Comment on "Regularized SCAN functional" Supplementary Material

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In this supplementary material we present the individual values for each one of the systems in the different test sets. All results are given as the difference between calculated values and experimental ones. Experimental results are taken from references [S1–S4]. Enthalpies of formation found in the active thermochemical tables [S4] were preferred over those found in reference [S1].

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TABLE S1: SCAN standard enthalpies of formation [kcal/mol] obtained with different grid qualities.

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
LiH	3.018	3.162	3.035	2.996	2.990	33.300
^{2}BeH	−9.878	−9.564	−9.687	−9.472	−9.514	81.700
^{2}CH	3.157	1.908	2.442	2.331	2.373	142.500
CH_2 ($^3B_1$)	−4.719	−6.169	−6.133	−6.165	−6.097	93.600
CH_2 ($^1A_1$)	6.426	5.204	6.167	5.990	6.036	102.600
$^3CH_3$	−3.888	−5.256	−4.686	−4.718	−4.675	35.000
CH_4	1.439	−0.585	0.717	0.543	0.605	−17.800
^{3}NH	−4.269	−2.218	−1.833	−1.466	−1.483	85.800
NH_2 ($^2B_1$)	−3.581	−1.532	−1.619	−1.345	−1.361	44.500
NH_3	1.619	4.186	3.929	4.332	4.296	−10.900
^{2}OH	0.577	−1.769	−1.237	−1.190	−1.174	9.000
H_2O	7.370	4.285	4.960	4.613	4.659	−57.800
HF	3.382	5.192	4.707	4.922	4.953	−65.200
SiH_2 ($^1A_1$)	3.056	2.623	2.068	2.069	2.114	65.200
SiH_2 ($^3B_1$)	−6.789	−7.258	−7.785	−7.816	−7.752	86.200
$^2SiH_3$	−4.182	−4.635	−5.188	−5.194	−5.138	47.900
SiH_4	−0.369	−0.859	−1.466	−1.477	−1.425	8.200
$^2PH_2$	−3.207	−3.009	−3.447	−3.471	−3.477	33.100
PH_3	0.705	0.904	0.485	0.463	0.435	1.300
H_2S	−0.525	0.195	0.281	0.432	0.331	−4.900
HCl	0.590	0.276	0.722	1.444	0.973	−22.000
Li_2	6.224	6.614	6.329	6.275	6.272	51.600
LiF	3.908	6.362	5.941	5.916	5.944	−80.100
HC≡CH	6.058	4.421	4.099	3.717	3.766	54.600
$H_2C{=}CH_2$	3.154	1.456	0.996	0.859	0.899	12.500
$H_3C{-}CH_3$	1.532	−0.357	−0.657	−0.830	−0.804	−20.100
CN	2.977	4.086	3.926	4.013	4.031	105.200
HCN	4.593	4.881	6.593	6.336	6.375	30.900
CO	7.598	2.891	5.107	5.155	5.226	−26.400
^{2}HCO	0.040	−4.542	−2.484	−3.039	−2.966	10.000
H_2CO	4.184	−1.113	1.581	0.928	0.989	−26.100
CH_3OH	2.314	−1.415	1.255	0.694	0.748	−48.000
N_2	4.712	9.130	8.837	9.747	9.657	0.000
H_2NNH_2	0.130	7.384	8.607	8.516	8.415	23.300
NO	1.605	0.756	1.764	1.715	1.733	21.800
$^3O_2$	−4.257	−8.531	−7.383	−7.123	−7.126	0.000
H_2O_2	3.292	−0.643	3.065	2.229	2.310	−32.400
F_2	−4.024	0.780	0.506	1.086	1.093	0.000
CO_2	2.870	−6.468	−2.602	−3.440	−3.287	−94.000
Na_2	1.548	1.115	3.386	2.788	3.102	34.000
Si_2	−0.054	3.019	0.576	0.077	0.966	139.900
P_2	6.594	7.124	6.131	4.816	5.687	34.300
$^3S_2$	−5.916	−5.529	−7.972	−7.450	−7.274	30.700
Cl_2	−3.102	0.648	−0.572	0.177	0.188	0.000
NaCl	−0.372	1.306	2.200	2.177	1.909	−43.600
SiO	5.254	4.137	6.379	5.804	5.832	−24.600
CS	6.630	4.199	3.336	3.969	3.911	66.900
SO	−8.578	−6.189	−5.947	−5.784	−5.905	1.200
ClO	−8.280	−5.479	−4.653	−4.119	−4.406	24.300
ClF	5.307	0.018	1.096	1.032	0.740	−13.300
Si_2H_6	−6.450	−5.619	−5.070	−6.263	−5.416	19.100
CH_3Cl	0.072	−1.151	−1.192	−1.204	−1.156	−19.600
$H_3C{-}SH$	3.300	−0.494	−0.925	−1.214	−1.148	−5.500
HOCl	3.778	0.832	1.027	1.336	1.387	−18.400
SO_2	6.830	−1.134	1.246	0.404	0.331	−71.000
BF_3	−19.439	2.082	−0.211	0.199	0.294	−271.400
BCl_3	−6.813	−10.996	−10.385	−8.563	−9.706	−96.300
AlF_3	0.582	2.004	6.059	6.343	6.220	−289.000
$AlCl_3$	−5.012	−8.925	−5.827	−5.783	−6.908	−139.700
CF_4	−29.195	−3.461	−2.747	−4.606	−4.526	−223.100
CCl_4	−9.759	−6.189	−5.985	−3.258	−4.673	−22.900

TABLE S1: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
OCS	−10.830	−8.777	−6.615	−6.986	−6.503	−33.100
CS_2	−5.195	−7.510	−8.832	−8.665	−8.481	28.000
F_2CO	−16.878	−3.537	−5.278	−4.809	−4.733	−145.000
SiF_4	2.127	9.948	8.450	8.473	8.659	−386.000
$SiCl_4$	−5.706	−5.848	−5.423	−6.651	−6.171	−158.400
NNO	−6.576	−2.918	−2.245	−1.347	−1.411	19.700
ClNO	−11.421	−5.302	−5.239	−5.049	−5.057	12.600
NF_3	3.170	−6.151	−4.836	−6.013	−6.034	−31.600
PF_3	−15.259	5.523	3.912	4.158	4.257	−229.100
O_3	0.898	−5.187	−1.260	−0.514	−0.401	33.900
F_2O	−14.689	−4.878	−4.565	−4.534	−4.465	5.900
ClF_3	−23.036	−15.617	−12.524	−11.098	−11.498	−38.000
$F_2C{=}CF_2$	−19.109	−11.859	−9.213	−8.668	−8.414	−161.300
$Cl_2C{=}CCl_2$	5.187	−7.062	−5.876	−7.745	−7.265	−5.500
$F_3C{-}CN$	−12.889	−8.702	−0.867	−1.634	−1.805	−118.400
$HC{\equiv}C{-}CH_3$	9.350	−0.993	0.843	0.657	0.735	44.400
$H_2C{=}C{=}CH_2$	−3.189	−0.799	−3.232	−2.984	−2.845	45.400
C_3H_4 (cyclopropene)	6.767	−2.056	−0.515	−1.055	−0.944	67.800
$H_2C{=}CH{-}CH_3$	3.884	−2.817	−1.479	−1.229	−1.176	4.800
C_3H_6 (cyclopropane)	0.745	−2.427	−2.613	−3.032	−2.991	12.800
$CH_3{-}CH_2{-}CH_3$	2.563	−3.482	−2.166	−1.967	−1.915	−25.100
C_4H_6 (Z-1,3-butadiene)	−6.937	0.658	−3.799	−2.648	−2.213	26.400
C_4H_6 (2-butyne)	−5.875	1.500	−2.595	−1.528	−1.127	34.800
C_4H_6 (methylenecyclopropane)	−0.240	−8.872	−7.084	−6.764	−6.689	47.900
C_4H_6 (bicyclo[1.1.0]butane)	−3.597	−0.832	−4.042	−3.894	−3.725	51.900
C_4H_6 (cyclobutene)	−3.474	−0.189	−2.059	−3.117	−2.956	38.200
C_4H_8 (cyclobutane)	−4.468	−8.464	−3.206	−4.193	−4.034	6.600
C_4H_8 (isobutene)	4.017	−4.640	−2.874	−2.539	−2.471	−4.100
C_4H_{10} (trans butane)	−7.763	0.003	−1.288	−3.427	−2.972	−30.100
C_4H_{10} (isobutane)	3.498	−4.575	−2.837	−2.559	−2.490	−32.200
C_5H_8 (spiropentane)	0.006	−10.127	−7.922	−7.597	−7.504	44.300
C_6H_6 (benzene)	8.747	−16.670	−9.030	−9.742	−9.210	19.900
CH_2F_2	−3.089	−1.410	−1.507	−1.507	−1.483	−107.700
CHF_3	−5.889	−2.592	−3.337	−3.240	−3.232	−166.300
CH_2Cl_2	−1.380	−3.089	−3.338	−1.953	−2.632	−22.600
$CHCl_3$	−1.626	−4.813	−4.752	−2.729	−3.774	−24.500
CH_3NH_2	8.334	7.737	9.614	9.542	9.518	−5.200
CH_3CN	0.418	3.650	2.285	2.697	2.666	18.000
CH_3NO_2 (nitromethane)	−4.264	−8.121	−4.805	−5.924	−5.884	−17.900
CH_3ONO (methyl nitrite)	−15.759	−2.924	−5.910	−4.220	−4.211	−16.100
CH_3SiH_3	−1.205	−2.560	−1.239	−1.529	−1.349	−7.000
HCO_2H	−10.904	−4.930	−2.970	−2.197	−2.132	−90.400
HCO_2CH_3	−14.434	−9.471	−6.510	−5.382	−5.181	−85.500
CH_3CONH_2	−2.468	−1.140	−2.966	−2.857	−2.783	−57.000
C_2H_5N (aziridine)	−0.801	−0.838	−0.370	−0.665	−0.657	30.200
NCCN (cyanogen)	−1.312	7.921	4.127	5.399	5.433	74.100
$NH(CH_3)_2$	0.891	1.045	0.248	0.263	0.289	−4.300
$CH_3CH_2NH_2$	−4.586	0.240	0.030	−0.133	0.000	−11.300
$H_2C{=}C{=}O$ (ketene)	0.828	−4.500	−4.043	−4.782	−4.713	−11.600
C_2H_4O (oxirane)	1.404	−3.898	−2.691	−3.344	−3.288	−12.600
CH_3CHO	3.003	−1.602	−2.159	−1.928	−1.863	−39.500
$O{=}CH{-}CH{=}O$	5.785	−6.611	−2.330	−1.629	−1.486	−50.800
CH_3CH_2OH	0.633	1.315	0.208	−0.857	−0.785	−56.100
$(CH_3)_2O$	−0.409	−2.310	−2.158	−2.538	−2.460	−44.000
C_2H_4S (thiooxirane)	−0.389	−3.491	−4.017	−4.386	−4.333	19.600
$(CH_3)_2S{=}O$	−4.741	−4.987	−5.093	−4.646	−4.593	−36.200
CH_3CH_2SH	2.091	−2.337	−2.491	−1.891	−2.048	−11.100
$(CH_3)_2S$	4.721	−3.896	−2.721	−2.845	−2.769	−8.900
$H_2C{=}CHF$	0.112	−3.590	−1.930	−2.154	−2.172	−34.000
CH_3CH_2Cl	0.510	−3.870	−2.877	−2.538	−2.750	−26.600
$H_2C{=}CHCl$	1.321	−3.271	−2.079	−1.788	−2.005	5.200
$H_2C{=}CHCN$	6.237	7.252	3.321	3.598	3.701	43.200

TABLE S1: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
$(CH_3)_2C{=}O$	3.663	−5.409	−4.465	−3.713	−3.629	−51.700
CH_3CO_2H	0.353	−2.772	−1.981	−3.744	−3.607	−103.400
CH_3CFO	1.022	−5.895	−4.367	−4.065	−4.076	−105.700
CH_3COCl	−0.355	−7.620	−6.965	−6.098	−6.283	−57.700
$CH_3CH_2CH_2Cl$	3.749	−8.301	−4.063	−3.971	−3.876	−31.500
$(CH_3)_2CHOH$	4.404	−2.623	−1.641	−2.075	−2.015	−65.200
$CH_3{-}O{-}CH_2CH_3$	−6.197	−3.019	−4.885	−4.592	−4.267	−51.700
$(CH_3)_3N$	−3.857	0.485	−1.080	−1.031	−0.964	−6.600
C_4H_4O (furan)	−5.758	−5.309	−7.547	−7.924	−7.735	−8.300
C_4H_4S (thiophene)	0.232	−9.020	−7.668	−7.433	−7.581	27.500
C_4H_5N (pyrrole)	−11.075	−2.523	−6.948	−5.989	−5.841	25.900
C_5H_5N (pyridine)	6.397	−12.222	−8.521	−8.304	−7.942	33.600
H_2	2.028	2.029	2.029	2.029	2.029	0.000
^2SH	−2.552	−1.811	−1.803	−1.626	−1.711	34.200
$^2C{\equiv}CH$	2.660	0.063	−0.090	−0.570	−0.387	135.800
$HC{=}CH_2$ ($^2A'$)	−2.426	−4.600	−4.697	−5.060	−4.933	71.000
$CH_3C{=}O$ ($^2A'$)	−0.773	−5.469	−5.992	−5.673	−5.577	−2.400
$CH_2{-}OH$ (^2A)	−2.447	−5.954	−3.978	−4.429	−4.354	−4.000
CH_3O ($^2A'$)	−5.650	−9.676	−7.412	−7.701	−7.591	5.200
CH_3CH_2O ($^2A''$)	−7.143	−9.386	−9.568	−9.967	−9.887	−2.900
CH_3S ($^2A'$)	−3.808	−6.156	−4.799	−4.774	−4.676	29.800
CH_2CH_3 ($^2A'$)	−4.163	−6.290	−6.272	−6.590	−6.496	28.600
$(CH_3)_2CH$ ($^2A'$)	−3.742	−9.983	−8.638	−8.527	−8.418	21.100
$^2C(CH_3)_3$	−3.022	−11.364	−9.544	−9.353	−9.229	12.000
NO_2 ($^2A_1$)	−10.449	−12.068	−9.047	−8.265	−8.223	8.100
$CH_3CH{=}C{=}CH_2$	−5.029	−3.108	−5.686	−4.030	−4.102	38.800
C_5H_8 (isoprene)	−9.223	0.298	−5.270	−3.827	−3.281	18.000
C_5H_{10} (cyclopentane twist)	2.741	−1.145	−5.038	−4.747	−4.645	−18.500
C_5H_{12} (n-pentane)	8.723	1.476	−1.887	−4.632	−4.062	−35.000
$C(CH_3)_4$ (neopentane)	4.414	−5.513	−3.380	−3.032	−2.945	−40.100
C_6H_8 (1,3-cyclohexadiene)	12.460	−12.949	−5.317	−5.884	−5.363	25.400
C_6H_8 (1,4-cyclohexadiene)	12.941	−12.493	−4.869	−5.434	−4.913	25.000
C_6H_{12} (cyclohexane chair)	12.083	−13.535	−4.140	−6.233	−5.714	−29.400
C_6H_{14} (n-hexane)	−1.157	−13.038	−0.908	−4.572	−5.162	−39.900
C_6H_{14} (3-methylpentane)	11.450	2.740	−1.294	−4.586	−3.905	−41.100
$C_6H_5{-}CH_3$ (toluene)	1.182	−19.322	−13.201	−11.109	−10.233	12.000
C_7H_{16} (n-heptane)	4.362	1.141	−6.319	−6.947	−6.263	−44.800
C_8H_8 (cyclooctatetraene)	−8.238	−4.805	−9.681	−6.415	−6.543	70.700
C_8H_{18} (n-octane)	4.924	1.187	−7.334	−8.049	−7.268	−49.800
$C_{10}H_8$ (naphtalene)	3.107	−6.456	−16.728	−19.610	−18.400	35.900
$C_{10}H_8$ (azulene)	−27.050	−7.071	−17.315	−18.820	−19.004	69.100
$CH_3CO_2CH_3$ (Z-methylacetate)	−18.579	−11.176	−8.650	−6.680	−6.228	−98.400
$(CH_3)_3COH$ (t-butanol)	5.248	−3.736	−2.339	−2.709	−2.633	−74.700
$C_6H_5NH_2$ (aniline)	−21.285	−6.721	−7.487	−10.913	−10.360	20.800
C_6H_5OH (phenol)	−19.333	−9.775	−13.458	−12.087	−11.342	−22.300
C_4H_6O (divinyl ether)	7.784	−3.972	−6.313	−5.229	−5.350	−3.300
C_4H_8O (tetrahydrofuran)	−4.205	−2.937	−4.881	−5.380	−5.238	−44.000
C_5H_8O (cyclopentanone)	2.508	−2.863	−8.655	−7.779	−7.480	−45.900
$C_6H_4O_2$ (benzoquinone)	12.902	−16.129	−10.776	−9.679	−9.298	−29.400
$C_6H_4N_2$ (pyrimidine)	2.477	−13.590	−9.717	−8.394	−8.345	46.800
$(CH_3)_2SO_2$	−9.993	−6.621	−8.101	−7.212	−7.002	−89.200
C_6H_5Cl (chlorobenzene)	−12.997	−11.408	−10.841	−11.780	−11.746	12.500
$NC(CH_2)_2CN$ (succinonitrile)	0.183	5.123	3.630	5.220	4.965	50.100
$C_4H_4N_2$ (pyrazine)	−1.401	−4.743	−5.441	−4.249	−4.234	46.900
C_4H_4O (3-butyn-2-one)	−4.379	4.175	−1.935	−0.195	0.306	15.600
C_4H_6O (E-crotonaldehyde)	−15.054	−7.636	−8.398	−6.351	−5.918	−24.000
$C_4H_6O_3$ (acetic anhydride)	9.877	−8.986	−10.549	−10.430	−10.755	−136.800
C_4H_6S (2,5-dihydrothiophene)	1.764	−2.605	−6.482	−5.675	−5.775	20.800
$(CH_3)_2CHCN$	6.037	2.056	2.113	2.412	2.534	5.600
C_4H_8O (methyl ethyl ketone)	−12.532	−4.549	−2.644	−5.238	−4.717	−57.100
$(CH_3)_2CHCHO$	3.829	−3.227	−2.592	−2.582	−2.399	−51.600
$C_4H_8O_2$ (1,4-dioxane)	7.095	−7.871	−7.207	−8.470	−8.151	−75.500

TABLE S1: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
C_4H_8S (tetrahydrothiophene)	2.189	−6.140	−5.612	−4.847	−4.947	−8.200
$(CH_3)_3CCl$	−0.605	−7.101	−5.281	−4.440	−4.654	−43.500
C_4H_9Cl (n-butyl chloride)	−6.183	−8.196	−2.801	−3.639	−4.284	−37.000
C_4H_9N (tetrahydropyrrole)	−1.422	0.641	−3.856	−3.063	−2.935	−0.800
$C_4H_9NO_2$ (2-nitrobutane)	−9.775	−3.684	−8.966	−8.974	−8.434	−39.100
$(CH_3CH_2)_2O$	8.113	−4.141	−6.278	−4.864	−5.063	−60.300
$CH_3CH(OCH_3)_2$ (dimethyl acetal)	−17.094	−11.628	−7.340	−7.029	−6.482	−93.100
$(CH_3)_3CSH$	6.330	−5.141	−4.281	−3.680	−3.803	−26.200
$C_4H_{10}S_2$ (diethyl disulfide)	−13.827	−12.620	−3.985	−7.554	−6.358	−17.900
$(CH_3)_3CNH_2$	2.098	−1.956	−0.874	−0.878	−0.825	−28.900
$(CH_3)_4Si$	12.976	−5.265	1.188	−0.465	−0.009	−55.700
C_5H_6S (2-methyl thiophene)	−9.268	−14.359	−7.165	−8.607	−8.954	20.000
C_5H_7N (N-methyl pyrrole)	−17.743	−3.039	−9.940	−7.786	−7.270	24.600
$C_5H_{10}O$ (tetrahydropyran)	5.286	−16.056	−6.566	−7.202	−6.723	−53.400
$(CH_3CH_2)_2C{=}O$	2.654	−3.797	−4.006	−7.245	−6.605	−61.600
$C_5H_{10}O_2$ (isopropyl acetate)	10.879	−7.306	−12.163	−8.132	−8.482	−115.100
$C_5H_{10}S$ (tetrahydrothiopyran)	−6.589	−11.744	−4.581	−6.432	−6.400	−15.200
$C_5H_{11}N$ (piperidine)	10.395	−10.500	−4.626	−4.085	−3.741	−11.300
$C_5H_{12}O$ (t-butyl methyl ether)	−9.355	−0.543	−6.488	−5.614	−5.062	−67.800
$C_6H_4F_2$ (1,3-difluorobenzene)	−1.531	−19.560	−15.552	−15.510	−15.392	−73.900
$C_6H_4F_2$ (1,4-difluorobenzene)	−6.609	−23.475	−15.815	−15.323	−15.074	−73.300
C_6H_5F (fluorobenzene)	3.746	−17.988	−12.198	−12.520	−12.196	−27.400
$C_6H_{14}O$ (diisopropyl ether)	12.334	−5.565	−8.599	−6.215	−6.525	−76.300
PF_5	29.289	16.541	6.140	4.262	4.135	−381.100
SF_6	17.381	6.331	−6.740	−8.849	−9.224	−291.700
P_4	−9.744	−1.942	−1.255	−2.841	−2.116	14.100
SO_3	4.974	−7.220	−3.664	−4.889	−4.967	−94.600
SCl_2	−0.921	−2.967	−4.406	−3.910	−3.591	−4.200
$POCl_3$	−7.350	−8.310	−7.069	−7.057	−6.589	−133.800
PCl_5	−3.720	−11.679	−11.527	−13.804	−13.179	−86.100
Cl_2O_2S	−11.427	−14.200	−10.139	−10.496	−10.037	−84.800
PCl_3	−3.759	−4.634	−6.222	−5.796	−5.348	−69.000
Cl_2S_2	−7.193	−11.208	−11.431	−11.918	−11.890	−4.000
$SiCl_2$ ($^1A_1$)	−1.675	−1.655	−1.807	−2.558	−2.137	−40.300
CF_3Cl	4.580	−12.025	−5.872	−6.263	−6.464	−169.700
C_2F_6	−35.498	−16.178	−12.444	−10.687	−10.370	−320.900
$^2CF_3$	−27.224	−8.326	−7.577	−9.048	−8.959	−111.800
$^2C_6H_5$ (phenyl radical)	2.096	−21.719	−14.663	−15.460	−14.923	80.500
M.D.	−1.542	−3.904	−3.500	−3.532	−3.428	
M.A.D.	6.130	5.647	5.004	5.013	4.926	

TABLE S2: SCAN bond lengths [Å] obtained with different grid qualities.

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
H_2	0.001	0.001	0.001	0.001	0.001	0.741
Li_2	0.082	0.076	0.084	0.083	0.083	2.673
LiH	0.013	0.008	0.007	0.008	0.008	1.595
LiF	0.005	0.005	0.007	0.006	0.006	1.564
LiCl	0.007	0.004	0.004	0.005	0.004	2.021
LiO	0.002	0.004	0.005	0.005	0.005	1.688
Be_2	0.063	0.049	0.051	0.046	0.047	2.440
BeH	0.011	0.012	0.012	0.012	0.012	1.343
BeF	0.008	0.010	0.011	0.011	0.011	1.361
BeO	0.001	0.000	0.002	0.001	0.001	1.331
BeS	0.004	0.003	0.004	0.004	0.004	1.742
B_2	0.028	0.028	0.025	0.028	0.026	1.590
BH	0.012	0.007	0.010	0.009	0.009	1.232
BF	0.001	0.002	0.002	0.002	0.002	1.263
BF_3	−0.000	−0.001	−0.000	−0.001	−0.001	1.313
BCl	0.002	0.004	0.006	0.005	0.005	1.715
BCl_3	−0.005	−0.004	−0.003	−0.002	−0.003	1.742
BN	0.041	0.038	0.038	0.039	0.038	1.281
BO	0.001	0.001	0.000	0.001	0.001	1.204
BS	0.000	0.002	0.000	0.001	0.001	1.609
C_2	0.000	0.006	0.005	0.006	0.006	1.242
CH	0.004	0.005	0.005	0.005	0.005	1.120
CH_4	0.002	−0.000	0.000	0.000	0.001	1.087
CF	0.003	0.004	0.004	0.003	0.003	1.272
CF_4	−0.002	−0.001	−0.001	−0.001	−0.001	1.323
CCl	0.008	0.009	0.007	0.006	0.008	1.645
CCl_4	0.003	0.005	0.003	0.003	0.003	1.767
CN	−0.007	−0.009	−0.010	−0.009	−0.009	1.172
CO	−0.003	−0.004	−0.002	−0.002	−0.002	1.128
CO^+	−0.005	−0.006	−0.004	−0.005	−0.005	1.115
CO_2	−0.003	−0.001	−0.001	−0.001	−0.001	1.160
CP	−0.008	−0.009	−0.007	−0.010	−0.008	1.562
CS	−0.000	−0.001	−0.001	−0.001	−0.001	1.535
CS_2	−0.003	−0.002	−0.003	−0.003	−0.003	1.553
N_2	−0.008	−0.007	−0.006	−0.006	−0.006	1.098
N_2^+	−0.014	−0.012	−0.011	−0.011	−0.011	1.116
NH	0.005	0.004	0.004	0.004	0.004	1.036
NH^+	0.008	0.007	0.007	0.007	0.007	1.070
NF	0.003	0.001	0.000	−0.000	0.001	1.317
NCl	0.011	0.005	0.007	0.004	0.007	1.611
NO	−0.005	−0.003	−0.004	−0.004	−0.004	1.151
NO^+	−0.004	−0.004	−0.005	−0.005	−0.005	1.063
NS	−0.000	−0.001	−0.001	−0.002	−0.001	1.494
O_2	−0.002	−0.001	−0.001	−0.001	−0.001	1.208
O_2^+	−0.006	−0.007	−0.007	−0.008	−0.008	1.116
OH	0.002	0.002	0.002	0.002	0.002	0.970
OH^+	0.005	0.004	0.005	0.005	0.005	1.029
OF	−0.004	−0.005	−0.006	−0.007	−0.006	1.358
F_2	−0.012	−0.011	−0.012	−0.012	−0.012	1.412
F_2^+	−0.024	−0.022	−0.023	−0.023	−0.023	1.322
HF	0.003	0.003	0.003	0.003	0.003	0.917
HF^+	0.007	0.008	0.008	0.008	0.008	1.001
Na_2	0.050	0.050	0.049	0.049	0.049	3.079
NaH	0.005	0.007	0.008	0.006	0.006	1.887
NaF	−0.000	−0.002	−0.003	−0.003	−0.003	1.926
NaCl	−0.000	−0.000	−0.000	−0.000	−0.000	2.361
NaO	0.000	−0.000	−0.000	−0.000	−0.000	2.052
MgH	0.012	0.012	0.012	0.013	0.012	1.730
MgF	0.013	0.013	0.013	0.013	0.013	1.750
MgCl	0.012	0.012	0.012	0.012	0.012	2.196
MgO	−0.011	−0.013	−0.015	−0.015	−0.015	1.748

TABLE S2: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
Al_2	0.000	0.004	0.005	0.008	0.004	2.466
AlH	0.009	0.010	0.012	0.012	0.012	1.648
AlF	0.010	0.007	0.008	0.008	0.008	1.654
AlCl	0.012	0.012	0.012	0.013	0.013	2.130
AlO	0.000	0.001	0.000	−0.000	−0.000	1.618
AlS	−0.000	−0.000	−0.000	−0.000	−0.000	2.029
Si_2	−0.096	−0.096	−0.096	−0.096	−0.096	2.246
SiH	0.011	0.010	0.008	0.009	0.008	1.520
SiH_4	0.003	0.001	0.000	0.001	0.001	1.480
SiF	0.009	0.011	0.011	0.010	0.011	1.601
SiF_4	0.009	0.008	0.008	0.008	0.009	1.553
SiCl	0.011	0.011	0.011	0.011	0.011	2.058
$SiCl_4$	0.004	0.004	0.004	0.004	0.004	2.019
SiN	−0.007	−0.004	−0.004	−0.005	−0.003	1.572
SiO	0.004	0.002	0.002	0.003	0.003	1.510
SiS	0.004	0.004	0.004	0.004	0.004	1.929
P_2	−0.004	−0.005	−0.005	−0.005	−0.005	1.893
P_4	−0.015	−0.014	−0.014	−0.014	−0.014	2.210
PH	0.003	0.003	0.004	0.005	0.004	1.421
PF	0.008	0.009	0.008	0.008	0.008	1.589
PCl	0.005	0.006	0.005	0.004	0.005	2.015
PN	−0.005	−0.006	−0.005	−0.006	−0.006	1.491
PO	0.002	0.004	0.003	0.003	0.003	1.476
S_2	0.005	0.006	0.006	0.006	0.006	1.889
SH	0.004	0.001	0.003	0.003	0.003	1.341
SF	0.001	0.002	0.001	0.001	0.001	1.601
SF_6	0.014	0.013	0.013	0.013	0.013	1.561
SO	0.006	0.007	0.005	0.006	0.006	1.481
SO_3	0.003	0.005	0.004	0.004	0.004	1.420
Cl_2	0.011	0.012	0.012	0.012	0.012	1.988
Cl_2^+	0.008	0.008	0.009	0.009	0.009	1.891
HCl	0.002	0.002	0.004	0.004	0.003	1.275
HCl^+	0.006	0.006	0.006	0.006	0.005	1.315
ClF	0.006	0.006	0.005	0.006	0.006	1.628
ClO	0.006	0.009	0.008	0.007	0.008	1.570
M.D.	0.004	0.004	0.004	0.004	0.004	
M.A.D.	0.009	0.009	0.009	0.009	0.009	

TABLE S3: SCAN harmonic vibrational frequencies [cm^{-1}] obtained with different grid qualities.

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
H_2	33.280	27.860	28.640	28.530	28.470	4401.200
Li_2	−25.040	−15.080	−15.540	−19.350	−17.960	351.400
LiH	57.050	−10.370	−34.290	−4.790	−6.990	1405.700
LiF	3.240	9.950	−4.410	−4.290	−4.370	910.600
LiCl	24.400	13.990	−11.600	−5.910	2.190	643.000
LiO	12.840	2.380	11.430	−5.520	−1.690	814.600
LiNa	−4.320	−18.230	−5.990	−6.640	−9.580	256.800
Be_2	56.830	56.250	64.470	59.820	60.700	267.900
BeH	35.620	5.020	−35.920	−31.970	−42.920	2060.800
BeH^+	−12.480	4.040	13.810	−18.270	−15.950	2221.700
BeF	9.220	−15.990	−9.310	−20.410	−17.910	1247.400
BeCl	−24.140	−27.990	−20.430	−26.470	−25.090	846.700
BeO	46.610	34.780	19.130	30.540	27.150	1487.300
BeS	10.260	35.130	12.940	17.860	14.730	997.900
B_2	−82.580	−47.140	−36.750	−48.480	−47.490	1051.300
BH	−90.050	−59.520	−47.250	−52.740	−68.870	2366.900
BF	−8.590	−4.360	7.160	0.120	0.610	1402.100
BCl	25.360	−13.440	0.300	−3.750	−2.160	840.300
BN	55.020	45.980	54.640	59.660	61.190	1514.600
BO	32.570	4.280	10.970	15.790	16.610	1885.700
BS	41.170	7.110	27.800	28.610	21.450	1180.200
C_2	41.150	53.440	31.700	42.920	40.990	1854.700
CH	−16.860	1.540	4.730	−36.410	−45.850	2858.500
CF	84.730	−11.580	−1.910	−3.660	−1.100	1308.100
CN	63.300	97.150	96.580	85.150	91.030	2068.600
CO	51.770	51.640	38.530	42.180	36.660	2169.800
CO^+	63.590	87.410	70.340	78.360	72.900	2214.200
CP	31.780	63.930	45.950	47.940	35.610	1239.700
CS	47.820	45.520	12.560	24.250	24.800	1285.200
N_2	69.610	409.860	84.050	77.100	79.660	2358.600
N_2^+	116.490	119.090	124.880	119.920	121.320	2207.000
NH	−83.740	−56.530	51.580	−25.770	−25.410	3282.300
NF	−122.780	47.310	22.230	38.410	19.280	1141.400
NCl	−19.870	−0.810	−4.380	4.170	0.660	828.000
NO	55.110	59.740	55.950	57.220	57.510	1904.200
NO^+	95.140	95.930	87.590	88.570	86.720	2376.400
NS	47.290	45.670	36.880	41.930	38.360	1218.700
O_2	37.970	39.840	43.180	43.190	42.880	1580.200
O_2^+	130.650	128.450	122.820	121.080	122.690	1904.800
OH	7.370	−6.240	−2.950	−10.090	−9.860	3737.800
OH^+	8.890	−157.500	−31.530	−44.340	−47.280	3113.400
F_2	134.160	128.100	124.200	128.840	128.310	916.600
F_2^+	134.360	139.930	136.480	136.760	137.650	1073.300
HF	55.050	−22.240	−30.920	−39.550	−36.360	4138.300
HF^+	−69.640	−69.830	−65.230	−65.080	−63.160	3090.500
Na_2	−20.250	−5.290	−1.670	−2.500	−3.900	159.100
NaH	36.130	78.250	−101.060	10.690	−1.050	1172.200
NaF	4.560	−0.540	6.100	6.010	5.360	535.700
NaO	1.770	−3.840	−8.240	−0.790	−3.700	492.300
MgH	−102.820	−57.140	20.290	−30.410	−27.620	1495.200
MgH^+	74.930	20.150	−8.670	16.950	20.050	1699.100
MgO	55.790	179.890	55.270	51.060	53.470	784.800
MgS	20.240	24.770	23.600	22.760	24.890	528.700
Al_2	9.860	5.200	−3.370	0.220	1.920	350.000
AlH	114.890	−30.800	−57.090	−39.620	−35.620	1682.600
AlF	3.410	−20.480	−12.690	−13.570	−12.120	802.300
AlCl	2.880	−6.570	−6.980	−5.940	−5.150	481.300
AlO	−14.930	−0.880	0.250	11.750	6.480	979.200
AlS	10.200	9.260	13.170	15.180	14.230	617.100
Si_2	62.890	51.330	48.580	51.920	50.830	511.000
SiH	−75.770	4.220	51.900	17.770	−14.350	2041.800

TABLE S3: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
SiH^+	27.320	57.080	−46.780	−49.290	−37.740	2157.200
SiF	−14.860	−13.800	−10.530	−10.400	−10.350	857.200
SiCl	−6.220	−8.210	−4.500	−6.250	−6.340	535.600
SiN	25.920	25.320	30.990	28.200	21.240	1151.400
SiO	28.040	31.050	20.440	12.820	11.270	1241.500
SiS	5.380	12.100	9.810	8.880	9.000	749.600
P_2	43.650	29.300	36.700	32.450	35.650	780.800
$P_2{}^+$	120.050	102.230	99.560	109.640	107.900	672.200
PH	−85.180	−7.340	−28.910	21.830	7.260	2365.200
PF	−13.700	1.330	−2.180	1.450	1.660	846.800
PCl	3.290	−1.140	1.550	−0.920	−1.840	551.400
PN	23.520	64.350	57.020	54.230	57.910	1337.200
PO	27.840	34.900	11.860	24.270	24.150	1233.300
S_2	−2.930	1.460	5.740	8.270	6.320	725.600
SO	31.140	30.200	10.890	16.070	16.350	1149.200
Cl_2	−8.570	−8.430	−6.820	−4.280	−7.200	559.700
$Cl_2{}^+$	7.630	−1.450	−1.900	−1.100	−0.330	645.600
HCl	70.050	42.110	−54.370	−14.180	−8.000	2990.900
HCl^+	22.540	8.430	−32.770	−26.630	−28.250	2673.700
ClF	19.310	7.070	3.250	1.750	2.860	786.100
ClO	23.540	7.450	5.760	8.030	5.720	853.800
M.D.	20.624	24.220	14.723	15.509	14.160	
M.A.D.	42.705	41.360	32.941	32.079	31.076	

TABLE S4: SCAN-L standard enthalpies of formation [kcal/mol] obtained with different grid qualities.

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
LiH	4.050	3.800	3.709	3.709	3.705	33.300
^{2}BeH	−10.853	−10.663	−10.177	−10.178	−10.259	81.700
^{2}CH	1.299	−0.159	0.605	0.522	0.509	142.500
CH_2 ($^3B_1$)	−1.994	−4.615	−3.973	−3.922	−3.960	93.600
CH_2 ($^1A_1$)	5.462	3.466	4.729	4.566	4.526	102.600
$^3CH_3$	−0.503	−2.539	−1.629	−1.671	−1.695	35.000
CH_4	4.871	2.817	4.651	4.472	4.455	−17.800
^{3}NH	−8.354	−6.005	−5.452	−4.951	−5.025	85.800
NH_2 ($^2B_1$)	−7.658	−5.496	−5.584	−5.386	−5.427	44.500
NH_3	−0.662	0.550	0.434	0.799	0.694	−10.900
^{2}OH	−3.035	−3.462	−2.867	−2.924	−2.853	9.000
H_2O	5.773	3.121	4.347	3.890	3.941	−57.800
HF	5.378	6.357	6.326	6.838	6.812	−65.200
SiH_2 ($^1A_1$)	2.939	3.147	3.116	2.897	3.238	65.200
SiH_2 ($^3B_1$)	−6.216	−6.411	−6.208	−6.416	−6.077	86.200
$^2SiH_3$	−2.302	−2.480	−2.244	−2.467	−2.121	47.900
SiH_4	3.369	3.291	3.475	3.272	3.633	8.200
$^2PH_2$	−2.310	−2.866	−2.552	−2.169	−2.301	33.100
PH_3	3.313	2.534	2.926	3.329	3.147	1.300
H_2S	0.377	1.297	2.012	2.140	2.061	−4.900
HCl	1.617	2.518	2.152	1.819	2.193	−22.000
Li_2	6.275	5.826	5.648	5.658	5.630	51.600
LiF	8.098	9.953	9.261	9.419	9.267	−80.100
HC≡CH	7.504	4.689	5.347	4.985	4.807	54.600
$H_2C{=}CH_2$	6.962	4.546	4.864	4.868	4.655	12.500
$H_3C{-}CH_3$	8.023	5.756	6.121	6.241	6.003	−20.100
CN	−5.670	−3.620	−3.183	−3.183	−3.316	105.200
HCN	−0.453	−0.872	1.779	1.322	1.316	30.900
CO	7.274	3.307	3.996	4.592	4.573	−26.400
^{2}HCO	−2.307	−6.370	−3.443	−4.064	−4.099	10.000
H_2CO	3.253	−1.062	2.115	1.488	1.449	−26.100
CH_3OH	3.786	0.670	3.799	3.320	3.256	−48.000
N_2	−4.272	−1.209	−1.489	−0.798	−1.048	0.000
H_2NNH_2	−8.999	−2.354	−0.109	−0.667	−0.779	23.300
NO	−7.117	−9.309	−7.608	−7.777	−7.785	21.800
$^3O_2$	−13.738	−15.292	−15.036	−15.058	−14.891	0.000
H_2O_2	−8.528	−7.178	−4.697	−5.519	−5.484	−32.400
F_2	−5.640	−6.412	−7.222	−6.524	−6.514	0.000
CO_2	0.092	−3.701	0.013	−1.083	−1.079	−94.000
Na_2	−2.329	2.936	3.565	3.176	3.579	34.000
Si_2	−8.609	−1.895	−2.580	−2.652	−2.952	139.900
P_2	6.523	3.313	3.998	4.219	3.905	34.300
$^3S_2$	−2.876	−7.862	−6.893	−7.603	−7.671	30.700
Cl_2	−6.394	−2.518	−1.733	−3.128	−2.356	0.000
NaCl	3.935	3.940	4.975	4.764	5.114	−43.600
SiO	5.070	5.156	6.699	5.794	5.935	−24.600
CS	7.094	2.669	1.939	2.296	2.152	66.900
SO	−9.775	−8.444	−7.809	−7.263	−7.566	1.200
ClO	−12.743	−10.479	−9.810	−9.996	−9.631	24.300
ClF	0.633	−2.557	−1.853	−2.563	−2.274	−13.300
Si_2H_6	−2.499	3.151	3.868	3.669	3.442	19.100
CH_3Cl	4.291	2.176	2.200	2.454	2.197	−19.600
$H_3C{-}SH$	9.599	2.236	3.399	3.529	2.897	−5.500
HOCl	−1.827	−3.697	−2.997	−3.807	−3.387	−18.400
SO_2	1.892	−2.158	1.174	0.617	0.232	−71.000
BF_3	9.850	15.917	12.096	13.346	13.298	−271.400
BCl_3	−3.014	−3.080	−3.766	−3.638	−3.565	−96.300
AlF_3	15.627	18.432	19.712	19.681	19.552	−289.000
$AlCl_3$	6.728	0.902	2.149	1.958	2.166	−139.700
CF_4	4.057	10.982	10.835	8.606	8.503	−223.100
CCl_4	−7.261	−3.840	−4.752	−4.070	−3.944	−22.900

TABLE S4: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
OCS	−9.198	−7.763	−4.571	−4.914	−5.365	−33.100
CS_2	−5.325	−7.236	−8.076	−7.141	−7.764	28.000
F_2CO	0.045	4.341	1.372	2.661	2.518	−145.000
SiF_4	22.499	31.716	29.225	29.159	28.791	−386.000
$SiCl_4$	12.017	5.866	5.704	3.198	5.093	−158.400
NNO	−23.821	−14.113	−14.869	−14.148	−14.372	19.700
ClNO	−21.907	−16.188	−16.568	−17.783	−17.329	12.600
NF_3	−11.020	−16.817	−15.798	−17.301	−17.411	−31.600
PF_3	9.249	15.887	12.010	13.484	13.324	−229.100
O_3	−22.273	−21.260	−19.416	−19.264	−19.236	33.900
F_2O	−20.781	−18.615	−18.952	−17.992	−18.009	5.900
ClF_3	−7.726	−14.692	−16.346	−17.671	−17.223	−38.000
$F_2C{=}CF_2$	21.432	7.196	4.323	2.844	2.504	−161.300
$Cl_2C{=}CCl_2$	−0.463	0.914	−5.731	−3.939	−4.170	−5.500
$F_3C{-}CN$	−3.488	−4.255	0.939	2.410	2.051	−118.400
$HC{\equiv}C{-}CH_3$	14.480	3.813	6.172	5.998	5.739	44.400
$H_2C{=}C{=}CH_2$	2.482	2.885	1.338	1.996	1.857	45.400
C_3H_4 (cyclopropene)	14.161	2.009	4.524	3.779	3.650	67.800
$H_2C{=}CH{-}CH_3$	12.703	4.278	5.704	6.384	6.090	4.800
C_3H_6 (cyclopropane)	9.020	5.418	6.781	6.207	5.849	12.800
$CH_3{-}CH_2{-}CH_3$	14.559	6.567	7.793	8.268	7.987	−25.100
C_4H_6 (Z-1,3-butadiene)	3.986	8.260	3.639	4.884	5.273	26.400
C_4H_6 (2-butyne)	6.706	10.820	6.033	7.363	7.697	34.800
C_4H_6 (methylenecyclopropane)	11.708	0.598	2.459	3.207	2.836	47.900
C_4H_6 (bicyclo[1.1.0]butane)	7.463	7.952	6.753	7.199	6.974	51.900
C_4H_6 (cyclobutene)	6.608	7.143	7.606	6.353	6.113	38.200
C_4H_8 (cyclobutane)	7.693	2.651	8.773	7.677	7.419	6.600
C_4H_8 (isobutene)	17.146	6.016	7.806	8.635	8.243	−4.100
C_4H_{10} (trans butane)	8.454	13.942	12.685	9.533	10.020	−30.100
C_4H_{10} (isobutane)	19.297	8.653	10.284	10.890	10.516	−32.200
C_5H_8 (spiropentane)	17.952	4.524	6.712	7.447	6.993	44.300
C_6H_6 (benzene)	22.195	−6.259	4.245	2.842	3.317	19.900
CH_2F_2	2.767	6.162	5.971	5.392	5.198	−107.700
CHF_3	2.429	8.369	7.564	6.770	6.502	−166.300
CH_2Cl_2	−0.110	0.463	−0.258	0.137	0.183	−22.600
$CHCl_3$	−1.907	−1.483	−2.364	−1.811	−1.733	−24.500
CH_3NH_2	7.643	6.526	9.214	9.050	8.890	−5.200
CH_3CN	0.446	1.856	1.627	2.317	1.921	18.000
CH_3NO_2 (nitromethane)	−17.182	−16.995	−11.338	−12.721	−12.880	−17.900
CH_3ONO (methyl nitrite)	−21.125	−11.649	−15.369	−13.939	−13.781	−16.100
CH_3SiH_3	5.208	5.005	6.421	6.608	6.601	−7.000
HCO_2H	−6.777	−3.596	−1.016	0.155	0.056	−90.400
HCO_2CH_3	−3.147	−2.309	−1.085	0.173	0.156	−85.500
CH_3CONH_2	3.435	2.198	0.246	0.739	0.579	−57.000
C_2H_5N (aziridine)	0.033	−0.668	1.172	0.653	0.418	30.200
NCCN (cyanogen)	−10.369	−2.080	−6.544	−5.071	−5.119	74.100
$NH(CH_3)_2$	4.893	3.012	3.396	3.461	3.270	−4.300
$CH_3CH_2NH_2$	−1.153	3.297	3.131	2.625	2.778	−11.300
$H_2C{=}C{=}O$ (ketene)	−0.340	−1.805	−0.789	−1.179	−1.448	−11.600
C_2H_4O (oxirane)	3.707	−0.999	1.289	0.575	0.381	−12.600
CH_3CHO	3.864	1.922	2.489	2.981	2.707	−39.500
$O{=}CH{-}CH{=}O$	−0.305	−5.584	−1.789	−0.763	−0.724	−50.800
CH_3CH_2OH	7.735	6.901	6.477	5.079	5.052	−56.100
$(CH_3)_2O$	5.005	3.176	3.724	3.680	3.542	−44.000
C_2H_4S (thiooxirane)	6.089	0.167	1.634	1.716	0.899	19.600
$(CH_3)_2S{=}O$	9.069	3.029	3.432	4.042	3.384	−36.200
CH_3CH_2SH	11.021	5.386	5.276	5.652	5.125	−11.100
$(CH_3)_2S$	13.486	2.869	4.210	4.615	3.836	−8.900
$H_2C{=}CHF$	1.709	2.240	4.951	4.034	3.810	−34.000
CH_3CH_2Cl	9.683	1.906	4.908	3.593	3.874	−26.600
$H_2C{=}CHCl$	7.527	−0.364	2.964	1.617	1.897	5.200
$H_2C{=}CHCN$	7.694	5.361	2.542	3.029	2.798	43.200

TABLE S4: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
$(CH_3)_2C{=}O$	9.981	2.416	3.612	5.013	4.672	−51.700
CH_3CO_2H	7.176	2.584	4.595	2.674	2.457	−103.400
CH_3CFO	0.021	2.017	4.251	4.054	3.764	−105.700
CH_3COCl	2.899	−3.953	−1.119	−1.692	−1.464	−57.700
$CH_3CH_2CH_2Cl$	10.217	1.849	5.247	4.907	5.817	−31.500
$(CH_3)_2CHOH$	15.640	6.667	7.644	7.233	7.077	−65.200
$CH_3{-}O{-}CH_2CH_3$	6.243	5.965	4.427	4.631	5.059	−51.700
$(CH_3)_3N$	3.150	5.487	5.494	5.692	5.448	−6.600
C_4H_4O (furan)	3.235	1.763	0.610	0.751	0.505	−8.300
C_4H_4S (thiophene)	12.771	0.324	0.809	2.028	1.241	27.500
C_4H_5N (pyrrole)	−3.017	2.445	−1.516	0.126	−0.054	25.900
C_5H_5N (pyridine)	12.708	−6.961	−1.583	−1.911	−1.625	33.600
H_2	3.345	3.359	3.335	3.339	3.342	0.000
^2SH	−2.547	−1.920	−1.225	−1.021	−1.084	34.200
$^2C{\equiv}CH$	2.839	−0.314	0.331	−0.104	−0.191	135.800
$HC{=}CH_2$ ($^2A'$)	0.661	−2.238	−1.470	−1.845	−1.970	71.000
$CH_3C{=}O$ ($^2A'$)	−1.330	−3.517	−3.287	−2.600	−2.753	−2.400
$CH_2{-}OH$ (^2A)	−2.346	−5.769	−2.883	−3.379	−3.411	−4.000
CH_3O ($^2A'$)	−4.104	−7.991	−5.239	−5.577	−5.495	5.200
CH_3CH_2O ($^2A''$)	−0.294	−4.042	−3.629	−4.247	−4.460	−2.900
CH_3S ($^2A'$)	0.711	−3.155	−1.692	−1.055	−1.644	29.800
CH_2CH_3 ($^2A'$)	2.166	−0.613	0.134	−0.208	−0.335	28.600
$(CH_3)_2CH$ ($^2A'$)	6.889	−0.814	0.844	1.200	0.981	21.100
$^2C(CH_3)_3$	11.539	1.155	3.184	3.716	3.394	12.000
NO_2 ($^2A_1$)	−22.684	−22.766	−20.590	−20.054	−20.023	8.100
$CH_3CH{=}C{=}CH_2$	1.862	3.526	2.134	4.501	3.853	38.800
C_5H_8 (isoprene)	5.830	11.557	5.374	7.024	7.533	18.000
C_5H_{10} (cyclopentane twist)	21.494	11.561	10.246	10.936	10.495	−18.500
C_5H_{12} (n-pentane)	22.650	17.752	15.524	11.444	12.014	−35.000
$C(CH_3)_4$ (neopentane)	23.920	10.670	12.772	13.545	13.077	−40.100
C_6H_8 (1,3-cyclohexadiene)	27.590	−1.479	9.013	7.938	8.399	25.400
C_6H_8 (1,4-cyclohexadiene)	28.707	−0.453	10.026	8.958	9.414	25.000
C_6H_{12} (cyclohexane chair)	33.243	2.802	15.666	12.644	13.124	−29.400
C_6H_{14} (n-hexane)	17.964	7.606	18.590	15.698	14.004	−39.900
C_6H_{14} (3-methylpentane)	27.740	21.872	19.185	14.303	14.983	−41.100
$C_6H_5{-}CH_3$ (toluene)	17.459	−5.267	2.847	4.784	5.693	12.000
C_7H_{16} (n-heptane)	19.707	19.707	15.686	15.368	15.982	−44.800
C_8H_8 (cyclooctatetraene)	4.694	7.526	4.929	9.520	8.245	70.700
C_8H_{18} (n-octane)	22.304	22.313	17.732	17.359	18.061	−49.800
$C_{10}H_8$ (naphtalene)	24.704	13.159	4.763	1.371	2.681	35.900
$C_{10}H_8$ (azulene)	−0.341	11.018	2.666	2.192	0.607	69.100
$CH_3CO_2CH_3$ (Z-methylacetate)	−2.063	−0.614	0.635	2.544	2.964	−98.400
$(CH_3)_3COH$ (t-butanol)	20.371	8.712	10.103	9.835	9.585	−74.700
$C_6H_5NH_2$ (aniline)	−6.050	3.900	3.366	−1.010	−0.513	20.800
C_6H_5OH (phenol)	1.214	4.652	−0.460	0.798	1.398	−22.300
C_4H_6O (divinyl ether)	14.403	3.401	1.799	3.310	2.658	−3.300
C_4H_8O (tetrahydrofuran)	9.663	7.146	7.128	6.793	6.629	−44.000
C_5H_8O (cyclopentanone)	16.546	7.798	5.159	6.736	6.522	−45.900
$C_6H_4O_2$ (benzoquinone)	17.509	−6.245	−1.151	−0.605	−0.046	−29.400
$C_6H_4N_2$ (pyrimidine)	1.847	−14.509	−8.767	−7.324	−7.858	46.800
$(CH_3)_2SO_2$	13.124	7.213	7.231	7.475	7.309	−89.200
C_6H_5Cl (chlorobenzene)	3.003	−1.584	2.401	1.584	0.977	12.500
$NC(CH_2)_2CN$ (succinonitrile)	−5.732	1.066	1.409	3.000	2.245	50.100
$C_4H_4N_2$ (pyrazine)	0.124	−4.394	−5.381	−4.077	−4.488	46.900
C_4H_4O (3-butyn-2-one)	1.138	8.606	3.214	5.355	5.778	15.600
C_4H_6O (E-crotonaldehyde)	−2.810	−0.698	−0.204	1.792	2.420	−24.000
$C_4H_6O_3$ (acetic anhydride)	22.253	4.811	−0.019	1.337	0.723	−136.800
C_4H_6S (2,5-dihydrothiophene)	14.958	6.277	3.622	4.719	4.015	20.800
$(CH_3)_2CHCN$	14.776	6.906	7.612	8.101	7.784	5.600
C_4H_8O (methyl ethyl ketone)	1.431	8.495	9.299	6.179	6.708	−57.100
$(CH_3)_2CHCHO$	12.958	6.127	8.510	8.533	8.252	−51.600
$C_4H_8O_2$ (1,4-dioxane)	20.859	3.137	5.116	2.870	3.357	−75.500

TABLE S4: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
C_4H_8S (tetrahydrothiophene)	18.006	6.601	6.985	7.886	7.193	−8.200
$(CH_3)_3CCl$	15.438	5.153	8.616	8.279	8.277	−43.500
C_4H_9Cl (n-butyl chloride)	6.646	2.104	11.064	9.105	8.467	−37.000
C_4H_9N (tetrahydropyrrole)	10.000	8.030	4.536	5.834	5.592	−0.800
$C_4H_9NO_2$ (2-nitrobutane)	−10.327	−2.616	−6.297	−6.589	−6.045	−39.100
$(CH_3CH_2)_2O$	19.505	8.511	6.637	8.298	7.582	−60.300
$CH_3CH(OCH_3)_2$ (dimethyl acetal)	−4.008	1.604	3.853	5.033	5.553	−93.100
$(CH_3)_3CSH$	22.023	8.900	9.698	10.221	9.501	−26.200
$C_4H_{10}S_2$ (diethyl disulfide)	8.464	0.133	10.434	7.634	6.618	−17.900
$(CH_3)_3CNH_2$	14.770	7.884	8.703	8.616	8.268	−28.900
$(CH_3)_4Si$	29.610	9.209	18.398	16.508	16.762	−55.700
C_5H_6S (2-methyl thiophene)	8.957	−4.272	6.371	4.567	3.316	20.000
C_5H_7N (N-methyl pyrrole)	−3.417	7.495	−1.060	1.464	1.974	24.600
$C_5H_{10}O$ (tetrahydropyran)	21.105	−1.574	8.742	8.086	8.521	−53.400
$(CH_3CH_2)_2C{=}O$	15.031	11.622	11.289	7.279	7.926	−61.600
$C_5H_{10}O_2$ (isopropyl acetate)	17.056	9.889	3.126	8.074	7.161	−115.100
$C_5H_{10}S$ (tetrahydrothiopyran)	5.736	0.698	11.077	8.788	9.120	−15.200
$C_5H_{11}N$ (piperidine)	23.524	−0.725	7.723	8.069	8.334	−11.300
$C_5H_{12}O$ (t-butyl methyl ether)	10.746	15.716	8.590	9.614	10.284	−67.800
$C_6H_4F_2$ (1,3-difluorobenzene)	18.161	2.358	2.977	1.782	1.957	−73.900
$C_6H_4F_2$ (1,4-difluorobenzene)	8.391	−12.580	1.080	2.028	2.050	−73.300
C_6H_5F (fluorobenzene)	20.208	−1.858	3.687	2.375	2.705	−27.400
$C_6H_{14}O$ (diisopropyl ether)	28.911	13.396	10.424	13.439	12.297	−76.300
PF_5	27.245	30.296	21.013	22.597	22.796	−381.100
SF_6	16.978	15.249	4.461	7.061	7.013	−291.700
P_4	−13.784	0.255	−0.915	0.046	−1.181	14.100
SO_3	0.905	−4.006	0.272	−0.976	−1.324	−94.600
SCl_2	−2.508	−4.688	−5.223	−5.889	−5.106	−4.200
$POCl_3$	−1.662	0.512	1.864	0.368	1.656	−133.800
PCl_5	−9.069	1.685	−9.651	−6.848	−7.088	−86.100
Cl_2O_2S	−6.755	−9.606	−4.633	−6.390	−5.353	−84.800
PCl_3	−3.155	−0.547	−2.196	−3.124	−1.945	−69.000
Cl_2S_2	−15.107	−10.242	−14.507	−13.750	−13.458	−4.000
$SiCl_2$ ($^1A_1$)	2.021	2.793	2.731	1.533	2.443	−40.300
CF_3Cl	5.800	1.411	2.301	3.132	3.394	−169.700
C_2F_6	29.278	15.494	10.234	9.418	8.850	−320.900
$^2CF_3$	−4.038	0.344	0.631	−1.155	−1.230	−111.800
$^2C_6H_5$ (phenyl radical)	14.284	−12.472	−2.520	−3.860	−3.494	80.500
M.D.	4.860	1.595	2.267	2.224	2.180	
M.A.D.	9.107	5.970	5.799	5.726	5.662	

TABLE S5: SCAN-L bond lengths [Å] obtained with different grid qualities.

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
H_2	0.001	0.001	0.001	0.001	0.001	0.741
Li_2	0.057	0.058	0.051	0.054	0.052	2.673
LiH	−0.000	−0.000	−0.004	−0.000	−0.001	1.595
LiF	0.003	0.000	0.000	0.001	0.001	1.564
LiCl	−0.007	−0.007	−0.008	−0.008	−0.009	2.021
LiO	−0.000	−0.002	−0.002	−0.002	−0.002	1.688
Be_2	−0.036	−0.049	−0.046	−0.048	−0.050	2.440
BeH	0.003	0.004	0.005	0.005	0.005	1.343
BeF	0.007	0.009	0.009	0.009	0.009	1.361
BeO	0.004	0.002	0.003	0.003	0.003	1.331
BeS	−0.001	−0.000	−0.002	−0.002	−0.002	1.742
B_2	0.015	0.019	0.016	0.016	0.016	1.590
BH	0.009	0.006	0.007	0.008	0.008	1.232
BF	0.005	0.005	0.005	0.005	0.005	1.263
BF_3	0.005	0.004	0.005	0.005	0.005	1.313
BCl	0.002	0.005	0.006	0.006	0.006	1.715
BCl_3	−0.006	−0.006	−0.005	−0.004	−0.005	1.742
BN	0.042	0.039	0.040	0.040	0.040	1.281
BO	0.003	0.004	0.003	0.003	0.003	1.204
BS	−0.002	−0.000	−0.001	−0.000	−0.000	1.609
C_2	0.148	0.151	0.149	0.149	0.149	1.242
CH	0.005	0.003	0.003	0.003	0.003	1.120
CH_4	0.002	0.001	0.000	0.001	0.001	1.087
CF	0.015	0.015	0.015	0.015	0.015	1.272
CF_4	0.011	0.011	0.011	0.011	0.011	1.323
CCl	0.015	0.015	0.014	0.014	0.014	1.645
CCl_4	0.014	0.013	0.013	0.012	0.012	1.767
CN	−0.004	−0.003	−0.005	−0.005	−0.005	1.172
CO	0.002	0.002	0.003	0.003	0.004	1.128
CO^+	0.001	−0.000	0.001	0.000	0.000	1.115
CO_2	0.006	0.008	0.008	0.008	0.008	1.160
CP	−0.008	−0.008	−0.007	−0.007	−0.007	1.562
CS	0.002	0.004	0.003	0.003	0.003	1.535
CS_2	−0.000	0.002	0.002	0.001	0.001	1.553
N_2	−0.003	−0.001	−0.001	0.000	−0.000	1.098
N_2^+	−0.009	−0.009	−0.008	−0.007	−0.007	1.116
NH	0.006	0.008	0.007	0.007	0.007	1.036
NH^+	0.008	0.009	0.009	0.009	0.009	1.070
NF	0.018	0.016	0.016	0.016	0.016	1.317
NCl	0.016	0.018	0.018	0.019	0.019	1.611
NO	0.005	0.006	0.005	0.005	0.005	1.151
NO^+	0.004	0.003	0.002	0.003	0.002	1.063
NS	0.008	0.008	0.007	0.007	0.007	1.494
O_2	0.012	0.014	0.014	0.014	0.014	1.208
O_2^+	0.007	0.007	0.006	0.006	0.006	1.116
OH	0.004	0.004	0.004	0.004	0.004	0.970
OH^+	0.009	0.008	0.008	0.009	0.009	1.029
OF	0.007	0.007	0.006	0.006	0.006	1.358
F_2	−0.001	0.001	0.001	0.001	0.001	1.412
F_2^+	−0.007	−0.004	−0.004	−0.004	−0.004	1.322
HF	0.005	0.007	0.007	0.007	0.007	0.917
HF^+	0.010	0.009	0.009	0.009	0.009	1.001
Na_2	0.001	0.003	0.004	0.004	0.003	3.079
NaH	−0.012	−0.008	−0.009	−0.006	−0.007	1.887
NaF	−0.006	−0.005	−0.006	−0.005	−0.005	1.926
NaCl	−0.013	−0.013	−0.013	−0.013	−0.013	2.361
NaO	−0.006	−0.007	−0.005	−0.005	−0.005	2.052
MgH	−0.000	0.003	0.001	0.003	0.003	1.730
MgF	0.013	0.013	0.013	0.013	0.013	1.750
MgCl	0.004	0.004	0.003	0.003	0.003	2.196
MgO	−0.009	−0.009	−0.011	−0.009	−0.010	1.748

TABLE S5: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
Al_2	−0.007	−0.003	−0.000	−0.000	−0.000	2.466
AlH	0.004	0.003	0.005	0.002	0.005	1.648
AlF	0.012	0.011	0.012	0.012	0.012	1.654
AlCl	0.008	0.009	0.009	0.009	0.009	2.130
AlO	0.004	0.002	0.004	0.003	0.003	1.618
AlS	−0.005	−0.004	−0.004	−0.004	−0.004	2.029
Si_2	0.012	0.012	0.012	0.011	0.012	2.246
SiH	0.004	0.003	0.002	0.003	0.003	1.520
SiH_4	−0.002	−0.003	−0.003	−0.003	−0.003	1.480
SiF	0.016	0.017	0.018	0.018	0.018	1.601
SiF_4	0.015	0.013	0.014	0.014	0.014	1.553
SiCl	0.010	0.010	0.010	0.010	0.010	2.058
$SiCl_4$	0.001	0.003	0.003	0.003	0.003	2.019
SiN	−0.002	−0.001	−0.002	−0.001	−0.001	1.572
SiO	0.009	0.008	0.009	0.009	0.009	1.510
SiS	0.006	0.006	0.006	0.006	0.006	1.929
P_2	−0.003	−0.003	−0.003	−0.003	−0.003	1.893
P_4	−0.009	−0.010	−0.010	−0.010	−0.010	2.210
PH	0.000	0.001	0.001	0.001	0.001	1.421
PF	0.019	0.021	0.021	0.021	0.021	1.589
PCl	0.011	0.011	0.011	0.011	0.011	2.015
PN	0.001	−0.002	0.000	−0.000	−0.000	1.491
PO	0.013	0.013	0.012	0.012	0.012	1.476
S_2	0.012	0.013	0.013	0.013	0.013	1.889
SH	−0.000	0.001	−0.001	0.000	0.000	1.341
SF	0.019	0.020	0.020	0.020	0.020	1.601
SF_6	0.028	0.030	0.030	0.030	0.030	1.561
SO	0.019	0.022	0.020	0.021	0.021	1.481
SO_3	0.019	0.020	0.020	0.020	0.020	1.420
Cl_2	0.023	0.024	0.024	0.024	0.024	1.988
Cl_2^+	0.025	0.026	0.026	0.026	0.026	1.891
HCl	0.003	0.003	0.001	0.001	0.001	1.275
HCl^+	0.004	0.004	0.004	0.004	0.003	1.315
ClF	0.025	0.028	0.027	0.027	0.027	1.628
ClO	0.026	0.030	0.027	0.027	0.027	1.570
M.D.	0.007	0.008	0.007	0.008	0.008	
M.A.D.	0.011	0.011	0.011	0.011	0.011	

TABLE S6: SCAN-L harmonic vibrational frequencies [cm^{-1}] obtained with different grid qualities.

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
H_2	41.750	27.310	37.850	35.020	32.380	4401.200
Li_2	−10.650	−19.140	0.510	−6.570	−13.490	351.400
LiH	−40.170	−131.650	−20.040	−15.400	−2.380	1405.700
LiF	−45.360	−13.080	−12.290	−9.160	−7.530	910.600
LiCl	29.320	−4.240	6.230	4.260	5.820	643.000
LiO	2.590	−5.650	−12.810	−6.560	−6.420	814.600
LiNa	10.190	−16.990	−7.560	−8.030	−4.100	256.800
Be_2	120.310	120.470	109.360	109.280	115.160	267.900
BeH	63.130	132.330	−15.980	6.190	−24.110	2060.800
BeH^+	47.990	58.200	23.440	−24.800	−15.420	2221.700
BeF	−9.640	−13.990	−38.270	−27.020	−30.080	1247.400
BeCl	−41.000	−17.910	−16.830	−20.190	−17.790	846.700
BeO	8.390	−17.280	−6.780	−0.900	−4.330	1487.300
BeS	23.870	30.380	4.930	−2.170	5.030	997.900
B_2	−46.160	−30.770	−35.070	−36.010	−40.130	1051.300
BH	53.380	−75.430	−31.440	−52.100	−59.050	2366.900
BF	−12.160	−14.810	−19.700	−27.460	−27.840	1402.100
BCl	−51.790	−13.090	−27.500	−18.870	−23.390	840.300
BN	44.980	24.250	24.270	36.570	34.110	1514.600
BO	−158.520	−8.400	−24.390	−20.810	−20.620	1885.700
BS	−4.500	−3.450	4.130	−0.550	4.130	1180.200
C_2	19.090	21.560	8.300	32.370	25.860	1854.700
CH	−2.050	−53.350	9.030	−43.470	−50.940	2858.500
CF	−82.340	−72.130	−70.770	−73.960	−74.400	1308.100
CN	55.390	20.000	49.460	44.700	44.750	2068.600
CO	−33.980	−20.470	−22.890	−14.440	−30.670	2169.800
CO^+	10.970	30.110	18.930	11.850	10.550	2214.200
CP	25.430	23.890	27.750	27.560	26.090	1239.700
CS	13.300	−28.410	12.710	−7.710	−8.280	1285.200
N_2	24.070	10.080	12.720	4.510	9.090	2358.600
N_2^+	68.370	70.800	77.710	65.150	70.450	2207.000
NH	−113.700	−70.950	−31.540	−56.460	−68.240	3282.300
NF	−27.990	−20.560	−27.370	−30.230	−29.350	1141.400
NCl	5.820	−21.990	−8.110	−15.590	−11.470	828.000
NO	−35.650	−35.330	−35.260	−30.450	−30.200	1904.200
NO^+	−9.940	−9.140	−4.430	−6.860	−6.840	2376.400
NS	−39.050	−20.800	−4.300	−10.520	−9.210	1218.700
O_2	−39.230	−58.920	−58.740	−59.450	−58.860	1580.200
O_2^+	−11.040	−13.860	−5.770	−6.030	−6.450	1904.800
OH	−27.230	−22.970	−60.330	−48.060	−50.630	3737.800
OH^+	−125.860	−204.990	−87.130	−95.860	−97.410	3113.400
F_2	137.390	97.120	88.000	96.100	94.110	916.600
F_2^+	90.100	104.150	98.970	99.310	98.810	1073.300
HF	−83.100	−119.120	−120.920	−118.200	−113.570	4138.300
HF^+	−125.650	−92.880	−103.940	−96.360	−96.880	3090.500
Na_2	−11.440	2.500	5.030	−0.020	1.310	159.100
NaH	63.130	−135.480	0.280	−14.330	5.560	1172.200
NaF	−0.720	0.130	2.770	−0.720	−0.170	535.700
NaO	−5.190	−1.280	−9.200	−5.310	−7.270	492.300
MgH	38.330	53.070	46.310	−20.730	−20.760	1495.200
MgH^+	−106.490	15.230	65.400	3.700	19.600	1699.100
MgO	29.800	−17.950	26.640	26.010	25.520	784.800
MgS	6.890	15.920	12.580	12.280	13.600	528.700
Al_2	−7.590	−5.760	1.550	−5.410	−5.770	350.000
AlH	169.380	102.880	−87.880	−39.660	−13.630	1682.600
AlF	−27.990	−30.620	−31.330	−30.240	−30.890	802.300
AlCl	−8.620	−10.730	−8.770	−11.450	−10.690	481.300
AlO	−28.360	−13.600	−21.620	−17.160	−16.530	979.200
AlS	10.620	6.490	10.160	11.280	8.650	617.100
Si_2	2.200	−12.160	−11.720	−19.090	−14.560	511.000
SiH	−88.830	69.520	40.250	−7.090	−0.660	2041.800

TABLE S6: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
SiH^+	−38.090	100.870	−175.840	−72.710	−45.360	2157.200
SiF	−30.250	−44.540	−38.580	−37.700	−37.470	857.200
SiCl	−17.410	−14.770	−15.500	−15.380	−14.760	535.600
SiN	−12.400	−20.390	−9.820	−17.090	−18.380	1151.400
SiO	−16.060	−19.750	−23.330	−32.410	−31.450	1241.500
SiS	−15.470	−8.180	−6.130	−8.410	−9.160	749.600
P_2	23.520	24.000	17.150	14.660	15.850	780.800
P_2^+	20.050	22.000	22.410	18.020	22.040	672.200
PH	83.250	125.130	134.900	−27.420	8.170	2365.200
PF	−41.900	−45.340	−40.790	−49.820	−46.510	846.800
PCl	−31.570	−24.630	−22.100	−16.550	−16.810	551.400
PN	27.540	36.460	31.740	19.990	19.710	1337.200
PO	−51.820	−26.540	−27.650	−31.000	−28.300	1233.300
S_2	−25.640	−21.640	−21.340	−22.400	−23.370	725.600
SO	−53.250	−61.500	−43.310	−52.830	−53.260	1149.200
Cl_2	−22.950	−19.840	−20.220	−22.650	−21.360	559.700
Cl_2^+	−26.870	−25.640	−26.830	−26.840	−26.120	645.600
HCl	21.130	−142.710	85.050	−13.540	−30.060	2990.900
HCl^+	−95.700	−61.210	64.430	−79.040	−39.130	2673.700
ClF	−16.030	−34.680	−15.450	−22.310	−19.800	786.100
ClO	−10.910	−23.070	−25.560	−21.770	−20.760	853.800
M.D.	−7.032	−8.889	−5.027	−12.836	−11.301	
M.A.D.	40.975	41.690	33.830	29.392	28.773	

TABLE S7: regSCAN standard enthalpies of formation [kcal/mol] obtained with different grid qualities.

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
LiH	2.678	2.602	2.646	2.639	2.640	33.300
^{2}BeH	−10.040	−10.045	−10.061	−10.062	−10.061	81.700
^{2}CH	1.702	1.753	1.733	1.736	1.736	142.500
CH_2 ($^3B_1$)	−8.611	−8.604	−8.622	−8.619	−8.620	93.600
CH_2 ($^1A_1$)	4.327	4.405	4.379	4.375	4.374	102.600
$^3CH_3$	−7.349	−7.337	−7.353	−7.352	−7.352	35.000
CH_4	−3.790	−3.632	−3.665	−3.668	−3.669	−17.800
^{3}NH	−1.987	−2.098	−2.072	−2.074	−2.074	85.800
NH_2 ($^2B_1$)	−2.754	−2.913	−2.851	−2.863	−2.862	44.500
NH_3	0.687	0.432	0.497	0.486	0.487	−10.900
^{2}OH	−2.660	−2.411	−2.463	−2.458	−2.456	9.000
H_2O	0.401	0.600	0.557	0.561	0.560	−57.800
HF	1.659	1.604	1.591	1.590	1.590	−65.200
SiH_2 ($^1A_1$)	1.095	1.120	1.116	1.116	1.116	65.200
SiH_2 ($^3B_1$)	−8.723	−8.732	−8.733	−8.732	−8.732	86.200
$^2SiH_3$	−6.374	−6.388	−6.394	−6.394	−6.394	47.900
SiH_4	−2.365	−2.361	−2.362	−2.362	−2.363	8.200
$^2PH_2$	−4.122	−4.108	−4.103	−4.103	−4.103	33.100
PH_3	−0.489	−0.478	−0.472	−0.473	−0.472	1.300
H_2S	−1.805	−1.806	−1.813	−1.812	−1.812	−4.900
HCl	−0.961	−0.961	−0.956	−0.957	−0.957	−22.000
Li_2	5.699	5.536	5.624	5.611	5.613	51.600
LiF	1.916	2.076	2.152	2.145	2.146	−80.100
HC≡CH	−3.258	−2.954	−2.965	−2.966	−2.968	54.600
H_2C=CH_2	−6.246	−5.961	−5.974	−5.977	−5.979	12.500
H_3C−CH_3	−7.836	−7.554	−7.563	−7.567	−7.569	−20.100
CN	−0.253	−0.221	−0.185	−0.197	−0.197	105.200
HCN	1.071	1.167	1.152	1.134	1.134	30.900
CO	0.754	0.877	0.870	0.876	0.875	−26.400
^{2}HCO	−7.700	−7.452	−7.533	−7.533	−7.533	10.000
H_2CO	−4.263	−3.993	−4.075	−4.078	−4.079	−26.100
CH_3OH	−4.654	−4.529	−4.611	−4.612	−4.613	−48.000
N_2	6.354	5.795	5.938	5.918	5.918	0.000
H_2NNH_2	3.506	3.014	3.049	3.024	3.025	23.300
NO	−1.957	−1.981	−2.001	−2.008	−2.007	21.800
$^3O_2$	−12.074	−11.754	−11.855	−11.846	−11.846	0.000
H_2O_2	−3.402	−2.904	−2.927	−2.928	−2.928	−32.400
F_2	−1.564	−1.750	−1.783	−1.781	−1.782	0.000
CO_2	−11.559	−11.274	−11.295	−11.293	−11.294	−94.000
Na_2	2.510	2.503	2.504	2.504	2.504	34.000
Si_2	−1.577	−1.575	−1.578	−1.577	−1.577	139.900
P_2	3.156	3.165	3.167	3.168	3.167	34.300
$^3S_2$	−10.368	−10.357	−10.358	−10.358	−10.358	30.700
Cl_2	−2.054	−2.063	−2.061	−2.062	−2.061	0.000
NaCl	−0.062	−0.068	−0.067	−0.067	−0.069	−43.600
SiO	2.347	2.535	2.540	2.542	2.541	−24.600
CS	0.184	0.212	0.209	0.216	0.216	66.900
SO	−8.808	−8.864	−8.882	−8.882	−8.882	1.200
ClO	−6.614	−6.719	−6.746	−6.739	−6.739	24.300
ClF	−1.535	−1.392	−1.401	−1.402	−1.403	−13.300
Si_2H_6	−6.850	−6.962	−6.946	−6.945	−6.946	19.100
CH_3Cl	−5.104	−5.199	−5.203	−5.199	−5.199	−19.600
H_3C−SH	−5.971	−5.922	−5.942	−5.941	−5.942	−5.500
HOCl	−2.541	−2.295	−2.321	−2.319	−2.319	−18.400
SO_2	−6.234	−5.793	−5.912	−5.909	−5.910	−71.000
BF_3	−7.377	−8.369	−8.417	−8.417	−8.417	−271.400
BCl_3	−13.755	−13.761	−13.769	−13.775	−13.777	−96.300
AlF_3	−3.366	−2.420	−2.504	−2.507	−2.507	−289.000
$AlCl_3$	−11.232	−11.296	−11.299	−11.299	−11.303	−139.700
CF_4	−12.365	−13.556	−13.601	−13.608	−13.608	−223.100
CCl_4	−10.204	−10.399	−10.396	−10.396	−10.400	−22.900

TABLE S7: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
OCS	−13.714	−13.602	−13.685	−13.681	−13.680	−33.100
CS_2	−14.910	−14.917	−14.933	−14.927	−14.928	28.000
F_2CO	−12.282	−12.731	−12.720	−12.719	−12.720	−145.000
SiF_4	−2.454	−1.504	−1.373	−1.378	−1.378	−386.000
$SiCl_4$	−10.190	−10.330	−10.303	−10.303	−10.308	−158.400
NNO	−9.378	−9.763	−9.698	−9.706	−9.706	19.700
ClNO	−10.060	−10.692	−10.598	−10.603	−10.603	12.600
NF_3	−13.646	−13.374	−13.396	−13.408	−13.408	−31.600
PF_3	−0.393	−1.508	−1.412	−1.411	−1.412	−229.100
O_3	−9.317	−8.642	−8.671	−8.664	−8.665	33.900
F_2O	−9.134	−9.391	−9.464	−9.461	−9.461	5.900
ClF_3	−16.647	−17.692	−17.678	−17.682	−17.682	−38.000
$F_2C{=}CF_2$	−17.290	−18.608	−18.595	−18.600	−18.602	−161.300
$Cl_2C{=}CCl_2$	−15.791	−15.818	−15.791	−15.789	−15.794	−5.500
$F_3C{-}CN$	−12.496	−12.819	−12.960	−12.970	−12.971	−118.400
$HC{\equiv}C{-}CH_3$	−9.025	−8.871	−8.943	−8.948	−8.951	44.400
$H_2C{=}C{=}CH_2$	−13.019	−12.967	−12.913	−12.899	−12.897	45.400
C_3H_4 (cyclopropene)	−11.245	−11.220	−11.245	−11.243	−11.246	67.800
$H_2C{=}CH{-}CH_3$	−11.322	−10.744	−10.827	−10.807	−10.811	4.800
C_3H_6 (cyclopropane)	−13.042	−12.605	−12.627	−12.625	−12.628	12.800
$CH_3{-}CH_2{-}CH_3$	−11.778	−11.265	−11.341	−11.321	−11.325	−25.100
C_4H_6 (Z-1,3-butadiene)	−14.257	−14.847	−14.776	−14.748	−14.754	26.400
C_4H_6 (2-butyne)	−13.223	−13.792	−13.735	−13.709	−13.714	34.800
C_4H_6 (methylenecyclopropane)	−19.872	−19.146	−19.252	−19.228	−19.233	47.900
C_4H_6 (bicyclo[1.1.0]butane)	−16.130	−16.031	−15.986	−15.968	−15.966	51.900
C_4H_6 (cyclobutene)	−14.070	−14.018	−13.922	−13.943	−13.941	38.200
C_4H_8 (cyclobutane)	−14.984	−14.650	−14.847	−14.867	−14.865	6.600
C_4H_8 (isobutene)	−15.518	−14.784	−14.892	−14.867	−14.872	−4.100
C_4H_{10} (trans butane)	−14.538	−15.152	−15.004	−15.040	−15.046	−30.100
C_4H_{10} (isobutane)	−15.243	−14.550	−14.649	−14.625	−14.630	−32.200
C_5H_8 (spiropentane)	−23.307	−22.498	−22.624	−22.594	−22.600	44.300
C_6H_6 (benzene)	−27.257	−26.588	−26.975	−26.991	−26.993	19.900
CH_2F_2	−7.346	−6.849	−6.800	−6.807	−6.808	−107.700
CHF_3	−11.115	−10.377	−10.291	−10.300	−10.301	−166.300
CH_2Cl_2	−7.044	−7.119	−7.117	−7.112	−7.115	−22.600
$CHCl_3$	−8.802	−8.872	−8.865	−8.860	−8.863	−24.500
CH_3NH_2	3.668	3.792	3.772	3.757	3.757	−5.200
CH_3CN	−5.552	−5.600	−5.563	−5.565	−5.566	18.000
CH_3NO_2 (nitromethane)	−17.445	−16.734	−16.784	−16.800	−16.800	−17.900
CH_3ONO (methyl nitrite)	−12.667	−13.642	−13.531	−13.518	−13.520	−16.100
CH_3SiH_3	−5.798	−5.818	−5.875	−5.871	−5.871	−7.000
HCO_2H	−8.927	−9.368	−9.523	−9.514	−9.515	−90.400
HCO_2CH_3	−13.167	−13.780	−13.916	−13.895	−13.893	−85.500
CH_3CONH_2	−13.131	−13.283	−13.178	−13.175	−13.174	−57.000
C_2H_5N (aziridine)	−9.163	−8.915	−8.914	−8.926	−8.927	30.200
NCCN (cyanogen)	−3.840	−4.280	−4.127	−4.129	−4.132	74.100
$NH(CH_3)_2$	−7.917	−7.693	−7.647	−7.651	−7.650	−4.300
$CH_3CH_2NH_2$	−8.286	−8.581	−8.509	−8.516	−8.516	−11.300
$H_2C{=}C{=}O$ (ketene)	−14.251	−13.487	−13.505	−13.510	−13.511	−11.600
C_2H_4O (oxirane)	−10.908	−10.439	−10.514	−10.511	−10.513	−12.600
CH_3CHO	−10.660	−9.946	−9.985	−9.978	−9.980	−39.500
$O{=}CH{-}CH{=}O$	−11.761	−10.527	−10.696	−10.684	−10.685	−50.800
CH_3CH_2OH	−8.950	−8.986	−8.905	−8.915	−8.914	−56.100
$(CH_3)_2O$	−9.496	−9.321	−9.335	−9.328	−9.327	−44.000
C_2H_4S (thiooxirane)	−12.051	−11.729	−11.756	−11.755	−11.757	19.600
$(CH_3)_2S{=}O$	−14.602	−14.659	−14.674	−14.670	−14.673	−36.200
CH_3CH_2SH	−9.535	−9.440	−9.472	−9.475	−9.479	−11.100
$(CH_3)_2S$	−10.462	−10.353	−10.389	−10.391	−10.394	−8.900
$H_2C{=}CHF$	−9.933	−9.219	−9.269	−9.273	−9.275	−34.000
CH_3CH_2Cl	−9.487	−9.445	−9.455	−9.453	−9.456	−26.600
$H_2C{=}CHCl$	−9.190	−9.156	−9.167	−9.167	−9.170	5.200
$H_2C{=}CHCN$	−7.416	−7.415	−7.245	−7.230	−7.232	43.200

TABLE S7: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
$(CH_3)_2C{=}O$	−15.641	−14.658	−14.762	−14.735	−14.739	−51.700
CH_3CO_2H	−13.863	−13.890	−13.874	−13.888	−13.887	−103.400
CH_3CFO	−14.454	−13.257	−13.327	−13.326	−13.328	−105.700
CH_3COCl	−15.720	−15.235	−15.270	−15.262	−15.265	−57.700
$CH_3CH_2CH_2Cl$	−13.337	−13.040	−13.230	−13.237	−13.238	−31.500
$(CH_3)_2CHOH$	−13.430	−12.970	−13.003	−12.987	−12.991	−65.200
$CH_3{-}O{-}CH_2CH_3$	−13.506	−13.975	−13.929	−13.908	−13.912	−51.700
$(CH_3)_3N$	−11.262	−11.245	−11.184	−11.185	−11.183	−6.600
C_4H_4O (furan)	−20.579	−20.551	−20.502	−20.487	−20.485	−8.300
C_4H_4S (thiophene)	−21.690	−20.917	−21.033	−21.008	−21.014	27.500
C_4H_5N (pyrrole)	−19.701	−20.117	−19.959	−19.943	−19.941	25.900
C_5H_5N (pyridine)	−24.369	−23.835	−23.955	−23.969	−23.971	33.600
H_2	2.028	2.029	2.029	2.029	2.029	0.000
^2SH	−2.655	−2.644	−2.642	−2.642	−2.642	34.200
$^2C{\equiv}CH$	−6.124	−5.936	−5.925	−5.930	−5.931	135.800
$HC{=}CH_2$ ($^2A'$)	−10.912	−10.695	−10.714	−10.717	−10.718	71.000
$CH_3C{=}O$ ($^2A'$)	−13.737	−13.048	−13.108	−13.101	−13.103	−2.400
$CH_2{-}OH$ (^2A)	−9.325	−9.178	−9.253	−9.252	−9.253	−4.000
CH_3O ($^2A'$)	−11.005	−10.776	−10.850	−10.853	−10.854	5.200
CH_3CH_2O ($^2A''$)	−16.205	−15.997	−15.989	−15.991	−15.994	−2.900
CH_3S ($^2A'$)	−8.501	−8.530	−8.573	−8.567	−8.568	29.800
CH_2CH_3 ($^2A'$)	−12.247	−12.013	−12.056	−12.054	−12.055	28.600
$(CH_3)_2CH$ ($^2A'$)	−17.401	−16.878	−16.930	−16.919	−16.922	21.100
$^2C(CH_3)_3$	−21.350	−20.652	−20.729	−20.713	−20.717	12.000
NO_2 ($^2A_1$)	−16.132	−15.899	−15.887	−15.895	−15.894	8.100
$CH_3CH{=}C{=}CH_2$	−16.337	−16.865	−16.831	−16.811	−16.810	38.800
C_5H_8 (isoprene)	−17.932	−18.672	−18.581	−18.545	−18.552	18.000
C_5H_{10} (cyclopentane twist)	−19.139	−18.491	−18.426	−18.392	−18.399	−18.500
C_5H_{12} (n-pentane)	−18.865	−19.068	−18.732	−18.778	−18.787	−35.000
$C(CH_3)_4$ (neopentane)	−18.711	−17.749	−17.851	−17.812	−17.819	−40.100
C_6H_8 (1,3-cyclohexadiene)	−22.365	−21.736	−22.119	−22.136	−22.138	25.400
C_6H_8 (1,4-cyclohexadiene)	−21.683	−21.103	−21.473	−21.488	−21.490	25.000
C_6H_{12} (cyclohexane chair)	−21.938	−21.349	−21.740	−21.736	−21.737	−29.400
C_6H_{14} (n-hexane)	−23.850	−22.151	−22.539	−22.555	−22.546	−39.900
C_6H_{14} (3-methylpentane)	−21.530	−21.750	−21.346	−21.404	−21.413	−41.100
$C_6H_5{-}CH_3$ (toluene)	−32.438	−30.300	−30.764	−30.749	−30.762	12.000
C_7H_{16} (n-heptane)	−28.906	−26.903	−26.410	−26.281	−26.297	−44.800
C_8H_8 (cyclooctatetraene)	−27.654	−28.772	−28.704	−28.665	−28.662	70.700
C_8H_{18} (n-octane)	−32.939	−30.649	−30.088	−29.940	−29.958	−49.800
$C_{10}H_8$ (naphtalene)	−46.233	−47.179	−46.792	−46.666	−46.684	35.900
$C_{10}H_8$ (azulene)	−44.786	−47.562	−47.172	−47.075	−47.068	69.100
$CH_3CO_2CH_3$ (Z-methylacetate)	−16.670	−17.701	−17.854	−17.820	−17.823	−98.400
$(CH_3)_3COH$ (t-butanol)	−17.023	−16.390	−16.444	−16.421	−16.426	−74.700
$C_6H_5NH_2$ (aniline)	−29.052	−30.126	−29.892	−29.962	−29.971	20.800
C_6H_5OH (phenol)	−29.430	−30.673	−30.670	−30.624	−30.633	−22.300
C_4H_6O (divinyl ether)	−18.992	−18.591	−18.454	−18.458	−18.455	−3.300
C_4H_8O (tetrahydrofuran)	−16.668	−16.636	−16.598	−16.581	−16.579	−44.000
C_5H_8O (cyclopentanone)	−24.120	−23.020	−22.902	−22.867	−22.864	−45.900
$C_6H_4O_2$ (benzoquinone)	−29.711	−28.197	−28.561	−28.561	−28.565	−29.400
$C_6H_4N_2$ (pyrimidine)	−23.102	−22.431	−22.550	−22.561	−22.564	46.800
$(CH_3)_2SO_2$	−17.958	−18.721	−18.701	−18.693	−18.694	−89.200
C_6H_5Cl (chlorobenzene)	−28.921	−29.749	−29.661	−29.663	−29.661	12.500
$NC(CH_2)_2CN$ (succinonitrile)	−9.872	−9.927	−9.846	−9.830	−9.827	50.100
$C_4H_4N_2$ (pyrazine)	−18.106	−18.591	−18.505	−18.518	−18.523	46.900
C_4H_4O (3-butyn-2-one)	−13.242	−13.411	−13.307	−13.273	−13.278	15.600
C_4H_6O (E-crotonaldehyde)	−18.516	−19.468	−19.535	−19.495	−19.502	−24.000
$C_4H_6O_3$ (acetic anhydride)	−27.857	−27.381	−27.228	−27.245	−27.243	−136.800
C_4H_6S (2,5-dihydrothiophene)	−18.552	−17.955	−17.891	−17.866	−17.872	20.800
$(CH_3)_2CHCN$	−11.123	−10.861	−10.860	−10.840	−10.844	5.600
C_4H_8O (methyl ethyl ketone)	−17.797	−18.408	−18.341	−18.377	−18.383	−57.100
$(CH_3)_2CHCHO$	−16.930	−15.781	−15.836	−15.810	−15.814	−51.600
$C_4H_8O_2$ (1,4-dioxane)	−19.727	−19.599	−19.581	−19.592	−19.593	−75.500

TABLE S7: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
C_4H_8S (tetrahydrothiophene)	−17.419	−16.710	−16.804	−16.780	−16.787	−8.200
$(CH_3)_3CCl$	−17.399	−16.669	−16.761	−16.738	−16.744	−43.500
C_4H_9Cl (n-butyl chloride)	−16.496	−16.062	−16.269	−16.309	−16.307	−37.000
C_4H_9N (tetrahydropyrrole)	−15.565	−15.394	−15.264	−15.249	−15.247	−0.800
$C_4H_9NO_2$ (2-nitrobutane)	−27.976	−27.565	−27.343	−27.358	−27.363	−39.100
$(CH_3CH_2)_2O$	−18.156	−17.580	−17.480	−17.479	−17.476	−60.300
$CH_3CH(OCH_3)_2$ (dimethyl acetal)	−18.945	−19.488	−19.613	−19.583	−19.588	−93.100
$(CH_3)_3CSH$	−16.763	−16.568	−16.636	−16.642	−16.648	−26.200
$C_4H_{10}S_2$ (diethyl disulfide)	−19.953	−20.077	−20.340	−20.332	−20.340	−17.900
$(CH_3)_3CNH_2$	−15.395	−14.825	−14.833	−14.822	−14.827	−28.900
$(CH_3)_4Si$	−15.603	−15.184	−15.417	−15.409	−15.410	−55.700
C_5H_6S (2-methyl thiophene)	−25.352	−24.699	−24.985	−25.039	−25.035	20.000
C_5H_7N (N-methyl pyrrole)	−22.474	−23.672	−23.495	−23.463	−23.470	24.600
$C_5H_{10}O$ (tetrahydropyran)	−20.624	−20.126	−20.497	−20.508	−20.509	−53.400
$(CH_3CH_2)_2C{=}O$	−22.749	−23.020	−22.767	−22.815	−22.823	−61.600
$C_5H_{10}O_2$ (isopropyl acetate)	−27.479	−25.787	−25.673	−25.654	−25.650	−115.100
$C_5H_{10}S$ (tetrahydrothiopyran)	−20.259	−20.351	−20.664	−20.667	−20.668	−15.200
$C_5H_{11}N$ (piperidine)	−18.836	−18.154	−18.460	−18.472	−18.473	−11.300
$C_5H_{12}O$ (t-butyl methyl ether)	−19.728	−20.519	−20.385	−20.345	−20.352	−67.800
$C_6H_4F_2$ (1,3-difluorobenzene)	−34.711	−33.265	−33.505	−33.512	−33.515	−73.900
$C_6H_4F_2$ (1,4-difluorobenzene)	−32.958	−32.758	−33.203	−33.215	−33.218	−73.300
C_6H_5F (fluorobenzene)	−30.891	−29.836	−30.150	−30.162	−30.164	−27.400
$C_6H_{14}O$ (diisopropyl ether)	−25.654	−24.718	−24.591	−24.590	−24.584	−76.300
PF_5	−7.831	−6.654	−6.461	−6.459	−6.460	−381.100
SF_6	−21.917	−20.606	−20.366	−20.368	−20.368	−291.700
P_4	−6.412	−6.389	−6.383	−6.383	−6.382	14.100
SO_3	−14.471	−13.865	−14.032	−14.029	−14.030	−94.600
SCl_2	−6.672	−6.660	−6.651	−6.650	−6.652	−4.200
$POCl_3$	−11.319	−11.076	−11.136	−11.138	−11.141	−133.800
PCl_5	−16.303	−16.352	−16.307	−16.310	−16.313	−86.100
Cl_2O_2S	−17.897	−17.415	−17.566	−17.570	−17.572	−84.800
PCl_3	−8.051	−8.022	−8.003	−8.003	−8.006	−69.000
Cl_2S_2	−16.542	−16.586	−16.575	−16.575	−16.578	−4.000
$SiCl_2$ ($^1A_1$)	−4.590	−4.574	−4.559	−4.560	−4.562	−40.300
CF_3Cl	−15.007	−14.240	−14.349	−14.341	−14.342	−169.700
C_2F_6	−21.225	−23.475	−23.468	−23.462	−23.465	−320.900
$^2CF_3$	−15.050	−15.881	−15.942	−15.942	−15.942	−111.800
$^2C_6H_5$ (phenyl radical)	−32.016	−31.408	−31.758	−31.775	−31.778	80.500
M.D.	−12.601	−12.476	−12.491	−12.488	−12.489	
M.A.D.	13.011	12.882	12.900	12.895	12.897	

TABLE S8: regSCAN bond lengths [Å] obtained with different grid qualities.

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
H_2	0.001	0.001	0.001	0.001	0.001	0.741
Li_2	0.083	0.081	0.081	0.081	0.081	2.673
LiH	0.006	0.006	0.006	0.006	0.006	1.595
LiF	0.006	0.006	0.006	0.006	0.006	1.564
LiCl	0.004	0.005	0.005	0.005	0.005	2.021
LiO	0.005	0.005	0.005	0.005	0.005	1.688
Be_2	0.029	0.029	0.029	0.029	0.029	2.440
BeH	0.012	0.012	0.012	0.012	0.012	1.343
BeF	0.011	0.011	0.011	0.011	0.011	1.361
BeO	0.002	0.002	0.001	0.001	0.001	1.331
BeS	0.006	0.005	0.006	0.006	0.006	1.742
B_2	0.023	0.024	0.024	0.024	0.024	1.590
BH	0.009	0.009	0.009	0.009	0.009	1.232
BF	0.002	0.002	0.002	0.002	0.002	1.263
BF_3	−0.001	−0.001	−0.001	−0.001	−0.001	1.313
BCl	0.008	0.007	0.007	0.007	0.007	1.715
BCl_3	−0.002	−0.002	−0.002	−0.002	−0.002	1.742
BN	0.038	0.038	0.038	0.038	0.038	1.281
BO	0.001	0.001	0.001	0.001	0.001	1.204
BS	0.001	0.001	0.001	0.001	0.001	1.609
C_2	0.006	0.006	0.006	0.006	0.006	1.242
CH	0.005	0.005	0.005	0.005	0.005	1.120
CH_4	0.000	0.000	0.000	0.000	0.000	1.087
CF	0.003	0.003	0.003	0.003	0.003	1.272
CF_4	−0.001	−0.001	−0.001	−0.001	−0.001	1.323
CCl	0.006	0.006	0.006	0.006	0.006	1.645
CCl_4	0.006	0.006	0.006	0.006	0.006	1.767
CN	−0.009	−0.009	−0.009	−0.009	−0.009	1.172
CO	−0.002	−0.002	−0.002	−0.002	−0.002	1.128
CO^+	−0.004	−0.004	−0.004	−0.004	−0.004	1.115
CO_2	0.000	0.000	0.000	0.000	0.000	1.160
CP	−0.009	−0.009	−0.009	−0.009	−0.009	1.562
CS	−0.000	−0.001	−0.001	−0.001	−0.001	1.535
CS_2	−0.002	−0.002	−0.002	−0.002	−0.002	1.553
N_2	−0.006	−0.006	−0.006	−0.006	−0.006	1.098
N_2^+	−0.011	−0.011	−0.011	−0.011	−0.011	1.116
NH	0.004	0.003	0.003	0.004	0.004	1.036
NH^+	0.007	0.007	0.007	0.007	0.007	1.070
NF	−0.001	−0.002	−0.002	−0.002	−0.002	1.317
NCl	0.000	0.001	0.001	0.001	0.001	1.611
NO	−0.004	−0.005	−0.005	−0.005	−0.005	1.151
NO^+	−0.005	−0.005	−0.005	−0.005	−0.005	1.063
NS	−0.001	−0.002	−0.002	−0.002	−0.002	1.494
O_2	−0.003	−0.003	−0.003	−0.003	−0.003	1.208
O_2^+	−0.008	−0.008	−0.008	−0.008	−0.008	1.116
OH	0.002	0.002	0.002	0.002	0.002	0.970
OH^+	0.005	0.005	0.005	0.005	0.005	1.029
OF	−0.011	−0.011	−0.011	−0.011	−0.011	1.358
F_2	−0.016	−0.017	−0.017	−0.017	−0.017	1.412
F_2^+	−0.028	−0.027	−0.027	−0.027	−0.027	1.322
HF	0.003	0.003	0.003	0.003	0.003	0.917
HF^+	0.008	0.008	0.008	0.008	0.008	1.001
Na_2	0.051	0.051	0.051	0.051	0.051	3.079
NaH	0.004	0.005	0.006	0.005	0.005	1.887
NaF	−0.002	−0.002	−0.002	−0.002	−0.002	1.926
NaCl	0.000	0.000	0.000	0.000	0.000	2.361
NaO	−0.000	0.000	0.000	0.000	0.000	2.052
MgH	0.011	0.012	0.012	0.012	0.012	1.730
MgF	0.013	0.014	0.014	0.014	0.014	1.750
MgCl	0.014	0.014	0.014	0.014	0.014	2.196
MgO	−0.014	−0.015	−0.015	−0.015	−0.015	1.748

TABLE S8: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
Al_2	−0.000	−0.000	−0.000	−0.000	−0.000	2.466
AlH	0.014	0.014	0.013	0.013	0.013	1.648
AlF	0.008	0.008	0.008	0.008	0.008	1.654
AlCl	0.014	0.014	0.014	0.014	0.014	2.130
AlO	−0.002	−0.002	−0.002	−0.002	−0.002	1.618
AlS	−0.000	−0.000	−0.000	−0.000	−0.000	2.029
Si_2	−0.097	−0.097	−0.097	−0.097	−0.097	2.246
SiH	0.008	0.008	0.008	0.008	0.008	1.520
SiH_4	0.002	0.001	0.001	0.001	0.001	1.480
SiF	0.010	0.010	0.010	0.010	0.010	1.601
SiF_4	0.009	0.009	0.009	0.009	0.009	1.553
SiCl	0.010	0.010	0.010	0.010	0.010	2.058
$SiCl_4$	0.005	0.005	0.005	0.005	0.005	2.019
SiN	−0.005	−0.005	−0.005	−0.005	−0.005	1.572
SiO	0.004	0.004	0.004	0.004	0.004	1.510
SiS	0.007	0.007	0.007	0.007	0.007	1.929
P_2	−0.003	−0.003	−0.003	−0.003	−0.003	1.893
P_4	−0.019	−0.019	−0.019	−0.019	−0.019	2.210
PH	0.004	0.004	0.004	0.004	0.004	1.421
PF	0.006	0.007	0.007	0.007	0.007	1.589
PCl	0.002	0.002	0.002	0.002	0.002	2.015
PN	−0.005	−0.005	−0.005	−0.005	−0.005	1.491
PO	0.004	0.004	0.004	0.004	0.004	1.476
S_2	0.006	0.006	0.006	0.006	0.006	1.889
SH	0.003	0.003	0.003	0.003	0.003	1.341
SF	0.001	0.001	0.001	0.001	0.001	1.601
SF_6	0.011	0.011	0.011	0.011	0.011	1.561
SO	0.007	0.007	0.007	0.007	0.007	1.481
SO_3	0.007	0.007	0.007	0.007	0.007	1.420
Cl_2	0.006	0.006	0.006	0.006	0.006	1.988
Cl_2^+	0.006	0.006	0.006	0.006	0.006	1.891
HCl	0.003	0.003	0.003	0.003	0.003	1.275
HCl^+	0.006	0.006	0.006	0.006	0.006	1.315
ClF	0.005	0.005	0.005	0.005	0.005	1.628
ClO	0.001	0.001	0.001	0.001	0.001	1.570
M.D.	0.003	0.003	0.003	0.003	0.003	
M.A.D.	0.009	0.009	0.009	0.009	0.009	

TABLE S9: regSCAN harmonic vibrational frequencies [cm^{-1}] obtained with different grid qualities.

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
H_2	33.380	27.950	28.730	28.620	28.620	4401.200
Li_2	−16.910	−17.620	−17.440	−17.590	−17.500	351.400
LiH	−4.960	−8.380	−5.420	−5.030	−5.120	1405.700
LiF	−17.520	−6.690	−4.710	−4.390	−4.440	910.600
LiCl	7.750	0.160	1.280	1.130	1.140	643.000
LiO	6.000	−0.770	−1.520	−1.800	−1.750	814.600
LiNa	−8.540	−8.970	−9.560	−9.480	−9.450	256.800
Be_2	72.910	70.880	71.890	71.750	71.740	267.900
BeH	−45.610	−39.930	−42.760	−42.850	−43.160	2060.800
BeH^+	−21.400	−13.720	−18.550	−16.150	−16.250	2221.700
BeF	−10.560	−17.830	−18.240	−17.870	−17.910	1247.400
BeCl	−27.540	−24.320	−24.570	−24.780	−24.740	846.700
BeO	28.440	26.190	27.110	27.130	27.070	1487.300
BeS	14.150	11.190	11.340	11.550	11.590	997.900
B_2	−28.210	−27.000	−32.670	−31.030	−31.260	1051.300
BH	−48.450	−55.270	−61.210	−59.700	−59.720	2366.900
BF	6.150	1.210	1.160	1.230	1.260	1402.100
BCl	−15.710	−12.920	−12.760	−12.660	−12.610	840.300
BN	62.830	61.570	61.230	61.270	61.210	1514.600
BO	11.930	15.910	15.840	15.890	15.900	1885.700
BS	19.050	17.680	17.740	17.730	17.710	1180.200
C_2	38.880	40.300	42.940	42.800	42.550	1854.700
CH	−44.450	−43.580	−42.950	−45.910	−46.110	2858.500
CF	−13.040	−3.560	−3.080	−3.060	−3.050	1308.100
CN	93.920	89.230	87.550	87.840	87.950	2068.600
CO	28.180	30.410	30.270	30.260	30.170	2169.800
CO^+	68.880	69.850	71.030	70.760	70.660	2214.200
CP	48.130	49.130	52.310	51.130	50.880	1239.700
CS	21.490	19.480	19.810	19.800	19.790	1285.200
N_2	77.600	73.190	77.720	77.760	77.720	2358.600
N_2^+	119.940	128.170	125.580	125.490	125.660	2207.000
NH	−3.610	−20.090	−11.710	−16.000	−16.030	3282.300
NF	4.580	22.190	32.000	31.860	25.630	1141.400
NCl	13.800	15.430	16.090	15.820	15.790	828.000
NO	59.160	60.810	60.890	60.870	60.870	1904.200
NO^+	86.160	84.050	84.330	84.360	84.350	2376.400
NS	40.060	39.220	38.660	38.860	38.870	1218.700
O_2	56.640	52.860	52.380	52.430	52.020	1580.200
O_2^+	130.220	127.520	126.390	126.360	126.350	1904.800
OH	−4.300	−6.250	−6.220	−5.940	−5.910	3737.800
OH^+	−48.090	−46.210	−45.510	−46.000	−45.960	3113.400
F_2	136.720	133.520	134.070	133.940	133.930	916.600
F_2^+	149.370	150.510	151.470	150.950	151.550	1073.300
HF	−30.570	−32.240	−32.380	−32.150	−32.160	4138.300
HF^+	−87.910	−59.770	−64.970	−64.440	−64.480	3090.500
Na_2	−3.120	−3.430	−3.420	−3.470	−3.460	159.100
NaH	13.210	−4.490	−1.790	−3.460	−3.330	1172.200
NaF	−4.330	3.760	3.350	3.160	3.270	535.700
NaO	0.520	−3.880	−3.600	−3.770	−3.820	492.300
MgH	−52.610	−28.000	−27.000	−26.420	−26.530	1495.200
MgH^+	48.830	27.600	20.650	19.590	19.820	1699.100
MgO	58.300	63.470	56.370	56.850	56.720	784.800
MgS	24.380	24.060	24.120	24.210	24.180	528.700
Al_2	6.420	7.300	6.930	6.920	7.030	350.000
AlH	−73.990	−36.500	−39.000	−38.760	−38.660	1682.600
AlF	−8.660	−13.870	−14.200	−13.940	−14.020	802.300
AlCl	−6.560	−6.910	−6.840	−6.870	−6.860	481.300
AlO	22.660	21.640	20.380	20.310	20.360	979.200
AlS	16.390	16.310	16.340	16.310	16.310	617.100
Si_2	54.740	54.930	54.410	54.700	54.620	511.000
SiH	−56.970	−23.410	−14.590	−16.160	−15.600	2041.800

TABLE S9: (continued)

System	Coarse	Medium	Fine	XFine	Huge	Exptl.
SiH^+	−75.440	−49.810	−36.330	−39.390	−39.520	2157.200
SiF	−10.400	−9.230	−8.530	−8.180	−8.240	857.200
SiCl	−5.280	−5.220	−5.190	−5.210	−5.220	535.600
SiN	28.650	39.160	35.300	34.250	34.250	1151.400
SiO	8.960	8.580	6.220	6.490	6.460	1241.500
SiS	3.080	3.260	3.180	3.140	3.210	749.600
P_2	31.530	31.920	31.910	32.300	31.910	780.800
P_2^+	34.890	34.790	34.890	34.990	34.840	672.200
PH	−29.150	−7.240	6.070	6.660	7.440	2365.200
PF	1.930	3.130	4.030	4.010	4.020	846.800
PCl	0.650	0.670	0.690	0.690	0.690	551.400
PN	57.200	55.640	56.040	55.960	55.900	1337.200
PO	22.710	22.060	20.900	21.310	21.250	1233.300
S_2	5.480	5.260	5.300	5.530	5.320	725.600
SO	13.390	13.960	13.740	14.000	13.970	1149.200
Cl_2	−1.890	−1.810	−1.850	−1.820	−1.860	559.700
Cl_2^+	4.540	4.780	4.690	4.690	4.690	645.600
HCl	−20.610	−9.080	−13.200	−9.090	−9.040	2990.900
HCl^+	−36.420	−34.970	−29.250	−29.210	−28.790	2673.700
ClF	9.490	6.590	7.140	6.990	6.970	786.100
ClO	25.340	26.310	25.790	26.070	26.030	853.800
M.D.	13.010	14.766	15.088	15.050	14.972	
M.A.D.	34.054	31.424	31.211	31.211	31.132	

TABLE S10: Equilibrium lattice constant [Å] obtained with SCAN, SCAN-L and regSCAN.

System	SCAN	SCAN-L	regSCAN	Exptl.
C	−0.003	0.013	−0.000	3.553
Si	0.007	−0.001	0.014	5.421
Ge	0.025	0.033	0.040	5.644
Sn	0.063	0.081	0.097	6.477
SiC	0.005	0.009	0.002	4.346
BN	0.014	0.022	0.012	3.592
BP	0.000	0.010	0.004	4.525
AlN	−0.008	−0.004	−0.008	4.368
AlP	0.015	−0.003	0.016	5.451
AlAs	0.022	0.014	0.026	5.649
GaN	−0.014	−0.008	−0.017	4.520
GaP	0.008	0.004	0.012	5.439
GaAs	0.018	0.042	0.032	5.640
InP	0.034	0.043	0.044	5.858
InAs	0.047	0.081	0.063	6.047
InSb	0.061	0.059	0.094	6.468
LiH	0.014	−0.007	0.019	3.979
LiF	0.006	0.010	0.010	3.972
LiCl	0.029	0.014	0.034	5.070
NaF	−0.028	−0.007	−0.014	4.582
NaCl	−0.006	−0.018	0.012	5.569
MgO	0.005	0.016	0.010	4.189
Li	0.012	0.023	0.023	3.443
Na	−0.018	−0.076	0.016	4.214
K	0.093	0.044	0.153	5.212
Rb	0.133	0.026	0.180	5.577
Cs	0.183	0.068	0.229	6.039
Ca	−0.011	−0.083	0.021	5.556
Ba	0.032	0.022	0.092	5.002
Sr	0.042	0.005	0.068	6.040
Al	−0.011	−0.009	−0.023	4.018
Fe	0.003	−0.046	0.005	2.853
Co	−0.018	−0.023	−0.017	3.524
Ni	−0.049	−0.016	−0.034	3.508
Sc	0.002	−0.008	0.004	3.270
Y	0.019	0.006	0.018	3.594
Ti	−0.018	−0.017	−0.017	2.915
Zr	0.014	0.013	0.011	3.198
Hf	−0.029	0.009	0.003	3.151
V	−0.048	−0.038	−0.043	3.021
Nb	0.002	0.013	0.004	3.294
Ta	−0.027	−0.001	0.001	3.299
Mo	0.004	0.010	0.008	3.141
W	−0.011	0.007	0.006	3.160
Tc	−0.005	0.006	0.001	2.716
Re	0.007	0.017	0.004	2.744
Ru	−0.006	0.010	0.002	2.669
Os	−0.013	0.011	0.007	2.699
Rh	−0.008	0.014	0.004	3.794
Ir	−0.017	0.024	0.013	3.831
Pd	0.020	0.042	0.030	3.876
Pt	−0.000	0.044	0.030	3.913
Cu	−0.032	−0.030	−0.029	3.595
Ag	0.019	0.039	0.036	4.062
Au	0.024	0.057	0.059	4.062
M.D.	0.011	0.010	0.025	
M.A.D.	0.025	0.025	0.032	

TABLE S11: Bulk modulus [GPa] obtained with SCAN, SCAN-L and regSCAN.

System	SCAN	SCAN-L	regSCAN	Exptl.
C	3.095	−12.590	0.797	454.700
Si	−1.649	−2.971	−4.184	101.300
Ge	−7.384	−2.898	−8.590	79.400
Sn	−3.639	−2.893	−1.406	42.800
SiC	−2.307	−11.859	−0.600	229.100
BN	−17.216	−28.842	−15.251	410.200
BP	5.549	−3.225	2.745	168.000
AlN	6.816	2.565	6.617	206.000
AlP	3.973	2.509	3.523	87.400
AlAs	1.507	0.979	0.911	75.000
GaN	−17.826	−34.448	−17.016	213.000
GaP	−0.902	−2.989	−1.676	89.600
GaAs	−3.392	−8.304	−4.474	76.700
InP	−3.161	−7.370	−3.608	72.000
InAs	−0.751	−6.168	−1.429	58.600
InSb	−2.488	−4.066	−3.227	46.100
LiH	−5.349	−2.002	−5.038	40.100
LiF	−0.237	8.997	−1.668	76.300
LiCl	−3.330	−2.697	−3.778	38.700
NaF	7.085	8.239	3.943	53.100
NaCl	0.702	3.481	−0.024	27.600
MgO	−3.459	−7.187	−5.253	169.800
Li	3.346	1.920	−0.447	13.100
Na	0.888	−2.499	0.717	7.900
K	−0.375	0.969	−0.551	3.800
Rb	−0.897	−0.498	−0.777	3.600
Cs	−0.378	1.087	−0.210	2.300
Ca	1.688	4.106	0.650	15.900
Ba	−2.243	−0.837	−2.690	10.600
Sr	−0.550	−5.657	−1.398	12.000
Al	0.101	8.793	11.253	77.100
Ni	40.355	34.173	25.315	192.500
V	31.583	28.800	27.461	165.800
Nb	3.170	13.324	1.562	173.200
Ta	4.467	−1.736	0.822	202.700
Mo	−0.924	−3.245	−4.724	276.200
W	0.145	−15.241	−7.291	327.500
Rh	15.420	−10.137	5.374	277.100
Ir	46.075	−10.307	14.549	362.200
Pd	5.799	−2.100	−1.790	187.200
Pt	6.222	−34.916	−14.449	285.500
Cu	23.455	24.708	21.888	144.300
Ag	4.706	−5.788	−0.173	105.700
Au	−12.777	−26.790	−26.084	182.000
M.D.	2.839	−2.628	−0.220	
M.A.D.	6.986	9.203	6.044	

TABLE S12: Cohesive energies [eV/atom] obtained with SCAN, SCAN-L and regSCAN.

System	SCAN	SCAN-L	regSCAN	Exptl.
C	−0.002	−0.130	0.073	7.550
Si	0.038	−0.094	0.034	4.680
Ge	0.099	−0.098	0.012	3.890
Sn	0.240	0.044	0.091	3.160
SiC	−0.018	−0.194	0.036	6.480
BN	0.084	0.023	0.136	6.760
BP	0.184	0.036	0.195	5.140
AlN	−0.030	−0.108	0.019	5.850
AlP	−0.052	−0.164	−0.033	4.320
AlAs	0.082	−0.115	0.085	3.820
GaN	−0.116	−0.199	−0.067	4.550
GaP	0.052	−0.116	0.056	3.610
GaAs	0.025	−0.215	−0.001	3.340
InP	−0.197	−0.365	−0.168	3.470
InAs	−0.030	−0.254	−0.022	3.080
InSb	0.008	−0.130	−0.052	2.810
LiH	−0.057	−0.070	−0.039	2.490
LiF	−0.076	−0.178	−0.023	4.460
LiCl	−0.069	−0.161	−0.057	3.590
NaF	−0.054	−0.171	−0.022	3.970
NaCl	−0.051	−0.157	−0.055	3.340
MgO	0.041	−0.050	0.092	5.200
Li	−0.104	−0.090	−0.053	1.670
Na	−0.053	−0.104	−0.045	1.120
K	−0.076	−0.145	−0.038	0.940
Rb	−0.102	−0.183	−0.054	0.860
Cs	−0.141	−0.193	−0.074	0.810
Ca	0.042	0.108	0.087	1.870
Ba	−0.293	−0.229	−0.051	1.910
Sr	0.072	−0.020	0.090	1.730
Al	0.169	0.077	0.187	3.430
Fe	0.328	0.227	0.416	4.300
Co	0.706	−0.048	1.558	4.420
Ni	0.882	0.971	1.133	4.480
Sc	0.055	−0.065	0.033	3.930
Y	−0.303	−0.506	−0.354	4.390
Ti	0.060	0.191	0.147	4.880
Zr	−1.805	−1.000	−2.021	6.270
Hf	0.474	−0.553	−0.106	6.460
V	−0.627	1.008	−0.663	5.350
Nb	−1.150	−1.264	−1.191	7.600
Ta	0.794	−0.356	−0.039	8.130
Mo	−0.975	−0.709	−1.242	6.860
W	−0.339	−1.311	−0.100	8.940
Tc	−0.379	−0.266	−0.586	6.880
Re	1.684	−1.020	−0.721	8.050
Ru	−0.457	−0.474	−0.460	6.770
Os	0.533	−0.114	−0.284	8.200
Rh	−0.479	−0.612	−0.328	5.780
Ir	0.330	−0.357	0.053	6.990
Pd	0.360	0.098	0.152	3.930
Pt	−0.086	−0.581	0.653	5.870
Cu	0.418	0.189	0.379	3.510
Ag	−0.073	−0.287	−0.098	2.960
Au	−0.260	−0.552	−0.431	3.830
M.D.	−0.013	−0.201	−0.068	
M.A.D.	0.295	0.309	0.276	

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