Basis-set correction for coupled-cluster estimation of dipole moments Supplementary information

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CONTENTS

I. GEOMETRIES

TABLE I. Input xyz geometries (in angstrm) and their references.

Molecules			
CO [1]			
C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.1282
BeH [1]			
Be	0.0000	0.0000	0.0000
H	0.0000	0.0000	1.3426
BF [1]			
B	0.0000	0.0000	0.0000
F	0.00000	0.0000	1.2669
BH [2]			
B	0.0000	0.0000	0.0000
H	0.0000	0.0000	1.2324
CH [1]			
C	0.0000	0.0000	0.0000
H	0.0000	0.0000	1.1199
NH [1]			
N	0.0000	0.0000	0.0000
H	0.0000	0.0000	1.0362
CH_2 (singlet) [1]			
C	0.0000	-0.0000	0.1734
H	0.0000	-0.8623	-0.5202
H	0.0000	-0.8623	-0.5202
FH [2]			
F	0.0000	0.0000	0.0000
H	0.0000	0.0000	0.9170
H_2O [1]			
O	0.0000	0.0000	0.1173
H	0.0000	0.7572	-0.4692
H	0.0000	-0.7572	-0.4692
BN [1]			
B	0.0000	0.0000	0.0000
N	0.0000	0.0000	1.3250
BO [1]			
B	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2045
LiH [1]			
Li	0.0000	0.0000	0.0000
H	0.0000	0.0000	1.5949
LiF [1]			
Li	0.0000	0.0000	0.0000
F	0.0000	0.0000	1.5639
LiN [1]			
Li	0.0000	0.0000	0.0000
N	0.0000	0.0000	1.8690

II. DETAILED RESULTS FOR THE MOLECULES

TABLE II. CO

Basis/Method	**HF**	**CCSD(T)**	**CCSD(T)+PBEUEG**
aug-cc-pVDZ	-0.10199	0.05550	0.04398
aug-cc-pVTZ	-0.10499	0.05000	0.04414
aug-cc-pVQZ	-0.10433	0.04600	0.04273
aug-cc-pV5Z	-0.10421	0.04500	0.04360
CBS		0.04485	

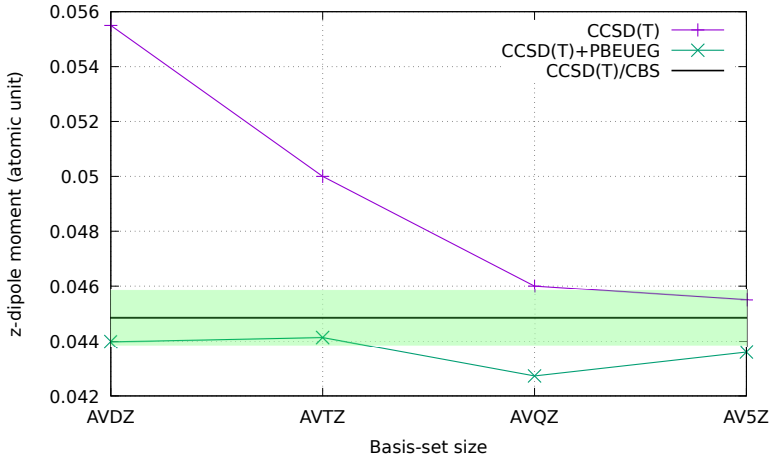

FIG. 1. CO

TABLE III. BeH

Basis/Method	**ROHF**	**ROCCSD(T)**	**ROCCSD(T)+PBEUEG**
aug-cc-pVDZ	0.11017	0.09550	0.08416
aug-cc-pVTZ	0.11076	0.09100	0.08746
aug-cc-pVQZ	0.11199	0.09050	0.08941
aug-cc-pV5Z	0.11218	0.09050	0.08980
CBS		0.09030	

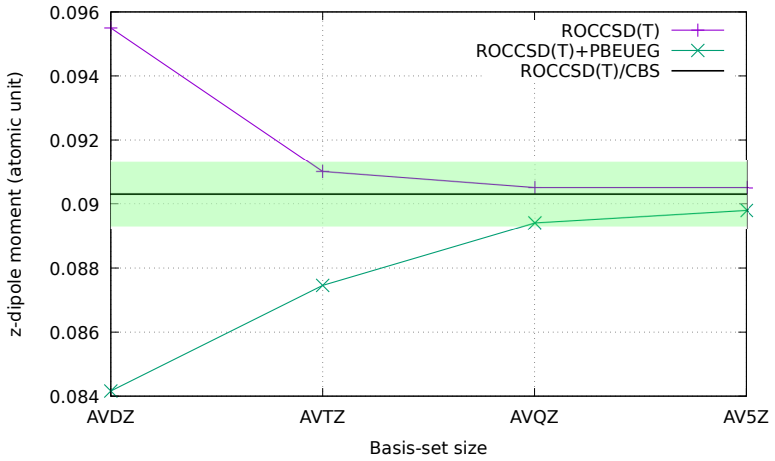

FIG. 2. BeH

TABLE IV. BF

Basis/Method	**HF**	**CCSD(T)**	**CCSD(T)+PBEUEG**
aug-cc-pVDZ	0.34436	0.34100	0.33287
aug-cc-pVTZ	0.33390	0.32700	0.32351
aug-cc-pVQZ	0.33314	0.32300	0.32082
aug-cc-pV5Z	0.33328	0.32200	0.32068
CBS		0.32081	

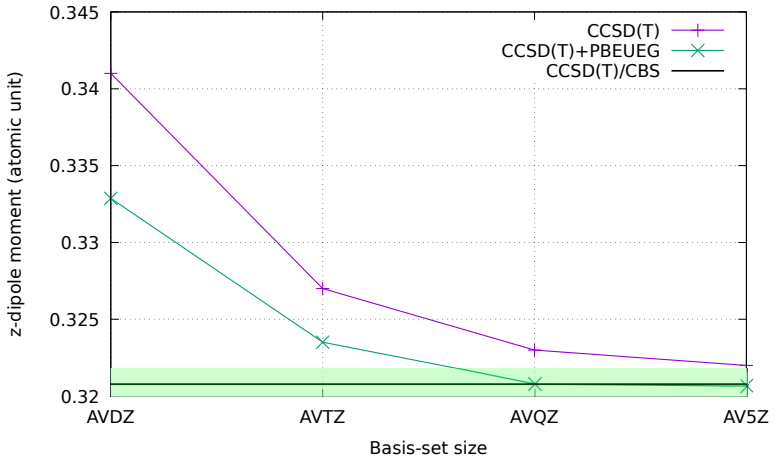

FIG. 3. BF

TABLE V. BH

Basis/ Method	**HF**	**CCSD(T)**	**CCSD(T)+PBEUEG**
aug-cc-pVDZ	0.68796	0.52950	0.54162
aug-cc-pVTZ	0.68649	0.54500	0.55002
aug-cc-pVQZ	0.68493	0.54750	0.54986
aug-cc-pV5Z	0.68496	0.54850	0.54980
CBS		0.54953	

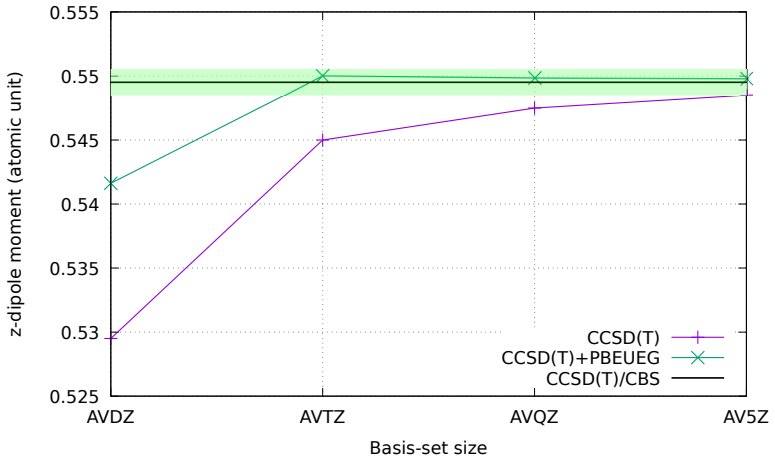

FIG. 4. BH

TABLE VI. CH

Basis/Method	**ROHF**	**ROCCSD(T)**	**ROCCSD(T)+PBEUEG**
aug-cc-pVDZ	0.62348	0.54150	0.55427
aug-cc-pVTZ	0.62000	0.54950	0.55481
aug-cc-pVQZ	0.61871	0.55150	0.55405
aug-cc-pV5Z	0.61858	0.55250	0.55396
CBS		0.55368	

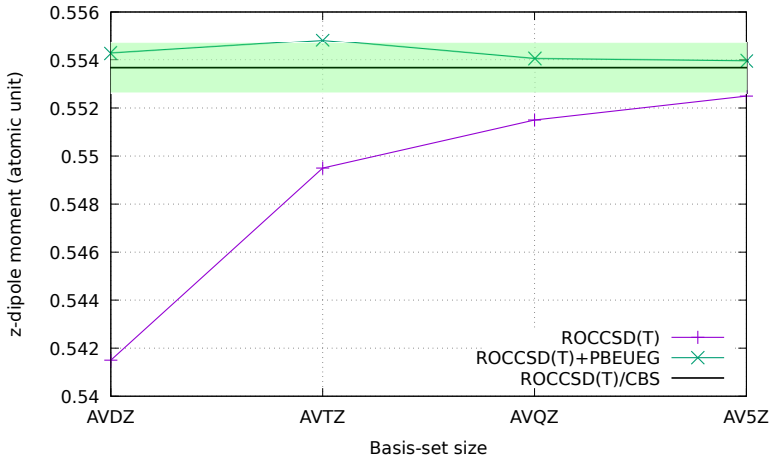

FIG. 5. CH

TABLE VII. NH

Basis/Method	**HF**	**CCSD(T)**	**CCSD(T)+PBEUEG**
aug-cc-pVDZ	0.63850	0.59350	0.60792
aug-cc-pVTZ	0.63505	0.59950	0.60519
aug-cc-pVQZ	0.63381	0.60200	0.60464
aug-cc-pV5Z	0.63384	0.60350	0.60506
CBS		0.60504	

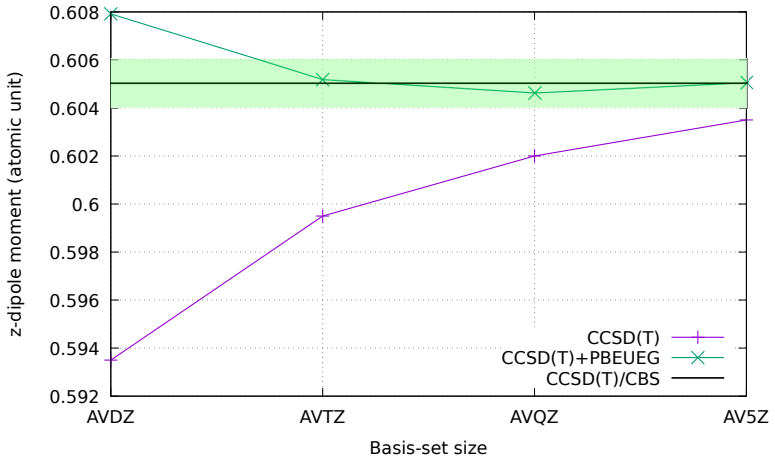

FIG. 6. NH

TABLE VIII. CH_2

Basis/Method	**HF**	**CCSD(T)**	**CCSD(T)+PBEUEG**
aug-cc-pVDZ	0.74877	0.65600	0.66666
aug-cc-pVTZ	0.74477	0.66000	0.66455
aug-cc-pVQZ	0.74355	0.66200	0.66420
aug-cc-pV5Z	0.74353	0.66350	0.66478
CBS		0.66510	

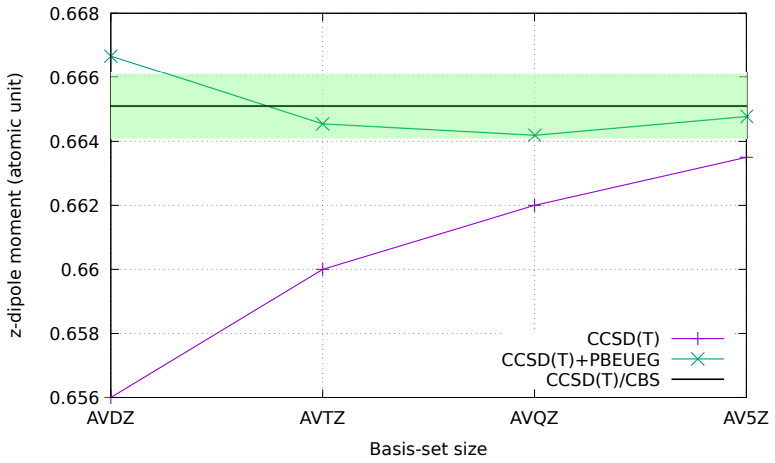

FIG. 7. CH_2

TABLE IX. FH

Basis/Method	**HF**	**CCSD(T)**	**CCSD(T)+PBEUEG**
aug-cc-pVDZ	0.75976	0.70350	0.71371
aug-cc-pVTZ	0.75751	0.70450	0.70903
aug-cc-pVQZ	0.75634	0.70700	0.70946
aug-cc-pV5Z	0.75617	0.70750	0.70900
CBS		0.70820	

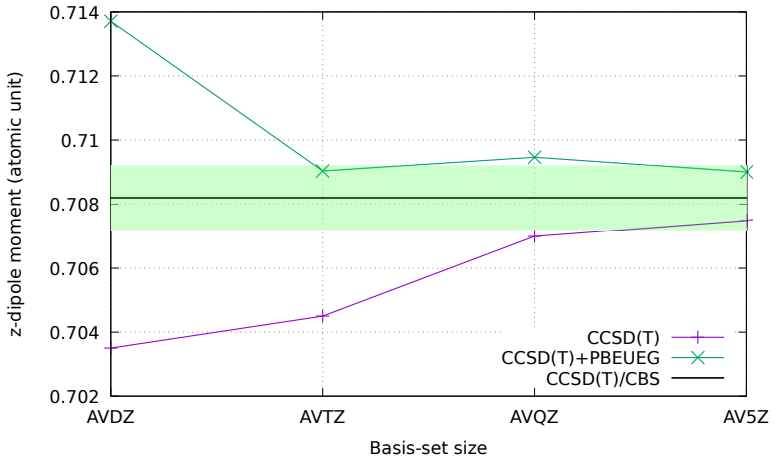

FIG. 8. FH

TABLE X. H_2O

Basis/Method	**HF**	**CCSD(T)**	**CCSD(T)+PBEUEG**
aug-cc-pVDZ	0.78671	0.72700	0.73891
aug-cc-pVTZ	0.78039	0.72400	0.72930
aug-cc-pVQZ	0.77956	0.72650	0.72912
aug-cc-pV5Z	0.77956	0.72800	0.72920
CBS		0.72957	

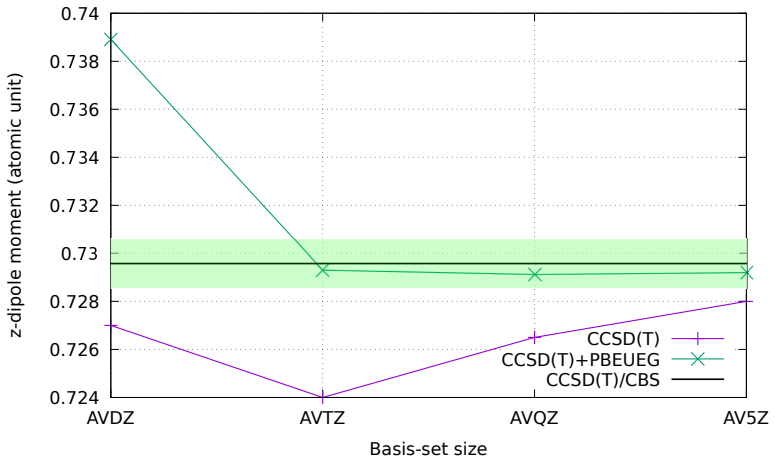

FIG. 9. H_2O

TABLE XI. BN

Basis/Method	**ROHF**	**ROCCSD(T)**	**ROCCSD(T)+PBEUEG**
aug-cc-pVDZ	1.13451	0.76250	0.77517
aug-cc-pVTZ	1.13862	0.77550	0.78145
aug-cc-pVQZ	1.13831	0.78400	0.78756
aug-cc-pV5Z	1.13840	0.78650	0.78846
CBS		0.78902	

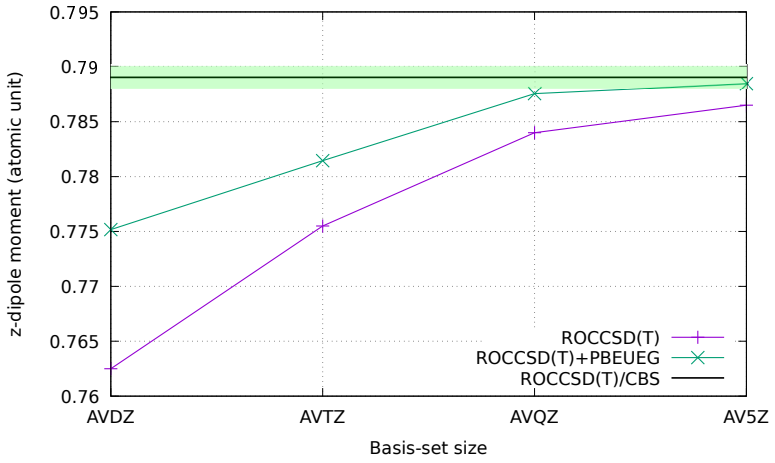

FIG. 10. BN

TABLE XII. BO

Basis/Method	**ROHF**	**ROCCSD(T)**	**ROCCSD(T)+PBEUEG**
aug-cc-pVDZ	1.17803	0.88300	0.89417
aug-cc-pVTZ	1.18533	0.89550	0.90153
aug-cc-pVQZ	1.18527	0.90250	0.90622
aug-cc-pV5Z	1.18539	0.90450	0.90698
CBS		0.90647	

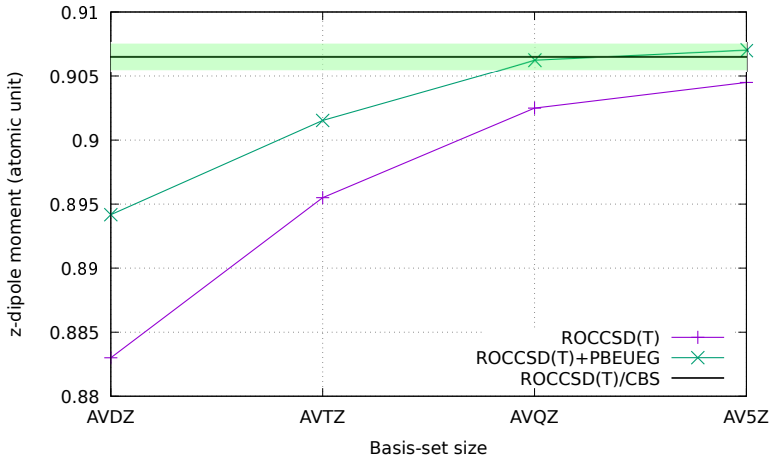

FIG. 11. BO

TABLE XIII. LiH

Basis/Method	**HF**	**CCSD(T)**	**CCSD(T)+PBEUEG**
aug-cc-pVDZ	2.37055	2.32500	2.32501
aug-cc-pVTZ	2.36235	2.31000	2.30965
aug-cc-pVQZ	2.36153	2.30800	2.30795
aug-cc-pV5Z	2.36129	2.30800	2.30802
CBS		2.30825	

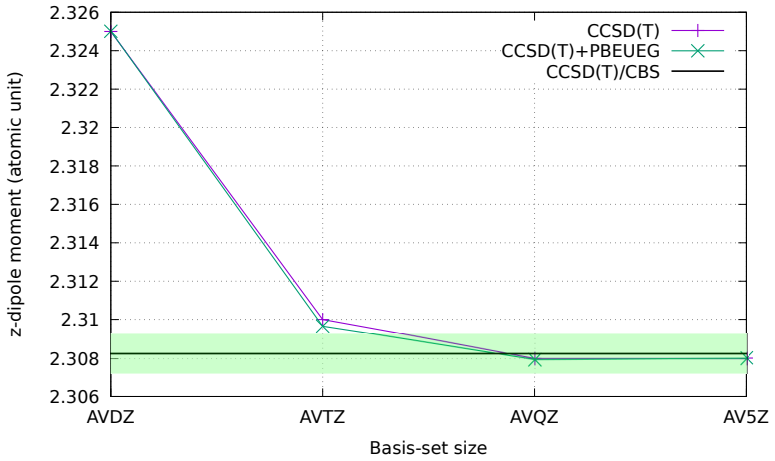

FIG. 12. LiH

TABLE XIV. LiF

Basis/Method	**HF**	**CCSD(T)**	**CCSD(T)+PBEUEG**
aug-cc-pVDZ	2.56111	2.50400	2.50942
aug-cc-pVTZ	2.54103	2.48300	2.48542
aug-cc-pVQZ	2.53949	2.48250	2.48367
aug-cc-pV5Z	2.53905	2.48250	2.48321
CBS		2.48297	

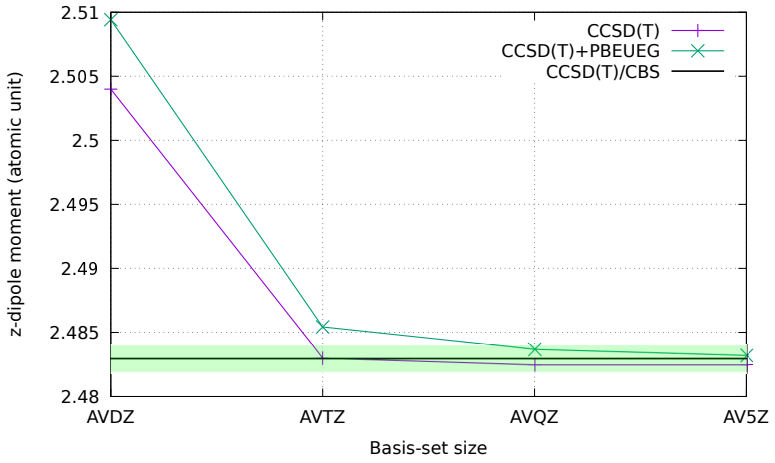

FIG. 13. LiF

TABLE XV. LiN

Basis/Method	**ROHF**	**ROCCSD(T)**	**ROCCSD(T)+PBEUEG**
aug-cc-pVDZ	2.90309	2.74200	2.75215
aug-cc-pVTZ	2.90379	2.77300	2.77714
aug-cc-pVQZ	2.90372	2.78250	2.78464
aug-cc-pV5Z	2.90317	2.78450	2.78583
CBS		2.78718	

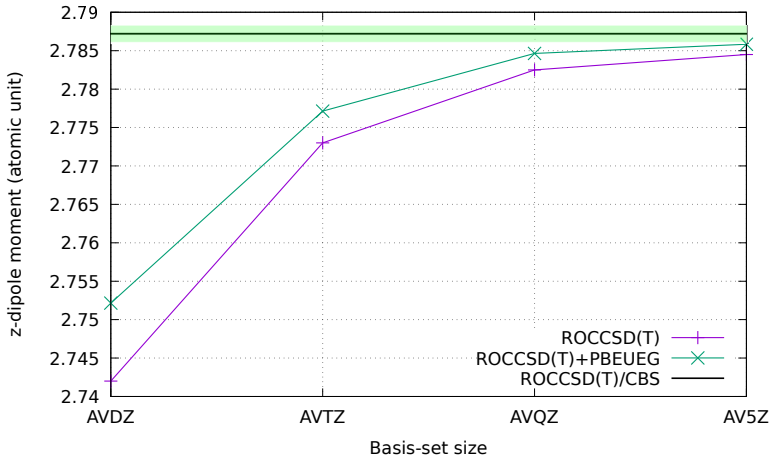

FIG. 14. LiN

III. TABLE OF ERRORS

TABLE XVI. Errors in dipole moments (in atomic units) with respect to CCSD(T)/CBS for frozen-core calculations for the entire set of molecules. For each Dunning basis set (AV*X*Z=aug-cc-pV*X*Z, *X* ∈{D,T,Q,5}), the first column contains the errors of the CCSD(T) dipole moments and the second column contains the errors after adding the PBEUEG basis-set correction.

	AVDZ		AVTZ		AVQZ		AV5Z	
	CCSD(T)	+PBEUEG	CCSD(T)	+PBEUEG	CCSD(T)	+PBEUEG	CCSD(T)	+PBEUEG
CO	0.01065	-0.00087	0.00515	-0.00071	0.00115	-0.00212	0.00065	-0.00125
BeH	0.00520	-0.00614	0.00070	-0.00284	0.00020	-0.00089	0.00020	-0.00050
BF	0.02019	0.01207	0.00619	0.00270	0.00219	0.00001	0.00119	-0.00013
BH	0.02003	0.00791	0.00453	-0.00049	0.00203	-0.00033	0.00103	-0.00027
CH	0.01218	-0.00059	0.00418	-0.00112	0.00218	-0.00036	0.00118	-0.00027
NH	0.01154	-0.00288	0.00554	-0.00015	0.00304	0.00041	0.00154	-0.00002
CH_2 (singlet)	0.00910	-0.00156	0.00510	0.00055	0.00310	0.00090	0.00160	0.00032
FH	0.00470	-0.00551	0.00370	-0.00083	0.00120	-0.00126	0.00070	-0.00080
H_2O	0.00257	-0.00934	0.00557	0.00027	0.00307	0.00045	0.00157	0.00037
BN	0.02652	0.013855	0.01352	0.00757	0.00502	0.00146	0.00252	0.00056
BO	0.02347	0.01230	0.01097	0.00494	0.00397	0.00025	0.00197	-0.00051
LiH	0.01675	0.01676	0.00175	0.00140	-0.00025	-0.00030	-0.00025	-0.00023
LiF	-0.02103	-0.02645	-0.00003	-0.00246	0.00047	-0.00070	0.00047	-0.00024
LiN	0.04518	0.03504	0.01418	0.01004	0.00468	0.00254	0.00268	0.00136

TABLE XVII. Relative errors (%) in dipole moments with respect to CCSD(T)/CBS for frozen-core calculations for the entire set of molecules. For each Dunning basis set (AV*X*Z=aug-cc-pV*X*Z, *X* ∈{D,T,Q,5}), the first column contains the errors of the CCSD(T) dipole moments and the second column contains the errors after adding the PBEUEG basis-set correction.

	AVDZ		AVTZ		AVQZ		AV5Z	
	CCSD(T)	+PBEUEG	CCSD(T)	+PBEUEG	CCSD(T)	+PBEUEG	CCSD(T)	+PBEUEG
CO	23.75	-1.95	11.48	-1.59	2.57	-4.74	1.45	-2.80
BeH	5.76	-6.79	0.78	-3.14	0.22	-0.99	0.22	-0.56
BF	6.29	3.76	1.93	0.84	0.68	0.00	0.37	-0.04
BH	-3.64	-1.44	-0.82	0.09	-0.37	0.06	-0.19	0.05
CH	-2.20	0.11	-0.76	0.20	-0.39	0.07	-0.21	0.05
NH	-1.91	0.48	-0.92	0.02	-0.50	-0.07	-0.25	0.00
CH_2 (singlet)	-1.37	0.23	-0.77	-0.08	-0.47	-0.14	-0.24	-0.05
FH	-0.66	0.78	-0.52	0.12	-0.17	0.18	-0.10	0.11
H_2O	-0.35	1.28	-0.76	-0.04	-0.42	-0.06	-0.22	-0.05
BN	-3.36	-1.76	-1.71	-0.96	-0.64	-0.19	-0.32	-0.07
BO	-2.59	-1.36	-1.21	-0.55	-0.44	-0.03	-0.22	0.06
LiH	0.73	0.73	0.08	0.06	-0.01	-0.01	-0.01	-0.01
LiF	0.85	1.07	0.00	0.10	-0.02	0.03	-0.02	0.01
LiN	-1.62	-1.26	-0.51	-0.36	-0.17	-0.09	-0.10	-0.05

[1] D. Hait and M. Head-Gordon, Journal of Chemical Theory and Computation **14**, 1969 (2018).
[2] A. Halkier, W. Klopper, T. Helgaker and P. Jorgensen, J. Chem. Phys. **111**, 4424 (1999).