Supporting information for "A systematic benchmark of the ab initio Bethe-Salpeter equation approach for low-lying optical excitations of small organic molecules"

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All the energies in the present document are in eV.

I. THIEL'S SET SINGLET RESULTS

	Molecule	Symmetry	BTE	TD-DFT B3LYP	BSE PBE	BSE B3LYP	BSE BHLYP	BSE tCAM-B3LYP
			Ref. 1	Ref. 2	MOLGW	MOLGW	MOLGW	MOLGW
Series 1	Ethene	B_{1u}	7.80	7.70	7.26	7.48	7.70	7.66
	E-Butadiene	B_u	6.18	5.74	5.31	5.60	5.89	5.85
		A_g	6.55	6.82	6.18	6.83	7.46	7.28
	all-E-Hexatriene	B_u	5.10	4.69	4.24	4.57	4.88	4.84
		A_g	5.09	5.69	4.94	5.73	6.49	6.34
	all-E-Octatetraene	A_g	4.47	4.84	4.06	4.91	5.71	5.60
		B_u	4.66	4.02	3.54	3.90	4.23	4.19
	Cyclopropene	B_1	6.76	6.46	6.03	6.30	6.66	6.48
		B_2	7.06	6.31	6.15	6.37	6.65	6.57
	Cyclopentadiene	B_2	5.55	5.02	4.49	4.79	5.08	5.00
		A_1	6.31	6.52	5.92	6.43	6.83	6.77
	Norbornadiene	A_2	5.34	4.79	4.64	4.91	5.19	5.11
		B_2	6.11	5.52	5.52	5.86	6.23	6.07
Series 2	Benzene	B_{2u}	5.08	5.40	4.60	4.88	5.21	5.10
		B_{1u}	6.54	6.10	5.53	5.79	6.05	6.03
		E_{1u}	7.13	7.07	6.31	6.60	6.93	6.84
		E_{2g}	8.41	8.91	7.38	8.11	8.83	8.79
	Naphthalene	A_g	5.87	6.18	5.26	5.68	6.12	6.04
		A_g	6.67	6.85	6.31	6.79	7.24	7.08
		B_{1g}	5.99	5.58	4.96	5.41	5.91	5.84
		B_{1g}	6.47	6.32	5.54	5.89	6.26	6.24
		B_{2u}	4.77	4.35	3.77	4.09	4.42	4.37
		B_{2u}	6.33	6.12	5.43	5.75	6.09	6.05
		B_{3u}	4.24	4.44	3.71	4.00	4.33	4.25
		B_{3u}	6.06	5.93	5.22	5.52	5.83	5.76
	Furan	B_2	6.32	6.16	5.54	5.86	6.17	6.05
		A_1	6.57	6.70	5.92	6.31	6.77	6.63
		A_1	8.13	8.25	7.45	7.80	8.17	8.06
	Pyrrole	A_1	6.37	6.53	6.50	6.10	6.76	6.66

		A_1	7.91	7.96	7.88	7.53	7.88	7.78
		B_2	6.57	6.40	5.80	6.09	6.37	6.29
	Imidazole	A'	6.19	6.45	5.76	6.10	6.45	6.33
		A'	6.93	7.04	6.27	6.60	6.97	6.87
		A''	6.81	6.46	5.79	6.06	6.59	6.43
	Pyridine	A_1	6.26	6.31	5.67	5.96	6.25	6.21
		A_1	7.18	7.32	6.48	6.82	7.13	7.08
		B_2	4.85	5.49	4.63	4.93	5.27	5.15
		B_2	7.27	7.30	6.42	6.76	7.18	7.03
		B_1	4.59	4.80	4.08	4.46	4.95	4.77
		A_2	5.11	5.11	4.33	4.73	5.29	5.11
	Pyrazine	B_{1u}	6.58	6.50	5.79	6.11	6.41	6.36
		B_{1u}	7.72	7.68	6.64	7.06	7.49	7.38
		B_{2u}	4.64	5.37	4.44	4.76	5.10	4.95
		B_{2u}	7.60	7.78	6.73	7.13	7.57	7.46
		A_u	4.81	4.69	3.93	4.32	4.86	4.67
		B_{1g}	6.60	6.38	5.36	5.89	6.58	6.38
		B_{2g}	5.56	5.55	4.62	5.10	5.66	5.47
		B_{3u}	3.95	3.96	3.25	3.62	4.08	3.88
	Pyrimidine	A_1	6.95	6.58	5.87	6.20	6.51	6.46
		B_2	5.44	5.74	4.79	5.13	5.48	5.36
		B_1	4.55	4.27	3.51	3.88	4.36	4.20
		A_2	4.91	4.60	3.83	4.21	4.72	4.56
	Pyridazine	A_1	5.18	5.61	4.58	5.13	5.34	5.21
		A_2	4.31	4.18	3.36	4.21	4.34	4.15
		A_2	5.77	5.44	4.66	5.35	5.69	5.45
		B_1	3.78	3.58	2.79	3.88	3.70	3.50
	s-Triazine	A_2'	5.79	6.14	5.07	5.44	5.83	5.71
		A_1''	4.60	4.45	3.65	4.04	4.54	4.39
		A_2''	4.66	4.64	3.82	4.20	4.68	4.52
		E''	4.70	4.64	3.76	4.15	4.64	4.48
	s-Tetrazine	A_u	3.51	3.51	2.67	3.08	3.64	3.41
		A_u	5.50	5.04	4.35	4.73	5.34	5.10
		B_{1g}	4.73	4.73	3.57	4.20	4.83	4.60
		B_{2g}	5.20	5.29	4.15	4.81	5.34	5.10
		B_{2u}	4.93	5.58	4.23	4.81	5.20	5.04
		B_{3u}	2.29	2.24	1.35	1.78	2.26	2.04
Series 3	Formaldehyde	A_2	3.88	3.89	3.08	3.36	3.77	3.59
		B_1	9.10	8.89	7.98	8.38	8.84	8.69
		A_1	9.30	9.17	8.99	9.30	9.70	9.06
	Acetone	A_2	4.40	4.34	3.36	3.72	4.19	3.97
		A_1	9.40	9.04	8.55	9.02	9.47	9.43
		B_1	9.10	8.60	8.43	8.60	9.20	8.79
	p-Benzoquinone	A_u	2.77	2.55	1.57	2.16	2.77	2.57
		B_{1g}	2.76	2.43	1.53	2.11	2.72	2.47
		B_{1u}	5.28	4.83	3.73	4.63	5.06	5.01
		B_{3g}	4.26	3.73	3.28	3.78	4.25	4.01
		B_{3g}	6.96	6.59	5.50	6.38	7.08	6.83
		B_{3u}	5.64	5.43	4.60	5.22	5.95	5.81
	Formamide	A''	5.63	5.55	4.64	4.96	5.36	5.26
		A'	7.39	8.13	7.45	7.76	8.18	8.20
	Acetamide	A''	5.69	5.56	4.63	4.95	5.39	5.26
		A'	7.27	7.46	6.81	7.16	7.56	7.54
	Propanamide	A''	5.72	5.59	4.64	4.96	5.41	5.27
		A'	7.20	7.76	6.77	7.13	7.56	7.52
Series 4	Cytosine	A'	4.66	4.64	3.78	4.17	4.59	4.56
		A'	5.62	5.42	4.60	5.10	5.55	5.51
		A''	4.87	4.76	4.12	4.54	4.96	5.05
		A''	5.26	5.11	4.26	4.91	5.59	5.40
	Thymine	A'	5.20	5.00	4.33	4.72	5.13	5.02

		A'	6.27	5.97	5.24	5.71	6.26	6.19
		A'	6.53	6.31	5.78	6.21	6.69	6.54
		A''	4.82	4.70	3.83	4.24	4.74	4.65
		A''	6.16	5.80	5.09	5.55	6.08	5.98
	Uracil	A'	5.35	5.19	4.43	4.82	5.24	5.13
		A'	6.26	5.87	5.17	5.65	6.21	6.13
		A'	6.70	6.50	5.89	6.33	6.82	6.66
		A''	4.80	4.63	3.80	4.21	4.70	4.62
		A''	6.10	5.74	5.02	5.48	6.01	5.92
		A''	6.56	6.14	5.52	6.14	6.71	6.56
	Adenine	A'	5.25	5.27	4.51	4.83	5.18	5.14
		A'	5.25	5.00	4.31	4.69	5.18	5.00
		A''	5.12	4.97	4.25	4.67	5.10	5.05
		A''	5.75	5.61	4.86	5.27	5.79	5.65
MSE			—	-0.08	-0.82	-0.41	0.03	-0.09
MAE			—	0.26	0.82	0.45	0.21	0.25

II. THIEL'S SET TRIPLET RESULTS

	Molecule	Symmetry	BTE	TD-DFT B3LYP	BSE PBE	BSE B3LYP	BSE BHLYP	BSE tCAM-B3LYP
			Ref. 1	Ref. 2	MOLGW	MOLGW	MOLGW	MOLGW
Series 1	Ethene	B_{1u}	4.50	4.03	3.58	3.75	3.97	3.76
	E-Butadiene	A_g	5.08	4.86	3.97	4.35	4.66	4.52
		B_u	3.20	2.76	2.37	2.59	2.81	2.62
	all-E-Hexatriene	A_g	4.15	3.92	3.00	3.43	3.79	3.64
		B_u	2.40	2.09	1.68	1.92	2.18	1.99
	all-E-Octatetraene	A_g	3.55	3.24	2.30	2.77	3.15	3.00
		B_u	2.20	1.68	1.23	1.50	1.79	1.61
	Cyclopropene	B_2	4.34	3.70	3.57	3.68	3.90	3.77
		B_1	6.62	6.01	5.51	5.79	6.15	5.96
	Cyclopentadiene	A_1	5.09	4.75	3.98	4.36	4.66	4.53
		B_2	3.25	2.71	2.30	2.51	2.73	2.55
	Norbornadiene	A_2	3.72	3.08	2.82	2.98	3.20	3.07
		B_2	4.16	3.62	3.23	3.40	3.64	3.48
Series 2	Benzene	B_{1u}	4.15	3.77	3.26	3.44	3.65	3.48
		B_{2u}	5.88	5.09	4.25	4.52	4.81	4.73
		E_{1u}	4.86	4.70	3.96	4.21	4.50	4.39
		E_{1g}	7.51	7.33	5.95	6.54	7.13	7.01
	Naphthalene	A_g	5.52	5.33	4.25	4.69	5.09	5.01
		A_g	6.47	5.95	4.99	5.40	5.88	5.77
		A_g	6.79	6.07	5.11	5.66	6.23	6.17
		B_{2u}	3.11	2.69	2.20	2.40	2.62	2.48
		B_{2u}	4.64	4.40	3.71	3.97	4.26	4.18
		B_{3u}	4.18	3.95	3.23	3.50	3.79	3.71
		B_{3u}	5.11	4.22	3.46	3.74	4.04	3.97
		B_{1g}	4.47	4.17	3.44	3.73	4.03	3.91
		B_{1g}	6.48	5.55	4.91	5.37	5.83	5.82

		B_{1g}	6.76	6.56	5.26	5.88	6.46	6.35
	Furan	A_1	5.48	5.21	4.43	4.69	4.97	4.87
		B_2	4.17	3.71	3.17	3.38	3.62	3.44
	Pyrrole	A_1	5.51	5.25	4.47	4.74	5.04	4.92
		B_2	4.48	4.07	3.48	3.70	3.94	3.78
	Imidazole	A'	4.69	4.24	3.65	3.87	4.12	3.96
		A'	5.79	5.44	4.65	4.94	5.29	5.11
		A'	6.55	5.95	5.01	5.32	5.74	5.56
		A''	6.37	5.83	5.01	5.37	5.88	5.67
	Pyridine	A_1	4.06	3.89	3.33	3.54	3.75	3.58
		A_1	4.91	4.84	4.04	4.31	4.62	4.51
		B_2	4.64	4.51	3.69	3.96	4.24	4.13
		B_2	6.08	5.64	4.71	5.01	5.36	5.27
		B_1	4.25	4.04	3.29	3.66	4.17	3.94
		A_2	5.28	4.98	4.17	4.57	5.12	4.95
	s-Tetrazine	A_u	3.52	3.10	2.26	2.66	3.20	2.96
		A_u	5.03	4.43	3.70	4.16	4.70	4.44
		B_{1g}	4.21	3.63	2.49	3.09	3.68	3.43
		B_{1u}	4.33	3.83	2.79	3.37	3.64	3.46
		B_{1u}	5.38	5.24	4.01	4.52	4.89	4.75
		B_{2g}	4.93	4.48	3.40	3.93	4.50	4.27
		B_{2u}	4.54	4.06	2.93	3.41	3.70	3.56
		B_{3u}	1.89	1.42	0.63	1.00	1.45	1.21
Series 3	Formaldehyde	A_2	3.50	3.13	2.31	2.58	3.00	2.80
		A_1	5.87	5.18	1.51	4.59	4.93	4.76
	Acetone	A_2	4.05	3.69	2.68	3.03	3.51	3.27
		A_1	6.03	5.39	4.53	4.96	5.30	5.17
	p-Benzoquinone	A_u	2.62	2.05	1.00	1.59	2.28	1.97
		B_{1g}	2.51	1.92	0.97	1.54	2.16	1.89
		B_{1u}	2.96	2.19	1.21	1.95	2.20	2.06
		B_{3g}	3.41	2.68	2.19	2.56	2.84	2.70
	Formamide	A''	5.36	4.97	4.03	4.34	4.74	4.62
		A'	5.74	5.13	4.17	4.44	4.80	4.64
	Acetamide	A''	5.42	5.01	4.04	4.36	4.81	4.65
		A'	5.88	5.26	4.27	4.59	4.99	4.80
	Propanamide	A''	5.45	5.04	4.06	4.38	4.84	4.68
		A'	5.90	5.28	4.31	4.61	5.02	4.83
MSE			—	-0.44	-1.28	-0.89	-0.52	-0.68
MAE			—	0.44	1.28	0.89	0.52	0.68

III. THIEL'S MOLECULES HOMO-LUMO GAP

	Molecule	CCSD(T)	gKS B3LYP	GW PBE	GW B3LYP	GW BHLYP	GW tCAM-B3LYP	GW HF
		Gaussian09	molgw	molgw	molgw	molgw	molgw	molgw
Series 1	Ethene	13.34	7.40	12.64	12.83	13.08	13.03	13.46
	E-Butadiene	10.66	5.45	9.66	9.98	10.34	10.24	10.80

	all-E-Hexatriene	9.14	4.39	7.94	8.32	8.76	8.64	9.28
	all-E-Octatetraene	8.17	3.74	6.81	7.24	7.73	7.61	8.31
	Cyclopropene	12.57	6.77	11.93	12.13	12.41	12.37	12.84
	Cyclopentadiene	10.44	5.33	9.47	9.77	10.11	9.99	10.57
	Norbornadiene	10.56	5.58	9.72	10.01	10.37	10.26	10.85
Series 2	Benzene	11.31	6.63	10.38	10.66	11.00	10.93	11.43
	Naphthalene	8.92	4.72	7.90	8.20	8.56	8.49	9.00
	Furan	11.46	6.36	10.65	10.96	11.30	11.18	11.74
	Pyrrole	10.87	6.61	10.35	11.01	10.83	10.80	11.25
	Imidazole	11.91	6.79	10.85	11.38	11.31	11.28	11.72
	Pyridine	11.06	6.12	9.88	10.35	10.83	10.74	11.25
	Pyrazine	10.92	5.31	9.25	9.71	10.62	10.08	11.03
	Pyrimidine	10.73	5.66	9.57	10.01	10.59	10.42	11.65
	Pyridazine	9.94	4.91	8.76	9.24	9.88	9.66	10.76
	s-Triazine	11.16	5.94	10.02	10.46	11.04	10.87	10.83
	s-Tetrazine	8.97	3.66	7.83	8.32	8.92	8.65	9.75
Series 3	Formaldehyde	12.45	5.87	11.62	11.97	12.44	12.32	13.10
	Acetone	11.81	6.24	10.59	11.13	11.79	11.56	13.03
	p-Benzoquinone	8.76	3.79	7.23	7.91	8.68	8.40	9.82
	Formamide	13.31	7.48	12.34	12.82	12.99	12.90	13.80
	Acetamide	12.31	7.42	11.84	12.34	12.30	12.80	13.25
	Propanamide	12.24	7.42	11.28	11.72	12.23	12.14	13.23
Series 4	Cytosine	9.80	5.29	8.83	9.20	9.65	9.59	10.24
	Thymine	9.97	5.40	9.03	9.41	9.88	9.72	10.50
	Uracil	10.30	5.60	9.61	9.74	10.21	10.06	10.83
	Adenine	9.75	5.34	8.68	9.05	9.51	9.38	10.12
	MSE	—	-5.06	-1.01	-0.61	-0.19	-0.31	0.41

[1]M. Schreiber, M. R. Silva-Junior, S. P. A. Sauer, and W. Thiel, J. Chem. Phys. **128**, 134110 (2008).
[2]M. R. Silva-Junior, M. Schreiber, S. P. A. Sauer, and W. Thiel, J. Chem. Phys. **129**, 104103 (2008).