Supplementary material for "Spin-unrestricted random-phase approximation with range separation: Benchmark on atomization energies and reaction barrier heights"

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The detailed results of the calculations on the AE49 and DBH24/08 datasets for the full-range and range-separated MP2, dRPA-I, and RPAx-SO2 methods at $\mu = 0.5$ are reported in Tables I and II.

[1]R. Haunschild and W. Klopper, J. Chem. Phys. **136**, 164102 (2012).
[2]J. Zheng, Y. Zhao and D. G. Truhlar, J. Chem. Theory Comput. **5**, 808 (2009).

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TABLE I. Atomization energies (in kcal/mol) of the AE49 dataset (molecules of the G2-1 dataset except for the six molecules containing Li, Be, and Na) calculated by full-range HF+MP2, HF+dRPA-I, HF+RPAx-SO2 and range-separated RSH+MP2, RSH+dRPA-I, RSH+RPAx-SO2. The calculations were carried out using the cc-pVQZ basis set, MP2(full)/6-31G* geometries, and with the srPBE functional and $\mu = 0.5$ in the case of the range-separated calculations. The reference values are the non-relativistic FC-CCSD(T)/cc-pVQZ-F12 values of Ref. 1. For each method, the value with the largest absolute error is indicated in boldface.

	HF+			RSH+			Reference
	MP2	dRPA-I	RPAx-SO2	MP2	dRPA-I	RPAx-SO2	
CH_2 (singlet)	174.45	165.75	197.04	171.39	170.64	172.69	180.62
CH_2 (triplet)	188.70	181.63	201.41	190.84	189.71	191.31	189.74
CH_3Cl	394.58	370.34	417.42	389.72	386.32	391.19	394.52
CH_3	303.36	291.30	318.89	303.79	302.23	304.71	306.59
CH_3SH	469.94	442.53	495.56	465.03	460.82	467.01	473.49
CH_4	414.84	397.27	432.29	411.74	409.65	413.14	418.87
CH	76.38	74.13	85.21	79.46	79.19	80.04	83.87
Cl_2	60.43	46.49	79.13	55.73	53.53	56.71	59.07
ClF	65.20	45.91	83.08	61.15	60.68	62.04	62.57
ClH	106.53	98.52	119.27	102.11	101.21	103.02	107.20
ClO	59.68	42.55	72.39	63.94	62.60	65.22	64.53
CN	168.84	141.95	164.00	176.12	173.99	177.86	180.06
CO_2	**409.33**	350.00	413.15	395.12	392.37	396.91	388.59
CO	269.30	234.43	276.58	257.79	256.26	259.24	258.88
F_2	42.18	15.59	59.82	36.60	36.99	37.84	38.75
FH	144.17	129.15	154.97	138.23	137.89	138.65	141.51
H_2CCH_2	561.39	528.59	582.70	556.69	552.92	558.80	561.34
H_2CO	379.20	343.30	392.00	370.88	368.85	372.48	373.21
H_2NNH_2	432.47	394.47	431.32	432.36	429.67	434.62	436.70
H_3CCH_3	707.16	673.49	**735.15**	703.80	699.25	705.86	710.20
H_3COH	513.32	477.43	534.34	507.36	504.60	509.06	511.83
HCCH	409.59	373.19	419.99	401.10	397.40	403.34	402.76
HCN	319.26	279.53	312.96	308.30	305.60	310.48	311.52
HCO	285.80	252.01	291.99	280.35	278.63	281.90	278.28
HOCl	168.50	141.01	184.05	161.23	159.81	162.68	165.79
HOOH	272.51	232.25	286.06	263.66	262.62	265.56	268.65
N_2	234.80	193.15	213.76	222.17	220.46	224.27	227.44
NH_2	176.66	165.16	179.49	178.54	177.84	179.51	181.96
NH_3	293.12	272.47	295.33	290.20	288.89	291.65	297.07
NH	78.57	74.39	80.62	82.08	81.82	82.54	82.79
NO	156.95	123.74	147.37	155.31	154.30	156.90	152.19
O_2	126.53	92.04	113.98	124.06	123.31	126.00	120.54
OH_2	233.83	212.21	243.34	226.55	225.77	227.54	232.56
OH	105.78	96.58	112.19	105.25	104.93	105.73	106.96
P_2	113.59	88.61	105.38	106.63	99.52	107.19	115.95
PH_2	144.95	141.41	152.46	146.95	146.30	147.68	153.97
PH_3	230.24	222.62	241.82	229.63	228.31	230.84	241.47
S_2	103.68	85.63	109.74	101.19	96.76	102.13	103.11
SC	175.16	146.58	186.41	164.13	159.64	166.22	170.98
SH_2	178.55	168.10	194.48	174.35	172.84	175.82	183.30
Si_2H_6	519.18	504.65	556.67	**517.31**	**512.50**	**520.68**	535.47
Si_2	59.29	50.71	67.94	72.31	69.20	75.82	73.41
SiH_2 (singlet)	145.90	141.61	165.21	143.64	142.93	145.89	153.68
SiH_2 (triplet)	128.93	126.44	141.38	129.82	128.58	131.14	133.26
SiH_3	220.51	216.07	237.96	220.33	218.83	221.84	228.08
SiH_4	314.28	307.46	336.62	311.98	310.07	313.73	324.59
SiO	200.09	165.92	203.39	187.97	185.75	190.47	192.36
SO_2	270.73	**207.21**	269.30	249.24	245.56	251.39	259.77
SO	129.29	101.94	127.35	125.02	123.21	126.41	125.80
MAD	5.63	23.23	12.20	5.09	6.80	4.06	

TABLE II. Forward (F) and reverse (R) reaction barrier heights (in kcal/mol) of the DBH24/08 dataset calculated by full-range HF+MP2, HF+dRPA-I, HF+RPAx-SO2 and range-separated RSH+MP2, RSH+dRPA-I, RSH+RPAx-SO2. The calculations were carried out using the aug-cc-pVQZ basis set, QCISD/MG3 geometries, and with the srPBE functional and $\mu = 0.5$ in the case of the range-separated calculations. The reference values are taken from Ref. 2. For each method, the value with the largest absolute error is indicated in boldface.

	HF+			RSH+			Reference
	MP2	dRPA-I	RPAx-SO2	MP2	dRPA-I	RPAx-SO2	
	F/R	F/R	F/R	F/R	F/R	F/R	F/R
Heavy-atom transfer							
$H+N_2O \rightarrow OH+N_2$	35.94/89.26	28.20/**100.80**	32.74/**100.57**	18.11/74.67	18.00/76.40	17.92/74.43	17.13/82.47
$H+ClH \rightarrow HCl+H$	22.79/22.79	24.07/24.07	23.33/23.33	19.07/19.07	19.36/19.36	18.44/18.44	18.00/18.00
$CH_3+FCl \rightarrow CH_3F+Cl$	19.74/74.29	17.63/75.16	21.67/66.18	7.19/61.68	7.38/61.98	7.40/61.25	6.75/60.00
Nucleophilic substitution							
$Cl^- \cdots CH_3Cl \rightarrow ClCH_3 \cdots Cl^-$	14.64/14.64	15.92/15.92	15.05/15.05	15.12/15.12	15.85/15.85	14.76/14.76	13.41/13.41
$F^- \cdots CH_3Cl \rightarrow FCH_3 \cdots Cl^-$	4.59/28.88	4.78/33.98	4.35/33.29	4.43/30.70	4.62/31.50	4.09/30.43	3.44/29.42
$OH^-+CH_3F \rightarrow HOCH_3+F^-$	-1.75/17.86	1.23/22.00	0.52/20.92	-2.33/20.59	-1.43/21.22	-2.60/19.81	-2.44/17.66
Unimolecular and association							
$H+N_2 \rightarrow HN_2$	27.60/8.06	22.54/12.53	23.36/12.59	13.23/12.66	13.34/12.59	12.81/12.47	14.36/10.61
$H+C_2H_4 \rightarrow CH_3CH_2$	9.32/46.54	6.67/48.13	7.80/49.83	2.38/45.29	2.62/45.24	2.20/44.74	1.72/41.75
$HCN \rightarrow HNC$	34.46/**52.09**	36.14/49.49	34.73/47.08	34.36/**47.93**	34.85/**48.15**	34.03/**47.70**	48.07/32.82
Hydrogen transfer							
$OH+CH_4 \rightarrow CH_3+H_2O$	7.66/25.01	13.65/24.16	9.28/25.55	4.63/18.62	4.77/18.82	4.14/18.16	6.70/19.60
$H+OH \rightarrow O+H_2$	17.56/15.58	15.42/20.08	16.13/15.90	12.44/8.22	12.07/8.03	11.88/7.64	10.70/13.10
$H+H_2S \rightarrow H_2+HS$	6.42/16.36	7.18/20.71	6.32/15.59	4.28/15.00	4.42/15.89	3.84/14.29	3.60/17.30
MAD	6.17	6.95	6.40	2.94	3.01	2.83	