Table 1: Bond lengths (in Å) of rare-gas dimers without counterpoise correction for BSSE. [a]

Method	He_2	Ne_2	Ar_2	Kr_2	HeNe	HeAr	HeKr	NeAr	NeKr	ArKr	MSE	MUE
Reference	2.97 [b]	3.09 [b]	3.76 [b]	4.01 [b]	3.03 [c]	3.48 [c]	3.69 [c]	3.49 [c]	3.62 [c]	3.88 [c]		
B97-1	2.70	3.02	3.88	4.21	2.85	3.35	3.53	3.46	3.64	4.05	**-0.03**	**0.14**
PBEPW91	2.74	3.09	3.98	4.30	2.92	3.43	3.59	3.54	3.69	4.14	**0.04**	**0.14**
B98	2.78	3.13	4.01	4.34	2.97	3.47	3.63	3.57	3.75	4.17	0.08	**0.14**
PBE	2.75	3.11	4.00	4.33	2.94	3.44	3.60	3.55	3.71	4.17	**0.06**	**0.15**
PBE0	2.80	3.14	4.04	4.37	2.98	3.48	3.72	3.59	3.75	4.20	0.11	**0.15**
PW6B95	3.04	3.22	3.72	4.27	3.00	3.39	3.83	3.57	4.08	4.15	0.13	0.16
M05-2X	2.73	2.87	3.81	4.12	2.79	3.29	3.45	3.34	3.52	3.97	-0.11	0.16
PBE1W	2.75	3.11	4.05	4.39	2.94	3.45	3.61	3.57	3.73	4.22	0.08	0.17
PW91	2.65	3.02	3.95	4.30	2.82	3.34	3.53	3.48	3.64	4.13	**-0.02**	0.17
PWB6K	2.77	2.94	3.71	4.26	2.98	3.38	3.81	3.56	4.07	4.14	**0.06**	0.17
MPW1B95	3.05	3.23	3.73	4.28	3.01	3.40	4.18	3.60	4.09	4.16	0.17	0.20
MPWB1K	3.05	3.23	3.72	4.28	3.01	3.40	4.19	3.60	4.10	4.16	0.17	0.20
M05	2.62	2.86	3.73	4.19	2.74	3.26	3.46	3.31	3.45	3.97	-0.14	0.20
TPSS	2.95	3.23	4.37	4.66	3.04	3.69	3.85	3.74	4.01	4.51	0.30	0.31
TPSSh	2.96	3.23	4.37	4.65	3.04	3.71	3.86	3.82	4.01	4.51	0.31	0.32
LSDA	2.40	2.61	3.40	3.69	2.47	2.93	3.12	3.01	3.16	3.55	-0.47	0.47
MPW1K	3.09	3.39	4.65	5.03	3.25	3.89	4.22	3.96	4.09	4.86	0.54	0.54
mPW1PW91	3.09	3.43	4.65	5.06	3.25	3.88	4.22	3.97	4.10	4.86	0.55	0.55
Average											0.10	0.24

[a] The aug-cc-pVTZ basis set are employed in all calculations in this table.
[b] Ref. [1] [c] Ref. [2]

Table 2: Binding energies (in kcal/mol) of rare-gas dimers without counterpoise correction for BSSE [a]

Method	He_2	Ne_2	Ar_2	Kr_2	HeNe	HeAr	HeKr	NeAr	NeKr	ArKr	MSE	MUE
Reference	0.022 [b]	0.084 [b]	0.285 [b]	0.400 [b]	0.041 [c]	0.057 [c]	0.057 [c]	0.134 [c]	0.142 [c]	0.361 [c]		
M05-2X	0.025	0.181	0.266	0.291	0.084	0.082	0.085	0.194	0.201	0.275	**0.010**	**0.053**
B97-1	0.072	0.124	0.185	0.224	0.100	0.099	0.101	0.144	0.152	0.201	**-0.018**	**0.069**
B98	0.051	0.089	0.121	0.148	0.072	0.067	0.068	0.100	0.105	0.132	-0.063	**0.080**
PBE	0.075	0.128	0.138	0.163	0.104	0.090	0.090	0.136	0.144	0.149	-0.037	**0.082**
PBEPW91	0.077	0.132	0.145	0.172	0.107	0.093	0.094	0.141	0.150	0.157	**-0.032**	**0.083**
M05	0.075	0.199	0.225	0.232	0.131	0.110	0.091	0.215	0.198	0.220	**0.011**	0.085
PBE1W	0.079	0.132	0.135	0.158	0.108	0.093	0.093	0.138	0.146	0.145	-0.036	0.086
PBE0	0.042	0.080	0.092	0.109	0.064	0.054	0.052	0.084	0.086	0.099	-0.082	0.091
PWB6K	0.150	0.269	0.271	0.309	0.177	0.188	0.154	0.240	0.174	0.291	0.064	0.099
TPSS	0.047	0.085	0.072	0.079	0.071	0.052	0.055	0.077	0.084	0.076	-0.089	0.100
PW6B95	0.095	0.189	0.132	0.206	0.148	0.133	0.125	0.190	0.166	0.202	**0.000**	0.101
MPWB1K	0.048	0.102	0.012	0.093	0.071	0.048	0.048	0.088	0.093	0.095	-0.089	0.103
TPSSh	0.039	0.073	0.064	0.070	0.061	0.044	0.046	0.066	0.072	0.067	-0.098	0.105
MPW1B95	0.057	0.116	-0.004	0.089	0.081	0.052	0.057	0.096	0.106	0.093	-0.084	0.105
mPW1PW91	0.038	0.069	0.053	0.050	0.055	0.043	0.040	0.064	0.065	0.052	-0.105	0.111
MPW1K	0.027	0.052	0.042	0.040	0.042	0.032	0.029	0.049	0.048	0.041	-0.118	0.119
PW91	0.231	0.337	0.305	0.324	0.284	0.250	0.251	0.335	0.347	0.314	0.139	0.164
LSDA	0.227	0.528	0.761	0.895	0.369	0.363	0.353	0.606	0.627	0.818	0.396	0.396
Average											-0.01	0.11

[a] The aug-cc-pVTZ basis set are employed in all calculations in this table.
[b] Ref. [1] [c] Ref. [2]

Table 3: Binding energies (in kcal/mol) of rare-gas dimers with counterpoise correction for BSSE [a b]

Method	He_2	Ne_2	Ar_2	Kr_2	HeNe	HeAr	HeKr	NeAr	NeKr	ArKr	MSE	MUE
Reference	0.022 [b]	0.084 [b]	0.285 [b]	0.400 [b]	0.041 [c]	0.057 [c]	0.057 [c]	0.134 [c]	0.142 [c]	0.361 [c]		
M05-2X	0.021	0.151	0.238	0.261	0.069	0.074	0.066	0.171	0.170	0.248	**-0.012**	**0.048**
B97-1	0.071	0.105	0.171	0.208	0.091	0.095	0.095	0.131	0.139	0.187	**-0.029**	**0.068**
PBEPW91	0.075	0.115	0.134	0.155	0.098	0.088	0.087	0.130	0.138	0.143	-0.042	**0.082**
PBE	0.073	0.111	0.127	0.146	0.095	0.085	0.084	0.125	0.133	0.136	-0.047	**0.084**
B98	0.049	0.070	0.109	0.133	0.062	0.062	0.063	0.087	0.093	0.119	-0.074	**0.086**
M05	0.074	0.165	0.198	0.204	0.118	0.107	0.103	0.193	0.195	0.196	**-0.003**	0.086
PBE1W	0.077	0.116	0.125	0.142	0.099	0.088	0.087	0.128	0.136	0.133	**-0.045**	0.086
PWB6K	0.149	0.246	0.259	0.301	0.167	0.184	0.148	0.228	0.168	0.283	0.055	0.095
PBE0	0.041	0.062	0.081	0.095	0.054	0.049	0.041	0.071	0.075	0.086	-0.093	0.099
PW6B95	0.094	0.174	0.118	0.196	0.139	0.130	0.122	0.178	0.160	0.193	**-0.008**	0.100
TPSS	0.045	0.068	0.061	0.065	0.059	0.049	0.049	0.068	0.074	0.063	-0.098	0.107
MPWB1K	0.047	0.085	-0.004	0.082	0.060	0.043	0.046	0.075	0.086	0.084	-0.098	0.107
MPW1B95	0.056	0.099	-0.019	0.077	0.070	0.048	0.055	0.083	0.100	0.082	-0.093	0.109
TPSSh	0.038	0.056	0.052	0.057	0.049	0.041	0.037	0.057	0.062	0.055	-0.108	0.113
mPW1PW91	0.037	0.060	0.042	0.040	0.049	0.038	0.037	0.055	0.057	0.042	-0.113	0.117
MPW1K	0.026	0.041	0.031	0.031	0.034	0.027	0.027	0.039	0.040	0.031	-0.126	0.127
PW91	0.229	0.315	0.293	0.307	0.273	0.245	0.244	0.320	0.333	0.300	0.128	0.158
LSDA	0.224	0.491	0.714	0.827	0.349	0.345	0.334	0.566	0.583	0.763	0.361	0.361
Average											-0.02	0.11

[a] The aug-cc-pVTZ basis set are employed in all calculations in this table.
Ref. [1] [c] Ref. [2]

Table 4: Bond lengths (in Å) of alkaline metal dimers, Zn_2, and Zn-rare-gas dimers without counterpoise correction for BSSE [a b]

Method	Be_2	Mg_2	Ca_2	Zn_2	ZnNe	ZnAr	ZnKr	MSE	MUE
Reference	2.45	3.89	4.28	4.19	4.42	4.38	4.20		
PWB6K	2.62	3.79	4.30	3.67	4.00	4.25	4.28	-0.13	**0.21**
M05-2X	2.66	3.86	4.41	3.85	3.93	4.27	4.38	**-0.06**	**0.21**
B98	2.53	3.68	4.26	3.51	3.99	4.36	4.47	-0.15	**0.25**
PW6B95	2.52	3.74	4.23	3.58	4.12	4.63	4.55	**-0.06**	**0.25**
B97-1	2.52	3.63	4.23	3.48	3.86	4.20	4.32	-0.22	**0.28**
MPWB1K	2.61	3.75	4.28	3.62	4.20	4.66	4.78	**0.01**	0.28
PBE0	2.50	3.59	4.20	3.32	4.06	4.45	4.53	-0.17	0.29
MPW1B95	2.54	3.70	4.23	3.52	4.17	4.65	4.78	**-0.03**	0.30
M05	2.54	3.63	4.23	3.55	3.57	4.11	4.25	-0.28	0.32
PBE1W	2.42	3.56	4.12	3.30	3.89	4.38	4.49	-0.23	0.32
PBE	2.42	3.50	4.10	3.17	3.87	4.28	4.38	-0.30	0.35
PBEPW91	2.42	3.51	4.10	3.18	3.85	4.25	4.34	-0.31	0.35
PW91	2.42	3.50	4.09	3.14	3.77	4.23	4.35	-0.33	0.37
TPSSh	2.47	3.55	4.15	3.18	4.23	4.75	4.99	**-0.07**	0.41
TPSS	2.44	3.51	4.11	3.10	4.19	4.72	4.88	-0.12	0.41
MPW1K	2.58	3.66	4.27	3.45	4.56	5.11	5.30	0.16	0.44
mPW1PW91	2.51	3.60	4.21	3.34	4.41	5.09	5.31	0.09	0.44
LSDA	2.40	3.40	3.99	2.85	3.19	3.51	3.60	-0.70	0.70
Average								-0.16	0.34

[a] The aug-CV(T+2d)Z (see text) is employed for Ca, and the aug-cc-pVTZ basis set is employed for all other elements.
[b] The reference data for Be_2: ref.[3]; Mg_2: ref. [4];Ca_2: ref. [5]; Zn_2:[6]; ZnNe: ref. [7]; ZnAr: ref. [8]; ZnKr: ref. [9].

Table 5: Binding energies (in kcal/mol) of alkaline metal dimers and Zn_2 without counterpoise correction for BSSE [a]

Method	X [b]	Be_2	Mg_2	Ca_2	Zn_2	MSE	MUE
Reference		2.72 [c]	1.21 [c]	3.13 [c]	0.80 [c]		
M05-2X	56	2.53	1.20	2.90	0.77	**-0.12**	**0.12**
PWB6K	46	3.07	1.38	3.34	0.74	**0.17**	**0.20**
MPWB1K	44	3.08	1.30	3.36	0.53	**0.10**	**0.24**
PW6B95	28	4.36	1.38	3.57	0.66	**0.53**	**0.59**
MPW1B95	31	4.22	1.45	3.68	0.59	**0.52**	**0.62**
M05	28	4.53	1.39	3.49	1.07	0.65	0.65
MPW1K	43	4.33	1.98	4.04	0.76	0.81	0.83
B98	22	5.49	2.04	4.15	0.93	1.19	1.19
mPW1PW91	25	6.09	2.28	4.60	0.91	1.50	1.50
B97-1	21	6.20	2.41	4.65	1.19	1.65	1.65
PBE0	25	6.60	2.61	4.93	1.27	1.89	1.89
TPSSh	10	6.93	2.66	5.56	1.36	2.16	2.16
PBE1W	0	9.04	2.51	5.48	1.18	2.58	2.58
TPSS	0	8.17	2.97	6.27	1.63	2.80	2.80
PBEPW91	0	9.86	3.20	6.24	1.77	3.30	3.30
PBE	0	9.89	3.28	6.32	1.80	3.36	3.36
PW91	0	10.05	3.41	6.50	2.04	3.53	3.53
LSDA	0	12.93	5.00	7.91	5.25	5.81	5.81
Average						1.80	1.83

[a] The aug-CV(T+2d)Z (see text) is employed for Ca, and the aug-cc-pVTZ basis set is employed for all other elements.
[b] *X* denotes the percentage of Hartree-Fock exchange in the functional.
[c] The reference data for Be_2: ref.[3]; Mg_2: ref. [4];Ca_2: ref. [5]; Zn_2: ref.[6].

Table 6: Binding energies (in kcal/mol) of alkaline metal dimers and Zn_2 with counterpoise correction for BSSE [a]

Method	X [b]	Be_2	Mg_2	Ca_2	Zn_2	MSE	MUE
Reference		2.72 [c]	1.21 [c]	3.13 [c]	0.80 [c]		
M05-2X	56	2.45	1.13	2.87	0.72	**-0.17**	**0.17**
PWB6K	46	3.04	1.37	3.33	0.72	**0.15**	**0.19**
MPWB1K	44	3.06	1.28	3.35	0.51	**0.08**	**0.23**
PW6B95	28	4.30	1.35	3.55	0.64	**0.49**	**0.57**
M05	28	4.46	1.33	3.43	1.01	0.59	**0.59**
MPW1B95	31	4.18	1.42	3.66	0.57	**0.49**	0.61
MPW1K	43	4.24	1.93	4.03	0.75	0.77	0.80
B98	22	5.40	1.98	4.14	0.84	1.12	1.12
mPW1PW91	25	5.95	2.22	4.58	0.88	1.44	1.44
B97-1	21	6.10	2.35	4.64	1.16	1.60	1.60
PBE0	25	6.49	2.55	4.91	1.24	1.83	1.83
TPSSh	10	6.73	2.56	5.54	1.33	2.08	2.08
PBE1W	0	8.87	2.43	5.45	1.13	2.50	2.50
TPSS	0	7.92	2.86	6.25	1.60	2.69	2.69
PBEPW91	0	9.68	3.10	6.22	1.72	3.22	3.22
PBE	0	9.71	3.19	6.32	1.75	3.27	3.27
PW91	0	9.86	3.33	6.46	1.99	3.44	3.44
LSDA	0	12.81	4.77	7.89	5.16	5.69	5.69
Average						1.74	1.78

[a] The aug-CV(T+2d)Z (see text) is employed for Ca, and the aug-cc-pVTZ basis set is employed for all other elements.
[b] *X* denotes the percentage of Hartree-Fock exchange in the functional.
[c] The reference data for Be_2: ref.[3]; Mg_2: ref. [4];Ca_2: ref. [5]; Zn_2: ref.[6].

Table 7: Binding energies (in kcal/mol) of zinc-rare-gas dimers without counterpoise corrections for BSSE [a]

Method	ZnNe	ZnAr	ZnKr	MSE	MUE
Reference	0.067 [b]	0.234 [b]	0.329 [b]		
B97-1	0.158	0.236	0.284	**0.016**	**0.046**
M05-2X	0.101	0.200	0.245	**-0.028**	**0.050**
PWB6K	0.213	0.254	0.272	0.037	**0.074**
PBEPW91	0.177	0.193	0.227	**-0.011**	**0.084**
B98	0.112	0.159	0.192	-0.056	**0.085**
PBE	0.170	0.182	0.215	**-0.021**	0.089
M05	0.295	0.276	0.306	0.082	0.098
PBE1W	0.173	0.173	0.197	-0.029	0.099
PW6B95	0.194	0.188	0.193	**-0.018**	0.103
PBE0	0.086	0.111	0.135	-0.099	0.112
MPWB1K	0.091	0.095	0.099	-0.115	0.131
MPW1B95	0.111	0.103	0.104	-0.104	0.133
TPSS	0.096	0.083	0.090	-0.120	0.139
TPSSh	0.078	0.071	0.078	-0.134	0.142
mPW1PW91	0.073	0.055	0.053	-0.149	0.153
PW91	0.388	0.344	0.366	0.156	0.156
MPW1K	0.049	0.041	0.040	-0.167	0.167
LSDA	0.641	0.978	1.199	0.729	0.729
Average				-0.043	0.099

[a] The aug-cc-pVTZ basis set are employed for all calculations.
[b] The reference data for ZnNe: ref. [7]; ZnAr: ref. [8]; ZnKr: ref. [9]

Table 8: Binding energies (in kcal/mol) of zinc-rare-gas dimers with counterpoise corrections for BSSE [a]

Method	ZnNe	ZnAr	ZnKr	MSE	MUE
Reference	0.067 [b]	0.234 [b]	0.329 [b]		
B97-1	0.150	0.224	0.269	**0.004**	**0.051**
M05-2X	0.088	0.177	0.212	-0.051	**0.065**
PWB6K	0.207	0.246	0.263	**0.029**	**0.073**
B98	0.106	0.147	0.178	-0.066	**0.092**
PBEPW91	0.169	0.179	0.208	**-0.024**	**0.092**
M05	0.274	0.263	0.273	0.060	0.097
PBE	0.162	0.170	0.196	**-0.034**	0.097
PBE1W	0.166	0.161	0.180	-0.041	0.107
PW6B95	0.190	0.181	0.183	**-0.025**	0.107
PBE0	0.081	0.101	0.122	-0.109	0.118
MPWB1K	0.084	0.088	0.091	-0.122	0.134
MPW1B95	0.105	0.095	0.095	-0.112	0.137
PW91	0.379	0.329	0.346	0.142	0.142
TPSS	0.089	0.072	0.075	-0.131	0.145
TPSSh	0.071	0.061	0.065	-0.144	0.147
mPW1PW91	0.068	0.047	0.043	-0.157	0.157
MPW1K	0.044	0.033	0.032	-0.173	0.173
LSDA	0.604	0.936	1.134	0.681	0.681
Average				-0.015	0.145

[a] The aug-cc-pVTZ basis set are employed for all calculations.
[b] The reference data for ZnNe: ref. [7]; ZnAr: ref. [8]; ZnKr: ref. [9]

Table 9: Mean percentage unsigned errors (M%UE) [a]

Method	Energetics										Geometry			MMMM%UE
	Rare Gas Dimers			Metal Dimers			Zn-rare-gas dimers			MMM%UE	Bond Length			
	no-CP	CP	MM%UE	no-CP	CP	MM%UE	no-CP	CP	MM%UE		no-CP	CP	MM%UE	
M05-2X	**49**	**34**	**41**	**5**	**9**	**7**	**30**	**30**	**30**	**26**	**5**	**5**	**5**	**16**
MPWB1K	58	**59**	**59**	**15**	**15**	**15**	55	53	54	**42**	6	6	6	**24**
B98	**49**	**51**	**50**	55	50	52	**47**	**47**	**47**	**50**	**5**	**5**	**5**	**27**
MPW1B95	63	63	63	**29**	29	**29**	63	62	63	**51**	6	6	6	**29**
B97-1	66	60	63	81	78	79	**50**	**49**	**49**	64	**5**	**5**	**5**	**34**
PBE0	**49**	**55**	**52**	94	90	92	**46**	**46**	**46**	**64**	5	6	6	35
MPW1K	62	69	66	39	38	38	66	70	68	58	13	14	14	36
mPW1PW91	60	64	62	68	65	66	56	56	56	61	13	14	14	37
PW6B95	114	108	111	**26**	**26**	**26**	83	83	83	73	**5**	**5**	**5**	39
TPSSh	**57**	62	60	106	101	103	**54**	**53**	**54**	72	9	10	9	41
M05	97	89	93	32	**27**	29	121	112	116	78	7	7	7	42
PWB6K	169	161	165	**10**	**10**	**10**	81	78	79	84	**5**	**5**	**5**	45
PBE1W	73	69	71	115	111	113	74	74	74	86	6	6	6	46
TPSS	**56**	**59**	**58**	138	132	135	60	59	60	84	9	9	9	46
PBEPW91	72	66	69	162	157	159	70	70	70	99	6	6	6	53
PBE	68	65	67	165	160	163	70	69	69	100	6	6	6	53
PW91	283	273	278	166	148	157	178	167	172	201	6	6	6	103
LSDA	458	428	443	350	341	345	478	447	462	412	15	15	15	213
Average	106	102	104	92	88	90	93	90	92	95	7	8	7	51

[a] see section 3.6 for the definitions of MM%UE, MMM%UE, and MMMM%UE. CP denotes the counterpoise correction for BSSE.

Table 10: Mean unsigned errors (kcal/mol) on a broad range of energetic databases.

Functional	WI17 [a]	NCBE31	TMAE4/05 [b]	MLBE4/05 [b]	MGT135	HTK57	NHTBH38	AMUEXM [c]	AMUE [d]
M05-2X	**0.07**	**0.3** [b]	29.4	15.2	**0.9** [b]	**1.0** [b]	**1.7** [a]	**0.8**	7.0
MPWB1K	**0.14**	**0.6** [e]	29.3	11.5	1.4 [f]	**1.3** [b]	**1.5** [g]	**1.0**	6.5
B98	0.34	0.8 [e]	**19.9**	8.0	**1.0** [f]	2.6 [b]	3.4 [g]	1.6	**5.1**
MPW1B95	0.23	0.7 [e]	25.1	7.6	**1.0** [e,f]	1.9 [b]	2.3 [g]	**1.2**	5.5
B97-1	0.43	0.7 [e]	**18.6**	8.4	1.1 [e]	2.9 [b,f]	3.5 [g]	1.7	**5.1**
PBE0	0.51	0.7 [e]	25.0	**6.3**	1.3 [e,f]	2.8 [b]	3.5 [g]	1.8	5.7
MPW1K	0.29	0.9 [e]	31.8	13.1	2.6 [e,f]	**1.3** [b]	**1.8** [g]	1.4	7.4
mPW1PW91	0.44	1.0 [e]	26.5	**7.0**	1.3 [e,f]	2.3 [f]	3.2 [g]	1.7	6.0
PW6B95	**0.22**	**0.6** [e]	**24.3**	**7.4**	**0.8** [f]	2.0 [a]	2.9 [a]	1.3	**5.5**
TPSSh	0.59	1.1 [e]	**16.0**	**4.6**	1.4 [f]	4.3 [b,f]	6.9 [g]	2.8	**5.0**
M05	**0.21**	**0.5** [h]	**7.3**	**5.0**	**1.0** [h]	**1.4** [b,f]	**2.1** [g]	**1.1**	**2.5**
PWB6K	**0.12**	**0.4** [f]	33.9	13.6	1.7 [e]	**1.4** [b,f]	**1.4** [a]	**1.0**	7.5

[a] present work
[b] Ref. [10]
[c] Average over mean errors for the WI17, NCBE31, MGT135, HTK57, and NHTBH databases.
[d] Average over mean errors for all seven databases.
[e] Ref. [11]
[f] Ref. [12]
[g] Ref. [13]
[h] Ref. [14]

Figure captions

Figure 1. Potential energy curves for the Be_2 dimer. The aug-cc-pVTZ basis set is used for all calculations in this figure, and no counterpoise corrections are applied. The reference curve is taken form Ref.[3].

Figure 2. Potential energy curves for the Ar_2 dimer. The aug-cc-pVTZ basis set is used for all calculations in this figure, and no counterpoise corrections are applied.

Figure 1.

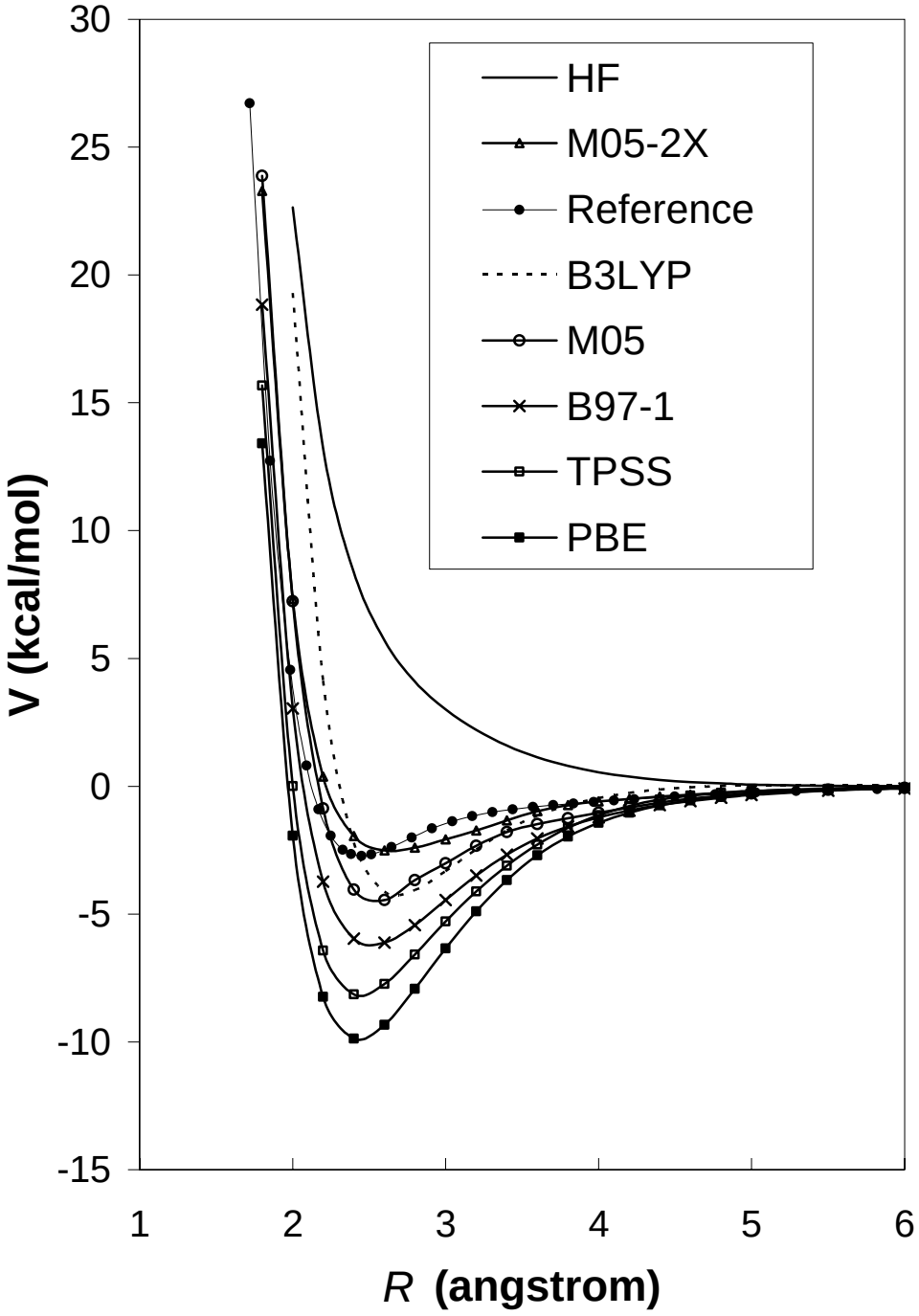
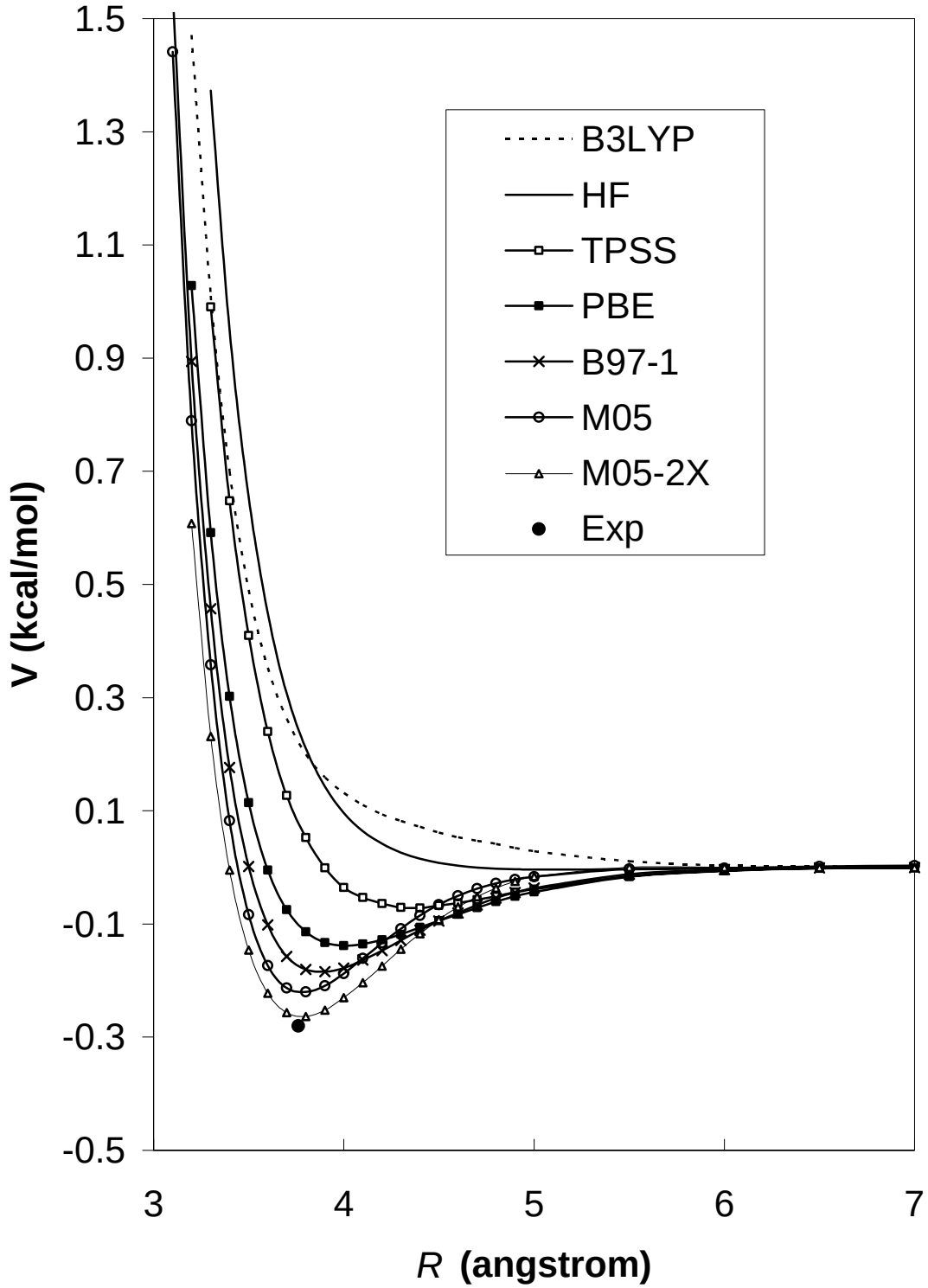

HF
M05-2X
Reference
B3LYP
M05
B97-1
TPSS
PBE
V (kcal/mol)
R (angstrom)
30
25
20
15
10
5
0
-5
-10
-15
1
2
3
4
5
6

Figure 2.


1.5
1.3
1.1
0.9
0.7
0.5
0.3
0.1
-0.1
-0.3
-0.5
V (kcal/mol)
3
4
5
6
7
R (angstrom)
B3LYP
HF
TPSS
PBE
B97-1
M05
M05-2X
Exp

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(14) Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Phys.* **2005**, *123*, 161103. Note that in this communication we interchanged $c_{C\alpha\beta,i}$ and $c_{C\sigma\sigma,i}$ in Table 1. In addition, "reduced density x_σ" before eq. (1) should read "reduced density gradient x_σ".