The meta-GGA level screened range-separated hybrid functional by employing short range Hartree-Fock with long range semilocal functional

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TABLE I: Total energies of atoms (hartree) computed using aug-cc-pVQZ basis set. The accurate reference values of each atomic systems are taken from ref. [1, 2].

Atom	Accurate	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
H	-0.500	-0.502	-0.501	-0.500	-0.503	-0.499
He	-2.904	-2.915	-2.895	-2.908	-2.902	-2.910
Li	-7.478	-7.492	-7.466	-7.487	-7.475	-7.490
Be	-14.667	-14.672	-14.636	-14.670	-14.647	-14.674
B	-24.654	-24.664	-24.619	-24.666	-24.632	-24.670
C	-37.845	-37.860	-37.806	-37.863	-37.821	-37.863
N	-54.589	-54.605	-54.545	-54.611	-54.562	-54.605
O	-75.067	-75.099	-75.021	-75.102	-75.040	-75.092
F	-99.734	-99.773	-99.679	-99.769	-99.700	-99.748
Ne	-128.938	-128.977	-128.868	-128.968	-128.890	-128.937
Na	-162.255	-162.298	-162.182	-162.288	-162.205	-162.253
Mg	-200.053	-200.098	-199.967	-200.082	-199.992	-200.042
Al	-242.346	-242.393	-242.254	-242.379	-242.280	-242.327
Si	-289.359	-289.399	-289.256	-289.391	-289.283	-289.327
P	-341.259	-341.288	-341.143	-341.287	-341.171	-341.212
S	-398.110	-398.142	-397.983	-398.139	-398.013	-398.053
Cl	-460.148	-460.178	-460.009	-460.175	-460.039	-460.074
MAE		0.026	0.063	0.022	0.044	0.021

TABLE II: Atomization energies of the G2 test set computed using aug-cc-pVQZ basis set. All quantities are in kcal/mol. CCSD(T) values are taken from ref [3]

Molecule	Name	CCSD(T)	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
$AlCl_3$	Aluminum trichloride	313.454	293.202	304.142	302.176	298.920	314.406
AlF_3	Aluminum trifluoride	432.192	415.208	411.605	412.195	406.825	415.663
BCl_3	Boron trichloride	323.172	312.892	328.359	318.887	321.741	328.278
BF_3	Boron trifluoride	469.403	464.873	466.460	459.390	459.986	459.737
BeH	Berilium monohydride	50.789	58.113	55.985	50.197	55.948	59.035
CCl_4	Tetrachloromethane	313.633	294.972	317.493	305.412	307.687	322.960
CF_4	Tetrafluoromethane	478.081	468.906	478.858	468.327	468.783	473.488
CH	Methylidyne radical	83.869	85.561	83.008	86.609	83.623	86.746
CH_2Cl_2	Dichloromethane	370.105	363.661	372.625	370.492	366.442	375.302
CH_2F_2	Difluoromethane	436.843	435.229	436.739	437.229	430.501	437.080
CH_2O_2	Formic acid	500.306	498.830	500.369	493.422	493.313	491.616
CH_2O	Formaldehyde	373.210	373.530	372.150	371.701	368.032	370.714
CH_2	Singlet carbene	180.619	181.028	176.432	180.619	175.233	180.033
CH_2	Triplet carbene	189.742	192.264	193.716	198.372	192.235	195.453
CH_3Cl	Chloromethane	394.518	392.717	395.368	397.937	390.766	398.126
CH_3	Methyl radical	306.590	310.204	308.517	313.852	306.314	310.930
CH_3O	Hydroxymethyl radical	408.552	411.164	410.924	410.911	405.986	406.028
CH_3O	Methoxy radical	398.894	403.937	403.132	405.078	398.573	400.955
CH_3S	Methylthio radical	381.246	382.346	384.332	386.415	379.841	381.979
CH_4	Methane	418.872	421.224	417.861	424.748	414.689	421.096
CH_4O	Methanol	511.829	511.982	510.089	511.973	504.388	507.297
CH_4S	Thiomethanol	473.495	471.634	472.869	477.136	467.419	475.058
$CHCl_3$	Trichloromethane	343.726	331.733	347.317	340.229	339.399	350.778
CHF_3	Trifluromethane	458.777	453.630	459.068	454.456	450.947	456.693
CHO	Formyl radical	278.282	280.381	280.297	278.037	276.853	277.268
CN	Cyano radical	180.065	178.840	178.247	175.409	175.927	178.971
CNH	Hydrogen cyanide	311.523	312.502	310.083	307.926	306.936	311.384
CNH_3O_2	Methyl nitrite	597.491	598.763	599.394	597.417	589.594	600.172
CNH_3O_2	Nitromethane	599.632	602.577	604.904	600.381	595.005	602.773
CNH_5	Methylamine	580.082	584.793	581.720	585.121	575.592	581.165
C_2Cl_4	Tetrachloroethylene	469.319	451.178	479.107	462.009	466.800	479.017
C_2F_4	Tetrafluroethylene	587.668	584.157	596.684	583.310	584.511	588.466
C_2H	Ethynyl radical	263.659	262.757	266.490	262.267	263.119	261.660
C_2H_2	Acetylene	402.763	403.153	404.139	401.988	399.953	402.015
$C_2H_2O_2$	Glyoxal	632.360	630.604	634.689	625.389	625.829	625.606
C_2H_2O	Ketene	530.603	533.813	537.741	531.309	531.043	530.538
C_2H_3Cl	Vinyl Chloride	541.516	539.705	546.643	544.055	539.583	545.584
C_2H_3	Vinyl radical	443.495	447.689	449.933	450.301	445.269	447.579
$C2H_3F$	Vinyl fluoride	571.223	572.586	575.603	574.272	568.497	573.267
C_2H_3O	Carbonyl methane	579.876	582.681	586.206	582.575	579.056	579.508
C_2H_3OCl	Acetyl chloride	666.141	663.119	672.060	665.272	662.502	667.383
C_2H_3OF	Acetyl fluoride	704.174	702.790	708.625	702.189	698.904	701.127
C_2H_4	Ethylene	561.341	563.715	564.026	566.248	558.549	563.460
$C_2H_4O_2$	Acetic acid	800.868	798.778	804.219	795.331	793.291	792.064
$C_2H_4O_2$	Methyl formate	784.033	782.802	786.502	781.639	775.770	779.339
C_2H_4O	Acetaldehyde	675.005	675.749	678.197	675.912	670.265	672.746
C_2H_4O	Oxirane	648.827	648.389	654.618	653.490	646.021	650.030
C_2H_4S	Thiirane	623.588	619.677	629.933	628.913	621.384	627.489
C_2H_5Cl	Ethyl chloride	690.032	687.116	693.581	694.724	685.145	693.489
C_2H_5	Ethyl radical	601.427	605.718	607.585	611.654	601.652	606.016
C_2H_5O	Ethoxy radical	695.120	695.919	698.855	699.301	690.471	693.688
C_2H_6	Ethane	710.204	712.113	712.371	718.143	705.519	712.034
C_2H_6O	Dimethyl ether	796.040	796.596	797.168	800.651	787.769	795.623
C_2H_6O	Ethanol	808.220	807.325	809.175	809.495	799.634	803.327
C_2H_6OS	Dimethyl sulfoxide	854.413	845.880	852.485	852.760	840.628	850.025
C_2H_6S	Dimethyl sulfide	766.299	763.395	768.400	772.005	759.221	768.416
C_2H_6S	Thioethanol	767.393	764.115	769.258	772.090	759.960	768.727
C_2N_2	Cyanogen	498.280	501.221	502.594	492.144	496.098	500.305

TABLE III: Atomization energies of the G2 test set computed using aug-cc-pVQZ basis set. All quantities are in kcal/mol. CCSD(T) values are taken from ref [3]

Molecule	Name	CCSD(T)	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
C_2NF_3	Trifluroacetonitril	639.494	633.221	643.356	628.465	631.486	636.709
C_2NH_3	Acetonitrile	613.275	615.730	617.186	613.745	610.351	614.196
C_2NH_5	Aziridine	717.130	720.420	726.284	725.154	717.109	722.287
C_2NH_5O	Acetamide	864.915	868.547	872.338	865.155	861.016	862.778
C_2NH_7	Dimethylamine	867.075	871.340	871.603	874.967	861.670	870.369
C_2NH_7	Ethaylamine	875.261	878.751	879.523	881.377	869.545	876.087
C_3H_4	Allene	699.982	704.981	709.655	706.774	701.792	704.232
C_3H_4	Cyclopropene	678.007	679.304	689.130	685.124	680.583	682.053
C_3H_4	Propyne	701.358	702.843	707.787	704.337	699.904	701.435
C_3H_6	Cyclopropane	849.824	850.449	860.044	859.272	849.966	853.668
C_3H_6O	Acetone	975.379	975.183	981.651	977.443	969.802	973.123
C_3H_6	Propene	857.410	859.388	863.671	864.342	854.387	859.575
C_3H_7Cl	1-Chloropropane	983.574	979.160	989.532	989.210	977.252	986.708
C_3H_7	Isopropyl radical	897.482	901.550	907.230	909.774	897.472	902.323
C_3H_8O	Methoxyethane	1092.532	1091.878	1096.215	1098.144	1082.975	1091.623
C_3H_8O	Isopropyl alcohol	1105.317	1102.360	1108.267	1106.745	1094.719	1100.294
C_3H_8	Propane	1003.629	1004.219	1008.352	1012.632	997.659	1005.243
C_3NH_3	Acrylontrile	758.512	761.469	766.395	758.771	757.308	760.737
C_3NH_9	Trimethylamine	1156.873	1159.400	1163.365	1166.420	1149.386	1162.611
C_4H_{10}	Isobutane	1298.551	1296.761	1305.079	1307.566	1290.357	1300.143
C_4H_{10}	n-Butane	1297.126	1296.254	1304.289	1307.093	1289.745	1298.453
C_4H_4O	Furan	990.051	988.793	1006.342	992.032	991.696	990.474
C_4H_4S	Thiophene	959.884	954.121	975.908	962.274	961.478	962.981
C_4H_6	1,3-Butadiene	1007.991	1010.584	1018.587	1014.761	1006.996	1011.609
C_4H_6	2-Butyne	999.002	1001.183	1010.107	1005.471	998.529	999.708
C_4H_6	Bicyclobutane	981.134	979.529	998.760	992.053	985.475	987.505
C_4H_6	Cyclobutene	996.655	995.318	1010.303	1004.075	997.495	999.252
C_4H_6	Methylenecyclopropane	988.022	990.275	1003.777	998.218	991.407	993.245
C_4H_8	Cyclobutane	1145.231	1142.726	1157.149	1154.374	1142.893	1147.500
C_4H_8	Isobutene	1154.236	1154.729	1163.187	1162.111	1149.961	1156.481
C_4H_9	tert-Butyl radical	1194.236	1197.132	1206.877	1207.749	1193.175	1199.450
C_4NH_5	Pyrrole	1067.054	1070.436	1087.746	1073.116	1072.486	1071.863
C_5H_8	Spiropentane	1278.794	1277.914	1300.528	1292.036	1283.538	1285.290
C_5NH_5	Pyridine	1232.274	1236.854	1256.774	1238.723	1239.437	1239.671
C_6H_6	Benzene	1361.588	1362.890	1386.658	1368.504	1368.384	1366.305
Cl_2	Dichlorine	59.073	54.819	58.792	58.400	56.531	65.282
CO	Carbon monoxide	258.877	254.690	254.661	249.394	251.854	251.872
CO_2	Carbon dioxide	388.592	387.229	390.682	380.854	385.210	382.137
COF_2	Carbonyl fluoride	419.501	415.705	422.000	412.298	414.299	414.866
COS	Carbonyl sulfide	334.288	332.011	337.079	330.313	331892	334.300
CS	Carbon monosulfide	170.985	165.664	167.371	165.176	164.873	169.891
CS_2	Carbon disulphide	278.664	275.291	282.292	278.128	277.486	284.925
FCl	Chlorine monofluoride	62.572	60.189	60.176	61.917	57.899	66.998
F_2	Difluorine	38.755	36.916	34.395	39.113	32.179	44.097
F_3Cl	Chlorine trifluoride	128.346	126.029	127.172	132.329	120.509	140.060
HCl	Hydrogen Chloride	107.199	104.859	104.744	106.276	103.607	108.920
HF	Hydrogen fluoride	141.513	139.300	136.814	137.582	135.536	137.245
HOCl	Hypochlorus acid	165.791	162.596	162.203	161.875	158.833	164.158
HO	Hydroxyl radical	106.955	108.307	105.743	105.745	104.782	102.992
HS	Mercapto radical	87.390	87.987	86.525	88.815	85.675	86.932
H_2	Dihydrgen	109.400	110.280	104.301	112.659	104.645	111.769
H_2O_2	Hydrogen peroxide	268.655	267.134	262.887	262.457	258.456	260.590
H_2O	Water	232.565	231.099	227.101	226.927	224.867	224.026
H_2S	Hydrogen sulphide	183.298	181.640	179.444	183.955	177.571	184.373
LiF	Lithium fluoride	139.369	137.167	132.051	133.653	131.248	132.606
LiH	Lithium hydride	57.904	5/.587	52.837	58.930	53.159	58.544
Li_2	Dilithium	24.197	20.893	19.428	22.802	19.427	21.801
Na_2	Disodium	17.101	17.171	15.846	18.621	16.09	18.502

TABLE IV: Atomization energies of the G2 test set computed using aug-cc-pVQZ basis set. All quantities are in kcal/mol. CCSD(T) values are taken from ref [3]

Molecule	Name	CCSD(T)	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
NaCl	Sodium chloride	98.466	92.408	93.233	95.450	92.396	98.813
NF_3	Trifluoroamine	206.212	208.298	209.523	209.636	202.512	218.529
NH_2	Amino radical	181.955	188.202	183.288	186.482	181.972	185.089
NH_3	Ammonia	297.070	301.308	295.236	298.214	292.708	296.254
NH	Imidogen	82.787	88.145	85.303	89.103	84.877	89.148
NO_2	Nitrogen dioxide	227.058	232.132	232.437	228.103	227.241	231.431
NOCl	Nitrosyl chloride	191.468	192.707	191.666	191.834	187.567	200.729
NO	Nitric oxide	152.187	155.495	153.713	150.182	151.113	153.316
N_2	Dinitrogen	227.436	227.445	222.948	219.968	220.728	227.207
N_2H_4	Hydrazine	436.699	444.594	438.495	439.404	433.072	437.764
N_2O	Nitrous oxide	269.474	273.123	272.142	267.847	267.285	274.542
OCl	Monochlorine monoxide	64.532	65.219	65.919	65.888	63.520	65.014
OF_2	Diflourine monoxide	93.772	93.550	90.927	95.662	86.399	101.661
OS	Sulpher monoxide	125.796	124.787	124.583	123.450	121.933	122.416
O_2	Dioxygen	120.545	122.512	122.239	119.475	119.352	120.215
O_2S	Sulpher dioxide	259.766	244.873	245.509	242.371	240.056	245.441
O_3	Ozone	146.819	138.562	135.859	137.995	130.688	142.984
P_2	Diphosphorus	115.951	114.437	109.760	111.021	107.831	118.659
PF_3	Phosphorus trifluoride	365.156	356.327	353.282	353.311	346.720	358.472
PH_2	Phosphino radical	153.970	158.278	152.688	160.081	151.574	158.581
PH_3	Phosphane	241.475	244.201	236.754	247.599	234.807	247.906
S_2	Disulpher	103.112	102.127	105.408	104.785	102.947	103.256
$SiCH_6$	Methylsilane	627.656	625.703	621.001	637.227	615.352	635.468
$SiCl_4$	Silicon tetrachloride	388.483	361.134	380.051	374.291	371.568	391.150
SiF_4	Silicon tetrafluoride	577.546	554.321	552.458	550.756	544.495	556.948
SiH_2	Singlet silylene	153.678	153.585	147.022	156.112	146.174	158.040
SiH_2	Triplet silylene	133.260	133.158	132.205	141.321	131.164	138.881
SiH_3	Silyl radical	228.083	228.539	223.423	237.069	221.988	235.663
SiH_4	Silane	324.589	323.671	315.092	333.551	313.157	335.321
SiO	Silicon monoxide	192.359	186.596	181.364	181.082	178.994	183.946
Si_2H_6	Disilane	535.471	530.474	522.354	548.331	517.857	550.941
Si_2	Disilicon	73.411	69.314	71.365	72.311	69.934	72.577
MAE	–	–	3.599	5.619	5.296	5.335	4.008

TABLE V: Atomization energies (kcal/mol) of the AE6 molecules. The experimental values are taken from [1, 4]. All calculations are done using aug-cc-pVQZ basis set.

Atom	Expt.	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
SiH_4	322.4	323.4	315.0	333.5	313.1	335.3
SiO	192.1	187.1	182.0	181.4	179.6	184.2
S_2	101.7	102.1	105.7	104.8	103.2	103.2
C_3H_4	704.8	703.2	708.1	704.6	700.2	701.6
$C_2H_2O_2$	633.4	631.4	635.8	625.9	626.9	626.0
C_4H_8	1149.0	1142.8	1157.1	1154.4	1142.9	1147.4
MAE	–	2.7	5.8	6.3	6.7	5.7

TABLE VI: Ionization potential for the test set IP13 for the exchange-correlation functional shown in each column using 6-311++G(3df,3pd) basis set. The experimental values are taken from [1, 4]. All quantities are in kcal/mol.

Molecule	Expt	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
C	259.74	266.08	265.57	264.06	265.53	261.54
S	238.34	242.89	239.89	240.79	239.84	240.35
SH	238.36	241.18	238.82	238.57	238.63	236.65
Cl	299.31	301.22	298.86	298.67	298.79	295.86
Cl_2	265.30	262.25	261.18	259.70	261.28	262.95
OH	298.90	282.93	300.57	297.69	300.63	295.58
O	313.67	326.21	319.66	321.62	320.15	322.35
O_2	278.90	289.60	286.30	284.33	286.64	280.21
P	242.80	239.30	242.78	242.66	242.63	240.83
PH	234.10	234.30	237.08	236.97	237.00	234.78
PH_2	226.30	228.72	230.75	230.67	230.70	226.05
S_2	216.00	219.88	221.19	220.20	221.07	217.66
Si	188.05	187.07	189.55	189.71	189.51	188.31
MAE	–	5.29	3.20	3.16	3.24	2.29

TABLE VII: Electron affinity for the test set EA13 for the exchange-correlation functional shown in each column using 6-311++G(3df,3pd) basis set. All quantities are in kcal/mol. The experimental values are taken from [1, 4]

Molecule	Expt	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
C	29.19	31.20	32.34	31.86	31.95	29.29
S	47.91	50.33	47.35	47.19	47.15	44.69
SH	53.84	53.50	51.30	51.03	51.03	51.99
Cl	84.24	84.65	82.51	82.24	82.09	83.81
Cl_2	55.60	64.43	59.21	60.46	59.93	53.72
OH	42.30	40.54	35.34	35.26	35.16	34.69
O	33.77	36.84	30.48	29.85	30.46	25.97
O_2	10.80	11.37	4.72	6.69	5.29	3.65
P	16.92	21.50	17.55	18.02	17.57	17.88
PH	23.20	24.96	21.83	21.51	21.69	19.77
PH_2	29.40	28.48	26.31	25.86	26.04	26.26
S_2	38.50	38.15	35.99	35.86	36.10	33.33
Si	32.33	30.44	33.13	32.34	32.92	31.14
MAE	–	2.22	2.79	2.85	2.87	3.37

TABLE VIII: Proton affinities for the test set PA8 for the exchange-correlation functional shown in each column using 6-311++G(3df,3pd) basis set. All quantities are in kcal/mol. The experimental values are taken from [1, 4]

Molecule	Expt	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
NH_3	211.90	210.99	212.64	213.74	213.10	214.42
H_2O	171.80	170.84	172.48	173.04	172.88	172.95
C_2H_2	156.60	158.67	161.07	162.92	161.51	161.97
SiH_4	156.50	157.53	156.61	159.03	157.65	159.43
PH_3	193.10	193.28	192.97	196.17	193.81	198.39
H_2S	173.70	174.92	175.07	176.88	175.85	177.77
HCl	137.10	138.15	139.15	140.39	139.48	140.84
H_2	105.90	104.53	106.35	108.14	106.62	106.46
MAE	–	1.10	1.25	2.84	1.79	3.20

TABLE IX: FORWARD barrier heights of hydrogen transfer reactions for the HTBH38 test set for the exchange-correlation functional shown in each column using aug-cc-pVQZ basis set. All quantities are in kcal/mol. The experimental values are taken from [1, 4]

	Molecule	Expt	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
1.	$H + HCl \rightarrow H_2 + Cl$	5.70	-1.00	2.72	-3.63	2.66	1.06
2.	$OH + H_2 \rightarrow H_2O + H$	4.90	0.72	0.18	0.41	1.56	0.99
3.	$CH_3 + H_2 \rightarrow CH_4 + H$	12.10	8.78	6.94	8.00	8.23	8.93
4.	$OH + CH_4 \rightarrow H_2O + CH_3$	6.50	2.27	2.01	1.70	3.28	3.62
5.	$H + H_2 \rightarrow H_2 + H$	9.60	4.28	5.66	1.16	6.09	2.04
6.	$OH + NH_3 \rightarrow H_2O + NH_2$	3.00	-2.26	-1.86	-3.63	-0.59	-2.33
7.	$HCl + CH_3 \rightarrow CH_4 + Cl$	1.70	-1.42	-2.26	-2.30	-1.24	3.44
8.	$OH + C_2H_6 \rightarrow H_2O + C_2H_5$	3.20	-0.68	-0.80	-1.26	0.44	0.27
9.	$F + H_2 \rightarrow HF + H$	1.42	-5.69	-4.54	-5.78	-3.52	-6.08
10.	$O + CH_4 \rightarrow OH + CH_3$	13.47	7.32	7.76	7.94	8.83	11.26
11.	$H + PH_3 \rightarrow H_2 + PH_2$	3.10	-1.06	0.38	-4.15	0.65	-0.35
12.	$H + HO \rightarrow H_2 + O$	10.50	4.10	7.11	-0.13	7.27	0.08
13.	$H + H_2S \rightarrow H_2 + HS$	3.50	-0.59	1.05	-3.76	1.33	0.52
14	$O + HCl \rightarrow OH + Cl$	9.57	1.13	2.44	1.22	3.56	7.49
15.	$CH_3 + NH_2 \rightarrow CH_4 + NH$	8.00	6.26	5.23	4.52	6.37	6.51
16.	$C_2H_5 + NH_2 \rightarrow C_2H_6 + NH$	7.50	8.83	7.14	6.45	8.28	7.80
17.	$NH_2 + C_2H_6 \rightarrow NH_3 + C_2H_5$	10.40	8.89	7.48	8.33	8.82	9.97
18.	$NH_2 + CH_4 \rightarrow NH_3 + CH_3$	14.50	11.41	10.05	10.86	11.36	12.91
19.	s-trans cis-$C_5H_8 \rightarrow$ s-trans cis-C_5H_8	38.40	38.81	35.59	36.20	36.71	37.77
	MAE	–	4.20	3.39	5.52	3.07	3.43

TABLE X: BACKWARD barrier heights of hydrogen transfer reactions for the HTBH38 test set for the exchange-correlation functional shown in each column using aug-cc-pVQZ basis set. All quantities are in kcal/mol. The experimental values are taken from [1, 4]

	Molecule	Expt	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
1.	$H + HCl \rightarrow H_2 + Cl$	7.86	3.41	2.38	2.76	3.72	3.94
2.	$OH + H_2 \rightarrow H_2O + H$	21.20	7.91	17.23	8.94	17.08	10.24
3.	$CH_3 + H_2 \rightarrow CH_4 + H$	15.30	5.77	11.88	6.23	11.94	7.30
4.	$OH + CH_4 \rightarrow H_2O + CH_3$	19.60	5.50	14.12	12.00	15.08	14.49
5.	$H + H_2 \rightarrow H_2 + H$	9.60	5.31	5.66	1.16	6.09	2.04
6.	$OH + NH_3 \rightarrow H_2O + NH_2$	12.70	5.25	7.61	5.83	8.81	7.54
7.	$HCl + CH_3 \rightarrow CH_4 + Cl$	7.06	2.30	2.34	2.32	3.53	4.69
8.	$OH + C_2H_6 \rightarrow H_2O + C_2H_5$	19.90	4.10	15.89	13.46	16.78	15.31
9.	$F + H_2 \rightarrow HF + H$	33.40	10.02	28.03	19.13	27.51	19.35
10.	$O + CH_4 \rightarrow OH + CH_3$	7.90	3.29	4.19	2.75	5.27	4.06
11.	$H + PH_3 \rightarrow H_2 + PH_2$	23.20	0.07	20.68	20.95	22.04	22.06
12.	$H + HO \rightarrow H_2 + O$	12.87	6.77	5.73	6.81	7.11	8.92
13.	$H + H_2S \rightarrow H_2 + HS$	16.76	0.72	12.53	13.75	14.09	14.86
14	$O + HCl \rightarrow OH + Cl$	9.36	4.76	3.48	0.67	4.78	1.54
15.	$CH_3 + NH_2 \rightarrow CH_4 + NH$	22.40	5.16	16.59	18.06	17.64	20.75
16.	$C_2H_5 + NH_2 \rightarrow C_2H_6 + NH$	18.30	3.60	13.90	15.56	15.02	17.87
17.	$NH_2 + C_2H_6 \rightarrow NH_3 + C_2H_5$	17.40	1.72	14.71	13.59	15.75	15.13
18.	$NH_2 + CH_4 \rightarrow NH_3 + CH_3$	17.80	4.26	12.69	11.69	13.75	13.89
19.	s-trans cis-$C_5H_8 \rightarrow$ s-trans cis-C_5H_8	38.40	0.41	35.59	36.20	36.71	37.77
	MAE	–	4.23	4.50	6.26	3.58	4.69

TABLE XI: FORWARD barrier heights of non-hydrogen transfer reactions for the NHTBH38/04 test set for the exchange-correlation functional shown in each column using aug-cc-pVQZ basis set. All quantities are in kcal/mol. The experimental values are taken from [1, 4].

	Molecule	Expt	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
1.	$H + N_2O \rightarrow OH + N_2$	17.13	11.39	13.93	9.41	14.42	11.06
2.	$H + HF \rightarrow HF + H$	42.18	30.91	33.64	29.08	34.21	32.18
3.	$H + ClH \rightarrow HCl + H$	18.00	12.75	13.69	9.06	14.25	14.84
4.	$H + FCH_3 \rightarrow HF + CH_3$	30.38	21.58	25.48	19.72	25.57	22.35
5.	$H + F_2 \rightarrow HF + F$	2.27	43.76	47.59	40.31	47.74	44.30
6.	$CH_3 + FCl \rightarrow CH_3F + Cl$	6.75	-1.05	1.47	-1.61	1.82	2.80
7.	$F^- + CH_3F \rightarrow FCH_3 + F^-$	-0.34	-2.21	-1.01	-4.67	-0.22	-5.09
8.	$F^-...CH_3F \rightarrow FCH_3...F^-$	13.38	10.46	11.90	8.19	12.09	8.88
9.	$Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$	3.10	-0.30	1.10	-2.77	1.48	-3.35
10.	$Cl^-...CH_3Cl \rightarrow ClCH_3...Cl^-$	13.41	9.12	11.14	7.21	11.09	7.65
11.	$F^- + CH_3Cl \rightarrow FCH_3 + Cl^-$	-12.54	-14.73	-13.73	-17.25	-13.08	-18.46
12.	$F^-...CH_3Cl \rightarrow FCH_3...Cl^-$	3.44	0.48	1.78	-1.23	1.81	-1.08
13.	$OH^- + CH_3F \rightarrow HOCH_3 + F^-$	-2.44	-4.00	-3.29	-6.56	-2.52	-6.53
14	$OH^-...CH_3F \rightarrow HOCH_3...F^-$	10.96	8.16	9.21	5.64	9.38	6.62
15.	$H + N_2 \rightarrow HN_2$	14.36	7.51	8.53	4.10	9.09	6.23
16.	$H + CO \rightarrow HCO$	3.17	-0.63	0.24	-4.27	0.67	-2.56
17.	$H + C_2H_4 \rightarrow CH_3CH_2$	1.72	-0.18	0.67	-3.93	1.06	-3.58
18.	$CH_3 + C_2H_4 \rightarrow CH_3CH_2CH_2$	6.85	6.05	4.12	4.16	5.24	4.72
19.	$HCN \rightarrow CNH$	48.07	47.39	46.30	47.41	46.55	47.49
	MAE	–	6.12	5.14	8.10	4.75	7.12

TABLE XII: BACKWARD barrier heights of non-hydrogen transfer reactions for the NHTBH38/04 test set for the exchange-correlation functional shown in each column using aug-cc-pVQZ basis set. All quantities are in kcal/mol. The experimental values are taken from [1, 4].

	Molecule	Expt	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
1.	$H + N_2O \rightarrow OH + N_2$	82.27	73.12	69.18	66.70	71.42	66.37
2.	$H + HF \rightarrow HF + H$	42.18	30.91	33.64	29.08	34.21	32.18
3.	$H + ClH \rightarrow HCl + H$	18.00	12.75	13.69	9.06	14.25	14.84
4.	$H + FCH_3 \rightarrow HF + CH_3$	57.02	48.61	49.82	45.83	51.06	47.17
5.	$H + F_2 \rightarrow HF + F$	105.80	145.94	149.45	138.61	150.61	137.39
6.	$CH_3 + FCl \rightarrow CH_3F + Cl$	59.16	51.06	53.51	47.81	53.81	48.25
7.	$F^- + CH_3F \rightarrow FCH_3 + F^-$	-0.34	-2.21	-1.01	-4.67	-0.22	-5.09
8.	$F^-...CH_3F \rightarrow FCH_3...F^-$	13.38	10.46	11.90	8.19	12.09	8.88
9.	$Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$	3.10	-0.30	1.10	-2.77	1.48	-3.35
10.	$Cl^-...CH_3Cl \rightarrow ClCH_3...Cl^-$	13.41	9.12	11.14	7.21	11.09	7.65
11.	$F^- + CH_3Cl \rightarrow FCH_3 + Cl^-$	20.11	18.42	19.68	16.76	20.16	16.70
12.	$F^-...CH_3Cl \rightarrow FCH_3...Cl^-$	29.42	26.42	28.19	25.01	28.26	25.86
13.	$OH^- + CH_3F \rightarrow HOCH_3 + F^-$	17.66	15.91	17.63	12.70	18.35	12.33
14	$OH^-...CH_3F \rightarrow HOCH_3...F^-$	47.20	45.08	48.73	42.72	48.29	41.24
15.	$H + N_2 \rightarrow HN_2$	10.61	10.76	11.54	9.40	11.43	8.01
16.	$H + CO \rightarrow HCO$	22.68	24.54	25.38	23.98	25.19	22.44
17.	$H + C_2H_4 \rightarrow CH_3CH_2$	41.75	41.80	44.19	41.46	44.14	38.96
18.	$CH_3 + C_2H_4 \rightarrow CH_3CH_2CH_2$	32.97	29.48	34.49	29.86	33.60	29.08
19.	$HCN \rightarrow CNH$	32.82	33.52	32.68	32.73	32.81	31.83
	MAE:		5.76	5.25	7.24	4.91	6.92

TABLE XIII: Thermochemistry of π system for the πTC13 test set for functional shown in each column. All quantities are in kcal/mol. The 6-311++G(3df,3pd) basis set is used. The experimental values are taken from [1, 4].

Molecule	Expt	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
E2-E1	-1.40	-2.23	-2.20	-2.58	-1.99	-2.99
E4-E3	-8.80	-2.40	-2.98	-1.38	-2.84	-0.57
E6-E5	-14.30	-5.54	-6.41	-3.93	-6.04	-2.68
P-2	167.81	168.54	170.77	172.06	171.29	172.13
P-4	193.45	198.54	198.25	200.96	199.21	201.24
P-6	209.68	216.32	215.73	218.84	216.79	230.76
P-8	219.67	227.62	226.90	230.31	228.01	239.01
P-10	225.95	235.68	234.83	238.44	236.04	217.41
SB-2	214.46	215.37	216.54	217.24	216.97	231.60
SB-4	226.15	229.77	230.63	231.63	231.15	241.36
SB-6	233.44	239.46	240.09	241.38	240.69	248.29
SB-8	238.16	246.22	246.69	248.23	247.38	248.29
SB-10	240.97	251.29	251.61	253.41	252.42	253.54
MAE	–	5.77	5.89	7.82	6.54	8.17

TABLE XIV: Alkyl Bond Dissociation Energies for the ABDE12 test set for functional shown in each column. All quantities are in kcal/mol. The aug-cc-pVQZ basis set is used. The experimental values are taken from [1, 4].

Molecule	Expt	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
C_2H_6	97.39	91.71	95.29	90.41	92.85	90.17
iPr-CH_3	95.00	84.99	89.16	83.90	86.46	86.79
C_2H_6O	89.79	82.33	85.30	81.57	82.71	83.49
iPr-OCH_3	91.51	79.68	83.07	78.90	80.16	83.65
Et-H	108.92	106.34	104.71	106.45	103.80	105.98
Et-CH_3	95.89	88.27	92.13	87.08	89.61	88.22
Et-OCH_3	95.26	82.09	85.23	81.27	82.55	84.38
Et-OH	100.29	93.34	95.88	92.10	93.25	94.27
tBu-H	103.86	99.59	98.08	99.76	97.10	100.71
tBu-CH_3	93.67	81.64	86.19	80.68	83.24	85.75
tBu-OCH_3	89.27	75.87	79.64	75.26	76.41	82.07
tBu-OH	115.02	90.95	93.92	89.60	90.92	95.13
MAE		9.91	7.26	10.73	9.73	7.93

TABLE XV: Isomerization Energies for the IsoL6 test set for functional shown in each column. All quantities are in kcal/mol. The 6-311++G(3df,3pd) basis set is used. The experimental values are taken from [1, 4].

Molecule	Expt	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
10-	6.82	2.72	5.85	2.50	5.31	2.64
13-	33.52	30.24	31.47	28.68	31.34	29.21
14-	5.30	3.96	5.75	3.40	5.14	3.42
20-	4.66	4.28	5.13	4.25	5.04	3.19
3-	9.77	7.39	11.40	8.22	10.27	8.39
9-	21.66	17.97	18.68	16.15	17.96	20.41
MAE		2.54	1.44	3.10	1.42	2.42

TABLE XVI: Reaction Energies for the HC7 test set for functional shown in each column. All quantities are in kcal/mol. The 6-311++G(3df,3pd) basis set is used. The experimental values are taken from [1, 4].

Molecule	Expt	B3LYP	PBE0	TPSSh	HSE06	DME-sc-TPSSc
E22 - E1	14.34	0.12	24.43	16.50	20.58	16.44
E31 - E1	25.02	2.67	33.42	21.35	28.22	20.98
$(CH_3)_3CC(CH_3)_3 \rightarrow$ n-C_8H_18	1.90	-7.86	-4.54	-5.80	-6.45	3.21
n-C_6H_14 + 4 $CH_4 \rightarrow 5C_2H_6$	9.81	4.64	5.85	4.36	5.15	9.11
n-C_8H_18 + 6 $CH_4 \rightarrow 7C_2H_6$	14.84	6.86	8.67	6.44	7.63	13.64
adamantane $\rightarrow$ 3 C_2H_4 + 2 C_2H_2	193.99	164.78	215.80	185.27	201.95	187.98
biclo[2.2.2]octane $\rightarrow$ 3 C_2H_4 + C_2H_2	127.22	104.36	140.87	119.13	131.04	120.04
MAE		15.93	10.07	6.31	5.92	3.21