Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting Information
to
Benchmarking B3LYP, PBE0 and M06L for nuclear spin–spin couplings against CC3: influence of geometry optimization
by

Elif Küçükefe, Rodrigo A. Cormanich and Stephan P. A. Sauer

April 17, 2026

Table S1 The SSCC values (in Hz) for all molecules and couplings in the study. All of the results reported are for for the ^{1}H, ^{13}C, ^{15}N, ^{17}O, and ^{19}F isotopes. CCSD(T)/aug-cc-pCVQZ optimized geometries from Faber et al. study.

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
CO	$^{1}J_{CO}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	11.64	-6.66	14.54	0.10	19.62
CO	$^{1}J_{CO}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	13.28	-6.70	14.50	0.10	21.19
CO	$^{1}J_{CO}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	11.85	-6.70	14.33	0.10	19.59
CO	$^{1}J_{CO}$	M06L/aug-pc-2	M06L/aug-pcJ-2	3.96	-6.59	13.74	0.10	11.21
F_2CO	$^{1}J_{CO}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	19.24	-5.00	7.50	-0.13	21.61
F_2CO	$^{1}J_{CO}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	19.35	-5.07	7.31	-0.13	21.47
F_2CO	$^{1}J_{CO}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	2.90	-4.32	6.48	-0.14	4.93
F_2CO	$^{1}J_{CO}$	B3LYP/pc-2	B3LYP/pcJ-2	20.00	-5.12	7.32	-0.13	22.08
F_2CO	$^{1}J_{CO}$	B3LYP/pc-2	PBE0/pcJ-2	20.07	-5.19	7.14	-0.13	21.90
F_2CO	$^{1}J_{CO}$	B3LYP/pc-2	M06L/pcJ-2	3.46	-4.42	6.35	-0.13	5.25
F_2CO	$^{1}J_{CO}$	PBE0/pc-2	B3LYP/pcJ-2	18.13	-4.96	7.49	-0.13	20.53
F_2CO	$^{1}J_{CO}$	PBE0/pc-2	PBE0/pcJ-2	18.27	-5.03	7.30	-0.13	20.42
F_2CO	$^{1}J_{CO}$	PBE0/pc-2	M06L/pcJ-2	2.27	-4.29	6.48	-0.14	4.33
F_2CO	$^{1}J_{CO}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	17.95	-5.02	7.30	-0.13	20.10
F_2CO	$^{1}J_{CO}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	2.18	-4.28	6.48	-0.14	4.24
F_2CO	$^{1}J_{CO}$	M06L/pc-2	B3LYP/pcJ-2	19.26	-5.01	7.43	-0.13	21.56
F_2CO	$^{1}J_{CO}$	M06L/pc-2	PBE0/pcJ-2	19.37	-5.08	7.25	-0.13	21.41
F_2CO	$^{1}J_{CO}$	M06L/pc-2	M06L/pcJ-2	2.96	-4.33	6.43	-0.13	4.93
F_2CO	$^{1}J_{CO}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	19.09	-5.08	7.25	-0.13	21.12
F_2CO	$^{1}J_{CO}$	M06L/aug-pc-2	M06L/aug-pcJ-2	2.90	-4.32	6.42	-0.13	4.86
F_2CO	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-353.34	-1.43	-47.41	1.16	-401.02
F_2CO	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-343.96	-1.99	-46.49	1.16	-391.28
F_2CO	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-241.24	-1.08	-41.72	1.17	-282.88
F_2CO	$^{1}J_{CF}$	B3LYP/pc-2	B3LYP/pcJ-2	-364.18	-1.24	-47.00	1.15	-411.28
F_2CO	$^{1}J_{CF}$	B3LYP/pc-2	PBE0/pcJ-2	-354.38	-1.80	-46.08	1.15	-401.11
F_2CO	$^{1}J_{CF}$	B3LYP/pc-2	M06L/pcJ-2	-248.49	-0.91	-41.38	1.15	-289.63
F_2CO	$^{1}J_{CF}$	PBE0/pc-2	B3LYP/pcJ-2	-350.85	-1.38	-47.20	1.17	-398.25
F_2CO	$^{1}J_{CF}$	PBE0/pc-2	PBE0/pcJ-2	-341.55	-1.93	-46.28	1.17	-388.59

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
F_2CO	$^1J_{CF}$	PBE0/pc-2	M06L/pcJ-2	-239.38	-1.04	-41.57	1.17	-280.82
F_2CO	$^1J_{CF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-339.95	-1.90	-46.49	1.17	-387.17
F_2CO	$^1J_{CF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-238.98	-1.01	-41.69	1.17	-280.51
F_2CO	$^1J_{CF}$	M06L/pc-2	B3LYP/pcJ-2	-354.13	-1.36	-47.35	1.16	-401.68
F_2CO	$^1J_{CF}$	M06L/pc-2	PBE0/pcJ-2	-344.71	-1.91	-46.43	1.16	-391.89
F_2CO	$^1J_{CF}$	M06L/pc-2	M06L/pcJ-2	-241.73	-1.01	-41.68	1.16	-283.26
F_2CO	$^1J_{CF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-343.33	-1.88	-46.63	1.16	-390.67
F_2CO	$^1J_{CF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-241.48	-0.98	-41.80	1.16	-283.09
F_2CO	$^2J_{OF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	6.97	-6.81	53.84	0.32	54.33
F_2CO	$^2J_{OF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	6.08	-6.88	53.96	0.32	53.48
F_2CO	$^2J_{OF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-10.61	-5.90	45.33	0.32	29.14
F_2CO	$^2J_{OF}$	B3LYP/pc-2	B3LYP/pcJ-2	7.38	-6.74	54.64	0.32	55.60
F_2CO	$^2J_{OF}$	B3LYP/pc-2	PBE0/pcJ-2	6.49	-6.82	54.75	0.32	54.74
F_2CO	$^2J_{OF}$	B3LYP/pc-2	M06L/pcJ-2	-10.21	-5.89	45.88	0.32	30.11
F_2CO	$^2J_{OF}$	PBE0/pc-2	B3LYP/pcJ-2	6.69	-6.74	53.51	0.32	53.78
F_2CO	$^2J_{OF}$	PBE0/pc-2	PBE0/pcJ-2	5.81	-6.81	53.63	0.32	52.96
F_2CO	$^2J_{OF}$	PBE0/pc-2	M06L/pcJ-2	-10.77	-5.85	45.07	0.33	28.78
F_2CO	$^2J_{OF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	5.74	-6.78	53.52	0.32	52.81
F_2CO	$^2J_{OF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-10.43	-5.84	44.88	0.32	28.94
F_2CO	$^2J_{OF}$	M06L/pc-2	B3LYP/pcJ-2	7.16	-6.76	53.75	0.32	54.48
F_2CO	$^2J_{OF}$	M06L/pc-2	PBE0/pcJ-2	6.27	-6.83	53.86	0.32	53.63
F_2CO	$^2J_{OF}$	M06L/pc-2	M06L/pcJ-2	-10.40	-5.87	45.24	0.32	29.30
F_2CO	$^2J_{OF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	6.22	-6.80	53.78	0.32	53.52
F_2CO	$^2J_{OF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-10.04	-5.86	45.06	0.32	29.48
F_2CO	$^2J_{FF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	49.02	26.94	-312.20	-1.10	-237.35
F_2CO	$^2J_{FF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	45.41	27.29	-307.82	-1.10	-236.23
F_2CO	$^2J_{FF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	199.08	27.85	-266.36	-1.11	-40.55
F_2CO	$^2J_{FF}$	B3LYP/pc-2	B3LYP/pcJ-2	34.17	28.70	-316.57	-1.06	-254.77
F_2CO	$^2J_{FF}$	B3LYP/pc-2	PBE0/pcJ-2	30.89	29.09	-311.89	-1.07	-252.97
F_2CO	$^2J_{FF}$	B3LYP/pc-2	M06L/pcJ-2	190.76	29.45	-269.26	-1.07	-50.12
F_2CO	$^2J_{FF}$	PBE0/pc-2	B3LYP/pcJ-2	51.08	26.86	-311.29	-1.11	-234.46
F_2CO	$^2J_{FF}$	PBE0/pc-2	PBE0/pcJ-2	47.42	27.21	-306.93	-1.11	-233.41
F_2CO	$^2J_{FF}$	PBE0/pc-2	M06L/pcJ-2	200.93	27.77	-265.59	-1.12	-38.01
F_2CO	$^2J_{FF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	49.97	27.41	-308.25	-1.11	-231.98
F_2CO	$^2J_{FF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	201.82	27.54	-266.77	-1.11	-38.53
F_2CO	$^2J_{FF}$	M06L/pc-2	B3LYP/pcJ-2	51.81	27.06	-314.57	-1.08	-236.79
F_2CO	$^2J_{FF}$	M06L/pc-2	PBE0/pcJ-2	48.19	27.40	-310.14	-1.09	-235.63
F_2CO	$^2J_{FF}$	M06L/pc-2	M06L/pcJ-2	202.56	27.91	-268.26	-1.09	-38.87
F_2CO	$^2J_{FF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	50.50	27.64	-311.56	-1.08	-234.51
F_2CO	$^2J_{FF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	203.32	27.72	-269.53	-1.09	-39.58
FCCF	$^1J_{CC}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	406.70	14.40	17.36	0.31	438.77
FCCF	$^1J_{CC}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	395.96	14.69	16.98	0.31	427.93
FCCF	$^1J_{CC}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	410.69	12.83	14.04	0.32	437.87
FCCF	$^1J_{CC}$	B3LYP/pc-2	B3LYP/pcJ-2	406.45	14.29	17.30	0.31	438.34
FCCF	$^1J_{CC}$	B3LYP/pc-2	PBE0/pcJ-2	395.69	14.57	16.91	0.31	427.48
FCCF	$^1J_{CC}$	B3LYP/pc-2	M06L/pcJ-2	409.64	12.74	14.02	0.32	436.71
FCCF	$^1J_{CC}$	PBE0/pc-2	B3LYP/pcJ-2	404.89	14.15	17.06	0.31	436.41
FCCF	$^1J_{CC}$	PBE0/pc-2	PBE0/pcJ-2	394.14	14.43	16.69	0.32	425.57
FCCF	$^1J_{CC}$	PBE0/pc-2	M06L/pcJ-2	407.87	12.61	13.82	0.32	434.63

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
FCCF	$^{1}J_{CC}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	394.80	14.46	16.73	0.32	426.30
FCCF	$^{1}J_{CC}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	408.14	12.55	13.80	0.32	434.81
FCCF	$^{1}J_{CC}$	M06L/pc-2	B3LYP/pcJ-2	404.63	14.13	17.02	0.31	436.10
FCCF	$^{1}J_{CC}$	M06L/pc-2	PBE0/pcJ-2	393.88	14.42	16.65	0.32	425.27
FCCF	$^{1}J_{CC}$	M06L/pc-2	M06L/pcJ-2	407.64	12.59	13.79	0.32	434.34
FCCF	$^{1}J_{CC}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	394.60	14.45	16.70	0.32	426.07
FCCF	$^{1}J_{CC}$	M06L/aug-pc-2	M06L/aug-pcJ-2	407.99	12.54	13.78	0.32	434.63
FCCF	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-355.00	-13.93	-17.88	0.58	-386.24
FCCF	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-352.88	-16.01	-19.04	0.58	-387.35
FCCF	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-179.63	-11.39	-12.38	0.59	-202.80
FCCF	$^{1}J_{CF}$	B3LYP/pc-2	B3LYP/pcJ-2	-353.99	-13.37	-17.07	0.58	-383.84
FCCF	$^{1}J_{CF}$	B3LYP/pc-2	PBE0/pcJ-2	-351.82	-15.42	-18.23	0.58	-384.89
FCCF	$^{1}J_{CF}$	B3LYP/pc-2	M06L/pcJ-2	-178.62	-10.92	-11.82	0.59	-200.77
FCCF	$^{1}J_{CF}$	PBE0/pc-2	B3LYP/pcJ-2	-342.33	-13.94	-18.52	0.58	-374.21
FCCF	$^{1}J_{CF}$	PBE0/pc-2	PBE0/pcJ-2	-340.38	-15.98	-19.64	0.58	-375.42
FCCF	$^{1}J_{CF}$	PBE0/pc-2	M06L/pcJ-2	-172.01	-11.39	-12.94	0.59	-195.75
FCCF	$^{1}J_{CF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-338.99	-15.88	-19.77	0.58	-374.06
FCCF	$^{1}J_{CF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-171.64	-11.26	-12.99	0.59	-195.29
FCCF	$^{1}J_{CF}$	M06L/pc-2	B3LYP/pcJ-2	-340.33	-14.09	-18.84	0.58	-372.68
FCCF	$^{1}J_{CF}$	M06L/pc-2	PBE0/pcJ-2	-338.42	-16.12	-19.95	0.58	-373.92
FCCF	$^{1}J_{CF}$	M06L/pc-2	M06L/pcJ-2	-170.90	-11.51	-13.18	0.59	-194.99
FCCF	$^{1}J_{CF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-337.43	-16.02	-20.06	0.58	-372.93
FCCF	$^{1}J_{CF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-170.77	-11.37	-13.21	0.59	-194.76
FCCF	$^{2}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	6.14	29.05	13.18	-0.69	47.68
FCCF	$^{2}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	8.70	29.51	12.54	-0.69	50.05
FCCF	$^{2}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	56.35	24.83	9.16	-0.69	89.65
FCCF	$^{2}J_{CF}$	B3LYP/pc-2	B3LYP/pcJ-2	5.73	28.65	12.73	-0.70	46.40
FCCF	$^{2}J_{CF}$	B3LYP/pc-2	PBE0/pcJ-2	8.22	29.09	12.10	-0.70	48.71
FCCF	$^{2}J_{CF}$	B3LYP/pc-2	M06L/pcJ-2	55.75	24.53	8.86	-0.70	88.44
FCCF	$^{2}J_{CF}$	PBE0/pc-2	B3LYP/pcJ-2	7.94	28.98	13.52	-0.70	49.74
FCCF	$^{2}J_{CF}$	PBE0/pc-2	PBE0/pcJ-2	10.40	29.41	12.88	-0.70	51.99
FCCF	$^{2}J_{CF}$	PBE0/pc-2	M06L/pcJ-2	56.92	24.75	9.40	-0.70	90.36
FCCF	$^{2}J_{CF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	10.63	29.20	12.69	-0.70	51.82
FCCF	$^{2}J_{CF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	56.16	24.57	9.32	-0.70	89.35
FCCF	$^{2}J_{CF}$	M06L/pc-2	B3LYP/pcJ-2	8.37	29.07	13.70	-0.70	50.43
FCCF	$^{2}J_{CF}$	M06L/pc-2	PBE0/pcJ-2	10.82	29.50	13.06	-0.70	52.67
FCCF	$^{2}J_{CF}$	M06L/pc-2	M06L/pcJ-2	57.18	24.81	9.52	-0.70	90.80
FCCF	$^{2}J_{CF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	10.99	29.29	12.85	-0.70	52.43
FCCF	$^{2}J_{CF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	56.39	24.64	9.43	-0.70	89.75
FCCF	$^{2}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	4.21	52.95	-24.74	-0.19	30.58
FCCF	$^{2}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	6.86	52.12	-32.67	-1.85	24.46
FCCF	$^{2}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	10.86	33.95	-46.23	-1.86	-3.28
FCCF	$^{2}J_{CF}$	B3LYP/pc-2	B3LYP/pcJ-2	4.11	52.23	-24.23	-1.85	30.26
FCCF	$^{2}J_{CF}$	B3LYP/pc-2	PBE0/pcJ-2	6.70	51.37	-32.15	-1.85	24.07
FCCF	$^{2}J_{CF}$	B3LYP/pc-2	M06L/pcJ-2	10.60	33.59	-45.51	-1.86	-3.18
FCCF	$^{2}J_{CF}$	PBE0/pc-2	B3LYP/pcJ-2	3.96	55.45	-16.64	-1.88	40.89
FCCF	$^{2}J_{CF}$	PBE0/pc-2	PBE0/pcJ-2	6.49	54.56	-24.64	-1.88	34.53
FCCF	$^{2}J_{CF}$	PBE0/pc-2	M06L/pcJ-2	10.81	36.36	-39.47	-1.89	5.81
FCCF	$^{2}J_{CF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	5.97	52.63	-27.03	-1.88	29.69

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
FCCF	$^{2}J_{CF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	9.95	35.69	-39.81	-1.89	3.95
FCCF	$^{2}J_{CF}$	M06L/pc-2	B3LYP/pcJ-2	3.95	56.08	-15.34	-1.89	42.80
FCCF	$^{2}J_{CF}$	M06L/pc-2	PBE0/pcJ-2	6.47	55.19	-23.35	-1.89	36.41
FCCF	$^{2}J_{CF}$	M06L/pc-2	M06L/pcJ-2	10.87	36.88	-38.47	-1.89	7.39
FCCF	$^{2}J_{CF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	5.96	53.16	-26.02	-1.89	31.22
FCCF	$^{2}J_{CF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	10.01	36.13	-39.01	-1.89	5.24
FCCH	$^{1}J_{CC}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	265.48	13.57	13.50	0.16	292.71
FCCH	$^{1}J_{CC}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	256.34	14.01	13.29	0.16	283.80
FCCH	$^{1}J_{CC}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	275.39	12.97	10.88	0.17	299.41
FCCH	$^{1}J_{CC}$	B3LYP/pc-2	B3LYP/pcJ-2	265.95	13.35	13.35	0.16	292.80
FCCH	$^{1}J_{CC}$	B3LYP/pc-2	PBE0/pcJ-2	256.78	13.78	13.13	0.16	283.85
FCCH	$^{1}J_{CC}$	B3LYP/pc-2	M06L/pcJ-2	274.73	12.78	10.79	0.17	298.47
FCCH	$^{1}J_{CC}$	PBE0/pc-2	B3LYP/pcJ-2	265.46	13.26	13.20	0.16	292.09
FCCH	$^{1}J_{CC}$	PBE0/pc-2	PBE0/pcJ-2	256.30	13.68	12.99	0.17	292.08
FCCH	$^{1}J_{CC}$	PBE0/pc-2	M06L/pcJ-2	274.09	12.68	10.66	0.18	297.62
FCCH	$^{1}J_{CC}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	256.55	13.71	13.01	0.17	283.45
FCCH	$^{1}J_{CC}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	273.72	12.60	10.62	0.17	297.11
FCCH	$^{1}J_{CC}$	M06L/pc-2	B3LYP/pcJ-2	265.12	13.24	13.14	0.16	291.67
FCCH	$^{1}J_{CC}$	M06L/pc-2	PBE0/pcJ-2	255.96	13.67	12.93	0.17	282.72
FCCH	$^{1}J_{CC}$	M06L/pc-2	M06L/pcJ-2	273.78	12.66	10.61	0.18	297.23
FCCH	$^{1}J_{CC}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	256.22	13.70	12.96	0.17	283.05
FCCH	$^{1}J_{CC}$	M06L/aug-pc-2	M06L/aug-pcJ-2	273.43	12.57	10.57	0.18	296.75
FCCH	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-352.85	-17.37	-32.88	0.48	-402.62
FCCH	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-350.14	-19.81	-34.06	0.47	-403.54
FCCH	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-210.40	-15.77	-25.63	0.48	-251.32
FCCH	$^{1}J_{CF}$	B3LYP/pc-2	B3LYP/pcJ-2	-349.04	-16.65	-31.96	0.48	-397.17
FCCH	$^{1}J_{CF}$	B3LYP/pc-2	PBE0/pcJ-2	-346.31	-19.03	-33.13	0.48	-397.99
FCCH	$^{1}J_{CF}$	B3LYP/pc-2	M06L/pcJ-2	-207.21	-15.14	-25.02	0.49	-246.88
FCCH	$^{1}J_{CF}$	PBE0/pc-2	B3LYP/pcJ-2	-338.45	-17.36	-33.74	0.48	-389.07
FCCH	$^{1}J_{CF}$	PBE0/pc-2	PBE0/pcJ-2	-336.01	-19.73	-34.85	0.48	-390.11
FCCH	$^{1}J_{CF}$	PBE0/pc-2	M06L/pcJ-2	-201.03	-15.74	-26.37	0.48	-242.66
FCCH	$^{1}J_{CF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-335.19	-19.59	-34.75	0.48	-389.05
FCCH	$^{1}J_{CF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-201.11	-15.48	-26.39	0.48	-242.49
FCCH	$^{1}J_{CF}$	M06L/pc-2	B3LYP/pcJ-2	-335.19	-17.62	-34.36	0.48	-386.69
FCCH	$^{1}J_{CF}$	M06L/pc-2	PBE0/pcJ-2	-332.84	-20.00	-35.46	0.48	-387.81
FCCH	$^{1}J_{CF}$	M06L/pc-2	M06L/pcJ-2	-199.12	-15.96	-26.84	0.48	-241.43
FCCH	$^{1}J_{CF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-332.18	-19.84	-35.33	0.48	-386.88
FCCH	$^{1}J_{CF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-199.31	-15.68	-26.83	0.48	-241.34
FCCH	$^{2}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	2.29	27.25	-0.07	-0.88	28.58
FCCH	$^{2}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	4.38	28.02	-0.66	-0.88	30.85
FCCH	$^{2}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	42.90	25.02	-3.37	-0.88	63.67
FCCH	$^{2}J_{CF}$	B3LYP/pc-2	B3LYP/pcJ-2	2.22	26.74	-0.32	-0.89	27.75
FCCH	$^{2}J_{CF}$	B3LYP/pc-2	PBE0/pcJ-2	4.22	27.47	-0.91	-0.89	29.89
FCCH	$^{2}J_{CF}$	B3LYP/pc-2	M06L/pcJ-2	42.47	24.56	-3.48	-0.89	62.67
FCCH	$^{2}J_{CF}$	PBE0/pc-2	B3LYP/pcJ-2	3.78	27.29	1.02	-0.90	31.18
FCCH	$^{2}J_{CF}$	PBE0/pc-2	PBE0/pcJ-2	5.77	28.01	0.41	-0.90	33.28
FCCH	$^{2}J_{CF}$	PBE0/pc-2	M06L/pcJ-2	43.44	25.03	-2.45	-0.90	65.12
FCCH	$^{2}J_{CF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	5.78	27.83	0.27	-0.90	32.98
FCCH	$^{2}J_{CF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	42.48	24.80	-2.52	-0.90	63.86

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
FCCH	$^{2}J_{CF}$	M06L/pc-2	B3LYP/pcJ-2	4.37	27.47	1.38	-0.91	32.32
FCCH	$^{2}J_{CF}$	M06L/pc-2	PBE0/pcJ-2	6.35	28.20	0.77	-0.90	34.41
FCCH	$^{2}J_{CF}$	M06L/pc-2	M06L/pcJ-2	43.87	25.18	-2.19	-0.90	65.96
FCCH	$^{2}J_{CF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	6.34	28.01	0.61	-0.90	34.06
FCCH	$^{2}J_{CF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	42.90	24.95	-2.28	-0.90	64.66
FCCH	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	304.12	0.56	-0.89	0.42	304.22
FCCH	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	287.84	0.48	-1.05	0.44	287.71
FCCH	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	353.16	0.33	-0.35	0.46	353.60
FCCH	$^{1}J_{CH}$	B3LYP/pc-2	B3LYP/pcJ-2	301.75	0.56	-0.83	0.43	301.91
FCCH	$^{1}J_{CH}$	B3LYP/pc-2	PBE0/pcJ-2	285.55	0.48	-0.99	0.45	285.49
FCCH	$^{1}J_{CH}$	B3LYP/pc-2	M06L/pcJ-2	350.60	0.34	-0.31	0.47	351.11
FCCH	$^{1}J_{CH}$	PBE0/pc-2	B3LYP/pcJ-2	302.07	0.56	-0.81	0.43	302.26
FCCH	$^{1}J_{CH}$	PBE0/pc-2	PBE0/pcJ-2	285.81	0.48	-0.97	0.45	285.77
FCCH	$^{1}J_{CH}$	PBE0/pc-2	M06L/pcJ-2	350.55	0.35	-0.29	0.47	351.08
FCCH	$^{1}J_{CH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	285.82	0.46	-0.98	0.45	285.74
FCCH	$^{1}J_{CH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	350.30	0.35	-0.30	0.47	350.82
FCCH	$^{1}J_{CH}$	M06L/pc-2	B3LYP/pcJ-2	301.00	0.56	-0.84	0.44	301.16
FCCH	$^{1}J_{CH}$	M06L/pc-2	PBE0/pcJ-2	284.87	0.48	-1.00	0.45	284.80
FCCH	$^{1}J_{CH}$	M06L/pc-2	M06L/pcJ-2	349.62	0.34	-0.32	0.47	350.12
FCCH	$^{1}J_{CH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	284.92	0.46	-1.02	0.45	284.81
FCCH	$^{1}J_{CH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	349.43	0.34	-0.33	0.47	349.91
FCCH	$^{2}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	67.66	1.19	6.26	-1.13	73.98
FCCH	$^{2}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	64.48	1.26	6.25	-1.12	70.87
FCCH	$^{2}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	65.39	1.29	5.52	-1.12	71.09
FCCH	$^{2}J_{CH}$	B3LYP/pc-2	B3LYP/pcJ-2	67.45	1.18	6.22	-1.14	73.71
FCCH	$^{2}J_{CH}$	B3LYP/pc-2	PBE0/pcJ-2	64.36	1.25	6.21	-1.13	70.68
FCCH	$^{2}J_{CH}$	B3LYP/pc-2	M06L/pcJ-2	65.31	1.28	5.50	-1.13	70.96
FCCH	$^{2}J_{CH}$	PBE0/pc-2	B3LYP/pcJ-2	67.39	1.17	6.17	-1.13	73.60
FCCH	$^{2}J_{CH}$	PBE0/pc-2	PBE0/pcJ-2	64.32	1.24	6.16	-1.12	70.60
FCCH	$^{2}J_{CH}$	PBE0/pc-2	M06L/pcJ-2	65.27	1.27	5.46	-1.12	70.88
FCCH	$^{2}J_{CH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	64.33	1.27	6.18	-1.12	70.66
FCCH	$^{2}J_{CH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	65.36	1.27	5.47	-1.12	70.97
FCCH	$^{2}J_{CH}$	M06L/pc-2	B3LYP/pcJ-2	67.15	1.20	6.23	-1.14	73.44
FCCH	$^{2}J_{CH}$	M06L/pc-2	PBE0/pcJ-2	64.11	1.27	6.22	-1.13	70.47
FCCH	$^{2}J_{CH}$	M06L/pc-2	M06L/pcJ-2	65.02	1.29	5.50	-1.13	70.69
FCCH	$^{2}J_{CH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	64.12	1.30	6.24	-1.13	70.52
FCCH	$^{2}J_{CH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	65.12	1.29	5.51	-1.13	70.80
FCCH	$^{3}J_{FH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	0.43	4.08	16.76	-2.62	18.64
FCCH	$^{3}J_{FH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-1.60	4.23	16.67	-2.62	16.68
FCCH	$^{3}J_{FH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	1.98	4.32	14.38	-2.62	18.06
FCCH	$^{3}J_{FH}$	B3LYP/pc-2	B3LYP/pcJ-2	0.44	4.03	16.61	-2.63	18.45
FCCH	$^{3}J_{FH}$	B3LYP/pc-2	PBE0/pcJ-2	-1.52	4.17	16.52	-2.63	16.55
FCCH	$^{3}J_{FH}$	B3LYP/pc-2	M06L/pcJ-2	1.96	4.27	14.28	-2.64	17.87
FCCH	$^{3}J_{FH}$	PBE0/pc-2	B3LYP/pcJ-2	0.66	4.04	16.80	-2.65	18.84
FCCH	$^{3}J_{FH}$	PBE0/pc-2	PBE0/pcJ-2	-1.28	4.19	16.71	-2.65	16.97
FCCH	$^{3}J_{FH}$	PBE0/pc-2	M06L/pcJ-2	1.94	4.28	14.43	-2.65	18.00
FCCH	$^{3}J_{FH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-1.18	4.19	16.57	-2.65	16.94
FCCH	$^{3}J_{FH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	2.38	4.23	14.37	-2.65	18.33
FCCH	$^{3}J_{FH}$	M06L/pc-2	B3LYP/pcJ-2	0.72	4.12	17.06	-2.67	19.24

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
FCCH	$^{3}J_{FH}$	M06L/pc-2	PBE0/pcJ-2	-1.21	4.28	16.97	-2.67	17.38
FCCH	$^{3}J_{FH}$	M06L/pc-2	M06L/pcJ-2	1.89	4.37	14.65	-2.67	18.24
FCCH	$^{3}J_{FH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-1.11	4.28	16.82	-2.66	17.33
FCCH	$^{3}J_{FH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	2.32	4.31	14.58	-2.67	18.55
FCN	$^{1}J_{CN}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	13.87	-8.11	-5.77	-0.03	-0.05
FCN	$^{1}J_{CN}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	14.86	-8.34	-5.74	-0.03	0.75
FCN	$^{1}J_{CN}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	1.05	-7.34	-4.42	-0.04	-10.75
FCN	$^{1}J_{CN}$	B3LYP/pc-2	B3LYP/pcJ-2	11.79	-7.93	-5.63	-0.03	-1.81
FCN	$^{1}J_{CN}$	B3LYP/pc-2	PBE0/pcJ-2	12.80	-8.15	-5.60	-0.03	-0.98
FCN	$^{1}J_{CN}$	B3LYP/pc-2	M06L/pcJ-2	0.17	-7.21	-4.33	-0.04	-11.41
FCN	$^{1}J_{CN}$	PBE0/pc-2	B3LYP/pcJ-2	10.61	-7.85	-5.49	-0.03	-2.77
FCN	$^{1}J_{CN}$	PBE0/pc-2	PBE0/pcJ-2	11.66	-8.06	-5.47	-0.03	-1.90
FCN	$^{1}J_{CN}$	PBE0/pc-2	M06L/pcJ-2	-0.64	-7.14	-4.22	-0.04	-12.03
FCN	$^{1}J_{CN}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	11.12	-8.08	-5.48	-0.03	-2.47
FCN	$^{1}J_{CN}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-0.81	-7.13	-4.22	-0.04	-12.20
FCN	$^{1}J_{CN}$	M06L/pc-2	B3LYP/pcJ-2	12.10	-7.98	-5.59	-0.03	-1.50
FCN	$^{1}J_{CN}$	M06L/pc-2	PBE0/pcJ-2	13.14	-8.20	-5.56	-0.04	-0.65
FCN	$^{1}J_{CN}$	M06L/pc-2	M06L/pcJ-2	-0.04	-7.22	-4.27	-0.04	-11.57
FCN	$^{1}J_{CN}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	12.64	-8.22	-5.58	-0.04	-1.19
FCN	$^{1}J_{CN}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-0.17	-7.22	-4.28	-0.04	-11.71
FCN	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-490.82	-16.87	-39.79	0.55	-546.94
FCN	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-481.59	-18.82	-41.03	0.55	-540.88
FCN	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-366.33	-13.40	-31.98	0.56	-411.16
FCN	$^{1}J_{CF}$	B3LYP/pc-2	B3LYP/pcJ-2	-484.85	-16.00	-38.26	0.56	-538.55
FCN	$^{1}J_{CF}$	B3LYP/pc-2	PBE0/pcJ-2	-475.73	-17.89	-39.50	0.56	-532.56
FCN	$^{1}J_{CF}$	B3LYP/pc-2	M06L/pcJ-2	-360.25	-12.77	-30.93	0.57	-403.38
FCN	$^{1}J_{CF}$	PBE0/pc-2	B3LYP/pcJ-2	-471.12	-16.44	-39.37	0.56	-526.37
FCN	$^{1}J_{CF}$	PBE0/pc-2	PBE0/pcJ-2	-462.50	-18.32	-40.56	0.56	-520.82
FCN	$^{1}J_{CF}$	PBE0/pc-2	M06L/pcJ-2	-350.26	-13.15	-31.77	0.57	-394.61
FCN	$^{1}J_{CF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-459.80	-18.30	-40.70	0.56	-518.24
FCN	$^{1}J_{CF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-349.78	-13.08	-31.71	0.56	-394.00
FCN	$^{1}J_{CF}$	M06L/pc-2	B3LYP/pcJ-2	-473.87	-17.20	-40.75	0.55	-531.27
FCN	$^{1}J_{CF}$	M06L/pc-2	PBE0/pcJ-2	-465.23	-19.11	-41.93	0.55	-525.73
FCN	$^{1}J_{CF}$	M06L/pc-2	M06L/pcJ-2	-353.63	-13.71	-32.73	0.56	-399.50
FCN	$^{1}J_{CF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-463.15	-19.07	-42.01	0.55	-523.68
FCN	$^{1}J_{CF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-353.61	-13.61	-32.62	0.56	-399.29
FCN	$^{2}J_{NF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	52.45	-15.24	16.16	0.41	53.78
FCN	$^{2}J_{NF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	50.46	-15.39	16.73	0.41	52.21
FCN	$^{2}J_{NF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	42.03	-12.94	16.97	0.41	46.48
FCN	$^{2}J_{NF}$	B3LYP/pc-2	B3LYP/pcJ-2	52.48	-14.86	15.99	0.42	54.03
FCN	$^{2}J_{NF}$	B3LYP/pc-2	PBE0/pcJ-2	50.47	-14.99	16.58	0.42	52.48
FCN	$^{2}J_{NF}$	B3LYP/pc-2	M06L/pcJ-2	42.58	-12.67	16.81	0.42	47.14
FCN	$^{2}J_{NF}$	PBE0/pc-2	B3LYP/pcJ-2	52.77	-15.19	14.90	0.42	52.91
FCN	$^{2}J_{NF}$	PBE0/pc-2	PBE0/pcJ-2	50.75	-15.32	15.50	0.42	51.36
FCN	$^{2}J_{NF}$	PBE0/pc-2	M06L/pcJ-2	42.73	-12.93	15.98	0.42	46.21
FCN	$^{2}J_{NF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	50.88	-15.23	15.56	0.42	51.63
FCN	$^{2}J_{NF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	43.13	-12.89	15.97	0.42	46.63
FCN	$^{2}J_{NF}$	M06L/pc-2	B3LYP/pcJ-2	52.81	-15.54	14.86	0.42	52.55
FCN	$^{2}J_{NF}$	M06L/pc-2	PBE0/pcJ-2	50.80	-15.69	15.46	0.42	50.99

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
FCN	$^{2}J_{NF}$	M06L/pc-2	M06L/pcJ-2	42.35	-13.18	15.98	0.42	45.56
FCN	$^{2}J_{NF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	50.92	-15.58	15.56	0.42	51.33
FCN	$^{2}J_{NF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	42.73	-13.13	16.01	0.42	46.04
FNO	$^{1}J_{NF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	147.25	-12.76	54.44	-0.27	188.67
FNO	$^{1}J_{NF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	154.36	-13.87	51.03	-0.27	191.26
FNO	$^{1}J_{NF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	201.19	-9.40	52.79	-0.27	244.31
FNO	$^{1}J_{NF}$	B3LYP/pc-2	B3LYP/pcJ-2	130.87	-13.96	54.32	-0.27	170.97
FNO	$^{1}J_{NF}$	B3LYP/pc-2	PBE0/pcJ-2	139.02	-15.32	50.68	-0.27	174.11
FNO	$^{1}J_{NF}$	B3LYP/pc-2	M06L/pcJ-2	185.53	-10.34	53.13	-0.26	228.06
FNO	$^{1}J_{NF}$	PBE0/pc-2	B3LYP/pcJ-2	167.63	-11.06	53.31	-0.28	209.60
FNO	$^{1}J_{NF}$	PBE0/pc-2	PBE0/pcJ-2	173.81	-11.88	50.20	-0.28	211.85
FNO	$^{1}J_{NF}$	PBE0/pc-2	M06L/pcJ-2	218.07	-8.11	51.40	-0.28	261.08
FNO	$^{1}J_{NF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	171.04	-11.94	49.76	-0.28	208.59
FNO	$^{1}J_{NF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	218.00	-8.12	51.35	-0.28	260.95
FNO	$^{1}J_{NF}$	M06L/pc-2	B3LYP/pcJ-2	113.11	-15.46	55.37	-0.26	152.76
FNO	$^{1}J_{NF}$	M06L/pc-2	PBE0/pcJ-2	122.10	-17.16	51.44	-0.26	156.12
FNO	$^{1}J_{NF}$	M06L/pc-2	M06L/pcJ-2	167.59	-11.46	54.48	-0.26	210.34
FNO	$^{1}J_{NF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	121.23	-17.14	50.86	-0.26	154.69
FNO	$^{1}J_{NF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	169.26	-11.46	54.39	-0.26	211.93
FNO	$^{1}J_{NO}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-23.82	0.22	-19.18	-0.01	-42.78
FNO	$^{1}J_{NO}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-23.17	0.15	-19.06	-0.01	-42.09
FNO	$^{1}J_{NO}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-12.20	1.04	-16.06	-0.01	-27.23
FNO	$^{1}J_{NO}$	B3LYP/pc-2	B3LYP/pcJ-2	-23.11	0.18	-18.95	-0.01	-41.90
FNO	$^{1}J_{NO}$	B3LYP/pc-2	PBE0/pcJ-2	-22.50	0.09	-18.82	-0.01	-41.23
FNO	$^{1}J_{NO}$	B3LYP/pc-2	M06L/pcJ-2	-11.84	0.98	-15.97	-0.01	-26.83
FNO	$^{1}J_{NO}$	PBE0/pc-2	B3LYP/pcJ-2	-23.35	0.10	-19.07	-0.01	-42.32
FNO	$^{1}J_{NO}$	PBE0/pc-2	PBE0/pcJ-2	-22.76	0.01	-18.97	-0.01	-41.72
FNO	$^{1}J_{NO}$	PBE0/pc-2	M06L/pcJ-2	-12.06	0.91	-15.95	-0.01	-27.11
FNO	$^{1}J_{NO}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-22.05	0.12	-18.77	-0.01	-40.71
FNO	$^{1}J_{NO}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-11.87	0.91	-15.87	-0.01	-26.84
FNO	$^{1}J_{NO}$	M06L/pc-2	B3LYP/pcJ-2	-23.11	0.20	-18.97	-0.01	-41.90
FNO	$^{1}J_{NO}$	M06L/pc-2	PBE0/pcJ-2	-22.47	0.11	-18.82	-0.01	-41.19
FNO	$^{1}J_{NO}$	M06L/pc-2	M06L/pcJ-2	-11.81	1.01	-16.02	-0.01	-26.84
FNO	$^{1}J_{NO}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-21.88	0.23	-18.63	-0.01	-40.30
FNO	$^{1}J_{NO}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-11.68	1.01	-15.95	-0.01	-26.63
FNO	$^{2}J_{OF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-21.69	7.70	206.55	0.26	192.82
FNO	$^{2}J_{OF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-23.20	9.61	204.88	0.26	191.56
FNO	$^{2}J_{OF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-61.52	1.74	157.39	0.26	97.87
FNO	$^{2}J_{OF}$	B3LYP/pc-2	B3LYP/pcJ-2	-20.86	5.17	205.05	0.26	189.63
FNO	$^{2}J_{OF}$	B3LYP/pc-2	PBE0/pcJ-2	-22.38	6.65	203.08	0.26	187.61
FNO	$^{2}J_{OF}$	B3LYP/pc-2	M06L/pcJ-2	-61.61	-0.22	156.37	0.26	94.80
FNO	$^{2}J_{OF}$	PBE0/pc-2	B3LYP/pcJ-2	-21.59	9.67	201.71	0.28	190.07
FNO	$^{2}J_{OF}$	PBE0/pc-2	PBE0/pcJ-2	-23.09	11.80	200.26	0.28	189.25
FNO	$^{2}J_{OF}$	PBE0/pc-2	M06L/pcJ-2	-59.59	3.74	154.13	0.28	98.56
FNO	$^{2}J_{OF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-22.24	11.26	199.14	0.28	188.44
FNO	$^{2}J_{OF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-58.77	3.53	153.82	0.28	98.85
FNO	$^{2}J_{OF}$	M06L/pc-2	B3LYP/pcJ-2	-20.45	2.60	207.50	0.25	189.91
FNO	$^{2}J_{OF}$	M06L/pc-2	PBE0/pcJ-2	-21.99	3.62	205.24	0.25	187.13
FNO	$^{2}J_{OF}$	M06L/pc-2	M06L/pcJ-2	-62.53	-2.37	158.09	0.25	93.44

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
FNO	$^{2}J_{OF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-21.44	3.22	203.96	0.25	186.00
FNO	$^{2}J_{OF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-62.09	-2.49	157.86	0.25	93.53
H_2CO	$^{1}J_{CO}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	14.59	-2.68	23.55	0.01	35.46
H_2CO	$^{1}J_{CO}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	14.84	-3.14	23.40	0.01	35.11
H_2CO	$^{1}J_{CO}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-1.71	-3.03	19.35	0.00	14.61
H_2CO	$^{1}J_{CO}$	B3LYP/pc-2	B3LYP/pcJ-2	13.47	-2.63	23.13	0.01	33.97
H_2CO	$^{1}J_{CO}$	B3LYP/pc-2	PBE0/pcJ-2	13.76	-3.04	22.97	0.01	33.70
H_2CO	$^{1}J_{CO}$	B3LYP/pc-2	M06L/pcJ-2	-2.19	-2.98	19.03	0.00	13.87
H_2CO	$^{1}J_{CO}$	PBE0/pc-2	B3LYP/pcJ-2	12.68	-2.58	22.97	0.01	33.08
H_2CO	$^{1}J_{CO}$	PBE0/pc-2	PBE0/pcJ-2	13.01	-2.98	22.81	0.01	32.86
H_2CO	$^{1}J_{CO}$	PBE0/pc-2	M06L/pcJ-2	-2.57	-2.93	18.92	0.00	13.42
H_2CO	$^{1}J_{CO}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	12.90	-2.96	22.80	0.01	32.74
H_2CO	$^{1}J_{CO}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-2.55	-2.88	18.93	0.00	13.51
H_2CO	$^{1}J_{CO}$	M06L/pc-2	B3LYP/pcJ-2	12.53	-2.59	22.73	0.01	32.69
H_2CO	$^{1}J_{CO}$	M06L/pc-2	PBE0/pcJ-2	12.87	-2.97	22.58	0.01	32.49
H_2CO	$^{1}J_{CO}$	M06L/pc-2	M06L/pcJ-2	-2.60	-2.94	18.74	0.01	13.20
H_2CO	$^{1}J_{CO}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	12.80	-2.96	22.58	0.01	32.42
H_2CO	$^{1}J_{CO}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-2.55	-2.89	18.75	0.01	13.32
H_2CO	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	182.67	0.50	-0.87	0.62	182.93
H_2CO	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	171.35	0.49	-0.94	0.64	171.54
H_2CO	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	213.58	0.37	-0.74	0.65	213.86
H_2CO	$^{1}J_{CH}$	B3LYP/pc-2	B3LYP/pcJ-2	182.38	0.48	-0.85	0.63	182.65
H_2CO	$^{1}J_{CH}$	B3LYP/pc-2	PBE0/pcJ-2	170.98	0.47	-0.92	0.65	171.17
H_2CO	$^{1}J_{CH}$	B3LYP/pc-2	M06L/pcJ-2	212.27	0.36	-0.73	0.66	212.56
H_2CO	$^{1}J_{CH}$	PBE0/pc-2	B3LYP/pcJ-2	182.20	0.47	-0.84	0.64	182.47
H_2CO	$^{1}J_{CH}$	PBE0/pc-2	PBE0/pcJ-2	170.77	0.46	-0.91	0.65	170.96
H_2CO	$^{1}J_{CH}$	PBE0/pc-2	M06L/pcJ-2	211.80	0.36	-0.73	0.67	212.09
H_2CO	$^{1}J_{CH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	171.06	0.46	-0.94	0.65	171.23
H_2CO	$^{1}J_{CH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	212.15	0.36	-0.75	0.66	212.42
H_2CO	$^{1}J_{CH}$	M06L/pc-2	B3LYP/pcJ-2	181.80	0.47	-0.84	0.64	182.08
H_2CO	$^{1}J_{CH}$	M06L/pc-2	PBE0/pcJ-2	170.36	0.46	-0.91	0.65	170.56
H_2CO	$^{1}J_{CH}$	M06L/pc-2	M06L/pcJ-2	210.77	0.35	-0.73	0.67	211.06
H_2CO	$^{1}J_{CH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	170.66	0.45	-0.94	0.65	170.83
H_2CO	$^{1}J_{CH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	211.16	0.36	-0.75	0.66	211.43
H_2CO	$^{2}J_{OH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-5.85	-1.10	3.55	0.50	-2.90
H_2CO	$^{2}J_{OH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-5.36	-1.23	3.58	0.50	-2.50
H_2CO	$^{2}J_{OH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-0.76	-0.78	3.04	0.50	2.01
H_2CO	$^{2}J_{OH}$	B3LYP/pc-2	B3LYP/pcJ-2	-5.96	-1.06	3.45	0.51	-3.07
H_2CO	$^{2}J_{OH}$	B3LYP/pc-2	PBE0/pcJ-2	-5.46	-1.18	3.47	0.51	-2.67
H_2CO	$^{2}J_{OH}$	B3LYP/pc-2	M06L/pcJ-2	-1.06	-0.74	2.95	0.50	1.65
H_2CO	$^{2}J_{OH}$	PBE0/pc-2	B3LYP/pcJ-2	-6.00	-1.05	3.41	0.51	-3.13
H_2CO	$^{2}J_{OH}$	PBE0/pc-2	PBE0/pcJ-2	-5.51	-1.16	3.44	0.51	-2.73
H_2CO	$^{2}J_{OH}$	PBE0/pc-2	M06L/pcJ-2	-1.17	-0.73	2.92	0.51	1.53
H_2CO	$^{2}J_{OH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-5.42	-1.16	3.44	0.51	-2.64
H_2CO	$^{2}J_{OH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-1.10	-0.73	2.93	0.51	1.59
H_2CO	$^{2}J_{OH}$	M06L/pc-2	B3LYP/pcJ-2	-6.06	-1.03	3.35	0.51	-3.23
H_2CO	$^{2}J_{OH}$	M06L/pc-2	PBE0/pcJ-2	-5.57	-1.14	3.37	0.51	-2.82
H_2CO	$^{2}J_{OH}$	M06L/pc-2	M06L/pcJ-2	-1.34	-0.71	2.86	0.51	1.32
H_2CO	$^{2}J_{OH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-5.48	-1.13	3.38	0.51	-2.73

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
H_2CO	$^2J_{OH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-1.26	-0.71	2.87	0.51	1.40
H_2CO	$^2J_{HH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	44.19	0.39	3.61	-3.54	44.65
H_2CO	$^2J_{HH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	40.20	0.42	3.60	-3.53	40.69
H_2CO	$^2J_{HH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	31.56	0.47	3.55	-3.52	32.06
H_2CO	$^2J_{HH}$	B3LYP/pc-2	B3LYP/pcJ-2	45.10	0.40	3.51	-3.44	45.57
H_2CO	$^2J_{HH}$	B3LYP/pc-2	PBE0/pcJ-2	41.04	0.43	3.50	-3.43	41.53
H_2CO	$^2J_{HH}$	B3LYP/pc-2	M06L/pcJ-2	31.88	0.48	3.45	-3.42	32.39
H_2CO	$^2J_{HH}$	PBE0/pc-2	B3LYP/pcJ-2	45.84	0.40	3.50	-3.43	46.31
H_2CO	$^2J_{HH}$	PBE0/pc-2	PBE0/pcJ-2	41.73	0.42	3.49	-3.42	42.22
H_2CO	$^2J_{HH}$	PBE0/pc-2	M06L/pcJ-2	32.46	0.47	3.44	-3.41	32.96
H_2CO	$^2J_{HH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	41.90	0.42	3.47	-3.43	42.35
H_2CO	$^2J_{HH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	33.02	0.46	3.42	-3.42	33.49
H_2CO	$^2J_{HH}$	M06L/pc-2	B3LYP/pcJ-2	45.10	0.42	3.40	-3.33	45.59
H_2CO	$^2J_{HH}$	M06L/pc-2	PBE0/pcJ-2	41.02	0.45	3.39	-3.31	41.54
H_2CO	$^2J_{HH}$	M06L/pc-2	M06L/pcJ-2	31.23	0.49	3.34	-3.31	31.76
H_2CO	$^2J_{HH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	41.16	0.44	3.37	-3.33	41.65
H_2CO	$^2J_{HH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	31.77	0.49	3.33	-3.32	32.26
H_2O	$^1J_{OH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-61.63	-0.55	-13.02	-0.03	-75.23
H_2O	$^1J_{OH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-58.39	-0.42	-12.80	-0.03	-71.64
H_2O	$^1J_{OH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-87.75	-0.47	-11.51	-0.03	-99.76
H_2O	$^1J_{OH}$	B3LYP/pc-2	B3LYP/pcJ-2	-61.77	-0.54	-12.92	-0.03	-75.25
H_2O	$^1J_{OH}$	B3LYP/pc-2	PBE0/pcJ-2	-58.53	-0.41	-12.71	-0.03	-71.68
H_2O	$^1J_{OH}$	B3LYP/pc-2	M06L/pcJ-2	-87.95	-0.46	-11.42	-0.03	-99.85
H_2O	$^1J_{OH}$	PBE0/pc-2	B3LYP/pcJ-2	-62.38	-0.56	-13.00	-0.03	-75.97
H_2O	$^1J_{OH}$	PBE0/pc-2	PBE0/pcJ-2	-59.11	-0.43	-12.78	-0.03	-72.36
H_2O	$^1J_{OH}$	PBE0/pc-2	M06L/pcJ-2	-88.35	-0.48	-11.49	-0.03	-100.35
H_2O	$^1J_{OH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-60.27	-0.56	-12.60	-0.03	-73.46
H_2O	$^1J_{OH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-89.04	-0.56	-11.41	-0.03	-101.04
H_2O	$^1J_{OH}$	M06L/pc-2	B3LYP/pcJ-2	-61.81	-0.57	-13.10	-0.03	-75.50
H_2O	$^1J_{OH}$	M06L/pc-2	PBE0/pcJ-2	-58.55	-0.44	-12.88	-0.03	-71.90
H_2O	$^1J_{OH}$	M06L/pc-2	M06L/pcJ-2	-87.82	-0.48	-11.59	-0.03	-99.91
H_2O	$^1J_{OH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-59.76	-0.57	-12.70	-0.03	-73.06
H_2O	$^1J_{OH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-88.55	-0.57	-11.50	-0.03	-100.65
H_2O	$^2J_{HH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-10.49	0.93	9.57	-7.20	-7.19
H_2O	$^2J_{HH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-10.51	0.96	9.52	-7.21	-7.23
H_2O	$^2J_{HH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-18.06	0.90	9.11	-7.21	-15.26
H_2O	$^2J_{HH}$	B3LYP/pc-2	B3LYP/pcJ-2	-9.69	0.89	9.64	-7.29	-6.45
H_2O	$^2J_{HH}$	B3LYP/pc-2	PBE0/pcJ-2	-9.76	0.92	9.60	-7.30	-6.54
H_2O	$^2J_{HH}$	B3LYP/pc-2	M06L/pcJ-2	-17.21	0.86	9.18	-7.30	-14.48
H_2O	$^2J_{HH}$	PBE0/pc-2	B3LYP/pcJ-2	-10.03	0.91	9.68	-7.30	-6.74
H_2O	$^2J_{HH}$	PBE0/pc-2	PBE0/pcJ-2	-10.08	0.94	9.63	-7.31	-6.82
H_2O	$^2J_{HH}$	PBE0/pc-2	M06L/pcJ-2	-17.57	0.88	9.21	-7.32	-14.79
H_2O	$^2J_{HH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-10.25	0.97	9.62	-7.29	-6.95
H_2O	$^2J_{HH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-17.74	0.88	9.22	-7.29	-14.92
H_2O	$^2J_{HH}$	M06L/pc-2	B3LYP/pcJ-2	-11.01	0.96	9.55	-7.16	-7.67
H_2O	$^2J_{HH}$	M06L/pc-2	PBE0/pcJ-2	-11.00	0.99	9.50	-7.17	-7.69
H_2O	$^2J_{HH}$	M06L/pc-2	M06L/pcJ-2	-18.61	0.93	9.08	-7.17	-15.77
H_2O	$^2J_{HH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-11.13	1.02	9.49	-7.16	-7.78
H_2O	$^2J_{HH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-18.73	0.93	9.10	-7.16	-15.86

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
HCCH	$^{1}J_{CC}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	182.08	12.91	8.49	0.01	203.48
HCCH	$^{1}J_{CC}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	174.44	13.59	8.45	0.01	196.48
HCCH	$^{1}J_{CC}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	200.68	13.48	6.56	0.02	220.75
HCCH	$^{1}J_{CC}$	B3LYP/pc-2	B3LYP/pcJ-2	182.85	12.58	8.29	0.01	203.73
HCCH	$^{1}J_{CC}$	B3LYP/pc-2	PBE0/pcJ-2	175.17	13.23	8.24	0.01	196.65
HCCH	$^{1}J_{CC}$	B3LYP/pc-2	M06L/pcJ-2	199.93	13.15	6.45	0.02	219.55
HCCH	$^{1}J_{CC}$	PBE0/pc-2	B3LYP/pcJ-2	182.95	12.59	8.32	0.01	203.87
HCCH	$^{1}J_{CC}$	PBE0/pc-2	PBE0/pcJ-2	175.27	13.24	8.27	0.01	196.79
HCCH	$^{1}J_{CC}$	PBE0/pc-2	M06L/pcJ-2	200.06	13.16	6.47	0.02	219.71
HCCH	$^{1}J_{CC}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	175.15	13.25	8.25	0.01	196.67
HCCH	$^{1}J_{CC}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	199.56	13.08	6.43	0.02	219.09
HCCH	$^{1}J_{CC}$	M06L/pc-2	B3LYP/pcJ-2	182.79	12.57	8.27	0.01	203.64
HCCH	$^{1}J_{CC}$	M06L/pc-2	PBE0/pcJ-2	175.11	13.22	8.22	0.01	196.56
HCCH	$^{1}J_{CC}$	M06L/pc-2	M06L/pcJ-2	199.86	13.14	6.43	0.02	219.44
HCCH	$^{1}J_{CC}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	175.00	13.23	8.21	0.01	196.45
HCCH	$^{1}J_{CC}$	M06L/aug-pc-2	M06L/aug-pcJ-2	199.37	13.06	6.38	0.02	218.83
HCCH	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	272.17	0.53	-0.94	0.29	272.05
HCCH	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	256.82	0.46	-1.12	0.30	256.47
HCCH	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	319.58	0.18	-0.35	0.32	319.74
HCCH	$^{1}J_{CH}$	B3LYP/pc-2	B3LYP/pcJ-2	269.60	0.54	-0.87	0.30	269.57
HCCH	$^{1}J_{CH}$	B3LYP/pc-2	PBE0/pcJ-2	254.32	0.46	-1.04	0.31	254.06
HCCH	$^{1}J_{CH}$	B3LYP/pc-2	M06L/pcJ-2	316.76	0.20	-0.29	0.33	317.00
HCCH	$^{1}J_{CH}$	PBE0/pc-2	B3LYP/pcJ-2	270.16	0.54	-0.85	0.30	270.14
HCCH	$^{1}J_{CH}$	PBE0/pc-2	PBE0/pcJ-2	254.82	0.46	-1.02	0.31	254.57
HCCH	$^{1}J_{CH}$	PBE0/pc-2	M06L/pcJ-2	317.19	0.20	-0.28	0.33	317.45
HCCH	$^{1}J_{CH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	254.87	0.44	-1.03	0.31	254.59
HCCH	$^{1}J_{CH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	316.64	0.21	-0.29	0.33	316.89
HCCH	$^{1}J_{CH}$	M06L/pc-2	B3LYP/pcJ-2	269.25	0.54	-0.88	0.30	269.21
HCCH	$^{1}J_{CH}$	M06L/pc-2	PBE0/pcJ-2	254.02	0.46	-1.05	0.31	253.74
HCCH	$^{1}J_{CH}$	M06L/pc-2	M06L/pcJ-2	316.49	0.20	-0.30	0.33	316.72
HCCH	$^{1}J_{CH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	254.10	0.44	-1.06	0.31	253.80
HCCH	$^{1}J_{CH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	315.96	0.20	-0.31	0.33	316.19
HCCH	$^{2}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	49.83	1.27	6.27	-1.35	56.02
HCCH	$^{2}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	47.12	1.35	6.28	-1.35	53.40
HCCH	$^{2}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	39.87	1.53	5.57	-1.35	45.63
HCCH	$^{2}J_{CH}$	B3LYP/pc-2	B3LYP/pcJ-2	50.09	1.25	6.22	-1.37	56.19
HCCH	$^{2}J_{CH}$	B3LYP/pc-2	PBE0/pcJ-2	47.46	1.33	6.23	-1.36	53.65
HCCH	$^{2}J_{CH}$	B3LYP/pc-2	M06L/pcJ-2	40.45	1.50	5.54	-1.36	46.13
HCCH	$^{2}J_{CH}$	PBE0/pc-2	B3LYP/pcJ-2	50.17	1.24	6.19	-1.36	56.23
HCCH	$^{2}J_{CH}$	PBE0/pc-2	PBE0/pcJ-2	47.53	1.31	6.20	-1.36	53.68
HCCH	$^{2}J_{CH}$	PBE0/pc-2	M06L/pcJ-2	40.54	1.49	5.52	-1.36	46.18
HCCH	$^{2}J_{CH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	47.55	1.35	6.22	-1.36	53.75
HCCH	$^{2}J_{CH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	40.67	1.49	5.54	-1.36	46.34
HCCH	$^{2}J_{CH}$	M06L/pc-2	B3LYP/pcJ-2	50.04	1.26	6.23	-1.37	56.16
HCCH	$^{2}J_{CH}$	M06L/pc-2	PBE0/pcJ-2	47.42	1.34	6.24	-1.37	53.63
HCCH	$^{2}J_{CH}$	M06L/pc-2	M06L/pcJ-2	40.40	1.51	5.56	-1.37	46.10
HCCH	$^{2}J_{CH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	47.45	1.37	6.26	-1.37	53.71
HCCH	$^{2}J_{CH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	40.54	1.51	5.58	-1.36	46.27
HCCH	$^{3}J_{HH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	9.19	0.67	4.89	-3.60	11.15

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
HCCH	$^{3}J_{HH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	10.42	0.72	4.91	-3.59	12.46
HCCH	$^{3}J_{HH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	19.70	0.68	4.71	-3.59	21.49
HCCH	$^{3}J_{HH}$	B3LYP/pc-2	B3LYP/pcJ-2	8.83	0.65	4.90	-3.63	10.75
HCCH	$^{3}J_{HH}$	B3LYP/pc-2	PBE0/pcJ-2	10.03	0.70	4.92	-3.62	12.03
HCCH	$^{3}J_{HH}$	B3LYP/pc-2	M06L/pcJ-2	19.12	0.66	4.73	-3.62	20.88
HCCH	$^{3}J_{HH}$	PBE0/pc-2	B3LYP/pcJ-2	8.88	0.65	4.87	-3.61	10.78
HCCH	$^{3}J_{HH}$	PBE0/pc-2	PBE0/pcJ-2	10.07	0.70	4.89	-3.60	12.05
HCCH	$^{3}J_{HH}$	PBE0/pc-2	M06L/pcJ-2	19.15	0.66	4.70	-3.61	20.90
HCCH	$^{3}J_{HH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	10.06	0.70	4.94	-3.60	12.09
HCCH	$^{3}J_{HH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	18.88	0.66	4.74	-3.60	20.67
HCCH	$^{3}J_{HH}$	M06L/pc-2	B3LYP/pcJ-2	8.81	0.65	4.91	-3.64	10.74
HCCH	$^{3}J_{HH}$	M06L/pc-2	PBE0/pcJ-2	10.00	0.70	4.94	-3.63	12.02
HCCH	$^{3}J_{HH}$	M06L/pc-2	M06L/pcJ-2	19.10	0.66	4.74	-3.63	20.87
HCCH	$^{3}J_{HH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	9.99	0.71	4.99	-3.63	12.06
HCCH	$^{3}J_{HH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	18.82	0.67	4.78	-3.63	20.64
HCN	$^{1}J_{CN}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-9.49	-7.64	-0.77	0.04	-17.86
HCN	$^{1}J_{CN}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-8.04	-8.01	-0.82	0.04	-16.83
HCN	$^{1}J_{CN}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-18.48	-7.88	0.09	0.03	-26.23
HCN	$^{1}J_{CN}$	B3LYP/pc-2	B3LYP/pcJ-2	-11.69	-7.32	-0.62	0.04	-19.59
HCN	$^{1}J_{CN}$	B3LYP/pc-2	PBE0/pcJ-2	-10.18	-7.65	-0.66	0.04	-18.46
HCN	$^{1}J_{CN}$	B3LYP/pc-2	M06L/pcJ-2	-19.44	-7.56	0.17	0.03	-26.80
HCN	$^{1}J_{CN}$	PBE0/pc-2	B3LYP/pcJ-2	-11.72	-7.30	-0.62	0.04	-19.60
HCN	$^{1}J_{CN}$	PBE0/pc-2	PBE0/pcJ-2	-10.21	-7.63	-0.67	0.04	-18.47
HCN	$^{1}J_{CN}$	PBE0/pc-2	M06L/pcJ-2	-19.40	-7.55	0.16	0.03	-26.76
HCN	$^{1}J_{CN}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-10.31	-7.65	-0.68	0.04	-18.61
HCN	$^{1}J_{CN}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-19.44	-7.51	0.18	0.03	-26.73
HCN	$^{1}J_{CN}$	M06L/pc-2	B3LYP/pcJ-2	-11.10	-7.40	-0.66	0.04	-19.12
HCN	$^{1}J_{CN}$	M06L/pc-2	PBE0/pcJ-2	-9.61	-7.74	-0.70	0.04	-18.02
HCN	$^{1}J_{CN}$	M06L/pc-2	M06L/pcJ-2	-19.19	-7.65	0.15	0.03	-26.65
HCN	$^{1}J_{CN}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-9.70	-7.77	-0.72	0.04	-18.15
HCN	$^{1}J_{CN}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-19.21	-7.61	0.17	0.03	-26.62
HCN	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	282.34	0.58	-0.77	0.39	282.53
HCN	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	264.50	0.51	-0.93	0.40	264.49
HCN	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	324.79	0.32	-0.19	0.42	325.34
HCN	$^{1}J_{CH}$	B3LYP/pc-2	B3LYP/pcJ-2	280.23	0.58	-0.68	0.41	280.54
HCN	$^{1}J_{CH}$	B3LYP/pc-2	PBE0/pcJ-2	262.44	0.52	-0.83	0.42	262.55
HCN	$^{1}J_{CH}$	B3LYP/pc-2	M06L/pcJ-2	322.87	0.34	-0.13	0.44	323.52
HCN	$^{1}J_{CH}$	PBE0/pc-2	B3LYP/pcJ-2	280.51	0.58	-0.66	0.41	280.83
HCN	$^{1}J_{CH}$	PBE0/pc-2	PBE0/pcJ-2	262.65	0.52	-0.81	0.42	262.78
HCN	$^{1}J_{CH}$	PBE0/pc-2	M06L/pcJ-2	322.92	0.35	-0.11	0.44	323.59
HCN	$^{1}J_{CH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	262.92	0.49	-0.82	0.42	263.01
HCN	$^{1}J_{CH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	323.03	0.35	-0.13	0.44	323.69
HCN	$^{1}J_{CH}$	M06L/pc-2	B3LYP/pcJ-2	280.70	0.58	-0.71	0.40	280.97
HCN	$^{1}J_{CH}$	M06L/pc-2	PBE0/pcJ-2	262.91	0.52	-0.86	0.42	262.98
HCN	$^{1}J_{CH}$	M06L/pc-2	M06L/pcJ-2	323.36	0.33	-0.15	0.43	323.98
HCN	$^{1}J_{CH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	263.20	0.49	-0.87	0.41	263.23
HCN	$^{1}J_{CH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	323.48	0.33	-0.16	0.43	324.09
HCN	$^{2}J_{NH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-3.26	-0.90	-3.89	0.62	-7.44
HCN	$^{2}J_{NH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-3.05	-0.96	-3.90	0.62	-7.30

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
HCN	$^{2}J_{NH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	5.36	-1.01	-3.32	0.61	1.65
HCN	$^{2}J_{NH}$	B3LYP/pc-2	B3LYP/pcJ-2	-3.99	-0.88	-3.85	0.63	-8.09
HCN	$^{2}J_{NH}$	B3LYP/pc-2	PBE0/pcJ-2	-3.76	-0.93	-3.85	0.63	-7.92
HCN	$^{2}J_{NH}$	B3LYP/pc-2	M06L/pcJ-2	4.53	-0.98	-3.30	0.63	0.89
HCN	$^{2}J_{NH}$	PBE0/pc-2	B3LYP/pcJ-2	-4.01	-0.87	-3.82	0.63	-8.07
HCN	$^{2}J_{NH}$	PBE0/pc-2	PBE0/pcJ-2	-3.77	-0.92	-3.83	0.63	-7.90
HCN	$^{2}J_{NH}$	PBE0/pc-2	M06L/pcJ-2	4.51	-0.97	-3.28	0.63	0.89
HCN	$^{2}J_{NH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-3.77	-0.94	-3.83	0.63	-7.92
HCN	$^{2}J_{NH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	4.52	-0.97	-3.28	0.63	0.90
HCN	$^{2}J_{NH}$	M06L/pc-2	B3LYP/pcJ-2	-3.80	-0.89	-3.86	0.63	-7.92
HCN	$^{2}J_{NH}$	M06L/pc-2	PBE0/pcJ-2	-3.57	-0.95	-3.87	0.63	-7.76
HCN	$^{2}J_{NH}$	M06L/pc-2	M06L/pcJ-2	4.76	-0.99	-3.31	0.62	1.09
HCN	$^{2}J_{NH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-3.56	-0.96	-3.88	0.63	-7.77
HCN	$^{2}J_{NH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	4.78	-0.99	-3.31	0.62	1.10
HFCO	$^{1}J_{CO}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	14.27	-4.61	12.74	-0.05	22.34
HFCO	$^{1}J_{CO}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	14.51	-4.81	12.54	-0.05	22.18
HFCO	$^{1}J_{CO}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	0.21	-4.26	10.98	-0.06	6.88
HFCO	$^{1}J_{CO}$	B3LYP/pc-2	B3LYP/pcJ-2	13.98	-4.65	12.57	-0.05	21.85
HFCO	$^{1}J_{CO}$	B3LYP/pc-2	PBE0/pcJ-2	14.23	-4.84	12.37	-0.05	21.70
HFCO	$^{1}J_{CO}$	B3LYP/pc-2	M06L/pcJ-2	0.21	-4.26	10.98	-0.06	6.88
HFCO	$^{1}J_{CO}$	PBE0/pc-2	B3LYP/pcJ-2	13.11	-4.53	12.61	-0.05	21.13
HFCO	$^{1}J_{CO}$	PBE0/pc-2	PBE0/pcJ-2	13.39	-4.72	12.41	-0.05	21.03
HFCO	$^{1}J_{CO}$	PBE0/pc-2	M06L/pcJ-2	-0.36	-4.19	10.89	-0.06	6.28
HFCO	$^{1}J_{CO}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	13.31	-4.72	12.41	-0.05	20.95
HFCO	$^{1}J_{CO}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-0.31	-4.17	10.89	-0.06	6.36
HFCO	$^{1}J_{CO}$	M06L/pc-2	B3LYP/pcJ-2	13.76	-4.57	12.59	-0.05	21.73
HFCO	$^{1}J_{CO}$	M06L/pc-2	PBE0/pcJ-2	14.02	-4.76	12.40	-0.05	21.60
HFCO	$^{1}J_{CO}$	M06L/pc-2	M06L/pcJ-2	0.03	-4.22	10.87	-0.06	6.62
HFCO	$^{1}J_{CO}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	13.96	-4.76	12.39	-0.05	21.54
HFCO	$^{1}J_{CO}$	M06L/aug-pc-2	M06L/aug-pcJ-2	0.09	-4.20	10.87	-0.06	6.71
HFCO	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-393.11	-1.04	-52.02	0.71	-445.45
HFCO	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-382.74	-1.71	-50.74	0.71	-434.47
HFCO	$^{1}J_{CF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-313.10	-1.36	-47.96	0.72	-361.71
HFCO	$^{1}J_{CF}$	B3LYP/pc-2	B3LYP/pcJ-2	-396.78	-0.48	-51.01	0.71	-447.55
HFCO	$^{1}J_{CF}$	B3LYP/pc-2	PBE0/pcJ-2	-386.23	-1.11	-49.71	0.71	-436.33
HFCO	$^{1}J_{CF}$	B3LYP/pc-2	M06L/pcJ-2	-317.24	-0.87	-47.21	0.72	-364.61
HFCO	$^{1}J_{CF}$	PBE0/pc-2	B3LYP/pcJ-2	-392.40	-1.04	-51.85	0.72	-444.56
HFCO	$^{1}J_{CF}$	PBE0/pc-2	PBE0/pcJ-2	-382.04	-1.69	-50.58	0.72	-433.58
HFCO	$^{1}J_{CF}$	PBE0/pc-2	M06L/pcJ-2	-312.10	-1.36	-47.81	0.72	-360.55
HFCO	$^{1}J_{CF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-381.94	-1.62	-50.69	0.72	-433.53
HFCO	$^{1}J_{CF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-312.73	-1.30	-47.88	0.72	-361.18
HFCO	$^{1}J_{CF}$	M06L/pc-2	B3LYP/pcJ-2	-394.14	-0.98	-51.86	0.72	-446.26
HFCO	$^{1}J_{CF}$	M06L/pc-2	PBE0/pcJ-2	-383.72	-1.63	-50.58	0.72	-435.21
HFCO	$^{1}J_{CF}$	M06L/pc-2	M06L/pcJ-2	-313.82	-1.31	-47.84	0.72	-362.26
HFCO	$^{1}J_{CF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-383.60	-1.55	-50.69	0.72	-435.13
HFCO	$^{1}J_{CF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-314.44	-1.24	-47.91	0.72	-362.87
HFCO	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	265.93	0.64	-0.85	1.17	266.88
HFCO	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	250.45	0.64	-0.92	1.19	251.36
HFCO	$^{1}J_{CH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	303.63	0.61	-0.73	1.21	304.71

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
HFCO	$^{1}J_{CH}$	B3LYP/pc-2	B3LYP/pcJ-2	268.67	0.63	-0.84	1.16	269.63
HFCO	$^{1}J_{CH}$	B3LYP/pc-2	PBE0/pcJ-2	252.93	0.63	-0.90	1.17	253.84
HFCO	$^{1}J_{CH}$	B3LYP/pc-2	M06L/pcJ-2	305.86	0.61	-0.71	1.19	306.95
HFCO	$^{1}J_{CH}$	PBE0/pc-2	B3LYP/pcJ-2	265.02	0.61	-0.84	1.18	265.98
HFCO	$^{1}J_{CH}$	PBE0/pc-2	PBE0/pcJ-2	249.49	0.61	-0.90	1.20	250.40
HFCO	$^{1}J_{CH}$	PBE0/pc-2	M06L/pcJ-2	301.43	0.59	-0.72	1.22	302.51
HFCO	$^{1}J_{CH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	250.11	0.61	-0.94	1.20	250.97
HFCO	$^{1}J_{CH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	302.61	0.59	-0.76	1.21	303.65
HFCO	$^{1}J_{CH}$	M06L/pc-2	B3LYP/pcJ-2	265.84	0.62	-0.84	1.18	266.80
HFCO	$^{1}J_{CH}$	M06L/pc-2	PBE0/pcJ-2	250.25	0.62	-0.90	1.19	251.16
HFCO	$^{1}J_{CH}$	M06L/pc-2	M06L/pcJ-2	302.25	0.59	-0.71	1.21	303.33
HFCO	$^{1}J_{CH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	250.89	0.61	-0.94	1.19	251.76
HFCO	$^{1}J_{CH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	303.48	0.60	-0.75	1.20	304.53
HFCO	$^{2}J_{OF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-7.27	-4.20	83.13	0.33	72.00
HFCO	$^{2}J_{OF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-8.49	-4.41	82.86	0.33	70.30
HFCO	$^{2}J_{OF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-28.88	-4.04	68.00	0.33	35.42
HFCO	$^{2}J_{OF}$	B3LYP/pc-2	B3LYP/pcJ-2	-6.99	-3.99	82.99	0.33	72.34
HFCO	$^{2}J_{OF}$	B3LYP/pc-2	PBE0/pcJ-2	-8.20	-4.18	82.70	0.33	70.65
HFCO	$^{2}J_{OF}$	B3LYP/pc-2	M06L/pcJ-2	-28.63	-3.90	67.79	0.33	35.60
HFCO	$^{2}J_{OF}$	PBE0/pc-2	B3LYP/pcJ-2	-7.04	-4.10	82.05	0.34	71.24
HFCO	$^{2}J_{OF}$	PBE0/pc-2	PBE0/pcJ-2	-8.27	-4.28	81.79	0.34	69.57
HFCO	$^{2}J_{OF}$	PBE0/pc-2	M06L/pcJ-2	-28.47	-3.96	67.18	0.34	35.10
HFCO	$^{2}J_{OF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-8.17	-4.21	81.24	0.34	69.19
HFCO	$^{2}J_{OF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-27.92	-3.92	66.88	0.34	35.38
HFCO	$^{2}J_{OF}$	M06L/pc-2	B3LYP/pcJ-2	-6.75	-4.09	82.18	0.34	71.67
HFCO	$^{2}J_{OF}$	M06L/pc-2	PBE0/pcJ-2	-7.98	-4.28	81.92	0.34	69.99
HFCO	$^{2}J_{OF}$	M06L/pc-2	M06L/pcJ-2	-28.25	-3.96	67.26	0.34	35.39
HFCO	$^{2}J_{OF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-7.89	-4.22	81.39	0.34	69.62
HFCO	$^{2}J_{OF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-27.71	-3.93	66.98	0.34	35.68
HFCO	$^{2}J_{OH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-10.83	-0.76	0.59	0.52	-10.49
HFCO	$^{2}J_{OH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-10.08	-0.82	0.58	0.52	-9.80
HFCO	$^{2}J_{OH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-7.82	-0.55	0.56	0.51	-7.30
HFCO	$^{2}J_{OH}$	B3LYP/pc-2	B3LYP/pcJ-2	-10.85	-0.76	0.53	0.52	-10.56
HFCO	$^{2}J_{OH}$	B3LYP/pc-2	PBE0/pcJ-2	-10.10	-0.81	0.53	0.52	-9.87
HFCO	$^{2}J_{OH}$	B3LYP/pc-2	M06L/pcJ-2	-7.85	-0.55	0.51	0.52	-7.38
HFCO	$^{2}J_{OH}$	PBE0/pc-2	B3LYP/pcJ-2	-11.13	-0.74	0.58	0.52	-10.78
HFCO	$^{2}J_{OH}$	PBE0/pc-2	PBE0/pcJ-2	-10.37	-0.79	0.57	0.52	-10.07
HFCO	$^{2}J_{OH}$	PBE0/pc-2	M06L/pcJ-2	-8.18	-0.53	0.54	0.51	-7.65
HFCO	$^{2}J_{OH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-10.35	-0.79	0.59	0.52	-10.04
HFCO	$^{2}J_{OH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-8.23	-0.54	0.56	0.51	-7.69
HFCO	$^{2}J_{OH}$	M06L/pc-2	B3LYP/pcJ-2	-11.08	-0.74	0.56	0.52	-10.75
HFCO	$^{2}J_{OH}$	M06L/pc-2	PBE0/pcJ-2	-10.32	-0.79	0.55	0.52	-10.05
HFCO	$^{2}J_{OH}$	M06L/pc-2	M06L/pcJ-2	-8.15	-0.53	0.53	0.51	-7.63
HFCO	$^{2}J_{OH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-10.30	-0.80	0.58	0.51	-10.01
HFCO	$^{2}J_{OH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-8.19	-0.54	0.54	0.51	-7.67
HFCO	$^{2}J_{FH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	206.18	-1.31	-4.97	-1.85	198.06
HFCO	$^{2}J_{FH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	195.04	-1.49	-4.83	-1.84	186.88
HFCO	$^{2}J_{FH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	233.27	-1.50	-5.17	-1.84	224.76
HFCO	$^{2}J_{FH}$	B3LYP/pc-2	B3LYP/pcJ-2	207.23	-1.41	-5.15	-1.78	198.89

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
HFCO	$^{2}J_{FH}$	B3LYP/pc-2	PBE0/pcJ-2	195.99	-1.59	-5.00	-1.78	187.62
HFCO	$^{2}J_{FH}$	B3LYP/pc-2	M06L/pcJ-2	235.27	-1.57	-5.34	-1.78	226.58
HFCO	$^{2}J_{FH}$	PBE0/pc-2	B3LYP/pcJ-2	209.75	-1.27	-4.99	-1.83	201.66
HFCO	$^{2}J_{FH}$	PBE0/pc-2	PBE0/pcJ-2	198.27	-1.45	-4.85	-1.82	190.16
HFCO	$^{2}J_{FH}$	PBE0/pc-2	M06L/pcJ-2	235.68	-1.47	-5.18	-1.82	227.21
HFCO	$^{2}J_{FH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	197.98	-1.38	-5.20	-1.83	189.57
HFCO	$^{2}J_{FH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	236.64	-1.44	-5.45	-1.82	227.92
HFCO	$^{2}J_{FH}$	M06L/pc-2	B3LYP/pcJ-2	209.46	-1.29	-5.12	-1.80	201.24
HFCO	$^{2}J_{FH}$	M06L/pc-2	PBE0/pcJ-2	197.98	-1.47	-4.97	-1.80	189.74
HFCO	$^{2}J_{FH}$	M06L/pc-2	M06L/pcJ-2	235.54	-1.48	-5.31	-1.80	226.96
HFCO	$^{2}J_{FH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	197.61	-1.40	-5.33	-1.80	189.07
HFCO	$^{2}J_{FH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	236.42	-1.46	-5.59	-1.80	227.58
OH_2	$^{1}J_{OF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	145.56	-210.77	-257.22	-0.40	-322.82
OH_2	$^{1}J_{OF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	139.27	-220.69	-263.20	-0.40	-345.01
OH_2	$^{1}J_{OF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	223.06	-183.03	-167.37	-0.40	-127.72
OH_2	$^{1}J_{OF}$	B3LYP/pc-2	B3LYP/pcJ-2	145.95	-209.79	-254.87	-0.40	-319.10
OH_2	$^{1}J_{OF}$	B3LYP/pc-2	PBE0/pcJ-2	139.58	-219.70	-260.90	-0.40	-341.41
OH_2	$^{1}J_{OF}$	B3LYP/pc-2	M06L/pcJ-2	225.12	-181.95	-165.33	-0.39	-122.55
OH_2	$^{1}J_{OF}$	PBE0/pc-2	B3LYP/pcJ-2	188.27	-188.41	-240.75	-0.42	-241.31
OH_2	$^{1}J_{OF}$	PBE0/pc-2	PBE0/pcJ-2	182.08	-195.85	-245.60	-0.41	-259.78
OH_2	$^{1}J_{OF}$	PBE0/pc-2	M06L/pcJ-2	250.16	-163.93	-159.51	-0.41	-73.69
OH_2	$^{1}J_{OF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	183.54	-194.53	-244.04	-0.42	-255.45
OH_2	$^{1}J_{OF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	251.78	-163.29	-158.97	-0.42	-70.90
OH_2	$^{1}J_{OF}$	M06L/pc-2	B3LYP/pcJ-2	146.04	-209.64	-254.53	-0.40	-318.53
OH_2	$^{1}J_{OF}$	M06L/pc-2	PBE0/pcJ-2	139.66	-219.54	-260.57	-0.40	-340.85
OH_2	$^{1}J_{OF}$	M06L/pc-2	M06L/pcJ-2	225.43	-181.78	-165.05	-0.39	-121.80
OH_2	$^{1}J_{OF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	140.49	-219.04	-259.60	-0.40	-338.55
OH_2	$^{1}J_{OF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	226.54	-181.81	-164.75	-0.40	-120.42
OH_2	$^{2}J_{FF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	29.87	711.08	1074.37	-1.01	1814.31
OH_2	$^{2}J_{FF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	24.61	717.54	1059.20	-1.01	1800.34
OH_2	$^{2}J_{FF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	190.47	641.56	802.92	-1.01	1633.94
OH_2	$^{2}J_{FF}$	B3LYP/pc-2	B3LYP/pcJ-2	30.08	726.80	1107.20	-1.04	1863.02
OH_2	$^{2}J_{FF}$	B3LYP/pc-2	PBE0/pcJ-2	24.86	734.20	1091.56	-1.05	1849.56
OH_2	$^{2}J_{FF}$	B3LYP/pc-2	M06L/pcJ-2	188.81	655.17	826.10	-1.05	1669.04
OH_2	$^{2}J_{FF}$	PBE0/pc-2	B3LYP/pcJ-2	36.43	645.67	1022.82	-1.12	1703.79
OH_2	$^{2}J_{FF}$	PBE0/pc-2	PBE0/pcJ-2	33.25	649.28	1008.98	-1.12	1690.39
OH_2	$^{2}J_{FF}$	PBE0/pc-2	M06L/pcJ-2	188.85	583.99	772.18	-1.12	1543.90
OH_2	$^{2}J_{FF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	33.28	642.59	991.24	-1.13	1665.98
OH_2	$^{2}J_{FF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	187.28	583.54	766.48	-1.13	1536.17
OH_2	$^{2}J_{FF}$	M06L/pc-2	B3LYP/pcJ-2	30.17	728.89	1111.68	-1.05	1869.69
OH_2	$^{2}J_{FF}$	M06L/pc-2	PBE0/pcJ-2	24.96	736.42	1095.98	-1.06	1856.30
OH_2	$^{2}J_{FF}$	M06L/pc-2	M06L/pcJ-2	188.64	656.98	829.26	-1.05	1673.82
OH_2	$^{2}J_{FF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	25.65	732.95	1082.41	-1.06	1839.95
OH_2	$^{2}J_{FF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	187.45	660.00	826.98	-1.06	1673.37
OHF	$^{1}J_{OF}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	131.92	-314.36	-552.08	-0.26	-734.78
OHF	$^{1}J_{OF}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	127.38	-325.52	-548.79	-0.26	-747.19
OHF	$^{1}J_{OF}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	193.13	-284.74	-387.75	-0.26	-479.61
OHF	$^{1}J_{OF}$	B3LYP/pc-2	B3LYP/pcJ-2	137.69	-309.96	-546.71	-0.26	-719.25
OHF	$^{1}J_{OF}$	B3LYP/pc-2	PBE0/pcJ-2	133.13	-320.70	-543.36	-0.26	-731.19

Continued on next page

(Continued)

Molecule	Coupling	Geometry optimization method	SSCC calculation method	FC	SD	PSO	DSO	Total
OHF	$^{1}J_{OF}$	B3LYP/pc-2	M06L/pcJ-2	197.83	-280.61	-384.31	-0.26	-467.35
OHF	$^{1}J_{OF}$	PBE0/pc-2	B3LYP/pcJ-2	170.52	-277.90	-513.32	-0.27	-620.97
OHF	$^{1}J_{OF}$	PBE0/pc-2	PBE0/pcJ-2	166.21	-285.50	-509.37	-0.27	-628.93
OHF	$^{1}J_{OF}$	PBE0/pc-2	M06L/pcJ-2	219.08	-251.12	-365.16	-0.27	-397.47
OHF	$^{1}J_{OF}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	167.50	-284.88	-508.21	-0.27	-625.86
OHF	$^{1}J_{OF}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	219.64	-251.22	-365.83	-0.27	-397.67
OHF	$^{1}J_{OF}$	M06L/pc-2	B3LYP/pcJ-2	133.77	-313.69	-551.04	-0.26	-731.23
OHF	$^{1}J_{OF}$	M06L/pc-2	PBE0/pcJ-2	129.19	-324.81	-547.74	-0.26	-743.62
OHF	$^{1}J_{OF}$	M06L/pc-2	M06L/pcJ-2	194.83	-284.13	-387.04	-0.26	-476.61
OHF	$^{1}J_{OF}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	130.13	-324.61	-547.24	-0.26	-741.98
OHF	$^{1}J_{OF}$	M06L/aug-pc-2	M06L/aug-pcJ-2	194.89	-284.69	-388.26	-0.26	-478.32
OHF	$^{1}J_{OH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	-41.50	1.67	6.51	-0.11	-33.43
OHF	$^{1}J_{OH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	-39.67	1.87	6.73	-0.11	-31.18
OHF	$^{1}J_{OH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	-68.82	1.54	3.92	-0.12	-63.48
OHF	$^{1}J_{OH}$	B3LYP/pc-2	B3LYP/pcJ-2	-40.14	1.65	6.17	-0.11	-32.43
OHF	$^{1}J_{OH}$	B3LYP/pc-2	PBE0/pcJ-2	-38.39	1.85	6.39	-0.11	-30.26
OHF	$^{1}J_{OH}$	B3LYP/pc-2	M06L/pcJ-2	-67.82	1.52	3.67	-0.12	-62.75
OHF	$^{1}J_{OH}$	PBE0/pc-2	B3LYP/pcJ-2	-42.75	1.44	4.58	-0.13	-36.86
OHF	$^{1}J_{OH}$	PBE0/pc-2	PBE0/pcJ-2	-40.96	1.63	4.78	-0.14	-34.69
OHF	$^{1}J_{OH}$	PBE0/pc-2	M06L/pcJ-2	-69.56	1.35	2.55	-0.14	-65.81
OHF	$^{1}J_{OH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	-42.06	1.58	4.84	-0.14	-35.77
OHF	$^{1}J_{OH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	-70.21	1.32	2.58	-0.14	-66.46
OHF	$^{1}J_{OH}$	M06L/pc-2	B3LYP/pcJ-2	-41.83	1.67	6.54	-0.11	-33.73
OHF	$^{1}J_{OH}$	M06L/pc-2	PBE0/pcJ-2	-39.98	1.87	6.77	-0.11	-31.46
OHF	$^{1}J_{OH}$	M06L/pc-2	M06L/pcJ-2	-68.96	1.54	3.94	-0.12	-63.59
OHF	$^{1}J_{OH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	-41.19	1.83	6.85	-0.11	-32.61
OHF	$^{1}J_{OH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	-69.72	1.52	3.99	-0.11	-64.32
OHF	$^{2}J_{FH}$	CCSD(T)/aug-cc-pCVQZ	B3LYP/pcJ-2	33.19	-6.73	89.53	-1.98	114.02
OHF	$^{2}J_{FH}$	CCSD(T)/aug-cc-pCVQZ	PBE0/pcJ-2	34.18	-6.74	90.23	-1.99	115.69
OHF	$^{2}J_{FH}$	CCSD(T)/aug-cc-pCVQZ	M06L/pcJ-2	14.18	-6.99	69.23	-1.98	74.44
OHF	$^{2}J_{FH}$	B3LYP/pc-2	B3LYP/pcJ-2	32.53	-6.73	88.62	-2.03	112.39
OHF	$^{2}J_{FH}$	B3LYP/pc-2	PBE0/pcJ-2	33.52	-6.76	89.27	-2.04	113.99
OHF	$^{2}J_{FH}$	B3LYP/pc-2	M06L/pcJ-2	13.94	-6.96	68.68	-2.03	73.63
OHF	$^{2}J_{FH}$	PBE0/pc-2	B3LYP/pcJ-2	32.83	-6.60	84.51	-2.17	108.57
OHF	$^{2}J_{FH}$	PBE0/pc-2	PBE0/pcJ-2	33.51	-6.63	84.99	-2.18	109.69
OHF	$^{2}J_{FH}$	PBE0/pc-2	M06L/pcJ-2	16.58	-6.61	66.54	-2.17	74.34
OHF	$^{2}J_{FH}$	PBE0/aug-pc-2	PBE0/aug-pcJ-2	32.32	-6.39	84.38	-2.19	108.12
OHF	$^{2}J_{FH}$	PBE0/aug-pc-2	M06L/aug-pcJ-2	15.80	-6.53	66.23	-2.18	73.32
OHF	$^{2}J_{FH}$	M06L/pc-2	B3LYP/pcJ-2	32.85	-6.61	89.97	-2.01	114.20
OHF	$^{2}J_{FH}$	M06L/pc-2	PBE0/pcJ-2	33.86	-6.62	90.66	-2.02	115.89
OHF	$^{2}J_{FH}$	M06L/pc-2	M06L/pcJ-2	13.95	-6.86	69.57	-2.01	74.65
OHF	$^{2}J_{FH}$	M06L/aug-pc-2	PBE0/aug-pcJ-2	32.78	-6.37	90.11	-2.02	114.50
OHF	$^{2}J_{FH}$	M06L/aug-pc-2	M06L/aug-pcJ-2	13.26	-6.78	69.30	-2.01	73.77