2.81	-3.03	-2.76
C_{10}	-6.27	-6.86	-6.41
C_{14}	-9.94	-10.77	-10.27
C_{18}	-13.66	-14.67	-14.19
C_{22}	-17.39	-18.53	-18.15
C_{26}	-21.13	-22.27	-22.15
C_{16}	-12.45	-13.05	-12.78
C_{20}	-17.47	-17.76	-17.38
C_{24}	-21.06	-20.81	-21.06
		σ-π	
C_6	-3.25	-3.44	-3.26
C_{10}	-6.40	-6.81	-6.44
C_{14}	-9.70	-10.29	-9.72
C_{18}	-12.74	-13.36	-12.72
C_{22}	-16.35	-17.27	-16.28
C_{26}	-19.67	-20.76	-19.01
C_{16}	-11.71	-12.11	-11.61
C_{20}	-15.10	-15.24	-14.77
C_{24}	-19.04	-18.89	-18.50
		σ-σ	
C_6	-2.71	-2.50	-2.57
C_{10}	-5.15	-4.70	-4.83
C_{14}	-7.67	-6.90	-7.07
C_{18}	-10.06	-8.82	-9.12
C_{22}	-12.78	-11.33	-11.54
C_{26}	-15.35	-13.56	-13.72
C_{16}	-9.29	-8.02	-8.46
C_{20}	-12.10	-10.39	-10.91
C_{24}	-15.27	-12.63	-13.53

Table S7. Contributions to the interaction energies (kcal mol^{-1}) at the minimum for the most stable dimers studied as obtained with SAPT(DFT). C_n as in Figure 1.

	E_{ele}	E_{rep}	E_{ind}	E_{dis}	E_{tot}
		π-π			
C_6	-0.81	4.73	-0.53	-6.15	-2.76
C_{10}	-2.90	11.16	-1.14	-13.54	-6.42
C_{14}	-5.23	18.07	-1.82	-21.29	-10.27
C_{18}	-7.55	25.00	-2.53	-29.08	-14.16
C_{22}	-9.91	32.02	-3.30	-36.92	-18.11
C_{26}	-12.04	39.05	-4.36	-44.78	-22.13
C_{16}	-6.78	22.13	-2.19	-25.91	-12.75
C_{20}	-9.34	30.11	-3.10	-34.99	-17.32
C_{24}	-11.37	34.75	-3.07	-41.33	-21.02
		σ-π			
C_6	-1.82	4.89	-0.48	-5.84	-3.25
C_{10}	-3.79	10.05	-0.87	-11.84	-6.45
C_{14}	-5.95	15.75	-1.27	-18.26	-9.73
C_{18}	-7.77	20.52	-1.60	-23.87	-12.72
C_{22}	-10.28	27.11	-2.05	-31.06	-16.28
C_{26}[a]	-12.45	32.81	-2.45	-36.92	-19.01
C_{16}	-7.25	19.09	-1.49	-21.96	-11.61
C_{20}	-9.31	24.61	-1.88	-28.19	-14.77
C_{24}	-12.00	31.57	-2.28	-35.78	-18.49
		σ-σ			
C_6	-1.33	4.43	-0.35	-5.32	-2.57
C_{10}	-2.95	9.53	-0.72	-10.69	-4.83
C_{14}	-4.55	14.57	-1.09	-15.99	-7.06
C_{18}	-6.11	19.64	-1.45	-21.20	-9.12
C_{22}	-7.78	24.71	-1.82	-26.65	-11.54
C_{26} [a]	-9.40	29.78	-2.18	-31.92	-13.72
C_{16}	-5.80	18.38	-1.36	-19.69	-8.47
C_{20}	-7.53	23.82	-1.73	-25.47	-10.91
C_{24}	-9.89	31.00	-2.26	-32.38	-13.53

[a] Dispersion contribution obtained from linear extrapolation using the values for smaller linear acenes.

Table S8. Contributions to the interaction energies (kcal mol^{-1}) for the different dimers at the distance of the minima obtained for the smallest dimers. C_n as in Figure 1.

	E_{ele}	E_{rep}	E_{ind}	E_{dis}	E_{tot}
		π-π			
C_6	-0.81	4.73	-0.53	-6.15	-2.76
C_{10}	-1.81	8.24	-0.88	-11.70	-6.15
C_{14}	-2.86	11.86	-1.25	-17.43	-9.68
C_{18}	-3.93	15.54	-1.63	-23.24	-13.26
C_{22}	-5.00	19.25	-2.04	-29.07	-16.86
C_{26}	-6.08	22.98	-2.43	-34.81	-20.34
C_{16}	-3.30	12.88	-1.22	-19.95	-11.59
C_{20}	-4.31	16.23	-1.64	-25.67	-15.39
C_{24}	-5.52	19.66	-1.82	-31.79	-19.47
		σ-π			
C_6	-1.82	4.89	-0.48	-5.84	-3.25
C_{10}	-3.42	9.06	-0.79	-11.23	-6.38
C_{14}	-5.03	13.27	-1.09	-16.75	-9.6
C_{18}	-6.85	18.05	-1.43	-22.38	-12.61
C_{22}	-8.29	21.81	-1.68	-27.87	-16.03
C_{26} [a]	-9.94	26.12	-1.95	-33.33	-19.1
C_{16}	-6.01	15.91	-1.27	-19.84	-11.21
C_{20}	-7.68	20.27	-1.57	-25.60	-14.58
C_{24}	-9.70	25.49	-1.87	-32.19	-18.27
		σ-σ			
C_6	-1.33	4.43	-0.35	-5.32	-2.57
C_{10}	-2.65	8.61	-0.65	-10.10	-4.79
C_{14}	-3.97	12.82	-0.96	-14.91	-7.02
C_{18}	-5.60	18.09	-1.33	-20.26	-9.1
C_{22}	-6.64	21.26	-1.56	-24.54	-11.48
C_{26} [a]	-7.96	25.45	-1.85	-29.26	-13.62
C_{16}	-4.92	15.73	-1.15	-18.08	-8.42
C_{20}	-6.35	20.26	-1.46	-23.31	-10.86
C_{24}	-8.09	25.63	-1.84	-29.19	-13.49

[a] Dispersion contribution obtained from linear extrapolation using the values for smaller linear acenes.

Table S9. Isotropic polarizabilities (a. u.) obtained for the molecules studied at the TPSS-D3BJ/def2-TZVPP level.

	α		α
C_6H_6	65.51	C_6H_{12}	70.24
$C_{10}H_8$	115.52	$C_{10}H_{18}$	113.62
$C_{14}H_{10}$	177.00	$C_{14}H_{24}$	158.03
$C_{18}H_{12}$	250.04	$C_{18}H_{30}$	203.22
$C_{22}H_{14}$	333.99	$C_{22}H_{36}$	248.97
$C_{26}H_{16}$	427.87	$C_{26}H_{42}$	295.05
$C_{16}H_{10}$	194.68	$C_{16}H_{26}$	176.16
$C_{20}H_{12}$	253.02	$C_{20}H_{32}$	219.74
$C_{24}H_{12}$	298.62	$C_{24}H_{36}$	258.77

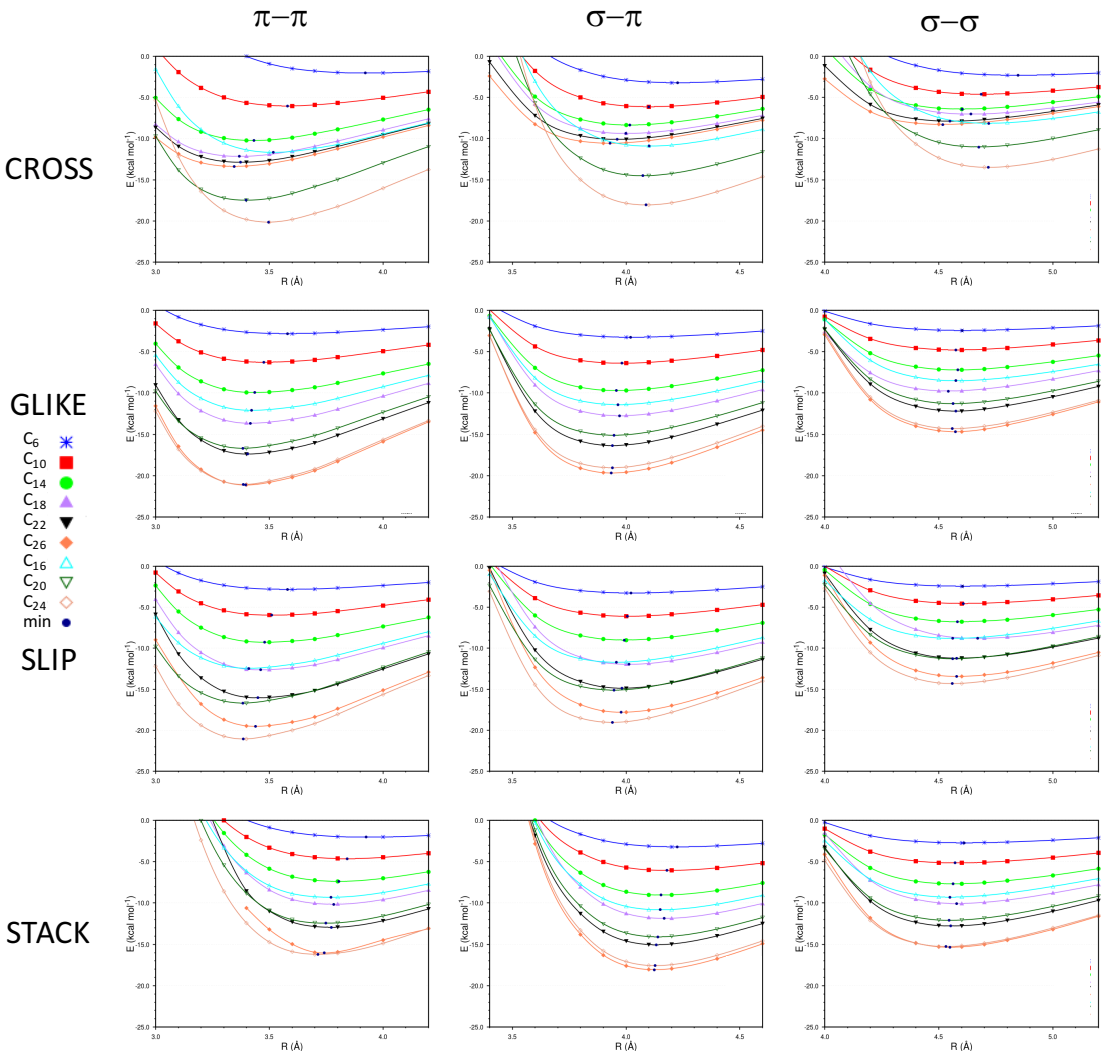

Figure S1. Potential energy curves for the different dimers studied at the TPSS-D3BJ/def2-TZVPP level.

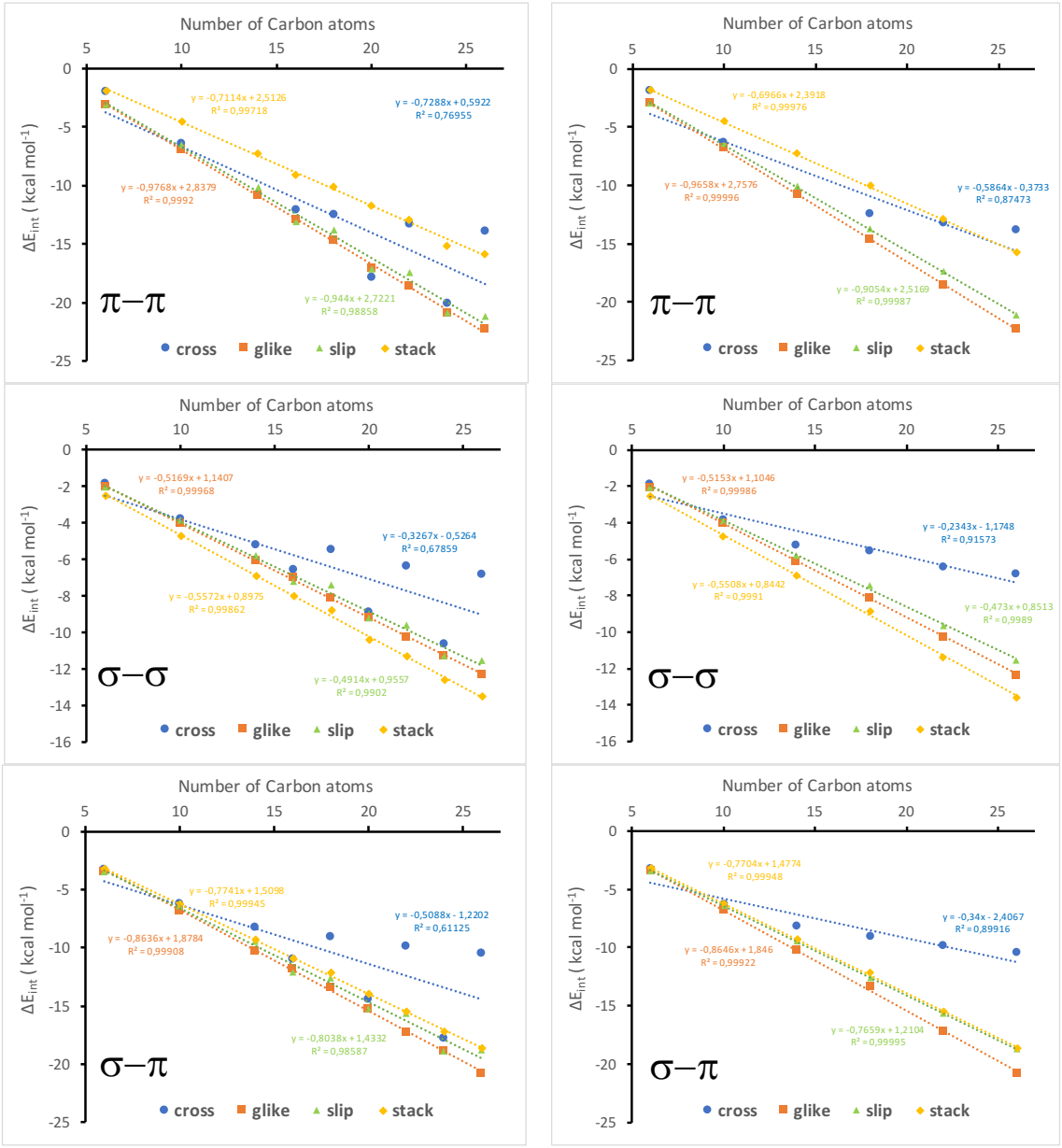

Figure S2. Linear fit of the interaction energy values obtained at the MP2.X level. On the left all values are employed; plots on the right employ only linear acenes.

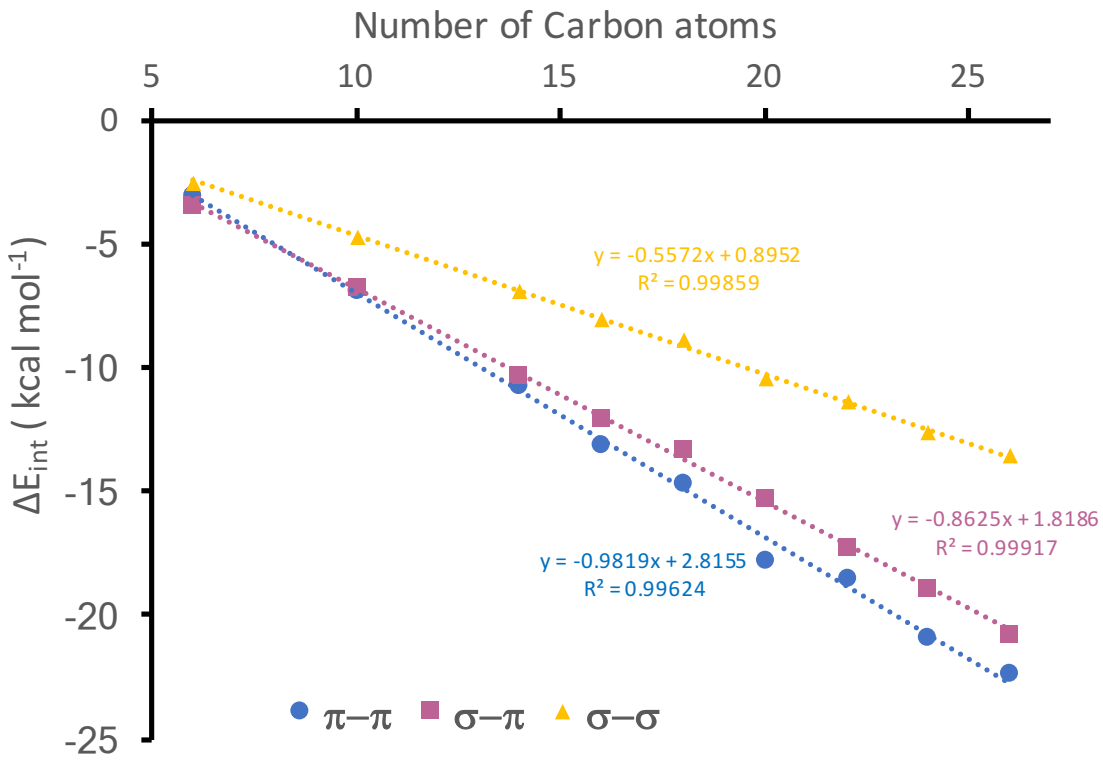

Figure S3. Interaction energies for the most stable structures as obtained at the MP2.X level.

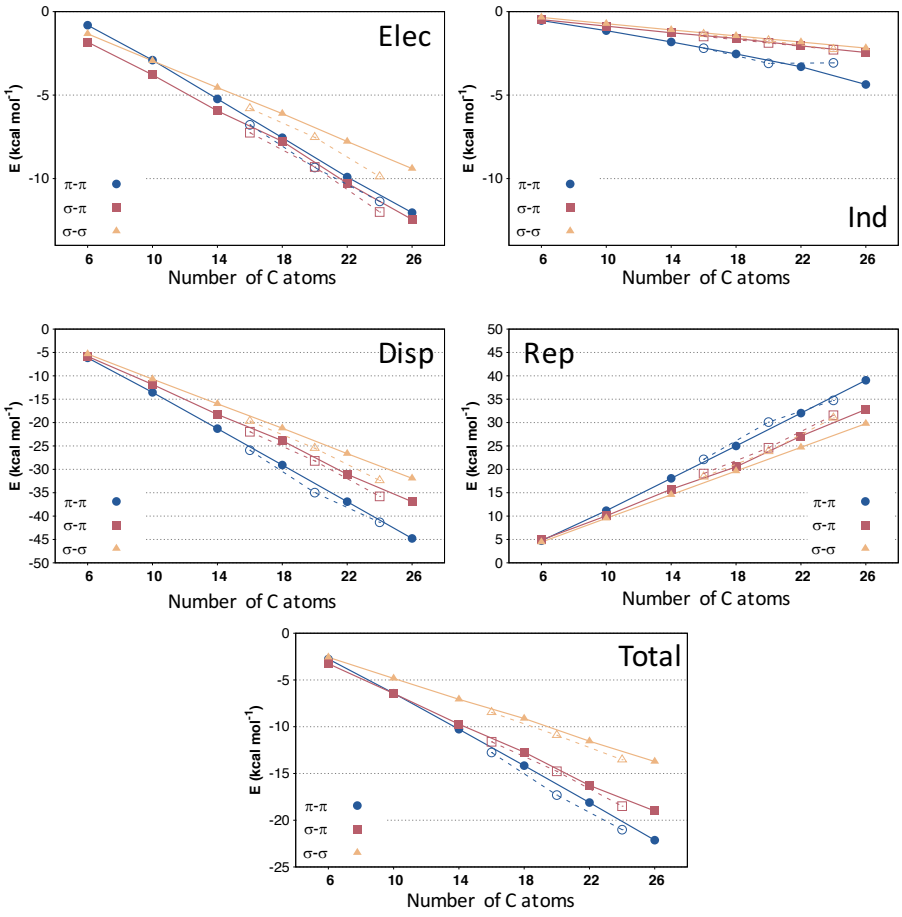

Figure S4. Variation of the components of the interaction energy as the size of the dimer grows.

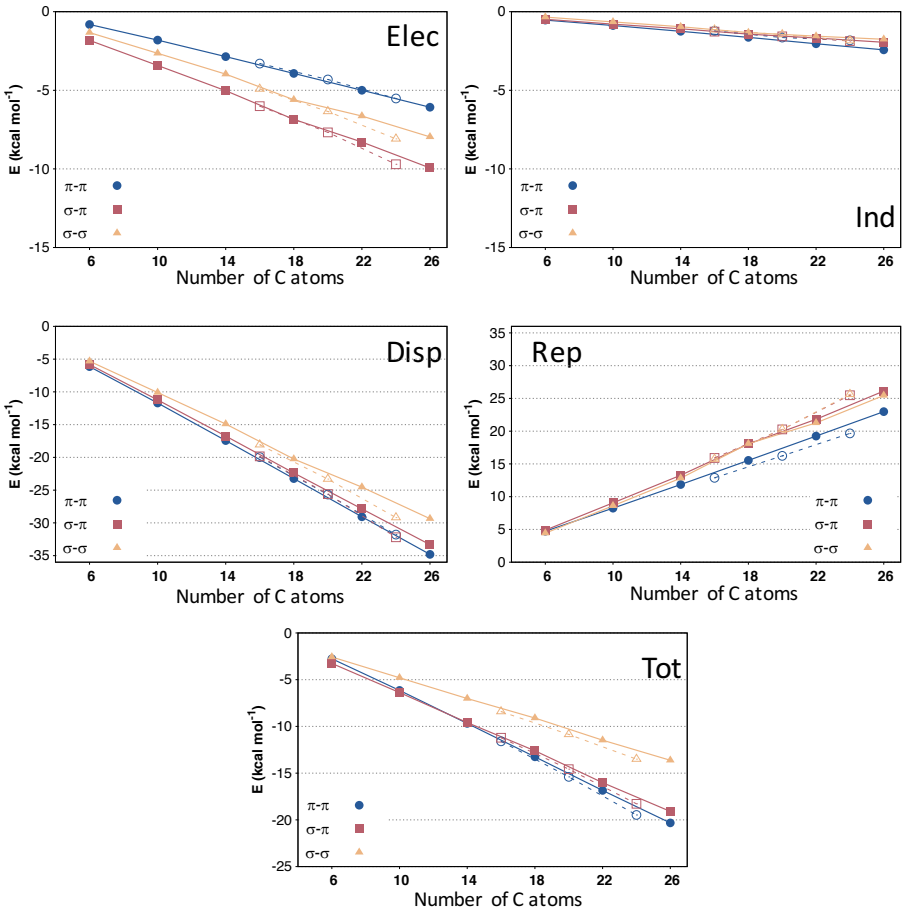

Figure S5. Variation of the components of the interaction energy as the size of the dimer grows. The intermolecular distance is kept at the value obtained for the smallest dimers.

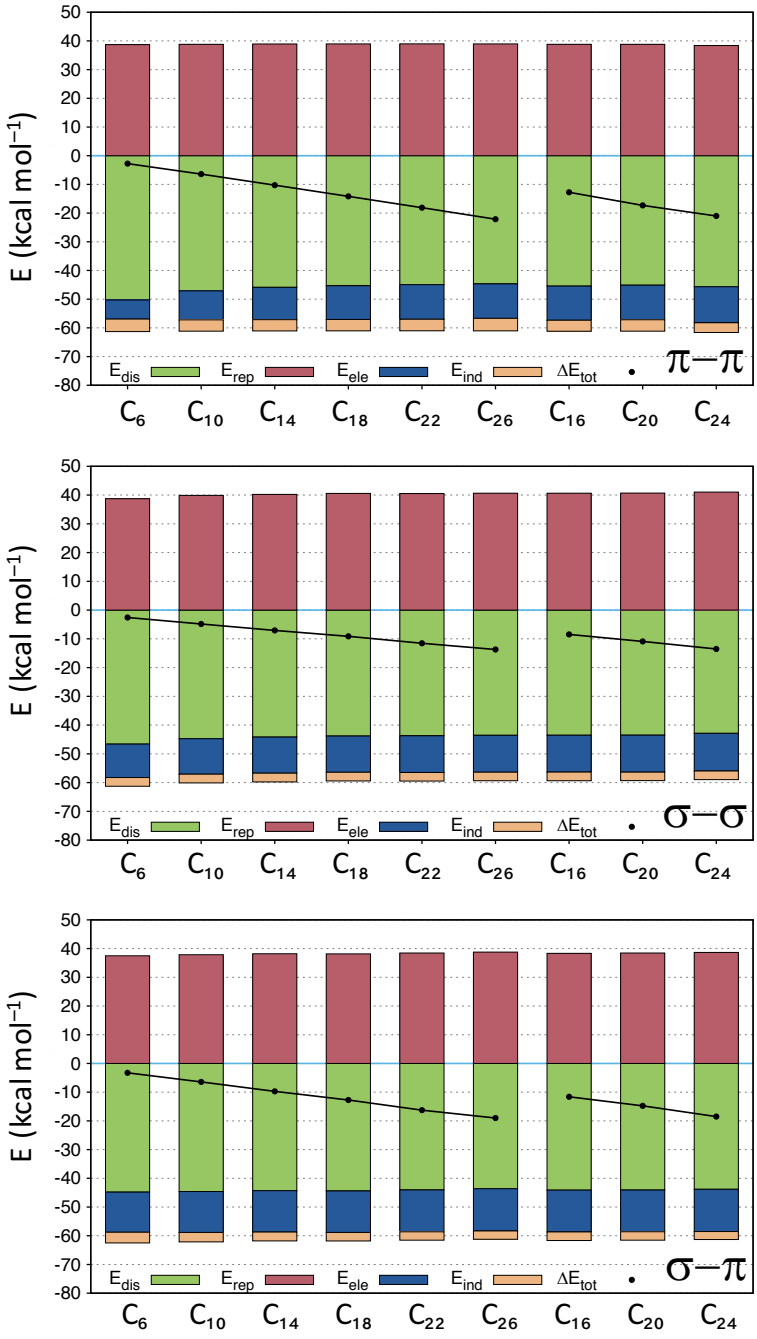

Figure S6. SAPT(DFT) percent contributions to the total interaction energy of the most stable dimers, obtained as $-E_i/(E_{ele}-E_{rep}+E_{ind}+E_{dis})*100$

Cartesian coordinates (Å) for isolated molecules at the TPSS-D3BJ/def2-TZVPP level.

C_6H_6

C	1.208832	0.697920	0.000000
C	1.208832	-0.697920	0.000000
C	0.000000	-1.395839	0.000000
C	-1.208832	-0.697920	0.000000
C	-1.208832	0.697920	0.000000
C	0.000000	1.395839	0.000000
H	2.149402	1.240958	0.000000
H	2.149402	-1.240958	0.000000
H	0.000000	-2.481916	0.000000
H	-2.149402	-1.240958	0.000000
H	-2.149402	1.240958	0.000000
H	0.000000	2.481916	0.000000

$C_{10}H_8$

C	-1.242676	1.402202	0.000000
C	-2.431680	0.707522	0.000000
C	0.000000	0.717236	0.000000
C	-2.431680	-0.707522	0.000000
C	0.000000	-0.717236	0.000000
C	1.242676	1.402202	0.000000
C	-1.242676	-1.402202	0.000000
C	1.242676	-1.402202	0.000000
C	2.431680	0.707522	0.000000
C	2.431680	-0.707522	0.000000
H	3.375844	1.243938	0.000000
H	3.375844	-1.243938	0.000000
H	1.239630	2.489188	0.000000
H	-1.239630	2.489188	0.000000
H	-3.375844	1.243938	0.000000
H	-3.375844	-1.243938	0.000000
H	1.239630	-2.489188	0.000000
H	-1.239630	-2.489188	0.000000

$C_{14}H_{10}$

C	-3.657400	-0.711752	0.000000
C	-2.475314	1.406308	0.000000
C	-1.222858	0.722863	0.000000
C	0.000000	1.404287	0.000000
H	-4.603239	-1.245089	0.000000
H	-2.472734	2.493180	0.000000
H	0.000000	2.492199	0.000000
C	3.657400	0.711752	0.000000
C	2.475314	-1.406308	0.000000
C	1.222858	-0.722863	0.000000
C	0.000000	-1.404287	0.000000
H	4.603239	1.245089	0.000000
H	2.472734	-2.493180	0.000000
H	0.000000	-2.492199	0.000000
C	-3.657400	0.711752	0.000000
C	-2.475314	-1.406308	0.000000
C	-1.222858	-0.722863	0.000000
H	-4.603239	1.245089	0.000000
H	-2.472734	-2.493180	0.000000
C	3.657400	-0.711752	0.000000
C	2.475314	1.406308	0.000000
C	1.222858	0.722863	0.000000
H	4.603239	-1.245089	0.000000
H	2.472734	2.493180	0.000000

$C_{18}H_{12}$

C	3.705158	-1.408243	0.000000
C	4.884357	-0.713725	0.000000
C	2.448535	-0.725816	0.000000
C	1.233201	-1.406971	0.000000
H	1.233629	-2.494780	0.000000
H	3.702838	-2.495092	0.000000
H	5.830924	-1.245703	0.000000
C	0.000000	-0.726795	0.000000
C	-3.705158	1.408243	0.000000
C	-4.884357	0.713725	0.000000
C	-2.448535	0.725816	0.000000
C	-1.233201	1.406971	0.000000
H	-1.233629	2.494780	0.000000
H	-3.702838	2.495092	0.000000
H	-5.830924	1.245703	0.000000
C	0.000000	0.726795	0.000000
C	3.705158	1.408243	0.000000
C	4.884357	0.713725	0.000000
C	2.448535	0.725816	0.000000
C	1.233201	1.406971	0.000000
H	1.233629	2.494780	0.000000
H	3.702838	2.495092	0.000000
H	5.830924	1.245703	0.000000
C	-3.705158	-1.408243	0.000000
C	-4.884357	-0.713725	0.000000
C	-2.448535	-0.725816	0.000000
C	-1.233201	-1.406971	0.000000
H	-1.233629	-2.494780	0.000000
H	-3.702838	-2.495092	0.000000
H	-5.830924	-1.245703	0.000000

$C_{22}H_{14}$

C	2.463478	-1.408362	0.000000
C	3.675389	-0.727300	0.000000
C	1.225565	-0.728976	0.000000
C	0.000000	-1.409170	0.000000
H	0.000000	-2.496836	0.000000
H	2.464131	-2.496132	0.000000
C	-1.225565	-0.728976	0.000000
C	-4.933993	1.409210	0.000000
C	-6.111839	0.714716	0.000000
C	-3.675389	0.727300	0.000000
C	-2.463478	1.408362	0.000000
H	-2.464131	2.496132	0.000000
H	-4.931933	2.496047	0.000000
H	-7.058676	1.246215	0.000000
C	-1.225565	0.728976	0.000000
C	2.463478	1.408362	0.000000
C	3.675389	0.727300	0.000000

C	1.225565	0.728976	0.000000
C	0.000000	1.409170	0.000000
H	0.000000	2.496836	0.000000
H	2.464131	2.496132	0.000000
C	-4.933993	-1.409210	0.000000
C	-6.111839	-0.714716	0.000000
C	-3.675389	-0.727300	0.000000
C	-2.463478	-1.408362	0.000000
H	-2.464131	-2.496132	0.000000
H	-4.931933	-2.496047	0.000000
H	-7.058676	-1.246215	0.000000
C	4.933993	1.409210	0.000000
H	4.931933	2.496047	0.000000
C	6.111839	0.714716	0.000000
H	7.058676	1.246215	0.000000
C	6.111839	-0.714716	0.000000
C	4.933993	-1.409210	0.000000
H	4.931933	-2.496047	0.000000
H	7.058676	-1.246215	0.000000

$C_{26}H_{16}$

C	-1.230354	-1.410278	0.000000
C	-2.452384	-0.730085	0.000000
C	0.000000	-0.730860	0.000000
C	1.230354	-1.410278	0.000000
H	1.230650	-2.497858	0.000000
H	-1.230650	-2.497858	0.000000
C	2.452384	-0.730085	0.000000
C	6.162477	1.409775	0.000000
C	7.339612	0.715264	0.000000
C	4.902837	0.728078	0.000000
C	3.692573	1.409095	0.000000
H	3.693386	2.496817	0.000000
H	6.160553	2.496596	0.000000
H	8.286644	1.246422	0.000000
C	2.452384	0.730085	0.000000
C	-1.230354	1.410278	0.000000
C	-2.452384	0.730085	0.000000
C	0.000000	0.730860	0.000000
C	1.230354	1.410278	0.000000
H	1.230650	2.497858	0.000000
H	-1.230650	2.497858	0.000000
C	6.162477	-1.409775	0.000000
C	7.339612	-0.715264	0.000000
C	4.902837	-0.728078	0.000000
C	3.692573	-1.409095	0.000000
H	3.693386	-2.496817	0.000000
H	6.160553	-2.496596	0.000000
H	8.286644	-1.246422	0.000000
C	-3.692573	1.409095	0.000000
H	-3.693386	2.496817	0.000000
C	-4.902837	0.728078	0.000000
C	-4.902837	-0.728078	0.000000
C	-3.692573	-1.409095	0.000000
H	-3.693386	-2.496817	0.000000
C	-6.162477	1.409775	0.000000
H	-6.160553	2.496596	0.000000
C	-7.339612	0.715264	0.000000
H	-8.286644	1.246422	0.000000
C	-7.339612	-0.715264	0.000000
C	-6.162477	-1.409775	0.000000
H	-8.286644	-1.246422	0.000000
H	-6.160553	-2.496596	0.000000

$C_{16}H_{10}$

C	-1.236145	1.426913	0.000000
C	-2.460959	0.681783	0.000000
C	0.000000	0.711302	0.000000
C	-1.210360	2.831188	0.000000
C	-2.460959	-0.681783	0.000000
C	0.000000	-0.711302	0.000000
C	1.236145	1.426913	0.000000
C	0.000000	3.521435	0.000000
C	-1.236145	-1.426913	0.000000
C	1.210360	2.831188	0.000000
C	1.236145	-1.426913	0.000000
C	2.460959	0.681783	0.000000
C	-1.210360	-2.831188	0.000000
C	2.460959	-0.681783	0.000000
C	1.210360	-2.831188	0.000000
C	0.000000	-3.521435	0.000000
H	0.000000	4.607386	0.000000
H	2.150318	3.376549	0.000000
H	3.398472	1.231672	0.000000
H	3.398472	-1.231672	0.000000
H	2.150318	-3.376549	0.000000
H	0.000000	-4.607386	0.000000
H	-3.398472	1.231672	0.000000
H	-2.150318	3.376549	0.000000
H	-3.398472	-1.231672	0.000000
H	-2.150318	-3.376549	0.000000

$C_{20}H_{12}$

C	0.013260	-1.447331	0.000000
C	-0.013260	1.447331	0.000000
C	-1.260055	-0.712182	0.000000
C	1.260055	0.712182	0.000000
C	1.243245	-0.717788	0.000000
C	-1.243245	0.717788	0.000000
C	-2.490611	-1.364559	0.000000
C	2.490611	1.364559	0.000000
C	2.486402	-1.435525	0.000000
C	-2.486402	1.435525	0.000000
C	0.063563	-2.839212	0.000000
C	-0.063563	2.839212	0.000000
C	2.475745	-2.851847	0.000000
C	-2.475745	2.851847	0.000000
C	-3.707644	0.718134	0.000000
C	3.707644	-0.718134	0.000000
C	1.281610	-3.537659	0.000000
C	-1.281610	3.537659	0.000000
C	-3.704508	-0.658923	0.000000
C	3.704508	0.658923	0.000000
H	-4.640364	-1.209605	0.000000
H	4.640364	1.209605	0.000000

H	-0.855507	-3.413877	0.000000
H	0.855507	3.413877	0.000000
H	-2.528751	-2.447829	0.000000
H	2.528751	2.447829	0.000000
H	-4.640998	1.274175	0.000000
H	4.640998	-1.274175	0.000000
H	1.272634	-4.623476	0.000000
H	-1.272634	4.623476	0.000000
H	3.423966	-3.382135	0.000000
H	-3.423966	3.382135	0.000000

$C_{24}H_{12}$

C	1.234072	0.712492	0.000000
C	1.234072	-0.712492	0.000000
C	0.000000	1.424983	0.000000
C	2.466181	1.423850	0.000000
C	0.000000	-1.424983	0.000000
C	-1.234072	0.712492	0.000000
C	2.466181	-1.423850	0.000000
C	0.000000	2.847701	0.000000
C	3.682207	0.686742	0.000000
C	2.435840	2.845514	0.000000
C	3.682207	-0.686742	0.000000
C	-1.234072	-0.712492	0.000000
C	1.246367	3.532256	0.000000
C	0.000000	-2.847701	0.000000
C	-2.466181	1.423850	0.000000
C	2.435840	-2.845514	0.000000
C	-1.246367	3.532256	0.000000
C	-2.466181	-1.423850	0.000000
C	1.246367	-3.532256	0.000000
C	-2.435840	2.845514	0.000000
C	-1.246367	-3.532256	0.000000
C	-3.682207	0.686742	0.000000
C	-2.435840	-2.845514	0.000000
C	-3.682207	-0.686742	0.000000
H	4.621501	1.233498	0.000000
H	3.378991	3.385588	0.000000
H	4.621501	-1.233498	0.000000
H	1.242510	4.619086	0.000000
H	3.378991	-3.385588	0.000000
H	-1.242510	4.619086	0.000000
H	1.242510	-4.619086	0.000000
H	-3.378991	3.385588	0.000000
H	-1.242510	-4.619086	0.000000
H	-4.621501	1.233498	0.000000
H	-3.378991	-3.385588	0.000000
H	-4.621501	-1.233498	0.000000

C_6H_{12}

C	1.266958	-0.731478	0.233157
C	1.266958	0.731478	-0.233157
C	0.000000	1.462957	0.233157
C	-1.266958	0.731478	-0.233157
C	-1.266958	-0.731478	0.233157
C	0.000000	-1.462957	-0.233157
H	1.313992	-0.758633	1.330978
H	2.161336	1.247848	0.134698
H	0.000000	1.517267	1.330978
H	-2.161336	1.247848	0.134698
H	-1.313992	-0.758633	1.330978
H	0.000000	-2.495696	0.134698
H	2.161336	-1.247848	-0.134698
H	1.313992	0.758633	-1.330978
H	0.000000	2.495696	-0.134698
H	-1.313992	0.758633	-1.330978
H	-2.161336	-1.247848	-0.134698
H	0.000000	-1.517267	-1.330978

$C_{10}H_{18}$

C	-2.542135	-0.726067	0.247844
C	1.272123	1.459802	0.200550
C	0.000000	0.728944	-0.250262
H	0.000000	-0.694433	1.352612
H	3.433499	-1.252541	-0.113097
H	-1.264533	-1.536370	-1.297694
H	-2.592756	-0.731869	1.345605
H	-1.266200	2.486483	-0.186789
C	-2.542135	0.726067	-0.247844
C	1.272123	-1.459802	-0.200550
C	0.000000	-0.728944	0.250262
H	0.000000	0.694433	-1.352612
H	3.433499	1.252541	0.113097
H	-1.264533	1.536370	1.297694
H	-2.592756	0.731869	-1.345605
H	-1.266200	-2.486483	0.186789
C	2.542135	0.726067	-0.247844
C	-1.272123	-1.459802	-0.200550
H	-3.433499	1.252541	0.113097
H	1.264533	1.536370	1.297694
H	2.592756	0.731869	-1.345605
H	1.266200	-2.486483	0.186789
C	2.542135	-0.726067	0.247844
C	-1.272123	1.459802	0.200550
H	-3.433499	-1.252541	-0.113097
H	1.264533	-1.536370	-1.297694
H	2.592756	-0.731869	1.345605
H	1.266200	2.486483	-0.186789

$C_{14}H_{24}$

C	2.544998	1.465688	0.157751
C	3.815207	0.718827	-0.268314
C	1.274383	0.720208	-0.272688
C	0.000000	-1.458363	-0.152855
H	-1.276980	0.651690	-1.373290
H	-4.706497	1.255120	0.078068
H	0.000000	1.569211	1.247820
H	-2.536419	-1.574692	-1.252140
H	-3.866527	0.693425	-1.365760
H	2.539307	2.480330	-0.259985
H	0.000000	2.474115	-0.264942
C	2.544998	-1.465688	-0.157751
C	3.815207	-0.718827	0.268314
C	1.274383	-0.720208	0.272688
C	0.000000	1.458363	0.152855
H	-1.276980	-0.651690	1.373290
H	-4.706497	-1.255120	-0.078068
H	0.000000	-1.569211	-1.247820
H	-2.536419	1.574692	1.252140
H	-3.866527	-0.693425	1.365760
H	2.539307	-2.480330	0.259985
H	0.000000	-2.474115	0.264942
C	-2.544998	-1.465688	-0.157751
C	-3.815207	-0.718827	0.268314
C	-1.274383	-0.720208	0.272688
H	1.276980	-0.651690	1.373290
H	4.706497	-1.255120	-0.078068
H	2.536419	1.574692	1.252140
H	3.866527	-0.693425	1.365760
H	-2.539307	-2.480330	0.259985
C	-2.544998	1.465688	0.157751
C	-3.815207	0.718827	-0.268314
C	-1.274383	0.720208	-0.272688
H	1.276980	0.651690	-1.373290
H	4.706497	1.255120	0.078068
H	2.536419	-1.574692	-1.252140
H	3.866527	0.693425	-1.365760
H	-2.539307	2.480330	-0.259985

$C_{18}H_{30}$

C	5.088467	-0.738925	0.206633
C	1.272742	1.442207	0.268754
C	2.547626	0.740189	-0.212905
H	2.552160	-0.761875	1.315506
H	3.807913	-1.464306	-1.378905
H	5.141123	-0.806523	1.302285
H	3.812270	2.493371	-0.051961
C	3.817722	-1.447262	-0.279289
H	5.979355	1.244051	0.184750
H	1.271213	1.466115	1.368955
H	1.273085	-2.487803	0.067427
C	0.000000	-0.738659	0.215764
H	0.000000	-0.756328	1.318275
C	5.088467	0.738925	-0.206633
C	1.272742	-1.442207	-0.268754
C	2.547626	-0.740189	0.212905
H	2.552160	0.761875	-1.315506
H	3.807913	1.464306	1.378905
H	5.141123	0.806523	-1.302285
H	3.812270	-2.493371	0.051961
C	3.817722	1.447262	0.279289
H	5.979355	-1.244051	-0.184750
H	1.271213	-1.466115	-1.368955

H	1.273085	2.487803	-0.067427
C	0.000000	0.738659	-0.215764
H	0.000000	0.756328	-1.318275
C	-5.088467	0.738925	-0.206633
C	-1.272742	-1.442207	-0.268754
C	-2.547626	-0.740189	0.212905
H	-2.552160	0.761875	-1.315506
H	-3.807913	1.464306	1.378905
H	-5.141123	0.806523	-1.302285
H	-3.812270	-2.493371	0.051961
C	-3.817722	1.447262	0.279289
H	-5.979355	-1.244051	-0.184750
H	-1.271213	-1.466115	-1.368955
H	-1.273085	2.487803	-0.067427
C	-5.088467	-0.738925	0.206633
C	-1.272742	1.442207	0.268754
C	-2.547626	0.740189	-0.212905
H	-2.552160	-0.761875	1.315506
H	-3.807913	-1.464306	-1.378905
H	-5.141123	-0.806523	1.302285
H	-3.812270	2.493371	-0.051961
C	-3.817722	-1.447262	-0.279289
H	-5.979355	1.244051	0.184750
H	-1.271213	1.466115	1.368955
H	-1.273085	-2.487803	0.067427

$C_{22}H_{36}$

C	6.361219	-0.716286	0.274984
C	2.546054	1.460237	0.139441
C	3.820438	0.717880	-0.279082
H	3.823113	-0.639238	1.379003
H	5.082611	-1.585386	-1.238156
H	6.412046	-0.680625	1.372171
H	5.085441	2.477962	-0.281622
C	5.091174	-1.466910	-0.144730
H	7.252738	1.255752	0.065863
H	2.545551	1.581215	1.233330
H	2.546108	-2.472021	0.287740
C	1.272969	-0.716768	0.280298
H	1.272803	-0.636467	1.379942
C	6.361219	0.716286	-0.274984
C	2.546054	-1.460237	-0.139441
C	3.820438	-0.717880	0.279082
H	3.823113	0.639238	-1.379003
H	5.082611	1.585386	1.238156
H	6.412046	0.680625	-1.372171
H	5.085441	-2.477962	0.281622
C	5.091174	1.466910	0.144730
H	7.252738	-1.255752	-0.065863
H	2.545551	-1.581215	-1.233330
H	2.546108	2.472021	-0.287740
C	1.272969	0.716768	-0.280298
H	1.272803	0.636467	-1.379942
C	-3.820438	0.717880	-0.279082
C	0.000000	-1.460772	-0.139454
C	-1.272969	-0.716768	0.280298
H	-1.272803	0.636467	-1.379942
H	-2.545551	1.581215	1.233330
H	-3.823113	0.639238	-1.379003
H	-2.546108	-2.472021	0.287740
C	-2.546054	1.460237	0.139441
H	0.000000	-1.581512	-1.233321
H	0.000000	2.472497	-0.287733
C	-3.820438	-0.717880	0.279082
C	0.000000	1.460772	0.139454
C	-1.272969	0.716768	-0.280298
H	-1.272803	-0.636467	1.379942
H	-2.545551	-1.581215	-1.233330
H	-3.823113	-0.639238	1.379003
H	-2.546108	2.472021	-0.287740
C	-2.546054	-1.460237	-0.139441
H	0.000000	1.581512	1.233321
H	0.000000	-2.472497	0.287733
C	-5.091174	-1.466910	-0.144730
H	-5.085441	-2.477962	0.281622
H	-5.082611	-1.585386	-1.238156
C	-6.361219	-0.716286	0.274984
H	-7.252738	-1.255752	-0.065863
H	-6.412046	-0.680625	1.372171
C	-6.361219	0.716286	-0.274984
H	-7.252738	1.255752	0.065863
H	-6.412046	0.680625	-1.372171
C	-5.091174	1.466910	0.144730
H	-5.085441	2.477962	-0.281622
H	-5.082611	1.585386	1.238156

$C_{26}H_{42}$

C	7.634563	-0.716868	0.273510
C	3.818727	1.460539	0.135519
C	5.093819	0.717611	-0.279710
H	5.098540	-0.638194	1.379559
H	6.354294	-1.583731	-1.239605
H	7.686714	-0.683610	1.370717
H	6.358378	2.478232	-0.279054
C	6.363916	-1.466647	-0.146040
H	8.525610	1.255760	0.069511
H	3.816360	1.584220	1.229102
H	3.819208	-2.471259	0.294189
C	2.546317	-0.715455	0.283586
H	2.548104	-0.630074	1.382840
C	7.634563	0.716868	-0.273510
C	3.818727	-1.460539	-0.135519
C	5.093819	-0.717611	0.279710
H	5.098540	0.638194	-1.379559
H	6.354294	1.583731	1.239605
H	7.686714	0.683610	-1.370717
H	6.358378	-2.478232	0.279054
C	6.363916	1.466647	0.146040
H	8.525610	-1.255760	-0.069511
H	3.816360	-1.584220	-1.229102
H	3.819208	2.471259	-0.294189
C	2.546317	0.715455	-0.283586
H	2.548104	0.630074	-1.382840
C	-2.546317	0.715455	-0.283586
C	1.272884	-1.461702	-0.130628
C	0.000000	-0.715088	0.284620

H	0.000000	0.628117	-1.383784
H	-1.272514	1.589900	1.223663
H	-2.548104	0.630074	-1.382840
H	-1.272902	-2.470548	0.303357
C	-1.272884	1.461702	0.130628
H	1.272514	-1.589900	-1.223663
H	1.272902	2.470548	-0.303357
C	-2.546317	-0.715455	0.283586
C	1.272884	1.461702	0.130628
C	0.000000	0.715088	-0.284620
H	0.000000	-0.628117	1.383784
H	-1.272514	-1.589900	-1.223663
H	-2.548104	-0.630074	1.382840
H	-1.272902	2.470548	-0.303357
C	-1.272884	-1.461702	-0.130628
H	1.272514	1.589900	1.223663
H	1.272902	-2.470548	0.303357
C	-3.818727	-1.460539	-0.135519
H	-3.819208	-2.471259	0.294189
H	-3.816360	-1.584220	-1.229102
C	-5.093819	-0.717611	0.279710
H	-5.098540	-0.638194	1.379559
C	-5.093819	0.717611	-0.279710
H	-5.098540	0.638194	-1.379559
C	-3.818727	1.460539	0.135519
H	-3.819208	2.471259	-0.294189
H	-3.816360	1.584220	1.229102
C	-6.363916	-1.466647	-0.146040
H	-6.358378	-2.478232	0.279054
H	-6.354294	-1.583731	-1.239605
C	-7.634563	-0.716868	0.273510
H	-8.525610	-1.255760	-0.069511
H	-7.686714	-0.683610	1.370717
C	-7.634563	0.716868	-0.273510
H	-8.525610	1.255760	0.069511
H	-7.686714	0.683610	-1.370717
C	-6.363916	1.466647	0.146040
H	-6.358378	2.478232	-0.279054
H	-6.354294	1.583731	1.239605

$C_{16}H_{26}$

C	2.529277	0.732799	0.221113
C	1.261493	-2.932920	-0.196130
C	-1.270429	-1.466830	0.255243
C	0.000000	-3.665440	0.273733
C	0.000000	-0.737771	-0.220026
H	0.000000	0.756012	1.324270
H	1.312074	-2.963590	-1.294390
H	-2.161059	-3.439980	0.175133
H	-3.423158	1.247180	-0.153878
H	0.000000	4.698880	0.092274
H	1.263128	1.449600	-1.357670
H	2.573475	0.782708	1.318790
H	0.000000	3.717480	-1.371250
C	2.529277	-0.732799	-0.221113
C	1.261493	2.932920	0.196130
C	-1.270429	1.466830	-0.255243
C	0.000000	3.665440	-0.273733
C	0.000000	0.737771	0.220026
H	0.000000	-0.756012	-1.324270
H	1.312074	2.963590	1.294390
H	-2.161059	3.439980	-0.175133
H	-3.423158	-1.247180	0.153878
H	0.000000	-4.698880	-0.092274
H	1.263128	-1.449600	1.357670
H	2.573475	-0.782708	-1.318790
H	0.000000	-3.717480	1.371250
C	-2.529277	-0.732799	-0.221113
C	-1.261493	2.932920	0.196130
C	1.270429	1.466830	-0.255243
H	-1.312074	2.963590	1.294390
H	2.161059	3.439980	-0.175133
H	3.423158	-1.247180	0.153878
H	-1.263128	-1.449600	1.357670
H	-2.573475	-0.782708	-1.318790
C	-2.529277	0.732799	0.221113
C	-1.261493	-2.932920	-0.196130
C	1.270429	-1.466830	0.255243
H	-1.312074	-2.963590	-1.294390
H	2.161059	-3.439980	0.175133
H	3.423158	1.247180	-0.153878
H	-1.263128	1.449600	-1.357670
H	-2.573475	0.782708	1.318790

$C_{20}H_{32}$

C	-2.559371	-1.443361	-0.229474
C	-3.822695	-0.714246	0.236049
C	-1.273906	-0.738282	0.235942
C	-2.545575	1.469688	0.240309
C	-0.029698	2.938161	-0.229474
C	2.559371	1.443361	0.229474
C	2.545575	-1.469688	-0.240309
C	0.029698	-2.938161	0.229474
C	-2.547640	2.928974	-0.227585
C	3.822695	0.714246	-0.236049
C	2.547640	-2.928974	0.227585
C	-1.270294	0.733405	-0.224406
C	0.002418	1.472376	0.235942
C	1.273906	0.738282	-0.235942
C	1.270294	-0.733405	0.224406
C	-0.002418	-1.472376	-0.235942
C	-3.810385	0.741834	-0.227585
C	1.292792	-3.667674	-0.236049
C	3.810385	-0.741834	0.227585
C	-1.292792	3.667674	0.236049
H	-1.292142	4.699031	-0.136291
H	1.273077	-0.735012	1.328666
H	0.019387	2.958206	-1.328418
H	-1.291272	3.726864	1.333370
H	4.697968	-1.273664	-0.137818
H	1.292142	-4.699031	0.136291
H	-4.697968	1.273664	0.137818
H	-0.006324	-1.466757	-1.339070
H	-1.267086	-0.738855	1.339070
H	-1.273077	0.735012	-1.328666
H	0.006324	1.466757	1.339070

H	1.267086	0.738855	-1.339070
H	2.552188	1.495893	1.328418
H	2.539035	-1.465913	-1.342974
H	-0.019387	-2.958206	1.328418
H	-2.552188	-1.495893	-1.328418
H	-2.539035	1.465913	1.342974
H	3.851244	-0.775731	1.326143
H	1.291272	-3.726864	-1.333370
H	-3.851244	0.775731	-1.326143
H	3.452009	-3.431728	-0.137818
H	4.715551	1.230487	0.136291
H	-3.452009	3.431728	0.137818
H	-4.715551	-1.230487	-0.136291
H	2.597424	-2.947410	1.326143
H	3.873195	0.745157	-1.333370
H	-2.597424	2.947410	-1.326143
H	-3.873195	-0.745157	1.333370
H	2.581011	2.474381	-0.135699
H	-0.852371	-3.472412	-0.135699
H	-2.581011	-2.474381	0.135699
H	0.852371	3.472412	0.135699

$C_{24}H_{36}$

C	2.540940	-1.467012	-0.237035
C	3.800958	-0.729717	0.229745
C	1.270492	-0.733519	0.230822
H	1.264022	4.689770	-0.139969
H	-1.273215	-0.735091	1.335230
H	0.000000	2.923688	-1.339800
H	1.258796	3.714032	1.327950
C	2.540940	1.467012	0.237035
C	0.000000	2.934025	-0.237035
C	-2.540940	1.467012	0.237035
C	-2.540940	-1.467012	-0.237035
C	0.000000	-2.934025	0.237035
C	2.532433	2.926868	-0.229745
C	-1.268526	3.656585	0.229745
C	-3.800958	0.729717	-0.229745
C	-2.532433	-2.926868	0.229745
C	1.268526	-3.656585	-0.229745
C	1.270492	0.733519	-0.230822
C	0.000000	1.467038	0.230822
C	-1.270492	0.733519	-0.230822
C	-1.270492	-0.733519	0.230822
C	0.000000	-1.467038	-0.230822
H	-3.429449	3.439560	0.139969
H	-4.693470	-1.250210	-0.139969
H	-1.264022	-4.689770	0.139969
H	3.429449	-3.439560	-0.139969
H	4.693470	1.250210	0.139969
H	0.000000	-1.470182	-1.335230
H	1.273215	-0.735091	1.335230
H	1.273215	0.735091	-1.335230
H	0.000000	1.470182	1.335230
H	-1.273215	0.735091	-1.335230
H	-2.531988	1.461844	1.339800
H	-2.531988	-1.461844	-1.339800
H	0.000000	-2.923688	1.339800
H	2.531988	-1.461844	-1.339800
H	2.531988	1.461844	1.339800
H	-2.587048	2.947165	-1.327950
H	-3.845844	-0.766867	1.327950
H	-1.258796	-3.714032	-1.327950
H	2.587048	-2.947165	1.327950
H	3.845844	0.766867	-1.327950
C	3.800958	0.729717	-0.229745
H	1.264022	-4.689770	0.139969
H	1.258796	-3.714032	-1.327950
C	2.532433	-2.926868	0.229745
C	-1.268526	-3.656585	-0.229745
C	-3.800958	-0.729717	0.229745
C	-2.532433	2.926868	-0.229745
C	1.268526	3.656585	0.229745
H	-3.429449	-3.439560	-0.139969
H	-4.693470	1.250210	0.139969
H	-1.264022	4.689770	-0.139969
H	3.429449	3.439560	0.139969
H	4.693470	-1.250210	-0.139969
H	-2.587048	-2.947165	1.327950
H	-3.845844	0.766867	-1.327950
H	-1.258796	3.714032	1.327950
H	2.587048	2.947165	-1.327950
H	3.845844	-0.766867	1.327950