

Supplementary Information for

Dipole Moment Propels π -Stacking of Hetero-Dimers of Fluoro-phenylacetylenes

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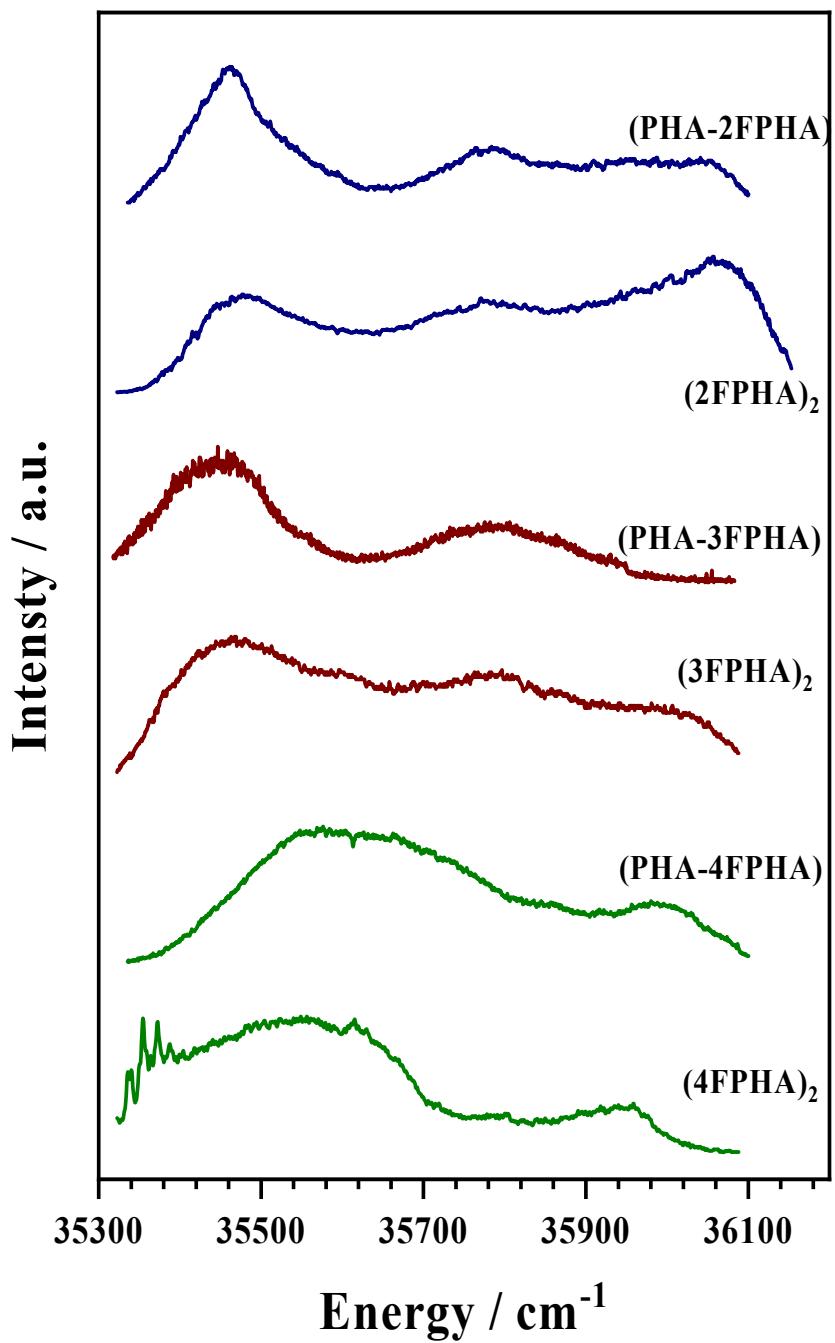


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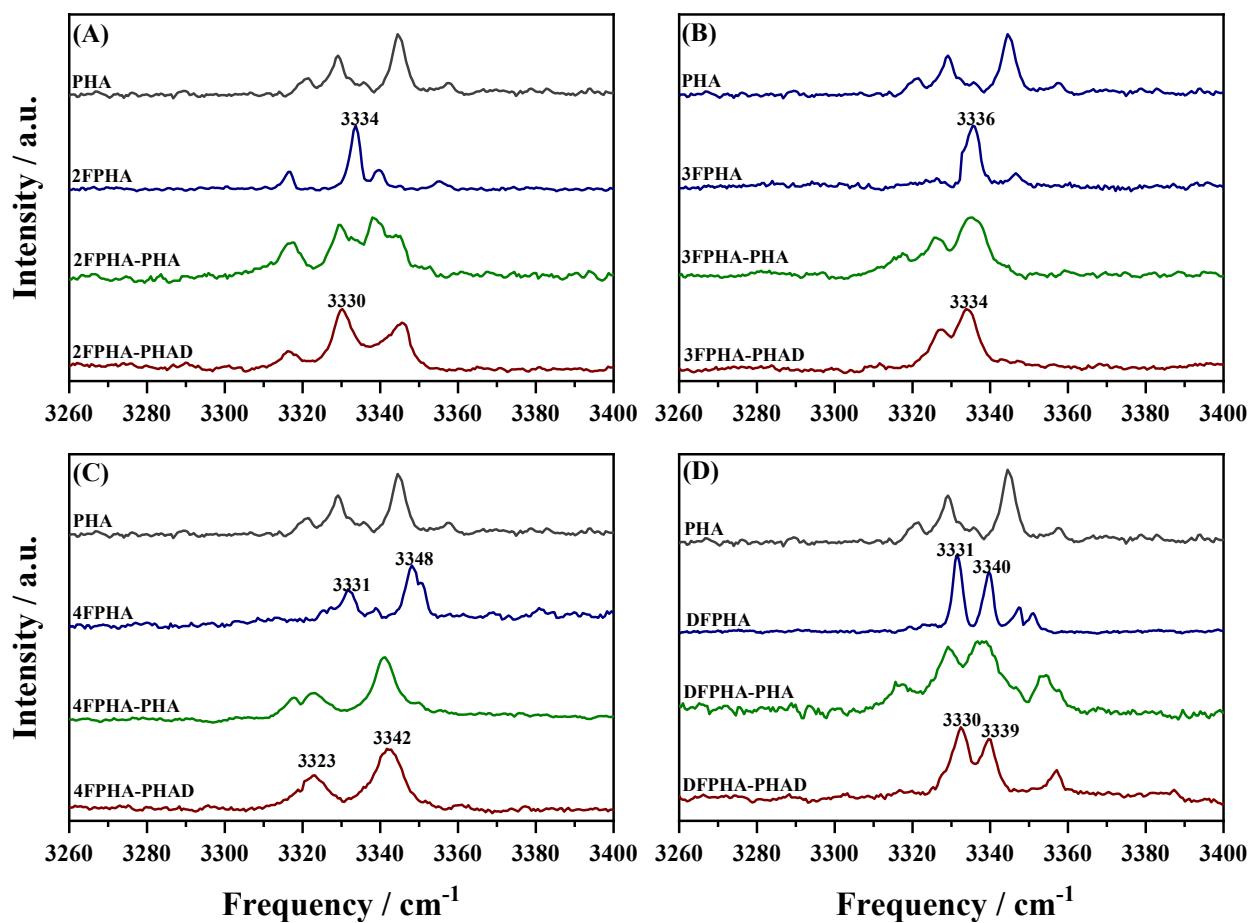


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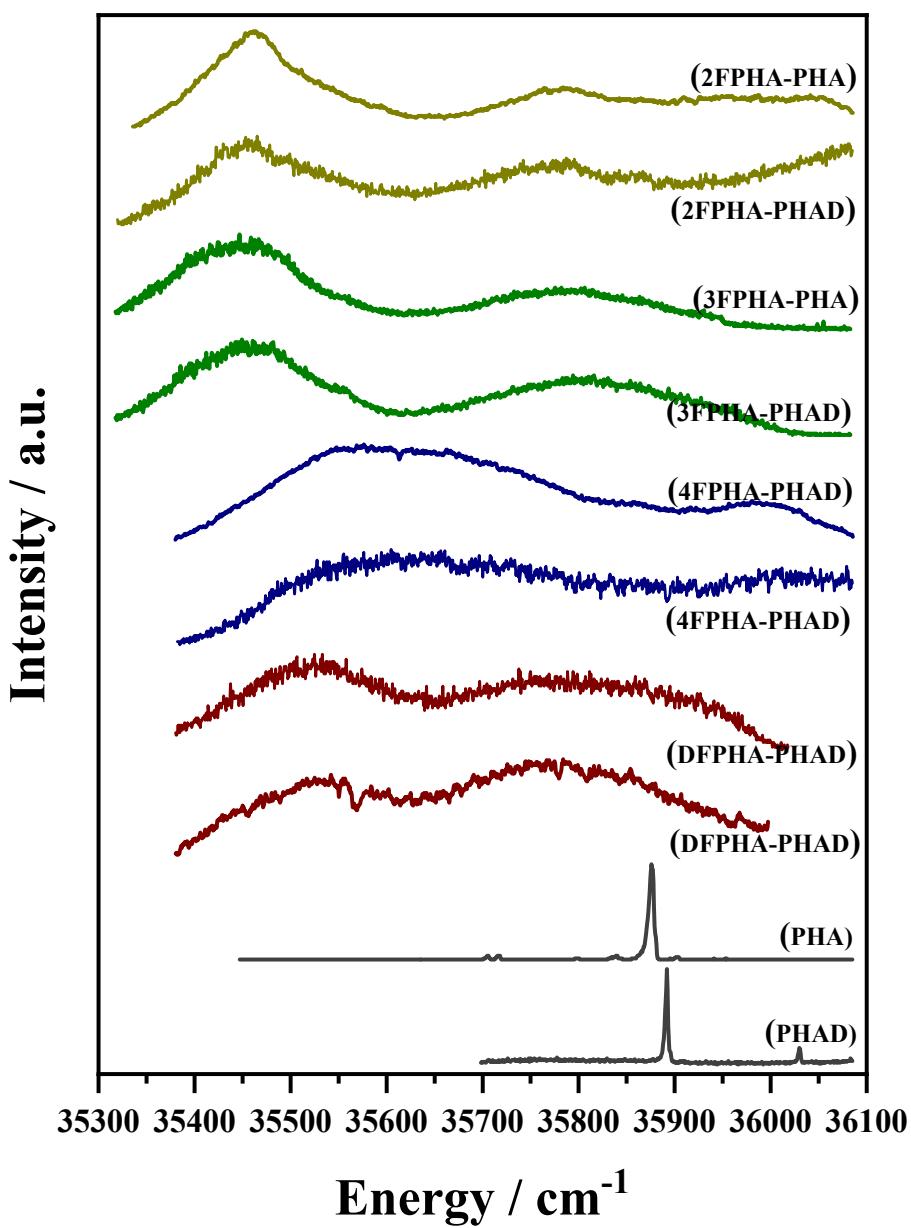


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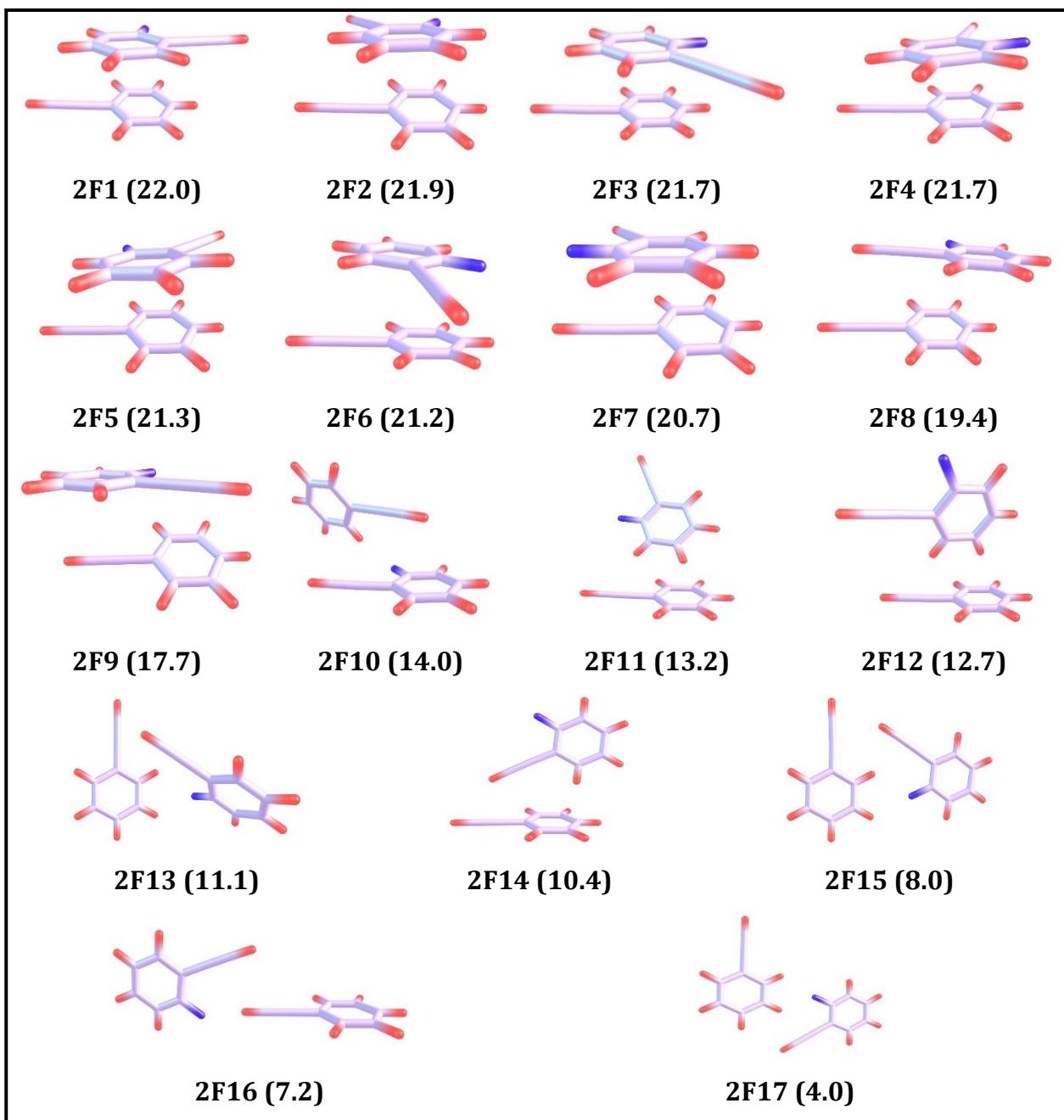


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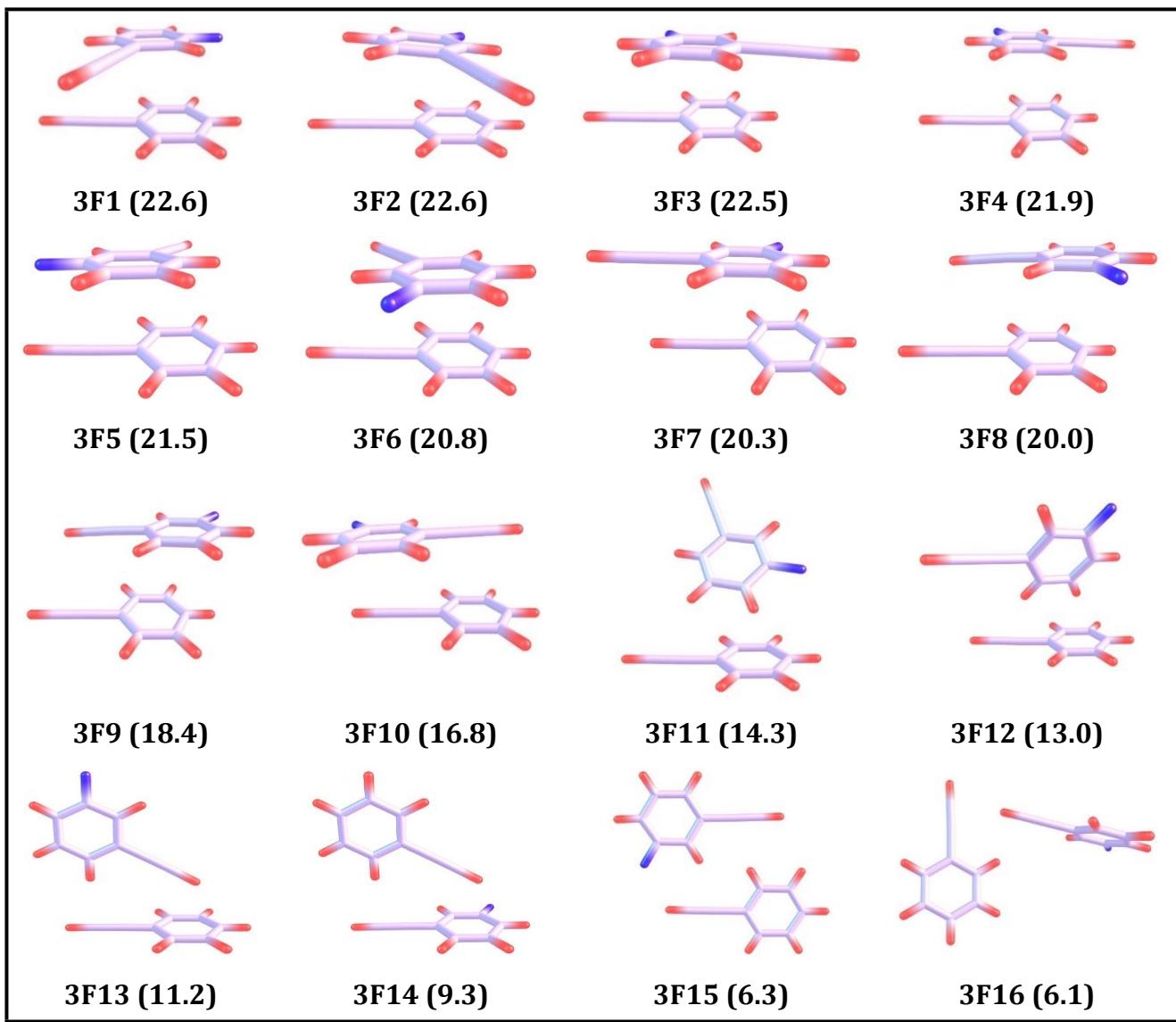


Figure S5. Structures of 3FPHA-PHA dimer optimized at M06-2X/aug-cc-pVDZ level. Structures are arranged in descending order with ZPE and BSSE corrected absolute value of stabilization energy (kJ mol^{-1}) (see Table S2).

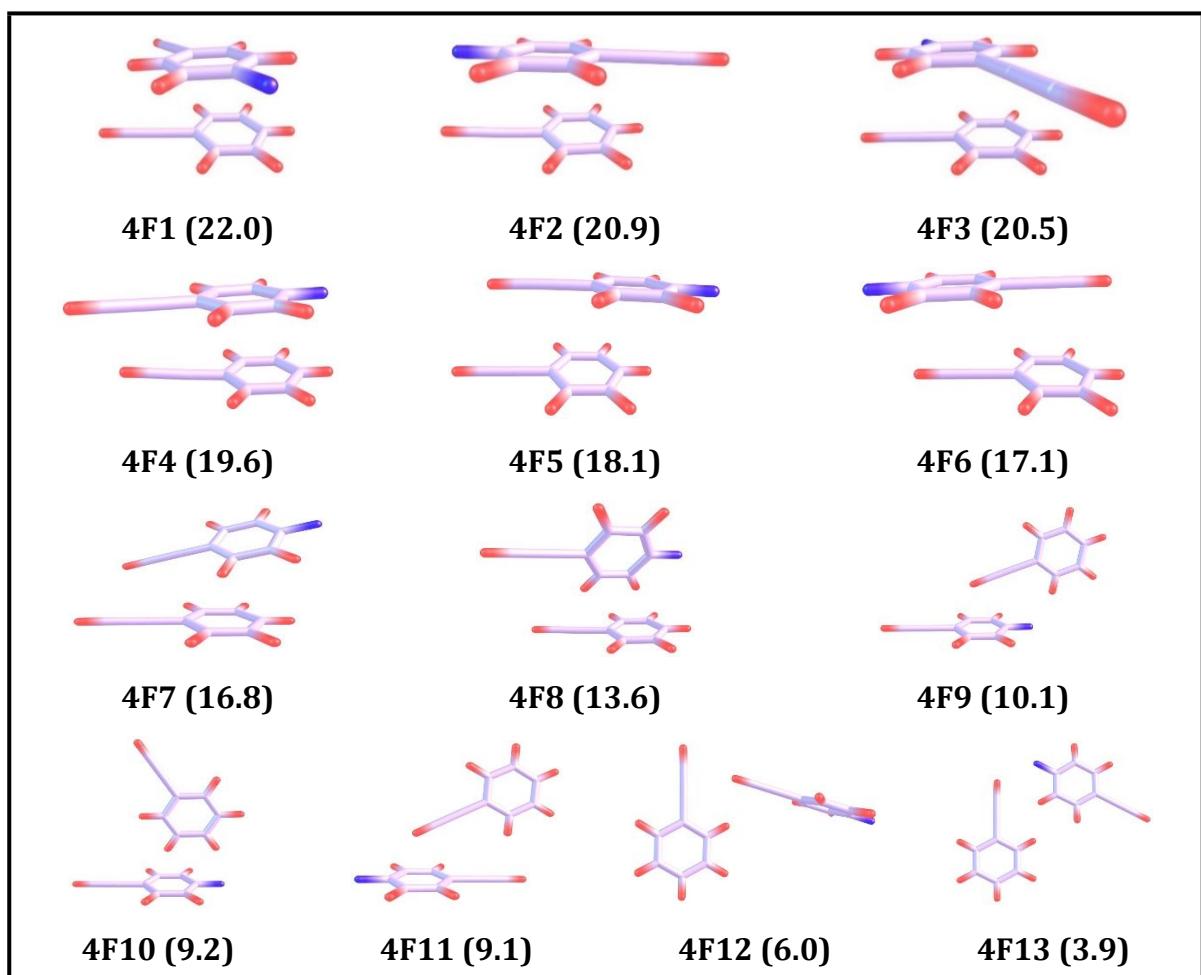


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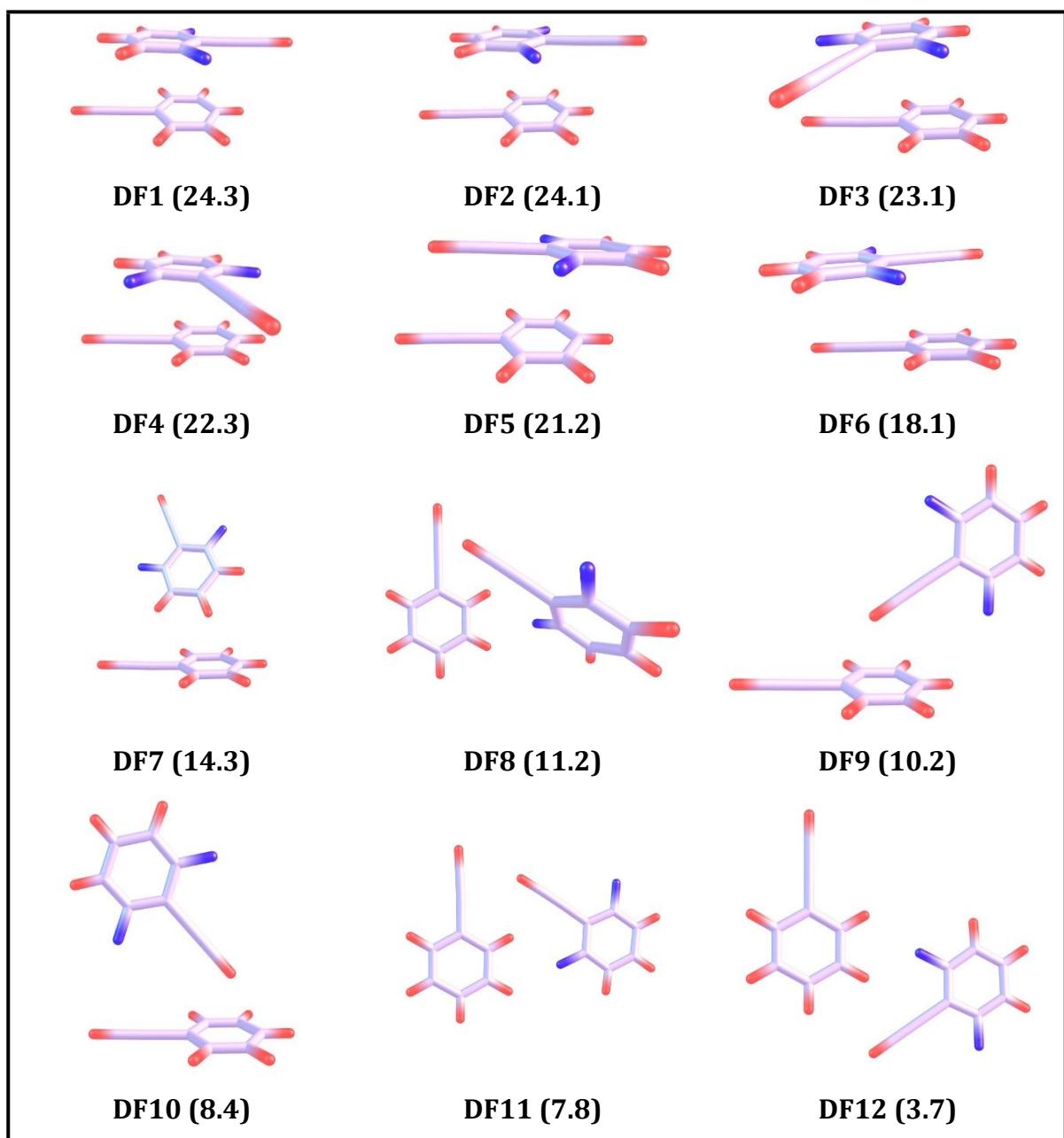


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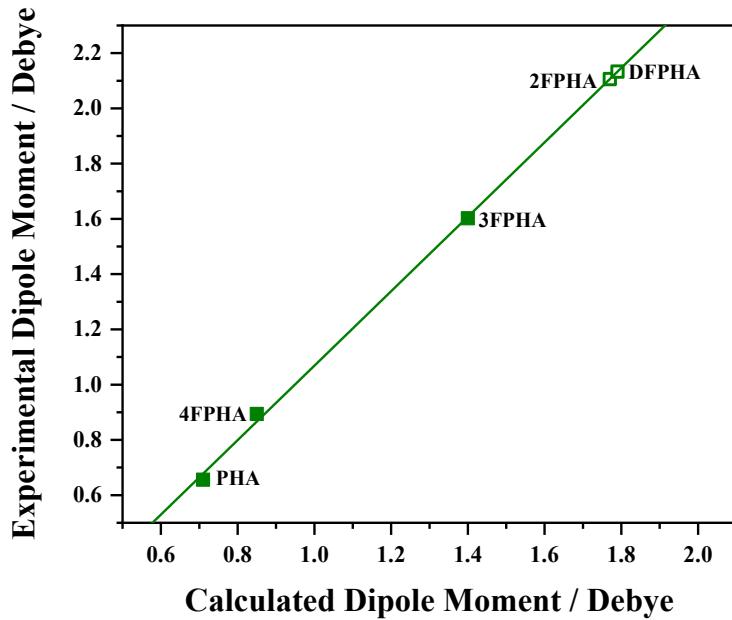


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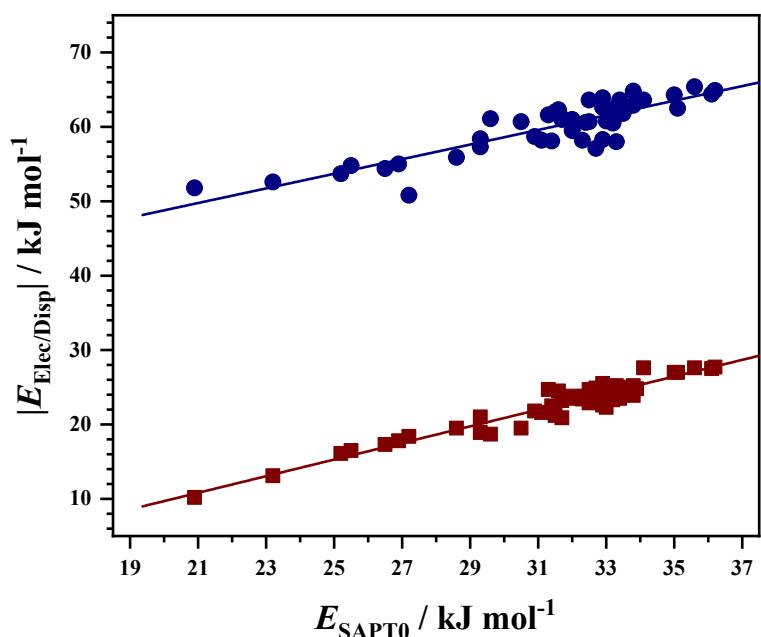


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Table S1. ZPE and BSSE corrected stabilization energies (kJ mol⁻¹), dipole moments (μ) and the scaled (0.9533) acetylenic C-H stretching frequencies (cm⁻¹) for various 2FPHA-PHA hetero-dimers calculated using aug-cc-pVDZ basis set.

Structure	M06-2X	MP2	$\nu_{\text{C-H}}$ (cm ⁻¹)	μ
PHA	-	-	3336	0.71
2FPHA	-	-	3333	1.77
2F1	-22.0	-31.6	3335,3335	1.3
2F2	-21.9	-31.8	3335,3337	1.5
2F3	-21.7	-31.1	3334,3335	1.0
2F4	-21.7	-31.8	3337,3336	1.0
2F5	-21.3	-31.4	3336,3339	1.7
2F6	-21.2	-31.0	3335,3336	1.2
2F7	-20.7	-30.2	3336,3336	2.1
2F8	-19.4	-28.9	3339,3338	2.0
2F9	-17.7	-24.7	3319,3336	1.1
2F10	-14.0	-19.0	3323,3334	1.2
2F11	-13.2	-17.5	3334,3338	2.6
2F12	-12.7	-17.7	33333336	2.6
2F13	-11.1	-13.4	3306,3333	2.1
2F14	-10.4	-16.3	3317,3331	2.4
2F15	-8.0	-10.3	3311,3331	2.0
2F16	-7.2	-8.4	3307,3329	1.7
2F17	-4.0	-6.3	3333,3337	2.8

Table S2. ZPE and BSSE corrected stabilization energies (kJ mol⁻¹), dipole moments (μ) and the scaled (0.9533) acetylenic C–H stretching frequencies (cm⁻¹) for various 3FPHA-PHA hetero-dimers calculated using aug-cc-pVDZ basis set.

Structure	M06-2X	MP2	$\nu_{\text{C-H}}$ (cm ⁻¹)	μ
PHA	-	-	3333	0.71
3FPHA	-	-	3337	1.40
3F1	-22.6	-32.5	3336,3338	0.8
3F2	-22.6	-32.7	3335,3337	0.9
3F3	-22.5	-32.1	3333,3335	1.4
3F4	-21.9	-31.1	3339,3339	1.7
3F5	-21.5	-31.1	3337,3337	1.8
3F6	-20.8	-30.4	3338,3338	1.9
3F7	-20.3	-29.6	3337,3338	1.3
3F8	-20.0	-29.5	3338,3339	1.5
3F9	-18.4	-27.3	3337,3339	1.3
3F10	-16.8	-24.6	3335,3340	1.7
3F11	-14.3	-19.1	3334,3339	1.1
3F12	-13.0	-18.2	3336,3337	1.9
3F13	-11.2	-15.8	3316,3331	2.0
3F14	-9.3	-14.1	3318,3330	1.6
3F15	-6.3	-9.77	3331,3334	1.6
3F16	-6.1	-8.09	3288,3329	1.7

Table S3. ZPE and BSSE corrected stabilization energies (kJ mol⁻¹), dipole moments (μ) and the scaled (0.9533) acetylenic C-H stretching frequencies (cm⁻¹) for various 4FPHA-PHA hetero-dimers calculated using aug-cc-pVDZ basis set.

Structure	M06-2X	MP2	$\nu_{\text{C-H}}$ (cm ⁻¹)	μ
PHA	-	-	3336	0.71
4FPHA	-	-	3338	0.85
4F1	-22.0	-31.7	3334,3338	0.9
4F2	-20.9	-30.1	3338,3338	1.4
4F3	-20.5	-30.6	3337,3338	1.2
4F4	-19.6	-28.7	3337,3337	0.2
4F5	-18.1	-27.1	3335,3343	0.4
4F6	-17.1	-25.2	3331,3342	1.6
4F7	-16.8	-22.1	3337,3344	0.8
4F8	-13.6	-19.0	3337,3338	0.6
4F9	-10.1	-14.3	3312,3337	1.8
4F10	-9.2	-13.1	3337,3338	1.2
4F11	-9.1	-13.7	3319,3333	1.4
4F12	-6.0	-8.05	3291,3330	1.2
4F13	-3.9	-6.44	3325,3332	1.3

Table S4. ZPE and BSSE corrected stabilization energies (kJ mol⁻¹), dipole moments (μ) and the scaled (0.9533) acetylenic C-H stretching frequencies (cm⁻¹) for various DFPHA-PHA hetero-dimers calculated using aug-cc-pVDZ basis set.

Structure	M06-2X	MP2	$\nu_{\text{C-H}}$ (cm ⁻¹)	μ
PHA	-	-	3333	0.71
DFPHA	-	-	3333	1.79
DF1	-24.3	-34.4	3337,3339	1.0
DF2	-24.1	-34.1	3336,3337	1.0
DF3	-23.1	-32.3	3334,3340	2.0
DF4	-22.3	-31.9	3334,3336	1.7
DF5	-21.2	-31.2	3337,3339	2.2
DF6	-18.1	-26.3	3338,3342	1.0
DF7	-14.3	-18.4	3334,3339	2.7
DF8	-11.2	-13.6	3305,3333	2.3
DF9	-10.2	-13.1	3308,3333	2.3
DF10	-8.4	-12.2	3308,3339	1.0
DF11	-7.8	-10.1	3311,3330	2.4
DF12	-3.7	-5.9	3332,3338	2.2

Table S5. SAPT0 interaction energy components (kJ mol⁻¹) for various 2FPHA-PHA hetero-dimer calculated using cc-pVTZ basis set.

Structure	E _{Elec}	E _{Disp}	E _{Ind}	E _{CT}	E _{Exch}	E _{SCS-Disp}	E _{SAPT0}	E _{SCS-SAPT0}
2F1	-23.8	-60.6	-5.0	-0.4	57.0	-47.3	-32.4	-19.2
2F2	-21.2	-62.0	-5.0	-0.5	56.7	-48.4	-31.5	-17.9
2F3	-24.9	-57.1	-5.1	-0.4	54.4	-44.6	-32.7	-20.2
2F4	-22.9	-60.7	-5.0	-0.5	56.1	-47.4	-32.5	-19.2
2F5	-23.2	-61.2	-5.2	-0.5	57.8	-47.8	-31.7	-18.4
2F6	-23.8	-59.5	-4.9	-0.5	56.3	-46.5	-32.0	-18.9
2F7	-21.9	-61.3	-5.3	-0.5	58.0	-47.9	-30.6	-17.1
2F8	-21.5	-58.8	-5.2	-0.5	56.6	-46.0	-29.0	-16.2
2F9	-15.3	-55.2	-4.5	-0.4	51.1	-43.1	-23.8	-11.7
2F10	-19.9	-38.7	-4.5	-0.6	41.8	-30.3	-21.4	-12.9
2F11	-15.3	-30.6	-4.4	-0.6	28.8	-23.9	-21.5	-14.8
2F12	-14.4	-31.3	-4.2	-0.6	28.7	-24.4	-21.1	-14.2
2F13	-16.9	-23.1	-5.0	-0.6	27.2	-18.0	-17.8	-12.7
2F14	-15.3	-30.0	-4.6	-0.6	30.8	-23.4	-19.1	-12.5
2F15	-17.4	-19.1	-5.4	-0.8	25.2	-14.9	-16.7	-12.5
2F16	-13.9	-12.1	-3.6	-0.4	16.9	-9.46	-12.7	-10.0
2F17	-8.3	-13.6	-2.7	-0.4	14.8	-10.6	-9.9	-6.84

Table S6. SAPT0 interaction energy components (kJ mol⁻¹) for various 3FPHA-PHA hetero-dimer calculated using cc-pVTZ basis set.

Structure	E _{Elec}	E _{Disp}	E _{Ind}	E _{CT}	E _{Exch}	E _{SCS-Disp}	E _{SAPT0}	E _{SCS-SAPT0}
3F1	-23.1	-63.9	-5.2	-0.6	59.4	-49.9	-32.9	-18.9
3F2	-24.3	-62.4	-5.2	-0.5	58.7	-48.8	-33.2	-19.6
3F3	-24.6	-61.8	-5.4	-0.6	58.7	-48.2	-33.1	-19.6
3F4	-23.4	-58.2	-5.1	-0.5	54.4	-45.5	-32.3	-19.6
3F5	-23.5	-61	-5.0	-0.5	57.6	-47.7	-32.0	-18.6
3F6	-19.5	-60.7	-4.9	-0.5	54.6	-47.4	-30.5	-17.3
3F7	-22.5	-59.3	-5.2	-0.5	57	-46.4	-30.0	-17.0
3F8	-21.5	-57.7	-5.0	-0.4	54.3	-45.1	-29.8	-17.1
3F9	-18.7	-54.8	-4.7	-0.4	50.6	-42.8	-27.6	-15.6
3F10	-12.7	-52.3	-3.9	-0.4	45.8	-40.9	-23.1	-11.7
3F11	-16.9	-32.7	-4.5	-0.6	31.4	-25.5	-22.8	-15.6
3F12	-15.1	-32.0	-4.3	-0.6	29.6	-24.9	-21.7	-14.7
3F13	-15.5	-30.0	-5.1	-0.8	31.2	-23.4	-19.5	-12.9
3F14	-12.9	-29.3	-4.4	-0.7	29.7	-22.9	-16.9	-10.4
3F15	-14.6	-20.2	-3.8	-0.6	24.1	-15.7	-14.4	-10.0
3F16	-14.8	-13.9	-4.5	-0.8	20.4	-10.9	-12.9	-9.8

Table S7. SAPT0 interaction energy components (kJ mol⁻¹) for various 4FPHA-PHA hetero-dimer calculated using cc-pVTZ basis set.

Structure	E _{Elec}	E _{Disp}	E _{Ind}	E _{CT}	E _{Exch}	E _{SCS-Disp}	E _{SAPT0}	E _{SCS-SAPT0}
4F1	-20.9	-61.0	-5.0	-0.5	55.2	-47.6	-31.7	-18.3
4F2	-21.8	-58.7	-4.9	-0.4	54.5	-45.9	-30.9	-18.0
4F3	-21.6	-58.2	-4.9	-0.5	53.7	-45.5	-31.1	-18.3
4F4	-21.0	-57.3	-4.9	-0.4	53.9	-44.7	-29.3	-16.8
4F5	-17.8	-55.0	-4.7	-0.4	50.7	-43.0	-26.9	-14.8
4F6	-13.1	-52.6	-3.8	-0.4	46.4	-41.1	-23.2	-11.7
4F7	-19.3	-43.7	-5.3	-0.6	43.6	-34.2	-24.7	-15.1
4F8	-15.9	-32.4	-4.5	-0.6	30.2	-25.3	-22.6	-15.5
4F9	-14.3	-26.0	-3.3	-0.6	27.0	-20.3	-16.6	-10.9
4F10	-10.8	-26.5	-2.8	-0.5	24.1	-20.6	-16.1	-10.2
4F11	-13.0	-29.1	-4.3	-0.7	29.5	-22.7	-16.9	-10.5
4F12	-14.9	-14.0	-4.5	-0.7	20.5	-10.9	-12.8	-9.8
4F13	-10.1	-13.4	-2.8	-0.4	16.1	-10.4	-10.2	-7.2

Table S8. SAPT0 interaction energy components (kJ mol⁻¹) for various DFPHA-PHA hetero-dimer calculated using cc-pVTZ basis set.

Structure	E _{Elec}	E _{Disp}	E _{Ind}	E _{CT}	E _{Exch}	E _{SCS-Disp}	E _{SAPT0}	E _{SCS-SAPT0}
DF1	-27.7	-64.9	-6.0	-0.6	62.4	-50.7	-36.2	-22.0
DF2	-27.5	-64.4	-5.8	-0.5	61.6	-50.3	-36.1	-22.0
DF3	-27.6	-63.6	-5.7	-0.6	62.7	-49.6	-34.1	-20.2
DF4	-25.2	-58.0	-4.9	-0.5	54.8	-45.3	-33.3	-20.6
DF5	-24.7	-61.6	-5.5	-0.5	60.5	-48.1	-31.3	-17.8
DF6	-16.5	-54.8	-4.3	-0.4	50.1	-42.8	-25.5	-13.4
DF7	-16.7	-31.0	-4.9	-0.6	29.6	-24.2	-23.1	-16.2
DF8	-16.5	-23.1	-4.8	-0.6	27.1	-18.0	-17.3	-12.2
DF9	-12.1	-24.0	-4.9	-0.6	24.5	-18.7	-16.5	-11.2
DF10	-9.23	-24.3	-5.3	-0.8	23.7	-18.9	-15.1	-9.74
DF11	-16.9	-19.0	-5.1	-0.8	25.0	-14.9	-16.1	-12.0
DF12	-7.7	-13.4	-2.5	-0.4	14.3	-10.4	-9.2	-6.26

Table S9. Dipole Moments of phenylacetylene and fluorophenylacetyles

	Calculated	Experimental	Estimated
PHA	0.71	0.656 [Ref.1]	
4FPHA	0.85	0.894 [Ref. 2]	
3FPHA	1.40	1.602 [Ref. 3]	
2FPHA	1.77		2.106
DFPHA	1.79		2.133

References

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Table S10. Optimized coordinates (Å) of various hetero-dimers of PHA with 2FPHA, 3FPHA, 4FPHA and DFPHA π-stacked PHA dimer calculated at M06-2X/aug-cc-pVDZ level of theory.

2FPHA-PHA Hetero-Dimer

2F1

C	-1.686129000000	0.835943000000	-0.052371000000
C	-0.824306000000	0.921522000000	1.044480000000
C	0.306930000000	1.721902000000	1.042095000000
C	0.596548000000	2.469011000000	-0.096838000000
C	-0.245623000000	2.412014000000	-1.209187000000
C	-1.376636000000	1.603601000000	-1.185627000000
C	-2.838505000000	-0.014458000000	-0.014406000000
C	-3.815158000000	-0.728597000000	0.001979000000
H	0.954044000000	1.731594000000	1.916495000000
F	-1.102405000000	0.197827000000	2.141153000000
H	1.492089000000	3.087077000000	-0.117159000000
H	-0.018042000000	2.997599000000	-2.097546000000
H	-2.039161000000	1.546406000000	-2.046955000000
H	-4.682628000000	-1.353642000000	0.024772000000
C	1.856533000000	-0.904774000000	-0.174420000000
C	1.308466000000	-1.677984000000	0.859420000000
C	0.151314000000	-2.418105000000	0.637369000000
C	-0.463678000000	-2.399329000000	-0.614746000000
C	0.081304000000	-1.634488000000	-1.646513000000
C	1.235468000000	-0.887325000000	-1.431547000000
C	3.030207000000	-0.110233000000	0.062316000000
C	4.007589000000	0.574545000000	0.269098000000
H	-0.279651000000	-3.001531000000	1.448859000000
H	1.788585000000	-1.678441000000	1.836168000000
H	-1.377794000000	-2.965918000000	-0.781177000000
H	-0.404299000000	-1.609282000000	-2.620771000000
H	1.658969000000	-0.275724000000	-2.225769000000
H	4.883584000000	1.161964000000	0.446090000000

2F2

C	-1.853913000000	-0.308097000000	-0.199209000000
C	-1.439045000000	-0.498090000000	1.126431000000
C	-0.527914000000	-1.504985000000	1.431958000000
C	-0.021721000000	-2.324084000000	0.422245000000
C	-0.430415000000	-2.135011000000	-0.898844000000
C	-1.344254000000	-1.134085000000	-1.212482000000
C	-2.780301000000	0.741212000000	-0.522521000000
C	-3.549294000000	1.634205000000	-0.800392000000
H	-0.206198000000	-1.646469000000	2.462688000000
H	-1.831420000000	0.152913000000	1.905138000000
H	0.694730000000	-3.107915000000	0.663497000000
H	-0.027491000000	-2.764006000000	-1.690493000000
H	-1.657159000000	-0.967010000000	-2.240980000000
H	-4.236628000000	2.414813000000	-1.048667000000
C	0.450411000000	1.760411000000	-1.236682000000
C	1.414345000000	0.821898000000	-0.856952000000
C	1.926986000000	0.759766000000	0.428635000000
C	1.463712000000	1.669258000000	1.377265000000
C	0.500983000000	2.619514000000	1.032123000000
C	-0.000240000000	2.665161000000	-0.264381000000
C	-0.074024000000	1.769551000000	-2.569382000000

C	-0.534474000000	1.783387000000	-3.688047000000
H	1.855054000000	1.631390000000	2.392473000000
H	0.139320000000	3.326138000000	1.776213000000
H	-0.761553000000	3.389383000000	-0.544892000000
H	-0.935315000000	1.798561000000	-4.679308000000
F	1.859072000000	-0.052611000000	-1.774167000000
H	2.670175000000	0.002203000000	0.666799000000

2F3

C	-1.221306000000	-0.567431000000	0.610830000000
C	-0.406668000000	-0.632957000000	1.749518000000
C	0.414255000000	-1.738053000000	1.956724000000
C	0.427837000000	-2.784678000000	1.034574000000
C	-0.389560000000	-2.727539000000	-0.095399000000
C	-1.212494000000	-1.625663000000	-0.309722000000
C	-2.036249000000	0.592090000000	0.373383000000
C	-2.706177000000	1.578848000000	0.163186000000
H	1.061993000000	-1.772648000000	2.831528000000
H	-0.411003000000	0.195285000000	2.455240000000
H	1.083284000000	-3.639493000000	1.190863000000
H	-0.382459000000	-3.544096000000	-0.815770000000
H	-1.848051000000	-1.569276000000	-1.191558000000
H	-3.313792000000	2.441251000000	-0.012533000000
C	2.873653000000	0.430795000000	1.186769000000
C	2.642835000000	-0.335057000000	0.040560000000
C	1.794360000000	0.078244000000	-0.973105000000
C	1.145401000000	1.304355000000	-0.843073000000
C	1.355288000000	2.097436000000	0.286186000000
C	2.215151000000	1.665466000000	1.290221000000
C	3.725770000000	-0.057485000000	2.229747000000
C	4.424365000000	-0.471824000000	3.126697000000
H	0.456581000000	1.633081000000	-1.619067000000
H	0.837437000000	3.048781000000	0.387849000000
H	2.383436000000	2.270416000000	2.178884000000
H	5.055587000000	-0.833037000000	3.910925000000
H	1.641642000000	-0.568843000000	-1.833729000000
F	3.256500000000	-1.524658000000	-0.072353000000

2F4

C	-1.268524000000	0.322506000000	0.925261000000
C	-1.951132000000	0.555529000000	-0.271928000000
C	-1.729243000000	1.680311000000	-1.050030000000
C	-0.779717000000	2.609083000000	-0.627426000000
C	-0.069013000000	2.402271000000	0.555865000000
C	-0.313846000000	1.270125000000	1.324892000000
C	-1.547589000000	-0.841517000000	1.712716000000
C	-1.787589000000	-1.810273000000	2.396620000000
H	-2.294186000000	1.808329000000	-1.970762000000
F	-2.855801000000	-0.347603000000	-0.685389000000
H	-0.592159000000	3.496138000000	-1.230038000000
H	0.685951000000	3.117224000000	0.875695000000
H	0.242945000000	1.092227000000	2.242876000000
H	-2.003385000000	-2.667504000000	2.998418000000
C	2.004746000000	-0.422746000000	-0.232029000000
C	1.608434000000	-1.633048000000	0.353714000000
C	0.676875000000	-2.444254000000	-0.287489000000
C	0.134983000000	-2.057829000000	-1.512909000000
C	0.533815000000	-0.856678000000	-2.102052000000
C	1.464868000000	-0.039945000000	-1.468587000000
C	2.932561000000	0.439011000000	0.447358000000
C	3.694444000000	1.175868000000	1.033343000000

H	0.358521000000	-3.373488000000	0.181158000000
H	2.022817000000	-1.919376000000	1.318423000000
H	-0.604930000000	-2.686902000000	-2.004593000000
H	0.107649000000	-0.549263000000	-3.055816000000
H	1.769570000000	0.905640000000	-1.912525000000
H	4.384985000000	1.814913000000	1.541753000000

2F5

C	1.647963000000	0.638466000000	-0.175234000000
C	0.599660000000	1.132502000000	-0.956345000000
C	-0.277756000000	2.103637000000	-0.500133000000
C	-0.111320000000	2.600616000000	0.790073000000
C	0.923355000000	2.127865000000	1.600706000000
C	1.794328000000	1.156695000000	1.120978000000
C	2.544837000000	-0.353379000000	-0.689915000000
C	3.320654000000	-1.179784000000	-1.113281000000
H	-1.084548000000	2.435478000000	-1.149145000000
F	0.434282000000	0.644718000000	-2.196362000000
H	-0.796959000000	3.358658000000	1.164511000000
H	1.050471000000	2.518400000000	2.608371000000
H	2.604724000000	0.778617000000	1.741055000000
H	4.004900000000	-1.907955000000	-1.494394000000
C	-1.791392000000	-0.849619000000	0.090810000000
C	-1.101432000000	-1.755488000000	-0.728686000000
C	-0.047101000000	-2.498729000000	-0.208356000000
C	0.327257000000	-2.347070000000	1.127386000000
C	-0.356978000000	-1.447368000000	1.944529000000
C	-1.413202000000	-0.699123000000	1.432362000000
C	-2.864660000000	-0.061288000000	-0.448794000000
C	-3.759192000000	0.613385000000	-0.908399000000
H	0.496976000000	-3.187104000000	-0.852213000000
H	-1.390190000000	-1.854897000000	-1.772845000000
H	1.162444000000	-2.920615000000	1.526232000000
H	-0.061776000000	-1.320509000000	2.984923000000
H	-1.945176000000	0.014275000000	2.058624000000
H	-4.559535000000	1.195281000000	-1.314069000000

2F6

C	-1.754605000000	0.588264000000	0.005318000000
C	-1.462093000000	-0.398481000000	0.952195000000
C	-0.659279000000	-0.157290000000	2.053319000000
C	-0.128025000000	1.120709000000	2.225693000000
C	-0.404402000000	2.130088000000	1.303983000000
C	-1.211503000000	1.865520000000	0.202189000000
C	-2.541847000000	0.274511000000	-1.149672000000
C	-3.176891000000	0.010819000000	-2.145462000000
H	-0.452660000000	-0.968615000000	2.747485000000
F	-1.967225000000	-1.630641000000	0.773966000000
H	0.511648000000	1.323763000000	3.082708000000
H	0.024445000000	3.121261000000	1.433007000000
H	-1.418002000000	2.638413000000	-0.535068000000
H	-3.757500000000	-0.217502000000	-3.014140000000
C	1.814331000000	0.117504000000	-0.699821000000
C	2.463316000000	-0.551945000000	0.347876000000
C	2.152151000000	-1.879962000000	0.624779000000
C	1.192015000000	-2.549245000000	-0.135558000000
C	0.546128000000	-1.888143000000	-1.180671000000
C	0.855115000000	-0.561507000000	-1.465526000000
C	2.127833000000	1.490460000000	-0.986054000000
C	2.392675000000	2.646701000000	-1.229754000000
H	2.659051000000	-2.394442000000	1.439740000000

H	3.205684000000	-0.019487000000	0.939537000000
H	0.942620000000	-3.584901000000	0.089803000000
H	-0.215936000000	-2.400500000000	-1.765268000000
H	0.342579000000	-0.034956000000	-2.268780000000
H	2.633579000000	3.664691000000	-1.451720000000

2F7

C	1.253932000000	0.835713000000	-0.213036000000
C	1.544085000000	1.550014000000	-1.377921000000
C	2.782983000000	1.489110000000	-1.996844000000
C	3.769212000000	0.675092000000	-1.443327000000
C	3.508814000000	-0.061097000000	-0.285884000000
C	2.262917000000	0.021074000000	0.324065000000
C	-0.021418000000	0.963570000000	0.425916000000
C	-1.085301000000	1.076825000000	0.990946000000
H	2.954177000000	2.074462000000	-2.897458000000
F	0.589111000000	2.321630000000	-1.919657000000
H	4.746603000000	0.618493000000	-1.919447000000
H	4.283097000000	-0.688998000000	0.149708000000
H	2.052378000000	-0.530375000000	1.237856000000
H	-2.033641000000	1.172376000000	1.475792000000
C	2.704559000000	3.174599000000	1.586439000000
C	4.052886000000	3.030472000000	1.232778000000
C	4.887111000000	2.209306000000	1.986750000000
C	4.385139000000	1.525334000000	3.093697000000
C	3.042190000000	1.667577000000	3.449384000000
C	2.202908000000	2.488610000000	2.703111000000
C	1.831456000000	3.994072000000	0.793268000000
C	1.088853000000	4.659781000000	0.107590000000
H	5.933454000000	2.099478000000	1.705497000000
H	4.432616000000	3.558712000000	0.360393000000
H	5.039505000000	0.883031000000	3.681302000000
H	2.647246000000	1.135325000000	4.313414000000
H	1.151310000000	2.595237000000	2.961895000000
H	0.425472000000	5.234887000000	-0.502863000000

2F8

C	2.160784000000	-0.668393000000	0.135805000000
C	1.504623000000	-0.540696000000	1.369066000000
C	0.360956000000	-1.288841000000	1.628664000000
C	-0.140963000000	-2.165123000000	0.664927000000
C	0.504737000000	-2.288400000000	-0.564831000000
C	1.651496000000	-1.544741000000	-0.832266000000
C	3.345757000000	0.097699000000	-0.134779000000
C	4.349537000000	0.736244000000	-0.360491000000
H	-0.148640000000	-1.177422000000	2.584590000000
H	1.893703000000	0.155299000000	2.109351000000
H	-1.042430000000	-2.741118000000	0.867650000000
H	0.110155000000	-2.963483000000	-1.322592000000
H	2.162094000000	-1.634403000000	-1.789127000000
H	5.241075000000	1.292588000000	-0.558723000000
C	-0.997394000000	1.095040000000	-0.535107000000
C	-1.748871000000	0.954235000000	0.634838000000
C	-2.872862000000	0.147929000000	0.709133000000
C	-3.266320000000	-0.557189000000	-0.427211000000
C	-2.536188000000	-0.446521000000	-1.611554000000
C	-1.413144000000	0.372651000000	-1.663350000000
C	0.157928000000	1.940575000000	-0.569831000000
C	1.142460000000	2.641586000000	-0.617521000000
H	-3.416628000000	0.080571000000	1.648968000000
F	-1.357557000000	1.617647000000	1.735519000000

H	-4.147589000000	-1.194960000000	-0.384900000000
H	-2.843601000000	-0.999705000000	-2.496709000000
H	-0.831508000000	0.464880000000	-2.578326000000
H	2.026158000000	3.242600000000	-0.652802000000

2F9

C	1.164117000000	-0.937084000000	0.662142000000
C	1.572733000000	-0.981784000000	-0.673875000000
C	2.704456000000	-0.327616000000	-1.131094000000
C	3.469772000000	0.398994000000	-0.220844000000
C	3.093811000000	0.463203000000	1.121361000000
C	1.950691000000	-0.197450000000	1.557271000000
C	-0.016508000000	-1.624808000000	1.091523000000
C	-1.013097000000	-2.197401000000	1.467816000000
H	2.970081000000	-0.396896000000	-2.183736000000
F	0.840337000000	-1.692511000000	-1.550521000000
H	4.364040000000	0.916818000000	-0.564266000000
H	3.692189000000	1.032686000000	1.829870000000
H	1.643420000000	-0.151569000000	2.600033000000
H	-1.899614000000	-2.700287000000	1.790560000000
C	-1.302596000000	1.251402000000	-0.244674000000
C	-2.213458000000	1.332136000000	0.818002000000
C	-3.340744000000	0.516354000000	0.831329000000
C	-3.567871000000	-0.384074000000	-0.210353000000
C	-2.660367000000	-0.470874000000	-1.266282000000
C	-1.532525000000	0.343042000000	-1.287579000000
C	-0.136946000000	2.091146000000	-0.262959000000
C	0.847912000000	2.795245000000	-0.275472000000
H	-4.046321000000	0.584663000000	1.658137000000
H	-2.027199000000	2.036265000000	1.626631000000
H	-4.451747000000	-1.020439000000	-0.197919000000
H	-2.828051000000	-1.180622000000	-2.074588000000
H	-0.815369000000	0.274614000000	-2.103013000000
H	1.719257000000	3.414775000000	-0.284890000000

2F10

C	1.125300000000	0.980747000000	-0.282237000000
C	2.265186000000	0.971249000000	0.525607000000
C	3.452126000000	0.372819000000	0.137469000000
C	3.510136000000	-0.246377000000	-1.110458000000
C	2.391527000000	-0.252214000000	-1.946402000000
C	1.210660000000	0.358725000000	-1.535865000000
C	-0.094389000000	1.560218000000	0.193489000000
C	-1.138471000000	2.009718000000	0.606903000000
H	4.302916000000	0.390616000000	0.814873000000
F	2.198729000000	1.549039000000	1.737152000000
H	4.434406000000	-0.724671000000	-1.429925000000
H	2.440394000000	-0.734556000000	-2.920614000000
H	0.328571000000	0.351497000000	-2.172670000000
H	-2.058649000000	2.403631000000	0.984458000000
C	-0.883594000000	-0.794138000000	3.079035000000
C	-0.601932000000	0.463354000000	3.633956000000
C	-1.455701000000	1.008152000000	4.588523000000
C	-2.593877000000	0.310030000000	4.995570000000
C	-2.877264000000	-0.940122000000	4.444462000000
C	-2.027241000000	-1.493170000000	3.490686000000
C	-0.003595000000	-1.356854000000	2.092088000000
C	0.745085000000	-1.822627000000	1.262156000000
H	-1.231551000000	1.983751000000	5.017347000000
H	0.280465000000	1.005347000000	3.299877000000
H	-3.259235000000	0.739404000000	5.743256000000

H	-3.764065000000	-1.487816000000	4.760022000000
H	-2.239916000000	-2.468320000000	3.056587000000
H	1.408582000000	-2.203009000000	0.512904000000

2F11

C	-2.787182000000	1.006564000000	0.042762000000
C	-2.479589000000	0.111684000000	1.078704000000
C	-1.960241000000	-1.145556000000	0.780958000000
C	-1.743249000000	-1.519399000000	-0.546496000000
C	-2.048212000000	-0.631409000000	-1.579106000000
C	-2.569352000000	0.626379000000	-1.289773000000
C	-3.300854000000	2.314349000000	0.344961000000
C	-3.702566000000	3.427747000000	0.598347000000
H	-1.722357000000	-1.835640000000	1.588573000000
H	-2.647683000000	0.414030000000	2.110317000000
H	-1.333864000000	-2.501896000000	-0.775800000000
H	-1.874794000000	-0.917939000000	-2.614777000000
H	-2.801215000000	1.328520000000	-2.088178000000
H	-4.068591000000	4.408120000000	0.820869000000
C	2.434529000000	3.370702000000	-1.442671000000
C	1.121316000000	3.678803000000	-1.074424000000
C	0.249303000000	2.735304000000	-0.555034000000
C	0.702088000000	1.426989000000	-0.391786000000
C	2.007648000000	1.083585000000	-0.748047000000
C	2.865356000000	2.046259000000	-1.269305000000
C	3.302063000000	4.378250000000	-1.977458000000
C	4.046220000000	5.216927000000	-2.431849000000
H	0.029745000000	0.672931000000	0.014325000000
H	2.357159000000	0.061118000000	-0.619757000000
H	3.885007000000	1.791751000000	-1.551471000000
H	4.699537000000	5.962850000000	-2.832539000000
F	0.689839000000	4.941521000000	-1.232418000000
H	-0.762167000000	3.035104000000	-0.285575000000

2F12

C	-2.548903000000	0.906794000000	0.012063000000
C	-2.349650000000	0.296210000000	1.259207000000
C	-2.744173000000	-1.023288000000	1.459768000000
C	-3.340737000000	-1.742988000000	0.423537000000
C	-3.541608000000	-1.138773000000	-0.818825000000
C	-3.148290000000	0.180497000000	-1.027856000000
C	-2.117905000000	2.260647000000	-0.203591000000
C	-1.721172000000	3.389366000000	-0.387658000000
H	-2.581062000000	-1.493663000000	2.427760000000
H	-1.874546000000	0.861656000000	2.058395000000
H	-3.646934000000	-2.775607000000	0.582915000000
H	-4.005459000000	-1.698073000000	-1.629429000000
H	-3.296137000000	0.658514000000	-1.994078000000
H	-1.378177000000	4.389868000000	-0.547662000000
C	2.280538000000	0.300986000000	-0.034150000000
C	3.056593000000	-0.861610000000	-0.013716000000
C	2.518230000000	-2.120668000000	-0.224887000000
C	1.149538000000	-2.229969000000	-0.466540000000
C	0.343615000000	-1.090730000000	-0.492544000000
C	0.904997000000	0.164040000000	-0.278087000000
C	2.880614000000	1.583310000000	0.189428000000
C	3.376174000000	2.670898000000	0.375976000000
H	3.173230000000	-2.988887000000	-0.197438000000
F	4.375591000000	-0.753516000000	0.219943000000
H	0.711810000000	-3.212644000000	-0.633920000000
H	-0.725250000000	-1.180972000000	-0.677269000000

H	0.288319000000	1.061122000000	-0.298510000000
H	3.820221000000	3.629448000000	0.542391000000

2F13

C	1.408265000000	4.840637000000	-0.128075000000
C	2.738589000000	4.862665000000	-0.573084000000
C	3.587642000000	3.800489000000	-0.278918000000
C	3.117358000000	2.710165000000	0.454856000000
C	1.794287000000	2.684248000000	0.896468000000
C	0.939345000000	3.744906000000	0.611224000000
C	0.529046000000	5.935693000000	-0.436132000000
C	-0.214585000000	6.854353000000	-0.702018000000
H	1.419489000000	1.833077000000	1.461643000000
H	-0.095876000000	3.723429000000	0.943945000000
H	-0.865721000000	7.674104000000	-0.921885000000
C	-2.592173000000	1.157225000000	-0.547734000000
C	-2.113673000000	0.629213000000	0.654493000000
C	-2.530130000000	-0.593422000000	1.154789000000
C	-3.464724000000	-1.328429000000	0.427257000000
C	-3.964796000000	-0.833614000000	-0.778332000000
C	-3.532655000000	0.397481000000	-1.260151000000
C	-2.129625000000	2.428310000000	-1.018615000000
C	-1.736297000000	3.503228000000	-1.410526000000
H	-4.694535000000	-1.409480000000	-1.343965000000
H	-3.915371000000	0.794061000000	-2.198273000000
H	-1.367539000000	4.459316000000	-1.726097000000
H	3.094757000000	5.716430000000	-1.146584000000
H	-2.121735000000	-0.949560000000	2.097872000000
H	4.619702000000	3.822165000000	-0.625490000000
H	3.783796000000	1.878849000000	0.680495000000
H	-3.802701000000	-2.291470000000	0.805932000000
F	-1.211756000000	1.340854000000	1.356325000000

2F14

C	-1.776275000000	0.466933000000	-0.006684000000
C	-3.104243000000	0.902026000000	0.003208000000
C	-4.176592000000	0.023818000000	-0.006302000000
C	-3.919908000000	-1.345981000000	-0.026520000000
C	-2.605145000000	-1.815463000000	-0.036626000000
C	-1.543630000000	-0.917033000000	-0.026832000000
C	-0.689879000000	1.399845000000	0.002524000000
C	0.256952000000	2.152571000000	0.008453000000
H	-5.188771100000	0.422442000000	0.001965000000
F	-3.351559000000	2.222029000000	0.022404000000
H	-4.752583000000	-2.047315000000	-0.034344000000
H	-2.407876000000	-2.885680000000	-0.052322000000
H	-0.512600000000	-1.266016000000	-0.033568000000
H	1.108944000000	2.800887000000	0.012030000000
C	2.947099000000	0.130912000000	-0.002746000000
C	2.643875000000	-0.482457000000	1.221123000000
C	2.116669000000	-1.770392000000	1.242510000000
C	1.886326000000	-2.454222000000	0.047562000000
C	2.170183000000	-1.839412000000	-1.173015000000
C	2.697588000000	-0.551532000000	-1.201818000000
C	3.510139000000	1.453037000000	-0.027595000000
C	3.987228000000	2.565939000000	-0.047976000000
H	1.886131000000	-2.242892000000	2.195761000000
H	2.826542000000	0.058438000000	2.147368000000
H	1.479023000000	-3.464132000000	0.067368000000
H	1.982077000000	-2.365937000000	-2.107087000000
H	2.922589000000	-0.064406000000	-2.148352000000

H	4.418231000000	3.544818000000	-0.066054000000
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2F15

C	-2.624645000000	0.670784000000	-0.011829000000
C	-2.476917000000	-0.718122000000	0.031539000000
C	-3.556694000000	-1.585595000000	0.038975000000
C	-4.842980000000	-1.049977000000	0.000955000000
C	-5.029120000000	0.332706000000	-0.043352000000
C	-3.929801000000	1.184639000000	-0.049522000000
C	-1.472768000000	1.522078000000	-0.016468000000
C	-0.492706000000	2.231372000000	-0.018916000000
H	-3.377675000000	-2.657771000000	0.074304000000
F	-1.233783000000	-1.232570000000	0.069108000000
H	-5.702640000000	-1.717795000000	0.006149000000
H	-6.034608000000	0.747597000000	-0.072779000000
H	-4.061478000000	2.264086000000	-0.083631000000
H	0.402037000000	2.821840000000	-0.020801000000
C	3.213948000000	0.473571000000	0.006194000000
C	4.473255000000	-0.144622000000	-0.020409000000
C	4.567125000000	-1.532633000000	-0.040606000000
C	3.410218000000	-2.313379000000	-0.034462000000
C	2.156995000000	-1.701108000000	-0.007929000000
C	2.052961000000	-0.313010000000	0.012325000000
C	3.131380000000	1.909686000000	0.027382000000
C	3.098209000000	3.120573000000	0.045943000000
H	5.547107000000	-2.007091000000	-0.061232000000
H	5.369688000000	0.472583000000	-0.025053000000
H	3.487192000000	-3.399582000000	-0.050343000000
H	1.251092000000	-2.304059000000	-0.003361000000
H	1.073811000000	0.161484000000	0.032462000000
H	3.078762000000	4.190051000000	0.063393000000

2F16

C	-3.007760000000	0.247245000000	0.150710000000
C	-2.914835000000	-0.413722000000	1.384606000000
C	-3.671682000000	-1.557224000000	1.623254000000
C	-4.526438000000	-2.052481000000	0.637860000000
C	-4.622297000000	-1.398530000000	-0.591048000000
C	-3.868519000000	-0.254604000000	-0.836828000000
C	-2.227936000000	1.428457000000	-0.100969000000
C	-1.575794000000	2.426296000000	-0.314232000000
H	-3.594617000000	-2.064270000000	2.583966000000
H	-2.247116000000	-0.020253000000	2.148736000000
H	-5.117711000000	-2.947039000000	0.827685000000
H	-5.288808000000	-1.781451000000	-1.362481000000
H	-3.938754000000	0.262035000000	-1.792193000000
H	-0.982910000000	3.297767000000	-0.511773000000
C	2.180453000000	4.690077000000	-1.788323000000
C	1.301708000000	5.694796000000	-1.375327000000
C	1.615461000000	7.041704000000	-1.444041000000
C	2.862537000000	7.408801000000	-1.947145000000
C	3.767232000000	6.433193000000	-2.369384000000
C	3.429056000000	5.086371000000	-2.290733000000
C	1.797228000000	3.313413000000	-1.691498000000
C	1.461166000000	2.155321000000	-1.596090000000
H	3.126857000000	8.463016000000	-2.008747000000
H	4.739718000000	6.724026000000	-2.761416000000
H	4.125422000000	4.316618000000	-2.616752000000
H	1.144389000000	1.137469000000	-1.498371000000
F	0.097776000000	5.334894000000	-0.889563000000
H	0.887710000000	7.776192000000	-1.106715000000

2F17

C	2.227159000000	-1.840693000000	5.686079000000
C	2.724476000000	-0.577753000000	5.354919000000
C	3.077306000000	0.361362000000	6.309977000000
C	2.929713000000	0.031292000000	7.655841000000
C	2.436179000000	-1.221445000000	8.024542000000
C	2.088224000000	-2.148469000000	7.048303000000
C	1.874545000000	-2.781687000000	4.664540000000
C	1.570943000000	-3.590483000000	3.817726000000
H	3.458899000000	1.327959000000	5.989353000000
F	2.866192000000	-0.262901000000	4.055112000000
H	3.202397000000	0.757808000000	8.419253000000
H	2.322555000000	-1.475752000000	9.076353000000
H	1.702520000000	-3.128191000000	7.322312000000
H	1.303168000000	-4.304470000000	3.067295000000
C	3.183358000000	0.394961000000	-0.587217000000
C	3.006290000000	-0.013230000000	0.742955000000
C	2.500244000000	-1.279225000000	1.023390000000
C	2.167925000000	-2.144955000000	-0.018898000000
C	2.341949000000	-1.744248000000	-1.344328000000
C	2.847572000000	-0.479733000000	-1.631276000000
C	3.705889000000	1.701646000000	-0.880460000000
C	4.145854000000	2.801876000000	-1.128712000000
H	2.366275000000	-1.587761000000	2.058253000000
H	3.267377000000	0.666934000000	1.551121000000
H	1.771825000000	-3.135764000000	0.200409000000
H	2.083145000000	-2.418796000000	-2.159147000000
H	2.987166000000	-0.157413000000	-2.661375000000
H	4.534680000000	3.773889000000	-1.347100000000

3FPHA-PHA Hetero-Dimer**3F1**

C	3.307584000000	0.286121000000	-0.043258000000
C	2.538660000000	0.207919000000	1.125144000000
C	1.874648000000	-0.976053000000	1.395424000000
C	1.945304000000	-2.085718000000	0.565619000000
C	2.715840000000	-1.992956000000	-0.593862000000
C	3.393401000000	-0.817779000000	-0.904147000000
C	3.986219000000	1.509625000000	-0.367690000000
C	4.546023000000	2.544792000000	-0.649994000000
H	1.400829000000	-2.990324000000	0.827342000000
H	2.782836000000	-2.848343000000	-1.263675000000
H	3.979497000000	-0.735366000000	-1.815961000000
H	5.050166000000	3.454412000000	-0.899130000000
C	0.733454000000	1.372718000000	-1.679106000000
C	0.754045000000	2.525837000000	-0.880771000000
C	0.015348000000	2.568432000000	0.297841000000
C	-0.748304000000	1.467434000000	0.689625000000
C	-0.773869000000	0.320977000000	-0.104858000000
C	-0.037062000000	0.269936000000	-1.284629000000
C	1.517233000000	1.312971000000	-2.881658000000
C	2.191964000000	1.256935000000	-3.885410000000
H	-1.318424000000	1.500468000000	1.616618000000
H	-1.361493000000	-0.542541000000	0.203038000000
H	-0.040211000000	-0.624890000000	-1.903994000000
H	2.779809000000	1.215693000000	-4.777680000000
H	1.364587000000	3.372446000000	-1.187355000000
H	2.443447000000	1.057209000000	1.796692000000
F	1.113247000000	-1.047365000000	2.507404000000

H	0.037876000000	3.464512000000	0.916139000000
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3F2

C	-1.665181000000	0.486344000000	0.107421000000
C	-1.281502000000	-0.401899000000	1.121056000000
C	-0.484365000000	0.079215000000	2.144592000000
C	-0.060492000000	1.399237000000	2.214313000000
C	-0.457220000000	2.272159000000	1.202730000000
C	-1.252503000000	1.825339000000	0.151416000000
C	-2.456190000000	0.009286000000	-0.992910000000
C	-3.104962000000	-0.391668000000	-1.932977000000
H	0.572676000000	1.719523000000	3.038590000000
H	-0.125469000000	3.308061000000	1.226638000000
H	-1.547976000000	2.500920000000	-0.647701000000
H	-3.694094000000	-0.741367000000	-2.754239000000
C	1.783358000000	0.112286000000	-0.686924000000
C	2.224845000000	-0.656465000000	0.400683000000
C	1.825420000000	-1.983644000000	0.524319000000
C	0.986015000000	-2.554453000000	-0.433680000000
C	0.544367000000	-1.793880000000	-1.517013000000
C	0.939158000000	-0.465618000000	-1.646005000000
C	2.195020000000	1.482914000000	-0.816550000000
C	2.546791100000	2.636236000000	-0.927808000000
H	2.163872000000	-2.571918000000	1.375428000000
H	2.874405000000	-0.200123000000	1.145354000000
H	0.673879000000	-3.592993000000	-0.334014000000
H	-0.121228000000	-2.231423000000	-2.259026000000
H	0.586382000000	0.138625000000	-2.479827000000
H	2.864369000000	3.652040000000	-1.031798000000
F	-0.087112000000	-0.778948000000	3.107227000000
H	-1.576358000000	-1.447598000000	1.098600000000

3F3

C	1.748036000000	0.900049000000	0.283972000000
C	1.012308000000	0.803959000000	-0.904182000000
C	-0.157370000000	1.536148000000	-1.013235000000
C	-0.625684000000	2.364146000000	-0.002527000000
C	0.122076000000	2.456666000000	1.170561000000
C	1.301599000000	1.731893000000	1.320752000000
C	2.941884000000	0.117332000000	0.445932000000
C	3.935493000000	-0.558453000000	0.592887000000
H	-1.562244000000	2.899669000000	-0.137263000000
H	-0.225098000000	3.097747000000	1.978823000000
H	1.881260000000	1.796628000000	2.238667000000
H	4.823924000000	-1.141163000000	0.716298000000
C	-1.861524000000	-0.906422000000	0.179652000000
C	-1.534702000000	-1.616776000000	-0.984587000000
C	-0.392404000000	-2.411797000000	-1.015596000000
C	0.431642000000	-2.503054000000	0.107125000000
C	0.107158000000	-1.799304000000	1.267396000000
C	-1.033961000000	-1.004266000000	1.307794000000
C	-3.026270000000	-0.065628000000	0.209919000000
C	-4.000123000000	0.653613000000	0.230020000000
H	-0.141476000000	-2.959187000000	-1.922873000000
H	-2.175583000000	-1.527562000000	-1.859321000000
H	1.332896000000	-3.113091000000	0.075720000000
H	0.757900000000	-1.856790000000	2.138557000000
H	-1.288476000000	-0.441681000000	2.203886000000
H	-4.869540000000	1.276184000000	0.247621000000
F	-0.881093000000	1.423787000000	-2.144623000000
H	1.330378000000	0.153679000000	-1.714831000000

3F4

C	-1.986730000000	-1.319443000000	0.324228000000
C	-1.853779000000	-1.753275000000	1.651001000000
C	-0.777496000000	-2.557269000000	2.016031000000
C	0.170972000000	-2.934847000000	1.064811000000
C	0.035717000000	-2.511700000000	-0.258033000000
C	-1.037240000000	-1.708781000000	-0.631596000000
C	-3.071392000000	-0.453138000000	-0.046760000000
C	-3.970057000000	0.297496000000	-0.355883000000
H	-0.676696000000	-2.887797000000	3.048688000000
H	-2.594960000000	-1.448264000000	2.387484000000
H	1.021704000000	-3.549048000000	1.354714000000
H	0.782196000000	-2.795168000000	-0.998500000000
H	-1.141635000000	-1.361243000000	-1.657765000000
H	-4.776522000000	0.942851000000	-0.633396000000
C	1.817277000000	0.200962000000	0.275395000000
C	1.713764000000	0.609333000000	-1.061448000000
C	0.632623000000	1.394265000000	-1.425865000000
C	-0.346606000000	1.792478000000	-0.527000000000
C	-0.225008000000	1.383757000000	0.800631000000
C	0.846854000000	0.595029000000	1.207146000000
C	2.904962000000	-0.647118000000	0.677971000000
C	3.817186000000	-1.371369000000	1.007678000000
H	-1.186018000000	2.392210000000	-0.870967000000
H	-0.991835000000	1.668171000000	1.519059000000
H	0.930780000000	0.258684000000	2.237739000000
H	4.630571000000	-1.999529000000	1.304141000000
H	2.453344000000	0.314800000000	-1.801960000000
F	0.525090000000	1.779732000000	-2.714908000000

3F5

C	1.499718000000	0.860096000000	-0.496234000000
C	0.610576000000	1.682527000000	-1.200921000000
C	-0.279767000000	2.458271000000	-0.477897000000
C	-0.328026000000	2.451791000000	0.908621000000
C	0.565083000000	1.629414000000	1.595406000000
C	1.477565000000	0.837508000000	0.905444000000
C	2.411816000000	0.015851000000	-1.217048000000
C	3.164229000000	-0.711308000000	-1.825913000000
H	-1.057343000000	3.072399000000	1.424152000000
H	0.540054000000	1.600156000000	2.683164000000
H	2.162417000000	0.183070000000	1.439055000000
H	3.842875000000	-1.338779000000	-2.364136000000
C	-1.527006000000	-0.925863000000	0.183591000000
C	-0.531390000000	-1.659646000000	-0.476419000000
C	0.346900000000	-2.457207000000	0.251488000000
C	0.238192000000	-2.532407000000	1.640163000000
C	-0.755350000000	-1.808145000000	2.301694000000
C	-1.635276000000	-1.007763000000	1.579928000000
C	-2.419074000000	-0.081400000000	-0.562003000000
C	-3.157227000000	0.646545000000	-1.187352000000
H	1.126836000000	-3.010591000000	-0.268647000000
H	-0.441274000000	-1.583137000000	-1.558567000000
H	0.926819000000	-3.156289000000	2.208051000000
H	-0.844126000000	-1.867373000000	3.385467000000
H	-2.408828000000	-0.433642000000	2.086688000000
H	-3.802754000000	1.295605000000	-1.740387000000
H	0.603230000000	1.708020000000	-2.287656000000
F	-1.139557000000	3.247213000000	-1.152266000000

3F6

C	1.402820000000	0.824523000000	-0.205128000000
C	1.717651000000	1.571918000000	-1.348479000000
C	2.957005000000	1.380929000000	-1.934504000000
C	3.894142000000	0.483062000000	-1.441784000000
C	3.566327000000	-0.251503000000	-0.302814000000
C	2.331424000000	-0.086474000000	0.317299000000
C	0.133234000000	1.010371000000	0.440345000000
C	-0.931543000000	1.167207000000	0.993791000000
H	4.852513000000	0.374734000000	-1.944876000000
H	4.287632000000	-0.955074000000	0.108958000000
H	2.079156000000	-0.648734000000	1.213062000000
H	-1.876569000000	1.305787000000	1.474721000000
C	2.551369000000	3.250120000000	1.615511000000
C	3.857961000000	3.065625000000	1.141763000000
C	4.726473000000	2.209079000000	1.811781000000
C	4.300958000000	1.530239000000	2.953937000000
C	2.999797000000	1.709818000000	3.426415000000
C	2.125677000000	2.565772000000	2.763423000000
C	1.647066000000	4.120230000000	0.916386000000
C	0.879446000000	4.841328000000	0.319205000000
H	5.738858000000	2.066898000000	1.436802000000
H	4.178156000000	3.592766000000	0.244959000000
H	4.982563000000	0.860327000000	3.476114000000
H	2.664358000000	1.180108000000	4.316691000000
H	1.105844000000	2.704360000000	3.115799000000
H	0.205899000000	5.486483000000	-0.203959000000
H	1.018988000000	2.296646000000	-1.757937000000
F	3.269249000000	2.102564000000	-3.031533000000

3F7

C	-0.854587000000	0.613856000000	-0.408824000000
C	-1.518884000000	0.254916000000	0.773163000000
C	-2.296228000000	-0.898774000000	0.813714000000
C	-2.417545000000	-1.703744000000	-0.320127000000
C	-1.761837000000	-1.348623000000	-1.499710000000
C	-0.985367000000	-0.194732000000	-1.547237000000
C	-0.032237000000	1.790942000000	-0.448926000000
C	0.680390000000	2.768989000000	-0.480376000000
H	-3.025523000000	-2.606577000000	-0.285035000000
H	-1.848861000000	-1.976538000000	-2.384734000000
H	-0.461945000000	0.083996000000	-2.460037000000
H	1.322794000000	3.623346000000	-0.506497000000
C	2.756958000000	0.015319000000	0.293960000000
C	2.166174000000	-0.354838000000	1.510222000000
C	1.333944000000	-1.469621000000	1.567327000000
C	1.076123000000	-2.226598000000	0.425668000000
C	1.667247000000	-1.831742000000	-0.765444000000
C	2.502480000000	-0.731783000000	-0.863895000000
C	3.618010000000	1.163293000000	0.226884000000
C	4.348526000000	2.126852000000	0.172354000000
H	0.870289000000	-1.750287000000	2.511310000000
H	2.362581000000	0.239607000000	2.399232000000
H	0.416214000000	-3.090781000000	0.440478000000
H	2.938193000000	-0.455586000000	-1.820746000000
H	5.001528000000	2.972660000000	0.126553000000
H	-1.411703000000	0.885232000000	1.653963000000
F	1.404976000000	-2.540093000000	-1.883951000000
H	-2.809800000000	-1.171824000000	1.734461000000

3F8

C	0.441211000000	1.242237000000	-1.372249000000
C	0.675235000000	1.323673000000	0.006346000000
C	1.797384000000	0.696641000000	0.519222000000
C	2.701031000000	0.001873000000	-0.272322000000
C	2.459110000000	-0.064013000000	-1.644470000000
C	1.338301000000	0.548658000000	-2.197610000000
C	-0.741336000000	1.842992000000	-1.922776000000
C	-1.762234000000	2.315914000000	-2.368459000000
H	3.565620000000	-0.473146000000	0.185881000000
H	3.154166000000	-0.601617000000	-2.287028000000
H	1.144140000000	0.492540000000	-3.266147000000
H	-2.663855000000	2.741726000000	-2.755136000000
C	-2.339422000000	-0.372795000000	0.483013000000
C	-1.867967000000	-1.044305000000	-0.653686000000
C	-0.757507000000	-1.878490000000	-0.558630000000
C	-0.114263000000	-2.055096000000	0.666670000000
C	-0.584572000000	-1.394261000000	1.802733000000
C	-1.691605000000	-0.556083000000	1.714611000000
C	-3.474494000000	0.503533000000	0.388384000000
C	-4.429664000000	1.243892000000	0.314960000000
H	-0.387992000000	-2.387597000000	-1.447159000000
H	-2.367359000000	-0.888319000000	-1.607688000000
H	0.758669000000	-2.702425000000	0.735102000000
H	-0.080175000000	-1.523739000000	2.758655000000
H	-2.063289000000	-0.032809000000	2.593569000000
H	-5.276636000000	1.893916000000	0.254551000000
F	2.013082000000	0.751378000000	1.849637000000
H	-0.015607000000	1.843275000000	0.665466000000

3F9

C	-1.279713000000	0.837287000000	-0.081966000000
C	-2.204210000000	0.415485000000	0.883460000000
C	-2.846990000000	-0.795686000000	0.691530000000
C	-2.619081000000	-1.602627000000	-0.414509000000
C	-1.698655000000	-1.167035000000	-1.367514000000
C	-1.029675000000	0.042730000000	-1.209448000000
C	-0.561617000000	2.067218000000	0.101813000000
C	0.079958000000	3.081000000000	0.259669000000
H	-3.153593000000	-2.544797000000	-0.513438000000
H	-1.494982000000	-1.786009000000	-2.239428000000
H	-0.298070000000	0.375479000000	-1.941961000000
H	0.648518000000	3.977522000000	0.388854000000
C	2.319872000000	-0.133447000000	0.008839000000
C	1.568469000000	-0.235930000000	1.187838000000
C	0.839542000000	-1.392473000000	1.451791000000
C	0.858218000000	-2.455443000000	0.549223000000
C	1.611365000000	-2.360911000000	-0.622414000000
C	2.338490000000	-1.206608000000	-0.895503000000
C	3.068394000000	1.060356000000	-0.273601000000
C	3.705471000000	2.061126000000	-0.515406000000
H	0.248859000000	-1.461732000000	2.363733000000
H	1.548671000000	0.604304000000	1.878978000000
H	0.281950000000	-3.355799000000	0.756419000000
H	1.630512000000	-3.190099000000	-1.328121000000
H	2.927994000000	-1.123211000000	-1.806653000000
H	4.272479000000	2.942324000000	-0.728966000000
H	-2.412550000000	1.014149000000	1.766740000000
F	-3.732687000000	-1.208709000000	1.622566000000

3F10

C	1.837667000000	-0.547459000000	1.387150000000
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C	2.821779000000	-0.631762000000	0.393631000000
C	3.822566000000	0.324478000000	0.377785000000
C	3.893483000000	1.356634000000	1.302182000000
C	2.903445000000	1.431721000000	2.281772000000
C	1.879756000000	0.490846000000	2.329332000000
C	0.787008000000	-1.525497000000	1.434815000000
C	-0.099541000000	-2.347943000000	1.475491000000
H	4.705116000000	2.078550000000	1.243613000000
H	2.934131000000	2.235415000000	3.015247000000
H	1.106379000000	0.546770000000	3.091973000000
H	-0.887533000000	-3.069958000000	1.507040000000
C	-0.632377000000	0.985062000000	-0.434585000000
C	-1.415136000000	1.151308000000	0.717304000000
C	-2.510709000000	0.323800000000	0.940984000000
C	-2.835367000000	-0.674488000000	0.021323000000
C	-2.055498000000	-0.847248000000	-1.122412000000
C	-0.957495000000	-0.023440000000	-1.352421000000
C	0.493386000000	1.845021000000	-0.673591000000
C	1.439766000000	2.571057000000	-0.879875000000
H	-3.115477000000	0.458315000000	1.836421000000
H	-1.153772000000	1.933543000000	1.427606000000
H	-3.695972000000	-1.318493000000	0.197162000000
H	-2.303975000000	-1.627310000000	-1.840453000000
H	-0.343723000000	-0.150354000000	-2.242127000000
H	2.278832000000	3.207999000000	-1.063148000000
F	4.768582000000	0.250482000000	-0.581639000000
H	2.805143000000	-1.422401000000	-0.352256000000

3F11

C	-1.682939000000	-1.009161000000	-0.183577000000
C	-2.041841000000	-1.680152000000	0.995372000000
C	-1.321616000000	-2.798821000000	1.406582000000
C	-0.241269000000	-3.255659000000	0.649583000000
C	0.115422000000	-2.592502000000	-0.525390000000
C	-0.600320000000	-1.474756000000	-0.944063000000
C	-2.407399000000	0.160973000000	-0.597763000000
C	-3.004314000000	1.159892000000	-0.931736000000
H	-1.601591000000	-3.313426000000	2.324063000000
H	-2.882147000000	-1.313562000000	1.581612000000
H	0.326164000000	-4.124283000000	0.978880000000
H	0.961621000000	-2.942575000000	-1.113750000000
H	-0.320787000000	-0.944147000000	-1.852030000000
H	-3.541606000000	2.033424000000	-1.235773000000
C	3.128575000000	2.000082000000	0.913199000000
C	3.499285000000	0.797853000000	1.531632000000
C	2.509298000000	-0.131168000000	1.806393000000
C	1.173215000000	0.076020000000	1.497196000000
C	0.818922000000	1.274928000000	0.878426000000
C	1.784306000000	2.234736000000	0.587223000000
C	4.129127000000	2.987907000000	0.615313000000
C	4.970157000000	3.821312000000	0.364791000000
H	0.438986000000	-0.692795000000	1.729713000000
H	-0.223053000000	1.455605000000	0.617066000000
H	1.510093000000	3.170789000000	0.106317000000
H	5.713251000000	4.558122000000	0.143006000000
H	4.534584000000	0.592322000000	1.792081000000
F	2.864623000000	-1.291447000000	2.398709000000

3F12

C	-2.549275000000	0.906770000000	0.011706000000
C	-2.279582000000	0.288520000000	1.241635000000

C	-2.635919000000	-1.041233000000	1.445805000000
C	-3.264403000000	-1.763706000000	0.430535000000
C	-3.536908000000	-1.151457000000	-0.794192000000
C	-3.182232000000	0.178257000000	-1.006684000000
C	-2.156860000000	2.271278000000	-0.210173000000
C	-1.796118000000	3.410897000000	-0.400998000000
H	-2.417114000000	-1.517723000000	2.399688000000
H	-1.778610000000	0.855791000000	2.023524000000
H	-3.540056000000	-2.804498000000	0.592541000000
H	-4.026736000000	-1.712521000000	-1.588181000000
H	-3.386140000000	0.662747000000	-1.959406000000
H	-1.486243000000	4.421264000000	-0.566443000000
C	2.276673000000	0.285625000000	-0.028346000000
C	3.052357000000	-0.879569000000	0.059376000000
C	2.436451000000	-2.096920000000	-0.175244000000
C	1.089722000000	-2.210578000000	-0.492221000000
C	0.330827000000	-1.043900000000	-0.574674000000
C	0.913293000000	0.200317000000	-0.345357000000
C	2.886657000000	1.565053000000	0.210387000000
C	3.402000000000	2.641487000000	0.410912000000
H	0.658200000000	-3.193854000000	-0.666255000000
H	-0.728809000000	-1.108882000000	-0.816741000000
H	0.320785000000	1.110917000000	-0.410221000000
H	3.857154000000	3.592936000000	0.588427000000
F	3.179394000000	-3.220583000000	-0.091241000000
H	4.110629000000	-0.837466000000	0.304763000000

3F13

C	-2.581041000000	0.920918000000	-0.022713000000
C	-3.033921000000	0.385232000000	1.191404000000
C	-3.926413000000	-0.683014000000	1.191616000000
C	-4.374194000000	-1.224444400000	-0.015086000000
C	-3.926308000000	-0.691694000000	-1.225609000000
C	-3.033807000000	0.376510000000	-1.232983000000
C	-1.649171000000	2.014468000000	-0.026639000000
C	-0.870369000000	2.941529000000	-0.029991000000
H	-4.272787000000	-1.096419000000	2.137367000000
H	-5.072623000000	-2.059695000000	-0.012126000000
H	-2.672166000000	0.791330000000	-2.171575000000
H	-0.192124000000	3.768713000000	-0.032967000000
C	1.823215000000	-0.980865000000	-0.011804000000
C	2.868532000000	-1.914710000000	-0.004739000000
C	4.170925000000	-1.444069000000	-0.003998000000
C	4.483332000000	-0.091916000000	-0.010006000000
C	3.432369000000	0.825338000000	-0.016982000000
C	2.109543000000	0.392593000000	-0.017910000000
C	0.457658000000	-1.426852000000	-0.012739000000
C	-0.700216000000	-1.778642000000	-0.013850000000
H	5.525270000000	0.220469000000	-0.009128000000
H	3.653008000000	1.891463000000	-0.021766000000
H	1.285638000000	1.103502000000	-0.023268000000
H	-1.732307000000	-2.066708000000	-0.010285000000
H	2.671577000000	-2.983885000000	0.000114000000
H	-2.672388000000	0.806808000000	2.127020000000
F	5.179179000000	-2.340660000000	0.002879000000
H	-4.272576000000	-1.111913000000	-2.168390000000

3F14

C	-2.577551000000	0.920025000000	-0.019535000000
C	-3.046056000000	0.384088000000	1.188632000000
C	-3.943491000000	-0.679703000000	1.174755000000

C	-4.386364000000	-1.221967000000	-0.032680000000
C	-3.908341000000	-0.669292000000	-1.213779000000
C	-3.013828000000	0.387654000000	-1.240054000000
C	-1.643413000000	2.011236000000	-0.011358000000
C	-0.865736000000	2.938569000000	-0.002115000000
H	-4.303417000000	-1.095752000000	2.113893000000
H	-5.088733000000	-2.051543000000	-0.071543000000
H	-2.657246000000	0.781235000000	-2.188499000000
H	-0.184171000000	3.763164000000	0.006700000000
C	1.821654000000	-0.982499000000	0.000602000000
C	2.877150000000	-1.905908000000	0.007665000000
C	4.195007000000	-1.458465000000	-0.011581000000
C	4.471848000000	-0.091099000000	-0.038218000000
C	3.423898000000	0.830371000000	-0.045385000000
C	2.103304000000	0.391440000000	-0.025992000000
C	0.457848000000	-1.434816000000	0.019959000000
C	-0.695276000000	-1.802879000000	0.035890000000
H	5.504009000000	0.255837000000	-0.053579000000
H	3.638110000000	1.897985000000	-0.066470000000
H	1.276386000000	1.099819000000	-0.031406000000
H	-1.720634000000	-2.111454000000	0.053167000000
H	2.652416000000	-2.970585000000	0.028006000000
H	-2.692972000000	0.800974000000	2.128571000000
H	5.010410000000	-2.180246000000	-0.006115000000
F	-4.330728000000	-1.184631000000	-2.384973000000

3F15

C	-6.869434000000	-2.598506000000	0.102392000000
C	-5.970909000000	-1.524080000000	0.051522000000
C	-6.490305000000	-0.243960000000	-0.042664000000
C	-7.851710000000	0.019770000000	-0.089177000000
C	-8.732142000000	-1.060719000000	-0.037907000000
C	-8.251463000000	-2.363311000000	0.057471000000
C	-6.374313000000	-3.944454000000	0.200697000000
C	-5.972137000000	-5.083000000000	0.283396000000
F	-5.631227000000	0.797400000000	-0.091414000000
H	-4.893299000000	-1.672162000000	0.083119000000
H	-8.200729000000	1.047169000000	-0.163529000000
H	-9.805194000000	-0.881170000000	-0.072921000000
H	-8.936907000000	-3.206570000000	0.097668000000
H	-5.621484000000	-6.090791000000	0.357408000000
C	-1.531625000000	-2.815256000000	0.147084000000
C	-2.393184000000	-3.920235000000	0.205459000000
C	-1.868818000000	-5.206837000000	0.282630000000
C	-0.487689000000	-5.404211000000	0.302572000000
C	0.371972000000	-4.306466000000	0.245024000000
C	-0.143945000000	-3.016129000000	0.167463000000
C	-2.071811000000	-1.485600000000	0.066452000000
C	-2.537904000000	-0.370159000000	-0.002467000000
H	-2.542215000000	-6.061529000000	0.327355000000
H	1.450440000000	-4.456336000000	0.260491000000
H	0.519414000000	-2.154586000000	0.122089000000
H	-2.968435000000	0.607772000000	-0.062621000000
H	-3.471260000000	-3.768051000000	0.190315000000
H	-0.080349000000	-6.412280000000	0.362795000000

3F16

C	1.862138000000	4.904439000000	-0.429792000000
C	3.165632000000	5.422762000000	-0.441155000000
C	4.251151000000	4.581986000000	-0.215721000000
C	4.047313000000	3.222144000000	0.022232000000

C	2.752075000000	2.703952000000	0.033939000000
C	1.660007000000	3.537480000000	-0.190711000000
C	0.745961000000	5.781010000000	-0.662883000000
C	-0.177146000000	6.539883000000	-0.861072000000
H	2.589579000000	1.643517000000	0.219522000000
H	0.648747000000	3.134191000000	-0.181667000000
H	-0.989025000000	7.214307000000	-1.037095000000
C	-3.090345000000	0.970106000000	-0.045504000000
C	-3.467062000000	0.548582000000	1.237391000000
C	-4.031450000000	-0.708169000000	1.378022000000
C	-4.238965000000	-1.565094000000	0.306126000000
C	-3.859186000000	-1.132846000000	-0.964232000000
C	-3.288692000000	0.123691000000	-1.146378000000
C	-2.502233000000	2.268662000000	-0.227442000000
C	-2.009061000000	3.363080000000	-0.383859000000
H	-4.012102000000	-1.786493000000	-1.821239000000
H	-2.993270000000	0.461478000000	-2.136948000000
H	-1.557219000000	4.326991000000	-0.522016000000
H	3.314902000000	6.484586000000	-0.627261000000
H	5.260809000000	4.989712000000	-0.225431000000
H	4.898652000000	2.566420000000	0.198781000000
H	-4.687074000000	-2.541684000000	0.475401000000
F	-4.395132000000	-1.115020000000	2.611022000000
H	-3.324464000000	1.186470000000	2.106207000000

4FPHA-PHA Hetero-Dimer

4F1

C	-0.918439000000	-6.611289000000	-1.667092000000
C	-1.985605000000	-6.752222000000	-2.566667000000
C	-1.911857000000	-7.692706000000	-3.589548000000
C	-0.779652000000	-8.498461000000	-3.723856000000
C	0.283402000000	-8.359639000000	-2.831240000000
C	0.218176000000	-7.420050000000	-1.806231000000
C	-0.983498000000	-5.632065000000	-0.618019000000
C	-1.033090000000	-4.798646000000	0.258731000000
H	-2.742521000000	-7.798369000000	-4.285651000000
H	-0.726446000000	-9.234145000000	-4.525093000000
H	1.171171000000	-8.981424000000	-2.936662000000
H	1.045445000000	-7.299501000000	-1.109546000000
H	-1.086876000000	-4.068334000000	1.037962000000
C	0.191415000000	-4.202361000000	-3.548618000000
C	0.405771000000	-5.117534000000	-4.589250000000
C	1.612887000000	-5.799884000000	-4.691388000000
C	2.591563000000	-5.554916000000	-3.739049000000
C	2.415408000000	-4.655155000000	-2.697163000000
C	1.204962000000	-3.975697000000	-2.606687000000
C	-1.069783000000	-3.526568000000	-3.432079000000
C	-2.140530000000	-2.971504000000	-3.326939000000
H	1.797620000000	-6.522381000000	-5.483069000000
H	-0.388370000000	-5.300702000000	-5.309708000000
H	3.214331000000	-4.501414000000	-1.975334000000
H	1.027842000000	-3.276337000000	-1.793029000000
H	-3.080820000000	-2.470745000000	-3.234839000000
H	-2.857549000000	-6.110465000000	-2.459699000000
F	3.758786000000	-6.227001000000	-3.823639000000

4F2

C	1.146744000000	0.699494000000	-1.000367000000
C	0.615847000000	0.597032000000	-2.294469000000
C	-0.666472000000	1.068512000000	-2.560269000000

C	-1.427040000000	1.646956000000	-1.542907000000
C	-0.896189000000	1.763000000000	-0.258439000000
C	0.384720000000	1.292983000000	0.015639000000
C	2.446358000000	0.162272000000	-0.706652000000
C	3.524442000000	-0.323444000000	-0.446993000000
H	-1.075852000000	0.981224000000	-3.565577000000
H	-2.436326000000	1.999547000000	-1.748144000000
H	-1.493437000000	2.202273000000	0.538998000000
H	0.800567000000	1.363022000000	1.018839000000
H	4.476039000000	-0.752763000000	-0.214857000000
C	-1.736944000000	-1.335928000000	0.670046000000
C	-1.100641000000	-1.894074000000	-0.447828000000
C	0.180568000000	-2.424078000000	-0.339263000000
C	0.811720000000	-2.384623000000	0.896021000000
C	0.214851000000	-1.832638000000	2.021721000000
C	-1.068105000000	-1.309131000000	1.902689000000
C	-3.054463000000	-0.777041000000	0.550531000000
C	-4.161628000000	-0.297040000000	0.450270000000
H	0.699747000000	-2.849944000000	-1.194965000000
H	-1.613937000000	-1.896409000000	-1.406947000000
H	0.752988000000	-1.822601000000	2.966835000000
H	-1.562048000000	-0.870925000000	2.767523000000
H	-5.145379000000	0.113547000000	0.364555000000
H	1.213161000000	0.136765000000	-3.079387000000
F	2.047322000000	-2.906463000000	1.011224000000

4F3

C	-1.015107000000	-6.877837000000	-1.723264000000
C	-2.071176000000	-7.065945000000	-2.628487000000
C	-2.036545000000	-8.126791000000	-3.527720000000
C	-0.951821000000	-9.006293000000	-3.534451000000
C	0.100073000000	-8.822487000000	-2.637188000000
C	0.071205000000	-7.763644000000	-1.733506000000
C	-1.051680000000	-5.784299000000	-0.791671000000
C	-1.089088000000	-4.862927000000	-0.007096000000
H	-2.859391000000	-8.268921000000	-4.226713000000
H	-0.927578000000	-9.835289000000	-4.240272000000
H	0.954983000000	-9.496493000000	-2.648073000000
H	0.893897000000	-7.607471000000	-1.038183000000
H	-1.128620000000	-4.052715000000	0.689808000000
C	2.068473000000	-6.142854000000	-3.784646000000
C	1.028584000000	-6.263070000000	-4.718021000000
C	-0.004480000000	-5.333859000000	-4.743438000000
C	0.022110000000	-4.289214000000	-3.829522000000
C	1.040793000000	-4.132599000000	-2.901220000000
C	2.068492000000	-5.069439000000	-2.882629000000
C	3.100844000000	-7.139071000000	-3.726386000000
C	3.955791000000	-7.993982000000	-3.657862000000
H	-0.831142000000	-5.415823000000	-5.445359000000
H	1.025956000000	-7.102989000000	-5.409105000000
H	1.007409000000	-3.303819000000	-2.198444000000
H	2.873992000000	-4.982660000000	-2.156551000000
H	4.723049000000	-8.737462000000	-3.609991000000
H	-2.909163000000	-6.371304000000	-2.617962000000
F	-0.989857000000	-3.399179000000	-3.837436000000

4F4

C	1.050082000000	0.932742000000	-0.390464000000
C	1.345924000000	-0.106734000000	-1.283320000000
C	2.515152000000	-0.845633000000	-1.128202000000
C	3.397013000000	-0.556931000000	-0.086253000000

C	3.110212000000	0.483861000000	0.798197000000
C	1.944141000000	1.229266000000	0.648457000000
C	-0.185377000000	1.654869000000	-0.512869000000
C	-1.251665000000	2.222001000000	-0.595009000000
H	2.733387000000	-1.660655000000	-1.816646000000
H	4.303784000000	-1.145907000000	0.039905000000
H	3.798079000000	0.714628000000	1.610246000000
H	1.709190000000	2.038376000000	1.337562000000
H	-2.192785000000	2.722568000000	-0.678545000000
C	-1.647641000000	-1.569583000000	0.186202000000
C	-1.178961000000	-2.657258000000	-0.566480000000
C	0.016903000000	-3.284078000000	-0.233586000000
C	0.731798000000	-2.807234000000	0.856855000000
C	0.298023000000	-1.737446000000	1.625711000000
C	-0.899245000000	-1.117853000000	1.282823000000
C	-2.888474000000	-0.934515000000	-0.159800000000
C	-3.944755000000	-0.416587000000	-0.445369000000
H	0.401347000000	-4.126134000000	-0.804847000000
H	-1.762229000000	-3.007862000000	-1.415381000000
H	0.902996000000	-1.393074000000	2.461196000000
H	-1.256911000000	-0.263469000000	1.853706000000
H	-4.877314000000	0.040799000000	-0.699660000000
H	0.641831000000	-0.338027000000	-2.080345000000
F	1.899096000000	-3.403003000000	1.173074000000

4F5

C	-3.244856000000	-5.209710000000	-3.077522000000
C	-2.833312000000	-6.140352000000	-4.042357000000
C	-1.794552000000	-7.022389000000	-3.760172000000
C	-1.157777000000	-6.986723000000	-2.518953000000
C	-1.563341000000	-6.060091000000	-1.558601000000
C	-2.600590000000	-5.172698000000	-1.832930000000
C	-4.320061000000	-4.300641000000	-3.363577000000
C	-5.229729000000	-3.538453000000	-3.603736000000
H	-1.476283000000	-7.740033000000	-4.514804000000
H	-0.340518000000	-7.673669000000	-2.304389000000
H	-1.064108000000	-6.024172000000	-0.591476000000
H	-2.921681000000	-4.445255000000	-1.090011000000
H	-6.040830000000	-2.873364000000	-3.811972000000
C	0.125479000000	-4.062164000000	-4.208036000000
C	0.643635000000	-5.052968000000	-5.055027000000
C	1.684665000000	-5.872545000000	-4.632550000000
C	2.196023000000	-5.684357000000	-3.355826000000
C	1.715788000000	-4.709355000000	-2.493503000000
C	0.673126000000	-3.897295000000	-2.927833000000
C	-0.963203000000	-3.232620000000	-4.641088000000
C	-1.893499000000	-2.543286000000	-4.993549000000
H	2.100758000000	-6.648080000000	-5.271804000000
H	0.216197000000	-5.179398000000	-6.047639000000
H	2.154410000000	-4.600551000000	-1.504053000000
H	0.267023000000	-3.130375000000	-2.271679000000
H	-2.730344000000	-1.948100000000	-5.291491000000
H	-3.331501000000	-6.157433000000	-5.009688000000
F	3.201320000000	-6.480800000000	-2.937705000000

4F6

C	-6.756709000000	-2.814833000000	0.599905000000
C	-5.895157000000	-1.727644000000	0.396112000000
C	-6.398220000000	-0.491299000000	0.006135000000
C	-7.767195000000	-0.364860000000	-0.178529000000
C	-8.650478000000	-1.417048000000	0.015891000000

C	-8.135773000000	-2.648105000000	0.406220000000
C	-6.231688000000	-4.090364000000	0.998128000000
C	-5.790174000000	-5.166389000000	1.332734000000
H	-4.825473000000	-1.861569000000	0.542845000000
H	-9.715218000000	-1.265608000000	-0.146648000000
H	-8.800475000000	-3.495460000000	0.561443000000
H	-5.399405000000	-6.119465000000	1.618918000000
C	-6.347606000000	-4.304078000000	-2.458306000000
C	-7.303621000000	-5.295236000000	-2.192662000000
C	-6.897933000000	-6.576862000000	-1.834355000000
C	-5.539683000000	-6.881546000000	-1.737203000000
C	-4.585736000000	-5.896053000000	-1.991839000000
C	-4.984065000000	-4.611690000000	-2.350148000000
C	-6.764164000000	-2.983417000000	-2.841495000000
C	-7.118011000000	-1.873059000000	-3.169557000000
H	-7.645050000000	-7.342574000000	-1.631410000000
H	-3.525032000000	-6.129155000000	-1.912059000000
H	-4.246912000000	-3.836884000000	-2.551985000000
H	-7.431854000000	-0.889543000000	-3.449892000000
H	-8.360613000000	-5.048337000000	-2.273997000000
H	-5.224976000000	-7.886735000000	-1.460236000000
F	-8.258911000000	0.827662000000	-0.576979000000
H	-5.748697000000	0.364512000000	-0.163698000000

4F7

C	2.609414000000	-0.396323000000	0.018279000000
C	2.436707000000	-1.503383000000	-0.825443000000
C	1.567643000000	-2.529908000000	-0.461539000000
C	0.866079000000	-2.460627000000	0.743143000000
C	1.032561000000	-1.358611000000	1.582941000000
C	1.899896000000	-0.330367000000	1.226768000000
C	3.514395000000	0.657069000000	-0.351036000000
C	4.273431000000	1.546581000000	-0.664211000000
H	1.441389000000	-3.388656000000	-1.119410000000
H	0.184074000000	-3.261589000000	1.024589000000
H	0.476575000000	-1.295915000000	2.517337000000
H	2.025289000000	0.537774000000	1.868311000000
H	4.954552000000	2.325125000000	-0.935834000000
C	-1.140802000000	1.371938000000	-0.082203000000
C	-2.398896000000	1.776528000000	0.390019000000
C	-3.494542000000	0.924527000000	0.299212000000
C	-3.310009000000	-0.330737000000	-0.265154000000
C	-2.081370000000	-0.762914000000	-0.745196000000
C	-0.993325000000	0.098325000000	-0.651810000000
C	-0.006335000000	2.245605000000	0.023457000000
C	0.960096000000	2.969000000000	0.111304000000
H	-4.479665000000	1.216363000000	0.657794000000
H	-2.511448000000	2.767124000000	0.827036000000
H	-1.986765000000	-1.757622000000	-1.177314000000
H	-0.015217000000	-0.217417000000	-1.011491000000
H	1.825951000000	3.592066000000	0.181335000000
H	2.989641000000	-1.549315000000	-1.761453000000
F	-4.368227000000	-1.163130000000	-0.351344000000

4F8

C	-0.035696000000	-6.397462000000	-1.539528000000
C	-1.399701000000	-6.596527000000	-1.801669000000
C	-1.803712000000	-7.632899000000	-2.639472000000
C	-0.855258000000	-8.475937000000	-3.221371000000
C	0.501904000000	-8.282215000000	-2.960105000000
C	0.913830000000	-7.249516000000	-2.122819000000

C	0.389776000000	-5.311584000000	-0.699768000000
C	0.755828000000	-4.378173000000	-0.021420000000
H	-2.862811000000	-7.780142000000	-2.843260000000
H	-1.173801000000	-9.279375000000	-3.883202000000
H	1.243753000000	-8.934455000000	-3.417302000000
H	1.970666000000	-7.083649000000	-1.923399000000
H	1.079508000000	-3.559780000000	0.586582000000
C	1.949239000000	-3.529126000000	-4.918168000000
C	2.057630000000	-3.699244000000	-6.306664000000
C	1.266884000000	-4.633523000000	-6.967118000000
C	0.372527000000	-5.387351000000	-6.219182000000
C	0.237974000000	-5.246479000000	-4.845863000000
C	1.035055000000	-4.309885000000	-4.195117000000
C	2.770839000000	-2.562810000000	-4.243149000000
C	3.463689000000	-1.747444000000	-3.677088000000
H	1.333728000000	-4.783445000000	-8.042398000000
H	2.768141000000	-3.092761000000	-6.864434000000
H	-0.475201000000	-5.865905000000	-4.305435000000
H	0.952854000000	-4.178272000000	-3.117356000000
H	4.075918000000	-1.027051000000	-3.177294000000
H	-2.131176000000	-5.930434000000	-1.348506000000
F	-0.395195000000	-6.296202000000	-6.855538000000

4F9

C	1.650771000000	-9.167531000000	-5.952939000000
C	2.453319000000	-10.316205000000	-6.011526000000
C	1.870191000000	-11.564865000000	-6.206498000000
C	0.486402000000	-11.679466000000	-6.344602000000
C	-0.315310000000	-10.538790000000	-6.286911000000
C	0.259737000000	-9.286220000000	-6.092068000000
C	2.244610000000	-7.874413000000	-5.751409000000
C	2.731024000000	-6.779749000000	-5.575924000000
H	2.498583000000	-12.453155000000	-6.250959000000
H	0.033019000000	-12.657779000000	-6.497233000000
H	-1.395491000000	-10.625193000000	-6.394361000000
H	-0.357765000000	-8.391019000000	-6.045528000000
H	3.140137000000	-5.801524000000	-5.423298000000
C	1.972884000000	-3.181389000000	-5.177434000000
C	1.551408000000	-3.491853000000	-6.479732000000
C	0.530389000000	-4.411938000000	-6.691090000000
C	-0.056891000000	-5.010981000000	-5.586096000000
C	0.328115000000	-4.725126000000	-4.284325000000
C	1.350002000000	-3.803512000000	-4.084241000000
C	3.033687000000	-2.236076000000	-4.965320000000
C	3.932908000000	-1.445812000000	-4.786987000000
H	0.197962000000	-4.679239000000	-7.691312000000
H	2.035540000000	-3.008710000000	-7.325756000000
H	-0.158039000000	-5.230948000000	-3.453535000000
H	1.678330000000	-3.561688000000	-3.075656000000
H	4.724777000000	-0.744147000000	-4.629311000000
H	3.531719000000	-10.217625000000	-5.902934000000
F	-1.033289000000	-5.918766000000	-5.786113000000

4F10

C	5.245140000000	-8.695543000000	-5.036335000000
C	4.773129000000	-7.375240000000	-5.000389000000
C	3.418359000000	-7.112699000000	-5.182929000000
C	2.524032000000	-8.161360000000	-5.402285000000
C	2.989848000000	-9.476603000000	-5.438625000000
C	4.343053000000	-9.746769000000	-5.257087000000
C	6.643479000000	-8.969986000000	-4.848425000000

C	7.821110000000	-9.201389000000	-4.689910000000
H	3.062299000000	-6.084147000000	-5.153154000000
H	1.463757000000	-7.958359000000	-5.544994000000
H	2.294636000000	-10.297069000000	-5.609407000000
H	4.714348000000	-10.769409000000	-5.284036000000
H	8.861479000000	-9.406161000000	-4.550321000000
C	2.059854000000	-3.476197000000	-5.165763000000
C	1.778783000000	-3.933580000000	-6.462333000000
C	0.868196000000	-4.965590000000	-6.665560000000
C	0.246574000000	-5.524720000000	-5.557729000000
C	0.500641000000	-5.100371000000	-4.260975000000
C	1.412955000000	-4.067517000000	-4.069830000000
C	3.005972000000	-2.414965000000	-4.961625000000
C	3.808624000000	-1.525837000000	-4.789288000000
H	0.640774000000	-5.341835000000	-7.660262000000
H	2.284955000000	-3.476832000000	-7.309901000000
H	-0.006646000000	-5.578763000000	-3.426464000000
H	1.635794000000	-3.714145000000	-3.065494000000
H	4.515146000000	-0.737161000000	-4.637159000000
H	5.476813000000	-6.562880000000	-4.828728000000
F	-0.630244000000	-6.531563000000	-5.748294000000

4F11

C	5.773006000000	-7.420347000000	-5.098845000000
C	6.382209000000	-8.679724000000	-5.196408000000
C	7.751871000000	-8.809703000000	-4.985187000000
C	8.523909000000	-7.689256000000	-4.675971000000
C	7.920708000000	-6.434698000000	-4.578226000000
C	6.551772000000	-6.295810000000	-4.787965000000
C	4.359610000000	-7.276335000000	-5.314491000000
C	3.170035000000	-7.141517000000	-5.493572000000
H	8.219452000000	-9.790175000000	-5.062221000000
H	9.595280000000	-7.794322000000	-4.511305000000
H	8.521696000000	-5.559052000000	-4.337017000000
H	6.068412000000	-5.322830000000	-4.714791000000
H	2.119392000000	-7.006585000000	-5.649234000000
C	2.480300000000	-3.932019000000	-5.074993000000
C	2.039770000000	-4.036520000000	-6.402130000000
C	0.812148000000	-4.621828000000	-6.695002000000
C	0.038939000000	-5.097239000000	-5.643840000000
C	0.445000000000	-5.013055000000	-4.318492000000
C	1.674644000000	-4.425562000000	-4.038796000000
C	3.751478000000	-3.332980000000	-4.779956000000
C	4.817426000000	-2.816303000000	-4.530077000000
H	0.450319000000	-4.714829000000	-7.716490000000
H	2.671433000000	-3.662174000000	-7.204724000000
H	-0.195992000000	-5.404001000000	-3.531510000000
H	2.024056000000	-4.353216000000	-3.011245000000
H	5.755728000000	-2.352566000000	-4.309053000000
H	5.772766000000	-9.548488000000	-5.437866000000
F	-1.151195000000	-5.665120000000	-5.921431000000

4F12

C	1.859121000000	4.904386000000	-0.432747000000
C	3.164799000000	5.417180000000	-0.444867000000
C	4.246884000000	4.571944000000	-0.219563000000
C	4.037378000000	3.213067000000	0.018992000000
C	2.739928000000	2.700422000000	0.031435000000
C	1.651177000000	3.538384000000	-0.193027000000
C	0.746548000000	5.785498000000	-0.665937000000
C	-0.173597000000	6.547906000000	-0.864211000000

H	2.573072000000	1.640684000000	0.217232000000
H	0.638071000000	3.139659000000	-0.183572000000
H	-0.983179000000	7.224882000000	-1.040896000000
C	-3.088485000000	0.974870000000	-0.039126000000
C	-3.480776000000	0.544068000000	1.237002000000
C	-4.046065000000	-0.714201000000	1.416128000000
C	-4.211067000000	-1.529119000000	0.304833000000
C	-3.834965000000	-1.136885000000	-0.972337000000
C	-3.270977000000	0.123544000000	-1.139125000000
C	-2.505407000000	2.275453000000	-0.218919000000
C	-2.016331000000	3.372321000000	-0.373247000000
H	-3.986184000000	-1.813019000000	-1.810919000000
H	-2.967054000000	0.459354000000	-2.128393000000
H	-1.568066000000	4.337819000000	-0.509768000000
H	-3.339415000000	1.205656000000	2.089120000000
H	3.318479000000	6.478272000000	-0.631601000000
H	-4.358024000000	-1.068422000000	2.396162000000
H	5.258260000000	4.975382000000	-0.229988000000
F	-4.757926000000	-2.749220000000	0.472305000000
H	4.886034000000	2.553778000000	0.195247000000

4F13

C	-1.211647000000	-6.653749000000	-1.970809000000
C	-2.197774000000	-6.778856000000	-2.959911000000
C	-2.073921000000	-7.750666000000	-3.948625000000
C	-0.970142000000	-8.604125000000	-3.960837000000
C	0.013535000000	-8.483191000000	-2.978683000000
C	-0.103853000000	-7.513664000000	-1.987421000000
C	-1.333083000000	-5.652862000000	-0.946458000000
C	-1.426194000000	-4.813715000000	-0.078531000000
H	-2.843113000000	-7.842645000000	-4.713881000000
H	-0.876563000000	-9.363345000000	-4.735805000000
H	0.876132000000	-9.147440000000	-2.985376000000
H	0.660967000000	-7.415333000000	-1.219091000000
H	-1.488576000000	-4.078571000000	0.697154000000
C	3.777107000000	-6.338649000000	2.558980000000
C	2.795013000000	-6.485862000000	1.567940000000
C	1.671542000000	-5.666201000000	1.555626000000
C	1.551047000000	-4.703252000000	2.547389000000
C	2.500089000000	-4.526938000000	3.544089000000
C	3.619115000000	-5.353536000000	3.544777000000
C	4.934469000000	-7.189432000000	2.563583000000
C	5.909942000000	-7.905929000000	2.567024000000
H	0.894297000000	-5.757967000000	0.799496000000
H	2.922756000000	-7.251809000000	0.805658000000
H	2.356396000000	-3.756379000000	4.298002000000
H	4.381506000000	-5.240613000000	4.312670000000
H	6.771969000000	-8.539067000000	2.570376000000
H	-3.055593000000	-6.109476000000	-2.943247000000
F	0.463589000000	-3.902293000000	2.543689000000

DFPHA-PHA Hetero-Dimer

DF1

C	2.851168000000	6.860448000000	-0.382912000000
C	4.053975000000	6.365293000000	-0.898600000000
C	4.578726000000	6.768550000000	-2.115065000000
C	3.872896000000	7.708171000000	-2.864064000000
C	2.663443000000	8.226795000000	-2.405509000000
C	2.179981000000	7.791881000000	-1.182920000000
C	2.342033000000	6.445608000000	0.885861000000

C	1.920085000000	6.114610000000	1.969532000000
H	5.515143000000	6.338578000000	-2.460826000000
F	4.715489000000	5.449690000000	-0.176423000000
H	4.260479000000	8.025068000000	-3.829490000000
H	2.087890000000	8.946813000000	-2.981363000000
H	1.548010000000	5.821470000000	2.928364000000
C	1.763149000000	4.932365000000	-3.375932000000
C	0.560299000000	5.449509000000	-2.872178000000
C	0.084780000000	5.029122000000	-1.633592000000
C	0.801517000000	4.091266000000	-0.889748000000
C	1.998567000000	3.574025000000	-1.385506000000
C	2.479946000000	3.990240000000	-2.623332000000
C	2.260686000000	5.367917000000	-4.651508000000
C	2.681561000000	5.734240000000	-5.726467000000
H	-0.842379000000	5.443955000000	-1.242248000000
H	0.012052000000	6.186180000000	-3.456715000000
H	0.435599000000	3.776397000000	0.085551000000
H	2.565564000000	2.851979000000	-0.800645000000
H	3.416175000000	3.597547000000	-3.015926000000
H	3.044598000000	6.046223000000	-6.682810000000
F	1.009265000000	8.271181000000	-0.739060000000

DF2

C	4.494782000000	8.305060000000	-1.062329000000
C	3.312086000000	9.048222000000	-1.134557000000
C	2.172469000000	8.728133000000	-0.414829000000
C	2.203990000000	7.610193000000	0.416450000000
C	3.352524000000	6.827488000000	0.520330000000
C	4.465590000000	7.187856000000	-0.219282000000
C	5.663956000000	8.667898000000	-1.798848000000
C	6.659102000000	8.988448000000	-2.406210000000
H	1.284639000000	9.346168000000	-0.520133000000
F	3.288671000000	10.112690000000	-1.949443000000
H	1.314382000000	7.332115000000	0.977070000000
H	3.390682000000	5.938535000000	1.144536000000
H	7.539777000000	9.272713000000	-2.942252000000
C	2.307657000000	5.672760000000	-2.554352000000
C	2.027170000000	6.796828000000	-3.344093000000
C	3.017970000000	7.344436000000	-4.155049000000
C	4.291621000000	6.777253000000	-4.184369000000
C	4.576302000000	5.658867000000	-3.399238000000
C	3.590978000000	5.105482000000	-2.588242000000
C	1.290684000000	5.110132000000	-1.709361000000
C	0.435521000000	4.637554000000	-0.993614000000
H	2.797274000000	8.223204000000	-4.758424000000
H	1.031944000000	7.236071000000	-3.308693000000
H	5.069094000000	7.217050000000	-4.806034000000
H	5.574369000000	5.224483000000	-3.408846000000
H	3.806491000000	4.238944000000	-1.965677000000
H	-0.324529000000	4.209862000000	-0.374559000000
F	5.570883000000	6.433055000000	-0.141740000000

DF3

C	2.939650000000	6.699566000000	0.084045000000
C	4.152878000000	6.002646000000	0.118418000000
C	5.133474000000	6.144583000000	-0.848230000000
C	4.899309000000	7.024283000000	-1.903727000000
C	3.712281000000	7.751172000000	-1.983467000000
C	2.762948000000	7.578183000000	-0.989836000000
C	1.923171000000	6.489414000000	1.065075000000
C	1.055931000000	6.288841000000	1.883314000000

H	6.045299000000	5.558112000000	-0.773287000000
F	4.354658000000	5.145403000000	1.129287000000
H	5.652462000000	7.141161000000	-2.680432000000
H	3.508895000000	8.440254000000	-2.799001000000
H	0.292698000000	6.124696000000	2.614354000000
C	2.385163000000	4.252394000000	-2.229363000000
C	2.655491000000	3.491017000000	-1.082240000000
C	3.818690000000	2.730913000000	-1.008753000000
C	4.717855000000	2.719515000000	-2.076238000000
C	4.450579000000	3.472224000000	-3.220563000000
C	3.290479000000	4.237582000000	-3.299882000000
C	1.199623000000	5.061432000000	-2.290828000000
C	0.211250000000	5.759844000000	-2.314829000000
H	4.028158000000	2.152544000000	-0.110657000000
H	1.956524000000	3.521983000000	-0.247759000000
H	5.626897000000	2.122847000000	-2.016517000000
H	5.150149000000	3.463774000000	-4.055177000000
H	3.076240000000	4.833927000000	-4.184801000000
H	-0.657135000000	6.383861000000	-2.328099000000
F	1.619359000000	8.271956000000	-1.054460000000

DF4

C	2.585095000000	7.121256000000	0.177145000000
C	3.724016000000	6.447463000000	-0.278148000000
C	4.483290000000	6.889805000000	-1.347201000000
C	4.096896000000	8.061866000000	-1.996188000000
C	2.976463000000	8.777864000000	-1.579284000000
C	2.247030000000	8.293975000000	-0.506620000000
C	1.780998000000	6.606003000000	1.239157000000
C	1.084494000000	6.150883000000	2.116636000000
H	5.344974000000	6.308859000000	-1.665191000000
F	4.070548000000	5.311048000000	0.343187000000
H	4.671313000000	8.416943000000	-2.849356000000
H	2.647943000000	9.682510000000	-2.083399000000
H	0.477514000000	5.762165000000	2.906887000000
C	1.749897000000	6.070861000000	-3.544787000000
C	1.204939000000	5.548048000000	-2.363606000000
C	1.738204000000	4.390795000000	-1.801925000000
C	2.813157000000	3.745604000000	-2.413082000000
C	3.353257000000	4.258005000000	-3.594222000000
C	2.827217000000	5.415171000000	-4.159913000000
C	1.215670000000	7.276073000000	-4.117008000000
C	0.769594000000	8.295567000000	-4.594356000000
H	1.323094000000	4.003322000000	-0.872730000000
H	0.373202000000	6.063071000000	-1.885492000000
H	3.233579000000	2.846412000000	-1.965857000000
H	4.189780000000	3.753767000000	-4.075639000000
H	3.244212000000	5.824483000000	-5.078245000000
H	0.363390000000	9.188125000000	-5.021254000000
F	1.152143000000	8.958332000000	-0.109416000000

DF5

C	2.895225000000	7.309642000000	0.016748000000
C	4.178476000000	6.786463000000	0.208463000000
C	5.333386000000	7.462331000000	-0.150310000000
C	5.212236000000	8.721996000000	-0.734783000000
C	3.958253000000	9.287989000000	-0.958984000000
C	2.833349000000	8.572184000000	-0.582823000000
C	1.720375000000	6.597011000000	0.405522000000
C	0.725370000000	5.995361000000	0.735450000000
H	6.299684000000	6.997803000000	0.029100000000

F	4.285205000000	5.569429000000	0.758637000000
H	6.107882000000	9.269289000000	-1.022054000000
H	3.838025000000	10.265651000000	-1.418793000000
H	-0.156313000000	5.452064000000	1.001792000000
C	1.532754000000	5.163157000000	-2.580603000000
C	1.439068000000	6.435107000000	-3.163381000000
C	2.594916000000	7.121148000000	-3.525666000000
C	3.849120000000	6.549486000000	-3.308716000000
C	3.945277000000	5.288767000000	-2.718420000000
C	2.794741000000	4.595690000000	-2.352870000000
C	0.342454000000	4.446155000000	-2.216175000000
C	-0.660705000000	3.836913000000	-1.918501000000
H	2.515607000000	8.110689000000	-3.973414000000
H	0.457507000000	6.876914000000	-3.321973000000
H	4.751427000000	7.091910000000	-3.586838000000
H	4.922522000000	4.844708000000	-2.534526000000
H	2.860957000000	3.615861000000	-1.884462000000
H	-1.547007000000	3.294794000000	-1.664943000000
F	1.623638000000	9.1024444000000	-0.807856000000

DF6

C	1.760576000000	6.803522000000	0.302540000000
C	0.428668000000	7.222563000000	0.384742000000
C	-0.573207000000	6.449625000000	0.948139000000
C	-0.241536000000	5.191715000000	1.447311000000
C	1.068572000000	4.719048000000	1.383311000000
C	2.036189000000	5.531767000000	0.818012000000
C	2.777601000000	7.622910000000	-0.275364000000
C	3.638530000000	8.313848000000	-0.767432000000
H	-1.588255000000	6.837225000000	0.981863000000
F	0.118292000000	8.429184000000	-0.107936000000
H	-1.015183000000	4.568813000000	1.892062000000
H	1.349818000000	3.741101000000	1.765308000000
H	4.397784000000	8.923706000000	-1.208866000000
C	1.961133000000	5.547614000000	-2.859588000000
C	2.043407000000	6.656654000000	-3.713315000000
C	3.287009000000	7.123700000000	-4.127596000000
C	4.454046000000	6.493329000000	-3.693884000000
C	4.375710000000	5.393711000000	-2.838645000000
C	3.136221100000	4.919172000000	-2.422448000000
C	0.680776000000	5.059077000000	-2.427277000000
C	-0.395834000000	4.647862000000	-2.056231000000
H	3.345433000000	7.984727000000	-4.791742000000
H	1.128136000000	7.145116000000	-4.041540000000
H	5.425818000000	6.861083000000	-4.020581000000
H	5.284442000000	4.905476000000	-2.490872000000
H	3.065904000000	4.065625000000	-1.751205000000
H	-1.347923000000	4.283878000000	-1.733747000000
F	3.302292000000	5.091181000000	0.761431000000

DF7

C	-2.781952000000	1.006653000000	0.035379000000
C	-2.481469000000	0.107879000000	1.070038000000
C	-1.950621000000	-1.144567000000	0.771843000000
C	-1.715270000000	-1.509797000000	-0.554933000000
C	-2.013999000000	-0.618226000000	-1.586394000000
C	-2.546385000000	0.634732000000	-1.296626000000
C	-3.305131000000	2.310429000000	0.338063000000
C	-3.714353000000	3.420985000000	0.592171000000
H	-1.718595000000	-1.837856000000	1.578405000000
H	-2.664106000000	0.403302000000	2.101176000000

H	-1.297458000000	-2.488644000000	-0.784545000000
H	-1.827245000000	-0.898525000000	-2.621451000000
H	-2.773574000000	1.339581000000	-2.093960000000
H	-4.088442000000	4.398193000000	0.815043000000
C	2.423770000000	3.374923000000	-1.446108000000
C	1.117120000000	3.686093000000	-1.049782000000
C	0.245367000000	2.752179000000	-0.515382000000
C	0.691794000000	1.439764000000	-0.362477000000
C	1.983287000000	1.073932000000	-0.739272000000
C	2.817308000000	2.043403000000	-1.271105000000
C	3.302869000000	4.358031000000	-1.996133000000
C	4.047020000000	5.189095000000	-2.461812000000
H	0.022075000000	0.690012000000	0.054699000000
H	2.350716000000	0.056774000000	-0.629395000000
H	4.705154000000	5.925063000000	-2.873230000000
F	0.702898000000	4.952095000000	-1.201792000000
H	-0.758341000000	3.058736000000	-0.227870000000
F	4.060819000000	1.702167000000	-1.639096000000

DF8

C	1.402696000000	4.841716000000	-0.128608000000
C	2.725068000000	4.841799000000	-0.597161000000
C	3.566837000000	3.773730000000	-0.303319000000
C	3.097216000000	2.699252000000	0.453822000000
C	1.781955000000	2.695060000000	0.918976000000
C	0.934413000000	3.761623000000	0.633824000000
C	0.530818000000	5.942555000000	-0.436734000000
C	-0.207166000000	6.864238000000	-0.707769000000
H	1.408216000000	1.856234000000	1.503061000000
H	-0.094978000000	3.757670000000	0.985079000000
H	-0.852632000000	7.687685000000	-0.930819000000
C	-2.578045000000	1.171851000000	-0.537446000000
C	-2.114434000000	0.630909000000	0.666921000000
C	-2.526580000000	-0.597265000000	1.155639000000
C	-3.448307000000	-1.331855000000	0.410616000000
C	-3.944472000000	-0.842608000000	-0.796613000000
C	-3.501906000000	0.392267000000	-1.242699000000
C	-2.131410000000	2.443159000000	-1.010613000000
C	-1.739192000000	3.521572000000	-1.391328000000
H	-4.663851000000	-1.397547000000	-1.393534000000
H	-1.375115000000	4.480956000000	-1.702869000000
H	3.080888000000	5.683340000000	-1.188638000000
H	-2.127416000000	-0.957866000000	2.100126000000
H	4.592716000000	3.778368000000	-0.668427000000
H	3.757990000000	1.863448000000	0.679506000000
H	-3.785219000000	-2.299677000000	0.776690000000
F	-1.228036000000	1.348136000000	1.376587000000
F	-3.973815000000	0.871658000000	-2.400721000000

DF9

C	-4.494208000000	3.702118000000	-4.067748000000
C	-4.939688000000	2.433430000000	-3.678670000000
C	-6.212024000000	1.960099000000	-3.952734000000
C	-7.092087000000	2.786832000000	-4.649856000000
C	-6.702432000000	4.060033000000	-5.062284000000
C	-5.419002000000	4.488468000000	-4.764268000000
C	-3.174642000000	4.158486000000	-3.766949000000
C	-2.053045000000	4.517725000000	-3.494741000000
H	-6.494076000000	0.964029000000	-3.621166000000
F	-4.084376000000	1.646489000000	-3.008203000000
H	-8.096434000000	2.433474000000	-4.874919000000

H	-7.371537000000	4.721571000000	-5.606718000000
H	-1.054764000000	4.820236000000	-3.246370000000
C	1.299352000000	4.239495000000	-1.951206000000
C	0.386301000000	4.054463000000	-0.901294000000
C	-0.478912000000	2.964078000000	-0.914087000000
C	-0.442415000000	2.049882000000	-1.967402000000
C	0.467117000000	2.226866000000	-3.010416000000
C	1.335908000000	3.314776000000	-3.006585000000
C	2.189338000000	5.368048000000	-1.946819000000
C	2.932501000000	6.323439000000	-1.948437000000
H	-1.194187000000	2.833830000000	-0.103930000000
H	0.361505000000	4.774611000000	-0.085828000000
H	-1.135894000000	1.211219000000	-1.984620000000
H	0.492713000000	1.519687000000	-3.837639000000
H	2.045780000000	3.462475000000	-3.818058000000
H	3.592320000000	7.165300000000	-1.947360000000
F	-5.035453000000	5.710533000000	-5.156364000000

DF10

C	1.975105000000	9.073505000000	-3.346951000000
C	3.308662000000	9.092932000000	-2.921078000000
C	4.113708000000	10.217088000000	-3.009767000000
C	3.572344000000	11.383559000000	-3.547671000000
C	2.250199000000	11.421135000000	-3.987762000000
C	1.484398000000	10.271880000000	-3.878556000000
C	1.163606000000	7.902036000000	-3.245056000000
C	0.477754000000	6.910376000000	-3.157567000000
H	5.141737000000	10.164322000000	-2.660387000000
F	3.820335000000	7.967919000000	-2.405855000000
H	4.189662000000	12.276427000000	-3.625155000000
H	1.806212000000	12.318764000000	-4.410727000000
H	-0.126721000000	6.028423000000	-3.078047000000
C	1.546460000000	4.013010000000	-1.807682000000
C	0.495264000000	4.268588000000	-0.914770000000
C	-0.822736000000	4.052106000000	-1.307798000000
C	-1.104660000000	3.579226000000	-2.591156000000
C	-0.060414000000	3.319184000000	-3.481223000000
C	1.259780000000	3.533561000000	-3.094380000000
C	2.905771000000	4.257354000000	-1.413343000000
C	4.051171000000	4.473865000000	-1.088973000000
H	-1.634067000000	4.257671000000	-0.611634000000
H	0.723131000000	4.647400000000	0.079387000000
H	-2.136198000000	3.413932000000	-2.897222000000
H	-0.276158000000	2.952044000000	-4.483129000000
H	2.078712000000	3.344160000000	-3.785204000000
H	5.062268000000	4.672203000000	-0.802354000000
F	0.212236000000	10.298386000000	-4.298977000000

DF11

C	-2.612774000000	0.674421000000	-0.005372000000
C	-2.473999000000	-0.717921000000	-0.009433000000
C	-3.551840000000	-1.586645000000	-0.011783000000
C	-4.837716000000	-1.046970000000	-0.009978000000
C	-5.035454000000	0.332790000000	-0.006009000000
C	-3.924674000000	1.160886000000	-0.003839000000
C	-1.475171000000	1.538048000000	-0.003152000000
C	-0.493695000000	2.243972000000	-0.000540000000
H	-3.374644000000	-2.658925000000	-0.015005000000
F	-1.229682000000	-1.222452000000	-0.011218000000
H	-5.698812000000	-1.712274000000	-0.011668000000
H	-6.028706000000	0.774585000000	-0.004596000000

H	0.399947000000	2.836189000000	0.001466000000
C	3.211720000000	0.471523000000	-0.005502000000
C	4.471493000000	-0.146211000000	-0.003691000000
C	4.566272000000	-1.534353000000	-0.002347000000
C	3.409858000000	-2.315762000000	-0.002788000000
C	2.156044000000	-1.704032000000	-0.004589000000
C	2.051221000000	-0.315804000000	-0.005919000000
C	3.127844000000	1.907701000000	-0.007087000000
C	3.093620000000	3.118694000000	-0.008673000000
H	5.546695000000	-2.008353000000	-0.000970000000
H	5.367623000000	0.471420000000	-0.003398000000
H	3.487557000000	-3.402027000000	-0.001740000000
H	1.250888000000	-2.308301000000	-0.004964000000
H	1.072059000000	0.159096000000	-0.007306000000
H	3.073269000000	4.188391000000	-0.009955000000
F	-4.102690000000	2.488010000000	-0.000122000000

DF12

C	2.226447000000	-1.838681000000	5.675500000000
C	2.731672000000	-0.572683000000	5.360046000000
C	3.085126000000	0.361695000000	6.318453000000
C	2.929946000000	0.024002000000	7.662202000000
C	2.431384000000	-1.223266000000	8.034995000000
C	2.091625000000	-2.124187000000	7.039196000000
C	1.868892000000	-2.785696000000	4.667149000000
C	1.563823000000	-3.592907000000	3.820592000000
H	3.471859000000	1.327759000000	6.004962000000
F	2.876328000000	-0.261154000000	4.063007000000
H	3.201996000000	0.744302000000	8.431146000000
H	2.302532000000	-1.507133000000	9.076403000000
H	1.292936000000	-4.309557000000	3.073684000000
C	3.182032000000	0.395161000000	-0.591494000000
C	3.007709000000	-0.013352000000	0.738940000000
C	2.505083000000	-1.280506000000	1.020084000000
C	2.173460000000	-2.147311000000	-0.021524000000
C	2.344850000000	-1.746281000000	-1.347151000000
C	2.846989000000	-0.480547000000	-1.634893000000
C	3.700886000000	1.703137000000	-0.885389000000
C	4.137729000000	2.804450000000	-1.134222000000
H	2.372871000000	-1.589737000000	2.054960000000
H	3.268424000000	0.668048000000	1.546205000000
H	1.780066000000	-3.139051000000	0.198339000000
H	2.086615000000	-2.421581000000	-2.161497000000
H	2.984379000000	-0.158052000000	-2.665220000000
H	4.523724000000	3.777386000000	-1.353547000000
F	1.611553000000	-3.325445000000	7.384284000000
