

The importance of solvent effects in calculations of NMR coupling constants at the doubles corrected Higher Random-Phase Approximation: Supporting Information

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Table S1: SSCC for all the molecules and methods in Hz.

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
Methanol	Chloroform	$^1J_{CH}$	SOPPA	140.11	140.42	140.95	141.28
			HRPA(D)	140.15	140.46	140.98	141.31
			B3LYP	145.63	145.98	146.40	146.76
			BHandH	135.62	135.89	136.24	136.53
			PBE0	135.41	135.71	136.07	136.38
			exp ¹				141.148
Propene	Chloroform	$^2J_{HH}$	SOPPA	-0.23	-0.17	-0.08	-0.02
			HRPA(D)	0.08	0.13	0.21	0.27
			B3LYP	2.58	2.67	2.77	2.85
			BHandH	1.17	1.23	1.34	1.41
			PBE0	1.03	1.10	1.20	1.28
			exp ²				2.24
		$^3J_{HH}$	SOPPA	16.96	16.96	17.08	17.07
			<i>trans</i> HRPA(D)	16.13	16.13	16.26	16.25
			B3LYP	18.36	18.33	18.53	18.51
			BHandH	17.62	17.61	17.75	17.74
			PBE0	18.11	18.09	18.26	18.25
			exp ²				17.03
		$^3J_{HH}$	SOPPA	11.29	11.26	11.36	11.33
			<i>cis</i> HRPA(D)	10.74	10.71	10.82	10.79
			B3LYP	11.89	11.84	12.00	11.95
			BHandH	12.42	12.38	12.52	12.47
			PBE0	11.68	11.63	11.77	11.73
			exp ²				10.089

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Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		$^3J_{HH}$	SOPPA	7.02	7.03	7.01	7.01
		<i>vic</i>	HRPA(D)	6.55	6.55	6.54	6.55
			B3LYP	7.58	7.59	7.57	7.58
			BHandH	7.94	7.95	7.92	7.94
			PBE0	7.59	7.60	7.58	7.60
			exp ²				6.482
	Carbon tetrachloride	$^2J_{HH}$	SOPPA	-0.23	-0.19	-0.13	-0.10
			HRPA(D)	0.08	0.12	0.16	0.20
			B3LYP	2.58	2.64	2.70	2.76
			BHandH	1.17	1.21	1.28	1.33
			PBE0	1.03	1.08	1.14	1.19
			exp ²				2.173
		$^3J_{HH}$	SOPPA	16.96	16.96	17.04	17.04
		<i>trans</i>	HRPA(D)	16.13	16.13	16.22	16.21
			B3LYP	18.36	18.34	18.48	18.46
			BHandH	17.62	17.61	17.71	17.70
			PBE0	18.11	18.10	18.21	18.20
			exp ²				16.98
		$^3J_{HH}$	SOPPA	11.29	11.27	11.34	11.32
		<i>cis</i>	HRPA(D)	10.74	10.72	10.80	10.77
			B3LYP	11.89	11.86	11.97	11.93
			BHandH	12.42	12.39	12.49	12.46
			PBE0	11.68	11.65	11.74	11.71
			exp ²				10.094
		$^3J_{HH}$	SOPPA	7.02	7.02	7.00	7.01

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Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		<i>vic</i>	HRPA(D)	6.55	6.55	6.54	6.55
			B3LYP	7.58	7.58	7.58	7.58
			BHandH	7.94	7.95	7.93	7.94
			PBE0	7.59	7.60	7.58	7.59
			exp ²				6.459
Acetonitrile	Acetone	¹ <i>J_{CC}</i>	SOPPA	62.69	62.03	59.29	58.65
			HRPA(D)	64.74	64.07	61.22	60.58
			B3LYP	63.37	62.75	60.94	60.33
			BHandH	67.25	66.73	64.21	63.71
			PBE0	59.99	59.48	57.62	57.12
			exp ³				56.94
		¹ <i>J_{CH}</i>	SOPPA	135.78	135.89	138.07	138.16
			HRPA(D)	135.47	135.58	137.74	137.82
			B3LYP	140.57	140.68	143.02	143.10
			BHandH	132.32	132.42	134.42	134.50
			PBE0	131.45	131.54	133.70	133.77
			exp ³				136.25
		² <i>J_{CH}</i>	SOPPA	-11.73	-11.91	-11.33	-11.51
			HRPA(D)	-11.25	-11.43	-10.87	-11.05
			B3LYP	-9.62	-9.84	-9.23	-9.45
			BHandH	-11.79	-12.00	-11.32	-11.54
			PBE0	-10.76	-10.97	-10.43	-10.64
			exp ³				-9.94
		¹ <i>J_{CN}</i>	SOPPA	-12.49	-12.62	-14.28	-14.40
			HRPA(D)	-15.78	-15.89	-17.10	-17.21

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			B3LYP	-19.32	-19.23	-21.19	-21.10
			BHandH	-28.98	-28.86	-30.18	-30.05
			PBE0	-18.22	-18.15	-19.96	-19.88
			exp ³				-17.53
		³ J _{NH}	SOPPA	-1.66	-1.66	-1.71	-1.71
			HRPA(D)	-1.45	-1.45	-1.50	-1.50
			B3LYP	-1.74	-1.75	-1.79	-1.80
			BHandH	-2.26	-2.28	-2.33	-2.35
			PBE0	-1.58	-1.59	-1.64	-1.65
			exp ³				-1.69
	Chloroform	¹ J _{CC}	SOPPA	62.69	62.14	60.01	59.47
			HRPA(D)	64.74	64.18	61.96	61.42
			B3LYP	63.37	62.85	61.48	60.97
			BHandH	67.25	66.81	64.85	64.43
			PBE0	59.99	59.55	58.15	57.72
			exp ⁴				56.48
		¹ J _{CH}	SOPPA	135.78	135.87	137.61	137.69
			HRPA(D)	135.47	135.56	137.28	137.35
			B3LYP	140.57	140.66	142.51	142.59
			BHandH	132.32	132.40	133.99	134.06
			PBE0	131.45	131.54	133.24	133.31
			exp ⁴				136.1
		² J _{CH}	SOPPA	-11.73	-11.88	-11.42	-11.57
			HRPA(D)	-11.25	-11.40	-10.95	-11.10
			B3LYP	-9.62	-9.79	-9.32	-9.50

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Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			BHandH	-11.79	-11.96	-11.42	-11.59
			PBE0	-10.76	-10.93	-10.50	-10.67
			exp ⁴				-9.87
		¹ <i>J_{CN}</i>	SOPPA	-12.49	-12.61	-13.97	-14.08
			HRPA(D)	-15.78	-15.88	-16.87	-16.96
			B3LYP	-19.32	-19.25	-20.87	-20.80
			BHandH	-28.98	-28.89	-29.98	-29.89
			PBE0	-18.22	-18.17	-19.66	-19.60
			exp ⁵				-17.8
		² <i>J_{CN}</i>	SOPPA	3.47	3.46	3.03	3.02
			HRPA(D)	2.42	2.41	2.12	2.12
			B3LYP	3.36	3.38	2.85	2.87
			BHandH	2.21	2.23	1.85	1.88
			PBE0	3.22	3.23	2.74	2.76
			exp ⁵				2.9
Acrylonitrile	Carbon tetrachloride	¹ <i>J_{CH}</i> (<i>CH</i>)	SOPPA	177.84	178.42	180.07	180.65
			HRPA(D)	176.58	177.15	178.79	179.37
			B3LYP	179.40	180.07	181.82	182.50
			BHandH	170.57	171.25	172.69	173.39
			PBE0	169.75	170.42	172.00	172.68
			exp ⁶				178.3
		¹ <i>J_{CH}</i> (<i>CH</i> ₂)	SOPPA	167.57	167.59	168.43	168.45
			HRPA(D)	166.71	166.73	167.60	167.62
			B3LYP	172.29	172.33	173.15	173.20
			BHandH	163.28	163.33	164.02	164.07

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Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
	Chloroform	$^1J_{CH}$ (CH)	PBE0	162.30	162.35	163.14	163.19
			exp ⁶				166.0
			SOPPA	177.84	178.69	181.19	182.06
			HRPA(D)	176.58	177.42	179.90	180.77
			B3LYP	179.40	180.39	183.07	184.08
			BHandH	170.57	171.58	173.78	174.81
			PBE0	169.75	170.73	173.16	174.17
			exp ⁶				179.0
		$^1J_{CH}$ (CH_2)	SOPPA	167.57	167.59	168.95	168.96
			HRPA(D)	166.71	166.74	168.13	168.14
			B3LYP	172.29	172.36	173.67	173.73
			BHandH	163.28	163.36	164.46	164.54
			PBE0	162.30	162.38	163.64	163.70
			exp ⁶				166.5
	THF	$^1J_{CH}$ (CH)	SOPPA	177.84	178.79	181.54	182.50
			HRPA(D)	176.58	177.52	180.25	181.22
			B3LYP	179.40	180.50	183.46	184.59
			BHandH	170.57	171.69	174.11	175.26
			PBE0	169.75	170.84	173.53	174.64
			exp ⁶				179.7
		$^1J_{CH}$ (CH_2)	SOPPA	167.57	167.59	169.12	169.13
			HRPA(D)	166.71	166.74	168.30	168.31
			B3LYP	172.29	172.36	173.84	173.91
			BHandH	163.28	163.37	164.61	164.69
			PBE0	162.30	162.39	163.80	163.87

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Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent	
	3-Pentanone		exp ⁶				165.5	
			¹ J _{CH}	SOPPA	177.84	178.88	181.90	182.96
			(CH)	HRPA(D)	176.58	177.61	180.61	181.67
				B3LYP	179.40	180.60	183.87	185.11
				BHandH	170.57	171.80	174.46	175.73
				PBE0	169.75	170.95	173.90	175.13
			exp ⁶					179.2
			¹ J _{CH}	SOPPA	167.57	167.59	169.30	169.31
			(CH ₂)	HRPA(D)	166.71	166.74	168.48	168.49
				B3LYP	172.29	172.37	174.03	174.09
				BHandH	163.28	163.37	164.77	164.85
				PBE0	162.30	162.39	163.98	164.05
		DMSO		exp ⁶				
	¹ J _{CH}			SOPPA	177.84	178.93	182.09	183.20
	(CH)			HRPA(D)	176.58	177.66	180.80	181.91
				B3LYP	179.40	180.66	184.09	185.39
				BHandH	170.57	171.86	174.65	175.98
				PBE0	169.75	171.00	174.11	175.40
			exp ⁶					180.9
			¹ J _{CH}	SOPPA	167.57	167.59	169.40	169.40
			(CH ₂)	HRPA(D)	166.71	166.74	168.59	168.59
				B3LYP	172.29	172.37	174.13	174.20
				BHandH	163.28	163.38	164.86	164.94
				PBE0	162.30	162.40	164.07	164.16
			exp ⁶				165.8	

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Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
Acetaldehyde	Cyclohexane	$^1J_{CH}$	SOPPA	172.83	172.73	175.17	175.08
		(CH)	HRPA(D)	172.85	172.74	175.16	175.06
			B3LYP	176.66	176.66	178.67	178.69
			BHandH	166.51	166.57	168.47	168.55
			PBE0	165.25	165.25	167.18	167.20
			exp ⁷				170.98
		$^1J_{CH}$	SOPPA	128.12	128.01	128.56	128.44
		(CH_3)	HRPA(D)	128.04	127.93	128.47	128.35
			B3LYP	133.36	133.25	133.82	133.71
			BHandH	125.15	125.07	125.53	125.45
			PBE0	124.25	124.17	124.66	124.58
			exp ⁷				126.88
	Chloroform	$^1J_{CH}$	SOPPA	172.83	172.70	176.79	176.68
		(CH)	HRPA(D)	172.85	172.71	176.76	176.64
			B3LYP	176.66	176.67	180.09	180.15
			BHandH	166.51	166.59	169.84	169.96
			PBE0	165.25	165.28	168.53	168.60
			exp ⁷				172.12
		$^1J_{CH}$	SOPPA	128.12	127.95	128.86	128.70
		(CH_3)	HRPA(D)	128.04	127.87	128.77	128.60
			B3LYP	133.36	133.17	134.15	133.97
			BHandH	125.15	125.01	125.81	125.66
			PBE0	124.25	124.10	124.96	124.82
			exp ⁷				127.26
	Acetone	$^1J_{CH}$	SOPPA	172.83	172.68	177.76	177.64

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Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		(CH)	HRPA(D)	172.85	172.70	177.71	177.59
			B3LYP	176.66	176.68	180.95	181.05
			BHandH	166.51	166.61	170.66	170.83
			PBE0	165.25	165.30	169.35	169.46
			exp ⁷				172.58
		¹ J _{CH}	SOPPA	128.12	127.91	129.05	128.85
		(CH ₃)	HRPA(D)	128.04	127.83	128.96	128.75
			B3LYP	133.36	133.12	134.35	134.13
			BHandH	125.15	124.96	125.97	125.79
			PBE0	124.25	124.06	125.15	124.96
			exp ⁷				127.10
	DMSO	¹ J _{CH}	SOPPA	172.83	172.68	177.93	177.82
		(CH)	HRPA(D)	172.85	172.69	177.88	177.77
			B3LYP	176.66	176.69	181.11	181.21
			BHandH	166.51	166.62	170.81	170.99
			PBE0	165.25	165.31	169.49	169.62
			exp ⁷				173.43
		¹ J _{CH}	SOPPA	128.12	127.91	129.08	128.87
		(CH ₃)	HRPA(D)	128.04	127.83	128.99	128.77
			B3LYP	133.36	133.11	134.39	134.15
			BHandH	125.15	124.95	126.01	125.82
			PBE0	124.25	124.05	125.18	124.99
			exp ⁷				127.11
Benzene	Acetone	¹ J _{CH}	SOPPA	162.12	162.36	163.59	163.84
			HRPA(D)	161.59	161.83	163.06	163.30

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Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
Carbon tetrachloride			B3LYP	166.07	166.32	167.48	167.74
			BHandH	156.03	156.31	157.41	157.70
			PBE0	156.12	156.38	157.54	157.80
			exp ⁸				158.8
			SOPPA	162.12	162.25	162.93	163.07
			HRPA(D)	161.59	161.72	162.41	162.54
			B3LYP	166.07	166.20	166.84	166.98
			BHandH	156.03	156.19	156.79	156.95
			PBE0	156.12	156.27	156.90	157.05
			exp ⁸				158.2
			SOPPA	-1.06	-1.06	-0.78	-0.76
			HRPA(D)	-0.52	-0.52	-0.32	-0.30
			B3LYP	0.22	0.23	0.54	0.57
			BHandH	-1.11	-1.11	-0.83	-0.82
Fluoro- benzene	Methanol	⁵ <i>J_{FH}</i>	PBE0	-0.33	-0.33	-0.03	-0.02
			exp ⁹				0.364
			SOPPA	5.06	5.10	5.40	5.45
			HRPA(D)	4.42	4.46	4.71	4.76
			B3LYP	5.49	5.53	5.94	6.01
			BHandH	5.37	5.41	5.64	5.70
		⁴ <i>J_{FH}</i>	PBE0	5.58	5.62	5.96	6.02
			exp ⁹				5.765
			SOPPA	6.01	5.96	7.18	7.17
			HRPA(D)	5.99	5.94	6.98	6.96
			B3LYP	9.30	9.21	10.72	10.68

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Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			BHandH	10.61	10.54	11.89	11.86
			PBE0	7.75	7.67	8.99	8.95
			exp ⁹				9.276
		³ J _{HH} (34 + 45)	SOPPA	8.05	8.02	8.09	8.06
			HRPA(D)	7.62	7.59	7.66	7.63
			B3LYP	8.74	8.71	8.80	8.76
			BHandH	9.46	9.42	9.52	9.48
			PBE0	8.55	8.51	8.61	8.57
			exp ⁹				7.452
		³ J _{HH} (23 + 56)	SOPPA	8.84	8.80	8.95	8.91
			HRPA(D)	8.33	8.29	8.43	8.39
			B3LYP	9.80	9.75	9.94	9.90
			BHandH	10.41	10.36	10.54	10.49
			PBE0	9.59	9.54	9.73	9.68
			exp ⁹				8.371
		⁴ J _{HH} (24 + 46)	SOPPA	0.65	0.65	0.63	0.63
			HRPA(D)	0.68	0.68	0.66	0.66
			B3LYP	0.95	0.94	0.92	0.91
			BHandH	0.53	0.53	0.51	0.51
			PBE0	0.77	0.76	0.75	0.74
			exp ⁹				1.051
		⁴ J _{HH} (35)	SOPPA	1.27	1.26	1.30	1.29
			HRPA(D)	1.20	1.19	1.23	1.22
			B3LYP	1.67	1.66	1.71	1.70
			BHandH	1.12	1.11	1.15	1.14

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Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			PBE0	1.50	1.50	1.54	1.54
			exp ⁹				1.812
			⁴ J _{HH}				
			SOPPA	2.21	2.20	2.32	2.32
			(26)				
			HRPA(D)	2.02	2.01	2.12	2.11
			B3LYP	2.90	2.89	3.03	3.04
			BHandH	2.45	2.44	2.57	2.57
			PBE0	2.66	2.66	2.79	2.79
			exp ⁹				2.779
			⁵ J _{HH}				
			SOPPA	0.90	0.91	0.89	0.89
			HRPA(D)	0.65	0.65	0.64	0.64
			B3LYP	0.51	0.51	0.50	0.50
			BHandH	0.77	0.78	0.75	0.76
			PBE0	0.70	0.71	0.69	0.70
			exp ⁹				0.417
Ethanol		⁵ J _{FH}	SOPPA	-1.06	-1.06	-0.78	-0.77
			HRPA(D)	-0.52	-0.52	-0.32	-0.31
			B3LYP	0.22	0.23	0.54	0.56
			BHandH	-1.11	-1.11	-0.83	-0.82
			PBE0	-0.33	-0.33	-0.03	-0.02
			exp ⁹				0.331
			⁴ J _{FH}				
			SOPPA	5.06	5.10	5.39	5.45
			HRPA(D)	4.42	4.46	4.71	4.75
			B3LYP	5.49	5.53	5.93	6.00
			BHandH	5.37	5.41	5.63	5.69
			PBE0	5.58	5.62	5.95	6.01

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Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent	
			exp ⁹				5.729	
			³ J _{FH}	SOPPA	6.01	5.96	7.17	7.15
				HRPA(D)	5.99	5.94	6.97	6.95
				B3LYP	9.30	9.21	10.70	10.66
				BHandH	10.61	10.54	11.87	11.84
				PBE0	7.75	7.67	8.97	8.94
				exp ⁹				9.165
			³ J _{HH}	SOPPA	8.05	8.02	8.09	8.06
			(34 + 45)	HRPA(D)	7.62	7.59	7.66	7.63
				B3LYP	8.74	8.71	8.80	8.76
				BHandH	9.46	9.42	9.51	9.48
				PBE0	8.55	8.51	8.61	8.57
				exp ⁹				7.454
			³ J _{HH}	SOPPA	8.84	8.80	8.95	8.91
			(23 + 56)	HRPA(D)	8.33	8.29	8.43	8.39
				B3LYP	9.80	9.75	9.94	9.89
				BHandH	10.41	10.36	10.53	10.49
				PBE0	9.59	9.54	9.72	9.68
				exp ⁹				8.350
			⁴ J _{HH}	SOPPA	0.65	0.65	0.63	0.63
			(24 + 46)	HRPA(D)	0.68	0.68	0.66	0.66
				B3LYP	0.95	0.94	0.92	0.91
				BHandH	0.53	0.53	0.51	0.51
				PBE0	0.77	0.76	0.75	0.74
				exp ⁹				1.053

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		$^4J_{HH}$	SOPPA	1.27	1.26	1.30	1.29
		(35)	HRPA(D)	1.20	1.19	1.23	1.22
			B3LYP	1.67	1.66	1.71	1.70
			BHandH	1.12	1.11	1.15	1.14
			PBE0	1.50	1.50	1.54	1.54
			exp ⁹				1.783
		$^4J_{HH}$	SOPPA	2.21	2.20	2.32	2.31
		(26)	HRPA(D)	2.02	2.01	2.12	2.11
			B3LYP	2.90	2.89	3.03	3.04
			BHandH	2.45	2.44	2.57	2.57
			PBE0	2.66	2.66	2.79	2.79
			exp ⁹				2.761
		$^5J_{HH}$	SOPPA	0.90	0.91	0.89	0.89
			HRPA(D)	0.65	0.65	0.64	0.64
			B3LYP	0.51	0.51	0.50	0.50
			BHandH	0.77	0.78	0.75	0.76
			PBE0	0.70	0.71	0.69	0.70
			exp ⁹				0.427
	Chloroform	$^5J_{FH}$	SOPPA	-1.06	-1.06	-0.84	-0.83
			HRPA(D)	-0.52	-0.52	-0.36	-0.35
			B3LYP	0.22	0.22	0.47	0.49
			BHandH	-1.11	-1.11	-0.89	-0.88
			PBE0	-0.33	-0.33	-0.09	-0.08
			exp ⁹				0.325
		$^4J_{FH}$	SOPPA	5.06	5.09	5.33	5.36

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			HRPA(D)	4.42	4.45	4.65	4.68
			B3LYP	5.49	5.52	5.84	5.89
			BHandH	5.37	5.40	5.58	5.62
			PBE0	5.58	5.61	5.88	5.92
			exp ⁹				5.742
			³ J _{FH}				
			SOPPA	6.01	5.97	6.94	6.93
			HRPA(D)	5.99	5.95	6.78	6.76
			B3LYP	9.30	9.23	10.43	10.39
			BHandH	10.61	10.56	11.63	11.60
			PBE0	7.75	7.69	8.73	8.70
			exp ⁹				9.114
			³ J _{HH}				
			SOPPA	8.05	8.02	8.08	8.05
			(34 + 45) HRPA(D)	7.62	7.59	7.65	7.63
			B3LYP	8.74	8.71	8.79	8.76
			BHandH	9.46	9.43	9.50	9.47
			PBE0	8.55	8.52	8.59	8.56
			exp ⁹				7.442
			³ J _{HH}				
			SOPPA	8.84	8.81	8.93	8.90
			(23 + 56) HRPA(D)	8.33	8.30	8.41	8.38
			B3LYP	9.80	9.76	9.91	9.88
			BHandH	10.41	10.37	10.51	10.47
			PBE0	9.59	9.55	9.70	9.66
			exp ⁹				8.362
			⁴ J _{HH}				
			SOPPA	0.65	0.65	0.64	0.63
			(24 + 46) HRPA(D)	0.68	0.68	0.67	0.66

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			B3LYP	0.95	0.94	0.93	0.92
			BHandH	0.53	0.53	0.52	0.51
			PBE0	0.77	0.76	0.75	0.75
			exp ⁹				1.068
		⁴ J _{HH} (35)	SOPPA	1.27	1.26	1.29	1.29
			HRPA(D)	1.20	1.19	1.22	1.22
			B3LYP	1.67	1.66	1.70	1.70
			BHandH	1.12	1.11	1.15	1.14
			PBE0	1.50	1.50	1.54	1.53
			exp ⁹				1.807
		⁴ J _{HH} (26)	SOPPA	2.21	2.20	2.30	2.29
			HRPA(D)	2.02	2.01	2.10	2.09
			B3LYP	2.90	2.89	3.01	3.01
			BHandH	2.45	2.45	2.55	2.55
			PBE0	2.66	2.66	2.76	2.76
			exp ⁹				2.807
		⁵ J _{HH}	SOPPA	0.90	0.91	0.89	0.89
			HRPA(D)	0.65	0.65	0.64	0.64
			B3LYP	0.51	0.51	0.50	0.50
			BHandH	0.77	0.78	0.76	0.76
			PBE0	0.70	0.71	0.69	0.70
			exp ⁹				0.403
	Acetone	⁵ J _{FH}	SOPPA	-1.06	-1.06	-0.78	-0.77
			HRPA(D)	-0.52	-0.52	-0.32	-0.31
			B3LYP	0.22	0.23	0.53	0.56

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			BHandH	-1.11	-1.11	-0.84	-0.82
			PBE0	-0.33	-0.33	-0.04	-0.02
			exp ⁹				0.385
		⁴ J _{FH}	SOPPA	5.06	5.10	5.39	5.44
			HRPA(D)	4.42	4.46	4.71	4.75
			B3LYP	5.49	5.53	5.93	6.00
			BHandH	5.37	5.41	5.63	5.69
			PBE0	5.58	5.62	5.95	6.01
			exp ⁹				5.815
		³ J _{FH}	SOPPA	6.01	5.96	7.16	7.14
			HRPA(D)	5.99	5.94	6.96	6.94
			B3LYP	9.30	9.21	10.69	10.65
			BHandH	10.61	10.54	11.86	11.83
			PBE0	7.75	7.67	8.96	8.93
			exp ⁹				9.338
		³ J _{HH} (34 + 45)	SOPPA	8.05	8.02	8.09	8.06
			HRPA(D)	7.62	7.59	7.66	7.63
			B3LYP	8.74	8.71	8.80	8.76
			BHandH	9.46	9.42	9.51	9.48
			PBE0	8.55	8.51	8.61	8.57
			exp ⁹				7.447
		³ J _{HH} (23 + 56)	SOPPA	8.84	8.80	8.95	8.91
			HRPA(D)	8.33	8.29	8.43	8.39
			B3LYP	9.80	9.75	9.94	9.89
			BHandH	10.41	10.36	10.53	10.49

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum-	vacuum-	solvent-	solvent-
				vacuum	solvent	vacuum	solvent
			PBE0	9.59	9.54	9.72	9.68
			exp ⁹				8.368
		⁴ J _{HH}	SOPPA	0.65	0.65	0.63	0.63
		(24 + 46)	HRPA(D)	0.68	0.68	0.66	0.66
			B3LYP	0.95	0.94	0.92	0.91
			BHandH	0.53	0.53	0.51	0.51
			PBE0	0.77	0.76	0.75	0.74
			exp ⁹				1.047
		⁴ J _{HH}	SOPPA	1.27	1.26	1.30	1.29
		(35)	HRPA(D)	1.20	1.19	1.23	1.22
			B3LYP	1.67	1.66	1.71	1.70
			BHandH	1.12	1.11	1.15	1.14
			PBE0	1.50	1.50	1.54	1.54
			exp ⁹				1.822
		⁴ J _{HH}	SOPPA	2.21	2.20	2.32	2.31
		(26)	HRPA(D)	2.02	2.01	2.12	2.11
			B3LYP	2.90	2.89	3.03	3.03
			BHandH	2.45	2.44	2.57	2.57
			PBE0	2.66	2.66	2.79	2.79
			exp ⁹				2.794
		⁵ J _{HH}	SOPPA	0.90	0.91	0.89	0.89
			HRPA(D)	0.65	0.65	0.64	0.64
			B3LYP	0.51	0.51	0.50	0.50
			BHandH	0.77	0.78	0.75	0.76
			PBE0	0.70	0.71	0.69	0.70

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			exp ⁹				0.419
1,2-difluoro- benzene	Methanol	$^3J_{FF}$	SOPPA	-18.89	-19.44	-18.92	-19.37
			HRPA(D)	-17.01	-17.10	-17.02	-17.04
			B3LYP	-18.41	-19.23	-18.46	-19.19
			BHandH	-13.51	-13.74	-14.27	-14.43
			PBE0	-17.96	-18.59	-18.23	-18.78
			exp ⁹				-20.478
		$^3J_{FH}$	SOPPA	6.93	6.59	8.69	8.39
			HRPA(D)	6.77	6.46	8.26	7.98
			B3LYP	11.04	10.60	13.17	12.79
			BHandH	12.23	11.78	14.18	13.77
			PBE0	9.59	9.20	11.46	11.12
			exp ⁹				10.949
		$^4J_{FH}$ (13 + 26)	SOPPA	6.99	6.91	7.65	7.57
			HRPA(D)	6.13	6.05	6.68	6.61
			B3LYP	7.97	7.86	8.83	8.74
			BHandH	8.50	8.41	9.17	9.09
			PBE0	8.11	8.01	8.87	8.79
			exp ⁹				8.151
		$^4J_{FH}$ (15 + 24)	SOPPA	4.04	4.11	4.34	4.42
			HRPA(D)	3.57	3.63	3.81	3.89
			B3LYP	4.10	4.18	4.47	4.58
			BHandH	4.20	4.28	4.41	4.51
			PBE0	4.23	4.30	4.54	4.64
			exp ⁹				4.531

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum-	vacuum-	solvent-	solvent-
				vacuum	solvent	vacuum	solvent
		$^5J_{FH}$	SOPPA	-2.38	-2.40	-2.25	-2.27
			HRPA(D)	-1.55	-1.56	-1.46	-1.47
			B3LYP	-1.49	-1.51	-1.38	-1.40
			BHandH	-2.69	-2.72	-2.57	-2.59
			PBE0	-1.96	-1.98	-1.85	-1.87
			exp ⁹				-1.388
		$^5J_{HH}$	SOPPA	0.79	0.79	0.77	0.77
			HRPA(D)	0.57	0.57	0.56	0.56
			B3LYP	0.35	0.34	0.34	0.33
			BHandH	0.64	0.64	0.63	0.63
			PBE0	0.53	0.53	0.52	0.52
			exp ⁹				0.269
		$^4J_{HH}$	SOPPA	1.13	1.11	1.12	1.11
			HRPA(D)	1.08	1.07	1.08	1.06
			B3LYP	1.49	1.47	1.49	1.47
			BHandH	0.96	0.95	0.96	0.94
			PBE0	1.32	1.31	1.32	1.31
			exp ⁹				1.591
		$^3J_{HH}$ (34 + 56)	SOPPA	8.81	8.80	8.92	8.92
			HRPA(D)	8.29	8.28	8.40	8.39
			B3LYP	9.71	9.70	9.85	9.84
			BHandH	10.37	10.35	10.50	10.49
			PBE0	9.50	9.48	9.64	9.63
			exp ⁹				8.313
		$^3J_{HH}$	SOPPA	8.20	8.19	8.24	8.24

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum-	vacuum-	solvent-	solvent-
				vacuum	solvent	vacuum	solvent
		(45)	HRPA(D)	7.74	7.74	7.79	7.79
			B3LYP	8.89	8.87	8.96	8.94
			BHandH	9.65	9.64	9.72	9.71
			PBE0	8.69	8.68	8.76	8.75
			exp ⁹				7.628
	Ethanol	³ J _{FF}	SOPPA	-18.89	-19.43	-18.92	-19.37
			HRPA(D)	-17.01	-17.10	-17.02	-17.04
			B3LYP	-18.41	-19.22	-18.46	-19.18
			BHandH	-13.51	-13.74	-14.26	-14.42
			PBE0	-17.96	-18.58	-18.23	-18.77
			exp ⁹				-20.634
		³ J _{FH}	SOPPA	6.93	6.59	8.66	8.37
			HRPA(D)	6.77	6.46	8.24	7.96
			B3LYP	11.04	10.61	13.14	12.77
			BHandH	12.23	11.78	14.15	13.75
			PBE0	9.59	9.20	11.44	11.10
			exp ⁹				10.822
		⁴ J _{FH}	SOPPA	6.99	6.91	7.64	7.57
			(13 + 26) HRPA(D)	6.13	6.05	6.67	6.61
			B3LYP	7.97	7.86	8.82	8.73
			BHandH	8.50	8.41	9.16	9.09
			PBE0	8.11	8.01	8.86	8.78
			exp ⁹				8.063
		⁴ J _{FH}	SOPPA	4.04	4.11	4.33	4.42
			(15 + 24) HRPA(D)	3.57	3.63	3.81	3.88

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			B3LYP	4.10	4.18	4.47	4.57
			BHandH	4.20	4.28	4.41	4.51
			PBE0	4.23	4.30	4.54	4.63
			exp ⁹				4.504
			⁵ J _{FH}				
			SOPPA	-2.38	-2.40	-2.25	-2.27
			HRPA(D)	-1.55	-1.56	-1.46	-1.47
			B3LYP	-1.49	-1.51	-1.38	-1.40
			BHandH	-2.69	-2.72	-2.57	-2.60
			PBE0	-1.96	-1.98	-1.85	-1.88
			exp ⁹				-1.401
			⁵ J _{HH}				
			SOPPA	0.79	0.79	0.77	0.77
			HRPA(D)	0.57	0.57	0.56	0.56
			B3LYP	0.35	0.34	0.34	0.33
			BHandH	0.64	0.64	0.63	0.64
			PBE0	0.53	0.53	0.52	0.52
			exp ⁹				0.262
			⁴ J _{HH}				
			SOPPA	1.13	1.11	1.12	1.11
			HRPA(D)	1.08	1.07	1.08	1.06
			B3LYP	1.49	1.47	1.49	1.47
			BHandH	0.96	0.95	0.96	0.94
			PBE0	1.32	1.31	1.32	1.31
			exp ⁹				1.602
			³ J _{HH}				
			SOPPA	8.81	8.80	8.92	8.91
			(34 + 56) HRPA(D)	8.29	8.28	8.40	8.39
			B3LYP	9.71	9.70	9.85	9.84

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			BHandH	10.37	10.35	10.50	10.49
			PBE0	9.50	9.48	9.64	9.63
			exp ⁹				8.296
		³ J _{HH}	SOPPA	8.20	8.19	8.24	8.24
		(45)	HRPA(D)	7.74	7.74	7.79	7.79
			B3LYP	8.89	8.87	8.96	8.94
			BHandH	9.65	9.64	9.72	9.71
			PBE0	8.69	8.68	8.76	8.74
			exp ⁹				7.609
	Acetone	³ J _{FF}	SOPPA	-18.89	-19.43	-18.92	-19.36
			HRPA(D)	-17.01	-17.09	-17.02	-17.04
			B3LYP	-18.41	-19.21	-18.46	-19.17
			BHandH	-13.51	-13.73	-14.26	-14.41
			PBE0	-17.96	-18.57	-18.22	-18.77
			exp ⁹				-20.781
		³ J _{FH}	SOPPA	6.93	6.59	8.65	8.35
			HRPA(D)	6.77	6.47	8.23	7.95
			B3LYP	11.04	10.61	13.12	12.75
			BHandH	12.23	11.79	14.13	13.73
			PBE0	9.59	9.21	11.42	11.09
			exp ⁹				11.082
		⁴ J _{FH}	SOPPA	6.99	6.91	7.63	7.56
			(13 + 26) HRPA(D)	6.13	6.05	6.67	6.6
			B3LYP	7.97	7.86	8.81	8.73
			BHandH	8.50	8.41	9.15	9.08

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum-	vacuum-	solvent-	solvent-
				vacuum	solvent	vacuum	solvent
			PBE0	8.11	8.01	8.85	8.77
			exp ⁹				8.167
		⁴ J _{FH} (15 + 24)	SOPPA	4.04	4.11	4.33	4.41
			HRPA(D)	3.57	3.62	3.81	3.88
			B3LYP	4.10	4.18	4.47	4.57
			BHandH	4.20	4.27	4.41	4.50
			PBE0	4.23	4.30	4.53	4.63
			exp ⁹				4.586
		⁵ J _{FH}	SOPPA	-2.38	-2.4	-2.25	-2.27
			HRPA(D)	-1.55	-1.56	-1.46	-1.47
			B3LYP	-1.49	-1.51	-1.38	-1.40
			BHandH	-2.69	-2.72	-2.57	-2.60
			PBE0	-1.96	-1.98	-1.85	-1.88
			exp ⁹				-1.367
		⁵ J _{HH}	SOPPA	0.79	0.79	0.77	0.77
			HRPA(D)	0.57	0.57	0.56	0.56
			B3LYP	0.35	0.34	0.34	0.33
			BHandH	0.64	0.64	0.63	0.64
			PBE0	0.53	0.53	0.52	0.52
			exp ⁹				0.264
		⁴ J _{HH}	SOPPA	1.13	1.11	1.12	1.11
			HRPA(D)	1.08	1.07	1.08	1.06
			B3LYP	1.49	1.47	1.49	1.47
			BHandH	0.96	0.95	0.96	0.94
			PBE0	1.32	1.31	1.32	1.31

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent	
		(34 + 56)	exp ⁹				1.601	
			³ J _{HH}	SOPPA	8.81	8.8	8.92	8.91
				HRPA(D)	8.29	8.28	8.4	8.39
				B3LYP	9.71	9.70	9.85	9.84
				BHandH	10.37	10.35	10.50	10.48
				PBE0	9.50	9.48	9.64	9.63
				exp ⁹				8.309
		(45)	³ J _{HH}	SOPPA	8.2	8.19	8.24	8.24
				HRPA(D)	7.74	7.74	7.79	7.79
				B3LYP	8.89	8.87	8.95	8.94
				BHandH	9.65	9.64	9.72	9.71
				PBE0	8.69	8.68	8.76	8.74
				exp ⁹				7.605
1,2-dichloro-ethene	Cyclohexane	² J _{CH}	SOPPA	11.91	12.00	12.10	12.19	
				HRPA(D)	11.40	11.48	11.55	11.64
				B3LYP	18.78	18.91	19.01	19.14
				BHandH	13.18	13.29	13.34	13.46
				PBE0	15.92	16.03	16.11	16.23
				exp ⁸				13.3
1,1,2-trichloro-ethane	Chloroform	¹ J _{CH} (CH)	SOPPA	172.99	173.38	177.59	178.14	
				HRPA(D)	172.71	173.10	177.26	177.82
				B3LYP	182.99	183.53	188.00	188.59
				BHandH	169.35	169.84	173.68	174.21
				PBE0	170.22	170.71	174.79	175.33
				exp ¹⁰				181.89

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		$^1J_{CH}$	SOPPA	152.35	152.55	155.48	155.78
		(CH_2)	HRPA(D)	152.22	152.41	155.32	155.62
			B3LYP	159.36	159.68	162.70	163.05
			BHandH	148.51	148.73	151.45	151.70
			PBE0	148.38	148.61	151.41	151.68
			exp ¹⁰				155.27
	Acetone	$^1J_{CH}$	SOPPA	172.99	173.48	178.66	179.21
		(CH)	HRPA(D)	172.71	173.20	178.32	178.88
			B3LYP	182.99	183.67	189.19	189.96
			BHandH	169.35	169.96	174.69	175.38
			PBE0	170.22	170.83	175.88	176.56
			exp ¹⁰				183.59
		$^1J_{CH}$	SOPPA	152.35	152.60	156.23	156.53
		(CH_2)	HRPA(D)	152.22	152.47	156.07	156.37
			B3LYP	159.36	159.77	163.51	163.98
			BHandH	148.51	148.79	152.17	152.50
			PBE0	148.38	148.68	152.15	152.51
			exp ¹⁰				155.88
	Acetonitrile	$^1J_{CH}$	SOPPA	172.99	173.49	178.81	179.38
		(CH)	HRPA(D)	172.71	173.21	178.47	179.04
			B3LYP	182.99	183.69	189.36	190.16
			BHandH	169.35	169.98	174.84	175.54
			PBE0	170.22	170.85	176.03	176.74
			exp ¹⁰				183.35
		$^1J_{CH}$	SOPPA	152.35	152.61	156.34	156.65

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
	DMSO	(CH ₂)	HRPA(D)	152.22	152.48	156.18	156.48
			B3LYP	159.36	159.78	163.63	164.11
			BHandH	148.51	148.80	152.27	152.61
			PBE0	148.38	148.69	152.25	152.62
			exp ¹⁰				156.25
		(CH)	SOPPA	172.99	173.49	178.85	179.43
			HRPA(D)	172.71	173.21	178.51	179.09
			B3LYP	182.99	183.70	189.40	190.21
			BHandH	169.35	169.98	174.88	175.59
			PBE0	170.22	170.85	176.07	176.79
			exp ¹⁰				184.04
		(CH ₂)	SOPPA	152.35	152.61	156.37	156.68
			HRPA(D)	152.22	152.48	156.21	156.52
			B3LYP	159.36	159.79	163.66	164.15
			BHandH	148.51	148.80	152.30	152.64
			PBE0	148.38	148.69	152.28	152.66
			exp ¹⁰				156.66
1,1,2,2-tetra- chloroethane	Chloroform	¹ J _{CH}	SOPPA	179.20	179.57	182.33	182.78
		(CH)	HRPA(D)	178.80	179.17	181.90	182.35
			B3LYP	190.69	191.10	194.10	194.63
			BHandH	175.44	175.90	178.35	178.91
			PBE0	177.24	177.66	180.38	180.90
			exp ¹⁰				181.15
	Acetone	¹ J _{CH}	SOPPA	179.20	179.65	183.04	183.61
		(CH)	HRPA(D)	178.80	179.26	182.59	183.17

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			B3LYP	190.69	191.20	194.89	195.57
			BHandH	175.44	176.02	179.02	179.74
			PBE0	177.24	177.71	181.10	181.64
			exp ¹⁰				184.08
			SOPPA	179.20	179.66	183.13	183.73
			(CH) HRPA(D)	178.80	179.27	182.69	183.28
			B3LYP	190.69	191.22	195.00	195.71
			BHandH	175.44	176.02	179.11	179.84
			PBE0	177.24	177.76	181.20	181.88
			exp ¹⁰				184.09
	DMSO	¹ J _{CH} (CH)	SOPPA	179.20	179.67	183.16	183.76
			HRPA(D)	178.80	179.27	182.72	183.31
			B3LYP	190.69	191.22	195.03	195.75
			BHandH	175.44	176.03	179.13	179.88
			PBE0	177.24	177.77	181.22	181.91
			exp ¹⁰				185.54
Imidazole	Chloroform	¹ J _{CH} (N \underline{C} N)	SOPPA	212.62	212.76	214.54	214.74
			HRPA(D)	211.08	211.23	213.10	213.3
			B3LYP	220.03	219.98	221.7	221.71
			BHandH	203.88	203.96	205.52	205.66
			PBE0	205.62	205.67	207.25	207.36
			exp ⁸				205.1
		¹ J _{CH} (N \underline{C} C)	SOPPA	194.15	195.02	192.46	193.32
			HRPA(D)	193.11	193.96	191.48	192.34
			B3LYP	201.24	202.07	199.59	200.42

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
	DMSO		BHandH	187.24	188.08	185.63	186.47
			PBE0	188.59	189.41	186.92	187.74
			exp ⁸				188.6
		¹ <i>J_{CH}</i> (<i>N\overline{C}N</i>)	SOPPA	212.62	212.80	215.04	215.32
			HRPA(D)	211.08	211.27	213.62	213.90
			B3LYP	220.03	219.97	222.12	222.17
			BHandH	203.88	203.99	205.93	206.14
			PBE0	205.62	205.68	207.67	207.83
			exp ⁸				206.1
		¹ <i>J_{CH}</i> (<i>N\overline{C}C</i>)	SOPPA	194.15	195.27	191.80	192.92
			HRPA(D)	193.11	194.22	190.85	191.96
			B3LYP	201.24	202.32	198.96	200.03
			BHandH	187.24	188.33	185.02	186.11
			PBE0	188.59	189.66	186.28	187.34
			exp ⁸				187.7
1-methyl- imidazole	Chloroform	¹ <i>J_{CH}</i> (<i>C</i> 2)	SOPPA	209.87	210.18	212.01	212.36
			HRPA(D)	208.41	208.72	210.63	210.98
			B3LYP	217.22	217.33	219.09	219.25
			BHandH	201.23	201.49	203.04	203.35
			PBE0	202.97	203.19	204.79	205.05
			exp ¹¹				206.8
		¹ <i>J_{CH}</i> (<i>C</i> 5)	SOPPA	189.62	189.22	193.10	192.73
			HRPA(D)	189.13	188.73	192.56	192.19
			B3LYP	195.61	195.22	199.40	199.04
			BHandH	182.29	182.00	185.69	185.42

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			PBE0	183.27	182.92	186.89	186.56
			exp ¹¹				188.0
		¹ J _{CH}	SOPPA	138.72	139.07	140.16	140.52
		(CH ₃)	HRPA(D)	138.60	138.96	140.02	140.39
			B3LYP	143.58	143.95	145.07	145.45
			BHandH	134.23	134.53	135.58	135.88
			PBE0	134.01	134.34	135.43	135.76
			exp ¹¹				139.8
		¹ J _{CH}	SOPPA	193.13	193.91	191.77	192.54
		(C4)	HRPA(D)	192.10	192.86	190.80	191.56
			B3LYP	199.91	200.67	198.63	199.38
			BHandH	186.15	186.91	184.94	185.70
			PBE0	187.42	188.17	186.12	186.88
			exp ¹¹				188.2
		² J _{CH}	SOPPA	8.42	8.35	9.14	9.07
		(45)	HRPA(D)	8.37	8.29	9.03	8.96
			B3LYP	10.20	10.11	10.96	10.88
			BHandH	8.49	8.43	9.18	9.13
			PBE0	8.94	8.86	9.69	9.61
			exp ¹¹				10.4
		³ J _{CH}	SOPPA	11.63	11.52	11.43	11.31
		(42)	HRPA(D)	10.78	10.67	10.63	10.51
			B3LYP	12.46	12.33	12.33	12.19
			BHandH	12.40	12.28	12.22	12.09
			PBE0	12.30	12.18	12.15	12.02

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
Pyridine		exp ¹¹					10.4
		¹ J _{CH}	SOPPA	209.87	210.24	212.39	212.83
		(C2)	HRPA(D)	208.41	208.78	211.02	211.46
			B3LYP	217.22	217.35	219.41	219.62
			BHandH	201.23	201.54	203.35	203.73
			PBE0	202.97	203.23	205.10	205.44
		exp ¹¹					204.5
		¹ J _{CH}	SOPPA	189.62	189.13	193.82	193.39
		(C5)	HRPA(D)	189.13	188.65	193.28	192.85
			B3LYP	195.61	195.13	200.20	199.77
			BHandH	182.29	181.93	186.40	186.09
			PBE0	183.27	182.84	187.65	187.27
		exp ¹¹					188.2
		¹ J _{CH}	SOPPA	138.72	139.15	140.46	140.90
		(CH ₃)	HRPA(D)	138.60	139.03	140.31	140.76
			B3LYP	143.58	144.03	145.39	145.85
			BHandH	134.23	134.59	135.85	136.22
			PBE0	134.01	134.41	135.72	136.13
		exp ¹¹					139.5
		¹ J _{CH}	SOPPA	193.13	194.06	191.41	192.34
		(C4)	HRPA(D)	192.10	193.01	190.45	191.37
			B3LYP	199.91	200.83	198.28	199.20
			BHandH	186.15	187.07	184.62	185.54
			PBE0	187.42	188.32	185.78	186.69
		exp ¹¹					187.4

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		$^2J_{CH}$	SOPPA	8.42	8.33	9.28	9.20
		(45)	HRPA(D)	8.37	8.28	9.15	9.07
			B3LYP	10.20	10.09	11.11	11.02
			BHandH	8.49	8.42	9.32	9.26
			PBE0	8.94	8.85	9.83	9.75
			exp ¹¹				10.6
		$^3J_{CH}$	SOPPA	11.63	11.49	11.39	11.24
		(42)	HRPA(D)	10.78	10.65	10.60	10.46
			B3LYP	12.46	12.31	12.30	12.14
			BHandH	12.40	12.26	12.19	12.03
			PBE0	12.30	12.16	12.12	11.97
			exp ¹¹				10.6
	Acetone	$^1J_{CH}$	SOPPA	209.87	210.25	212.48	212.93
		(C2)	HRPA(D)	208.41	208.79	211.11	211.56
			B3LYP	217.22	217.36	219.48	219.71
			BHandH	201.23	201.55	203.42	203.82
			PBE0	202.97	203.24	205.18	205.53
			exp ¹¹				206.7
		$^1J_{CH}$	SOPPA	189.62	189.11	194.00	193.55
		(C5)	HRPA(D)	189.13	188.63	193.45	193.00
			B3LYP	195.61	195.11	200.39	199.95
			BHandH	182.29	181.92	186.57	186.25
			PBE0	183.27	182.82	187.83	187.44
			exp ¹¹				186.2
		$^1J_{CH}$	SOPPA	138.72	139.17	140.53	140.99

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		(CH ₃)	HRPA(D)	138.60	139.05	140.39	140.85
			B3LYP	143.58	144.05	145.46	145.94
			BHandH	134.23	134.60	135.92	136.30
			PBE0	134.01	134.43	135.79	136.21
			exp ¹¹				139.8
		¹ J _{CH}	SOPPA	193.13	194.09	191.32	192.28
		(C4)	HRPA(D)	192.10	193.05	190.36	191.31
			B3LYP	199.91	200.87	198.20	199.15
			BHandH	186.15	187.10	184.54	185.49
			PBE0	187.42	188.36	185.70	186.64
			exp ¹¹				187.1
		² J _{CH}	SOPPA	8.42	8.33	9.31	9.23
		(45)	HRPA(D)	8.37	8.27	9.18	9.10
			B3LYP	10.20	10.09	11.15	11.05
			BHandH	8.49	8.42	9.35	9.28
			PBE0	8.94	8.84	9.87	9.78
			exp ¹¹				10.6
		³ J _{CH}	SOPPA	11.63	11.49	11.38	11.23
		(42)	HRPA(D)	10.78	10.64	10.59	10.44
			B3LYP	12.46	12.30	12.30	12.12
			BHandH	12.40	12.25	12.18	12.02
			PBE0	12.30	12.15	12.11	11.95
			exp ¹¹				10.6
	DMSO	¹ J _{CH}	SOPPA	209.87	210.26	212.56	213.03
		(C2)	HRPA(D)	208.41	208.81	211.19	211.67

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			B3LYP	217.22	217.37	219.55	219.79
			BHandH	201.23	201.57	203.49	203.91
			PBE0	202.97	203.25	205.24	205.60
			exp ¹¹				207.0
		¹ J _{CH} (C5)	SOPPA	189.62	189.10	194.16	193.69
			HRPA(D)	189.13	188.62	193.61	193.14
			B3LYP	195.61	195.10	200.57	200.12
			BHandH	182.29	181.90	186.73	186.39
			PBE0	183.27	182.81	188.00	187.60
			exp ¹¹				189.0
		¹ J _{CH} (CH ₃)	SOPPA	138.72	139.18	140.60	141.07
			HRPA(D)	138.60	139.07	140.45	140.93
			B3LYP	143.58	144.06	145.53	146.03
			BHandH	134.23	134.62	135.98	136.38
			PBE0	134.01	134.44	135.86	136.30
			exp ¹¹				139.8
		¹ J _{CH} (C4)	SOPPA	193.13	194.13	191.23	192.23
			HRPA(D)	192.10	193.08	190.28	191.26
			B3LYP	199.91	200.89	198.12	199.10
			BHandH	186.15	187.14	184.46	185.45
			PBE0	187.42	188.39	185.62	186.59
			exp ¹¹				187.0
		² J _{CH} (45)	SOPPA	8.42	8.33	9.34	9.26
			HRPA(D)	8.37	8.27	9.21	9.12
			B3LYP	10.20	10.09	11.18	11.08

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			BHandH	8.49	8.41	9.38	9.31
			PBE0	8.94	8.84	9.90	9.81
			exp ¹¹				10.7
		³ <i>J_{CH}</i> (42)	SOPPA	11.63	11.48	11.37	11.21
			HRPA(D)	10.78	10.64	10.58	10.43
			B3LYP	12.46	12.30	12.29	12.11
			BHandH	12.40	12.25	12.17	12.00
			PBE0	12.30	12.15	12.11	11.94
			exp ¹¹				10.7
	Water	¹ <i>J_{CH}</i> (<i>C</i> 2)	SOPPA	209.87	210.27	212.59	213.06
			HRPA(D)	208.41	208.81	211.22	211.70
			B3LYP	217.22	217.37	219.57	219.82
			BHandH	201.23	201.57	203.51	203.93
			PBE0	202.97	203.25	205.26	205.63
			exp ¹¹				206.7
		¹ <i>J_{CH}</i> (<i>C</i> 5)	SOPPA	189.62	189.09	194.21	193.74
			HRPA(D)	189.13	188.61	193.66	193.20
			B3LYP	195.61	195.09	200.63	200.18
			BHandH	182.29	181.90	186.78	186.45
			PBE0	183.27	182.80	188.06	187.65
			exp ¹¹				189.5
		¹ <i>J_{CH}</i> (<i>CH</i> ₃)	SOPPA	138.72	139.19	140.62	141.10
			HRPA(D)	138.60	139.08	140.47	140.96
			B3LYP	143.58	144.07	145.56	146.06
			BHandH	134.23	134.63	136.01	136.41

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			PBE0	134.01	134.44	135.88	136.32
			exp ¹¹				140.7
		¹ J _{CH}	SOPPA	193.13	194.14	191.21	192.21
		(C4)	HRPA(D)	192.10	193.09	190.25	191.24
			B3LYP	199.91	200.90	198.09	199.08
			BHandH	186.15	187.14	184.44	185.43
			PBE0	187.42	188.40	185.59	186.57
			exp ¹¹				190.1
		² J _{CH}	SOPPA	8.42	8.33	9.35	9.27
		(45)	HRPA(D)	8.37	8.27	9.22	9.13
			B3LYP	10.20	10.09	11.19	11.09
			BHandH	8.49	8.41	9.39	9.32
			PBE0	8.94	8.84	9.91	9.82
			exp ¹¹				10.3
		³ J _{CH}	SOPPA	11.63	11.48	11.37	11.21
		(42)	HRPA(D)	10.78	10.64	10.58	10.43
			B3LYP	12.46	12.29	12.29	12.11
			BHandH	12.40	12.24	12.17	12.00
			PBE0	12.30	12.15	12.11	11.94
			exp ¹¹				10.3
Triethylamine		¹ J _{CH}	SOPPA	138.72	138.97	139.71	139.96
		(CH ₃)	HRPA(D)	138.60	138.85	139.57	139.83
			B3LYP	143.58	143.83	144.60	144.86
			BHandH	134.23	134.44	135.15	135.36
			PBE0	134.01	134.24	134.98	135.21

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		exp ¹¹					138.6
		¹ J _{CH}	SOPPA	193.13	193.69	192.28	192.83
		(C4)	HRPA(D)	192.10	192.64	191.28	191.83
			B3LYP	199.91	200.45	199.11	199.65
			BHandH	186.15	186.69	185.39	185.93
			PBE0	187.42	187.95	186.60	187.13
		exp ¹¹					187.9
1-methyl- pyrazole	n-Hexane	¹ J _{CH}	SOPPA	189.28	189.77	189.12	189.6
		(C3)	HRPA(D)	188.31	188.8	188.18	188.65
			B3LYP	195.74	196.13	195.47	195.85
			BHandH	183.01	183.38	182.76	183.12
			PBE0	183.64	184.03	183.37	183.75
		exp ¹¹					183.8
		² J _{CH}	SOPPA	5.22	5.20	5.43	5.41
		(C3)	HRPA(D)	5.09	5.06	5.28	5.26
			B3LYP	6.39	6.37	6.60	6.58
			BHandH	4.95	4.93	5.15	5.13
			PBE0	5.23	5.21	5.44	5.42
		exp ¹¹					5.7
		³ J _{CH}	SOPPA	8.49	8.49	8.47	8.48
		(C3)	HRPA(D)	7.81	7.81	7.81	7.81
			B3LYP	8.80	8.78	8.81	8.79
			BHandH	8.72	8.70	8.73	8.71
			PBE0	8.82	8.80	8.82	8.80
		exp ¹¹					8.3

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum-	vacuum-	solvent-	solvent-
				vacuum	solvent	vacuum	solvent
		$^1J_{CH}$	SOPPA	178.16	178.15	178.90	178.90
		(C4)	HRPA(D)	177.61	177.60	178.35	178.34
			B3LYP	185.10	185.12	185.86	185.89
			BHandH	173.24	173.28	173.90	173.96
			PBE0	174.08	174.11	174.79	174.82
			exp ¹¹				174.8
		$^2J_{CH}$	SOPPA	10.79	10.76	10.66	10.63
		(43)	HRPA(D)	10.43	10.40	10.31	10.28
			B3LYP	12.12	12.09	11.99	11.97
			BHandH	10.63	10.60	10.52	10.49
			PBE0	10.87	10.85	10.77	10.74
			exp ¹¹				10.5
		$^2J_{CH}$	SOPPA	7.80	7.84	7.94	7.98
		(45)	HRPA(D)	7.58	7.62	7.71	7.75
			B3LYP	9.30	9.32	9.45	9.47
			BHandH	7.51	7.54	7.67	7.70
			PBE0	8.16	8.18	8.31	8.34
			exp ¹¹				9.0
		$^1J_{CH}$	SOPPA	188.54	188.34	190.83	190.64
		(C5)	HRPA(D)	188.07	187.87	190.33	190.14
			B3LYP	193.28	193.00	195.54	195.26
			BHandH	180.05	179.86	182.11	181.93
			PBE0	181.15	180.91	183.31	183.08
			exp ¹¹				184.9
		$^1J_{CH}$	SOPPA	139.39	139.53	139.92	140.06

Continued on next page

Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		(CH ₃)	HRPA(D)	139.23	139.36	139.75	139.89
			B3LYP	144.21	144.33	144.79	144.91
			BHandH	134.84	134.93	135.35	135.45
			PBE0	134.61	134.71	135.15	135.25
			exp ¹¹				140.6
		¹ J _{CH}	SOPPA	189.28	190.14	188.82	189.67
			(C3)	HRPA(D)	188.31	189.15	187.90
			B3LYP	195.74	196.47	195.06	195.77
			BHandH	183.01	183.68	182.39	183.05
			PBE0	183.64	184.29	182.96	183.60
			exp ¹¹				184.7
	Chloroform	² J _{CH}	SOPPA	5.22	5.17	5.61	5.56
			(C3)	HRPA(D)	5.09	5.03	5.45
			B3LYP	6.39	6.35	6.77	6.74
			BHandH	4.95	4.92	5.32	5.30
			PBE0	5.23	5.21	5.61	5.59
			exp ¹¹				5.7
		³ J _{CH}	SOPPA	8.49	8.48	8.47	8.47
			(C3)	HRPA(D)	7.81	7.81	7.82
			B3LYP	8.80	8.76	8.84	8.79
			BHandH	8.72	8.68	8.74	8.70
			PBE0	8.82	8.78	8.84	8.80
			exp ¹¹				8.3
		¹ J _{CH}	SOPPA	178.16	178.04	179.55	179.39
			(C4)	HRPA(D)	177.61	177.50	178.98
						178.98	178.82

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			B3LYP	185.10	185.11	186.52	186.50
			BHandH	173.24	173.31	174.47	174.52
			PBE0	174.08	174.14	175.39	175.43
			exp ¹¹				175.4
		² <i>J_{CH}</i> (43)	SOPPA	10.79	10.74	10.55	10.50
			HRPA(D)	10.43	10.38	10.20	10.16
			B3LYP	12.12	12.08	11.88	11.84
			BHandH	10.63	10.58	10.42	10.37
			PBE0	10.87	10.83	10.67	10.63
			exp ¹¹				10.2
		² <i>J_{CH}</i> (45)	SOPPA	7.80	7.89	8.03	8.13
			HRPA(D)	7.58	7.66	7.80	7.89
			B3LYP	9.30	9.33	9.56	9.60
			BHandH	7.51	7.55	7.79	7.84
			PBE0	8.16	8.20	8.43	8.47
			exp ¹¹				8.9
		¹ <i>J_{CH}</i> (<i>C</i> 5)	SOPPA	188.54	188.14	192.82	192.48
			HRPA(D)	188.07	187.68	192.29	191.95
			B3LYP	193.28	192.72	197.53	197.02
			BHandH	180.05	179.74	183.90	183.65
			PBE0	181.15	180.74	185.20	184.86
			exp ¹¹				186.3
		¹ <i>J_{CH}</i> (<i>CH</i> ₃)	SOPPA	139.39	139.63	140.35	140.60
			HRPA(D)	139.23	139.47	140.17	140.42
			B3LYP	144.21	144.40	145.27	145.47

Continued on next page

Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
	Pyridine		BHandH	134.84	134.99	135.77	135.93
			PBE0	134.61	134.78	135.60	135.79
			exp ¹¹				139.6
		¹ <i>J_{CH}</i> (<i>C3</i>)	SOPPA	189.28	190.31	188.65	189.67
			HRPA(D)	188.31	189.32	187.73	188.74
			B3LYP	195.74	196.60	194.83	195.67
			BHandH	183.01	183.80	182.18	182.96
			PBE0	183.64	184.43	182.74	183.51
			exp ¹¹				183.7
		² <i>J_{CH}</i> (<i>C3</i>)	SOPPA	5.22	5.16	5.68	5.63
			HRPA(D)	5.09	5.03	5.52	5.46
			B3LYP	6.39	6.35	6.85	6.81
			BHandH	4.95	4.92	5.39	5.37
			PBE0	5.23	5.20	5.68	5.66
			exp ¹¹				5.7
		³ <i>J_{CH}</i> (<i>C3</i>)	SOPPA	8.49	8.48	8.47	8.47
			HRPA(D)	7.81	7.80	7.83	7.82
			B3LYP	8.80	8.75	8.85	8.79
			BHandH	8.72	8.67	8.75	8.70
			PBE0	8.82	8.77	8.85	8.80
			exp ¹¹				8.3
		¹ <i>J_{CH}</i> (<i>C4</i>)	SOPPA	178.16	178.03	179.83	179.65
			HRPA(D)	177.61	177.48	179.26	179.08
			B3LYP	185.10	185.11	186.81	186.79
			BHandH	173.24	173.31	174.73	174.79

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			PBE0	174.08	174.14	175.66	175.70
			exp ¹¹				175.5
		² J _{CH}	SOPPA	10.79	10.73	10.49	10.43
		(43)	HRPA(D)	10.43	10.38	10.15	10.10
			B3LYP	12.12	12.07	11.82	11.77
			BHandH	10.63	10.57	10.37	10.31
			PBE0	10.87	10.82	10.62	10.58
			exp ¹¹				10.6
		² J _{CH}	SOPPA	7.80	7.90	8.07	8.18
		(45)	HRPA(D)	7.58	7.67	7.84	7.94
			B3LYP	9.30	9.34	9.60	9.66
			BHandH	7.51	7.56	7.84	7.89
			PBE0	8.16	8.21	8.47	8.53
			exp ¹¹				8.9
		¹ J _{CH}	SOPPA	188.54	188.05	193.70	193.28
		(C5)	HRPA(D)	188.07	187.58	193.15	192.74
			B3LYP	193.28	192.61	198.43	197.83
			BHandH	180.05	179.68	184.70	184.40
			PBE0	181.15	180.66	186.05	185.64
			exp ¹¹				186.4
		¹ J _{CH}	SOPPA	139.39	139.68	140.53	140.82
		(CH ₃)	HRPA(D)	139.23	139.51	140.35	140.65
			B3LYP	144.21	144.44	145.48	145.73
			BHandH	134.84	135.02	135.95	136.15
			PBE0	134.61	134.81	135.79	136.02

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
	Acetone	exp ¹¹					139.3
		¹ J _{CH}	SOPPA	189.28	190.35	188.60	189.66
		(C3)	HRPA(D)	188.31	189.36	187.69	188.73
			B3LYP	195.74	196.62	194.77	195.64
			BHandH	183.01	183.83	182.13	182.93
			PBE0	183.64	184.46	182.68	183.48
		exp ¹¹					183.7
		² J _{CH}	SOPPA	5.22	5.16	5.70	5.64
		(C3)	HRPA(D)	5.09	5.03	5.54	5.48
			B3LYP	6.39	6.35	6.86	6.83
			BHandH	4.95	4.92	5.41	5.38
			PBE0	5.23	5.20	5.70	5.68
		exp ¹¹					5.7
		³ J _{CH}	SOPPA	8.49	8.48	8.47	8.47
		(C3)	HRPA(D)	7.81	7.80	7.83	7.82
			B3LYP	8.80	8.74	8.85	8.79
			BHandH	8.72	8.67	8.76	8.70
			PBE0	8.82	8.77	8.85	8.80
		exp ¹¹					8.3
		¹ J _{CH}	SOPPA	178.16	178.02	179.90	179.71
		(C4)	HRPA(D)	177.61	177.48	179.33	179.14
			B3LYP	185.10	185.11	186.88	186.86
			BHandH	173.24	173.32	174.79	174.85
			PBE0	174.08	174.13	175.72	175.76
		exp ¹¹					175.3

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		$^2J_{CH}$	SOPPA	10.79	10.73	10.48	10.42
		(43)	HRPA(D)	10.43	10.37	10.14	10.08
			B3LYP	12.12	12.06	11.81	11.76
			BHandH	10.63	10.57	10.36	10.30
			PBE0	10.87	10.82	10.61	10.56
			exp ¹¹				10.5
		$^2J_{CH}$	SOPPA	7.80	7.90	8.08	8.19
		(45)	HRPA(D)	7.58	7.67	7.84	7.95
			B3LYP	9.30	9.34	9.61	9.67
			BHandH	7.51	7.56	7.85	7.90
			PBE0	8.16	8.21	8.48	8.54
			exp ¹¹				9.1
		$^1J_{CH}$	SOPPA	188.54	188.03	193.91	193.47
		(C5)	HRPA(D)	188.07	187.56	193.36	192.93
			B3LYP	193.28	192.59	198.64	198.03
			BHandH	180.05	179.66	184.89	184.58
			PBE0	181.15	180.64	186.26	185.82
			exp ¹¹				186.7
		$^1J_{CH}$	SOPPA	139.39	139.68	140.57	140.88
		(CH ₃)	HRPA(D)	139.23	139.52	140.39	140.70
			B3LYP	144.21	144.45	145.53	145.78
			BHandH	134.84	135.03	135.99	136.19
			PBE0	134.61	134.82	135.84	136.07
			exp ¹¹				139.7
	DMSO	$^1J_{CH}$	SOPPA	189.28	190.38	188.56	189.65

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		(C3)	HRPA(D)	188.31	189.40	187.65	188.72
			B3LYP	195.74	196.65	194.71	195.61
			BHandH	183.01	183.86	182.08	182.91
			PBE0	183.64	184.48	182.63	183.45
			exp ¹¹				183.8
		² J _{CH}	SOPPA	5.22	5.16	5.72	5.66
		(C3)	HRPA(D)	5.09	5.02	5.55	5.50
			B3LYP	6.39	6.35	6.88	6.85
			BHandH	4.95	4.92	5.42	5.40
			PBE0	5.23	5.20	5.72	5.69
			exp ¹¹				5.7
		³ J _{CH}	SOPPA	8.49	8.48	8.48	8.47
		(C3)	HRPA(D)	7.81	7.80	7.83	7.82
			B3LYP	8.80	8.74	8.85	8.79
			BHandH	8.72	8.66	8.76	8.70
			PBE0	8.82	8.77	8.85	8.80
			exp ¹¹				8.3
		¹ J _{CH}	SOPPA	178.16	178.02	179.97	179.77
		(C4)	HRPA(D)	177.61	177.47	179.40	179.20
			B3LYP	185.10	185.11	186.95	186.93
			BHandH	173.24	173.32	174.84	174.91
			PBE0	174.08	174.13	175.78	175.82
			exp ¹¹				175.7
		² J _{CH}	SOPPA	10.79	10.73	10.47	10.40
		(43)	HRPA(D)	10.43	10.37	10.13	10.07

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			B3LYP	12.12	12.06	11.80	11.74
			BHandH	10.63	10.56	10.35	10.29
			PBE0	10.87	10.82	10.60	10.55
			exp ¹¹				9.9
		² <i>J_{CH}</i> (45)	SOPPA	7.80	7.90	8.08	8.20
			HRPA(D)	7.58	7.68	7.85	7.96
			B3LYP	9.30	9.34	9.62	9.68
			BHandH	7.51	7.56	7.86	7.91
			PBE0	8.16	8.21	8.49	8.55
			exp ¹¹				9.4
		¹ <i>J_{CH}</i> (<i>C</i> 5)	SOPPA	188.54	188.01	194.11	193.66
			HRPA(D)	188.07	187.55	193.56	193.11
			B3LYP	193.28	192.57	198.85	198.21
			BHandH	180.05	179.65	185.08	184.76
			PBE0	181.15	180.62	186.45	186.00
			exp ¹¹				186.0
		¹ <i>J_{CH}</i> (<i>CH</i> ₃)	SOPPA	139.39	139.70	140.61	140.93
			HRPA(D)	139.23	139.53	140.43	140.75
			B3LYP	144.21	144.46	145.57	145.84
			BHandH	134.84	135.03	136.03	136.24
			PBE0	134.61	134.83	135.88	136.13
			exp ¹¹				139.7
	Water	¹ <i>J_{CH}</i> (<i>C</i> 3)	SOPPA	189.28	190.40	188.54	189.65
			HRPA(D)	188.31	189.41	187.63	188.72
			B3LYP	195.74	196.66	194.70	195.60

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			BHandH	183.01	183.86	182.06	182.90
			PBE0	183.64	184.49	182.61	183.44
			exp ¹¹				186.0
		² J _{CH}	SOPPA	5.22	5.16	5.72	5.66
		(C3)	HRPA(D)	5.09	5.02	5.56	5.50
			B3LYP	6.39	6.35	6.89	6.85
			BHandH	4.95	4.92	5.43	5.41
			PBE0	5.23	5.20	5.72	5.70
			exp ¹¹				6.2
		³ J _{CH}	SOPPA	8.49	8.48	8.48	8.47
		(C3)	HRPA(D)	7.81	7.80	7.83	7.82
			B3LYP	8.80	8.74	8.85	8.79
			BHandH	8.72	8.66	8.76	8.70
			PBE0	8.82	8.77	8.85	8.80
			exp ¹¹				8.0
		¹ J _{CH}	SOPPA	178.16	178.02	179.99	179.79
		(C4)	HRPA(D)	177.61	177.47	179.42	179.22
			B3LYP	185.10	185.11	186.97	186.95
			BHandH	173.24	173.32	174.86	174.93
			PBE0	174.08	174.13	175.80	175.84
			exp ¹¹				178.3
		² J _{CH}	SOPPA	10.79	10.73	10.46	10.40
		(43)	HRPA(D)	10.43	10.37	10.12	10.06
			B3LYP	12.12	12.06	11.79	11.74
			BHandH	10.63	10.56	10.35	10.28

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			PBE0	10.87	10.82	10.60	10.55
			exp ¹¹				9.5
		² J _{CH}	SOPPA	7.80	7.90	8.09	8.20
		(45)	HRPA(D)	7.58	7.68	7.85	7.97
			B3LYP	9.30	9.34	9.63	9.68
			BHandH	7.51	7.56	7.86	7.92
			PBE0	8.16	8.21	8.50	8.56
			exp ¹¹				9.5
		¹ J _{CH}	SOPPA	188.54	188.00	194.17	193.72
		(C5)	HRPA(D)	188.07	187.54	193.62	193.17
			B3LYP	193.28	192.56	198.91	198.27
			BHandH	180.05	179.64	185.14	184.81
			PBE0	181.15	180.61	186.51	186.06
			exp ¹¹				186.6
		¹ J _{CH}	SOPPA	139.39	139.70	140.63	140.94
		(Me)	HRPA(D)	139.23	139.54	140.44	140.77
			B3LYP	144.21	144.46	145.58	145.86
			BHandH	134.84	135.04	136.04	136.26
			PBE0	134.61	134.83	135.90	136.14
			exp ¹¹				140.9
Triethylamine		¹ J _{CH}	SOPPA	189.28	189.89	189.04	189.64
		(C3)	HRPA(D)	188.31	188.91	188.10	188.69
			B3LYP	195.74	196.28	195.35	195.88
			BHandH	183.01	183.50	182.65	183.14
			PBE0	183.64	184.09	183.26	183.69

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent	
			exp ¹¹				183.8	
			² J _{CH}	SOPPA	5.22	5.18	5.49	5.45
			(C3)	HRPA(D)	5.09	5.05	5.34	5.30
				B3LYP	6.39	6.36	6.65	6.63
				BHandH	4.95	4.93	5.20	5.19
				PBE0	5.23	5.22	5.49	5.48
			exp ¹¹					5.6
			³ J _{CH}	SOPPA	8.49	8.48	8.47	8.47
			(C3)	HRPA(D)	7.81	7.81	7.82	7.81
				B3LYP	8.80	8.77	8.82	8.79
				BHandH	8.72	8.69	8.73	8.70
				PBE0	8.82	8.79	8.83	8.80
			exp ¹¹					8.4
			¹ J _{CH}	SOPPA	178.16	178.07	179.11	178.99
			(C4)	HRPA(D)	177.61	177.52	178.55	178.43
				B3LYP	185.10	185.11	186.07	186.06
				BHandH	173.24	173.29	174.08	174.12
				PBE0	174.08	174.13	174.98	175.02
			exp ¹¹					174.7
			² J _{CH}	SOPPA	10.79	10.76	10.63	10.59
			(43)	HRPA(D)	10.43	10.40	10.28	10.24
				B3LYP	12.12	12.09	11.96	11.93
				BHandH	10.63	10.60	10.49	10.46
				PBE0	10.87	10.85	10.74	10.71
			exp ¹¹					10.6

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		$^2J_{CH}$	SOPPA	7.80	7.87	7.97	8.04
		(45)	HRPA(D)	7.58	7.64	7.74	7.81
			B3LYP	9.30	9.32	9.48	9.52
			BHandH	7.51	7.54	7.71	7.75
			PBE0	8.16	8.18	8.35	8.38
			exp ¹¹				8.9
		$^1J_{CH}$	SOPPA	188.54	188.27	191.47	191.24
		(C5)	HRPA(D)	188.07	187.81	190.96	190.74
			B3LYP	193.28	192.87	196.18	195.80
			BHandH	180.05	179.84	182.68	182.51
			PBE0	181.15	180.87	183.91	183.67
			exp ¹¹				184.3
		$^1J_{CH}$	SOPPA	139.39	139.57	140.07	140.24
		(CH ₃)	HRPA(D)	139.23	139.41	139.89	140.07
			B3LYP	144.21	144.34	144.95	145.09
			BHandH	134.84	134.95	135.49	135.60
			PBE0	134.61	134.73	135.29	135.43
			exp ¹¹				138.6
2-methyl- aziridine	Chloroform	$^3J_{HH}$	SOPPA	6.34	6.34	6.45	6.45
		<i>cis</i>	HRPA(D)	6.19	6.18	6.29	6.29
			B3LYP	6.94	6.96	7.08	7.10
			BHandH	7.04	7.06	7.17	7.19
			PBE0	6.61	6.63	6.75	6.76
			exp ^{12a}				5.5
		$^3J_{HH}$	SOPPA	2.96	3.03	3.04	3.10

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		<i>trans</i>	HRPA(D)	2.89	2.95	2.96	3.02
			B3LYP	3.33	3.43	3.43	3.53
			BHandH	2.94	3.02	3.03	3.11
			PBE0	3.02	3.10	3.11	3.20
			exp ^{12a}				3.5
Spiropentane	Benzene	² <i>J_{HH}</i>	SOPPA	-6.20	-6.14	-6.18	-6.12
			HRPA(D)	-5.93	-5.87	-5.91	-5.85
			B3LYP	-4.31	-4.24	-4.29	-4.22
			BHandH	-5.04	-4.98	-5.04	-4.97
			PBE0	-5.29	-5.23	-5.29	-5.23
			exp ¹³				-3.9
		³ <i>J_{HH}</i>	SOPPA	4.93	4.92	4.94	4.93
			<i>trans</i> HRPA(D)	4.69	4.68	4.70	4.69
			B3LYP	5.58	5.57	5.60	5.58
			BHandH	5.56	5.54	5.57	5.56
			PBE0	5.43	5.41	5.44	5.43
			exp ¹³				5.2
		³ <i>J_{HH}</i>	SOPPA	9.12	9.09	9.14	9.11
			<i>cis</i> HRPA(D)	8.75	8.73	8.77	8.74
			B3LYP	10.03	10.00	10.06	10.03
			BHandH	10.39	10.36	10.43	10.39
			PBE0	9.74	9.71	9.78	9.75
			exp ¹³				8.9
Spirohexane	Benzene	² <i>J_{HH}</i>	SOPPA	-6.79	-6.67	-6.70	-6.59
			HRPA(D)	-6.53	-6.42	-6.45	-6.34

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			B3LYP	-5.23	-5.11	-5.15	-5.03
			BHandH	-5.92	-5.81	-5.85	-5.73
			PBE0	-6.25	-6.14	-6.18	-6.06
			exp ¹³				-4.6
			³ J _{HH}	SOPPA	5.71	5.69	5.72
			<i>trans</i>	HRPA(D)	5.41	5.39	5.42
				B3LYP	6.70	6.67	6.71
				BHandH	6.53	6.50	6.54
				PBE0	6.46	6.43	6.47
				exp ¹³			6.3
			³ J _{HH}	SOPPA	10.02	9.98	10.03
			<i>cis</i>	HRPA(D)	9.57	9.52	9.58
				B3LYP	11.23	11.18	11.26
				BHandH	11.48	11.43	11.51
				PBE0	10.86	10.81	10.89
				exp ¹³			9.7
1,1-dimethyl- cyclopropane	Benzene	² J _{HH}	SOPPA	-6.26	-6.14	-6.17	-6.04
			HRPA(D)	-6.09	-5.96	-5.99	-5.87
			B3LYP	-4.71	-4.57	-4.61	-4.47
			BHandH	-5.16	-5.03	-5.07	-4.94
			PBE0	-5.69	-5.56	-5.60	-5.47
			exp ¹³				-4.5
			³ J _{HH}	SOPPA	5.14	5.11	5.14
			<i>trans</i>	HRPA(D)	4.88	4.86	4.88
			B3LYP	5.95	5.92	5.96	5.93

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent	
			BHandH	5.78	5.75	5.78	5.75	
			PBE0	5.76	5.73	5.76	5.73	
			exp ¹³				5.4	
		³ J _{HH}	SOPPA	9.48	9.44	9.49	9.45	
		<i>cis</i>	HRPA(D)	9.07	9.03	9.08	9.05	
			B3LYP	10.51	10.46	10.53	10.49	
			BHandH	10.73	10.68	10.75	10.71	
			PBE0	10.17	10.13	10.19	10.15	
			exp ¹³				9.2	
		1,1-dichloro- cyclopropane	Benzene	² J _{HH}	SOPPA	-8.56	-8.57	-8.81
HRPA(D)	-8.14				-8.15	-8.37	-8.38	
B3LYP	-7.34				-7.40	-7.63	-7.70	
BHandH	-7.69				-7.74	-7.95	-7.99	
PBE0	-8.15				-8.18	-8.40	-8.44	
exp ¹³							-6.0	
³ J _{HH}	SOPPA			7.48	7.49	7.59	7.60	
	<i>trans</i>			HRPA(D)	7.04	7.04	7.13	7.13
				B3LYP	8.86	8.88	9.00	9.03
				BHandH	8.65	8.67	8.76	8.79
				PBE0	8.59	8.60	8.73	8.73
				exp ¹³				8.0
³ J _{HH}	SOPPA			11.31	11.34	11.46	11.49	
	<i>cis</i>			HRPA(D)	10.68	10.70	10.81	10.83
				B3LYP	13.02	13.06	13.22	13.27
				BHandH	13.17	13.22	13.35	13.40

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
			PBE0	12.60	12.67	12.79	12.86
			exp ¹³				11.2
Trans-1,2-di- chlorocyclo- pentane	Carbon tetrachloride	$^3J_{HH}(12)$	SOPPA	10.11	10.17	10.06	10.13
			HRPA(D)	9.66	9.72	9.63	9.69
			B3LYP	10.80	10.89	10.73	10.82
			BHandH	10.97	11.04	10.94	11.02
			PBE0	10.67	10.76	10.62	10.71
			exp ¹⁴				2.510
		$^3J_{HH}$	SOPPA	7.93	7.91	7.98	7.96
		(23c + 15c)	HRPA(D)	7.62	7.60	7.67	7.65
			B3LYP	9.35	9.33	9.41	9.39
			BHandH	9.19	9.16	9.25	9.22
			PBE0	8.81	8.79	8.88	8.85
			exp ¹⁴				5.980
		$^3J_{HH}$	SOPPA	12.03	12.03	11.94	11.94
		(23t + 15t)	HRPA(D)	11.48	11.48	11.41	11.41
			B3LYP	12.61	12.61	12.51	12.51
			BHandH	13.24	13.24	13.17	13.16
			PBE0	12.48	12.48	12.40	12.40
			exp ¹⁴				2.080
		$^3J_{HH}$	SOPPA	2.04	2.02	2.04	2.02
		(34t + 45t)	HRPA(D)	1.92	1.90	1.92	1.90
			B3LYP	2.32	2.29	2.32	2.29
			BHandH	2.10	2.07	2.10	2.07
			PBE0	2.19	2.16	2.19	2.17

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		exp ¹⁴					7.470
		³ J _{HH}	SOPPA	12.80	12.76	12.81	12.77
		(34c + 45c)	HRPA(D)	12.25	12.21	12.25	12.22
			B3LYP	14.21	14.17	14.24	14.20
			BHandH	14.73	14.69	14.76	14.71
			PBE0	13.70	13.66	13.74	13.69
		exp ¹⁴					8.880
		³ J _{HH}	SOPPA	10.58	10.57	10.59	10.58
		(34c + 45c)	HRPA(D)	10.15	10.14	10.15	10.15
			B3LYP	11.80	11.79	11.82	11.81
			BHandH	12.09	12.08	12.10	12.09
			PBE0	11.29	11.28	11.31	11.30
		exp ¹⁴					10.030
		³ J _{HH}	SOPPA	9.13	9.06	9.09	9.02
		(34t + 45t)	HRPA(D)	8.70	8.63	8.65	8.59
			B3LYP	9.41	9.34	9.37	9.29
			BHandH	10.02	9.95	9.99	9.91
			PBE0	9.30	9.22	9.26	9.19
		exp ¹⁴					4.040
	Benzene	³ J _{HH} (12)	SOPPA	10.11	10.17	10.06	10.13
			HRPA(D)	9.66	9.72	9.63	9.69
			B3LYP	10.80	10.89	10.73	10.82
			BHandH	10.97	11.05	10.94	11.02
			PBE0	10.67	10.76	10.62	10.71
		exp ¹⁴					2.860

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum-	vacuum-	solvent-	solvent-
				vacuum	solvent	vacuum	solvent
		$^3J_{HH}$	SOPPA	7.93	7.91	7.98	7.96
		(23c + 15c)	HRPA(D)	7.62	7.61	7.67	7.65
			B3LYP	9.35	9.33	9.41	9.39
			BHandH	9.19	9.16	9.25	9.22
			PBE0	8.81	8.79	8.88	8.85
			exp ¹⁴				6.610
		$^3J_{HH}$	SOPPA	12.03	12.03	11.94	11.94
		(23t + 15t)	HRPA(D)	11.48	11.48	11.41	11.41
			B3LYP	12.61	12.61	12.51	12.51
			BHandH	13.24	13.24	13.17	13.16
			PBE0	12.48	12.49	12.40	12.40
			exp ¹⁴				3.280
		$^3J_{HH}$	SOPPA	2.04	2.02	2.04	2.02
		(34t + 45t)	HRPA(D)	1.92	1.90	1.92	1.90
			B3LYP	2.32	2.29	2.33	2.30
			BHandH	2.10	2.07	2.10	2.07
			PBE0	2.19	2.16	2.19	2.17
			exp ¹⁴				7.080
		$^3J_{HH}$	SOPPA	12.80	12.76	12.81	12.77
		(34c + 45c)	HRPA(D)	12.25	12.21	12.25	12.22
			B3LYP	14.21	14.17	14.24	14.20
			BHandH	14.73	14.69	14.76	14.71
			PBE0	13.70	13.66	13.74	13.70
			exp ¹⁴				9.090
		$^3J_{HH}$	SOPPA	10.58	10.57	10.59	10.58

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum- vacuum	vacuum- solvent	solvent- vacuum	solvent- solvent
		(34c + 45c)	HRPA(D)	10.15	10.14	10.15	10.15
			B3LYP	11.80	11.80	11.82	11.81
			BHandH	12.09	12.08	12.10	12.09
			PBE0	11.29	11.28	11.31	11.30
			exp ¹⁴				9.830
		³ J _{HH}	SOPPA	9.13	9.06	9.08	9.02
		(34t + 45t)	HRPA(D)	8.70	8.64	8.65	8.60
			B3LYP	9.41	9.34	9.37	9.29
			BHandH	10.02	9.95	9.99	9.91
			PBE0	9.30	9.22	9.26	9.19
			exp ¹⁴				4.210
	Acetonitrile	³ J _{HH} (12)	SOPPA	10.11	10.23	10.01	10.14
			HRPA(D)	9.66	9.78	9.59	9.71
			B3LYP	10.80	10.99	10.66	10.84
			BHandH	10.97	11.12	10.91	11.06
			PBE0	10.67	10.84	10.56	10.73
			exp ¹⁴				3.340
		³ J _{HH}	SOPPA	7.93	7.89	8.03	7.99
		(23c + 15c)	HRPA(D)	7.62	7.59	7.71	7.68
			B3LYP	9.35	9.31	9.47	9.43
			BHandH	9.19	9.13	9.30	9.24
			PBE0	8.81	8.76	8.93	8.88
			exp ¹⁴				6.310
		³ J _{HH}	SOPPA	12.03	12.03	11.87	11.86
		(23t + 15t)	HRPA(D)	11.48	11.48	11.34	11.33

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum-	vacuum-	solvent-	solvent-
				vacuum	solvent	vacuum	solvent
			B3LYP	12.61	12.62	12.41	12.41
			BHandH	13.24	13.23	13.10	13.08
			PBE0	12.48	12.49	12.32	12.32
			exp ¹⁴				3.910
		³ J _{HH}	SOPPA	2.04	2.00	2.05	2.01
		(34 <i>t</i> + 45 <i>t</i>)	HRPA(D)	1.92	1.88	1.93	1.89
			B3LYP	2.32	2.26	2.33	2.27
			BHandH	2.10	2.05	2.11	2.06
			PBE0	2.19	2.14	2.20	2.15
			exp ¹⁴				6.540
		³ J _{HH}	SOPPA	12.80	12.73	12.82	12.75
		(34 <i>c</i> + 45 <i>c</i>)	HRPA(D)	12.25	12.18	12.26	12.20
			B3LYP	14.21	14.13	14.27	14.20
			BHandH	14.73	14.64	14.78	14.69
			PBE0	13.70	13.62	13.77	13.69
			exp ¹⁴				9.140
		³ J _{HH}	SOPPA	10.58	10.57	10.59	10.59
		(34 <i>c</i> + 45 <i>c</i>)	HRPA(D)	10.15	10.14	10.16	10.15
			B3LYP	11.80	11.79	11.84	11.82
			BHandH	12.09	12.07	12.12	12.10
			PBE0	11.29	11.28	11.33	11.32
			exp ¹⁴				9.810
		³ J _{HH}	SOPPA	9.13	9.00	9.05	8.92
		(34 <i>t</i> + 45 <i>t</i>)	HRPA(D)	8.70	8.58	8.62	8.50
			B3LYP	9.41	9.26	9.33	9.18

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Table S1 – *Continued from previous page*

Molecule	Solvent	SSCC	Method	vacuum-	vacuum-	solvent-	solvent-
				vacuum	solvent	vacuum	solvent
			BHandH	10.02	9.88	9.95	9.81
			PBE0	9.30	9.15	9.23	9.08
			exp ¹⁴				5.030

^a Assuming that they have switched cis and trans in the article

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