Supplementary Information

Balance of attraction and repulsion in nucleic-acid base stacking: reference quantum-chemical calculations on uracil dimer and a comparison with the force-field description

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When constructing the non-planar structures (NP1-NP4), the first uracil monomer was placed on the xy plane with its center of mass coinciding with the origin, but the orientation of the N1-H1 "glycosidic" bond was slightly different than for the P1-P9 geometries. The initial position of both monomers (before all the other parameters were applied) was rotated by 8° clockwise (opposite direction to that of the positive ω angle) with respect to the geometry having N1-H1 parallel to the y axis (described in the text and shown in Figure 1). This is a subtle technical detail about the way how the geometries were obtained and slightly affects the results or the direction of the α and γ rotations and of the Δx and Δy shifts. This information is relevant only for those readers interested in building the same structures via their own code.

Table S1: Structural parameters of parallel (P) and non-parallel (NP) dimers.

Dimer	Struct. N°	ω [°]	Δx [Å]	Δy [Å]	Δz [Å]	α [°]	γ [°]
P1	1-12	0.0	0.0	0.0	2.9-4.0	0.0	0.0
P2	13-24	180.0	0.0	0.0	2.9-4.0	0.0	0.0
P3	25-29	30.0-150.0	0.0	0.0	3.3	0.0	0.0
P4	30-35	0.0	1.5	0.0	2.9-3.9	0.0	0.0
P5	36-41	0.0	0.0	1.5	2.9-3.9	0.0	0.0
P6	42-47	180.0	1.5	0.0	2.9-3.9	0.0	0.0
P7	48-53	180.0	-1.5	0.0	2.9-3.9	0.0	0.0
P8	54-59	180.0	0.0	1.5	2.9-3.9	0.0	0.0
P9	60-65	180.0	0.0	-1.5	2.9-3.9	0.0	0.0
NP1	66-75	180.0	0.0	1.5	3.0-3.9	0.0	-25.0
NP2	76-85	180.0	0.0	-1.5	3.4-4.3	0.0	-25.0
NP3	86-95	180.0	-1.4	-0.3	3.4-4.3	0.0	-25.0
NP4	96-105	180.0	-1.0	0.3	3.3-4.2	30.0	10.0

Table S2: Interaction energies (kcal mol^{-1}) for the parallel dimers, calculated with the AMBER, DFT-D, SCS(MI)-MP2, DFT-SAPT, and CBS(T) methods.

Dimer	n	*r* [Å]*	AMBER	DFT-D	SCS(MI)-MP2	DFT-SAPT	CBS(T)
P1	1	2.9	13.03	14.59	15.54	15.17	13.09
	2	3.0	6.68	9.20	10.44	10.28	8.35
	3	3.1	2.83	5.52	6.89	6.87	5.12
	4	3.2	0.54	3.08	4.44	4.53	2.93
	5	3.3	-0.78	1.50	2.79	2.93	1.50
	6	3.4	-1.48	0.52	1.70	1.88	0.59
	7	3.5	-1.81	-0.05	0.99	1.19	0.05
	8	3.6	-1.90	-0.37	0.56	0.77	-0.24
	9	3.7	-1.86	-0.54	0.31	0.53	-0.38
	10	3.8	-1.74	-0.61	0.19	0.40	-0.41
	11	3.9	-1.57	-0.63	0.15	0.35	-0.36
	12	4.0	-1.39	-0.59	0.16	0.35	-0.30
P2	13	2.9	1.49	-2.04	-1.94	-0.63	-3.03
	14	3.0	-2.89	-4.46	-3.99	-2.90	-4.94
	15	3.1	-5.35	-5.94	-5.20	-4.29	-6.02
	16	3.2	-6.61	-6.68	-5.81	-5.07	-6.51
	17	3.3	-7.13	-6.90	-6.03	-5.42	-6.62
	18	3.4	-7.20	-6.82	-5.99	-5.50	-6.49
	19	3.5	-7.01	-6.56	-5.78	-5.39	-6.20
	20	3.6	-6.67	-6.19	-5.48	-5.16	-5.83
	21	3.7	-6.26	-5.78	-5.13	-4.87	-5.41
	22	3.8	-5.81	-5.39	-4.76	-4.54	-4.98
	23	3.9	-5.36	-5.01	-4.38	-4.21	-4.56
	24	4.0	-4.93	-4.65	-4.02	-3.88	-4.16
P3	25	30.0	-3.22	-2.25	-1.24	-0.66	-2.17
	26	60.0	-6.31	-6.02	-5.10	-4.39	-5.79
	27	90.0	-6.85	-6.54	-5.72	-5.06	-6.37
	28	120.0	-6.09	-6.00	-5.26	-4.52	-5.94
	29	150.0	-6.42	-6.07	-5.24	-4.64	-5.93
P4	30	2.9	3.88	2.07	2.14	3.65	0.85
	31	3.1	-1.17	-1.30	-0.57	0.51	-1.58
	32	3.3	-2.65	-2.22	-1.44	-0.67	-2.22
	33	3.5	-2.76	-2.15	-1.48	-0.93	-2.09
	34	3.7	-2.39	-1.78	-1.19	-0.79	-1.66
	35	3.9	-1.91	-1.39	-0.81	-0.52	-1.17

Table S2 (Cont.): Interaction energies (kcal mol^{-1}) for the parallel dimers, calculated with the AMBER, DFT-D, SCS(MI)-MP2, DFT-SAPT, and CBS(T) methods.

Dimer	n	*r* [Å]*	AMBER	DFT-D	SCS(MI)-MP2	DFT-SAPT	CBS(T)
P5	36	2.9	3.79	1.64	1.92	3.37	0.62
	37	3.1	-1.43	-1.55	-0.72	0.30	-1.77
	38	3.3	-2.92	-2.34	-1.55	-0.84	-2.37
	39	3.5	-2.99	-2.26	-1.55	-1.06	-2.20
	40	3.7	-2.58	-1.88	-1.24	-0.89	-1.74
	41	3.9	-2.05	-1.50	-0.85	-0.59	-1.24
P6	42	2.9	-0.58	-4.17	-4.37	-2.75	-4.87
	43	3.1	-5.93	-7.51	-7.01	-5.79	-7.34
	44	3.3	-7.21	-8.06	-7.50	-6.59	-7.69
	45	3.5	-6.96	-7.45	-7.02	-6.35	-7.11
	46	3.7	-6.19	-6.52	-6.19	-5.70	-6.20
	47	3.9	-5.34	-5.60	-5.30	-4.94	-5.26
P7	48	2.9	0.25	-1.19	-1.53	-0.24	-2.90
	49	3.1	-4.21	-3.58	-3.33	-2.54	-4.41
	50	3.3	-5.25	-4.17	-3.66	-3.20	-4.50
	51	3.5	-5.04	-4.02	-3.38	-3.14	-4.03
	52	3.7	-4.44	-3.56	-2.91	-2.79	-3.41
	53	3.9	-3.77	-3.13	-2.43	-2.38	-2.81
P8	54	2.9	-1.20	-3.20	-3.50	-2.40	-4.42
	55	3.1	-5.77	-6.12	-5.69	-4.90	-6.34
	56	3.3	-6.74	-6.64	-6.03	-5.50	-6.48
	57	3.5	-6.40	-6.15	-5.58	-5.24	-5.90
	58	3.7	-5.63	-5.45	-4.86	-4.65	-5.08
	59	3.9	-4.81	-4.73	-4.12	-3.99	-4.27
P9	60	2.9	1.51	0.46	1.06	1.48	-0.27
	61	3.1	-4.23	-3.96	-2.96	-2.54	-3.92
	62	3.3	-5.82	-5.28	-4.36	-4.02	-5.06
	63	3.5	-5.81	-5.23	-4.54	-4.28	-5.04
	64	3.7	-5.24	-4.82	-4.19	-4.02	-4.55
	65	3.9	-4.54	-4.25	-3.67	-3.56	-3.93

(*) For P3 the values correspond to the twist angle ω.

Table S3: Interaction energies (kcal mol^{-1}) for the non-parallel dimers, calculated with the AMBER, DFT-D, SCS(MI)-MP2, DFT-SAPT, and CBS(T) methods.

Dimer	n	*r* [Å]	AMBER	DFT-D	SCS(MI)-MP2	DFT-SAPT	CBS(T)
NP1	66	3.0	9.01	1.44	1.62	2.05	0.61
	67	3.1	2.04	-1.28	-1.11	-0.70	-1.95
	68	3.2	-1.94	-3.06	-2.87	-2.50	-3.58
	69	3.3	-4.14	-4.22	-3.94	-3.62	-4.54
	70	3.4	-5.26	-4.94	-4.53	-4.25	-5.03
	71	3.5	-5.74	-5.30	-4.79	-4.56	-5.21
	72	3.6	-5.83	-5.40	-4.82	-4.64	-5.17
	73	3.7	-5.70	-5.31	-4.70	-4.57	-4.99
	74	3.8	-5.45	-5.09	-4.50	-4.40	-4.75
	75	3.9	-5.13	-4.82	-4.25	-4.18	-4.46
NP2	76	3.4	3.85	1.62	2.08	2.38	0.77
	77	3.5	-0.15	-0.87	-0.32	-0.07	-1.47
	78	3.6	-2.45	-2.52	-1.88	-1.66	-2.87
	79	3.7	-3.71	-3.56	-2.84	-2.66	-3.71
	80	3.8	-4.33	-4.16	-3.38	-3.24	-4.13
	81	3.9	-4.57	-4.42	-3.64	-3.53	-4.29
	82	4.0	-4.57	-4.43	-3.70	-3.63	-4.28
	83	4.1	-4.43	-4.31	-3.64	-3.60	-4.14
	84	4.2	-4.22	-4.11	-3.51	-3.48	-3.94
	85	4.3	-3.97	-3.90	-3.33	-3.32	-3.70
NP3	86	3.4	0.96	-1.24	-1.19	-0.37	-2.38
	87	3.5	-1.74	-2.38	-2.17	-1.54	-3.24
	88	3.6	-3.20	-3.07	-2.74	-2.27	-3.69
	89	3.7	-3.93	-3.42	-3.01	-2.67	-3.87
	90	3.8	-4.21	-3.56	-3.09	-2.85	-3.86
	91	3.9	-4.23	-3.56	-3.05	-2.89	-3.73
	92	4.0	-4.10	-3.47	-2.92	-2.83	-3.54
	93	4.1	-3.89	-3.33	-2.76	-2.71	-3.30
	94	4.2	-3.64	-3.15	-2.57	-2.56	-3.07
	95	4.3	-3.38	-2.95	-2.38	-2.39	-2.82
NP4	96	3.3	3.81	2.79	2.47	3.37	0.91
	97	3.4	0.11	0.47	0.59	1.31	-0.79
	98	3.5	-2.00	-1.10	-0.60	-0.04	-1.82
	99	3.6	-3.14	-2.08	-1.31	-0.89	-2.39

Table S3 (Cont.): Interaction energies (kcal mol^{-1}) for the non-parallel dimers, calculated with the AMBER, DFT-D, SCS(MI)-MP2, DFT-SAPT, and CBS(T) methods.

Dimer	n	*r* [Å]	AMBER	DFT-D	SCS(MI)-MP2	DFT-SAPT	CBS(T)
NP4	100	3.7	-3.67	-2.56	-1.70	-1.39	-2.65
	101	3.8	-3.84	-2.70	-1.87	-1.65	-2.71
	102	3.9	-3.79	-2.69	-1.90	-1.75	-2.64
	103	4.0	-3.62	-2.62	-1.85	-1.75	-2.49
	104	4.1	-3.39	-2.52	-1.74	-1.68	-2.31
	105	4.2	-3.13	-2.36	-1.61	-1.58	-2.10

Table S4: Interaction energies (kcal mol^{-1}) for the H-bonded dimers, calculated with the AMBER, DFT-D, SCS(MI)-MP2, DFT-SAPT, and CBS(T) methods.

Dimer	n	*r* [Å]	AMBER	DFT-D	SCS(MI)-MP2	DFT-SAPT	CBS(T)
HB1	106	2.43	27.81	-1.90	-2.07	1.02	-0.92
	107	2.53	4.15	-8.25	-8.23	-4.94	-7.46
	108	2.63	-5.70	-11.64	-11.60	-8.51	-11.13
	109	2.73	-9.56	-13.16	-13.15	-10.44	-12.92
	110	2.83	-10.73	-13.54	-13.55	-11.28	-13.50
	111	2.93	-10.67	-13.25	-13.23	-11.42	-13.31
	112	3.03	-10.05	-12.57	-12.51	-11.12	-12.67
HB2	113	2.48	48.27	-2.66	-2.78	-0.63	-1.94
	114	2.58	18.24	-6.55	-6.67	-4.59	-6.08
	115	2.68	4.17	-8.69	-8.81	-6.97	-8.43
	116	2.78	-2.41	-9.68	-9.79	-8.26	-9.58
	117	2.88	-5.36	-9.94	-10.04	-8.82	-9.95
	118	2.98	-6.49	-9.77	-9.82	-8.91	-9.82
	119	3.08	-6.73	-9.31	-9.34	-8.68	-9.39

Figure S1: Interaction-Energy Gradient of P1

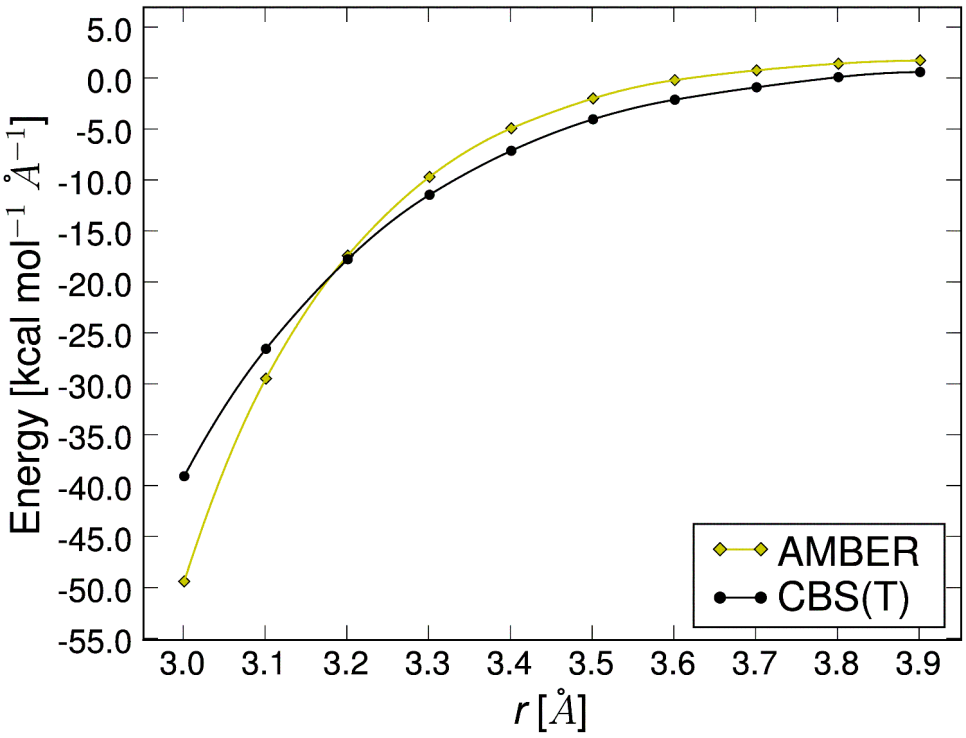

Figure S2: Interaction-Energy Gradient of P2

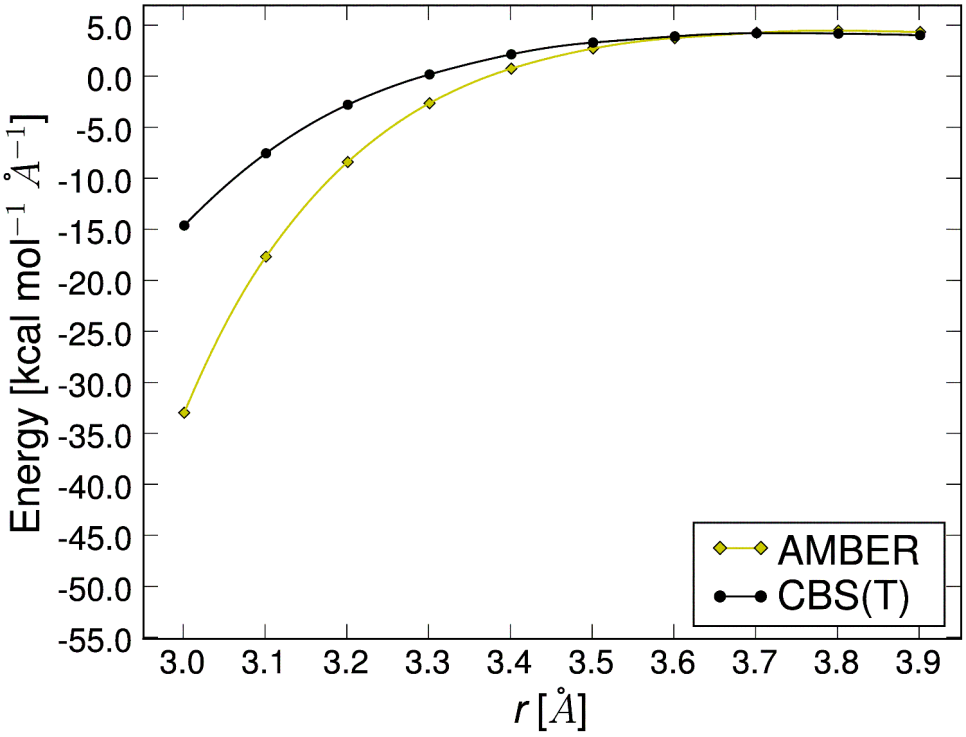

Figure S3: Interaction-Energy Gradient of P4

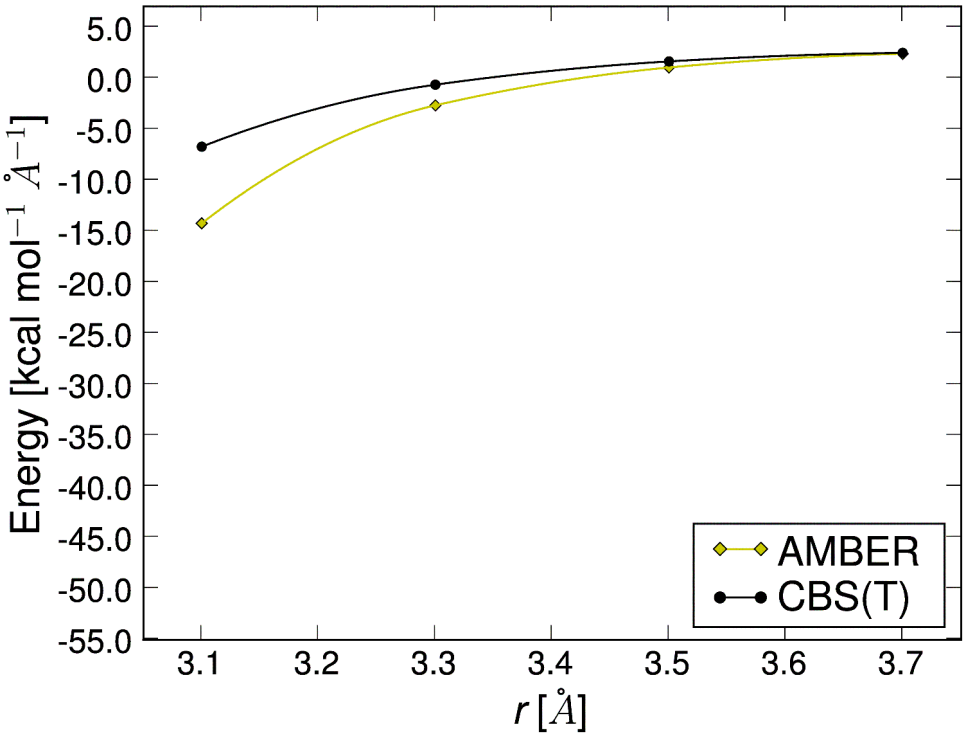

Figure S4: Interaction-Energy Gradient of P5

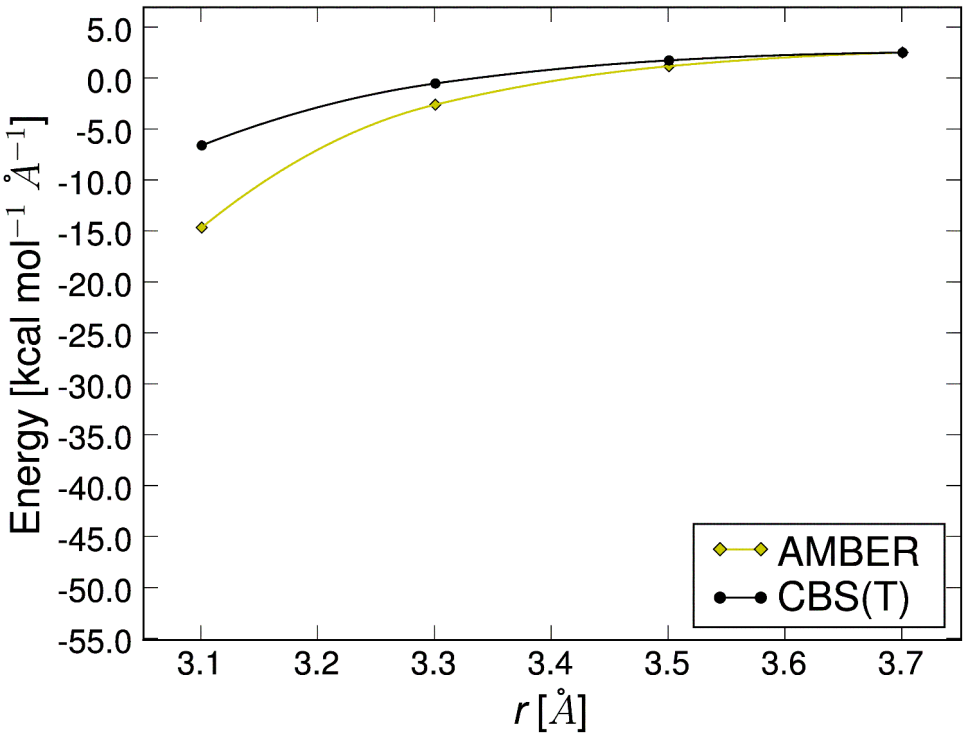

Figure S5: Interaction-Energy Gradient of P6

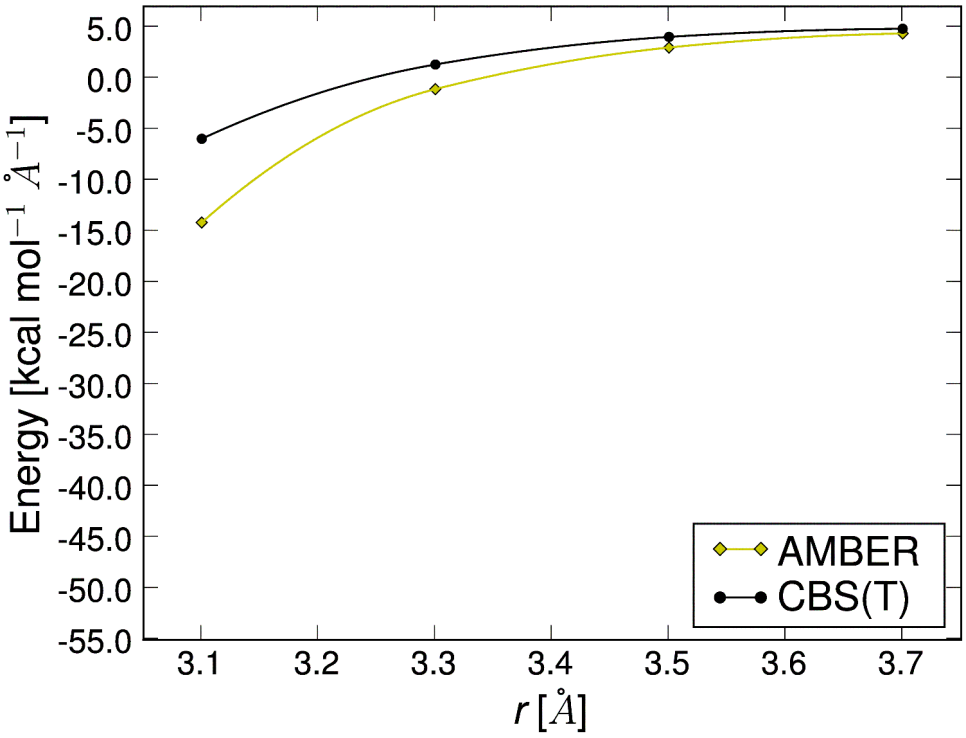

Figure S6: Interaction-Energy Gradient of P7

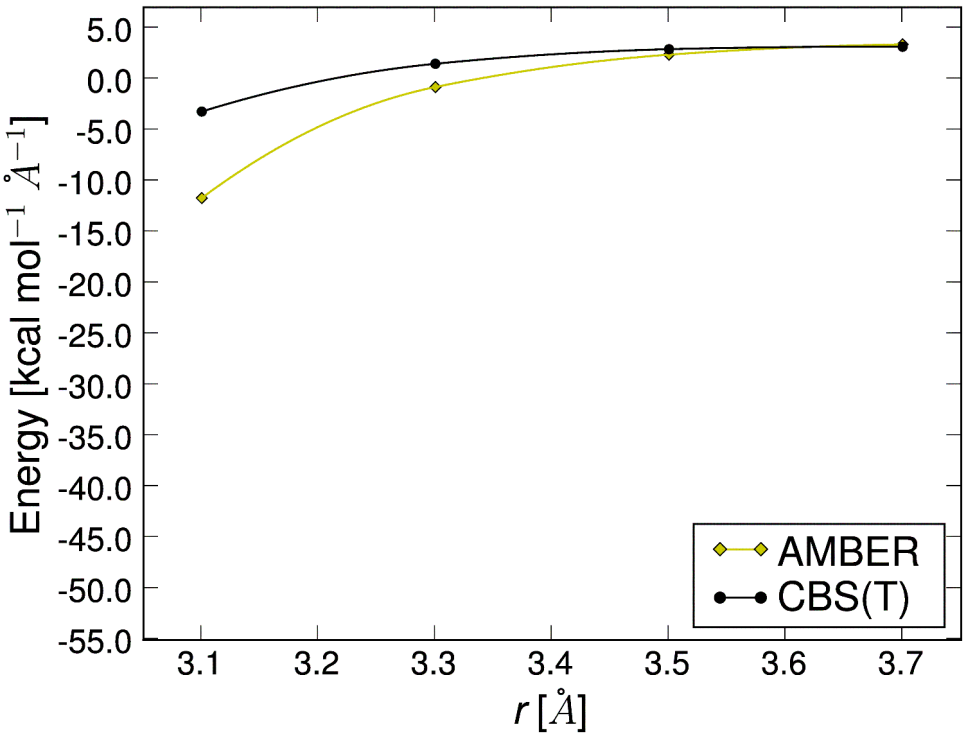

Figure S7: Interaction-Energy Gradient of P8

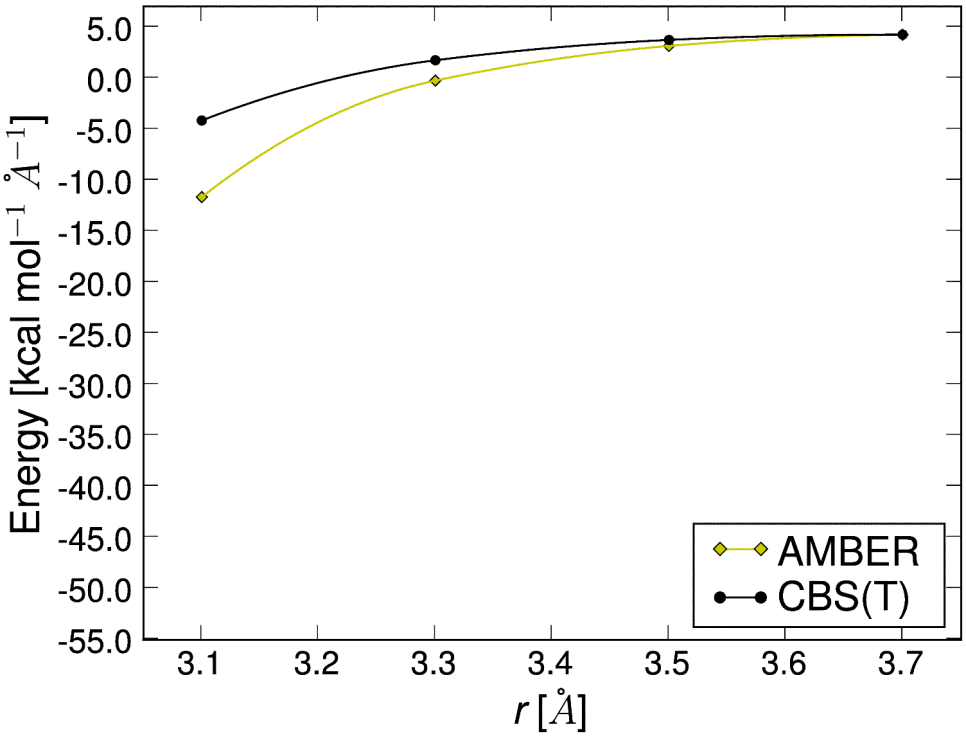

Figure S8: Interaction-Energy Gradient of P9

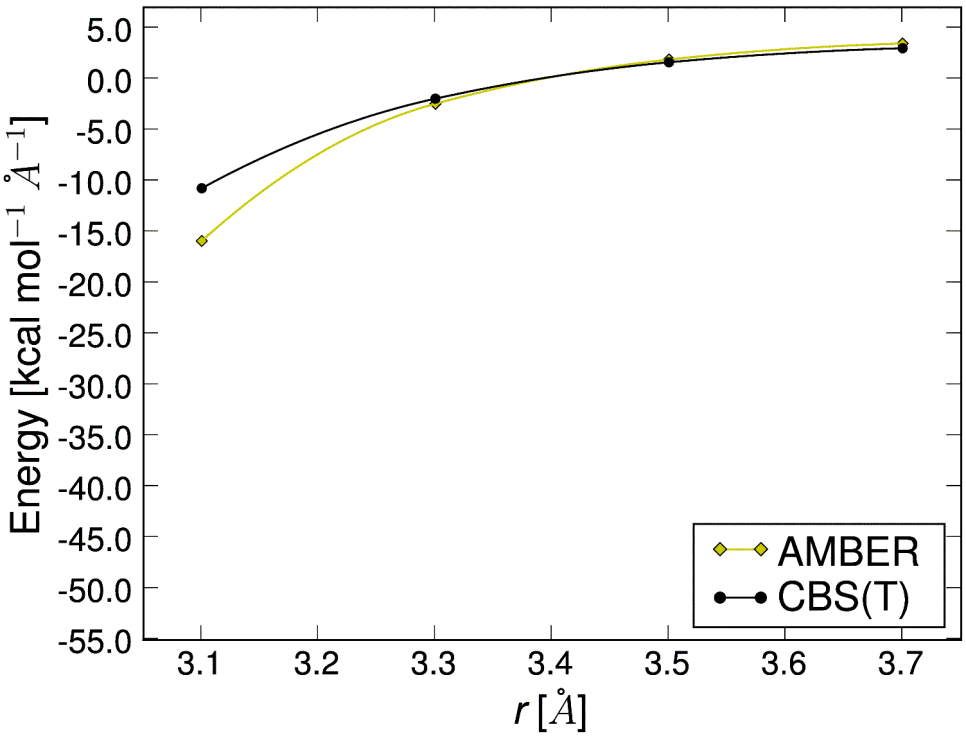

Figure S9: Interaction-Energy Gradient of NP1

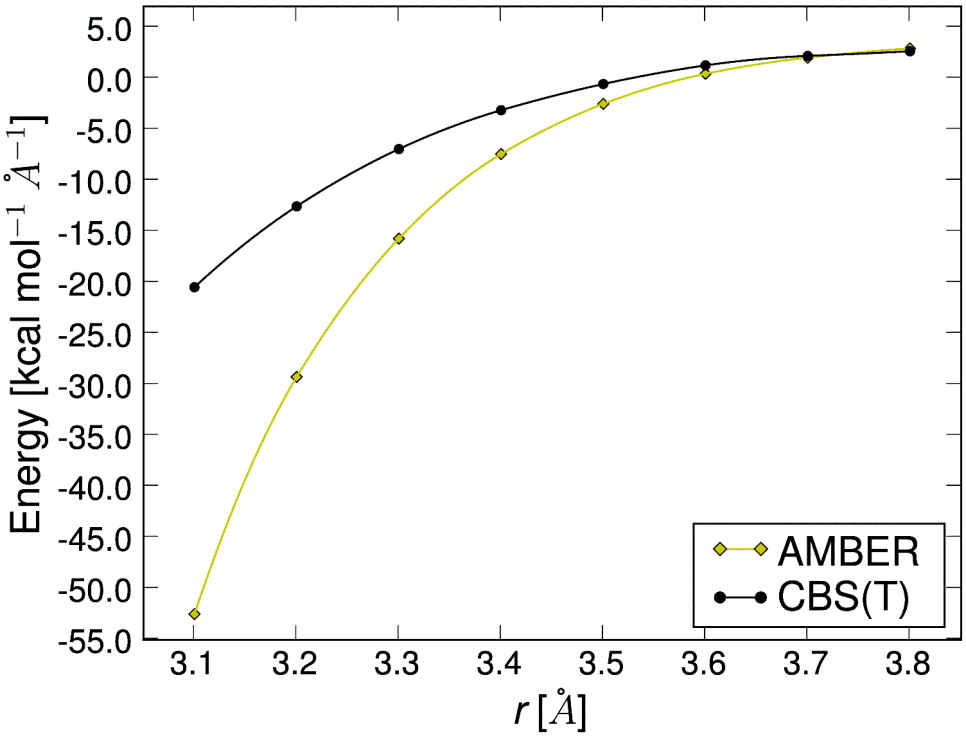

Figure S10: Interaction-Energy Gradient of NP2

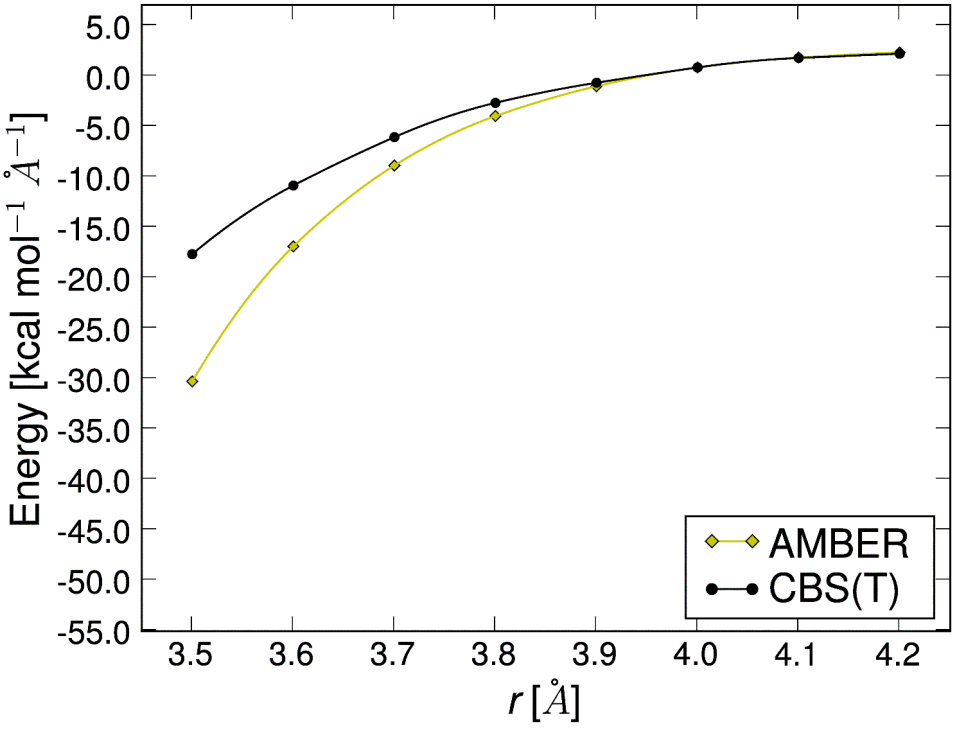

Figure S11: Interaction-Energy Gradient of NP4

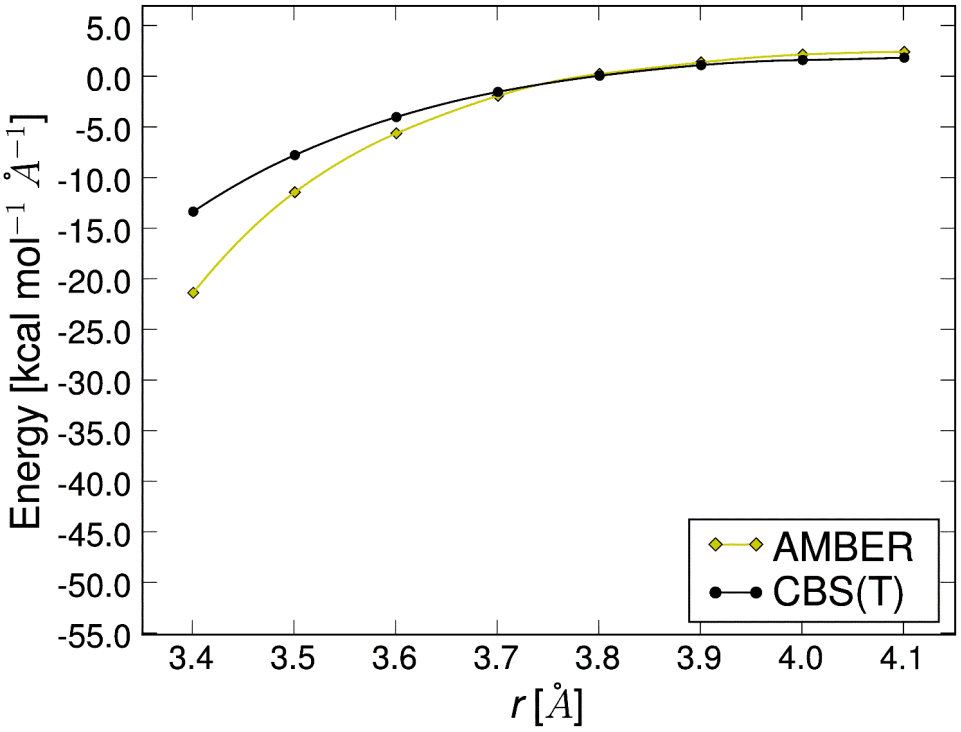

Figure S12: Interaction-Energy Gradient of HB1

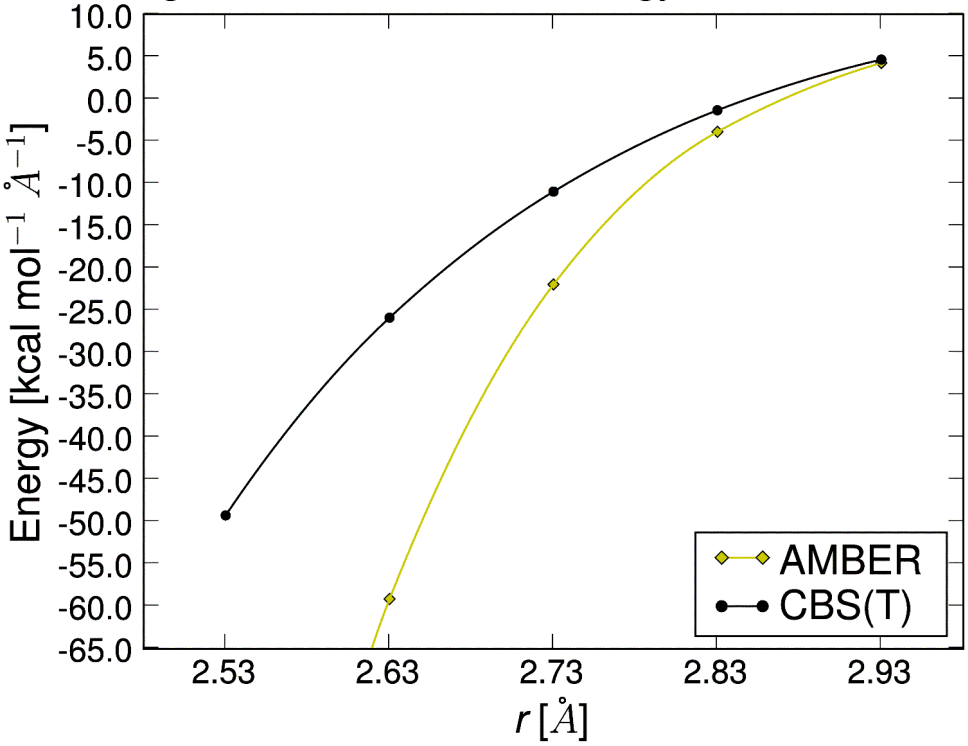

Figure S13: Interaction-Energy Gradient of HB2

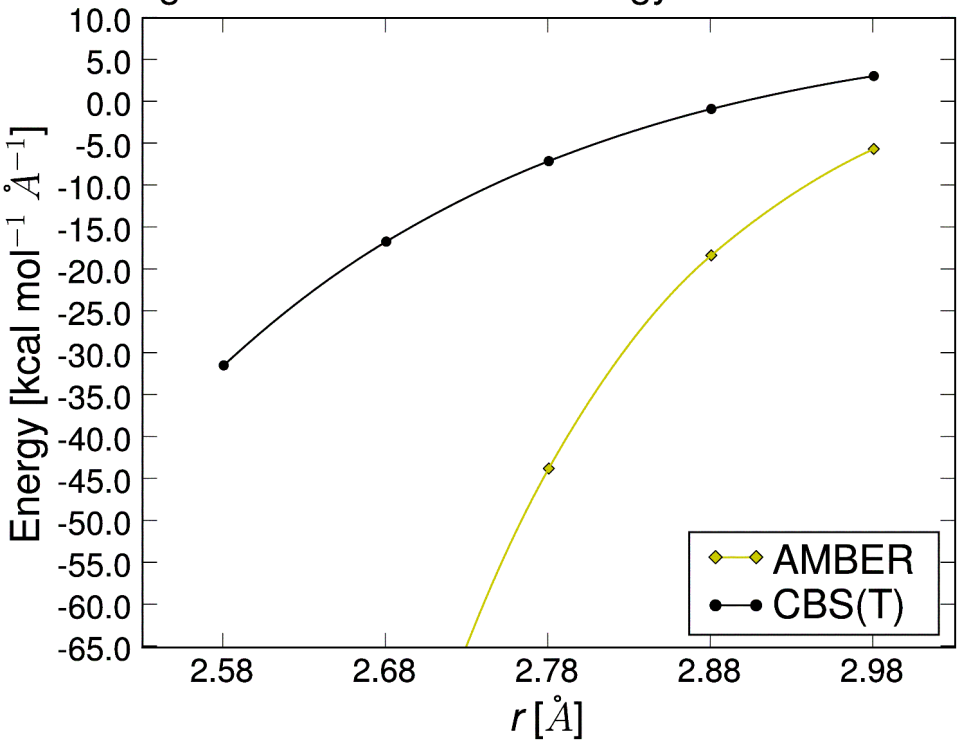

Figure S14: DFT-SAPT Energy Terms of P4

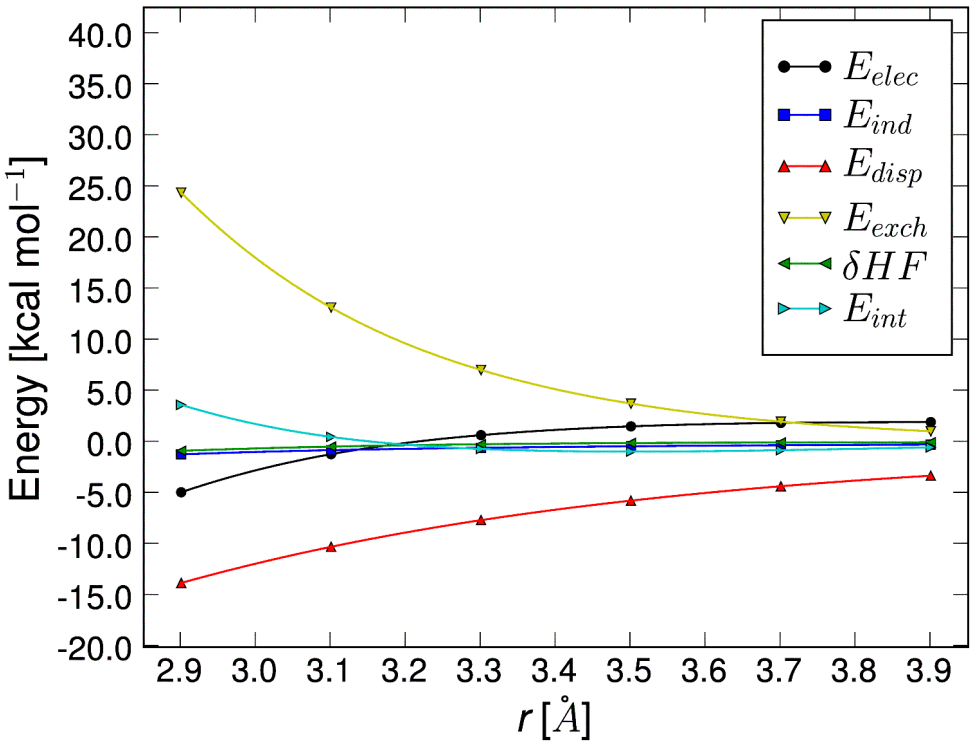

Figure S15: DFT-SAPT Energy Terms of P5

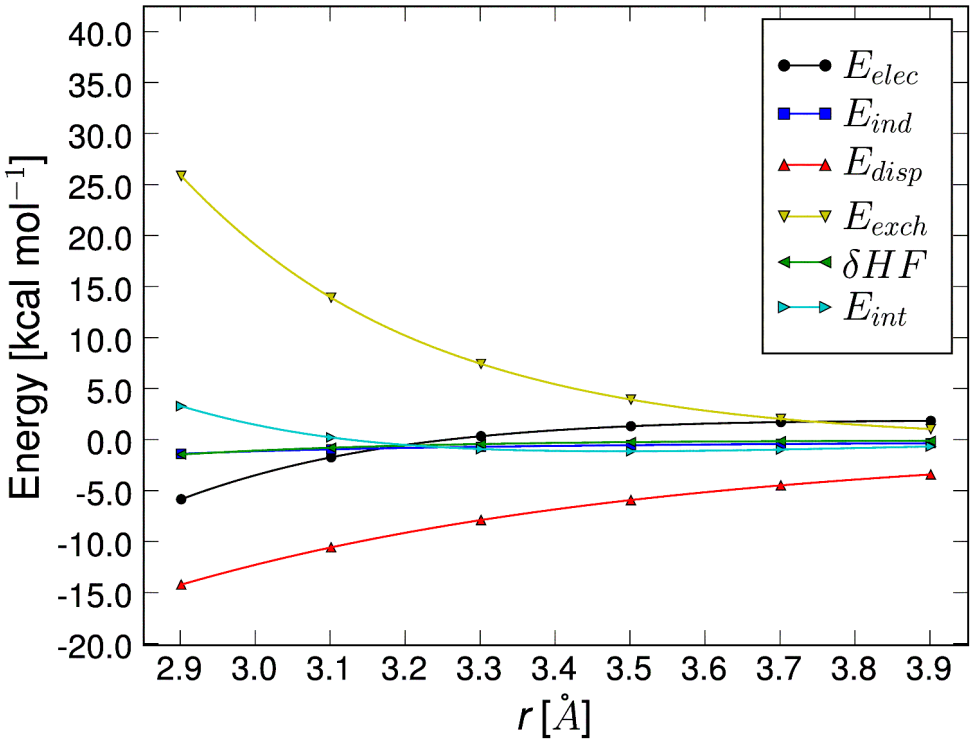

Figure S16: DFT-SAPT Energy Terms of P6

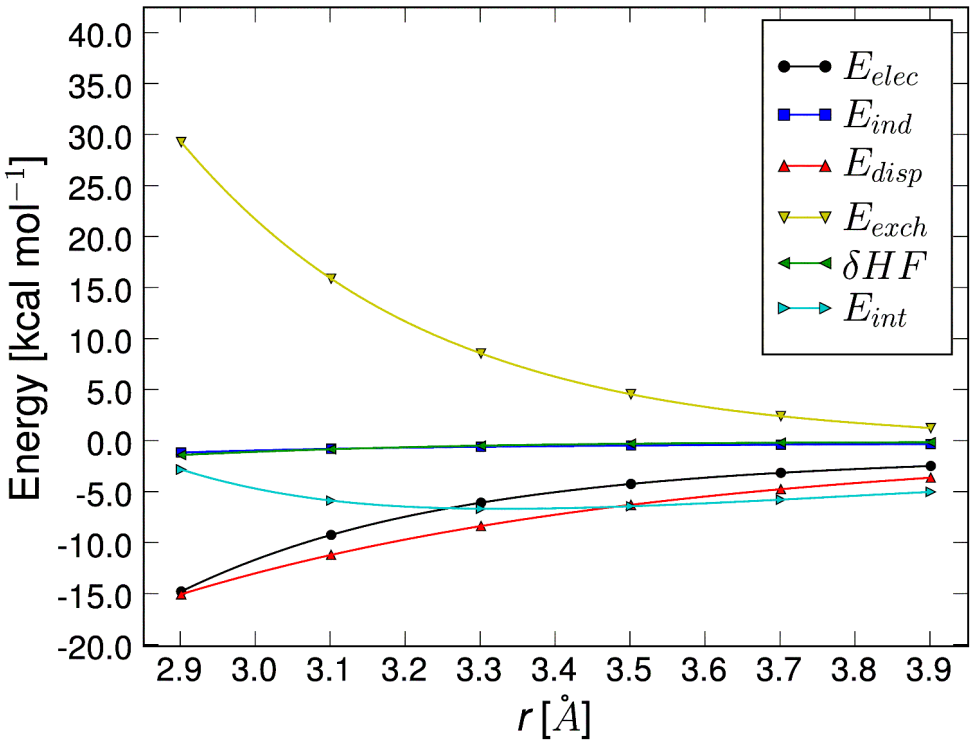

Figure S17: DFT-SAPT Energy Terms of P7

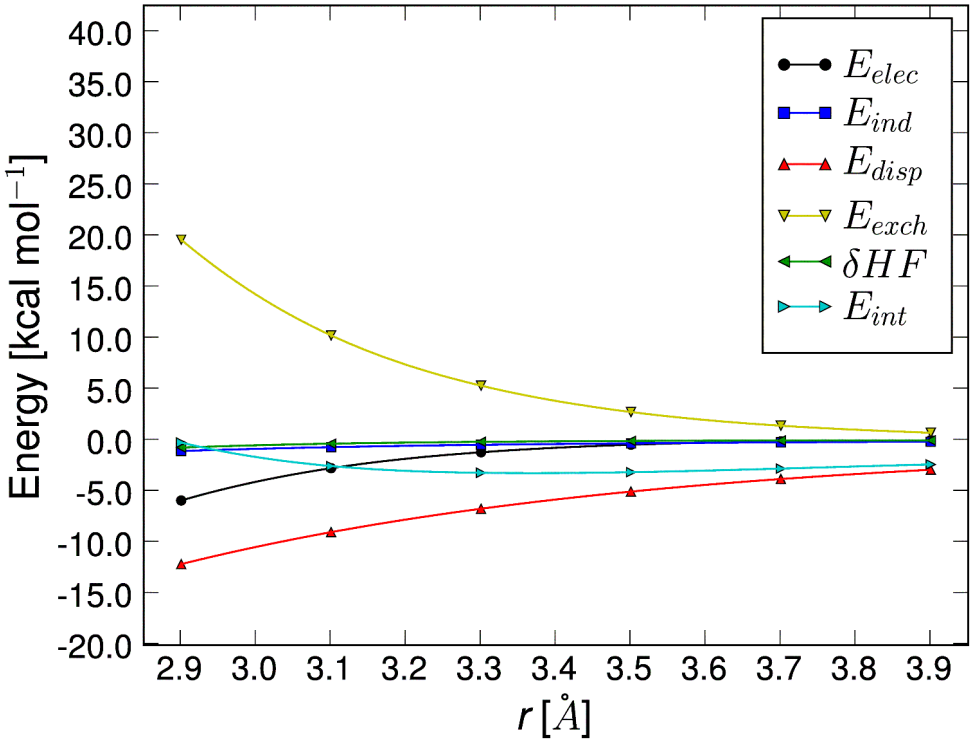

Figure S18: DFT-SAPT Energy Terms of P8

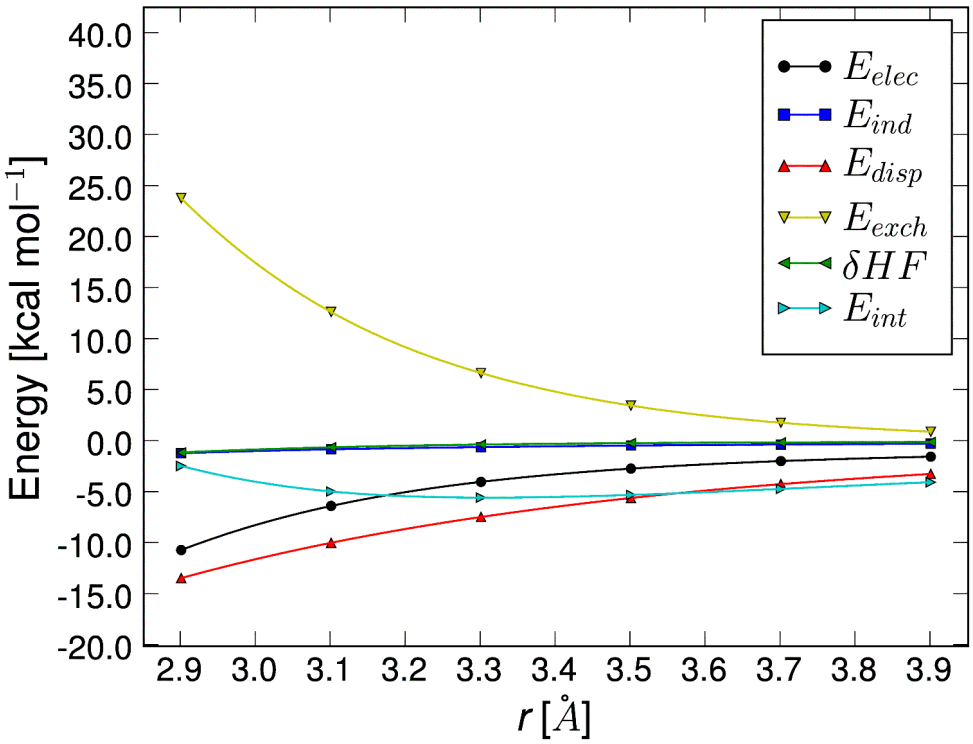

Figure S19: DFT-SAPT Energy Terms of P9

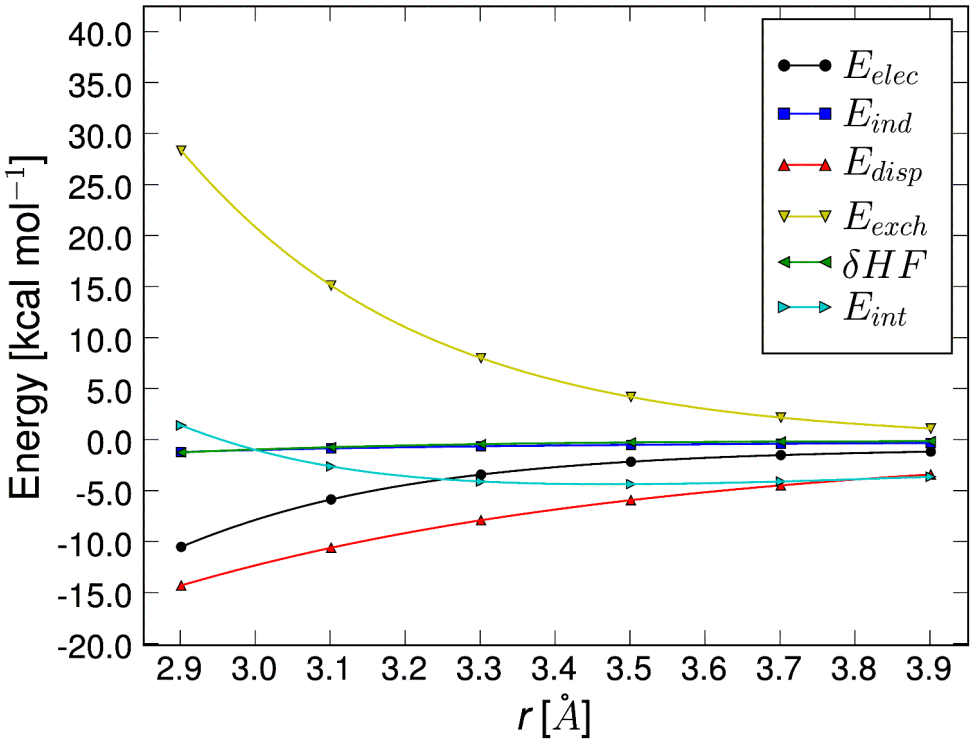

Figure S20: DFT-SAPT Energy Terms of NP1

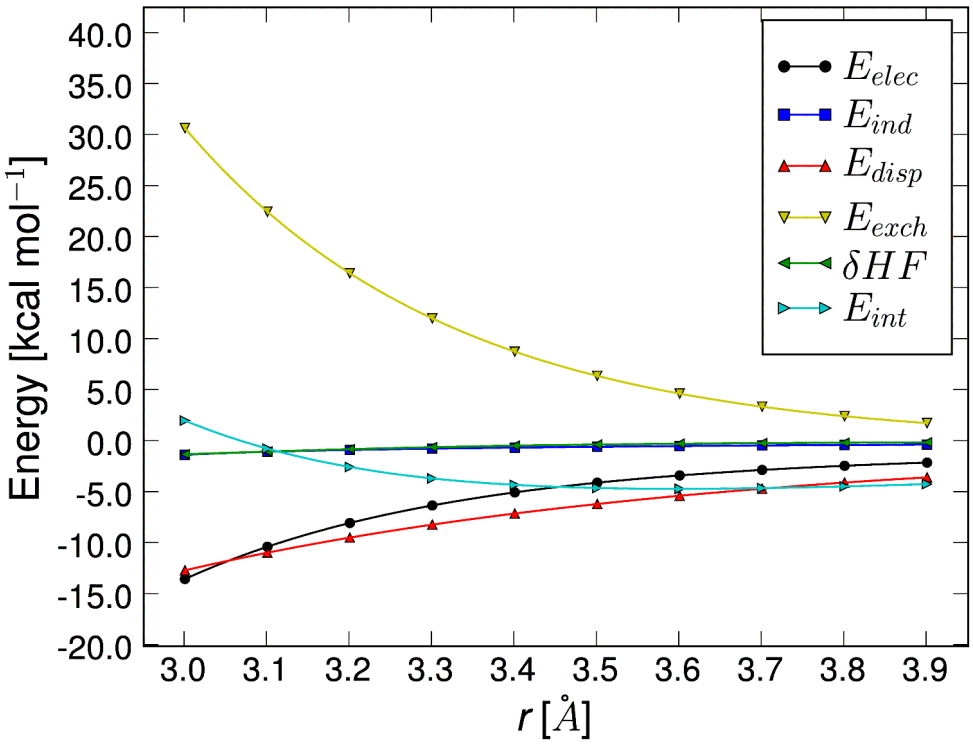

Figure S21: DFT-SAPT Energy Terms of NP2

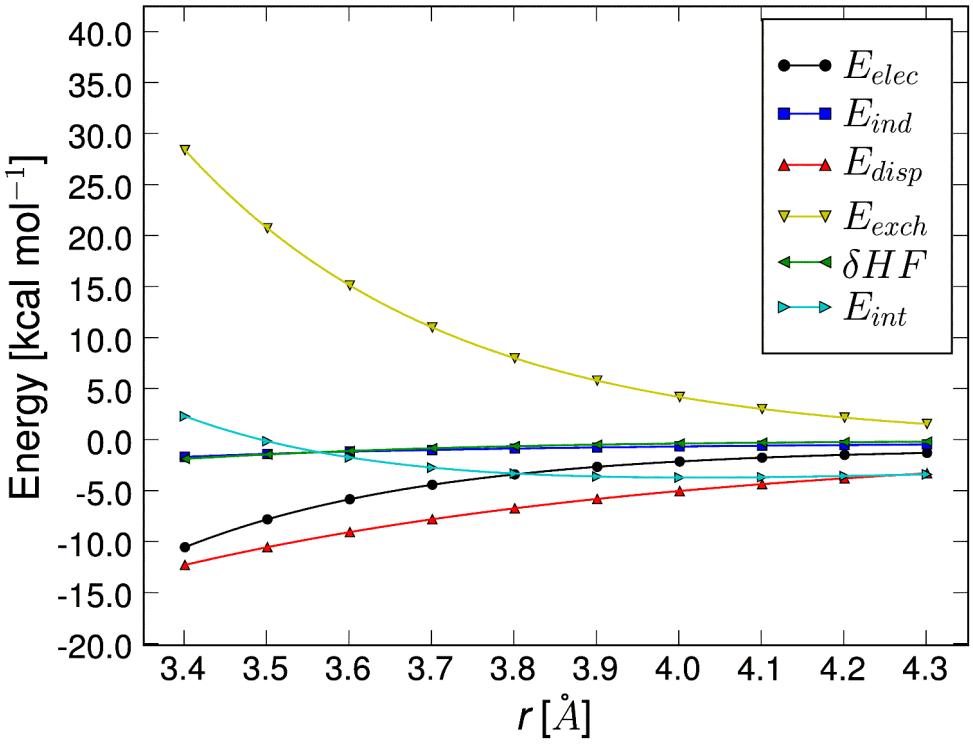

Figure S22: DFT-SAPT Energy Terms of NP3

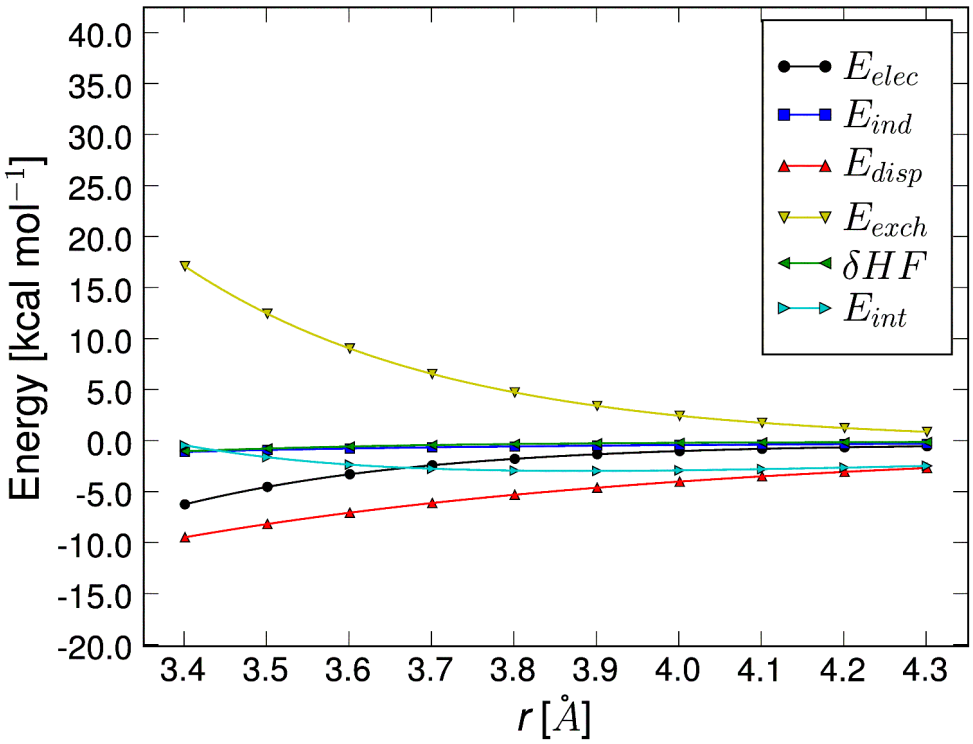

Figure S23: DFT-SAPT Energy Terms of NP4

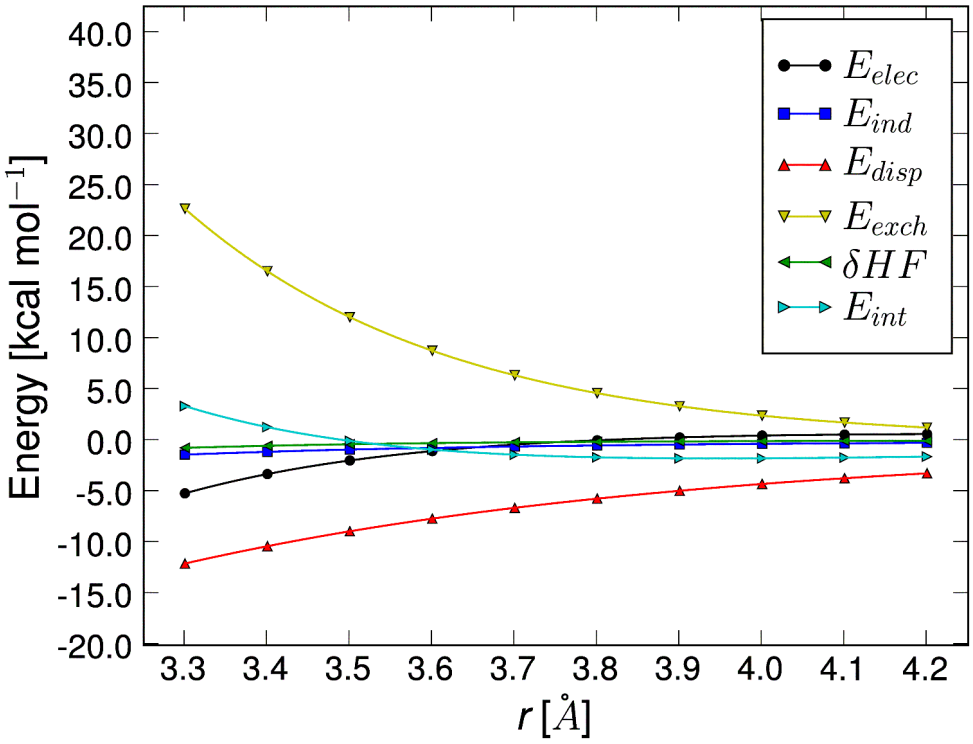

Figure S24: DFT-SAPT Energy Terms of HB1

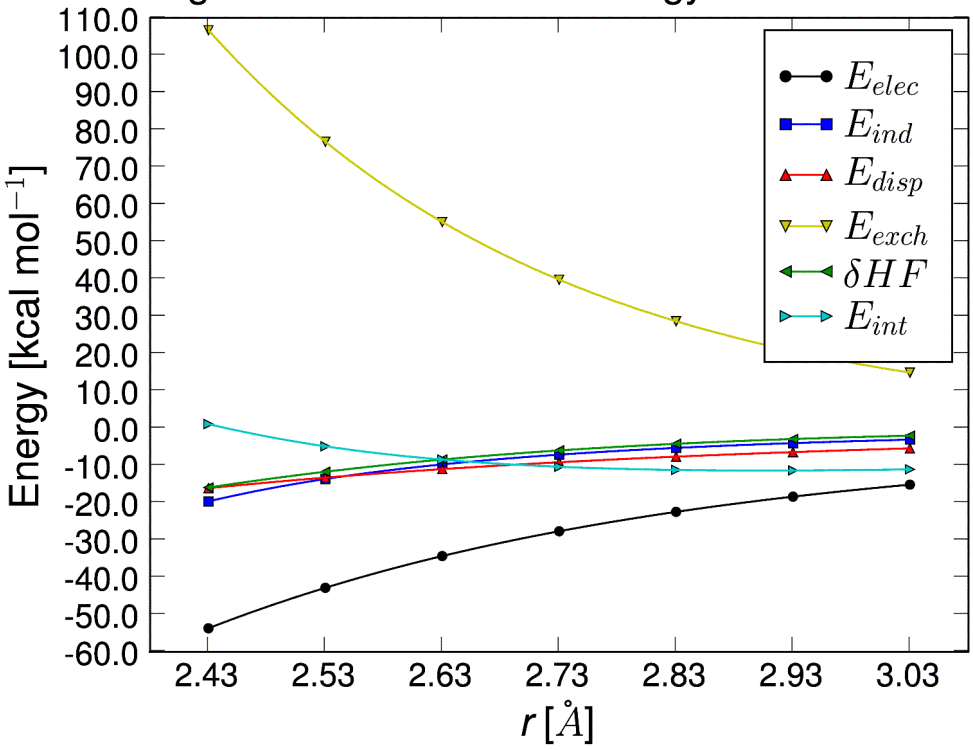

Figure S25: DFT-SAPT Energy Terms of HB2