Scope and Limitations of the SCS-MP2 Method for Stacking Interactions — Supplementary Information

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TABLE I: MP2 binding energies and counterpoise corrections (in kJ/mol) of the π-stacked 2-pyridone$\cdot n$-fluorobenzene complexes.

System	ΔE_{bin}	ΔE_{CP}	Σ	ΔE_{bin}	ΔE_{CP}	Σ
	aug-cc-pVTZ			aug-cc-pVQZ		
2PY·1-FB	40.12	−8.82	31.30	35.45	−3.34	32.11
2PY·12-FB	42.67	−10.28	32.39	37.13	−3.86	33.27
2PY·13-FB	41.31	−9.55	31.76	36.32	−3.69	32.63
2PY·14-FB	39.55	−9.30	30.25	34.57	−3.52	31.05
2PY·123-FB	45.88	−11.38	34.50	39.72	−4.25	35.47
2PY·124-FB	44.88	−10.82	34.06	39.09	−4.09	35.00
2PY·135-FB	41.32	−9.92	31.40	36.10	−3.87	32.23
2PY·1234-FB	49.10	−11.89	37.21	42.75	−4.53	38.22
2PY·1235-FB	46.45	−11.90	34.55	40.00	−4.47	35.53
2PY·1245-FB	47.17	−11.46	35.71	41.05	−4.38	36.67
2PY·5-FB	50.87	−12.73	38.14	44.03	−4.85	39.18
2PY·6-FB	50.42	−13.78	36.64	42.85	−5.13	37.72

TABLE II: SCS-MP2 binding energies and counterpoise corrections (in kJ/mol) of the π-stacked 2-pyridone$\cdot n$-fluorobenzene complexes.

System	ΔE_{bin}	ΔE_{CP}	Σ	ΔE_{bin}	ΔE_{CP}	Σ
	aug-cc-pVTZ			aug-cc-pVQZ		
2PY·1-FB	30.30	−9.44	20.86	25.30	−3.68	21.62
2PY·12-FB	32.13	−11.00	21.13	26.19	−4.25	21.94
2PY·13-FB	31.36	−10.22	21.14	26.01	−4.06	21.95
2PY·14-FB	29.81	−9.94	19.87	24.48	−3.88	20.60
2PY·123-FB	35.06	−12.17	22.89	28.46	−4.67	23.79
2PY·124-FB	34.39	−11.57	22.82	28.19	−4.50	23.69
2PY·135-FB	31.38	−10.62	20.76	25.80	−4.26	21.54
2PY·1234-FB	38.44	−12.72	25.72	31.64	−4.98	26.66
2PY·1235-FB	35.64	−12.72	22.92	28.73	−4.91	23.82
2PY·1245-FB	36.69	−12.26	24.43	30.14	−4.81	25.33
2PY·5-FB	39.91	−13.62	26.29	32.59	−5.33	27.26
2PY·6-FB	39.50	−14.73	24.77	31.41	−5.63	25.78

TABLE III: MP2-R12 binding energies and counterpoise corrections (in kJ/mol) of the π-stacked 2-pyridone·n-fluorobenzene complexes.

System	ΔE_{bin}	ΔE_{CP}	Σ	ΔE_{bin}	ΔE_{CP}	Σ
	aug-cc-pVTZ			aug-cc-pVQZ		
2PY·1-FB	35.58	−3.10	32.48	33.63	−0.96	32.67
2PY·12-FB	37.49	−3.79	33.70	35.07	−1.18	33.89
2PY·13-FB	36.50	−3.47	33.03	34.35	−1.11	33.24
2PY·14-FB	34.79	−3.36	31.43	32.65	−1.04	31.61
2PY·123-FB	40.26	−4.30	35.96	37.51	−1.35	36.16
2PY·124-FB	39.53	−4.05	35.48	36.95	−1.28	35.67
2PY·135-FB	36.35	−3.66	32.69	34.03	−1.19	32.84
2PY·1234-FB	43.32	−4.52	38.80	40.44	−1.46	38.98
2PY·1235-FB	40.59	−4.54	36.05	37.68	−1.45	36.23
2PY·1245-FB	41.55	−4.32	37.23	38.79	−1.40	37.39
2PY·5-FB	44.71	−4.90	39.81	41.57	−1.60	39.97
2PY·6-FB	43.79	−5.47	38.32	40.25	−1.74	38.51

TABLE IV: SCS-MP2-R12 binding energies and counterpoise corrections (in kJ/mol) of the π-stacked 2-pyridone·n-fluorobenzene complexes.

System	ΔE_{bin}	ΔE_{CP}	Σ	ΔE_{bin}	ΔE_{CP}	Σ
	aug-cc-pVTZ			aug-cc-pVQZ		
2PY·1-FB	25.19	−3.12	22.07	23.20	−0.97	22.23
2PY·12-FB	26.29	−3.82	22.47	23.80	−1.21	22.59
2PY·13-FB	25.95	−3.50	22.45	23.73	−1.13	22.60
2PY·14-FB	24.46	−3.38	21.08	22.26	−1.07	21.19
2PY·123-FB	28.74	−4.34	24.40	25.90	−1.38	24.52
2PY·124-FB	28.38	−4.09	24.29	25.72	−1.31	24.41
2PY·135-FB	25.79	−3.70	22.09	23.41	−1.22	22.19
2PY·1234-FB	31.95	−4.58	27.37	28.98	−1.51	27.47
2PY·1235-FB	29.05	−4.59	24.46	26.06	−1.49	24.57
2PY·1245-FB	30.37	−4.37	26.00	27.53	−1.43	26.10
2PY·5-FB	33.00	−4.97	28.03	29.76	−1.65	28.11
2PY·6-FB	32.05	−5.55	26.50	28.41	−1.80	26.61

TABLE V: MP2 binding energies and counterpoise corrections (in kJ/mol) of the H-bonded 2-pyridone·n-fluorobenzene complexes.

System	ΔE_{bin}	ΔE_{CP}	Σ	ΔE_{bin}	ΔE_{CP}	Σ
	aug-cc-pVTZ			aug-cc-pVQZ		
2PY·1-FB	30.60	−4.91	25.69	28.29	−1.96	26.33
2PY·12-FB	31.17	−5.09	26.08	28.78	−2.05	26.73
2PY·13-FB	30.57	−4.95	25.62	28.25	−1.99	26.26
2PY·14-FB	31.57	−5.04	26.53	29.24	−2.05	27.19
2PY·123-FB	31.30	−5.11	26.19	28.88	−2.06	26.82
2PY·124-FB	32.35	−5.19	27.16	29.93	−2.11	27.82
2PY·135-FB	30.33	−5.12	25.21	27.95	−2.10	25.85
2PY·1234-FB	32.62	−5.28	27.34	30.14	−2.15	27.99
2PY·1235-FB	31.46	−5.26	26.20	29.00	−2.16	26.84
2PY·1245-FB	32.70	−5.42	27.28	30.18	−2.21	27.97
2PY·5-FB	33.12	−5.47	27.65	30.57	−2.24	28.33
2PY·6-FB	33.61	−7.28	26.33	29.85	−2.83	27.02

TABLE VI: SCS-MP2 binding energies and counterpoise corrections (in kJ/mol) of the H-bonded 2-pyridone·n-fluorobenzene complexes.

System	ΔE_{bin}	ΔE_{CP}	Σ	ΔE_{bin}	ΔE_{CP}	Σ
	aug-cc-pVTZ			aug-cc-pVQZ		
2PY·1-FB	27.16	−5.30	21.86	24.70	−2.18	22.52
2PY·12-FB	27.91	−5.49	22.42	25.37	−2.27	23.10
2PY·13-FB	27.16	−5.34	21.82	24.70	−2.21	22.49
2PY·14-FB	28.12	−5.43	22.69	25.65	−2.27	23.38
2PY·123-FB	28.07	−5.51	22.56	25.51	−2.28	23.23
2PY·124-FB	29.07	−5.59	23.48	26.51	−2.34	24.17
2PY·135-FB	26.79	−5.52	21.27	24.26	−2.33	21.93
2PY·1234-FB	29.38	−5.69	23.69	26.76	−2.38	24.38
2PY·1235-FB	28.07	−5.67	22.40	25.46	−2.40	23.06
2PY·1245-FB	29.25	−5.84	23.41	26.57	−2.45	24.12
2PY·5-FB	29.69	−5.88	23.81	26.99	−2.48	24.51
2PY·6-FB	29.22	−7.78	21.44	25.21	−3.11	22.10

TABLE VII: MP2-R12 binding energies and counterpoise corrections (in kJ/mol) of the H-bonded 2-pyridone·n-fluorobenzene complexes.

System	ΔE_{bin}	ΔE_{CP}	Σ	ΔE_{bin}	ΔE_{CP}	Σ
	aug-cc-pVTZ			aug-cc-pVQZ		
2PY·1-FB	28.10	−1.55	26.55	27.24	−0.47	26.77
2PY·12-FB	28.62	−1.63	26.99	27.70	−0.51	27.19
2PY·13-FB	28.07	−1.57	26.50	27.18	−0.47	26.71
2PY·14-FB	29.03	−1.60	27.43	28.15	−0.49	27.66
2PY·123-FB	28.75	−1.65	27.10	27.80	−0.51	27.29
2PY·124-FB	29.77	−1.67	28.10	28.83	−0.52	28.31
2PY·135-FB	27.75	−1.66	26.09	26.80	−0.51	26.29
2PY·1234-FB	30.02	−1.71	28.31	29.03	−0.54	28.49
2PY·1235-FB	28.85	−1.72	27.13	27.85	−0.53	27.32
2PY·1245-FB	30.02	−1.77	28.25	29.01	−0.55	28.46
2PY·5-FB	30.45	−1.81	28.64	29.41	−0.57	28.84
2PY·6-FB	30.11	−2.85	27.26	28.46	−0.96	27.50

TABLE VIII: SCS-MP2-R12 binding energies and counterpoise corrections (in kJ/mol) of the H-bonded 2-pyridone·n-fluorobenzene complexes.

System	ΔE_{bin}	ΔE_{CP}	Σ	ΔE_{bin}	ΔE_{CP}	Σ
	aug-cc-pVTZ			aug-cc-pVQZ		
2PY·1-FB	24.37	−1.58	22.79	23.50	−0.48	23.02
2PY·12-FB	25.07	−1.66	23.41	24.14	−0.52	23.62
2PY·13-FB	24.37	−1.60	22.77	23.48	−0.49	22.99
2PY·14-FB	25.29	−1.62	23.67	24.40	−0.50	23.90
2PY·123-FB	25.24	−1.68	23.56	24.28	−0.52	23.76
2PY·124-FB	26.21	−1.69	24.52	25.25	−0.53	24.72
2PY·135-FB	23.90	−1.68	22.22	22.95	−0.52	22.43
2PY·1234-FB	26.49	−1.74	24.75	25.49	−0.55	24.94
2PY·1235-FB	25.16	−1.75	23.41	24.15	−0.55	23.60
2PY·1245-FB	26.26	−1.80	24.46	25.24	−0.56	24.68
2PY·5-FB	26.72	−1.82	24.90	25.67	−0.58	25.09
2PY·6-FB	25.30	−2.89	22.41	23.61	−0.99	22.62

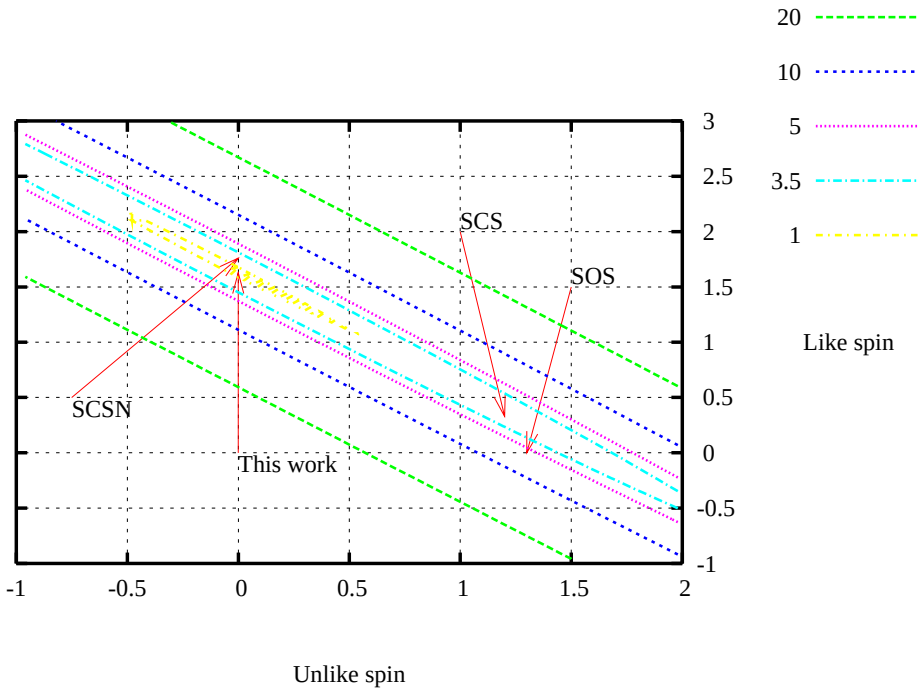

FIG. 1: Contour plot of the RMS deviation of the SCS-MP2-R12 binding energy as a function of the like and unlike spin scaling factors. The reference values are the CCSD(T) energies computed within the additivity scheme. The red arrows point to the scaling factors of the original Grimme SCS (spin-component-scaled), the SOS (spin-opposite-scaled), the SCSN (spin-component-scaled for the nucleic acid bases) approaches and to those of the present work.