Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material: How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?

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I. Figures and Tables

Fig. S1 shows the distribution of the relative errors in static polarizabilities computed using LSDA, SIC-LSDA and LSIC-LSDA with respect to CCSD(T) reference values.[1] The Gaussian curves have the same mean and standard deviation as the data. Fig. S2 and Fig. S3 show the relative errors in the static polarizabilities computed using the tested methods for the individual species of the NSP and SP subsets, respectively. Table S1 reports the effect of FOD optimization in the presence of an applied electric field on FLOSIC polarizabilities. Table S2 and S3 report the isotropic static polarizabilities (in $Å^3$) for all 132 species. Table S4 shows linear response isotropic dipole polarizabilities calculated with the PBE density functional[2] and different GTO basis sets[3–7] and with multi-wavelets, which are said to represent the infinite basis set limit.[8] All GTO basis linear response calculations were carried out using the Gaussian package and Cartesian GTO representation.[9] Table S5 shows total energies for the GTO calculations in Table S4. Table S6 compares PBE polarizabilities computed using the NRLMOL[10] basis set[11] (which uses a Cartesian form of the d-functions) and the finite field method for various values of the applied field for molecules of the NSP subset. The finite difference polarizabilities computed[8] with the MW basis and a field strength of 0.001 a.u. are also shown. Finally, Table S7 shows the values of PBE polarizabilities for a selection of molecules from the SP subset computed using the NRLMOL basis set and finite field strengths of 0.001 a.u. and 0.01 a.u. Hait and Head-Gordon[1] used 0.01 a.u. to obtain results for these molecules in their benchmark study.

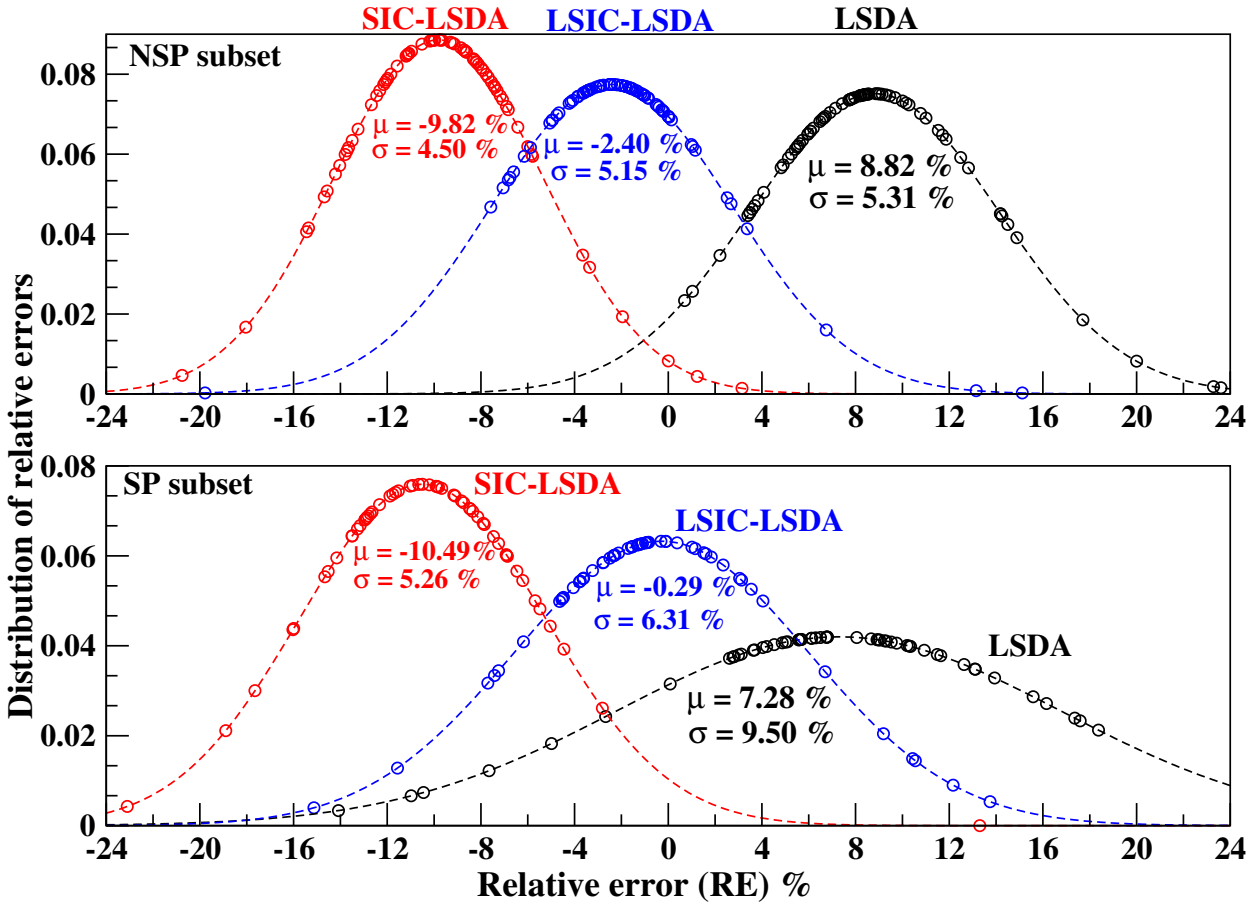

FIG. S1. Gaussian functions representing the relative errors (RE, in %) with respect to CCSD(T) for the calculated LSDA (black), SIC–LSDA (red), and LSIC–LSDA (blue) static polarizabilities of the 75 species in the NSP subset (upper panel) and the 57 species in the SP subset (lower panel). The means (μ) and standard deviations (σ) of the Gaussians are identical to those of the respective RE distributions. The circles indicate the REs of the individual species.

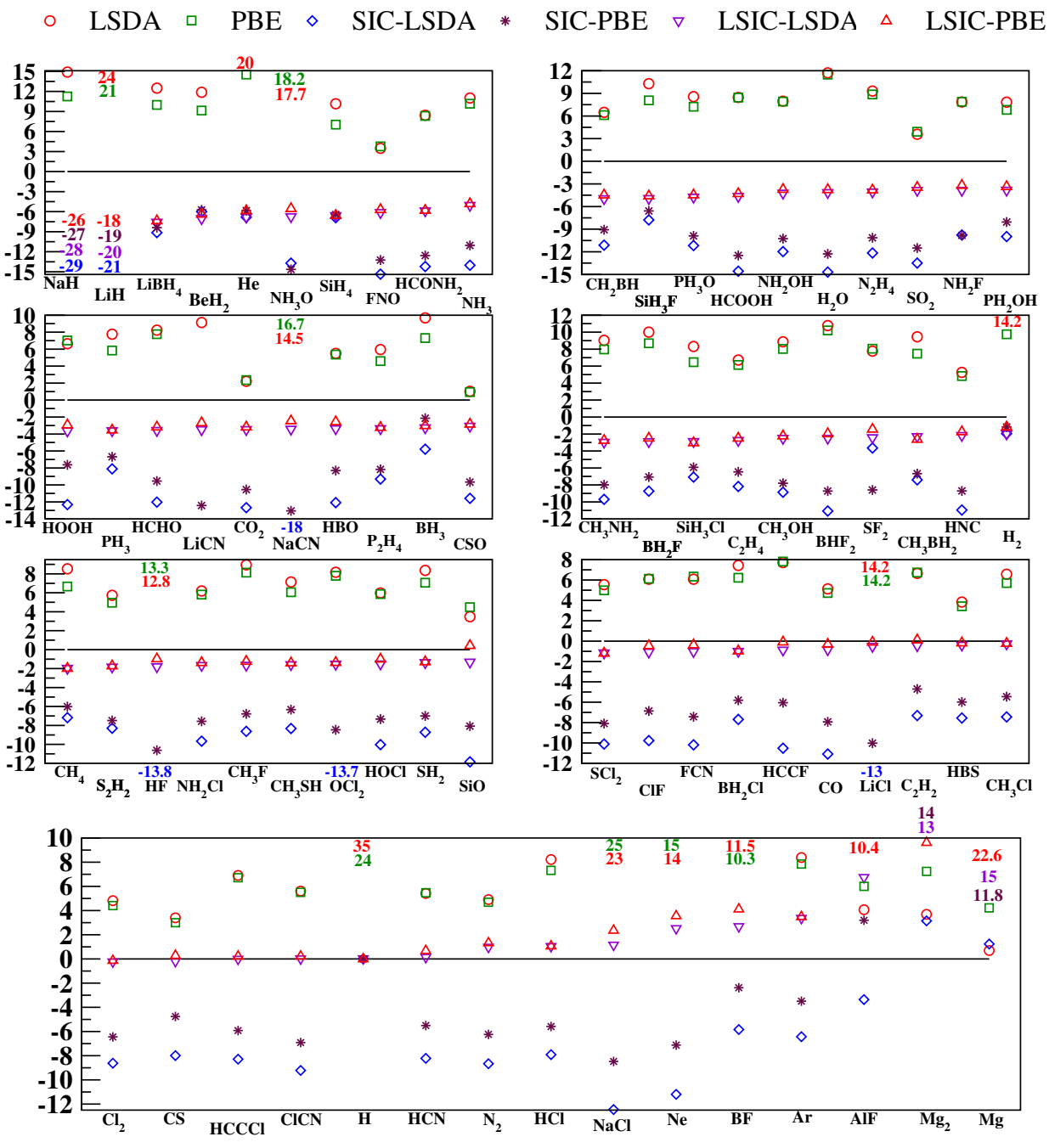

FIG. S2. The relative errors (in %) of the tested methods over the NSP subset. To avoid an expanded scale, some data points are replaced by the corresponding RE values.

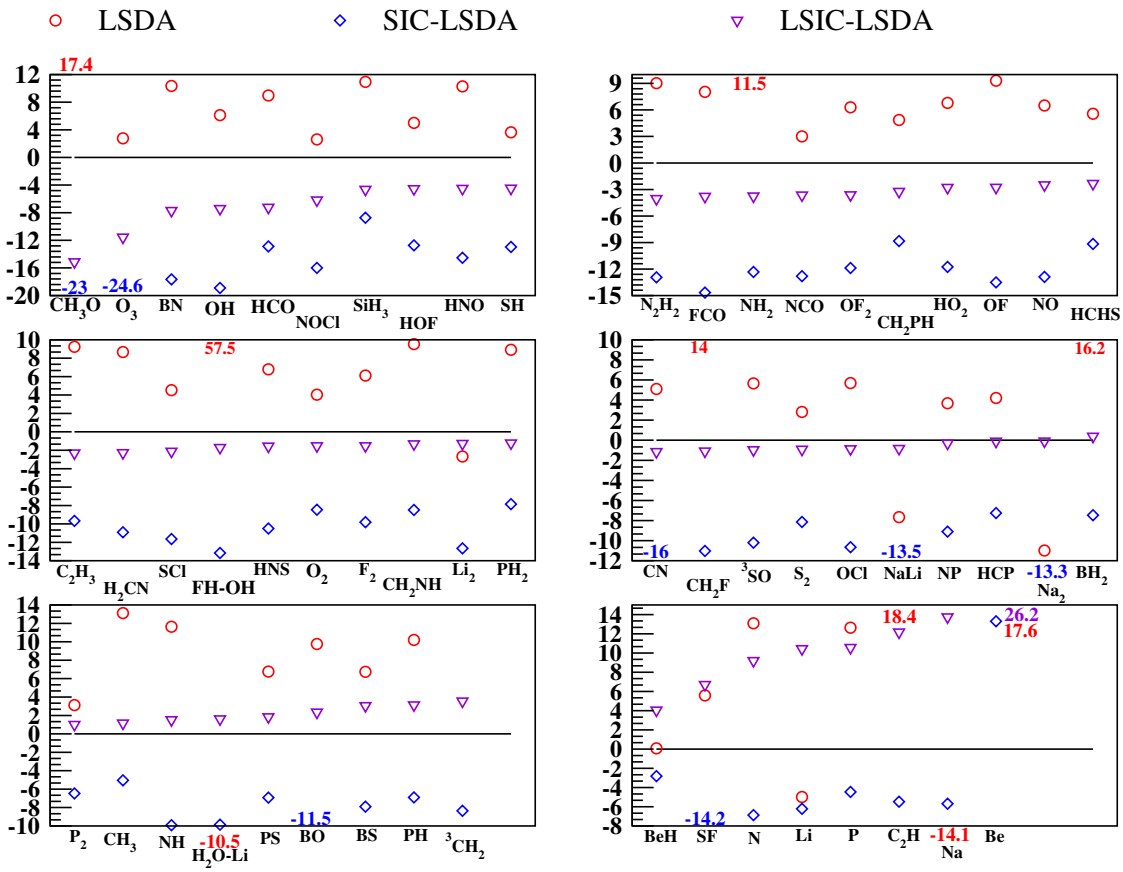

FIG. S3. The relative errors (in %) of the tested methods over the SP subset. To avoid an expanded scale, some data points are replaced by the corresponding RE values.

TABLE S1. Comparison of MAE (in Å^3) with respect to CCSD(T) reference values for different methods with FOD optimization (WFO) and without FOD optimization (WOFO) in the presence of the applied electric field of 0.005 a.u. N is the number of molecules used for the calculations with each method. The final row shows the MARD (mean absolute relative difference) (in %) between the WFO and WOFO polarizabilities. (MARD $= \frac{1}{N}\sum_n^N |\frac{\alpha_{n,\mathrm{WOFO}}-\alpha_{n,\mathrm{WFO}}}{\alpha_{n,\mathrm{WFO}}}| \times 100\%$)

Method (N)	FLO-LDA (31)	LSIC-LDA (31)	FLO-PBE (60)	LSIC-PBE (51)
MAE (WOFO)	0.446	0.321	0.364	0.219
MAE (WFO)	0.380	0.332	0.303	0.259
MARD	2.89	1.92	2.52	1.69

TABLE S2: Comparison of average polarizabilities (NSP subset) with CCSD(T) values taken from Ref. 1. All values in $Å^3$. The field strength used in calculating the polarizabilities was set to 0.005 a.u.

System	DFA-LDA	FLO-LDA	LSIC-LDA	DFA-PBE	FLO-PBE	LSIC-PBE	CCSD(T)[1]
AlF	5.923	5.500	6.0751	6.0330	5.873	6.281	5.691
Ar	1.771	1.529	1.6891	1.7623	1.577	1.691	1.634
BeH_2	3.281	2.757	2.7262	3.2010	2.765	2.746	2.933
BF	3.192	2.695	2.9388	3.1557	2.794	2.980	2.862
BH_2Cl	4.684	4.025	4.3160	4.6312	4.107	4.318	4.360
BH_2F	2.695	2.236	2.3787	2.6629	2.277	2.389	2.450
BH_3	2.764	2.374	2.4375	2.7043	2.466	2.444	2.520
BHF_2	2.642	2.121	2.3253	2.6283	2.177	2.338	2.385
C_2H_2	3.561	3.095	3.3237	3.5637	3.182	3.343	3.339
C_2H_4	4.276	3.679	3.8963	4.2530	3.748	3.907	4.007
CH_2BH	4.787	3.996	4.2729	4.7710	4.088	4.295	4.496
CH_3BH_2	4.676	3.956	4.1737	4.5911	3.987	4.160	4.272
CH_3Cl	4.707	4.088	4.4048	4.6691	4.176	4.407	4.417
CH_3F	2.653	2.225	2.3948	2.6330	2.270	2.405	2.435
CH_3NH_2	4.081	3.380	3.6320	4.0412	3.444	3.640	3.743
CH_3OH	3.379	2.829	3.0259	3.3533	2.862	3.035	3.104
CH_3SH	5.804	4.966	5.3312	5.7455	5.074	5.341	5.417
CH_4	2.633	2.252	2.3780	2.5877	2.280	2.378	2.426
Cl_2	4.719	4.114	4.4915	4.7006	4.212	4.496	4.502
ClCN	4.722	4.059	4.4719	4.7171	4.162	4.481	4.471
ClF	2.846	2.421	2.6540	2.8472	2.499	2.671	2.683
CO	2.029	1.716	1.9138	2.0211	1.777	1.924	1.930
CO_2	2.636	2.252	2.4892	2.6396	2.307	2.497	2.579
CS	4.350	3.871	4.1989	4.3333	4.007	4.219	4.207
CSO	5.166	4.521	4.9551	5.1611	4.619	4.968	5.113

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TABLE S2 – *Continued from previous page*

System	DFA-LDA	FLO-LDA	LSIC-LDA	DFA-PBE	FLO-PBE	LSIC-PBE	CCSD(T)[1]
FCN	2.845	2.409	2.6545	2.8520	2.483	2.672	2.682
FNO	2.641	2.160	2.3951	2.6485	2.214	2.407	2.552
H	0.900	0.667	0.6672	0.8277	0.667	0.667	0.667
H_2	0.877	0.753	0.7527	0.8429	0.759	0.759	0.768
H_2O	1.574	1.202	1.3505	1.5707	1.236	1.356	1.409
HBO	2.592	2.160	2.3739	2.5888	2.253	2.394	2.457
HBS	5.226	4.653	5.0131	5.2052	4.732	5.024	5.033
HCCCl	5.743	4.927	5.3716	5.7329	5.054	5.384	5.372
HCCF	3.687	3.063	3.3928	3.6903	3.216	3.420	3.423
HCHO	2.826	2.297	2.5173	2.8137	2.362	2.528	2.611
HCl	2.751	2.341	2.5685	2.7283	2.400	2.569	2.542
HCN	2.606	2.269	2.4754	2.6073	2.336	2.489	2.472
$HCONH_2$	4.425	3.501	3.8409	4.4211	3.568	3.844	4.081
HCOOH	3.589	2.827	3.1546	3.5881	2.896	3.167	3.309
He	0.246	0.191	0.1910	0.2348	0.193	0.193	0.205
HF	0.924	0.706	0.8042	0.9277	0.732	0.811	0.819
HNC	2.842	2.404	2.6413	2.8306	2.465	2.653	2.700
HOCl	3.510	2.980	3.2618	3.5060	3.069	3.279	3.312
HOOH	2.363	1.943	2.1353	2.3716	2.047	2.151	2.216
$LiBH_4$	4.972	4.016	4.085	4.861	4.049	4.094	4.420
LiCl	4.387	3.333	3.822	4.387	3.457	3.838	3.842
LiCN	3.908	3.028	3.456	3.946	3.136	3.485	3.581
LiH	5.174	3.317	3.358	5.061	3.401	3.442	4.186
Mg	10.665	10.722	12.1925	11.0383	11.839	12.981	10.591
Mg_2	23.919	23.795	26.1018	24.7380	26.306	25.288	23.068
N_2	1.817	1.582	1.7490	1.8133	1.624	1.755	1.732
N_2H_4	3.643	2.928	3.1972	3.6281	2.995	3.206	3.333

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TABLE S2 – *Continued from previous page*

System	DFA-LDA	FLO-LDA	LSIC-LDA	DFA-PBE	FLO-PBE	LSIC-PBE	CCSD(T)[1]
NaCl	5.427	3.854	4.4529	5.5048	4.029	4.506	4.402
NaCN	4.588	3.284	3.8695	4.6769	3.484	3.909	4.007
NaH	7.578	4.702	4.7508	7.3382	4.814	4.904	6.596
Ne	0.449	0.349	0.4029	0.4513	0.365	0.407	0.393
NH_2Cl	4.199	3.572	3.8880	4.1837	3.655	3.900	3.954
NH_2F	2.361	1.975	2.1046	2.3616	1.974	2.119	2.189
NH_2OH	3.011	2.455	2.6709	3.0096	2.503	2.685	2.789
NH_3	2.310	1.789	1.9757	2.2924	1.851	1.981	2.081
NH_3O	3.543	2.597	2.8066	3.5574	2.569	2.843	3.010
OCl_2	5.974	4.769	5.4377	5.9535	5.056	5.448	5.523
P_2H_4	9.005	7.708	8.2118	8.8888	7.805	8.225	8.499
PH_2OH	5.275	4.404	4.7039	5.2251	4.498	4.728	4.892
PH_3	4.822	4.112	4.3133	4.7363	4.176	4.317	4.475
PH_3O	4.741	3.879	4.1592	4.6831	3.935	4.172	4.367
$S2H_2$	6.897	5.982	6.4032	6.8462	6.035	6.411	6.523
SCl_2	7.982	6.799	7.4755	7.9404	6.951	7.473	7.563
SF_2	3.748	3.351	3.3935	3.7579	3.179	3.428	3.478
SH_2	3.887	3.274	3.5379	3.8404	3.336	3.541	3.587
SiH_3Cl	6.672	5.724	5.9822	6.5583	5.795	5.973	6.160
SiH_3F	4.537	3.794	3.9105	4.4459	3.843	3.925	4.114
SiH_4	5.055	4.272	4.2860	4.9121	4.294	4.287	4.589
SiO	4.524	3.854	4.3145	4.5682	4.019	4.391	4.372
SO_2	3.899	3.256	3.6183	3.9112	3.331	3.634	3.764

TABLE S3: Comparison of average polarizabilities (SP subset) with CCSD(T) polarizabilities taken from Ref. 1. All values in $Å^3$. The applied field strength used for these calculations was set to 0.01 a.u. except for the **bold faced** species, for which the field strength was set to 0.001 a.u.

System	DFA	FLOSIC	LSIC	CCSD(T)[1]	System	DFA	FLOSIC	LSIC	CCSD(T)[1]
Be	6.611	6.370	7.096	5.622	Na	20.895	22.937	27.662	24.320
BeH	4.876	4.735	5.069	4.872	**Na_2**	34.416	33.530	38.624	38.661
BH_2	3.394	2.704	2.933	2.922	**NaLi**	32.436	30.385	34.831	35.124
BN	3.839	2.865	3.211	3.479	NH	1.621	1.308	1.474	1.452
BO	2.667	2.150	2.487	2.430	NH_2	1.989	1.564	1.717	1.784
BS	5.323	4.593	5.139	4.987	NO	1.835	1.501	1.680	1.723
C_2H	3.911	3.123	3.706	3.304	NOCl	5.177	4.238	4.733	5.045
C_2H_3	4.211	3.482	3.766	3.855	NP	4.305	3.774	4.139	4.152
CH_2F	2.698	2.107	2.342	2.368	O_2	1.624	1.429	1.537	1.561
CH_2NH	3.565	2.979	3.212	3.255	O_3	2.897	2.124	2.493	2.819
CH_2PH	6.355	5.525	5.864	6.060	OCl	3.175	2.684	2.978	3.004
CH_2-t	2.477	1.964	2.219	2.143	OF	1.538	1.217	1.368	1.407
CH_3O	4.049	2.653	2.928	3.450	OF_2	2.263	1.876	2.052	2.129
F_2	1.320	1.122	1.225	1.244	OH	1.230	0.940	1.073	1.159
FH-OH	3.028	1.670	1.890	1.923	P	4.173	3.540	4.096	3.705
H_2CN	3.148	2.581	2.831	2.897	PH	4.473	3.779	4.186	4.059
H_2O-Li	34.561	34.788	39.216	38.594	PH_2	4.715	3.989	4.276	4.329
HCHS	5.326	4.583	4.927	5.045	S_2	6.169	5.512	5.945	6.000
HCO	2.708	2.165	2.305	2.485	SCl	5.566	4.705	5.212	5.325
HCP	5.479	4.877	5.252	5.258	SF	3.514	2.857	3.551	3.328
HNO	2.445	1.895	2.117	2.217	SH	3.567	2.996	3.288	3.442
HNS	4.621	3.873	4.259	4.327	SO-trip	3.605	3.064	3.379	3.412
HO_2	2.106	1.740	1.917	1.972	CN	3.010	2.405	2.831	2.864
HOF	1.824	1.516	1.658	1.737	P_2	7.563	6.860	7.408	7.334
Li	23.092	22.794	26.840	24.304	PS	6.974	6.080	6.652	6.532

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TABLE S3 – *Continued from previous page*

Li_2	30.105	27.019	30.537	30.932		CH_3	2.648	2.223	2.368	2.341
N	1.218	1.003	1.176	1.077		NCO	3.225	2.730	3.017	3.131
N_2H_2	3.067	2.449	2.699	2.813		FCO	2.792	2.205	2.486	2.584
						SiH_3	5.549	4.565	4.770	5.002

TABLE S4: Comparison of PBE linear-response polarizabilities (in $Å^3$) using different basis sets. Polarizabilities were computed using GAUSSIAN[9] for consistency, using Cartesian forms of the basis sets. The rightmost column indicates the multi-wavelet (MW) reference results taken from Ref. 8

	NRLMOL	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ	aug-cc-pV5Z	MW
BeH	5.2174	5.1072	5.1799	5.2008	5.2142	N.A.
CO	2.0186	1.9853	2.0152	2.0204	2.0215	N.A.
FH-OH	2.52803	2.36340	2.43922	2.47716	2.48510	N.A.
HO_2	2.1112	1.9648	2.0568	2.0907	2.1002	N. A.
Li	20.9604	20.9710	21.0494	21.0741	21.0562	N.A.
NaCl	5.4583	5.2002	5.4212	5.4676	5.4673	N.A.
NaCN	4.6448	4.6339	4.6410	4.6492	4.6513	N.A.
Li_2	29.9385	29.9382	29.9927	29.9661	29.9613	29.9608
NaLi	32.8369	33.0903	33.0108	32.9274	32.8952	32.8879
CO_2	2.6392	2.5508	2.6119	2.6327	2.6382	2.6411
F_2	1.3278	1.1548	1.2538	1.3043	1.3176	1.3282
H_2	0.8422	0.8062	0.8391	0.8414	0.8419	0.8422
HBO	2.5910	2.5611	2.5873	2.5910	2.5926	2.5931
HCN	2.6057	2.5522	2.5971	2.6056	2.6070	2.6080
He	0.2347	0.2185	0.2275	0.2323	0.2339	0.2348
HF	0.9262	0.8012	0.8743	0.9063	0.9163	0.9269
LiH	4.9762	5.0727	4.9590	4.9627	4.9623	4.9626
NaH	7.2067	7.3864	7.2979	7.2480	7.2107	7.1908

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TABLE S4 – *Continued from previous page*

	NRLMOL	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ	aug-cc-pV5Z	MW
Mg	10.9422	10.8876	10.9498	10.9492	10.9625	10.9661
Ne	0.4553	0.3176	0.3897	0.4310	0.4459	0.4557
NH_3	2.2879	2.1983	2.2609	2.2738	2.2810	2.2863
SiH_4	4.9074	4.8897	4.9116	4.9067	4.9052	4.9051
RMS(15) w.r.t MW	0.0161	0.1078	0.0515	0.0209	0.0072	–
RMS%(15) w.r.t MW	0.1309	9.3156	4.2478	1.5756	0.6576	–

TABLE S5: Comparison of PBE total energies (in Hartree) calculated with different basis sets. The last row shows the RMS difference with respect to the aug-cc-pV5Z basis. All energies were computed using GAUSSIAN[9] for consistency, using Cartesian forms of the basis sets.

Basis set	NRLMOL	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ	aug-cc-pV5Z
BeH	-15.2160099	-15.2147543	-15.2174880	-15.2183178	-15.2184426
CO	-113.2389527	-113.2061407	-113.2329857	-113.2408256	-113.2423520
FH-OH	-176.1009653	-176.0408629	-176.0871418	-176.1003922	-176.1026061
HO_2	-150.8372576	-150.7924741	-150.8282489	-150.8388051	-150.8411675
Li	-7.4621449	-7.4612451	-7.4618459	-7.4620734	-7.4621468
NaCl	-622.2930510	-622.2644418	-622.2829758	-622.2925230	-622.2951239
NaCN	-254.9676515	-254.9321695	-254.9589637	-254.9683910	-254.9689245
Li_2	-14.9559008	-14.9539604	-14.9553963	-14.9558966	-14.9559951
NaLi	-169.6620224	-169.6512753	-169.6582199	-169.6615944	-169.6629834
CO_2	-188.4852422	-188.4295512	-188.4765437	-188.4894595	-188.4919672
F_2	-199.4328979	-199.3639881	-199.4182097	-199.4328730	-199.4362266
H_2	-1.1665090	-1.1604473	-1.1661120	-1.1665636	-1.1666824
HBO	-100.6347928	-100.6018480	-100.6282350	-100.6357165	-100.6370742
HCN	-93.3518630	-93.3242421	-93.3479630	-93.3535405	-93.3545789
He	-2.8928768	-2.8869533	-2.8924351	-2.8927834	-2.8928871

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TABLE S5 – *Continued from previous page*

Basis set	NRLMOL	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ	aug-cc-pV5Z
HF	-100.4012733	-100.3646301	-100.3926066	-100.4005353	-100.4022872
LiH	-8.0470373	-8.0432914	-8.0467243	-8.0472143	-8.0473177
NaH	-162.7385017	-162.7264028	-162.7338411	-162.7376816	-162.7394621
Mg	-199.9530556	-199.9439553	-199.9493939	-199.9533960	-199.9543803
Ne	-128.8659964	-128.8158617	-128.8526684	-128.8638552	-128.8661349
NH_3	-56.5160773	-56.4950744	-56.5123715	-56.5163545	-56.5171480
SiH_4	-291.7304577	-291.7071179	-291.7239596	-291.7311326	-291.7325852
RMS(22) w.r.t 5Z	0.00234	0.03482	0.00924	0.00162	–

TABLE S6: Comparison of PBE polarizabilities (in $Å^3$) computed using the NRLMOL basis and the finite-field method for different field strengths, F = 0.001, 0.005, and 0.01 with corresponding values computed[8] with MW (multi-wavelet) basis sets. In the last row, RMSRE(%) is the root mean square relative difference with respect to NRLMOL-PBE (F = 0.001). The comparison of NRLMOL-PBE (F = 0.001) and the MW (F = 0.001) in the last row gives another indication of the quality of the NRLMOL basis relative to the basis-set-limit MW basis.

Code	NRLMOL	NRLMOL	NRLMOL	MW
Electric field	0.001	0.005	0.01	0.001
AlF	6.013	6.033	6.099	6.038
Ar	1.762	1.762	1.765	1.769
BeH_2	3.196	3.201	3.215	3.196
BF	3.149	3.156	3.178	3.157
BH_2Cl	4.626	4.631	4.632	4.637
BH_2F	2.661	2.663	2.670	2.662
BH_3	2.699	2.704	2.714	2.702
BHF_2	2.627	2.628	2.634	2.628
C_2H_2	3.557	3.564	3.577	3.558

Continued on next page

TABLE S6 – *Continued from previous page*

Code	NRLMOL	NRLMOL	NRLMOL	MW
Electric field	0.001	0.005	0.01	0.001
C_2H_4	4.249	4.253	4.270	4.247
CH_2BH	4.746	4.771	4.799	4.761
CH_3BH_2	4.586	4.591	4.610	4.587
CH_3Cl	4.663	4.669	4.682	4.676
CH_3F	2.631	2.633	2.639	2.632
CH_3NH_2	4.036	4.041	4.063	4.035
CH_3OH	3.350	3.353	3.364	3.349
CH_3SH	5.736	5.746	5.777	5.742
CH_4	2.584	2.588	2.595	2.585
Cl_2	4.689	4.701	4.712	4.72
ClCN	4.714	4.717	4.727	4.733
ClF	2.845	2.847	2.854	2.855
CO	2.020	2.021	2.025	2.022
CO_2	2.638	2.64	2.642	2.641
CS	4.327	4.333	4.350	4.344
CSO	5.159	5.161	5.175	5.17
FCN	2.850	2.852	2.856	2.853
FNO	2.647	2.649	2.654	2.649
H	0.826	0.828	0.834	0.825
H_2	0.842	0.843	0.845	0.843
H_2O	1.569	1.571	1.577	1.569
HBO	2.567	2.589	2.593	2.593
HBS	5.185	5.205	5.223	5.208
HCCCl	5.727	5.733	5.752	5.749
HCCF	3.695	3.69	3.709	3.695
HCHO	2.810	2.814	2.826	2.811

Continued on next page

TABLE S6 – *Continued from previous page*

Code	NRLMOL	NRLMOL	NRLMOL	MW
Electric field	0.001	0.005	0.01	0.001
HCl	2.722	2.728	2.737	2.73
HCN	2.603	2.607	2.613	2.608
$HCONH_2$	4.411	4.421	4.456	4.409
HCOOH	3.583	3.588	3.604	3.583
He	0.234	0.235	0.235	0.235
HF	0.919	0.928	0.928	0.927
HNC	2.827	2.831	2.843	2.83
HOCl	3.503	3.506	3.516	3.514
HOOH	2.370	2.372	2.378	2.37
$LiBH_4$	4.848	4.86	4.899	4.848
LiCl	4.343	4.403	4.454	4.385
LiCN	3.931	3.946	4.002	3.935
LiH	4.968	5.072	5.402	4.966
Mg	10.950	11.038	11.397	10.97
Mg_2	24.432	24.738	26.606	24.488
N_2	1.812	1.813	1.816	1.815
N_2H_4	3.622	3.628	3.653	3.621
NaCl	5.463	5.505	5.674	5.472
NaCN	4.645	4.677	4.798	4.655
NaH	7.212	7.338	7.911	7.196
Ne	0.452	0.451	0.451	0.456
NH_2Cl	4.179	4.184	4.200	4.19
NH_2F	2.359	2.362	2.371	2.36
NH_2OH	3.005	3.01	3.023	3.005
NH_3	2.313	2.292	2.307	2.286
NH_3O	3.544	3.557	3.595	3.54

Continued on next page

TABLE S6 – *Continued from previous page*

Code	NRLMOL	NRLMOL	NRLMOL	MW
Electric field	0.001	0.005	0.01	0.001
OCl_2	5.944	5.9535	5.980	5.962
P_2H_4	8.870	8.8888	8.948	8.878
PH_2OH	5.215	5.2251	5.259	5.216
PH_3	4.729	4.7363	4.761	4.726
PH_3O	4.678	4.6831	4.700	4.661
S_2H_2	6.836	6.8462	6.880	6.851
SCl_2	7.933	7.9404	7.968	7.96
SF_2	3.753	3.7579	3.775	3.766
SH_2	3.834	3.8404	3.862	3.834
SiH_3Cl	6.522	6.5583	6.579	6.558
SiH_3F	4.440	4.4459	4.460	4.44
SiH_4	4.905	4.9121	4.931	4.905
SiO	4.566	4.5682	4.588	4.574
SO_2	3.912	3.9112	3.921	3.9
RMSRE (%)	–	0.48	2.09	0.22

TABLE S7: Comparison of PBE polarizabilities (in $Å^3$) computed using the NRLMOL basis and the finite-field method for different field strengths F = 0.001 and 0.01 a.u.. In the last row, MARE (%) is the mean asbolute relative difference (in %) with respect to NRLMOL-PBE (F = 0.001 a.u.).

Electric field	0.001	0.01
BeH	5.219	5.387
BS	5.255	5.278
F_2	1.328	1.329
FCO	2.783	2.797

Continued on next page

TABLE S7 – *Continued from previous page*

Electric field	0.001	0.01
FH-OH	2.542	2.685
HCO	2.676	2.711
HCP	5.447	5.478
HNO	2.429	2.447
HNS	4.578	4.615
HO_2	2.111	2.119
HOF	1.829	1.833
NCO	3.201	3.207
NH	1.600	1.609
OF	1.574	1.509
OH	1.330	1.335
MARE (%)	–	1.28

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Basis in Gaussian Format

August 9, 2021

1 Introduction

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 0.5074092930E+03      0.9926141120E+00
 0.1658509660E+03     0.1482142820E+01
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 0.5984476610E+02     0.1955456810E+01
 0.2313469890E+02      0.2084929520E+01
 0.9418458910E+01     0.1512370950E+01
 0.3941794820E+01     0.5193947420E+00
 0.1622742640E+01      0.3717803360E-01
 0.6526657200E+00    -0.3809234080E-03
 0.2543715500E+00     0.3073830710E-04
 0.9411174000E-01     -0.1145079080E-05
S 13 1.0
 0.5175062370E+05    -0.4460788650E-01
 0.7806165340E+04   -0.8300555230E-01
 0.1785836240E+04   -0.1434592140E+00
 0.5074092930E+03    -0.2322378010E+00
 0.1658509660E+03   -0.3540798740E+00
 0.5984476610E+02   -0.4868621960E+00
 0.2313469890E+02    -0.5838257510E+00
 0.9418458910E+01   -0.5302733550E+00
 0.3941794820E+01   -0.2930227470E+00
 0.1622742640E+01     0.1017905400E+00
 0.6526657200E+00    0.2510234710E+00
 0.2543715500E+00    0.1235542910E+00
 0.9411174000E-01     0.1100946650E-01
S 1 1.0
 0.6526657200E+00   1.0
S 1 1.0
 0.2543715500E+00   1.0
S 1 1.0
 0.9411174000E-01   1.0
S 1 1.00
0.3481922253E-01    1.00
P 13 1.0
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 0.7806165340E+04     0.4794149630E-01
 0.1785836240E+04     0.9624701750E-01
 0.5074092930E+03    0.1412402870E+00
 0.1658509660E+03     0.2364183380E+00
 0.5984476610E+02     0.3189381040E+00
 0.2313469890E+02    0.4349960350E+00
 0.9418458910E+01     0.4842569670E+00
 0.3941794820E+01     0.4789960860E+00
 0.1622742640E+01    0.3663209510E+00
 0.6526657200E+00     0.1751237860E+00
 0.2543715500E+00     0.5187149180E-01
 0.9411174000E-01    0.7247309710E-02
P 1 1.0
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P 1 1.0
 0.2543715500E+00   1.0
P 1 1.0
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P 1 1.00
0.3481922253E-01    1.00
D 1 1.0
 0.1622742640E+01  1.0
D 1 1.0
 0.6526657200E+00  1.0
D 1 1.0
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D 1 1.0
 0.9411174000E-01  1.0
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-Na 0
S 16  1.0
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 0.3800758270E+05    0.5106827640E+00
 0.8715688450E+04    0.8799275060E+00
 0.2483133950E+04    0.1429422300E+01
 0.8135133250E+03    0.2193187980E+01
 0.2945696940E+03    0.3119941430E+01
 0.1149592610E+03    0.3904449050E+01
 0.4746043120E+02    0.3916234120E+01
 0.2041045840E+02    0.2576144260E+01
 0.9026008680E+01    0.7644203210E+00
 0.3998081980E+01    0.4535571520E-01
 0.1734809260E+01    0.5917155430E-03
 0.7379976200E+00   -0.2249938550E-03
 0.2969419100E+00    0.4878174190E-04
 0.7115394000E-01   -0.5418108810E-05
 0.2685790000E-01    0.1024029380E-05
S 16  1.0
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 0.3800758270E+05  -0.1255177030E+00
 0.8715688450E+04  -0.2167577330E+00
 0.2483133950E+04   -0.3527634130E+00
 0.8135133250E+03  -0.5476913090E+00
 0.2945696940E+03  -0.7969802310E+00
 0.1149592610E+03   -0.1063505890E+01
 0.4746043120E+02  -0.1215709730E+01
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 0.9026008680E+01   -0.4524548060E+00
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 0.7115394000E-01  -0.1530594040E-03
 0.2685790000E-01    0.3481779060E-04
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 0.8715688450E+04    0.4010390870E-01
 0.2483133950E+04     0.6536929340E-01
 0.8135133250E+03    0.1013683360E+00
 0.2945696940E+03    0.1480359290E+00
 0.1149592610E+03     0.1976652170E+00
 0.4746043120E+02    0.2285401320E+00
 0.2041045840E+02    0.2018209460E+00
 0.9026008680E+01     0.9019295550E-01
 0.3998081980E+01   -0.6155933610E-01
 0.1734809260E+01   -0.1207921530E+00
 0.7379976200E+00    -0.9810404730E-01
 0.2969419100E+00   -0.1555457760E-01
 0.7115394000E-01    0.5285447120E-01
 0.2685790000E-01     0.2691995250E-01
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S 1 1.0
 0.7115394000E-01  1.0
S 1 1.0
 0.2685790000E-01  1.0
S 1 1.0
 0.1013783344E-01  1.0
S 1 1.000
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P 16  1.0
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 0.8715688450E+04   0.2454134210E+00
 0.2483133950E+04    0.4169011860E+00
 0.8135133250E+03   0.6328444070E+00
 0.2945696940E+03   0.9630351770E+00
 0.1149592610E+03    0.1314378410E+01
 0.4746043120E+02   0.1713220100E+01
 0.2041045840E+02   0.1886850410E+01
 0.9026008680E+01    0.1788343490E+01
 0.3998081980E+01   0.1242364900E+01
 0.1734809260E+01   0.5739846420E+00
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 0.7379976200E+00    0.1705305970E+00
 0.2969419100E+00   0.2295712250E-01
 0.7115394000E-01   0.2234358930E-03
 0.2685790000E-01   -0.1555094750E-04
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! 0.7379976200E+00  1.0
P 1 1.0
 0.2969419100E+00  1.0
P 1 1.0
 0.7115394000E-01  1.0
P 1 1.0
 0.2685790000E-01  1.0
P 1 1.000
0.1013783344e-01 1.00000000000
!D 1 1.0
! 0.1734809260E+01 1.0
D 1 1.0
 0.7379976200E+00 1.0
D 1 1.0
 0.2969419100E+00 1.0
D 1 1.0
 0.7115394000E-01 1.0
D 1 1.0
 0.2685790000E-01 1.0
D 1 1.000
0.1013783344e-01 1.00000000000
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-Cl 0
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0.1156452380E+06      0.8803816070E+00
0.2650416860E+05      0.1518922810E+01
0.7546165150E+04      0.2472308980E+01
0.2471893990E+04      0.3813762320E+01
0.8955334270E+03      0.5511242440E+01
0.3502018090E+03      0.7169615360E+01
0.1452812440E+03      0.7760870250E+01
0.6311107360E+02      0.5933825840E+01
0.2842186910E+02      0.2371148900E+01
0.1295952600E+02      0.2768854050E+00
0.5938778000E+01     -0.6086912280E-04
0.2723597280E+01      0.4511226240E-03
0.1217237400E+01     -0.7419490690E-04
0.5380555600E+00      0.1244793470E-04
0.2218100500E+00     -0.1836734320E-05
0.8549084000E-01      0.1926362200E-06
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0.1156452380E+06     -0.2451372520E+00
0.2650416860E+05     -0.4236909770E+00
0.7546165150E+04     -0.6907905800E+00
0.2471893990E+04     -0.1076075890E+01
0.8955334270E+03     -0.1585594950E+01
0.3502018090E+03     -0.2176949650E+01
0.1452812440E+03     -0.2635079970E+01
0.6311107360E+02     -0.2563322680E+01
0.2842186910E+02     -0.1483648060E+01
0.1295952600E+02      0.2412830390E+00
0.5938778000E+01      0.1261105160E+01
0.2723597280E+01      0.7743913000E+00
0.1217237400E+01      0.1031951090E+00
0.5380555600E+00     -0.1080473290E-02
0.2218100500E+00      0.2954365990E-03
0.8549084000E-01     -0.3286570230E-04
S 17 1.0
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0.1156452380E+06      0.8017024150E-01
0.2650416860E+05      0.1383085710E+00
0.7546165150E+04      0.2261389170E+00
0.2471893990E+04      0.3513898800E+00
0.8955334270E+03      0.5209143100E+00
0.3502018090E+03      0.7149733910E+00
0.1452812440E+03      0.8808754430E+00
0.6311107360E+02      0.8687494720E+00
0.2842186910E+02      0.5385814620E+00
0.1295952600E+02     -0.1040518410E+00
0.5938778000E+01     -0.5993299400E+00
0.2723597280E+01     -0.5687659480E+00
0.1217237400E+01     -0.1726383870E-01
0.5380555600E+00      0.2717702610E+00
0.2218100500E+00      0.1215359850E+00
0.8549084000E-01      0.7456514150E-02
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0.5380555600E+00     1.00000
S 1 1.00
0.2218100500E+00     1.00000
S 1 1.00
0.8549084000E-01     1.00000
S 1 1.00
0.3295019195E-01     1.00000
P 17 1.0
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0.2471893990E+04      0.2193025490D+01
0.8955334270E+03      0.3353237010D+01
0.3502018090E+03      0.4680446020D+01
0.1452812440E+03      0.6270699110D+01
0.6311107360E+02      0.7287465380D+01
0.2842186910E+02      0.7367579690D+01
0.1295952600E+02      0.5613192300D+01
0.5938778000E+01      0.2889937070D+01
0.2723597280E+01      0.8063782520D+00
0.1217237400E+01      0.7444713490D-01
0.5380555600E+00     -0.6145532010D-04
0.2218100500E+00      0.9671962940D-04
0.8549084000E-01     -0.8265756710D-05
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0.1156452380E+06    -0.1437854490D+00
0.2650416860E+05    -0.2474340600D+00
0.7546165150E+04    -0.4059995640D+00
0.2471893990E+04    -0.6340056560D+00
0.8955334270E+03    -0.9533552000D+00
0.3502018090E+03    -0.1352842270D+01
0.1452812440E+03    -0.1802719810D+01
0.6311107360E+02    -0.2142763550D+01
0.2842186910E+02    -0.2197555690D+01
0.1295952600E+02    -0.1761529840D+01
0.5938778000E+01    -0.9427501270D+00
0.2723597280E+01    -0.2057292640D+00
0.1217237400E+01     0.1762314060D+00
0.5380555600E+00     0.1606983270D+00
0.2218100500E+00     0.5386056450D-01
0.8549084000E-01     0.6083841020D-02
P 1 1.000
0.5380555600E+00    1.000
P 1 1.000
0.2218100500E+00    1.000
P 1 1.000
0.8549084000E-01    1.000
P 1 1.000
0.3295019195e-01 1.000
D 1 1.00
0.1217237400E+01     1.000
D 1 1.000
0.5380555600E+00    1.000
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D 1 1.000
0.2218100500E+00    1.000
D 1 1.000
0.8549084000E-01    1.000
D 1 1.000
0.3295019195e-01 1.000
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-Li  0
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1.37916632e+03   -0.6001848738E-01
5.24950092e+02   -0.1002233904
1.79461008e+02   -0.1789313215
6.25244982e+01   -0.2786274379
2.33568013e+01   -0.3946603663
9.29375078e+00   -0.4880090038
3.79280557e+00   -0.5085738904
1.65598231e+00   -0.2880409710
1.10428577e+00   -0.1157827695
6.17106999e-01   -0.1026195663
2.98891332e-01   -0.1942268562E-01
9.55240908e-02   -0.1977155092E-03
3.91891205e-02   0.1988484732E-04
1.76690597e-02   -0.2681193753E-05
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1.37916632e+03     -0.1007550449E-01
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1.79461008e+02     -0.3027494317E-01
6.25244982e+01     -0.5299430541E-01
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1.65598231e+00     -0.1351592616
1.10428577e+00     0.4343848450E-01
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S 1 1.000
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S 1 1.000
9.55240908e-02   1.000
S 1 1.000
3.91891205e-02   1.000
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P 1 1.000
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6.17106999e-01   1.000
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P 1 1.000
1.76690597e-02   1.000
D 1 1.000
1.10428577e+00   1.000
D 1 1.000
6.17106999e-01   1.000
D 1 1.000
2.98891332e-01   1.000
D 1 1.000
9.55240908e-02   1.000
D 1 1.000
3.91891205e-02   1.000
****
-Be 0
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0.8776208410E+03      0.2539566910E+00
0.1991723400E+03      0.4342912580E+00
0.5626307070E+02      0.6750290760E+00
0.1826961590E+02      0.8917820500E+00
0.6473667150E+01      0.9024922970E+00
0.2445688700E+01      0.5799824540E+00
0.9341739200E+00      0.1536025430E+00
0.1817039200E+00      0.2107594360E-02
0.5906470000E-01     -0.2247270500E-03
S 10 1.0000
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0.8776208410E+03    -0.5170663340E-01
0.1991723400E+03    -0.9062186920E-01
0.5626307070E+02    -0.1392359400E+00
0.1826961590E+02    -0.1988883660E+00
0.6473667150E+01    -0.2142827010E+00
0.2445688700E+01    -0.1942901520E+00
0.9341739200E+00    -0.6634498410E-01
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S 1 1.00
0.1817039200E+00  1.00
S 1 1.00
0.5906470000E-01  1.00
S 1 1.00
0.1919957911E-01  1.00
P 1 1.000
0.2445688700E+01  1.000
P 1 1.00
0.9341739200E+00  1.00
P 1 1.00
0.1817039200E+00  1.00
P 1 1.00
0.5906470000E-01  1.00
P 1 1.00
0.1919957911E-01  1.00
D 1 1.00
0.9341739200E+00  1.00
D 1 1.00
0.1817039200E+00  1.00
D 1 1.00
0.5906470000E-01  1.00
D 1 1.00
0.1919957911E-01  1.00
****
-F  0
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 0.1223150920E+04        0.1216638020E+01
 0.4016733760E+03        0.1845316540E+01
 0.1457852270E+03        0.2551384850E+01
 0.5694551760E+02        0.3004077050E+01
 0.2349311190E+02        0.2682876730E+01
 0.1003418550E+02        0.1405497250E+01
 0.4343769680E+01        0.2609771830E+00
 0.1868203030E+01        0.2555561480E-02
 0.7806879100E+00        0.7546130340E-03
 0.3149846100E+00       -0.1646029690E-03
 0.1181861600E+00        0.2082887950E-04
S  14 1.000
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 0.1223150920E+04    -0.2894265580E+00
 0.4016733760E+03    -0.4466115800E+00
 0.1457852270E+03    -0.6343658820E+00
 0.5694551760E+02    -0.8145208580E+00
 0.2349311190E+02    -0.8538368980E+00
 0.1003418550E+02    -0.6447789780E+00
 0.4343769680E+01    -0.1142431720E+00
 0.1868203030E+01     0.3167190590E+00
 0.7806879100E+00     0.3041863400E+00
 0.3149846100E+00     0.1005780670E+00
 0.1181861600E+00     0.4817488440E-02
S 1 1.000
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S 1 1.000
 0.3149846100E+00  1.00
S 1 1.000
 0.1181861600E+00  1.00
S 1 1.000
 0.4434492344E-01  1.00
P  14 1.000
 0.1231742220E+06      0.4900854750E-01
 0.1865493160E+05      0.9059901630E-01
 0.4284660370E+04      0.1569389330E+00
 0.1223150920E+04      0.2549422150E+00
 0.4016733760E+03      0.3969983700E+00
 0.1457852270E+03      0.5817501900E+00
 0.5694551760E+02      0.7854593500E+00
 0.2349311190E+02      0.9713952850E+00
 0.1003418550E+02      0.1017485400E+01
 0.4343769680E+01      0.8881348760E+00
 0.1868203030E+01      0.5325776020E+00
 0.7806879100E+00      0.2097448310E+00
 0.3149846100E+00      0.5358788830E-01
 0.1181861600E+00      0.5596492130E-02
P 1 1.000
 0.7806879100E+00  1.00
P 1 1.000
 0.3149846100E+00  1.00
P 1 1.000
 0.1181861600E+00  1.00
P 1 1.000
 0.4434492344E-01  1.00
D 1 1.00
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0.1868203030E+01   1.000
D 1 1.000
 0.7806879100E+00  1.00
D 1 1.000
 0.3149846100E+00  1.00
D 1 1.000
 0.1181861600E+00  1.00
D 1 1.000
 0.4434492344E-01  1.00
****
-B 0
S  12 1.000
0.1715154660E+05      0.1419218390E+00
0.2539347650E+04      0.2671949380E+00
0.5729100010E+03      0.4615325680E+00
0.1610864570E+03      0.7384083450E+00
0.5218849780E+02      0.1065015950E+01
0.1861757420E+02      0.1279087950E+01
0.7055424410E+01      0.1147442970E+01
0.2776149160E+01      0.5697916130E+00
0.1086598520E+01      0.8508472600E-01
0.4101434300E+00     -0.9886062860E-03
0.1518772300E+00      0.3248798750E-03
0.5476114000E-01     -0.4304233470E-04
S  12 1.000
0.1715154660E+05     -0.3117877050E-01
0.2539347650E+04     -0.5904321360E-01
0.5729100010E+03     -0.1015094520E+00
0.1610864570E+03     -0.1655624640E+00
0.5218849780E+02     -0.2418845040E+00
0.1861757420E+02     -0.3163422910E+00
0.7055424410E+01     -0.3269134950E+00
0.2776149160E+01     -0.2400824900E+00
0.1086598520E+01     -0.4173518940E-01
0.4101434300E+00      0.1397861410E+00
0.1518772300E+00      0.1050968580E+00
0.5476114000E-01      0.1274604460E-01
S 1 1.000
0.4101434300E+00  1.000
S 1 1.000
0.1518772300E+00  1.000
S 1 1.000
0.5476114000E-01  1.000
S 1 1.000
0.1974477974E-01  1.000
P  12 1.000
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0.1715154660E+05      0.1404435530E-01
0.2539347650E+04      0.1991509840E-01
0.5729100010E+03      0.4282434150E-01
0.1610864570E+03      0.6012095370E-01
0.5218849780E+02      0.1025729050E+00
0.1861757420E+02      0.1270304500E+00
0.7055424410E+01      0.1691154860E+00
0.2776149160E+01      0.1651506840E+00
0.1086598520E+01      0.1490724420E+00
0.4101434300E+00      0.9284969190E-01
0.1518772300E+00      0.3277756630E-01
0.5476114000E-01      0.5491094980E-02
P 1 1.000
0.4101434300E+00  1.000
P 1 1.000
0.1518772300E+00  1.000
P 1 1.000
0.5476114000E-01  1.000
P 1 1.000
0.1974477974E-01  1.000
D 1 1.00
0.1086598520E+01   1.000
D 1 1.000
0.4101434300E+00  1.000
D 1 1.000
0.1518772300E+00  1.000
D 1 1.000
0.5476114000E-01  1.000
D 1 1.000
0.1974477974E-01  1.000
****
-Mg 0
S 16 1.00
0.3153321870E+06      0.3056554300E+00
0.4765445370E+05      0.5686534590E+00
0.1092476220E+05      0.9797500480E+00
0.3114792500E+04      0.1590029240E+01
0.1022187830E+04      0.2439436660E+01
0.3709118900E+03      0.3480275970E+01
0.1451174260E+03      0.4396579360E+01
0.6009075460E+02      0.4499103510E+01
0.2595462450E+02      0.3084056080E+01
0.1155775900E+02      0.9979481430E+00
0.5171717200E+01      0.7380006550E-01
0.2280794010E+01      0.4096687060E-03
0.1001940640E+01     -0.1936928560E-03
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0.4254800000E+00      0.5247771960E-04
0.1182550200E+00     -0.6743999680E-05
0.4268006000E-01      0.1089693040E-05
S 16 1.00
0.3153321870E+06      -0.7734719840E-01
0.4765445370E+05      -0.1438318890E+00
0.1092476220E+05      -0.2483266640E+00
0.3114792500E+04      -0.4037641680E+00
0.1022187830E+04      -0.6264518010E+00
0.3709118900E+03      -0.9135558670E+00
0.1451174260E+03      -0.1226942060E+01
0.6009075460E+02      -0.1423448410E+01
0.2595462450E+02      -0.1278406030E+01
0.1155775900E+02      -0.6001402410E+00
0.5171717200E+01       0.2857192830E+00
0.2280794010E+01       0.6067798050E+00
0.1001940640E+01       0.3334560380E+00
0.4254800000E+00       0.4578459520E-01
0.1182550200E+00      -0.3243905570E-04
0.4268006000E-01       0.2247599340E-04
S 16 1.00
0.3153321870E+06      0.1759757530E-01
0.4765445370E+05      0.3278208410E-01
0.1092476220E+05      0.5645678260E-01
0.3114792500E+04      0.9212899440E-01
0.1022187830E+04      0.1424040470E+00
0.3709118900E+03      0.2091277870E+00
0.1451174260E+03      0.2799712870E+00
0.6009075460E+02      0.3306215770E+00
0.2595462450E+02      0.2982511300E+00
0.1155775900E+02      0.1501677560E+00
0.5171717200E+01     -0.7865217670E-01
0.2280794010E+01     -0.1822319050E+00
0.1001940640E+01     -0.1592505240E+00
0.4254800000E+00     -0.2283353620E-01
0.1182550200E+00      0.9048542010E-01
0.4268006000E-01      0.3396371100E-01
S 1 1.000
0.4254800000E+00   1.000
S 1 1.000
0.1182550200E+00   1.000
S 1 1.000
0.4268006000E-01   1.000
S 1 1.00
0.1540389170E-01     1.000
P 16 1.000
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 0.3153321870E+06    0.9712614360E-01
 0.4765445370E+05    0.1942569660E+00
 0.1092476220E+05    0.3186309670E+00
 0.3114792500E+04    0.5398099040E+00
 0.1022187830E+04    0.8194347350E+00
 0.3709118900E+03    0.1246844620E+01
 0.1451174260E+03    0.1710414370E+01
 0.6009075460E+02    0.2243742190E+01
 0.2595462450E+02    0.2504071910E+01
 0.1155775900E+02    0.2410974990E+01
 0.5171717200E+01    0.1721927720E+01
 0.2280794010E+01    0.8233781440E+00
 0.1001940640E+01    0.2432462160E+00
 0.4254800000E+00    0.3242440120E-01
 0.1182550200E+00    0.3278498780E-03
 0.4268006000E-01   -0.1602123180E-04
P 1 1.000
0.4254800000E+00   1.000
P 1 1.000
0.1182550200E+00   1.000
P 1 1.000
0.4268006000E-01   1.000
P 1 1.00
0.1540389170E-01     1.000
D 1 1.000
0.1001940640E+01   1.0000
D 1 1.000
0.4254800000E+00   1.000
D 1 1.000
0.1182550200E+00   1.000
D 1 1.000
0.4268006000E-01   1.000
D 1 1.00
0.1540389170E-01     1.000
****
-Ne 0
S 14 1.000
0.1570064170E+06      0.2736595150E+00
0.2357202230E+05      0.5107683190E+00
0.5384378010E+04      0.8802155190E+00
0.1530177090E+04      0.1426612960E+01
0.5004819910E+03      0.2169207470E+01
0.1809504500E+03      0.3009228460E+01
0.7042869550E+02      0.3555665000E+01
0.2897948950E+02      0.3167599420E+01
0.1236590420E+02      0.1639436320E+01
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0.5350932040E+01      0.2944830460E+00
0.2301383830E+01      0.2383620200E-02
0.9613489300E+00      0.8564161010E-03
0.3866276500E+00     -0.1829687680E-03
0.1443326200E+00      0.2291426580E-04
S 14 1.000
0.1570064170E+06    -0.6521178170E-01
0.2357202230E+05    -0.1215738770E+00
0.5384378010E+04    -0.2102592370E+00
0.1530177090E+04    -0.3413226520E+00
0.5004819910E+03    -0.5277200320E+00
0.1809504500E+03    -0.7531077920E+00
0.7042869550E+02    -0.9705330410E+00
0.2897948950E+02    -0.1019814810E+01
0.1236590420E+02    -0.7623231240E+00
0.5350932040E+01    -0.1156185120E+00
0.2301383830E+01     0.3817250920E+00
0.9613489300E+00     0.3534878530E+00
0.3866276500E+00     0.1150470970E+00
0.1443326200E+00     0.5472659590E-02
S 1 1.000
0.9613489300E+00   1.000
S 1 1.000
0.3866276500E+00   1.000
S 1 1.000
0.1443326200E+00   1.000
S 1 1.000
0.5388105376E-01   1.000
P 14 1.000
0.1570064170E+06    0.6621720420E-01
0.2357202230E+05     0.1199414270E+00
0.5384378010E+04     0.2118454780E+00
0.1530177090E+04     0.3407103530E+00
0.5004819910E+03     0.5367356260E+00
0.1809504500E+03     0.7835796870E+00
0.7042869550E+02     0.1070897510E+01
0.2897948950E+02     0.1318317980E+01
0.1236590420E+02     0.1389828660E+01
0.5350932040E+01     0.1196385250E+01
0.2301383830E+01     0.6990196210E+00
0.9613489300E+00     0.2693808550E+00
0.3866276500E+00     0.6764143130E-01
0.1443326200E+00     0.7068470970E-02
P 1 1.000
0.9613489300E+00   1.000
P 1 1.000
```

```
0.3866276500E+00   1.000
P 1 1.000
0.1443326200E+00   1.000
P 1 1.000
0.5388105376E-01   1.000
D 1 1.000
0.2301383830E+01 1.000
D 1 1.000
0.9613489300E+00   1.000
D 1 1.000
0.3866276500E+00   1.000
D 1 1.000
0.1443326200E+00   1.000
D 1 1.000
0.5388105376E-01   1.000
****
-He 0
S 8 1.000
0.1064328140D+04     0.5162833960D-01
0.1595241650D+03     0.9661130170D-01
0.3611871570D+02     0.1649044020D+00
0.1016995400D+02     0.2492102630D+00
0.3274689320D+01     0.3028858630D+00
0.1125428480D+01     0.2646230430D+00
0.3956613500D+00     0.1458877990D+00
0.1382103700D+00     0.2884591850D-01
S 1 1.000
0.1125428480D+01  1.000
S 1 1.000
0.3956613500D+00  1.000
S 1 1.000
0.1382103700D+00  1.000
S 1 1.000
0.4827892938D-01 1.000
P 1 1.000
0.3274689320D+01  1.0000
P 1 1.000
0.1125428480D+01  1.000
P 1 1.000
0.3956613500D+00  1.000
P 1 1.000
0.1382103700D+00  1.000
P 1 1.000
0.4827892938D-01 1.000
D 1 1.000
0.1125428480D+01  1.000
```

```
D 1 1.000
0.3956613500D+00  1.000
D 1 1.000
0.1382103700D+00  1.000
D 1 1.000
0.4827892938D-01 1.000
****
```