Supporting Information: Benchmark tests and spin adaptation for the particle-particle Random Phase Approximation

Yang Yang,[1] Helen van Aggelen,[1,2,a)] Stephan Steinmann,[1] Degao Peng,[1] and Weitao Yang[3,b)]

[1)] *Department of Chemistry, Duke University, NC 27708, U.S.*

[2)] *Department of Inorganic and Physical Chemistry, Ghent University, 9000 Ghent, Belgium*

[3)] *Department of Chemistry and Department of Physics, Duke University, NC 27708, U.S.*

(Dated: 27 August 2013)

[a)] Helen.VanAggelen@UGent.be

[b)] weitao.yang@duke.edu

TABLE I. Basis convergence test (H_2O) for atomization energy and total energy (in kcal/mol)

Basis	Atomization energy		Total energy	
	ph-RPA	pp-RPA	ph-RPA	pp-RPA
cc-pVDZ	-201.70	-207.96	-47902.01	-47831.65
cc-pVTZ	-218.79	-225.33	-47992.78	-47890.96
cc-pVQZ	-225.06	-230.24	-48037.90	-47916.65
cc-pV5Z	-224.71	-230.65	-48054.01	-47925.35

TABLE II. Basis convergence test (HCN) for atomization energy and total energy (in kcal/mol)

Basis	Atomization energy		Total energy	
	ph-RPA	pp-RPA	ph-RPA	pp-RPA
cc-pVDZ	-278.85	-291.47	-58558.51	-58459.93
cc-pVTZ	-300.80	-312.17	-58663.40	-58521.58
cc-pVQZ	-299.15	-313.13	-58728.03	-58555.81
cc-pV5Z	-296.89	-312.56	-58752.07	-58567.76

TABLE VI: G2/97 atomization energy and enthalpies of formation (in kcal/mol) calculated by pp-RPA and ph-RPA. Numbers in the parenthesis indicate the error.

Molecule	Atomization energy		Enthalpies of formation		
	pp-RPA	ph-RPA	pp-RPA	ph-RPA	Expt
G2-1 test set					
LiH	48.0	52.6	43.2 (9.9)	38.5 (5.2)	33.3
BeH	54.7	49.7	76.8 (-4.9)	81.8 (0.1)	81.7
CH	76.5	81.7	149.9 (7.4)	144.6 (2.1)	142.5
$CH_2(^3B_1)$	188.1	181.5	95.6 (1.9)	102.2 (8.5)	93.7
$CH_2(^1A_1)$	168.4	176.5	115.0 (12.2)	106.9 (4.1)	102.8
CH_3	300.3	298.0	41.3 (6.3)	43.7 (8.7)	35.0

TABLE III. Basis convergence test ($H+OH \rightarrow O+H_2$) for forward and backward reaction barriers (in kcal/mol)

Basis	Forward		Backward	
	ph-RPA	pp-RPA	ph-RPA	pp-RPA
aug-cc-pVDZ	8.06	14.46	13.93	11.79
aug-cc-pVTZ	7.26	13.85	12.66	11.40
aug-cc-pVQZ	6.43	13.93	9.09	10.55

TABLE IV. Basis convergence test ($HCN \rightarrow HNC$) for forward and backward reaction barriers (in kcal/mol)

Basis	Forward		Backward	
	ph-RPA	pp-RPA	ph-RPA	pp-RPA
aug-cc-pVDZ	44.64	48.88	31.27	30.86
aug-cc-pVTZ	50.08	49.24	35.51	32.55
aug-cc-pVQZ	45.60	49.13	31.70	32.60

Molecule	Atomization energy		Enthalpies of formation		
	pp-RPA	ph-RPA	pp-RPA	ph-RPA	Expt
CH_4	410.3	410.8	-9.0 (8.9)	-9.6 (8.3)	-17.9
NH	75.3	81.4	93.4 (8.2)	87.3 (2.1)	85.2
NH_2	169.9	177.5	56.7 (11.6)	49.1 (4.0)	45.1
NH_3	283.8	288.9	2.7 (13.7)	-2.5 (8.5)	-11.0
OH	101.3	101.0	14.4 (5.0)	14.8 (5.4)	9.4
OH_2	225.3	218.8	-50.9 (6.9)	-44.4 (13.4)	-57.8
FH	139.1	128.5	-63.4 (1.7)	-52.8 (12.3)	-65.1
$SiH_2(^1A_1)$	138.2	148.1	78.4 (13.2)	68.4 (3.2)	65.2
$SiH_2(^3B_1)$	125.0	125.8	91.8 (5.6)	91.0 (4.8)	86.2
SiH_3	213.0	219.2	60.0 (12.1)	53.8 (5.9)	47.9

TABLE V. Basis convergence test for selected nonbonded systems (in kcal/mol)

pp-RPA	HF-HF	H2O-ClF	HCl-HCl	CH4-Ne
aug-cc-pVDZ	-4.87	-5.87	-2.38	-0.23
aug-cc-pVTZ	-5.12	-5.62	-2.67	-0.33
aug-cc-pVQZ	-5.24	-5.56	-2.28	-0.22

Molecule	Atomization energy		Enthalpies of formation		
	pp-RPA	ph-RPA	pp-RPA	ph-RPA	Expt
SiH_4	303.4	314.1	26.2 (18.0)	15.5 (7.3)	8.2
PH_2	141.5	155.4	44.4 (11.3)	30.5 (-2.6)	33.1
PH_3	225.8	243.8	17.3 (16.0)	-0.7 (-2.0)	1.3
SH_2	170.5	174.2	6.9 (11.8)	3.2 (8.1)	-4.9
ClH	102.0	98.3	-17.7 (4.4)	-14.0 (8.1)	-22.1
Li_2	13.5	18.0	62.4 (10.8)	57.9 (6.3)	51.6
LiF	139.2	119.8	-81.7 (-1.6)	-62.3 (17.8)	-80.1
C_2H_2	406.2	387.3	53.3 (-0.9)	72.2 (18.0)	54.2
C_2H_4	557.4	546.2	17.7 (5.2)	28.8 (16.3)	12.5
C_2H_6	703.3	696.5	-12.7 (7.4)	-5.9 (14.2)	-20.1
CN	182.2	169.6	103.6 (-1.3)	116.2 (11.3)	104.9
HCN	312.2	300.8	31.8 (0.3)	43.2 (11.7)	31.5
CO	264.8	243.6	-31.9 (-5.5)	-10.7 (15.7)	-26.4
HCO	283.0	263.1	5.7 (-4.3)	25.7 (15.7)	10.0
H_2CO	373.1	356.6	-25.4 (0.6)	-8.9 (17.1)	-26.0
H_3COH	505.3	492.7	-41.4 (6.6)	-28.8 (19.2)	-48.0
N_2	224.8	221.8	3.8 (3.8)	6.8 (6.8)	0.0
H_2NNH_2	419.3	424.2	41.3 (18.5)	36.4 (13.6)	22.8
NO	154.0	145.8	20.4 (-1.2)	28.6 (7.0)	21.6
O_2	129.4	111.3	-8.9 (-8.9)	9.2 (9.2)	0.0
HOOH	262.1	250.6	-25.9 (6.6)	-14.3 (18.2)	-32.5

Molecule	Atomization energy		Enthalpies of formation		
	pp-RPA	ph-RPA	pp-RPA	ph-RPA	Expt
F_2	37.6	27.9	0.9 (0.9)	10.6 (10.6)	0.0
CO_2	407.9	364.1	-112.8 (-18.7)	-69.1 (25.0)	-94.1
Na_2	9.0	14.9	41.9 (7.9)	36.1 (2.1)	34.0
Si_2	69.6	67.3	145.0 (5.1)	147.3 (7.4)	139.9
P_2	109.6	117.5	42.0 (7.7)	34.1 (-0.2)	34.3
S_2	102.5	90.8	29.9 (-0.8)	41.5 (10.8)	30.7
Cl_2	56.7	44.2	1.2 (1.2)	13.7 (13.7)	0.0
NaCl	94.5	82.2	-40.0 (3.6)	-27.8 (15.8)	-43.6
SiO	193.9	173.5	-26.2 (-1.6)	-5.8 (18.8)	-24.6
SC	170.5	157.9	67.7 (0.8)	80.4 (13.5)	66.9
SO	128.8	110.9	-2.5 (-3.7)	15.5 (14.3)	1.2
ClO	65.0	52.4	23.6 (-0.6)	36.3 (12.1)	24.2
FCl	60.6	47.0	-12.4 (0.8)	1.2 (14.4)	-13.2
Si_2H_6	503.2	513.6	45.6 (26.5)	35.2 (16.1)	19.1
CH_3Cl	389.9	378.0	-15.5 (4.1)	-3.6 (16.0)	-19.6
H_3CSH	462.1	456.8	5.4 (10.9)	10.6 (16.1)	-5.5
HOCl	161.3	148.5	-14.7 (3.1)	-1.9 (15.9)	-17.8
SO_2	262.7	222.4	-75.2 (-4.2)	-34.8 (36.2)	-71.0
G2-2 test set					
Nonhydrogen systems					
BF_3	491.9	430.3	-293.5 (-22.1)	-231.8 (39.6)	-271.4
BCl_3	338.1	290.8	-111.8 (-15.5)	-64.5 (31.8)	-96.3
AlF_3	438.5	378.8	-300.9 (-11.9)	-241.2 (47.8)	-289.0
$AlCl_3$	316.6	273.2	-150.1 (-10.4)	-106.7 (33.0)	-139.7
CF_4	501.5	428.0	-248.3 (-25.3)	-174.8 (48.2)	-223.0
CCl_4	330.4	271.4	-40.5 (-17.6)	18.5 (41.4)	-22.9
COS	347.5	311.0	-47.3 (-14.2)	-10.8 (22.3)	-33.1

Molecule	Atomization energy		Enthalpies of formation		
	pp-RPA	ph-RPA	pp-RPA	ph-RPA	Expt
CS_2	287.0	256.7	18.6 (-9.4)	48.8 (20.8)	28.0
COF_2	439.1	381.5	-165.0 (-15.9)	-107.4 (41.7)	-149.1
SiF_4	585.0	509.7	-398.2 (-12.2)	-322.8 (63.2)	-386.0
$SiCl_4$	393.3	334.6	-168.4 (-10.0)	-109.6 (48.8)	-158.4
N_2O	282.9	257.1	7.2 (-12.4)	33.1 (13.5)	19.6
ClNO	194.2	175.9	9.5 (-2.9)	27.8 (15.4)	12.4
NF_3	212.6	176.0	-38.9 (-7.3)	-2.3 (29.3)	-31.6
PF_3	371.2	328.1	-236.4 (-7.3)	-193.3 (35.8)	-229.1
O_3	163.7	129.7	17.5 (-16.6)	51.5 (17.4)	34.1
F_2O	95.9	74.3	3.2 (-2.7)	24.8 (18.9)	5.9
ClF_3	131.5	85.6	-43.8 (-5.8)	2.1 (40.1)	-38.0
C_2F_4	614.9	531.3	-188.5 (-31.1)	-104.8 (52.6)	-157.4
C_2Cl_4	493.9	418.5	-30.1 (-27.1)	45.2 (48.2)	-3.0
CF_3CN	667.8	305.6	-146.5 (-28.1)	-73.5 (44.9)	-118.4
Hydrocarbons					
CH_3CCH(propyne)	708.6	681.3	39.7 (-4.5)	67.1 (22.9)	44.2
$CH_2 = C = CH_2$(allene)	704.1	679.0	43.8 (-1.7)	68.9 (23.4)	45.5
C_3H_4(cyclopropene)	685.9	658.9	62.2 (-4.0)	89.3 (23.1)	66.2
$CH_3CH = CH_2$(propylene)	856.5	836.5	7.5 (2.7)	27.5 (22.7)	4.8
C_3H_6(cyclopropane)	854.4	831.4	10.1 (-2.6)	33.1 (20.4)	12.7
C_3H_8(propane)	999.3	984.1	-19.7 (5.3)	-4.5 (20.5)	-25.0
$CH_2CHCHCH_2$(butadiene)	1014.0	979.8	23.6 (-2.7)	57.8 (31.5)	26.3
C_4H_6(2-butyne)	1010.3	974.4	27.3 (-7.5)	63.2 (28.4)	34.8
C_4H_6(methylene cyclopropane)	999.6	963.1	37.7 (-10.2)	74.2 (26.3)	47.9
C_4H_6(bicyclobutane)	998.4	958.6	39.4 (-12.5)	79.2 (27.3)	51.9
C_4H_6(cyclobutene)	1008.7	972.2	29.1 (-8.3)	65.6 (28.2)	37.4
C_4H_8(cyclobutane)	1153.3	1122.5	0.5 (-6.3)	31.2 (24.4)	6.8
C_4H_8(isobutene)	1157.3	1127.9	-4.7 (-0.7)	24.8 (28.8)	-4.0

Molecule	Atomization energy		Enthalpies of formation		
	pp-RPA	ph-RPA	pp-RPA	ph-RPA	Expt
C_4H_{10}(trans butane)	1295.7	1272.0	-27.1 (2.9)	-3.5 (26.5)	-30.0
C_4H_{10}(isobutane)	1298.0	1273.5	-29.7 (2.4)	-5.2 (26.9)	-32.1
C_5H_8(spiropentane)	1299.2	1250.7	27.4 (-16.9)	75.9 (31.6)	44.3
C_6H_6(benzene)	1397.2	1322.2	-11.3 (-31.0)	63.7 (44.0)	19.7
Substituted hydrocarbons					
CH_2F_2	442.0	407.7	-113.4 (-5.7)	-79.2 (28.5)	-107.7
CHF_3	473.2	419.0	-182.0 (-15.4)	-127.8 (38.8)	-166.6
CH_2Cl_2	371.2	345.1	-24.4 (-1.6)	1.7 (24.5)	-22.8
$CHCl_3$	352.1	310.2	-33.5 (-8.8)	8.4 (33.1)	-24.7
CH_3NH_2(methylamine)	567.8	566.0	7.9 (13.4)	9.7 (15.2)	-5.5
CH_3CN(methylcyanide)	617.0	596.2	16.1 (-1.9)	36.9 (18.9)	18.0
CH_3NO_2(nitromethane)	610.0	573.5	-27.2 (-9.4)	9.4 (27.2)	-17.8
CH_3ONO(methylnitrite)	606.1	571.2	-23.7 (-7.8)	11.1 (27.0)	-15.9
CH_3SiH_3(methylsilane)	608.0	608.3	11.1 (18.1)	10.8 (17.8)	-7.0
HCOOH(formic acid)	508.3	471.7	-98.1 (-7.6)	-61.6 (28.9)	-90.5
$HCOOCH_3$(methyl formate)	794.5	750.2	-95.3 (-10.3)	-51.0 (34.0)	-85.0
CH_3CONH_2(acetamide)	868.8	833.9	-58.6 (-1.6)	-23.8 (33.2)	-57.0
C_2H_4NH(aziridine)	716.4	699.9	32.8 (2.6)	49.3 (19.1)	30.2
NCCN(cyanogen)	514.9	482.1	60.7 (-12.6)	93.6 (20.3)	73.3
$(CH_3)_2NH$(dimethylamine)	857.4	847.3	7.0 (11.4)	17.1 (21.5)	-4.4
$CH_3CH_2NH_2$(trans ethylamine)	865.8	855.4	-1.3 (10.0)	9.1 (20.4)	-11.3
CH_2CO(ketene)	542.5	508.1	-21.8 (-10.4)	12.6 (24.0)	-11.4
C_2H_4O(oxirane)	654.2	627.1	-16.8 (-4.2)	10.3 (22.9)	-12.6
CH_3CHO(acetaldehyde)	677.9	651.1	-41.3 (-1.6)	-14.6 (25.1)	-39.7
HCOCOH(glyoxal)	644.5	600.2	-61.8 (-11.1)	-17.5 (33.2)	-50.7
CH_3CH_2OH(ethanol)	804.5	783.3	-51.9 (4.3)	-30.6 (25.6)	-56.2
CH_3OCH_3(dimethylether)	792.2	771.6	-39.4 (4.6)	-18.8 (25.2)	-44.0
C_2H_4S(thiirane)	625.1	602.2	17.4 (-2.2)	40.3 (20.7)	19.6

Molecule	Atomization energy		Enthalpies of formation		
	pp-RPA	ph-RPA	pp-RPA	ph-RPA	Expt
$(CH_3)_2SO$(dimethylsulfoxide)	847.9	812.1	-29.9 (6.3)	5.9 (42.1)	-36.2
C_2H_5SH(ethanethiol)	759.0	744.9	-2.5 (8.6)	11.7 (22.8)	-11.1
CH_3SCH_3(dimethylsulfide)	757.4	742.0	-0.4 (8.5)	15.1 (24.0)	-8.9
$CH_2 = CHF$(vinylfluoride)	575.1	545.5	-36.8 (-3.6)	-7.2 (26.0)	-33.2
C_2H_5Cl(ethylchloride)	688.4	667.6	-25.0 (1.8)	-4.3 (22.5)	-26.8
CH2 = CHCl(vinylchloride)	543.5	517.5	4.0 (-4.9)	30.0 (21.1)	8.9
CH2 = CHCN(acrylonitrile)	768.8	734.9	37.8 (-5.4)	71.6 (28.4)	43.2
CH_3COCH_3(acetone)	981.5	944.9	-56.3 (-4.4)	-19.7 (32.2)	-51.9
CH_3COOH(acetic acid)	811.6	765.7	-112.8 (-9.4)	-66.9 (36.5)	-103.4
CH_3COF(acetylfluoride)	717.3	669.4	-117.5 (-11.8)	-69.7 (36.0)	-105.7
CH_3COCl(acetylchloride)	677.3	633.7	-68.4 (-10.4)	-24.8 (33.2)	-58.0
$CH_3CH_2CH_2Cl$(propylchloride)	984.8	955.5	-32.5 (-1.0)	-3.2 (28.3)	-31.5
$(CH_3)_2CHOH$(isopropanol)	1105.4	1074.7	-64.3 (0.9)	-33.6 (31.6)	-65.2
$C_2H_5OCH_3$(methylethylether)	1091.9	1062.6	-50.5 (1.2)	-21.1 (30.6)	-51.7
$(CH_3)_3N$(trimethylamine)	1151.9	1132.1	1.0 (6.7)	20.8 (26.5)	-5.7
C_4H_4O(furan)	1018.3	953.8	-33.5 (-25.2)	31.0 (39.3)	-8.3
C_4H_4S(thiophene)	984.0	921.9	5.5 (-22.0)	67.6 (40.1)	27.5
C_4H_5N(pyrrole)	1090.0	1034.5	6.4 (-19.5)	61.9 (36.0)	25.9
C_5H_5N(pyridine)	1264.2	1195.3	5.7 (-27.9)	74.6 (41.0)	33.6
Inorganic hydrides					
H_2	100.5	108.3	8.7 (8.7)	0.9 (0.9)	0.0
HS	80.1	83.4	40.8 (6.6)	37.6 (3.4)	34.2
Radicals					
CCH	268.4	248.2	132.5 (-2.6)	152.7 (17.6)	135.1
$C_2H_3(^2A')$	442.4	427.7	73.1 (1.5)	87.9 (16.3)	71.6
$CH_3CO(^2A')$	586.5	556.6	-8.0 (-5.6)	21.9 (24.3)	-2.4
$H_2COH(^2A)$	405.5	389.2	-0.7 (3.4)	15.6 (19.7)	-4.1
$CH_3O(^2A')$	393.9	384.5	10.7 (6.6)	20.1 (16.0)	4.1

Molecule	Atomization energy		Enthalpies of formation		
	pp-RPA	ph-RPA	pp-RPA	ph-RPA	Expt
$CH_3CH_2O(^2A'')$	692.5	674.4	0.9 (4.6)	19.0 (22.7)	-3.7
$CH_3S(^2A')$	374.8	368.4	35.5 (5.7)	42.0 (12.2)	29.8
$C_2H_5(^2A')$	596.5	586.4	34.7 (5.8)	44.9 (16.0)	28.9
$(CH_3)_2CH(^2A')$	894.9	876.0	25.4 (3.9)	44.3 (22.8)	21.5
$(CH_3)_3C$ (t-butyl radical)	1195.3	1167.0	14.0 (1.7)	42.3 (30.0)	12.3
NO_2	242.3	211.9	-6.9 (-14.8)	23.4 (15.5)	7.9

TABLE VII. Detailed interaction data (in kcal/mol) for HB6/04. Data unavailable in space left blank owing to large computational cost.

	Benchmark	phPBE	phHF	ppPBE	ppHF	cp-phPBE	cp-phHF	cp-ppPBE	cp-ppHF	ppHF-augqz
NH_3-NH_3	-3.15	-4.11	-3.97	-4.23	-3.68	-2.03	-2.21	-3.15	-2.71	-3.08
HF−HF	-4.57	-4.63	-5.01	-5.03	-5.01	-3.14	-3.85	-4.23	-4.36	-4.83
H_2O-H_2O	-4.97	-5.22	-5.48	-5.88	-5.51	-3.46	-4.00	-4.93	-4.67	-4.72
NH_3-H_2O	-6.41	-7.31	-7.40	-7.85	-7.18	-4.57	-5.14	-6.47	-6.01	-6.77
$(HCONH_2)_2$	-14.94	-17.31	-16.65	-18.93	-16.58	-12.44	-13.14	-16.48	-15.11	
$(HCOOH)_2$	-16.15	-17.80	-18.01	-20.31	-18.36	-13.64	-15.02	-18.74	-17.52	-17.75

TABLE VIII. Detailed interaction data (in kcal/mol) for CT7/04. Data unavailable in space left blank owing to large computational cost.

	Benchmark	phPBE	phHF	ppPBE	ppHF	cp-phPBE	cp-phHF	cp-ppPBE	cp-ppHF	ppHF-augqz
$C_2H_4-F_2$	-1.06	0.81	-1.90	-0.57	-1.71	2.81	-0.49	0.47	-0.98	-0.89
NH_3-F_2	-1.81	0.14	-2.27	-0.79	-2.01	2.23	-1.08	0.09	-1.60	-1.04
C_2H_2-ClF	-3.81	-2.95	-4.32	-5.79	-4.75	0.64	-1.68	-3.85	-3.27	-4.31
$HCN-ClF$	-4.86	-5.72	-6.88	-8.63	-6.97	-1.36	-3.24	-6.08	-4.72	-5.74
NH_3-Cl_2	-4.88	-4.74	-5.68	-7.21	-5.94	-1.35	-3.11	-5.59	-4.57	-4.87
H_2O-ClF	-5.36	-4.29	-5.77	-6.89	-6.19	-1.52	-3.73	-5.36	-5.00	-5.56
NH_3-ClF	-10.62	-10.31	-10.19	-15.94	-11.44	-4.79	-7.14	-13.75	-10.42	-10.70

TABLE IX. Detailed interaction data (in kcal/mol) for DI6/04. Data unavailable in space left blank owing to large computational cost.

	Benchmark	phPBE	phHF	ppPBE	ppHF	cp-phPBE	cp-phHF	cp-ppPBE	cp-ppHF	ppHF-augqz
H_2S-H_2S	-1.66	-2.59	-2.40	-3.04	-2.37	-0.60	-0.72	-1.83	-1.28	-1.81
$HCl-HCl$	-2.01	-2.60	-2.54	-3.06	-2.53	-0.66	-0.91	-1.92	-1.51	-2.28
H_2S-HCl	-3.35	-4.28	-4.22	-5.06	-4.31	-1.53	-1.97	-3.47	-2.90	-3.67
$CH_3Cl-HCl$	-3.55	-4.57	-4.27	-5.45	-4.34	-1.46	-1.72	-3.71	-2.80	
$HCN-CH_3SH$	-3.59	-5.93	-5.52	-6.19	-5.17	-2.28	-2.48	-4.05	-3.32	
$CH_3SH-HCl$	-4.16	-6.42	-6.07	-7.68	-6.22	-2.37	-2.77	-5.39	-4.23	

TABLE X. Detailed interaction data (in kcal/mol) for WI9/04. Data unavailable in space left blank owing to large computational cost.

	Benchmark	phPBE	phHF	ppPBE	ppHF	cp-phPBE	cp-phHF	cp-ppPBE	cp-ppHF	ppHF-augqz
HeNe	-0.04	-0.05	-0.08	-0.02	-0.05	0.04	0.01	0.03	0.00	-0.03
HeAr	-0.06	-0.06	-0.07	-0.05	-0.06	0.03	0.01	0.00	-0.01	-0.06
NeNe	-0.08	-0.13	-0.17	-0.06	-0.11	0.07	0.02	0.04	0.00	-0.07
NeAr	-0.13	-0.16	-0.17	-0.14	-0.13	0.05	0.03	-0.02	-0.01	-0.13
CH_4−Ne	-0.22	-0.55	-0.48	-0.39	-0.33	-0.02	-0.03	-0.10	-0.06	-0.21
C_6H_6−Ne	-0.47	-1.24	-0.95	-1.10	-0.74	-0.08	0.03	-0.45	-0.16	
CH_4−CH_4	-0.51	-1.85	-1.51	-1.51	-1.06	-0.25	-0.10	-0.63	-0.25	-0.43
C_2H_2−C_2H_2	-1.34	-2.54	-2.37	-2.55	-2.07	-0.83	-0.90	-1.64	-1.27	-1.53
C_2H_4−C_2H_4	-1.42	-3.49	-2.88	-3.30	-2.26	-0.71	-0.46	-1.85	-0.95	-1.45

TABLE XI. Mean Signed Errors (MSEs) and Mean Unsigned Errors (MUEs) (in kcal/mol) of HB6/04, CT7/04, DI6/04 and WI9/04 nonbonded interaction by pp-RPA and ph-RPA

Database	ph-RPA								pp-RPA							
	HF				PBE				HF				PBE			
	MSE		MUE		MSE		MUE		MSE		MUE		MSE		MUE	
	nocp	cp	nocp	cp	nocp	cp	nocp	cp	nocp	cp	nocp	cp	nocp	cp	nocp	cp
HB8/04	-1.05	1.14	1.05	1.14	-1.03	1.82	1.03	1.82	-1.02	-0.03	1.02	0.48	-2.01	-0.63	2.01	0.76
CT7/04	-0.66	1.70	0.78	1.70	0.76	4.15	1.01	4.15	-0.95	0.26	0.95	0.26	-1.92	-0.24	2.35	1.22
DI6/04	-1.12	1.29	1.12	1.29	-1.34	1.57	1.34	1.57	-1.10	0.38	1.10	0.40	-2.02	-0.34	2.02	0.37
WI9/04	-0.49	0.32	0.49	0.32	-0.65	0.29	0.65	0.29	-0.28	0.17	0.28	0.17	-0.54	-0.04	0.55	0.15
Total	-0.79	1.05	0.82	1.05	-0.53	1.86	0.97	1.86	-0.78	0.20	0.78	0.31	-1.52	-0.28	1.63	0.60