

Name dmc error(dmc) b3lyp lda m06 pbe

H2 -1.175167745 3.607893017e-05 -1.17594931 -1.13356652 -1.16709894 -1.16252620
0.009878

Al -1.936573844 5.041507623e-05 -1.94305855 -1.92199913 -1.93546968 -1.94072762 N/A

Mg -0.8188014595 3.569799429e-05 -0.82435466 -0.81234988 -0.83436481 -0.82105215 N/A

Mg2Al2 -5.643229551 0.0001180233441 -5.63864436 -5.63509989 -5.61984618 -5.66418262
0.002645

Mg3Al3 -8.511870899 0.0002975291007 -8.49491384 -8.50626746 -8.47204974 -8.54732940
0.004972

Mg4Al4 -11.45430699 0.0001271540904 -11.41078482 -11.45444056 -11.41786060 -
11.49962029 0.008683

Mg5Al5 -14.309331 0.0001529518671 -14.25459146 -14.31211855 -14.25365247 -14.36836383
0.010716

Mg6Al6 -17.20794712 0.0002302955374 -17.13219290 -17.21464710 -17.15227852 -
17.27691056 0.013201

Mg7Al7 -20.13423612 0.0002788854436 -20.03596121 -20.14312086 -20.07041278 -
20.21307406 0.015858

Mg8Al8 -23.10143083 0.0002959700883 -22.96852220 -23.10841666 -23.03148322 -
23.18221665 0.019553

Mg9Al9 -25.9588011 0.0003198097782 -25.81263116 -25.96903553 -25.87621267 -26.05359733
0.021500

Mg2Al2H10 -11.70442006 0.0001558506797 -11.72059263 -11.49281080 -11.67624450 -
11.63771259 0.070446

Mg3Al3H15 -17.62576114 0.0001989188274 -17.63782416 -17.31593287 -17.58097108 -
17.51998253 0.109739

Mg4Al4H20 -23.53381225 0.0002421743943 -23.55191309 -23.12614525 -23.47778703 -
23.39744377 0.146183

Mg5Al5H25 -29.42615404 0.0002527830997 -29.44618157 -28.91753634 -29.36436584 -
29.24667208 0.181356

Mg6Al6H30 -35.33568174 0.0003196582082 -35.35067764 -34.71899728 -35.25669806 -
35.11953802 0.217487

Mg7Al7H35 -41.21780959 0.0004246553726 -41.24346988 -40.49089863 -41.12746051 -
40.96296105 0.252072

Mg8Al8H40	-47.13296989	0.001099958153	-47.14770033	-46.30533887	-47.02534167	-46.83513359	0.292323
Mg9Al9H45	-53.0830052	0.0006158467245	-53.09831337	-52.13345990	-52.96790268	-52.73812671	0.329586
Mg1Al2	-4.78093871	0.0001049179828	-4.77803560	N/A	N/A	N/A	0.001874
Mg2Al4	-9.687129972	0.0001654076828	-9.67002739	N/A	N/A	N/A	0.004992
Mg3Al6	-14.64727262	0.00021485086	-14.59451945	N/A	N/A	N/A	0.009519
Mg4Al8	-19.56942295	0.0002576546499	-19.49061343	N/A	N/A	N/A	0.012923
Mg5Al10	-24.5985247	0.0003009321857	-24.46438242	N/A	N/A	N/A	0.018989
Mg6Al12	-29.50587203	0.0003362165533	-29.34731497	N/A	N/A	N/A	0.022402
Mg1Al2H8	-9.672736492	0.000137070686	-9.68726759	N/A	N/A	N/A	0.055574
Mg2Al4H16	-19.38893508	0.0002234273112	-19.39872056	N/A	N/A	N/A	0.118669
Mg3Al6H24	-29.11873891	0.000268785081	-29.13230441	N/A	N/A	N/A	0.175842
Mg4Al8H32	-38.84947861	0.0003509600288	-38.86939519	N/A	N/A	N/A	0.234825
Mg5Al10H40	-48.53246739	0.0005282920556	-48.54973204	N/A	N/A	N/A	0.286205
Mg6Al12H48	-58.30671029	0.0008930566091	-58.30015220	N/A	N/A	N/A	0.354309
Mg1	-0.8188014595	3.569799429e-05	-0.82435466	-0.81234988	-0.83436481	-0.82105215	N/A
Mg2	-1.641795769	5.612201251e-05	-1.64939717	-1.63255815	-1.63970043	-1.64755717	0.000219
Mg4	-3.325870465	9.958207095e-05	-3.32443734	-3.32310977	-3.31083253	-3.34464050	0.002374
Mg6	-4.991547303	0.0001341476248	-4.98536313	-4.99453793	-4.97556712	-5.02407087	0.003485
Mg8	-6.685879713	0.0001710526727	-6.66427148	-6.69515986	-6.66870558	-6.73040627	0.005720
Mg10	-8.420506487	0.0002043924685	-8.37817614	-8.43101606	-8.39051043	-8.47111960	0.008902
Mg12	-10.09858554	0.0002363145431	-10.04955780	-10.11259831	-10.06675353	-10.16037912	0.010311
Mg14	-11.79645643	0.0001425138127	-11.72899644	-11.81977210	-11.77029508	-11.87143079	0.011690

Mg16 -13.52134012 0.0001594527944 -13.42920742 -13.54779108 -13.49272712 -13.60449157
0.014450

Mg18 -15.26107645 0.0001764308696 -15.14551451 -15.28630024 -15.21879412 -15.34806587
0.017085

Mg1H2 -1.99289111 6.554614064e-05 -2.00373274 -1.94789343 -1.98858719 -1.98243880
0.009173

Mg2H4 -4.006586659 0.0001157188672 -4.02130050 -3.92480963 -3.99701264 -3.98503520
0.021189

Mg4H8 -8.136575363 0.0001435929376 -8.15880515 -7.97350200 -8.12121987 -8.08765041
0.051114

Mg6H12 -12.26207546 0.0002091405255 -12.27950296 -12.03324054 -12.23991144 -
12.18678846 0.081797

Mg8H16 -16.38695522 0.0002736503399 -16.41735435 -16.08447541 -16.36954989 -
16.28961841 0.109841

Mg10H20 -20.55723967 0.000312064267 -20.58727049 -20.16671494 -20.53376163 -
20.42357705 0.139638

Mg12H24 -24.67600726 0.0005010721179 -24.70660994 -24.21786945 -24.64850921 -
24.51709204 0.167706

Mg14H28 -28.81789758 0.0002964701887 -28.83758461 -28.25820398 -28.76891263 -
28.60957119 0.194606

Mg16H32 -32.9901989 0.000700695428 -32.99648046 -32.35592435 -32.92488424 -32.74825995
0.224627

Mg18H36 -37.14544979 0.0003931817103 -37.16367665 -36.41776358 -37.08716039 -
36.86827063 0.253529

Al1 -1.936573844 5.041507623e-05 -1.94305855 -1.92199913 -1.93546985 -1.94072762 N/A

Al2 -3.904991946 9.020762742e-05 -3.90877769 -3.89052980 -3.89051308 -3.91983420
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Al4 -7.959927685 0.0001879194275 -7.95137380 -7.95696460 -7.92686300 -7.95725199
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Al6 -12.04761194 0.0001762733834 -12.01864058 -12.04140424 -12.01550530 -12.09181090
0.005371

Al8 -16.12190119 0.0002189606825 -16.07867230 -16.12030259 -16.08759980 -16.18332348
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Al10 -20.18760901 0.0002545703584 -20.11854708 -20.19242116 -20.14199291 -20.26565231
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Al12 -24.30428342 0.0002622416568 -24.20530438 -24.30621746 -24.25421861 -24.38838911
0.014732

Al14 -28.42221547 0.0003099649826 -28.28464564 -28.42994150 -28.38423991 -28.51879805
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Al16 -32.50076116 0.0003328184326 -32.34100761 -32.50686627 -32.44411899 -32.60700176
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Al18 -36.56484584 0.0003484042062 -36.39350891 -36.57276431 -36.49018744 -36.68640443
0.023575

Al1H3 -3.780444275 0.0001055871523 -3.79018034 -3.70978770 -3.77516156 -3.76162755
0.017644

Al2H6 -7.622173883 0.0001113351328 -7.63325581 -7.49129051 -7.60273125 -7.58449098
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Al4H12 -15.25826409 0.0001714002427 -15.27627190 -15.00437712 -15.22543369 -15.17986548
0.086067

Al6H18 -22.89195042 0.0002109841062 -22.91719798 -22.53034745 -22.84494117 -22.77410821
0.129254

Al8H24 -30.54243493 0.0002765505813 -30.55558016 -30.07724172 -30.46715377 -30.38556185
0.178102

Al10H30 -38.19321983 0.0003345657681 -38.20170480 -37.61535762 -38.10084988 -
37.99844270 0.220942

Al12H36 -45.81884495 0.0004312970045 -45.81744717 -45.11604593 -45.69860465 -
45.57910551 0.262457

Al14H42 -53.48049276 0.0006063527448 -53.48468716 -52.66307908 -53.34763466 -
53.19747232 0.312587

Al16H48 -61.13862339 0.0007198112505 -61.13780315 -60.20804815 -60.97784757 -
60.80623335 0.356360

Al18H54 -68.76203626 0.0009021468859 -68.75811735 -67.73071172 -68.58074332 -
68.39919305 0.400040

Li1 -7.478227804 5.78747428e-05 -7.49269178 -7.34374333 -7.48561491 -7.46182860 N/A

Li2 -14.99178849 0.0001011605887 -15.01840549 -14.72510903 -15.01076578 -14.95537968
0.000758

Li4 -30.01558375 0.0001571690225 -30.06359811 -29.48624799 -30.05043420 -29.94384698
0.002978

Li6 -45.05720028 0.0002138410951 -45.12435120 -44.27417279 -45.10839644 -44.95511223
0.006338

Li8 -60.10750763 0.0002530899436 -60.19261991 -59.06548633 -60.17203784 -59.97208635
0.008214

Li9 -67.62271125 0.0002949666798 -67.71807462 -66.45833594 -67.69751636 -67.47729074
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Li10 -75.14697648 0.000296474038 -75.25425669 -73.85298901 -75.23290252 -74.98393498
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Li12 -90.19323682 0.0003320440938 -90.31577901 -88.64311929 -90.29594598 -89.99783463
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Li14 -105.2461066 0.0003683689309 -105.38400559 -103.43956673 -105.36629458 -
105.01757954 0.016782

Li15 -112.767537 0.0005727078277 -112.91589919 -110.83648480 -112.89537543 -
112.52796891 0.018307

Li16 -120.2949681 0.000714265885 -120.45107015 -118.23514132 -120.43292839 -
120.03696710 0.019355

Li18 -135.3543354 0.0008277853993 -135.52470477 -133.04107639 -135.51103321 -
135.06584735 0.023148

Li24 -180.4900476 0.0005251272515 -180.71660141 -177.41140974 -180.69970412 -
180.11063022 0.030443

Li1H1 -8.069808656 9.747963269e-05 -8.08791989 -7.91882930 -8.07811065 -8.04651640
0.003134

Li2H2 -16.21754702 0.0001464332317 -16.25256594 -15.91950695 -16.23337114 -16.17049747
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Li4H4 -32.51727053 0.0002265204022 -32.57988801 -31.93071500 -32.54371318 -32.42165513
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Li6H6 -48.80978471 0.0002994808213 -48.90018420 -47.93173743 -48.84842373 -48.66421137
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Li8H8 -65.10270792 0.0003446901244 -65.21979605 -63.93291222 -65.15205483 -64.90657600
0.061404

Li9H9 -73.26421648 0.0003647667377 -73.38604965 -71.94400845 -73.31155432 -73.03572601
0.069846

Li10H10 -81.39389647 0.0003620214299 -81.53970437 -79.93409925 -81.45588136 -
81.14910141 0.077435

Li12H12 -97.70108878 0.0004740010481 -97.87139326 -95.95171877 -97.77500721 -
97.40665015 0.094044

Li14H14 -113.9780349 0.000458524546 -114.17948384 -111.93486942 -114.06417102 -
113.63094833 N/A

Li15H15 -122.1476434 0.000506881407 -122.35702865 -119.96784040 -122.23853462 -
121.77790113 0.118044

Li16H16 -130.2994827 0.0005356500223 -130.52207970 -127.97836383 -130.39673921 -
129.90613099 0.126239

Li18H18 -146.6092061 0.0005550505792 -146.85328415 -144.00422695 -146.71791799 -
146.16516102 0.143879

Li24H24 -195.5249615 0.0009683020978 -195.84247244 -192.05911261 -195.66798857 -
194.93059654 N/A