

Supporting Information

for

Steric “attraction”: not by dispersion alone

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Additional figures, complete set of computed data and geometries of the studied monomers and dimers

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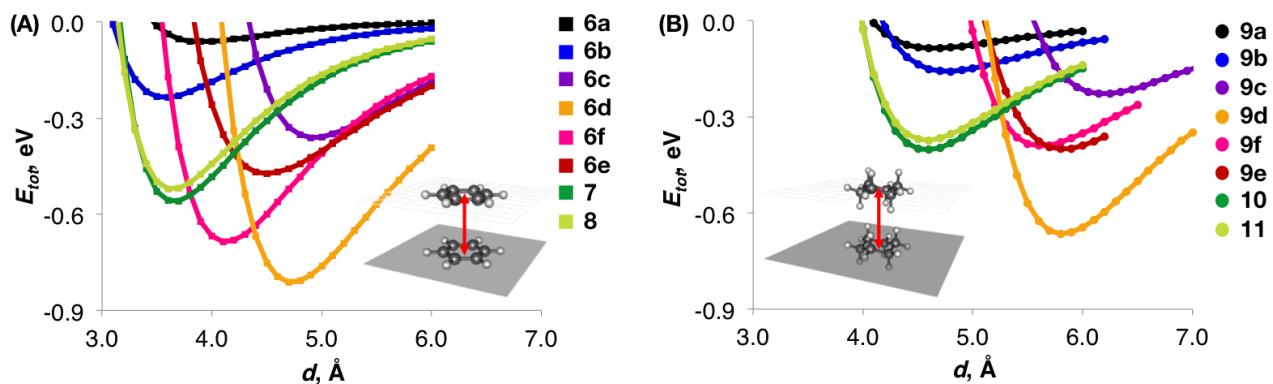


Figure S1: Computed SAPT0/jun-cc-pVDZ interaction energies E_{tot} for varied intermonomer distances d (schematically illustrated with red arrows for **6a** and **9a** dimers, see insets) for all investigated systems.

The interaction energy plots, shown in Figure S1, reveal a diverse interaction behavior: from rather shallow in smaller species, e.g., benzene (**6a**) and cyclohexane (**9a**), to pronounced deep minima in bulky **6d** and **9d**. Considering the various contributions to the total interaction energies, exchange is, of course, the dominant factor at short range but gives way to dispersion as d increases (Figure S2). In all species, charge penetration is appreciable at smaller d and decays with increasing separation. In contrast, the multipolar electrostatics, quantified by E_{DMA} , is negligible in all dimers, except **6a**, **6b**, **7** and **8**. In the latter systems, its contribution instead increases with larger d . The reason is that the multipolar electrostatics arising from quadrupole-quadrupole interactions (repelling π -clouds in the case of these π -conjugated monomers) decays slower (as $1/d^5$) than the exchange and charge penetration [1], and, at sufficiently large distances, than even dispersion (which decays as $1/d^6$). This effect vanishes moving from **6b** to **6c** due to much larger interaction distances, imposed by the steric bulk.

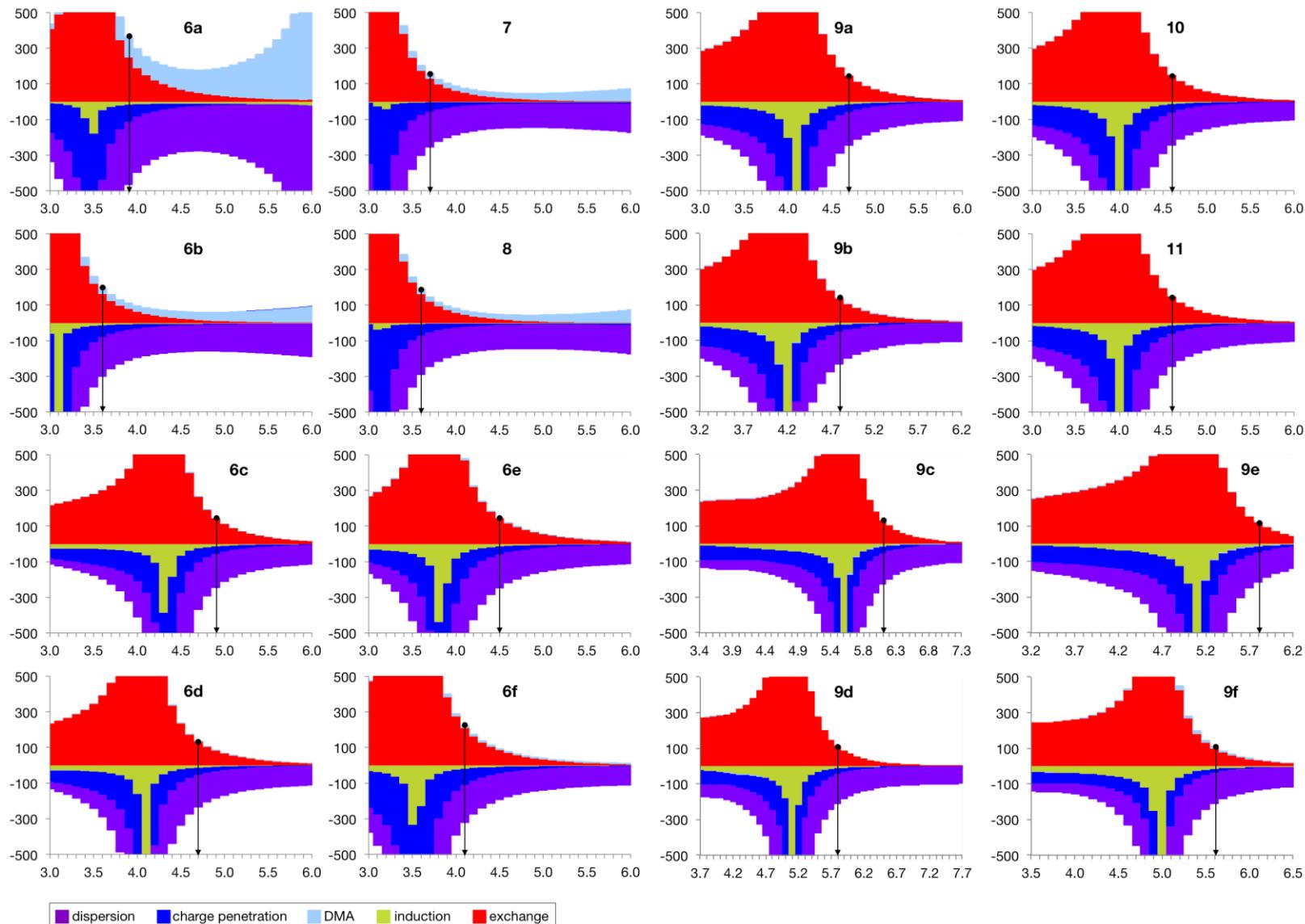


Figure S2: Percentile contributions to the total SAPTO/jun-cc-pVDZ interaction energies for the studied dimers with varied intermonomer separation (x-axis, in Å). Separations corresponding to the lowest E_{tot} are denoted with an arrow. y-Axis range is fixed to allow comparison and enhance the visibility around the lowest E_{tot} .

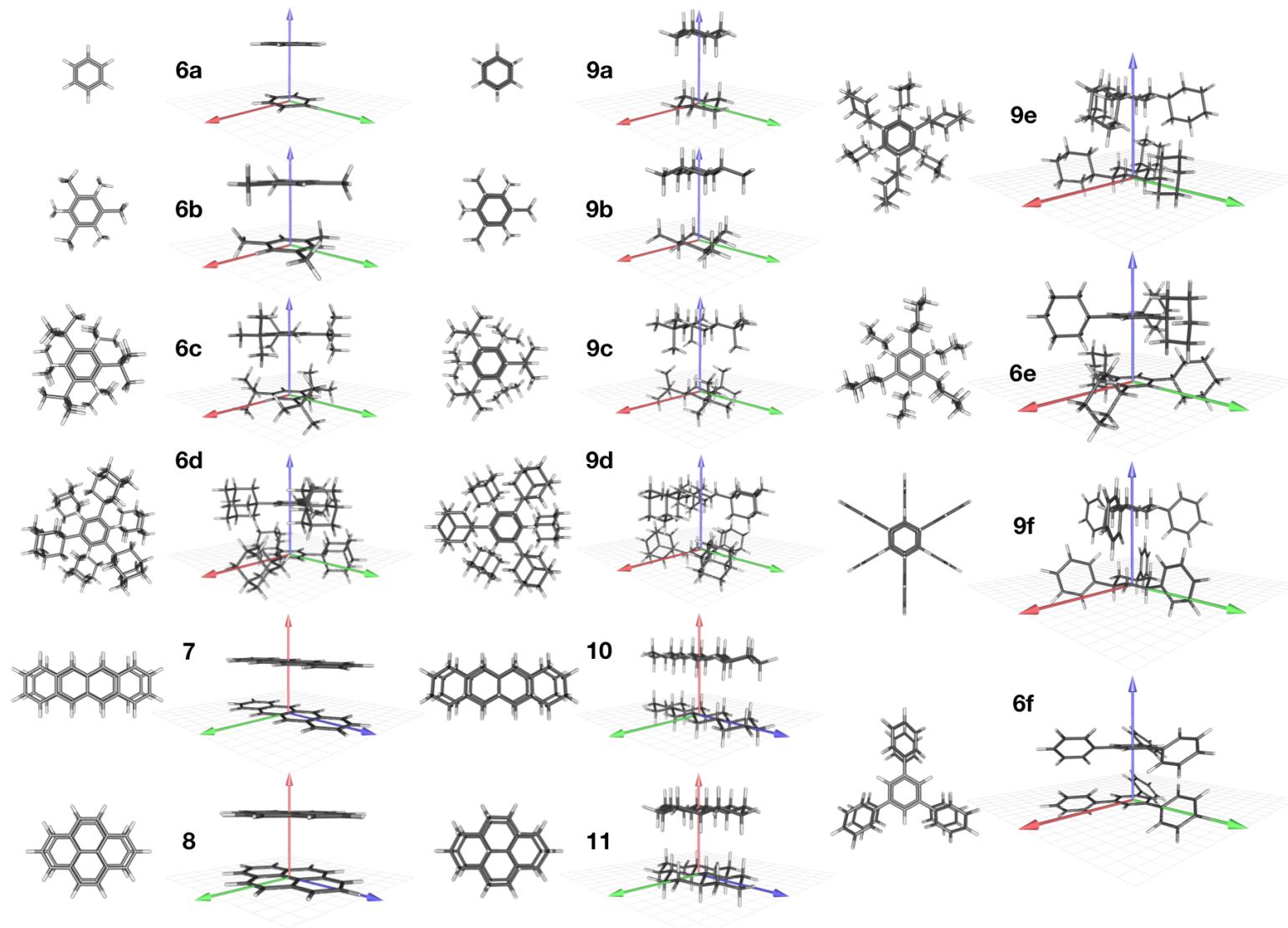


Figure S3: Frozen dimer geometries, assembled from M06-2X/def2-SVP optimized monomers. Systems are shown along the perpendicular axis (*i.e.*, top view, left) and from the side (right). Energy decomposition analysis was performed for changing intermonomer distance (0.1 Å step size along red axis for **7**, **8**, **10** and **11**, and blue axis for the rest).

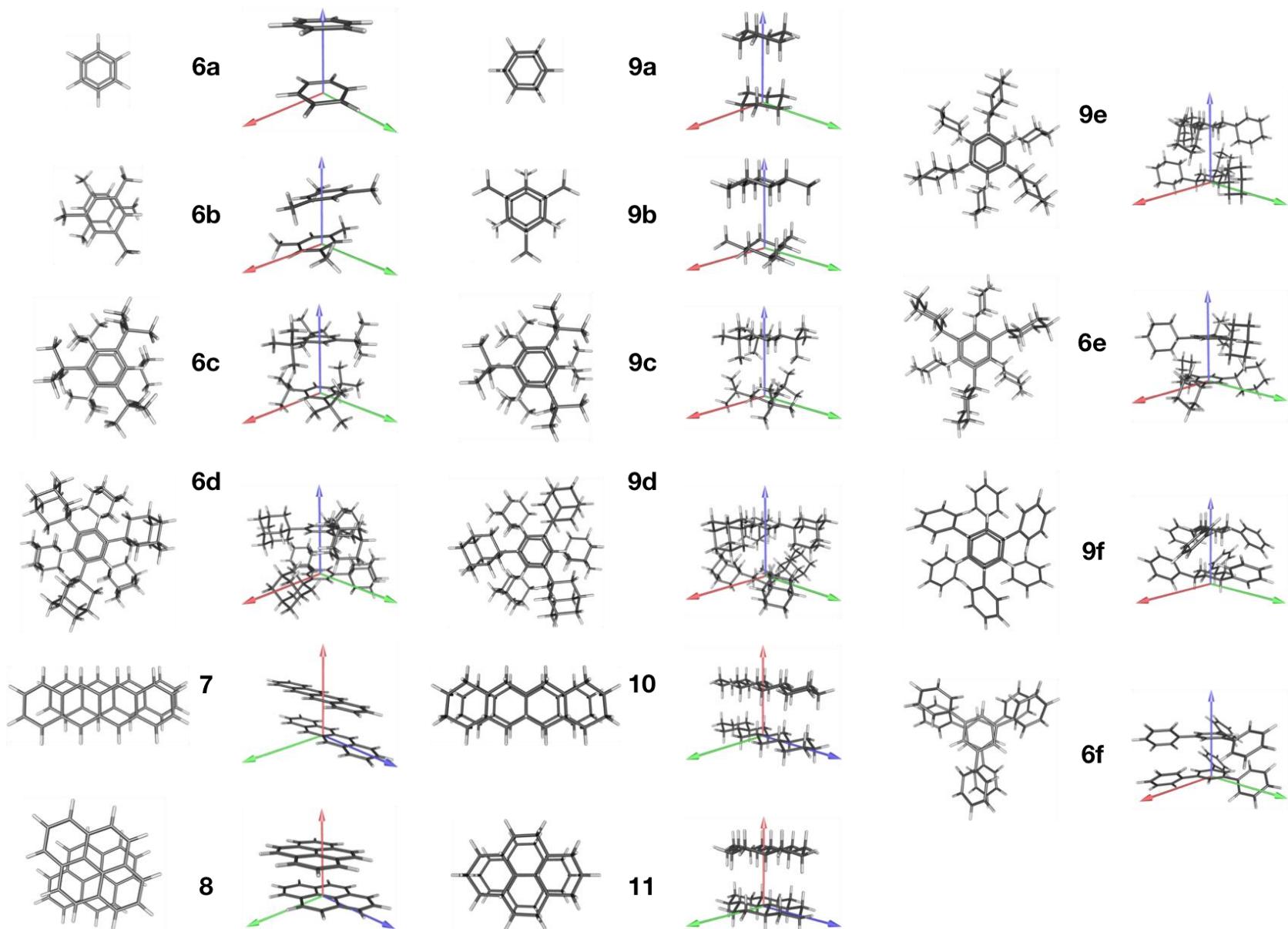


Figure S4: Optimized dimer geometries (M06-2X/def2-SVP level). Systems are shown along the perpendicular axis (*i.e.*, top view, left) and from the side (right).

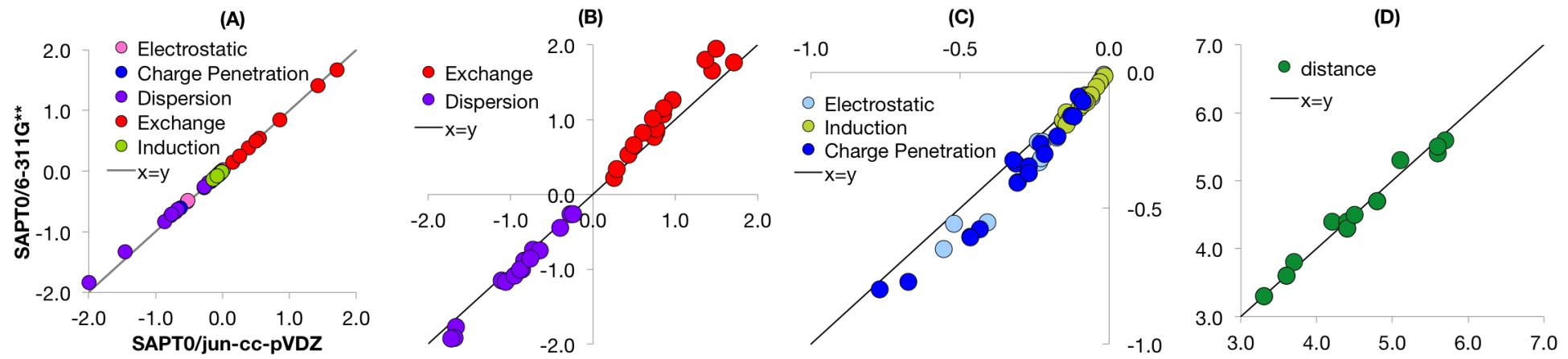


Figure S5: Comparison of the total interaction energies and their components for frozen and optimized dimers of **6a**, **6f**, **9f** and **11**, computed at SAPTO/jun-cc-pVDZ and SAPTO/6-311G** level in conjunction with HF/6-311G** DMA (A). Comparison of M06-2X/def2-SVP (x-axis) and PBE0-dDsC/def2-SVP (y-axis) optimized dimers: (B) exchange and dispersion energy components, in eV; (C) total electrostatic, charge penetration and induction energy components, in eV; (D) intermonomer distances, in Å.

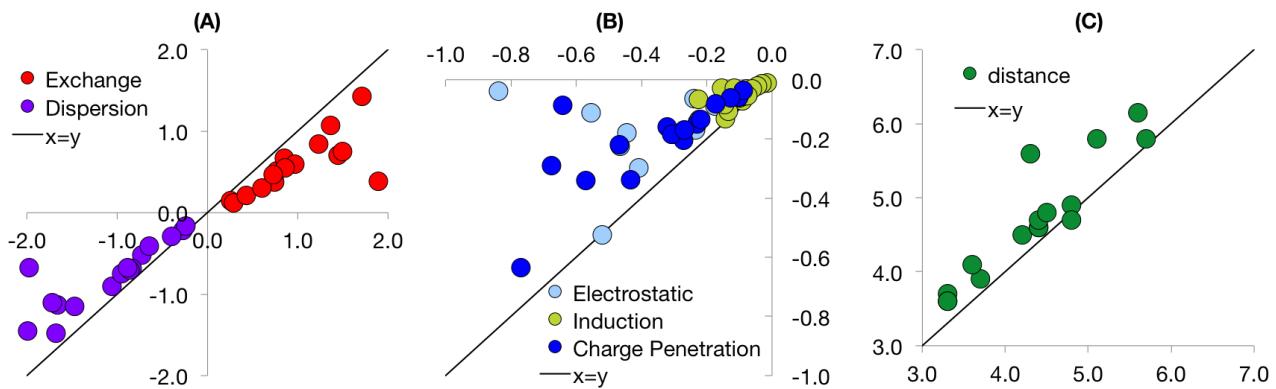


Figure S6: Comparison of the M06-2X/def2-SVP optimized (x-axis) and frozen (y-axis) dimers: (A) exchange and dispersion energy components, in eV; (B) total electrostatic, charge penetration and induction energy components, in eV; (C) intermonomer distances, in Å.

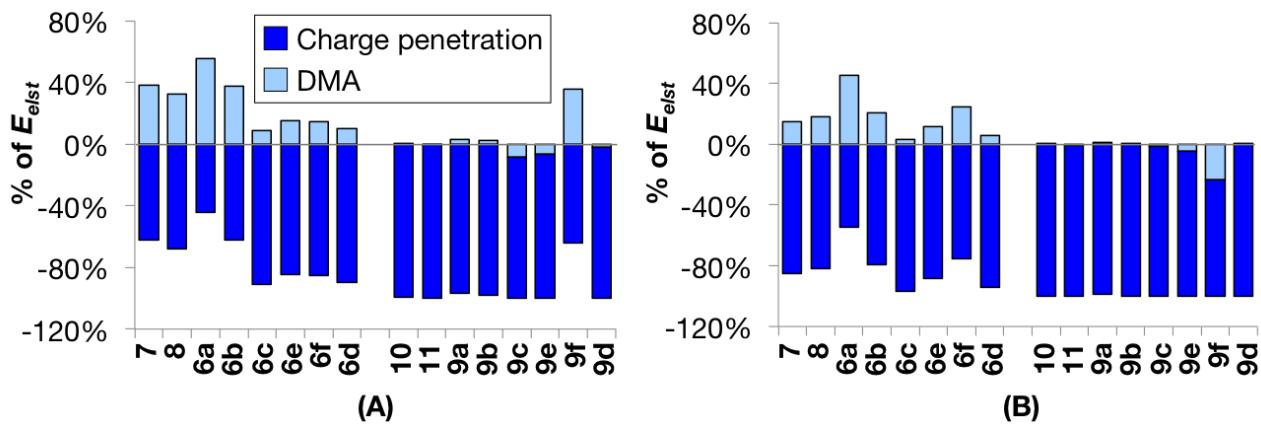


Figure S7: Percentages of the E_{Cpen} and E_{DMA} contributions to the total electrostatic energy in the frozen (A) and optimized dimers (B).

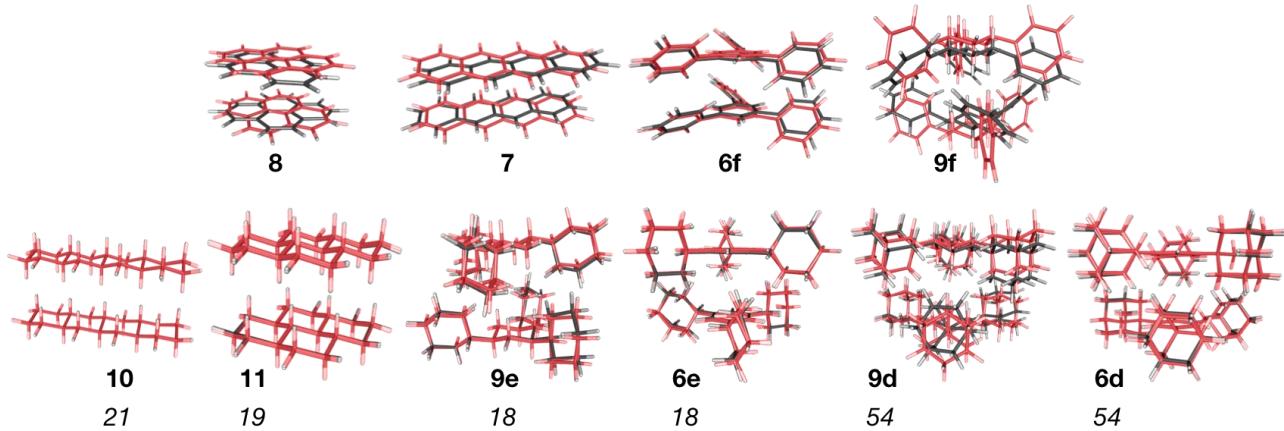


Figure S8: Structures of the frozen (in red) and optimized dimers in classes (II) and (III), top and bottom respectively. Numbers in italics for class (III) are quantities of intermolecular $\text{CH}\cdots\text{HC}$ contacts $< 3\text{\AA}$.

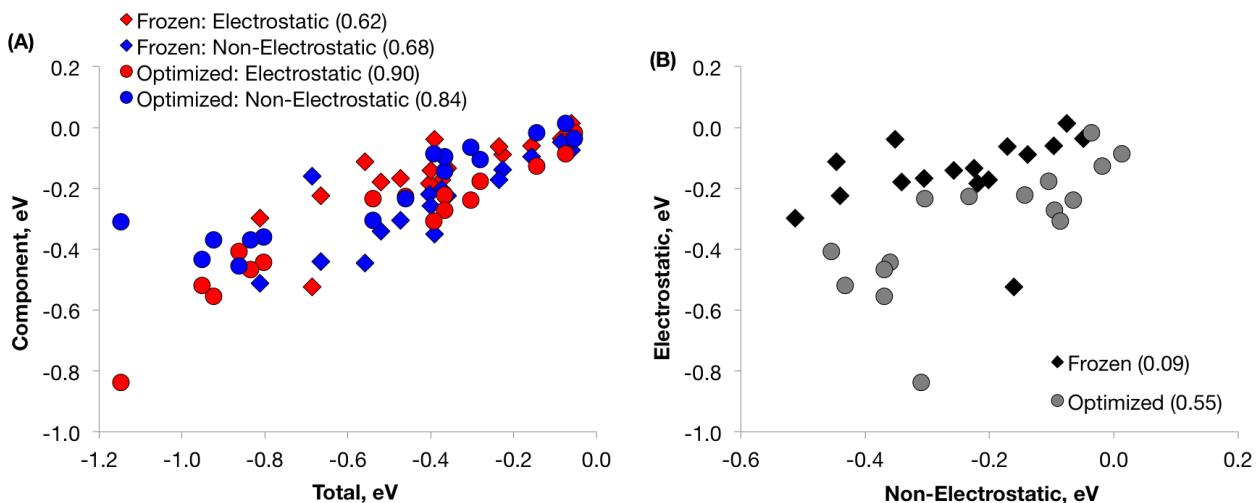


Figure S9: Probing the linear regression between the SAPT0/jun-cc-pVDZ total interaction energies and their electrostatic and non-electrostatic components in the frozen and optimized dimers. Numbers in brackets are R^2 values.

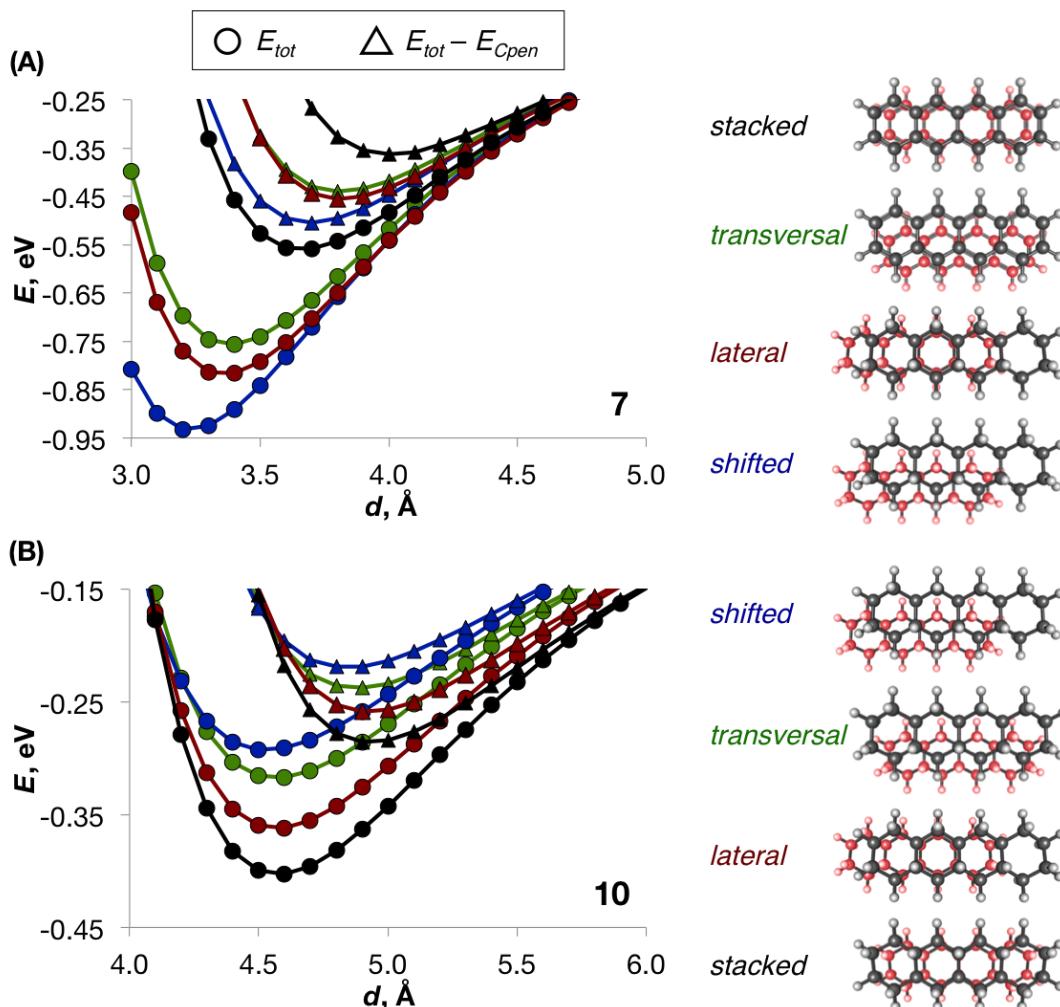


Figure S10: SAPT0/jun-cc-pVDZ interaction energy profiles with and without the charge penetration contribution for different dimers of tetracene (**7**, A) and perhydrotetracene (**10**, B): perfectly π -stacked (black), laterally (red) shifted by 1.24 Å in **7** and 2.54 Å in **10**, transversally (green) shifted by 1.12 Å in **7** and 2.17 Å in **10**, shifted (blue) both laterally and transversally by the aforementioned amounts.

Table S1: Computed properties of the frozen dimers.

Monomer	Volume, Å ³ mol ⁻¹	<i>d</i> , Å	<i>E</i> _{DMA} , eV	SAPT0/jun-cc-pVDZ energy decomposition, eV					<i>E</i> _{Copen} , eV
				<i>E</i> _{elst}	<i>E</i> _{exch}	<i>E</i> _{ind}	<i>E</i> _{disp}	<i>E</i> _{tot}	
7	302	3.7	0.18	-0.11	0.71	-0.03	-1.13	-0.56	-0.29
8	259	3.6	0.16	-0.18	0.84	-0.03	-1.15	-0.52	-0.34
6a	120	3.9	0.07	0.01	0.15	-0.01	-0.22	-0.06	-0.06
6b	195	3.6	0.10	-0.06	0.38	-0.03	-0.52	-0.23	-0.16
6c	409	4.9	0.01	-0.14	0.51	-0.05	-0.69	-0.36	-0.15
6e	461	4.5	0.04	-0.17	0.67	-0.07	-0.91	-0.47	-0.20
6f	441	4.1	0.11	-0.52	1.43	-0.13	-1.46	-0.69	-0.63
6d	639	4.7	0.04	-0.30	1.07	-0.11	-1.48	-0.81	-0.34
10	356	4.6	0.00	-0.18	0.59	-0.06	-0.75	-0.40	-0.18
11	307	4.6	0.00	-0.17	0.55	-0.06	-0.70	-0.37	-0.17
9a	131	4.7	0.00	-0.04	0.12	-0.01	-0.16	-0.08	-0.04
9b	233	4.8	0.00	-0.06	0.21	-0.02	-0.29	-0.16	-0.06
9c	417	6.1	-0.01	-0.09	0.30	-0.03	-0.41	-0.23	-0.08
9e	486	5.8	-0.01	-0.14	0.47	-0.05	-0.67	-0.40	-0.13
9f	383	5.6	0.05	-0.04	0.39	-0.07	-0.68	-0.39	-0.09
9d	601	5.8	0.00	-0.22	0.75	-0.08	-1.11	-0.66	-0.22

Table S2: Computed properties of the optimized dimers.

Monomer	<i>d</i> , Å	<i>E</i> _{DMA} , eV	SAPT0/jun-cc-pVDZ energy decomposition, eV					<i>E</i> _{Copen} , eV	
			<i>E</i> _{elst}	<i>E</i> _{exch}	<i>E</i> _{ind}	<i>E</i> _{disp}	<i>E</i> _{tot}		
M06-2X/def2-SVP									
7	3.3	0.12	-0.55	1.45	-0.16	-1.66	-0.92	-0.67	
8	3.3	0.13	-0.44	1.23	-0.12	-1.47	-0.80	-0.57	
8 (stuck)²	3.6	0.16	-0.16	0.77	-0.03	-1.11	-0.52	-0.31	
6a	3.7	0.08	-0.02	0.26	-0.01	-0.28	-0.05	-0.10	
6b	3.3	0.08	-0.24	0.74	-0.08	-0.73	-0.30	-0.32	
6c	4.8	0.01	-0.22	0.77	-0.07	-0.84	-0.37	-0.23	
6e	4.2	0.04	-0.23	0.85	-0.09	-1.06	-0.54	-0.27	
6f	3.6	0.25	-0.52	1.71	-0.14	-2.00	-0.95	-0.77	
6d	4.8	0.03	-0.41	1.36	-0.13	-1.68	-0.86	-0.43	
10	4.4	0.00	-0.31	0.97	-0.10	-0.96	-0.39	-0.31	
11	4.4	0.00	-0.27	0.86	-0.09	-0.86	-0.37	-0.27	
9a	4.4	0.00	-0.09	0.29	-0.03	-0.24	-0.07	-0.09	
9b	4.5	0.00	-0.13	0.43	-0.04	-0.40	-0.14	-0.13	
9c	5.6	0.00	-0.18	0.61	-0.06	-0.65	-0.28	-0.17	
9e	5.7	-0.01	-0.23	0.73	-0.07	-0.89	-0.46	-0.22	
9f	4.3	-0.20	-0.84	1.89	-0.23	-1.97	-1.15	-0.64	
9f (stuck)²	5.6	0.06	-0.06	0.50	-0.08	-0.76	-0.41	-0.12	
9d	5.1	0.00	-0.47	1.50	-0.14	-1.72	-0.84	-0.47	

PBE0-dDsC/def2-SVP

² The ‘stuck’ local minimum is very similar to the frozen geometry; this is the structure captured at the PBE0 level and used for comparisons in Figure S5.

7	3.3	0.12	-0.65	1.65	-0.18	-1.77	-0.94	-0.77
8	3.6	0.16	-0.18	0.83	-0.03	-1.15	-0.53	-0.34
6a	3.8	0.08	-0.01	0.22	-0.01	-0.26	-0.06	-0.09
6b	3.3	0.07	-0.25	0.77	-0.08	-0.73	-0.31	-0.32
6c	4.7	0.01	-0.25	0.88	-0.09	-0.89	-0.35	-0.26
6e	4.4	0.02	-0.33	1.07	-0.11	-1.17	-0.54	-0.35
6f	3.6	0.24	-0.56	1.77	-0.15	-2.01	-0.95	-0.80
6d	4.7	0.03	-0.55	1.81	-0.17	-1.92	-0.84	-0.58
10	4.3	0.00	-0.40	1.26	-0.13	-1.09	-0.36	-0.41
11	4.4	0.00	-0.37	1.16	-0.12	-1.00	-0.33	-0.37
9a	4.3	0.00	-0.10	0.34	-0.04	-0.27	-0.07	-0.11
9b	4.5	0.00	-0.16	0.53	-0.05	-0.45	-0.13	-0.16
9c	5.4	0.00	-0.24	0.83	-0.08	-0.75	-0.24	-0.24
9e	5.6	-0.01	-0.32	1.01	-0.11	-1.01	-0.41	-0.30
9f	5.5	0.07	-0.09	0.66	-0.11	-0.86	-0.39	-0.16
9d	5.3	0.00	-0.60	1.95	-0.19	-1.93	-0.78	-0.61

Geometries of the studied species

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on top of the right column)

Monomers (M06-2X/def2-SVP)

7

30

0 1

C 0.0000000013 0.7229984214 -2.4446946599
C -0.0000000013 -0.7229984214 -2.4446946599
C 0. -1.4094335199 -3.7084720514
C -0.0000000044 -0.7174238937 -4.8813880483
C 0.0000000045 0.7174238937 -4.8813880483
C -0.0000000007 1.4094335199 -3.7084720514
C 0.0000000002 1.4051504752 -1.2346796945
C 0.0000000002 -1.4051504752 -1.2346796945
H -0.0000000004 -2.5012416025 -3.7053575762
H -0.0000000041 -1.2518046335 -5.8324011925
H 0.0000000045 1.2518046335 -5.8324011925
H -0.0000000002 2.5012416025 -3.7053575762
C -0.0000000001 -0.7223507702 0.
C 0.0000000013 0.7223507702 0.
H 0.0000000007 2.497865981 -1.2353750297
H -0.0000000005 -2.497865981 -1.2353750297
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C -0.0000000013 1.4051504752 1.2346796945
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C 0.0000000001 -0.7229984214 2.4446946599
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8

26

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6a

12

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6b

21

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6c

48

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 C 2.9967881971 2.3503004596 0.1716729195
 C 0.5033732875 -3.7665672563 0.2762232243
 C 2.1950003346 -2.5451748861 1.6310746222
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 C -3.5581509012 -0.6423543684 0.9753422126
 C -3.3194908283 -0.7853329894 -1.5197412328
 C -3.5202924117 1.4285793237 -0.4028239246
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 H 1.7619900275 4.2319184254 -1.3335084199
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 H 2.9130788221 -1.7145004476 1.6842629593

H 2.7553673927 -3.4850294667 1.7528700915
 H 1.9067845614 -2.6870633514 -1.830931612
 H 2.9952123811 -3.6271362611 -0.7738318581
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 H -4.655435078 -0.6634989046 0.8876451177
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6e

60

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48

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90

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Frozen dimers

7
60

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52

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6a

24

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6b

42

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 C -0.691187 1.217751 3.600020
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 H 1.192005 3.128300 -0.882950
 H 0.803865 -3.385130 0.008180
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6c

96

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 H 2.6112187072 -2.559862563 -2.0524276625
 C 3.6124763267 -3.8972972163 -0.6626019685
 H -0.2626697664 -3.8540837477 -0.0189223971
 C 1.4614170029 -5.1131413134 -0.2921177417
 H 0.4167356711 -3.7683879031 -1.6561327831
 C 3.9094512151 3.9615098023 0.8418347677
 C 2.7801946028 5.1174947422 -1.0738045818
 C 1.7556025438 5.1817756684 1.2125715381
 H 2.7997413431 4.0045389934 2.7042186877
 H 0.8509487705 5.9802461853 -0.5895209547
 H 4.5584549964 3.8855964491 -1.2264748714
 H 4.5256297469 3.0978861897 1.1419124305
 H 4.4872668887 4.8709142622 1.0753168641
 H 2.5777011395 5.0879910798 -2.1570475254
 H 3.3385609896 6.0462001168 -0.8707884786
 H 0.8109138373 5.2036201408 1.7805339831
 H 2.3011997128 6.1095249274 1.4513437638
 C 2.7801984734 -5.1174960066 -1.0737992107
 C 3.9094534089 -3.9615083024 0.8418394621
 C 1.7556053436 -5.181775175 1.2125764721
 H 2.7997426579 -4.0045362485 2.7042228899
 H 4.5584581467 -3.8855967246 -1.2264699398
 H 0.8509529569 -5.9802481738 -0.5895156151
 H 2.5777055284 -5.0879936332 -2.1570422857
 H 3.3385653568 -6.0462008056 -0.8707818377
 H 4.5256312222 -3.0978839614 1.1419165045
 H 4.487269569 -4.8709121322 1.0753228091
 H 0.8109163733 -5.2036196443 1.7805384774
 H 2.3012029879 -6.1095238327 1.4513499519
 C -5.4572401535 -1.2506577893 0.8423874328
 C -5.4572347893 1.2506539891 0.8424008995
 C -5.8305149411 0.0000104019 -1.2980740877
 H -5.0075402813 -0.0000120423 2.555668142
 H -5.6380731236 -2.1524162338 -1.1218531022
 H -5.6380637885 2.1524342767 -1.1218299986
 H -5.0269021499 -2.1587460507 1.2959161322
 H -6.541120658 -1.2681819951 1.0431669699
 H -5.0268928976 2.1587355392 1.2959393435
 H -6.5411152174 1.2681806637 1.043180632
 H -5.6643673645 0.0000159077 -2.3879219141
 H -6.9206654984 0.0000118923 -1.1335290654

Optimized dimers (M06-2X/def2-SVP)

7

60

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 C 3.6644306461 -0.4514270319 -2.9495061073
 C 3.6422354932 -1.1255562059 -4.2187416548
 C 3.8397052225 -0.44144923 -5.3798806165
 C 4.0725147447 0.9741528656 -5.3587460363
 C 4.1092793444 1.653447467 -4.1784196309
 C 3.9464614277 1.6411490042 -1.710212804
 C 3.452790528 -1.1253055375 -1.7532836754
 H 3.4539192165 -2.2011384227 -4.2285853226
 H 3.8200532065 -0.96558682 -6.3366231517
 H 4.2266173262 1.5039737326 -6.3002096008
 H 4.2924857743 2.729950217 -4.1595932263
 C 3.4852761645 -0.4566606598 -0.511292438
 C 3.7445277694 0.9641156407 -0.4888018152
 H 4.137778176 2.7172278941 -1.693806135
 H 3.2507092334 -2.1993607499 -1.7710159942
 C 3.2695716388 -1.1314969789 0.709032467
 C 3.7806402204 1.6314477447 0.7535938255
 C 3.5749757266 0.9554765365 1.9496180003
 C 3.3095756179 -0.4655212975 1.927418165
 H 3.0597227781 -2.2040694048 0.6904368135
 H 3.9798014986 2.7060615376 0.7720583035
 C 3.6101848969 1.625671202 3.2214967149
 C 3.0878414123 -1.1436326492 3.1760745428
 C 3.4001736438 0.9401998897 4.3794971311
 C 3.1332135067 -0.4691935212 4.3581295208
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 H 3.4258553165 1.4619976774 5.33762405
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 C 0.3907163761 0.465547683 -1.927368327
 C 0.1251180214 -0.9554065223 -1.9496321423
 C 0.0896917816 -1.6254912206 -3.2215618208
 C 0.2996458486 -0.9399540737 -4.3795365915
 C 0.5668078095 0.4693953893 -4.3581055492
 C 0.6124510769 1.1437180304 -3.1759949491
 C 0.4308099452 1.1314644565 -0.7089513728
 C -0.0805508443 -1.6314305956 -0.7536336113
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 H 0.7475926047 0.9945122794 -5.297120319
 H 0.8283049552 2.2141024518 -3.1520126713
 C -0.0443535184 -0.9641557292 0.488789417
 C 0.2150041239 0.4565988796 0.5113362802
 H 0.6407818073 2.2040103028 -0.6903047296

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 C -0.4095194814 -1.6535408975 4.1783567655
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 H 0.2459964427 2.2010048813 4.2286542002
 H -0.5927725065 -2.7300347141 4.1594811461
 H -0.1205741924 0.9654709782 6.3366262781
 H -0.5272367377 -1.5040819547 6.3001292859

8

52

0 1

C 3.2009172099 -0.8899989836 2.1286080991
 C 3.1541589925 -1.7587434043 1.0872049052
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 C 3.359413034 0.098410534 -0.5211930755
 C 3.4043168913 1.0144884182 0.5750674072
 C 3.3244839857 0.5299699577 1.9104335306
 C 3.1926348873 -2.1781445226 -1.3667868877
 C 3.2736927275 -1.69918052 -2.6721688105
 C 3.3924230427 -0.3333082956 -2.9171855208
 C 3.4373255919 0.5820880827 -1.8569611812
 H 3.1319425352 -1.2516163021 3.1564416898
 H 3.047442023 -2.8310479758 1.2646878112
 C 3.5269749008 2.4116306105 0.331337942
 C 3.3524829582 1.4475622562 2.9694466133
 H 3.0911004511 -3.2489033909 -1.1783701172
 H 3.2408145754 -2.3989326967 -3.508852242
 H 3.4491729391 0.0396446194 -3.9420492849
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 H 3.2826021626 1.0754248333 3.9939520935
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 H 3.6201321704 2.3635678998 -3.1019472936
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 H 3.6536681855 4.3657160717 1.2328104609
 H 3.4916417502 3.5141284414 3.561288568
 H 3.7043861058 3.9455579975 -1.2105306894
 C -0.2644987933 -2.7203384344 -0.2572994801
 C -0.220263747 -2.1586683944 -1.4918945479
 C -0.0952601134 -0.7324966021 -1.6621194654
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 C -0.0636146065 -0.5009713623 0.7971574548

C -0.1848209732 -1.9127167788 0.9345624555
 C -0.0497857022 -0.1328993704 -2.9279904405
 C 0.067651926 1.2489404092 -3.055908798
 C 0.1474298886 2.0586664174 -1.9253804549
 C 0.106281827 1.5009024004 -0.6402812549
 H -0.36040486 -3.802219312 -0.1427333351
 H -0.2758730601 -2.7814706642 -2.3873795712
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 H 0.2483760736 3.1409625621 -2.0292818645
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 C -0.1240932571 -1.6632273996 3.3482687063
 H 0.2905214446 3.3895805142 0.436972026
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 H 0.0587976116 0.3512592394 4.1087279056
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 H 0.2064634051 2.3713477301 2.6812270767

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52

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 H 3.62519276 -0.0000121489 -4.6101382573
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 H 3.6186798946 -2.1547743974 3.3740998198
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H 3.6105751536 3.4048621926 1.2330150438
 C -0.0096420558 -2.4641258049 0.6783253833
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6a

24

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 C -1.20826064 -0.699752322 0.0922582086
 C -0.0010540781 -1.3978430305 0.094913395
 H 2.1518876977 -1.247851538 0.099555462
 H 2.1537428654 1.2380625825 0.0927235146
 H 0.0017653785 2.4825315442 0.0896278547
 H -2.1519730058 1.2412003714 0.0913450251
 H -2.1538071874 -1.2447287303 0.0979022311
 H -0.0018201924 -2.4891989759 0.1027189381
 C 1.2083401723 -0.6929274 3.8116073953
 C 1.2071431883 0.7016396577 3.8078383451
 C -0.0011558631 1.3978680952 3.8053033347
 C -1.2082702344 0.6996039442 3.80652064
 C -1.2070807475 -0.6949570492 3.8097600563
 C 0.0012150612 -1.3911755977 3.8121280895
 H 2.1539617314 -1.2377981063 3.8099989762

H 2.1518348102 1.2481056205 3.802915397
 H -0.0020648789 2.4892268001 3.7981351347
 H -2.1538849047 1.2444549239 3.8002611038
 H -2.1517650061 -1.2414428793 3.8058727833
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6b

42

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 C -0.9321497352 -0.9166663176 3.4687813594
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 C -0.9065477209 1.4995587422 3.7877140215
 H 0.9896518845 -1.8235855984 3.0925187046
 C -1.6724988602 -2.2243222677 3.373449784
 H -2.6860657894 0.2763287596 3.8339355797
 C -1.6589378427 2.7853927873 4.0147892628
 H 1.0324305491 2.4300721313 3.7081798511
 C 2.6726858619 0.3199877325 3.2014402082
 H -2.7488662197 -2.0926219907 3.5481535273
 H -1.2934319853 -2.9481958746 4.1099392543
 H -1.534078833 -2.6710473976 2.3760637558
 H -0.975251943 3.6172836372 4.229188478
 H -2.3617782798 2.6924830542 4.855117389
 H -2.2489096645 3.0551079106 3.1246699394
 H 3.0508840355 -0.6700233989 2.9136705787
 H 3.1783192771 0.6244958177 4.1305492423
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 C 1.6195254951 -0.2883698222 -0.1082031513
 C 0.9268354397 -1.5051855376 -0.1888420238
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 H 2.2686868051 -3.0615184799 0.4733166231

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6c
 96
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 C 0.704893484 -1.2059275153 4.8301250631
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 C -1.5013421925 2.5193065492 4.8223744012
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 C 3.4125318589 0.7393611898 3.5338965109
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 H -1.2667130927 -2.8715432183 6.9840805837
 H 0.0323480517 -3.5677066549 3.5182859317
 H -1.2808078584 -2.732107215 2.6569464206
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 H -3.4222072265 -3.4129004426 4.8674663293
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 H -3.0205668438 3.4893206751 6.0443479122
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 H -2.8886620171 3.5216344095 3.4659596457
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 H 3.1343840458 0.3256276902 6.9763251072
 H 3.068384158 1.8464498914 6.055927805
 H 4.5529601884 0.8675904329 6.0390711231
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 H 4.5114789597 0.7323319511 3.459934301

H 3.2740792074 -1.9138094443 5.7620250447
 H 4.6706171912 -1.2790127766 4.8630807136
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 C 1.4043650836 0.0043367374 0.0697938289
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 C -0.6703263241 -1.2023145699 0.071332488
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 H -3.0417918127 -1.854740882 -1.1554548228
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 H -3.2472119806 1.9056542733 -0.8618471264
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C	1.52970	0.00476	5.44196	H	-2.90102	-0.12354	-1.43845
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