

SUPPLEMENTARY MATERIAL: THE FULL NUMERICAL RESULT IN APPENDIX E OF PAPER “SELF-CONSISTENT GRADIENT-LIKE EIGEN DECOMPOSITION IN SOLVING SCHRÖDINGER EQUATIONS”

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Paper under double-blind review

Molecule Name	Exact HF Energy (Unit: Hartree)	H_{core}	minao	atom	huckel	SCGLED $T = 200$	SCGLED $T = 500$	SCGLED $T = 1000$	SCGLED $T = 2000$	SCGLED $T = 5000$	SCGLED $T = 10000$
acetaldehyde	-152.842695	-130.487235 (+22.355460) 0.9 ms ✗	-153.222210 (-0.379515) 37.2 ms ✓, 59 iters	-153.723694 (-0.880999) 43.9 ms ✓, 58 iters	-151.013594 (+1.829101) 46.7 ms ✓, 66 iters	-146.731514 (+6.111181) 5.0 ms ✗	-152.597728 (+0.244967) 11.7 ms ✓, 47 iters	-152.875331 (-0.032636) 21.9 ms ✓, 39 iters	-152.842690 (+0.000005) 47.5 ms ✓, 14 iters	-152.842695 (+0.000000) 124.4 ms ✓, 1 iters	-152.842695 (-0.000000) 231.7 ms ✓, 0 iters
acetic	-227.698712	-195.939403 (+31.759310) 1.0 ms ✗	-228.436062 (-0.737350) 33.7 ms ✓, 60 iters	-229.017397 (-1.318685) 45.9 ms ✓, 59 iters	-225.710577 (+1.988135) 52.5 ms ✓, 68 iters	-219.321388 (+8.377325) 7.7 ms ✗	-227.380581 (+0.318132) 16.3 ms ✓, 44 iters	-227.700111 (-0.001399) 36.9 ms ✓, 41 iters	-227.698848 (-0.000136) 67.5 ms ✓, 25 iters	-227.698712 (-0.000000) 178.4 ms ✓, 1 iters	-227.698712 (-0.000000) 349.7 ms ✓, 0 iters
alcl	-701.416908	-697.363310 (+4.053598) 0.8 ms ✗	-701.365129 (+0.051779) 25.3 ms ✓, 11 iters	-701.421442 (-0.004534) 46.1 ms ✓, 11 iters	-701.312615 (+0.104292) 49.4 ms ✓, 10 iters	-698.109164 (+3.307744) 4.2 ms ✗	-700.429691 (+0.987217) 10.0 ms ✓, 13 iters	-701.407504 (+0.009404) 18.5 ms ✓, 9 iters	-701.416897 (+0.000011) 37.9 ms ✓, 6 iters	-701.416909 (-0.000002) 97.4 ms ✓, 2 iters	-701.416908 (-0.000001) 193.9 ms ✓, 2 iters
alcl3	-1620.461846	-1611.231641 (+9.230204) 1.5 ms ✓, 12 iters	-1620.837026 (-0.375181) 25.1 ms ✓, 9 iters	-1620.938891 (-0.477045) 45.4 ms ✓, 9 iters	-1620.113643 (+0.348203) 45.2 ms ✓, 9 iters	-1613.394902 (+7.066943) 12.9 ms ✓, 11 iters	-1618.465135 (+1.996711) 30.7 ms ✓, 10 iters	-1620.436260 (+0.025586) 63.6 ms ✓, 9 iters	-1620.462297 (-0.000451) 124.7 ms ✓, 7 iters	-1620.461851 (-0.000005) 312.2 ms ✓, 3 iters	-1620.461853 (-0.000007) 615.0 ms ✓, 4 iters
alf	-341.372481	-332.777287 (+8.595194) 0.7 ms ✗	-341.184261 (+0.188220) 22.5 ms ✓, 25 iters	-341.175841 (+0.196640) 43.4 ms ✓, 25 iters	-341.216095 (+0.156385) 44.5 ms ✓, 24 iters	-337.326280 (+4.046200) 3.3 ms ✗	-341.143775 (+0.282706) 8.5 ms ✓, 24 iters	-341.365957 (+0.006524) 16.8 ms ✓, 14 iters	-341.372509 (-0.000028) 30.8 ms ✓, 7 iters	-341.372540 (-0.000059) 75.6 ms ✓, 7 iters	-341.372540 (-0.000000) 154.8 ms ✓, 7 iters
alf3	-540.340281	-521.188584 (+19.151697) 1.0 ms ✓, 32 iters	-540.193601 (+0.146680) 23.0 ms ✓, 21 iters	-540.099917 (+0.240364) 41.7 ms ✓, 22 iters	-539.957282 (+0.382999) 44.5 ms ✓, 21 iters	-531.290901 (+9.049380) 6.3 ms ✓, 28 iters	-539.900935 (+0.439346) 16.2 ms ✓, 21 iters	-540.330273 (+0.010008) 32.6 ms ✓, 13 iters	-540.341125 (-0.000844) 62.6 ms ✓, 11 iters	-540.340301 (-0.000020) 154.5 ms ✓, 6 iters	-540.340281 (-0.000000) 312.2 ms ✓, 1 iters
alh	-242.426380	-241.169937 (+1.256443) 0.7 ms ✓, 10 iters	-242.202780 (+0.223600) 22.7 ms ✓, 9 iters	-242.260623 (+0.165756) 24.3 ms ✓, 9 iters	-242.367860 (+0.058520) 28.4 ms ✓, 9 iters	-241.419954 (+1.006425) 3.2 ms ✓, 9 iters	-242.173320 (+0.253060) 6.2 ms ✓, 8 iters	-242.419485 (+0.006894) 13.8 ms ✓, 7 iters	-242.426375 (+0.000005) 21.6 ms ✓, 4 iters	-242.426380 (+0.000000) 54.2 ms ✓, 0 iters	-242.426380 (-0.000000) 111.0 ms ✓, 0 iters
alh3	-243.587761	-241.286329 (+2.301432) 0.7 ms ✓, 8 iters	-243.210264 (+0.377497) 23.6 ms ✓, 8 iters	-243.335237 (+0.252524) 25.0 ms ✓, 8 iters	-243.393303 (+0.194458) 25.4 ms ✓, 8 iters	-241.764754 (+1.823007) 1.2 ms ✓, 8 iters	-243.205226 (+0.382535) 6.3 ms ✓, 7 iters	-243.581977 (+0.005783) 12.9 ms ✓, 5 iters	-243.587759 (+0.000002) 24.7 ms ✓, 3 iters	-243.587761 (-0.000000) 60.0 ms ✓, 1 iters	-243.587762 (-0.000001) 126.8 ms ✓, 2 iters
allene	-115.820914	-98.473564 (+17.347350) 1.0 ms ✗	-116.307122 (-0.486208) 22.4 ms ✓, 13 iters	-116.861841 (-1.040927) 20.9 ms ✓, 14 iters	-114.388774 (+1.432140) 21.4 ms ✓, 17 iters	-109.461219 (+6.359695) 5.0 ms ✗	-115.617963 (+0.202951) 13.8 ms ✓, 15 iters	-115.818848 (+0.002066) 24.7 ms ✓, 12 iters	-115.821865 (-0.000952) 47.0 ms ✓, 12 iters	-115.820914 (-0.000000) 118.6 ms ✓, 6 iters	-115.820914 (-0.000000) 238.3 ms ✓, 1 iters
b2h6	-52.774881	-43.835427 (+8.939454) 0.9 ms ✓, 10 iters	-52.943715 (-0.168834) 25.9 ms ✓, 8 iters	-53.376930 (-0.602049) 23.2 ms ✓, 8 iters	-51.320838 (+1.454043) 22.2 ms ✓, 9 iters	-49.045525 (+3.729356) 3.8 ms ✓, 10 iters	-51.984252 (+0.790629) 8.7 ms ✓, 9 iters	-52.517218 (+0.257663) 17.4 ms ✓, 14 iters	-52.777013 (-0.002132) 33.8 ms ✓, 10 iters	-52.774881 (+0.000000) 87.7 ms ✓, 0 iters	-52.774881 (-0.000000) 159.9 ms ✓, 0 iters
benzene	-230.623825	-203.993141 (+26.630684) 1.9 ms ✓, 23 iters	-232.354772 (-1.730947) 23.9 ms ✓, 9 iters	-233.683144 (-3.059319) 22.6 ms ✓, 9 iters	-228.070443 (+2.553382) 23.8 ms ✓, 10 iters	-211.964590 (+18.659236) 17.4 ms ✗	-230.215189 (+0.408636) 40.9 ms ✓, 26 iters	-230.615998 (+0.007827) 87.3 ms ✓, 16 iters	-230.623789 (+0.000036) 169.2 ms ✓, 14 iters	-230.623826 (-0.000000) 426.4 ms ✓, 4 iters	-230.623825 (-0.000000) 837.3 ms ✓, 2 iters
beta-lactim	-245.646165	-209.854368 (+35.791796) 1.4 ms ✗	-246.932707 (-1.286543) 50.5 ms ✓, 44 iters	-247.982362 (-2.336198) 63.4 ms ✓, 46 iters	-243.196721 (+2.449444) 68.0 ms ✓, 52 iters	-232.347018 (+13.299147) 13.4 ms ✗	-244.654303 (+0.991862) 29.8 ms ✓, 41 iters	-245.602598 (+0.043566) 59.2 ms ✓, 36 iters	-245.645403 (+0.000761) 120.4 ms ✓, 16 iters	-245.646167 (-0.000002) 302.5 ms ✓, 4 iters	-245.646165 (-0.000000) 599.1 ms ✓, 0 iters
bf	-124.057391	-115.853479 (+8.203912) 0.8 ms ✗	-124.123147 (-0.065756) 23.1 ms ✓, 24 iters	-124.172813 (-0.115422) 40.5 ms ✓, 24 iters	-123.788632 (+0.268759) 43.9 ms ✓, 25 iters	-119.460262 (+4.597129) 2.3 ms ✗	-123.442889 (+0.614501) 7.3 ms ✓, 25 iters	-123.625609 (+0.431781) 12.6 ms ✓, 18 iters	-124.006451 (+0.050939) 24.2 ms ✓, 15 iters	-124.057391 (+0.000000) 59.9 ms ✓, 3 iters	-124.057391 (-0.000000) 115.8 ms ✓, 1 iters
bf3	-323.083876	-304.403095 (+18.680781) 0.9 ms ✓, 26 iters	-323.550027 (-0.466151) 23.8 ms ✓, 19 iters	-323.620542 (-0.536665) 40.5 ms ✓, 19 iters	-322.258547 (+0.825329) 41.5 ms ✓, 19 iters	-313.813968 (+9.269909) 4.7 ms ✓, 22 iters	-322.675593 (+0.408283) 11.9 ms ✓, 19 iters	-323.086211 (-0.002335) 23.4 ms ✓, 13 iters	-323.084097 (-0.000220) 48.9 ms ✓, 11 iters	-323.083876 (-0.000000) 114.6 ms ✓, 2 iters	-323.083876 (-0.000000) 243.0 ms ✓, 0 iters

bh	-25.108974	-23.514271 (+1.594702) 0.7 ms ✓, 10 iters	-24.897850 (+0.211124) 23.3 ms ✓, 9 iters	-24.962099 (+0.146875) 21.7 ms ✓, 9 iters	-25.013282 (+0.095692) 24.8 ms ✓, 9 iters	-24.250903 (+0.858070) 2.2 ms ✓, 9 iters	-24.829163 (+0.279810) 4.1 ms ✓, 8 iters	-24.874847 (+0.234127) 9.2 ms ✓, 7 iters	-24.875456 (+0.233518) 17.3 ms ✓, 4 iters	-24.875457 (+0.233517) 41.9 ms ✗, 0 iters	-24.875457 (+0.233517) 74.3 ms ✓, 0 iters
bh3	-26.376765	-23.340462 (+3.036303) 0.6 ms ✓, 8 iters	-26.099230 (+0.277535) 22.7 ms ✓, 8 iters	-26.253321 (+0.123444) 23.5 ms ✓, 8 iters	-25.859660 (+0.517105) 23.0 ms ✓, 9 iters	-25.241343 (+1.135422) 2.0 ms ✓, 7 iters	-26.370195 (+0.006570) 4.5 ms ✓, 7 iters	-26.377280 (-0.000516) 9.2 ms ✓, 5 iters	-26.376765 (+0.000000) 18.4 ms ✓, 3 iters	-26.376765 (-0.000000) 45.6 ms ✗, 0 iters	-26.376765 (+0.000000) 90.0 ms ✓, 0 iters
bhf2	-224.187016	-209.148734 (+15.038283) 1.0 ms ✗	-224.388498 (-0.201482) 34.8 ms ✓, 20 iters	-224.494862 (-0.307846) 44.5 ms ✓, 20 iters	-223.457386 (+0.729630) 44.3 ms ✓, 21 iters	-215.841942 (+8.345074) 4.0 ms ✗	-223.007455 (+1.179561) 9.7 ms ✓, 20 iters	-224.187065 (-0.000048) 22.7 ms ✓, 13 iters	-224.187003 (+0.000013) 43.7 ms ✓, 8 iters	-224.187029 (-0.000012) 92.3 ms ✓, 9 iters	-224.187016 (-0.000000) 186.8 ms ✓, 0 iters
borole	-178.940722	-154.493281 (+24.447440) 1.6 ms ✗	-180.076021 (-1.135300) 37.2 ms ✓, 29 iters	-181.069227 (-2.128505) 47.2 ms ✓, 28 iters	-176.908868 (+2.031854) 51.0 ms ✓, 30 iters	-169.551770 (+9.388952) 13.1 ms ✗	-177.388757 (+1.551965) 27.3 ms ✓, 30 iters	-179.071761 (-0.131039) 57.3 ms ✓, 23 iters	-178.941014 (-0.000292) 113.6 ms ✓, 16 iters	-178.940722 (-0.000001) 282.3 ms ✓, 2 iters	-178.940722 (-0.000000) 563.0 ms ✓, 1 iters
c-hcoh	-113.714969	-104.101835 (+9.613134) 0.8 ms ✗	-113.822094 (-0.107125) 34.4 ms ✓, 26 iters	-114.062328 (-0.347359) 43.4 ms ✓, 26 iters	-113.315364 (+0.399605) 43.4 ms ✓, 24 iters	-107.988049 (+5.726920) 2.6 ms ✗	-113.565420 (+0.149549) 6.8 ms ✓, 25 iters	-113.713011 (+0.001958) 13.4 ms ✓, 13 iters	-113.714957 (+0.000012) 25.9 ms ✓, 7 iters	-113.714969 (+0.000000) 64.1 ms ✗, 0 iters	-113.714969 (-0.000000) 128.7 ms ✓, 0 iters
c-hono	-204.518517	-191.510455 (+13.008062) 0.8 ms ✗	-204.943947 (-0.425430) 36.9 ms ✗	-205.241426 (-0.722909) 44.7 ms ✗	-203.716118 (+0.802399) 48.3 ms ✗	-197.644594 (+6.873923) 3.7 ms ✗	-204.178061 (+0.340456) 9.0 ms ✓, 152 iters	-204.514620 (+0.003897) 18.5 ms ✓, 87 iters	-204.518437 (+0.000080) 41.0 ms ✓, 40 iters	-204.518517 (+0.000000) 102.5 ms ✗, 0 iters	-204.518517 (-0.000000) 204.4 ms ✓, 0 iters
c-n2h2	-109.913041	-100.608217 (+9.304823) 0.8 ms ✓, 14 iters	-110.021877 (-0.108836) 25.1 ms ✓, 10 iters	-110.367326 (-0.454285) 21.2 ms ✓, 10 iters	-109.490583 (+0.422458) 21.1 ms ✓, 11 iters	-103.614440 (+6.298601) 2.8 ms ✗	-109.872615 (+0.040426) 6.8 ms ✓, 42 iters	-109.906551 (+0.006490) 13.2 ms ✓, 23 iters	-109.912875 (+0.000165) 24.5 ms ✓, 13 iters	-109.913041 (-0.000000) 64.4 ms ✓, 6 iters	-109.913041 (-0.000000) 128.6 ms ✓, 3 iters
c2c12	-994.503905	-985.576209 (+8.927696) 1.1 ms ✓, 16 iters	-995.523119 (-1.019214) 26.5 ms ✓, 12 iters	-995.902732 (-1.398826) 41.7 ms ✓, 10 iters	-993.479411 (+1.024495) 45.6 ms ✓, 14 iters	-985.180968 (+9.322937) 8.6 ms ✗	-991.915619 (+2.588286) 21.7 ms ✓, 54 iters	-994.208929 (+0.294977) 43.9 ms ✓, 49 iters	-994.500629 (+0.000000) 89.7 ms ✓, 33 iters	-994.503906 (-0.000000) 233.1 ms ✓, 12 iters	-994.503905 (-0.000000) 455.1 ms ✓, 1 iters
c2c14	-1913.460496	-1882.025268 (+31.435228) 1.8 ms ✗	-1914.917127 (-1.456631) 27.4 ms ✓, 23 iters	-1915.487661 (-2.027165) 45.4 ms ✓, 22 iters	-1911.732894 (+1.727601) 49.9 ms ✓, 26 iters	-1903.925727 (+9.534768) 28.7 ms ✓, 23 iters	-1910.890142 (+2.570353) 62.9 ms ✓, 18 iters	-1913.437762 (+0.022733) 125.6 ms ✓, 16 iters	-1913.461041 (-0.000545) 260.7 ms ✓, 8 iters	-1913.460509 (-0.000013) 631.4 ms ✓, 10 iters	-1913.460496 (-0.000000) 1233.8 ms ✓, 4 iters
c2c16	-2832.359449	-2795.661600 (+36.697849) 2.9 ms ✗	-2834.069671 (-1.710222) 25.4 ms ✓, 44 iters	-2834.760311 (-2.400862) 51.2 ms ✓, 42 iters	-2829.782166 (+2.577283) 49.8 ms ✗	-2816.515709 (+15.843740) 63.8 ms ✗	-2828.271639 (+4.087810) 133.7 ms ✓, 35 iters	-2832.327584 (+0.031865) 266.8 ms ✓, 25 iters	-2984.237760 (-151.878311) 524.8 ms ✗	-2985.696188 (-153.336739) 1367.8 ms ✗	-3222.117477 (-389.758028) 2737.2 ms ✓, 42 iters
c2clh	-535.649074	-522.399737 (+13.249337) 1.0 ms ✗	-536.244496 (-0.595422) 36.9 ms ✓, 60 iters	-536.566867 (-0.917793) 45.7 ms ✓, 61 iters	-534.605364 (+1.043710) 44.2 ms ✓, 68 iters	-529.482299 (+6.166775) 6.5 ms ✗	-534.836895 (+0.812179) 14.2 ms ✓, 44 iters	-535.709507 (-0.060433) 24.5 ms ✓, 61 iters	-535.649077 (-0.000004) 51.5 ms ✓, 5 iters	-535.649078 (-0.000004) 137.5 ms ✓, 2 iters	-535.649074 (-0.000000) 249.4 ms ✓, 0 iters
c2clh3	-536.879268	-521.726546 (+15.152722) 1.0 ms ✗	-537.303315 (-0.424047) 33.9 ms ✓, 19 iters	-537.751997 (-0.872728) 46.2 ms ✓, 19 iters	-535.609606 (+1.269662) 51.3 ms ✓, 21 iters	-529.814691 (+7.064577) 5.9 ms ✗	-535.989889 (+0.889379) 12.6 ms ✓, 13 iters	-536.873472 (+0.005796) 26.6 ms ✓, 11 iters	-536.879259 (+0.000010) 54.1 ms ✓, 8 iters	-536.879268 (-0.000001) 135.1 ms ✓, 1 iters	-536.879268 (-0.000000) 263.1 ms ✓, 0 iters
c2clh5	-538.077271	-522.805650 (+15.271621) 1.2 ms ✗	-538.365042 (-0.287771) 34.3 ms ✓, 14 iters	-538.929320 (-0.852049) 43.7 ms ✓, 12 iters	-536.513626 (+1.563645) 50.4 ms ✓, 16 iters	-529.988247 (+8.089024) 7.3 ms ✗	-537.235598 (+0.841673) 18.2 ms ✓, 12 iters	-538.071370 (+0.005901) 39.3 ms ✓, 9 iters	-538.077275 (-0.000004) 69.3 ms ✓, 6 iters	-538.077272 (-0.000001) 174.0 ms ✓, 3 iters	-538.077271 (-0.000000) 369.2 ms ✓, 2 iters
c2f4	-473.253828	-448.860140 (+24.393689) 1.2 ms ✓, 29 iters	-474.600170 (-1.346341) 24.5 ms ✓, 23 iters	-475.007082 (-1.753254) 41.6 ms ✓, 22 iters	-471.483866 (+1.769962) 42.2 ms ✓, 25 iters	-459.451965 (+13.801863) 13.8 ms ✓, 24 iters	-472.451843 (+0.801985) 33.3 ms ✓, 23 iters	-473.252419 (+0.001409) 67.4 ms ✓, 15 iters	-473.254802 (-0.000974) 126.2 ms ✓, 11 iters	-473.253828 (-0.000000) 324.9 ms ✓, 5 iters	-473.253828 (-0.000000) 605.3 ms ✓, 2 iters
c2f6	-672.141936	-629.517307 (+42.624629) 2.1 ms ✓, 27 iters	-673.865498 (-1.723563) 27.3 ms ✓, 23 iters	-674.297246 (-2.155311) 41.4 ms ✓, 23 iters	-669.708808 (+2.433127) 47.9 ms ✓, 24 iters	-653.945789 (+18.196147) 22.0 ms ✓, 25 iters	-669.646933 (+2.495002) 60.1 ms ✓, 21 iters	-672.139882 (+0.002053) 113.0 ms ✓, 15 iters	-672.142699 (-0.000763) 229.1 ms ✓, 12 iters	-672.141937 (-0.000001) 578.3 ms ✓, 6 iters	-672.141936 (-0.000000) 1172.7 ms ✓, 5 iters
c2h2	-76.792255	-67.920019 (+8.872236) 1.1 ms ✓, 10 iters	-76.968199 (-0.175944) 27.6 ms ✓, 8 iters	-77.233359 (-0.441105) 26.1 ms ✓, 8 iters	-75.980169 (+0.812086) 26.1 ms ✓, 9 iters	-70.261807 (+6.530448) 3.7 ms ✓, 10 iters	-75.390506 (+1.401749) 8.5 ms ✓, 68 iters	-76.619989 (+0.172266) 13.2 ms ✓, 46 iters	-76.787334 (+0.004920) 26.8 ms ✓, 21 iters	-76.792253 (+0.000002) 67.7 ms ✓, 10 iters	-76.792255 (-0.000000) 129.6 ms ✓, 2 iters
c2h3f	-176.826080	-157.691856 (+19.134224) 1.1 ms ✗	-177.202842 (-0.376762) 39.9 ms ✓, 21 iters	-177.612815 (-0.786735) 46.7 ms ✓, 19 iters	-175.532764 (+1.293316) 44.9 ms ✓, 23 iters	-169.247640 (+7.578440) 4.3 ms ✗	-175.774126 (+1.051954) 10.4 ms ✓, 23 iters	-176.060698 (+0.765382) 21.7 ms ✓, 21 iters	-176.824786 (+0.001294) 44.9 ms ✓, 10 iters	-176.826088 (-0.000009) 109.6 ms ✓, 8 iters	-176.826080 (-0.000000) 214.4 ms ✓, 1 iters
c2h4	-78.004021	-66.875657 (+11.128364) 0.7 ms ✓, 13 iters	-78.130797 (-0.126777) 23.1 ms ✓, 8 iters	-78.537452 (-0.533431) 22.5 ms ✓, 9 iters	-76.917588 (+1.086433) 24.2 ms ✓, 10 iters	-73.482578 (+4.521442) 3.0 ms ✓, 12 iters	-77.634628 (+0.369392) 7.3 ms ✓, 12 iters	-77.482859 (+0.521162) 14.0 ms ✓, 23 iters	-78.004000 (+0.514020) 27.9 ms ✓, 18 iters	-78.004020 (+0.000000) 69.6 ms ✓, 5 iters	-78.004021 (-0.000000) 144.9 ms ✓, 2 iters
c2h5f	-178.020838	-158.755423 (+19.265415) 1.2 ms ✗	-178.247754 (-0.226916) 36.8 ms ✓, 21 iters	-178.773272 (-0.752434) 42.3 ms ✓, 20 iters	-176.432794 (+1.588044) 44.0 ms ✓, 23 iters	-169.112681 (+8.908157) 5.4 ms ✗	-177.774113 (+0.246725) 12.3 ms ✓, 20 iters	-178.018998 (+0.001840) 26.8 ms ✓, 13 iters	-178.021392 (-0.000554) 54.7 ms ✓, 10 iters	-178.020838 (-0.000000) 136.2 ms ✓, 1 iters	-178.020838 (-0.000000) 253.4 ms ✓, 0 iters

c2h6	-79.197407	-66.825667 (+12.371740) 0.9 ms ✓, 16 iters	-79.249498 (-0.052092) 22.9 ms ✓, 9 iters	-79.780338 (-0.582931) 24.1 ms ✓, 11 iters	-77.807287 (+1.390120) 24.3 ms ✓, 13 iters	-73.543908 (+5.653499) 3.9 ms ✓, 15 iters	-79.078860 (+0.118547) 8.8 ms ✓, 11 iters	-79.196263 (+0.001143) 17.5 ms ✓, 7 iters	-79.197741 (-0.000334) 34.6 ms ✓, 6 iters	-79.197407 (-0.000000) 87.9 ms ✓, 0 iters	-79.197407 (-0.000000) 173.6 ms ✓, 1 iters
cc12	-956.627379	-949.635690 (+6.991689) 0.9 ms ✗	-956.969017 (-0.341638) 22.5 ms ✓, 19 iters	-957.196141 (-0.568762) 42.8 ms ✓, 18 iters	-956.120175 (+0.507204) 47.6 ms ✓, 19 iters	-951.329038 (+5.298341) 6.0 ms ✓, 24 iters	-955.065877 (+1.561502) 15.0 ms ✓, 56 iters	-956.416414 (+0.210965) 28.9 ms ✓, 70 iters	-956.428679 (+0.198700) 60.5 ms ✓, 58 iters	-956.428907 (+0.198472) 150.9 ms ✓, 45 iters	-956.625916 (+0.001463) 312.7 ms ✓, 24 iters
cc12h2	-957.918317	-948.674382 (+9.243935) 1.0 ms ✗	-958.251759 (-0.333442) 33.2 ms ✓, 16 iters	-958.577571 (-0.659254) 44.2 ms ✓, 16 iters	-956.808020 (+1.110297) 46.9 ms ✓, 18 iters	-950.468566 (+7.449751) 7.4 ms ✓, 20 iters	-956.413879 (+1.504438) 17.4 ms ✓, 12 iters	-957.908750 (+0.009567) 34.1 ms ✓, 9 iters	-957.920820 (-0.002503) 68.2 ms ✓, 7 iters	-957.918318 (-0.000001) 179.5 ms ✓, 3 iters	-957.918318 (-0.000001) 364.3 ms ✓, 3 iters
cc12o	-1031.558511	-1014.829944 (+16.728567) 1.0 ms ✗	-1032.344968 (-0.786457) 33.2 ms ✓, 85 iters	-1032.638370 (-1.079859) 64.0 ms ✓, 85 iters	-1030.103930 (+1.454581) 62.1 ms ✓, 92 iters	-1024.152694 (+7.405817) 8.3 ms ✗	-1029.352366 (+2.206145) 23.9 ms ✓, 68 iters	-1031.537068 (+0.021443) 40.5 ms ✓, 29 iters	-1031.558353 (+0.00158) 85.7 ms ✓, 15 iters	-1031.558514 (-0.000003) 200.2 ms ✓, 9 iters	-1031.558511 (-0.000000) 400.2 ms ✓, 1 iters
cc13h	-1416.773529	-1404.272889 (+12.500640) 1.2 ms ✓, 28 iters	-1417.403918 (-0.630390) 34.5 ms ✓, 22 iters	-1417.759385 (-0.985857) 46.3 ms ✓, 21 iters	-1415.476654 (+1.296875) 49.5 ms ✓, 24 iters	-1408.689068 (+8.084460) 12.3 ms ✓, 18 iters	-1414.732183 (+2.041345) 28.3 ms ✓, 15 iters	-1416.754639 (+0.018890) 60.8 ms ✓, 11 iters	-1416.773773 (-0.000244) 126.8 ms ✓, 7 iters	-1416.773545 (-0.000017) 299.8 ms ✓, 5 iters	-1416.773529 (-0.000001) 567.4 ms ✓, 4 iters
cc14	-1875.619526	-1856.254392 (+19.365135) 1.6 ms ✓, 54 iters	-1876.540267 (-0.920741) 25.1 ms ✓, 31 iters	-1876.916724 (-1.297198) 44.1 ms ✓, 31 iters	-1874.125908 (+1.493618) 51.7 ms ✓, 34 iters	-1867.356678 (+8.262848) 21.0 ms ✓, 25 iters	-1873.175968 (+2.443559) 45.9 ms ✓, 24 iters	-1875.607347 (+0.012179) 88.9 ms ✓, 8 iters	-1875.621038 (-0.001511) 194.5 ms ✓, 14 iters	-1875.619543 (-0.000016) 448.3 ms ✓, 3 iters	-1875.619526 (-0.000000) 916.7 ms ✓, 1 iters
cc1h3	-499.054132	-491.014086 (+8.040046) 0.9 ms ✓, 16 iters	-499.112104 (-0.057972) 35.7 ms ✓, 13 iters	-499.403283 (-0.349151) 46.3 ms ✓, 11 iters	-498.115005 (+0.939127) 44.8 ms ✓, 14 iters	-493.489858 (+5.564274) 4.0 ms ✓, 18 iters	-498.166824 (+0.887308) 9.8 ms ✓, 11 iters	-499.049119 (+0.005013) 19.7 ms ✓, 9 iters	-499.054124 (+0.000008) 38.9 ms ✓, 6 iters	-499.054134 (-0.000002) 93.8 ms ✓, 1 iters	-499.054132 (-0.000000) 185.1 ms ✓, 0 iters
cf2	-236.570043	-222.416287 (+14.153757) 0.8 ms ✗	-236.911356 (-0.341312) 22.9 ms ✓, 23 iters	-237.071734 (-0.501691) 39.2 ms ✓, 22 iters	-235.976261 (+0.593783) 42.2 ms ✓, 23 iters	-229.899973 (+6.670071) 3.7 ms ✓, 29 iters	-235.887613 (+0.682430) 8.7 ms ✓, 34 iters	-236.208701 (+0.361343) 15.9 ms ✓, 32 iters	-236.231442 (+0.338602) 30.8 ms ✓, 27 iters	-236.569695 (+0.000348) 77.0 ms ✓, 15 iters	-236.570043 (-0.000000) 163.6 ms ✓, 0 iters
cf2cl2	-1155.542628	-1125.904565 (+29.638063) 1.3 ms ✗	-1156.475353 (-0.932725) 34.2 ms ✓, 23 iters	-1156.766727 (-1.224099) 63.5 ms ✓, 23 iters	-1154.088035 (+1.454593) 64.0 ms ✓, 24 iters	-1144.956439 (+10.586189) 12.3 ms ✓, 21 iters	-1153.968661 (+1.573967) 33.0 ms ✓, 21 iters	-1155.529595 (+0.013033) 61.7 ms ✓, 12 iters	-1155.542992 (-0.000364) 125.1 ms ✓, 7 iters	-1155.542632 (-0.000004) 313.9 ms ✓, 2 iters	-1155.542628 (-0.000000) 620.6 ms ✓, 1 iters
cf4	-435.484482	-409.106502 (+26.377980) 1.3 ms ✓, 19 iters	-436.486070 (-1.001588) 24.3 ms ✓, 19 iters	-436.688508 (-1.204026) 40.3 ms ✓, 19 iters	-434.034994 (+1.449488) 44.3 ms ✓, 20 iters	-424.914505 (+10.569977) 9.6 ms ✓, 21 iters	-434.771277 (+0.713205) 24.3 ms ✓, 18 iters	-435.514927 (-0.030445) 50.1 ms ✓, 16 iters	-435.484576 (-0.001274) 90.4 ms ✓, 12 iters	-435.484482 (-0.000000) 221.1 ms ✓, 1 iters	-435.484482 (-0.000000) 457.4 ms ✓, 0 iters
ch2-sing	-38.852978	-35.217474 (+3.635503) 0.6 ms ✓, 12 iters	-38.587396 (+0.265581) 25.1 ms ✓, 11 iters	-38.729770 (+0.123207) 22.4 ms ✓, 11 iters	-38.599733 (+0.253245) 22.8 ms ✓, 11 iters	-37.362543 (+1.490435) 1.7 ms ✓, 11 iters	-38.804695 (+0.048283) 4.6 ms ✓, 8 iters	-38.852755 (+0.000223) 8.4 ms ✓, 6 iters	-38.852977 (+0.000000) 17.1 ms ✓, 3 iters	-38.852978 (+0.000000) 40.9 ms ✓, 0 iters	-38.852978 (-0.000000) ✓, 0 iters
ch2c	-76.735107	-67.925566 (+8.809541) 0.8 ms ✗	-76.790274 (-0.055167) 24.1 ms ✓, 14 iters	-77.083340 (-0.348233) 22.9 ms ✓, 16 iters	-76.011147 (+0.723960) 21.8 ms ✓, 20 iters	-73.805679 (+2.929427) 2.7 ms ✓, 33 iters	-76.270821 (+0.464286) 6.8 ms ✓, 34 iters	-76.403947 (+0.331160) 13.9 ms ✓, 31 iters	-76.413535 (+0.321571) 26.2 ms ✓, 28 iters	-76.734935 (+0.000172) 66.0 ms ✓, 15 iters	-76.735107 (+0.000000) 137.3 ms ✓, 0 iters
ch2clf	-597.865880	-584.907146 (+12.95735) 0.9 ms ✗	-598.152964 (-0.287084) 45.9 ms ✓, 21 iters	-598.441366 (-0.575486) 64.3 ms ✓, 20 iters	-596.752420 (+1.113460) 69.4 ms ✓, 22 iters	-589.668975 (+8.196905) 6.5 ms ✗	-596.946464 (+0.919417) 14.2 ms ✓, 20 iters	-597.859969 (+0.005911) 28.6 ms ✓, 10 iters	-597.865867 (-0.000013) 58.4 ms ✓, 6 iters	-597.865880 (-0.000000) 139.6 ms ✓, 1 iters	-597.865880 (-0.000000) 282.7 ms ✓, 1 iters
ch2f2	-237.821294	-221.034483 (+16.786811) 0.8 ms ✗	-238.084063 (-0.262769) 38.2 ms ✓, 20 iters	-238.335638 (-0.514344) 45.9 ms ✓, 20 iters	-236.690525 (+1.130769) 47.2 ms ✓, 21 iters	-228.591679 (+9.229615) 4.2 ms ✗	-237.518330 (+0.302963) 11.9 ms ✓, 19 iters	-237.820164 (+0.001130) 21.2 ms ✓, 12 iters	-237.821295 (-0.000001) 41.0 ms ✓, 7 iters	-237.821294 (+0.000000) 108.1 ms ✓, 0 iters	-237.821294 (-0.000000) 212.4 ms ✓, 0 iters
ch2nh	-93.979893	-82.474432 (+11.505461) 0.9 ms ✗	-94.103938 (-0.124044) 38.0 ms ✓, 31 iters	-94.477452 (-0.497559) 42.1 ms ✓, 33 iters	-92.910294 (+1.069599) 45.4 ms ✓, 35 iters	-90.264238 (+3.715655) 2.8 ms ✓, 41 iters	-93.833808 (+0.146085) 6.6 ms ✓, 28 iters	-93.978828 (+0.001065) 12.1 ms ✓, 15 iters	-93.979886 (+0.000008) 25.0 ms ✓, 8 iters	-93.979893 (+0.000000) 64.0 ms ✓, 0 iters	-93.979893 (-0.000000) 118.5 ms ✓, 0 iters
ch3f	-138.993245	-127.039241 (+11.954004) 0.9 ms ✗	-138.993224 (+0.000021) 34.5 ms ✓, 20 iters	-139.250801 (-0.257557) 43.6 ms ✓, 19 iters	-138.034350 (+0.958894) 42.4 ms ✓, 21 iters	-132.273081 (+6.720164) 2.9 ms ✗	-138.825022 (+0.168222) 6.2 ms ✓, 19 iters	-138.991899 (+0.001345) 12.6 ms ✓, 12 iters	-138.993242 (+0.000002) 25.5 ms ✓, 5 iters	-138.993245 (-0.000000) 64.3 ms ✓, 3 iters	-138.993245 (-0.000000) 127.5 ms ✓, 1 iters
ch3nh2	-95.167402	-82.350152 (+12.817251) 0.9 ms ✗	-95.239397 (-0.071994) 37.2 ms ✓, 14 iters	-95.731513 (-0.564110) 46.3 ms ✓, 16 iters	-94.154052 (+1.013350) 45.1 ms ✓, 16 iters	-89.758977 (+5.408426) 3.2 ms ✓, 17 iters	-95.034712 (+0.132690) 9.4 ms ✓, 16 iters	-95.166948 (+0.000455) 20.5 ms ✓, 9 iters	-95.167402 (+0.000000) 33.3 ms ✓, 5 iters	-95.167402 (+0.000000) 82.2 ms ✓, 0 iters	-95.167402 (-0.000000) 157.1 ms ✓, 0 iters
ch3ph2	-381.421525	-372.031475 (+9.390050) 1.4 ms ✓, 15 iters	-381.393204 (+0.028321) 39.4 ms ✓, 11 iters	-381.818543 (-0.397018) 48.1 ms ✓, 12 iters	-380.525024 (+0.896501) 44.5 ms ✓, 14 iters	-374.996364 (+6.425161) 4.2 ms ✓, 14 iters	-380.775955 (+0.645569) 10.5 ms ✓, 13 iters	-381.416283 (+0.005242) 21.7 ms ✓, 9 iters	-381.421513 (+0.000012) 41.7 ms ✓, 6 iters	-381.421525 (-0.000000) 101.8 ms ✓, 1 iters	-381.421525 (-0.000000) 207.2 ms ✓, 1 iters
ch4	-40.180463	-33.783430 (+6.397032) 0.6 ms ✓, 14 iters	-40.015070 (+0.165393) 25.4 ms ✓, 7 iters	-40.271569 (-0.091106) 24.1 ms ✓, 10 iters	-39.393953 (+0.786509) 22.7 ms ✓, 12 iters	-37.711423 (+2.469040) 2.3 ms ✓, 13 iters	-40.142041 (+0.038422) 6.5 ms ✓, 10 iters	-40.180272 (+0.000191) 12.0 ms ✓, 6 iters	-40.180463 (+0.000000) 24.0 ms ✓, 3 iters	-40.180463 (-0.000000) 58.6 ms ✓, 0 iters	-40.180463 (-0.000000) 98.5 ms ✓, 0 iters

chf3	-336.655909	-315.825054 (+20.830855) 1.0 ms ✓, 31 iters	-337.269245 (-0.613336) 36.9 ms ✓, 20 iters	-337.502879 (-0.846970) 41.3 ms ✓, 19 iters	-335.363781 (+1.292128) 43.8 ms ✓, 21 iters	-326.237121 (+10.418788) 6.3 ms ✓, 25 iters	-336.185971 (+0.469938) 15.5 ms ✓, 19 iters	-336.653578 (+0.002331) 29.5 ms ✓, 13 iters	-336.656158 (-0.000249) 63.0 ms ✓, 11 iters	-336.655909 (-0.000000) 165.7 ms ✓, 5 iters	-336.655909 (-0.000000) 298.2 ms ✓, 0 iters
cis-c2f2cl2	-1193.351418	-1169.555391 (+23.796026) 3.5 ms ✓, 25 iters	-1194.735840 (-1.384422) 35.2 ms ✓, 25 iters	-1195.224597 (-1.873180) 70.5 ms ✓, 24 iters	-1191.617933 (+1.733484) 70.7 ms ✓, 27 iters	-1181.142967 (+12.208451) 17.1 ms ✓, 23 iters	-1191.764580 (+1.586838) 42.0 ms ✓, 24 iters	-1204.579424 (-11.228006) 92.0 ms ✓, 25 iters	-1213.400929 (-20.049511) 172.1 ms ✓, 29 iters	-1193.351440 (-0.000022) 436.3 ms ✓, 7 iters	-1237.555265 (-44.203847) 869.4 ms ✓, 0 iters
cl2	-918.862956	-913.975979 (+4.886977) 0.8 ms ✓, 8 iters	-919.010481 (-0.147525) 12.2 ms ✓, 7 iters	-919.056701 (-0.193746) 25.1 ms ✓, 7 iters	-918.820921 (+0.042035) 27.4 ms ✓, 7 iters	-914.693364 (+4.169591) 4.9 ms ✓, 8 iters	-916.990279 (+1.872676) 11.5 ms ✓, 10 iters	-918.221525 (+0.641430) 20.0 ms ✓, 19 iters	-918.862449 (+0.000507) 37.3 ms ✓, 16 iters	-918.862959 (-0.000003) 95.6 ms ✓, 6 iters	-918.862956 (-0.000001) 188.2 ms ✓, 2 iters
clcn	-551.679111	-539.967463 (+11.711648) 1.0 ms ✓, 25 iters	-552.196746 (-0.517636) 33.9 ms ✓, 25 iters	-552.483339 (-0.804228) 60.5 ms ✓, 25 iters	-550.245372 (+1.433739) 73.9 ms ✓, 25 iters	-546.629752 (+5.049358) 4.8 ms ✓, 25 iters	-553.892988 (-2.213877) 11.5 ms ✓, 25 iters	-551.671323 (+0.007787) 41.0 ms ✓, 25 iters	-551.679087 (+0.000024) 50.0 ms ✓, 7 iters	-551.679111 (-0.000000) 137.0 ms ✓, 1 iters	-551.679111 (-0.000000) 582.8 ms ✓, 0 iters
clcof	-671.516915	-651.409403 (+20.107512) 1.3 ms ✓, 66 iters	-672.324750 (-0.807835) 51.9 ms ✓, 66 iters	-672.581173 (-1.064258) 94.1 ms ✓, 66 iters	-670.065540 (+1.451375) 99.1 ms ✓, 70 iters	-663.854989 (+7.661926) 6.8 ms ✓, 71 iters	-670.537424 (+0.979492) 16.2 ms ✓, 59 iters	-671.507248 (+0.009667) 33.4 ms ✓, 25 iters	-671.516908 (+0.000007) 69.9 ms ✓, 20 iters	-671.516918 (-0.000003) 167.7 ms ✓, 2 iters	-671.516915 (-0.000000) 332.6 ms ✓, 3 iters
clf	-558.775217	-551.769225 (+7.005992) 0.7 ms ✓, 30 iters	-558.824557 (-0.049340) 26.6 ms ✓, 24 iters	-558.843113 (-0.067896) 46.7 ms ✓, 24 iters	-558.690304 (+0.084913) 45.4 ms ✓, 26 iters	-554.459302 (+4.315914) 3.4 ms ✓, 23 iters	-558.038206 (+0.737010) 8.1 ms ✓, 25 iters	-558.769341 (+0.005876) 16.1 ms ✓, 14 iters	-558.775212 (+0.000005) 31.7 ms ✓, 6 iters	-558.775223 (-0.000007) 78.1 ms ✓, 2 iters	-558.775217 (-0.000000) 180.5 ms ✓, 0 iters
clno	-588.581841	-579.301316 (+9.280525) 0.9 ms ✓, 25 iters	-588.862912 (-0.281071) 35.2 ms ✓, 25 iters	-589.068084 (-0.486243) 72.1 ms ✓, 25 iters	-587.768288 (+0.813553) 62.5 ms ✓, 25 iters	-582.877278 (+5.704562) 4.8 ms ✓, 25 iters	-587.219647 (+1.362194) 11.5 ms ✓, 25 iters	-588.290981 (+0.290860) 22.3 ms ✓, 25 iters	-588.328461 (+0.253380) 46.5 ms ✓, 25 iters	-588.511810 (+0.070031) 118.3 ms ✓, 25 iters	-588.581826 (+0.000015) 234.0 ms ✓, 20 iters
co	-112.667221	-103.595808 (+9.071413) 0.7 ms ✓, 157 iters	-112.796500 (-0.129279) 25.1 ms ✓, 157 iters	-112.915490 (-0.248269) 39.8 ms ✓, 155 iters	-112.045092 (+0.622128) 39.5 ms ✓, 173 iters	-109.655463 (+3.011758) 2.6 ms ✓, 134 iters	-112.541176 (+0.126045) 5.9 ms ✓, 134 iters	-112.665975 (+0.001245) 13.8 ms ✓, 66 iters	-112.667220 (+0.000001) 26.3 ms ✓, 6 iters	-112.667221 (-0.000000) 62.7 ms ✓, 3 iters	-112.667221 (-0.000000) 120.4 ms ✓, 1 iters
co2	-187.514942	-176.634435 (+10.880507) 0.7 ms ✓, 39 iters	-188.163180 (-0.648238) 26.2 ms ✓, 32 iters	-188.364376 (-0.849433) 42.7 ms ✓, 32 iters	-186.095802 (+1.419141) 39.7 ms ✓, 34 iters	-180.323489 (+7.191453) 3.9 ms ✓, 34 iters	-187.298198 (+0.216744) 10.5 ms ✓, 34 iters	-187.513861 (+0.001081) 17.7 ms ✓, 34 iters	-187.514989 (+0.000047) 36.6 ms ✓, 34 iters	-187.514995 (-0.000005) 96.1 ms ✓, 13 iters	-187.514942 (-0.000000) 198.3 ms ✓, 3 iters
cs	-435.239631	-430.216995 (+5.022636) 0.8 ms ✓, 158 iters	-435.331672 (-0.092041) 26.7 ms ✓, 158 iters	-435.488324 (-0.248693) 41.5 ms ✓, 139 iters	-434.716442 (+0.523190) 44.3 ms ✓, 139 iters	-431.813065 (+3.426566) 3.5 ms ✓, 124 iters	-434.177192 (+1.062439) 9.6 ms ✓, 124 iters	-434.856190 (+0.383441) 20.1 ms ✓, 66 iters	-434.901271 (+0.338360) 34.8 ms ✓, 75 iters	-435.239568 (+0.000063) 77.3 ms ✓, 28 iters	-435.239631 (-0.000000) 155.6 ms ✓, 3 iters
cs2	-832.788299	-824.844474 (+7.943824) 1.0 ms ✓, 75 iters	-833.358008 (-0.569710) 24.1 ms ✓, 58 iters	-833.635426 (-0.847128) 41.3 ms ✓, 54 iters	-831.388610 (+1.399688) 44.1 ms ✓, 67 iters	-827.553350 (+5.234949) 6.5 ms ✓, 67 iters	-831.442010 (+1.346289) 17.4 ms ✓, 44 iters	-832.393476 (+0.394823) 35.7 ms ✓, 44 iters	-832.773990 (+0.014308) 69.3 ms ✓, 29 iters	-832.788296 (+0.000003) 155.7 ms ✓, 12 iters	-832.788301 (-0.000003) 311.3 ms ✓, 16 iters
cyclobutadiene	-153.574148	-136.183353 (+17.390794) 1.1 ms ✓, 14 iters	-154.561877 (-0.987729) 23.2 ms ✓, 9 iters	-155.413665 (-1.839517) 21.5 ms ✓, 9 iters	-151.997662 (+1.576486) 21.9 ms ✓, 10 iters	-139.986260 (+13.587888) 7.0 ms ✓, 51 iters	-153.260081 (+0.314067) 16.2 ms ✓, 43 iters	-153.394159 (+0.179988) 33.1 ms ✓, 43 iters	-153.395504 (+0.178644) 73.2 ms ✓, 49 iters	-153.573528 (+0.000619) 169.9 ms ✓, 24 iters	-153.574148 (-0.000001) 333.0 ms ✓, 8 iters
cyclobutane	-156.029831	-132.005436 (+24.024395) 1.5 ms ✓, 20 iters	-156.858703 (-0.828872) 26.5 ms ✓, 11 iters	-157.960556 (-1.930724) 25.3 ms ✓, 13 iters	-153.822923 (+2.206909) 21.5 ms ✓, 15 iters	-144.160037 (+11.869795) 8.8 ms ✓, 19 iters	-156.054963 (-0.025131) 22.5 ms ✓, 13 iters	-156.025717 (+0.004115) 43.9 ms ✓, 9 iters	-156.029917 (-0.000085) 95.4 ms ✓, 6 iters	-156.029831 (-0.000000) 215.6 ms ✓, 1 iters	-156.029831 (-0.000000) 471.8 ms ✓, 1 iters
cyclobutene	-154.832248	-134.255722 (+20.576526) 1.2 ms ✓, 10 iters	-155.780713 (-0.948465) 23.7 ms ✓, 10 iters	-156.764059 (-1.931811) 26.4 ms ✓, 11 iters	-152.901796 (+1.930453) 27.3 ms ✓, 13 iters	-142.383829 (+12.448419) 7.5 ms ✓, 26 iters	-154.118396 (+0.713852) 20.5 ms ✓, 23 iters	-154.809554 (+0.022694) 37.0 ms ✓, 16 iters	-154.832001 (+0.000247) 75.0 ms ✓, 12 iters	-154.832249 (-0.000001) 194.3 ms ✓, 6 iters	-154.832248 (-0.000000) 408.1 ms ✓, 2 iters
cyclopentadiene	-192.718214	-169.065388 (+23.652827) 1.5 ms ✓, 20 iters	-194.065942 (-1.347728) 29.0 ms ✓, 20 iters	-195.233653 (-2.515439) 26.4 ms ✓, 21 iters	-190.470735 (+2.247480) 27.3 ms ✓, 25 iters	-178.978390 (+13.739824) 13.9 ms ✓, 18 iters	-192.403683 (+0.314531) 61.2 ms ✓, 18 iters	-192.760369 (-0.042155) 61.2 ms ✓, 24 iters	-192.718425 (-0.000210) 120.2 ms ✓, 15 iters	-192.718215 (-0.000000) 294.5 ms ✓, 3 iters	-192.718214 (-0.000000) 595.9 ms ✓, 2 iters
cyclopropane	-117.007644	-99.258395 (+17.749250) 1.1 ms ✓, 17 iters	-117.678897 (-0.671253) 26.6 ms ✓, 10 iters	-118.454512 (-1.446867) 23.8 ms ✓, 11 iters	-115.262745 (+1.744900) 24.2 ms ✓, 13 iters	-107.802386 (+9.205258) 5.6 ms ✓, 18 iters	-116.821123 (+0.186522) 13.3 ms ✓, 12 iters	-117.006244 (+0.001400) 26.9 ms ✓, 8 iters	-117.007641 (+0.000003) 54.8 ms ✓, 5 iters	-117.007645 (-0.000000) 133.0 ms ✓, 2 iters	-117.007644 (-0.000000) 254.2 ms ✓, 1 iters
cyclopropene	-115.765808	-101.091458 (+14.674350) 0.9 ms ✓, 25 iters	-116.519846 (-0.754038) 23.5 ms ✓, 9 iters	-117.159039 (-1.393231) 22.2 ms ✓, 11 iters	-114.284785 (+1.481023) 22.4 ms ✓, 13 iters	-107.777708 (+7.988100) 4.9 ms ✓, 27 iters	-115.121923 (+0.643885) 11.9 ms ✓, 22 iters	-115.116975 (+0.648833) 24.0 ms ✓, 17 iters	-115.672590 (+0.093218) 46.9 ms ✓, 17 iters	-115.765805 (+0.000003) 125.6 ms ✓, 8 iters	-115.765808 (-0.000000) 237.0 ms ✓, 0 iters
dioxetan2one	-301.283713	-269.598604 (+31.685108) 1.3 ms ✓, 62 iters	-302.724883 (-1.441170) 33.7 ms ✓, 62 iters	-303.348049 (-2.064336) 44.1 ms ✓, 62 iters	-298.754263 (+2.529449) 42.7 ms ✓, 65 iters	-288.360428 (+12.923285) 10.7 ms ✓, 49 iters	-300.766571 (+0.517142) 23.3 ms ✓, 49 iters	-301.286647 (-0.002934) 46.8 ms ✓, 40 iters	-301.284327 (-0.000614) 90.9 ms ✓, 24 iters	-301.283714 (-0.000001) 230.8 ms ✓, 5 iters	-301.283713 (-0.000000) 476.0 ms ✓, 1 iters
dioxetane	-227.599550	-205.616411 (+21.983139) 1.2 ms ✓, 23 iters	-228.489653 (-0.890103) 37.8 ms ✓, 23 iters	-229.139819 (-1.540269) 45.1 ms ✓, 23 iters	-225.379930 (+2.219620) 50.1 ms ✓, 25 iters	-213.038447 (+14.561102) 7.0 ms ✓, 21 iters	-227.195748 (+0.403802) 32.9 ms ✓, 21 iters	-227.603739 (-0.004189) 68.4 ms ✓, 17 iters	-227.599543 (+0.000007) 68.4 ms ✓, 5 iters	-227.599550 (+0.000000) 166.5 ms ✓, 0 iters	-227.599550 (-0.000000) 348.9 ms ✓, 0 iters

dioxirane	-188.501623	-171.093838 (+17.407785) 0.8 ms ✗	-188.929616 (-0.427993) 35.4 ms ✓, 16 iters	-189.279573 (-0.777950) 41.2 ms ✓, 16 iters	-187.247070 (+1.254553) 41.9 ms ✓, 18 iters	-180.306779 (+8.194843) 4.0 ms ✗	-188.086171 (+0.415452) 10.4 ms ✓, 178 iters	-188.494596 (+0.007026) 20.6 ms ✓, 143 iters	-188.501621 (+0.000001) 44.1 ms ✓, 27 iters	-188.501623 (+0.000000) 98.7 ms ✓, 3 iters	-188.501623 (-0.000000) 200.1 ms ✓, 1 iters
dithiotane	-872.942829	-859.257909 (+13.684920) 1.4 ms ✓, 20 iters	-873.699682 (-0.756853) 36.0 ms ✓, 16 iters	-874.381625 (-1.438796) 45.2 ms ✓, 15 iters	-871.034257 (+1.908572) 50.1 ms ✓, 18 iters	-861.772456 (+11.170373) 11.5 ms ✓, 22 iters	-871.390010 (+1.552819) 25.8 ms ✓, 15 iters	-872.930862 (+0.011967) 54.3 ms ✓, 9 iters	-872.942812 (+0.000017) 104.6 ms ✓, 6 iters	-872.942830 (-0.000001) 274.5 ms ✓, 1 iters	-872.942829 (-0.000000) 514.8 ms ✓, 0 iters
ethanol	-154.011874	-134.214577 (+19.797297) 1.4 ms ✗	-154.311215 (-0.299341) 38.4 ms ✓, 21 iters	-154.923133 (-0.911259) 49.8 ms ✓, 21 iters	-152.446015 (+1.565860) 42.8 ms ✓, 22 iters	-145.762071 (+8.249803) 9.3 ms ✗	-153.805045 (+0.206829) 15.7 ms ✓, 20 iters	-154.010912 (+0.000962) 33.5 ms ✓, 13 iters	-154.011917 (-0.000043) 68.7 ms ✓, 6 iters	-154.011875 (-0.000000) 155.2 ms ✓, 2 iters	-154.011874 (-0.000000) 311.1 ms ✓, 0 iters
f2	-198.646097	-189.022850 (+9.623247) 0.7 ms ✓, 12 iters	-198.463017 (-0.847726) 13.8 ms ✓, 9 iters	-198.493132 (+0.152965) 23.6 ms ✓, 9 iters	-198.623690 (+0.022407) 21.1 ms ✓, 8 iters	-193.173794 (+5.472303) 2.3 ms ✓, 12 iters	-197.558236 (+1.087861) 6.6 ms ✓, 11 iters	-198.017546 (+0.628551) 11.7 ms ✓, 70 iters	-198.645997 (+0.000100) 23.7 ms ✓, 29 iters	-198.646097 (-0.000000) 64.8 ms ✓, 4 iters	-198.646097 (-0.000000) 137.6 ms ✓, 1 iters
f2co	-311.476901	-289.241291 (+22.235611) 0.9 ms ✗	-312.324627 (-0.847726) 33.4 ms ✓, 51 iters	-312.541718 (-1.064817) 59.2 ms ✓, 51 iters	-310.029142 (+1.447759) 60.2 ms ✓, 54 iters	-303.116192 (+8.360709) 4.5 ms ✓, 70 iters	-310.985921 (+0.490981) 11.2 ms ✓, 48 iters	-311.518999 (-0.042098) 22.9 ms ✓, 39 iters	-311.476859 (+0.000043) 45.5 ms ✓, 19 iters	-311.476901 (-0.000000) 111.5 ms ✓, 1 iters	-311.476901 (-0.000000) 222.7 ms ✓, 0 iters
fccf	-274.362968	-258.236825 (+16.126143) 0.9 ms ✗	-275.298312 (-0.935344) 26.0 ms ✓, 21 iters	-275.600288 (-1.237320) 46.0 ms ✓, 20 iters	-273.229415 (+1.133553) 43.9 ms ✓, 24 iters	-265.619063 (+8.743905) 4.9 ms ✓, 28 iters	-273.214476 (+1.148492) 12.1 ms ✓, 33 iters	-274.314540 (+0.048428) 24.8 ms ✓, 33 iters	-274.361982 (+0.000986) 51.6 ms ✓, 23 iters	-274.362969 (-0.000001) 129.1 ms ✓, 12 iters	-274.362968 (-0.000000) 247.6 ms ✓, 7 iters
fno	-228.509837	-215.648013 (+12.861825) 0.8 ms ✗	-228.787436 (-0.277599) 36.7 ms ✗	-228.983449 (-0.473612) 59.9 ms ✗	-227.618866 (+0.890972) 66.9 ms ✗	-222.005895 (+6.503942) 3.4 ms ✗	-228.173198 (+0.336639) 8.8 ms ✗	-228.504190 (+0.005648) 17.6 ms ✓, 137 iters	-228.509769 (+0.000069) 33.3 ms ✓, 124 iters	-228.509837 (-0.000000) 82.8 ms ✓, 2 iters	-228.509837 (-0.000000) 178.4 ms ✓, 0 iters
formamide	-168.854315	-152.598228 (+16.256088) 1.0 ms ✗	-169.373319 (-0.519004) 46.6 ms ✓, 58 iters	-169.835121 (-0.980806) 60.8 ms ✓, 57 iters	-167.365118 (+1.489197) 60.9 ms ✓, 65 iters	-161.804081 (+7.050234) 4.2 ms ✗	-167.644622 (+1.209693) 10.5 ms ✓, 47 iters	-168.296353 (+0.557962) 20.3 ms ✓, 30 iters	-168.853885 (+0.000430) 40.9 ms ✓, 11 iters	-168.854315 (+0.000000) 102.8 ms ✓, 0 iters	-168.854315 (-0.000000) 231.3 ms ✓, 0 iters
formic-anhydride	-301.311704	-278.556963 (+22.754740) 1.4 ms ✗	-302.459694 (-1.147990) 35.5 ms ✓, 119 iters	-302.986531 (-1.674828) 46.3 ms ✓, 118 iters	-298.796556 (+2.515148) 44.2 ms ✓, 132 iters	-289.602257 (+11.709447) 10.1 ms ✗	-300.130732 (+1.180972) 24.3 ms ✓, 95 iters	-301.282294 (+0.029409) 47.9 ms ✓, 84 iters	-301.311087 (+0.000617) 91.4 ms ✓, 55 iters	-301.311704 (+0.000000) 230.2 ms ✓, 5 iters	-301.311704 (-0.000000) 464.6 ms ✓, 0 iters
formic	-188.662894	-173.876317 (+14.786577) 0.9 ms ✗	-189.174302 (-0.511408) 33.8 ms ✓, 64 iters	-189.490255 (-0.827361) 40.7 ms ✓, 63 iters	-187.319034 (+1.343861) 41.6 ms ✓, 70 iters	-182.215499 (+6.447396) 5.0 ms ✓, 73 iters	-188.351153 (+0.311741) 10.6 ms ✓, 51 iters	-188.660829 (+0.002065) 20.3 ms ✓, 23 iters	-188.662821 (+0.000073) 42.1 ms ✓, 27 iters	-188.662894 (+0.000000) 101.0 ms ✓, 1 iters	-188.662894 (-0.000000) 200.0 ms ✓, 0 iters
furan	-228.523788	-202.958914 (+25.564875) 1.8 ms ✗	-230.063898 (-1.540110) 37.8 ms ✓, 38 iters	-231.015642 (-2.491854) 48.6 ms ✓, 28 iters	-226.351717 (+2.172072) 44.7 ms ✓, 47 iters	-212.177976 (+16.345812) 11.9 ms ✗	-228.195892 (+0.327896) 28.3 ms ✓, 40 iters	-228.530204 (-0.006415) 55.2 ms ✓, 23 iters	-228.523758 (+0.000030) 108.4 ms ✓, 11 iters	-228.523788 (-0.000000) 269.7 ms ✓, 2 iters	-228.523788 (-0.000000) 546.3 ms ✓, 1 iters
glyoxal	-226.474933	-207.807743 (+18.667190) 1.1 ms ✗	-227.144285 (-0.669352) 34.3 ms ✓, 73 iters	-227.610210 (-1.135277) 41.6 ms ✓, 72 iters	-224.232266 (+2.242667) 44.8 ms ✓, 83 iters	-218.095303 (+8.379631) 6.4 ms ✓, 86 iters	-225.409139 (+1.065794) 15.4 ms ✓, 63 iters	-225.824403 (+0.650531) 32.1 ms ✓, 62 iters	-226.472228 (+0.002705) 59.3 ms ✓, 31 iters	-226.474932 (+0.000001) 161.6 ms ✓, 10 iters	-226.474938 (-0.000004) 353.9 ms ✓, 15 iters
h2	-1.126726	-1.074200 (+0.052525) 0.7 ms ✓, 5 iters	-0.806938 (+0.319788) 12.8 ms ✓, 5 iters	-0.846739 (+0.279986) 2.0 ms ✓, 5 iters	-1.090206 (+0.036519) 2.4 ms ✓, 5 iters	-0.044400 (+1.082326) 1.7 ms ✓, 5 iters	-0.045503 (+1.081223) 3.8 ms ✓, 5 iters	-1.125658 (+0.001068) 8.8 ms ✓, 6 iters	-1.126725 (+0.000001) 14.5 ms ✓, 3 iters	-1.126726 (-0.000000) 37.3 ms ✓, 0 iters	-1.126726 (-0.000000) 62.5 ms ✓, 0 iters
h2co	-113.807811	-102.694122 (+11.113689) 0.8 ms ✗	-113.950195 (-0.142384) 39.8 ms ✓, 57 iters	-114.181871 (-0.374060) 45.5 ms ✓, 57 iters	-112.635331 (+1.172480) 48.9 ms ✓, 62 iters	-109.619773 (+4.188038) 2.6 ms ✗	-113.662647 (+0.145164) 6.3 ms ✓, 48 iters	-113.805871 (+0.001940) 12.3 ms ✓, 23 iters	-113.807794 (+0.000016) 25.3 ms ✓, 9 iters	-113.807811 (+0.000000) 62.4 ms ✓, 0 iters	-113.807811 (-0.000000) 125.2 ms ✓, 0 iters
h2o	-75.983831	-69.622812 (+6.361019) 1.2 ms ✓, 24 iters	-75.834360 (+0.149471) 28.1 ms ✓, 18 iters	-75.937782 (+0.046049) 25.8 ms ✓, 19 iters	-75.866020 (+0.117811) 24.2 ms ✓, 14 iters	-72.358780 (+3.625051) 2.2 ms ✓, 23 iters	-75.898398 (+0.085434) 7.6 ms ✓, 18 iters	-75.983081 (+0.000750) 12.3 ms ✓, 11 iters	-75.983826 (+0.000005) 28.1 ms ✓, 6 iters	-75.983831 (+0.000000) 48.9 ms ✓, 0 iters	-75.983831 (-0.000000) 86.4 ms ✓, 0 iters
h2s	-398.626802	-395.123588 (+3.503214) 0.8 ms ✓, 11 iters	-398.502608 (+0.124194) 23.0 ms ✓, 9 iters	-398.633888 (-0.007086) 25.0 ms ✓, 9 iters	-398.518339 (+0.108463) 26.2 ms ✓, 9 iters	-395.579564 (+3.047238) 3.0 ms ✓, 13 iters	-397.872076 (+0.754726) 7.7 ms ✓, 9 iters	-398.624013 (+0.002789) 14.0 ms ✓, 7 iters	-398.626801 (+0.000001) 25.8 ms ✓, 4 iters	-398.626802 (-0.000000) 61.4 ms ✓, 1 iters	-398.626802 (-0.000000) 109.9 ms ✓, 1 iters
hccf	-175.581615	-158.806255 (+16.775361) 0.9 ms ✗	-176.146356 (-0.564741) 33.6 ms ✓, 46 iters	-176.430977 (-0.849362) 43.9 ms ✓, 47 iters	-174.525767 (+1.055848) 43.6 ms ✓, 48 iters	-169.591589 (+5.990026) 3.9 ms ✗	-174.850662 (+0.730953) 9.8 ms ✓, 52 iters	-175.568953 (+0.012662) 19.3 ms ✓, 34 iters	-175.581513 (+0.000102) 38.5 ms ✓, 14 iters	-175.581615 (-0.000000) 100.0 ms ✓, 2 iters	-175.581615 (-0.000000) 203.4 ms ✓, 1 iters
hcl	-460.036945	-456.927365 (+3.109580) 0.7 ms ✓, 9 iters	-459.956728 (+0.080218) 25.5 ms ✓, 8 iters	-460.031781 (+0.005164) 27.1 ms ✓, 8 iters	-459.966640 (+0.070305) 27.9 ms ✓, 7 iters	-457.404151 (+2.632794) 2.4 ms ✓, 9 iters	-459.329005 (+0.707940) 5.8 ms ✓, 9 iters	-460.034008 (+0.002937) 13.3 ms ✓, 6 iters	-460.036945 (+0.000000) 22.1 ms ✓, 3 iters	-460.036945 (-0.000000) 54.2 ms ✓, 0 iters	-460.036945 (+0.000000) 109.9 ms ✓, 0 iters
hclo4	-758.511760	-738.762538 (+19.749222) 1.4 ms ✗	-761.491686 (-2.979927) 41.4 ms ✓, 42 iters	-761.726301 (-3.214541) 51.3 ms ✓, 41 iters	-757.027325 (+1.484435) 50.3 ms ✓, 47 iters	-744.515029 (+13.996731) 10.8 ms ✗	-756.731322 (+1.780438) 33.1 ms ✓, 32 iters	-758.486764 (+0.024996) 61.9 ms ✓, 31 iters	-758.511976 (-0.000216) 113.1 ms ✓, 31 iters	-758.511774 (-0.000014) 281.5 ms ✓, 20 iters	-758.511760 (-0.000000) 550.1 ms ✓, 0 iters

hcn	-92.827778	-81.914741 (+10.913037) 0.6 ms X	-92.924982 (-0.097204) 33.9 ms X	-93.153960 (-0.326181) 41.9 ms X	-91.540891 (+1.286887) 42.8 ms X	-90.645247 (+2.182532) 2.7 ms X	-92.656290 (+0.171489) 6.2 ms X	-92.846259 (-0.018481) 13.5 ms X	-92.827823 (-0.000045) 24.2 ms X	-92.827779 (-0.000001) 60.8 ms ✓, 5 iters	-92.827778 (-0.000000) 122.5 ms ✓, 1 iters
hcno	-167.536848	-149.050242 (+18.486605) 0.9 ms X	-168.293277 (-0.756430) 48.0 ms X	-168.630976 (-1.094129) 62.4 ms X	-166.030164 (+1.506684) 69.1 ms X	-162.478476 (+5.058372) 4.0 ms X	-167.271996 (+0.264852) 9.5 ms X	-167.537145 (-0.000298) 20.1 ms X	-167.536843 (+0.000005) 44.1 ms ✓, 13 iters	-167.536867 (-0.000020) 106.2 ms X	-167.536849 (-0.000002) 206.6 ms X
hcof	-212.653427	-198.122387 (+14.531040) 0.8 ms X	-213.100084 (-0.446656) 45.8 ms ✓, 59 iters	-213.328164 (-0.674736) 62.0 ms ✓, 59 iters	-211.337422 (+1.316005) 66.2 ms ✓, 64 iters	-205.166843 (+7.486584) 4.3 ms X	-211.757262 (+0.896165) 8.8 ms ✓, 49 iters	-212.101357 (+0.552071) 18.5 ms ✓, 27 iters	-212.624320 (+0.029107) 37.9 ms ✓, 37 iters	-212.653422 (+0.000005) 90.9 ms ✓, 10 iters	-212.653427 (+0.000000) 191.4 ms ✓, 0 iters
hf	-99.983397	-93.679547 (+6.303850) 0.6 ms ✓, 21 iters	-99.807365 (+0.176032) 22.1 ms ✓, 16 iters	-99.862595 (+0.120802) 22.2 ms ✓, 16 iters	-99.882955 (+0.100441) 25.3 ms ✓, 15 iters	-96.568815 (+3.414582) 1.7 ms ✓, 20 iters	-99.907200 (+0.076197) 4.6 ms ✓, 16 iters	-99.983229 (+0.000168) 9.1 ms ✓, 10 iters	-99.983396 (+0.000001) 19.6 ms ✓, 4 iters	-99.983397 (-0.000000) 34.2 ms ✓, 0 iters	-99.983397 (-0.000000) 80.2 ms ✓, 0 iters
hnc	-92.814612	-83.440650 (+9.373962) 0.7 ms X	-92.958657 (-0.144044) 34.1 ms ✓, 39 iters	-93.191766 (-0.377154) 41.7 ms ✓, 51 iters	-92.118171 (+0.696441) 41.4 ms ✓, 56 iters	-90.723657 (+2.090955) 3.2 ms ✓, 58 iters	-92.667346 (+0.147266) 7.5 ms ✓, 48 iters	-92.813485 (+0.001127) 13.1 ms ✓, 38 iters	-92.814630 (-0.000017) 24.7 ms ✓, 9 iters	-92.814613 (-0.000001) 58.7 ms ✓, 6 iters	-92.814612 (-0.000000) 122.9 ms ✓, 2 iters
hnco	-167.662159	-151.012754 (+16.649405) 0.8 ms X	-168.300336 (-0.638178) 44.0 ms X	-168.634212 (-0.972053) 62.7 ms X	-166.286108 (+1.376050) 64.1 ms X	-162.894395 (+4.767764) 4.7 ms X	-166.793407 (+0.868752) 10.1 ms X	-167.436862 (+0.225297) 20.4 ms ✓, 125 iters	-167.658420 (+0.003739) 38.1 ms ✓, 61 iters	-167.662158 (+0.000001) 107.9 ms ✓, 8 iters	-167.662159 (+0.000000) 216.2 ms ✓, 0 iters
hnnn	-163.728413	-147.741571 (+15.986842) 0.9 ms X	-164.416008 (-0.687595) 23.7 ms X	-164.867358 (-1.138945) 24.0 ms X	-162.651408 (+1.077005) 25.1 ms X	-159.261638 (+4.466776) 4.5 ms X	-163.404928 (+0.323485) 9.6 ms X	-163.714294 (+0.014119) 23.3 ms X	-163.726705 (+0.001708) 39.9 ms X	-163.728409 (+0.000004) 98.0 ms X	-163.728413 (+0.000000) 189.4 ms ✓, 0 iters
hno	-129.712437	-119.819422 (+9.893015) 0.7 ms X	-129.834734 (-0.122297) 33.5 ms ✓, 142 iters	-130.043730 (-0.331293) 45.6 ms ✓, 136 iters	-129.040421 (+0.672016) 42.0 ms ✓, 156 iters	-126.065517 (+3.646920) 2.5 ms ✓, 136 iters	-129.509623 (+0.202814) 6.0 ms ✓, 105 iters	-129.710558 (+0.001879) 11.7 ms ✓, 15 iters	-129.712407 (+0.000030) 23.2 ms ✓, 24 iters	-129.712437 (+0.000000) 61.1 ms ✓, 0 iters	-129.712437 (-0.000000) 117.4 ms ✓, 0 iters
hocl	-534.788222	-527.817879 (+6.970343) 0.7 ms ✓, 31 iters	-534.847037 (-0.058815) 33.7 ms ✓, 24 iters	-534.945273 (-0.157051) 44.5 ms ✓, 26 iters	-534.676666 (+0.111556) 46.1 ms ✓, 25 iters	-530.043413 (+4.744809) 3.2 ms ✓, 33 iters	-533.853244 (+0.934978) 7.1 ms ✓, 21 iters	-534.776525 (+0.011697) 15.0 ms ✓, 16 iters	-534.787997 (+0.000225) 30.7 ms ✓, 12 iters	-534.788222 (-0.000000) 71.7 ms ✓, 2 iters	-534.788222 (-0.000000) 155.7 ms ✓, 0 iters
hoclo	-609.398163	-598.416888 (+10.981275) 1.1 ms X	-610.041019 (-0.642856) 37.4 ms ✓, 64 iters	-610.183862 (-0.785699) 49.0 ms ✓, 63 iters	-609.012593 (+0.385569) 48.1 ms ✓, 65 iters	-602.534131 (+6.864032) 6.6 ms X	-607.888368 (+1.509795) 13.0 ms X	-609.204011 (+0.194152) 25.6 ms ✓, 33 iters	-609.387477 (+0.010686) 51.9 ms ✓, 31 iters	-609.398159 (+0.000004) 132.1 ms ✓, 10 iters	-609.398163 (-0.000000) 271.8 ms ✓, 0 iters
hoclo2	-683.971111	-668.704381 (+15.266730) 1.1 ms X	-685.668435 (-1.697325) 36.7 ms ✓, 61 iters	-685.859428 (-1.888318) 47.0 ms ✓, 61 iters	-683.121255 (+0.849856) 40.8 ms ✓, 60 iters	-673.395487 (+10.575624) 7.8 ms X	-682.531706 (+1.439405) 20.0 ms ✓, 51 iters	-683.950549 (+0.020562) 38.5 ms ✓, 40 iters	-683.970791 (+0.000319) 77.6 ms ✓, 37 iters	-683.971111 (-0.000000) 196.1 ms ✓, 7 iters	-683.971111 (-0.000000) 390.9 ms ✓, 0 iters
hocn	-167.632543	-152.811194 (+14.821349) 0.9 ms X	-168.146723 (-0.514180) 46.8 ms X	-168.475057 (-0.842514) 65.3 ms X	-166.180519 (+1.452024) 63.3 ms X	-162.503036 (+5.129507) 4.9 ms X	-166.768668 (+0.863874) 9.7 ms X	-167.258343 (+0.374200) 19.3 ms X	-167.627981 (+0.004561) 38.2 ms X	-167.632541 (+0.000002) 96.7 ms ✓, 10 iters	-167.632543 (+0.000000) 199.8 ms ✓, 0 iters
hof	-174.684623	-164.373819 (+10.310803) 0.8 ms X	-174.534454 (+0.150169) 38.3 ms ✓, 41 iters	-174.621431 (+0.063192) 39.8 ms ✓, 37 iters	-174.477726 (+0.206897) 39.4 ms ✓, 46 iters	-169.063385 (+5.621237) 2.7 ms X	-174.424961 (+0.259661) 6.9 ms ✓, 37 iters	-174.675471 (+0.009151) 13.5 ms ✓, 23 iters	-174.684300 (+0.000322) 25.2 ms ✓, 14 iters	-174.684623 (+0.000000) 63.3 ms ✓, 4 iters	-174.684623 (-0.000000) 127.1 ms ✓, 0 iters
honc	-167.541956	-151.723233 (+15.818723) 0.9 ms X	-168.023420 (-0.481464) 44.9 ms ✓, 80 iters	-168.366734 (-0.824778) 60.8 ms ✓, 74 iters	-166.682299 (+0.859657) 60.1 ms ✓, 86 iters	-160.558446 (+6.983510) 4.0 ms X	-167.295690 (+0.246266) 9.6 ms ✓, 74 iters	-167.540511 (+0.001445) 20.0 ms ✓, 36 iters	-167.541951 (+0.000005) 36.7 ms ✓, 6 iters	-167.541956 (+0.000000) 95.5 ms ✓, 0 iters	-167.541956 (-0.000000) 190.8 ms ✓, 0 iters
hooh	-150.707714	-140.737502 (+9.970212) 0.7 ms ✓, 18 iters	-150.624273 (+0.083441) 25.3 ms ✓, 14 iters	-150.780343 (-0.072628) 24.0 ms ✓, 14 iters	-150.510037 (+0.197677) 24.3 ms ✓, 16 iters	-144.739940 (+5.967774) 3.2 ms ✓, 22 iters	-149.698079 (+1.009636) 7.5 ms ✓, 19 iters	-149.994354 (+0.713360) 16.6 ms ✓, 38 iters	-150.706045 (+0.001669) 30.6 ms ✓, 24 iters	-150.707714 (+0.000000) 70.9 ms ✓, 4 iters	-150.707714 (-0.000000) 137.1 ms ✓, 1 iters
ketene	-151.648743	-130.883087 (+20.765656) 0.9 ms X	-152.232662 (-0.583919) 38.3 ms ✓, 98 iters	-152.610015 (-0.961272) 43.8 ms ✓, 95 iters	-150.119608 (+1.529136) 43.7 ms ✓, 128 iters	-147.067371 (+4.581373) 4.6 ms X	-150.983046 (+0.665697) 11.7 ms ✓, 87 iters	-151.262589 (+0.386155) 23.0 ms ✓, 53 iters	-151.602606 (+0.046137) 42.5 ms ✓, 55 iters	-151.648721 (+0.000022) 108.0 ms ✓, 14 iters	-151.648743 (+0.000000) 214.9 ms ✓, 0 iters
methanol	-114.986865	-102.677064 (+12.309801) 0.8 ms X	-115.048256 (-0.061392) 33.9 ms ✓, 21 iters	-115.388516 (-0.401651) 42.6 ms ✓, 21 iters	-114.023620 (+0.963245) 42.0 ms ✓, 21 iters	-108.932061 (+6.054804) 3.2 ms X	-114.942273 (+0.044592) 7.8 ms ✓, 20 iters	-114.987308 (-0.000443) 16.5 ms ✓, 12 iters	-114.986862 (+0.000003) 31.7 ms ✓, 5 iters	-114.986865 (+0.000000) 81.8 ms ✓, 0 iters	-114.986865 (-0.000000) 157.2 ms ✓, 0 iters
mr_bn	-78.851376	-71.928593 (+6.922783) 0.7 ms X	-78.922782 (-0.071406) 23.2 ms X	-79.055949 (-0.204573) 38.4 ms X	-78.185750 (+0.665626) 40.8 ms X	-76.245010 (+2.606366) 2.3 ms X	-78.741568 (+0.109808) 4.8 ms X	-78.849951 (+0.001425) 10.6 ms X	-78.851266 (+0.000110) 21.4 ms X	-78.851392 (-0.000016) 54.0 ms X	-78.851391 (-0.000015) 119.1 ms X
mr_c2	-75.348392	-70.857729 (+4.490663) 0.7 ms ✓, 10 iters	-75.519534 (-0.171142) 12.5 ms ✓, 9 iters	-75.688656 (-0.340264) 22.8 ms ✓, 9 iters	-74.882390 (+0.466002) 20.8 ms ✓, 10 iters	-72.421236 (+2.927156) 2.7 ms ✓, 9 iters	-73.965648 (+1.382744) 6.3 ms X	-75.299323 (+0.049069) 12.1 ms X	-75.363227 (-0.014835) 21.2 ms X	-75.364058 (-0.015666) 54.3 ms X	-75.364090 (-0.015698) 109.9 ms X

mr_cl2o	-993.591313	-981.902364 (+11.688948) 0.9 ms ✗	-993.846106 (-0.254794) 22.5 ms ✓, 55 iters	-993.928351 (-0.337038) 44.2 ms ✓, 52 iters	-993.478425 (+0.112887) 42.2 ms ✓, 55 iters	-987.920281 (+5.671032) 7.1 ms ✓, 56 iters	-992.202874 (+1.388439) 16.2 ms ✓, 51 iters	-993.571410 (+0.019903) 33.3 ms ✓, 26 iters	-993.591035 (+0.000277) 61.4 ms ✓, 19 iters	-993.591331 (-0.000018) 165.1 ms ✓, 7 iters	-993.591313 (-0.000000) 320.1 ms ✓, 1 iters
mr_clf3	-757.324492	-739.832688 (+17.491804) 1.0 ms ✗	-757.921673 (-0.597182) 27.0 ms ✓, 24 iters	-757.904289 (-0.579797) 42.6 ms ✓, 24 iters	-756.827886 (+0.496605) 44.5 ms ✓, 24 iters	-747.616802 (+9.707689) 7.2 ms ✓, 30 iters	-756.107993 (+1.216498) 18.6 ms ✓, 28 iters	-757.316310 (+0.008182) 36.9 ms ✓, 33 iters	-757.324441 (+0.000051) 72.8 ms ✓, 18 iters	-757.324507 (-0.000015) 183.4 ms ✓, 13 iters	-757.324492 (-0.000000) 356.6 ms ✓, 19 iters
mr_clf5	-955.814817	-928.578172 (+27.236645) 1.7 ms ✗	-957.298984 (-1.484167) 23.5 ms ✓, 36 iters	-957.187290 (-1.372474) 43.9 ms ✓, 36 iters	-954.683141 (+1.131675) 46.2 ms ✓, 37 iters	-940.003060 (+15.811756) 18.8 ms ✗	-953.986680 (+1.828137) 42.8 ms ✓, 42 iters	-955.801279 (+0.013537) 81.5 ms ✓, 21 iters	-955.815561 (-0.000744) 177.6 ms ✓, 33 iters	-955.814817 (-0.000000) 408.1 ms ✓, 16 iters	-955.814817 (-0.000000) 814.9 ms ✓, 0 iters
mr_cloocl	-1068.321164	-1053.147190 (+15.173974) 1.1 ms ✗	-1068.676536 (-0.355371) 24.7 ms ✓, 31 iters	-1068.799395 (-0.478231) 41.2 ms ✓, 30 iters	-1068.112319 (+0.208845) 44.9 ms ✓, 31 iters	-1060.151938 (+8.169226) 9.1 ms ✓, 64 iters	-1066.034982 (+2.286182) 22.2 ms ✓, 63 iters	-1068.271992 (+0.049172) 41.6 ms ✓, 36 iters	-1068.320815 (+0.000349) 82.8 ms ✓, 41 iters	-1068.321164 (-0.000000) 225.2 ms ✓, 13 iters	-1068.321166 (-0.000002) 427.8 ms ✓, 4 iters
mr_f2o	-273.381615	-258.456303 (+14.925311) 0.9 ms ✓, 133 iters	-273.339084 (+0.042531) 26.9 ms ✓, 94 iters	-273.407484 (-0.025869) 46.9 ms ✓, 92 iters	-273.038923 (+0.342692) 42.4 ms ✓, 99 iters	-266.417045 (+6.964569) 4.0 ms ✓, 103 iters	-273.006718 (+0.374897) 9.8 ms ✓, 70 iters	-273.383076 (-0.001461) 18.8 ms ✓, 43 iters	-273.381558 (+0.000056) 37.2 ms ✓, 10 iters	-273.381614 (+0.000000) 91.6 ms ✓, 6 iters	-273.381615 (-0.000000) 210.3 ms ✓, 0 iters
mr_foof	-348.092213	-329.493654 (+18.598559) 1.0 ms ✗	-348.252832 (-0.160619) 23.9 ms ✗	-348.352446 (-0.260233) 39.3 ms ✗	-347.401056 (+0.691157) 44.4 ms ✗	-338.365235 (+9.726977) 5.2 ms ✗	-346.896552 (+1.195661) 12.5 ms ✗	-347.535360 (+0.556853) 25.0 ms ✗	-348.068092 (+0.024121) 56.9 ms ✗	-348.092214 (-0.000001) 129.0 ms ✓, 193 iters	-348.092213 (-0.000000) 247.6 ms ✓, 2 iters
mr_o3	-224.137650	-210.962220 (+13.175430) 0.7 ms ✗	-224.597961 (-0.460311) 13.8 ms ✗	-224.741077 (-0.603427) 21.2 ms ✗	-223.515073 (+0.622577) 20.8 ms ✗	-218.453927 (+5.683723) 3.4 ms ✗	-223.633385 (+0.504265) 8.6 ms ✗	-223.992456 (+0.145194) 18.7 ms ✗	-223.996897 (+0.140753) 33.1 ms ✗	-223.997015 (+0.140635) 96.4 ms ✗	-224.023168 (+0.114482) 194.8 ms ✗
mr_s3	-1192.329712	-1184.497788 (+7.831923) 1.0 ms ✓, 32 iters	-1192.944624 (-0.614912) 14.0 ms ✓, 24 iters	-1193.104945 (-0.775233) 23.8 ms ✓, 24 iters	-1191.966434 (+0.363278) 24.2 ms ✓, 24 iters	-1185.937713 (+6.391999) 7.3 ms ✗	-1190.747042 (+1.582670) 17.1 ms ✓, 83 iters	-1192.202812 (+0.126900) 35.2 ms ✓, 80 iters	-1192.221206 (+0.108506) 70.0 ms ✓, 79 iters	-1192.221225 (+0.108487) 182.5 ms ✓, 62 iters	-1192.308410 (+0.021302) 345.7 ms ✗
mr_s4-c2v	-1589.764467	-1578.255384 (+11.509083) 1.4 ms ✗	-1590.652459 (-0.887991) 12.7 ms ✗	-1590.878763 (-1.114296) 23.1 ms ✗	-1589.312508 (+0.451960) 23.6 ms ✗	-1581.553057 (+8.211410) 12.3 ms ✗	-1587.486080 (+2.278387) 31.2 ms ✗	-1589.657206 (+0.107261) 65.5 ms ✗	-1589.745479 (+0.018988) 124.3 ms ✗	-1589.763737 (+0.000730) 327.0 ms ✗	-1589.764467 (+0.000000) 655.2 ms ✗
n-butane	-157.234261	-129.493006 (+27.741256) 1.7 ms ✗	-157.754492 (-0.520230) 27.9 ms ✓, 10 iters	-158.842064 (-1.607803) 25.4 ms ✓, 12 iters	-154.704743 (+2.529518) 25.3 ms ✓, 13 iters	-147.873632 (+9.360629) 11.9 ms ✓, 17 iters	-156.976764 (+0.257497) 29.0 ms ✓, 12 iters	-157.241778 (-0.007517) 56.2 ms ✓, 9 iters	-157.236522 (-0.002260) 115.6 ms ✓, 7 iters	-157.234262 (-0.000001) 273.7 ms ✓, 2 iters	-157.234261 (-0.000000) 553.0 ms ✓, 1 iters
n-pentane	-196.252633	-159.766386 (+36.486247) 2.4 ms ✗	-197.002699 (-0.750066) 24.9 ms ✓, 10 iters	-198.367522 (-2.114889) 22.2 ms ✓, 12 iters	-193.161242 (+3.091391) 24.3 ms ✓, 13 iters	-181.597457 (+14.655176) 19.8 ms ✗	-195.909787 (+0.342846) 46.2 ms ✓, 12 iters	-196.250994 (+0.001639) 95.0 ms ✓, 8 iters	-196.252949 (-0.000316) 194.3 ms ✓, 6 iters	-196.252636 (-0.000003) 473.2 ms ✓, 4 iters	-196.252633 (-0.000000) 966.4 ms ✓, 0 iters
n2	-108.867597	-102.046230 (+6.821367) 0.8 ms ✓, 10 iters	-108.975693 (-0.108096) 12.1 ms ✓, 8 iters	-109.173566 (-0.305969) 19.6 ms ✓, 8 iters	-107.567016 (+1.300581) 19.9 ms ✓, 10 iters	-102.444534 (+6.423063) 2.8 ms ✗	-107.922110 (+0.945487) 6.5 ms ✗	-108.850691 (+0.016906) 14.9 ms ✗	-108.866980 (+0.000617) 24.3 ms ✗	-108.867597 (+0.000000) 61.4 ms ✗	-108.867597 (-0.000000) 118.5 ms ✓, 0 iters
n2h4	-111.117357	-99.849559 (+11.267799) 0.9 ms ✓, 19 iters	-111.186037 (-0.068680) 25.2 ms ✓, 12 iters	-111.637606 (-0.520249) 25.7 ms ✓, 14 iters	-110.559946 (+0.557411) 26.4 ms ✓, 15 iters	-104.792444 (+6.324913) 3.3 ms ✓, 18 iters	-110.192271 (+0.925087) 9.6 ms ✓, 15 iters	-111.099092 (+0.018265) 18.1 ms ✓, 12 iters	-111.117207 (+0.000150) 36.3 ms ✓, 9 iters	-111.117357 (-0.000000) 85.4 ms ✓, 1 iters	-111.117357 (-0.000000) 158.3 ms ✓, 1 iters
n2o	-183.555025	-165.564884 (+17.990142) 0.8 ms ✗	-184.306683 (-0.751658) 23.0 ms ✗	-184.618652 (-1.063626) 38.8 ms ✗	-182.336824 (+1.218201) 42.5 ms ✗	-179.788774 (+3.766251) 4.0 ms ✗	-183.243713 (+0.311312) 9.1 ms ✗	-183.554028 (+0.000997) 18.6 ms ✗	-183.555014 (+0.000012) 35.1 ms ✗	-183.555026 (-0.000000) 101.4 ms ✓, 4 iters	-183.555026 (-0.000000) 193.4 ms ✓, 3 iters
n2o4	-407.774952	-378.579547 (+29.195405) 1.4 ms ✗	-409.519021 (-1.744069) 23.7 ms ✗	-410.074583 (-2.299631) 39.6 ms ✗	-404.815877 (+2.959075) 44.7 ms ✗	-394.819768 (+12.955184) 12.5 ms ✗	-406.692234 (+1.082718) 30.1 ms ✗	-407.763647 (+0.011305) 63.5 ms ✗	-407.774554 (+0.000398) 119.0 ms ✗	-407.774952 (+0.000000) 302.4 ms ✓, 4 iters	-407.774952 (-0.000000) 625.4 ms ✓, 1 iters
nccn	-184.498883	-167.256597 (+17.242286) 0.9 ms ✗	-185.193809 (-0.694926) 26.7 ms ✗	-185.670757 (-1.171874) 42.5 ms ✗	-181.778301 (+2.720582) 42.9 ms ✗	-179.700177 (+4.798707) 4.6 ms ✗	-182.898228 (+1.600655) 11.4 ms ✗	-184.502408 (-0.003525) 22.0 ms ✗	-184.499845 (-0.000961) 48.0 ms ✗	-184.498884 (-0.000001) 109.6 ms ✓, 3 iters	-184.498883 (-0.000000) 225.5 ms ✓, 1 iters
nh2cl	-514.988669	-507.653084 (+7.335586) 0.9 ms ✓, 24 iters	-515.035513 (-0.046843) 37.8 ms ✓, 19 iters	-515.285671 (-0.297002) 46.6 ms ✓, 16 iters	-514.593384 (+0.395285) 47.1 ms ✓, 22 iters	-510.330833 (+4.657837) 3.8 ms ✓, 22 iters	-513.478602 (+1.510068) 9.4 ms ✓, 22 iters	-514.942207 (+0.046462) 18.1 ms ✓, 18 iters	-514.987351 (+0.001318) 37.1 ms ✓, 15 iters	-514.988669 (+0.000000) 86.9 ms ✓, 5 iters	-514.988669 (+0.000000) 176.4 ms ✓, 0 iters
nh2f	-154.907456	-144.094900 (+10.812557) 0.8 ms ✗	-154.817794 (+0.089662) 35.6 ms ✓, 27 iters	-155.036951 (-0.129495) 40.7 ms ✓, 25 iters	-154.401904 (+0.505552) 46.6 ms ✓, 29 iters	-148.717551 (+6.189905) 3.1 ms ✗	-154.702002 (+0.205454) 7.2 ms ✓, 23 iters	-154.902942 (+0.004515) 15.0 ms ✓, 15 iters	-154.907345 (+0.000111) 29.1 ms ✓, 12 iters	-154.907456 (+0.000000) 76.2 ms ✓, 2 iters	-154.907456 (-0.000000) 172.5 ms ✓, 0 iters
nh2oh	-130.923056	-119.783877 (+11.139179) 0.8 ms ✗	-130.915061 (+0.007995) 34.1 ms ✓, 25 iters	-131.215609 (-0.292553) 41.7 ms ✓, 24 iters	-130.437112 (+0.485944) 46.1 ms ✓, 26 iters	-124.827132 (+6.095924) 4.2 ms ✗	-130.813095 (+0.109961) 6.8 ms ✓, 21 iters	-130.918035 (+0.005021) 13.7 ms ✓, 13 iters	-130.922971 (+0.000085) 27.4 ms ✓, 10 iters	-130.923056 (+0.000000) 81.3 ms ✓, 0 iters	-130.923056 (-0.000000) 163.2 ms ✓, 0 iters

nh3	-56.160561	-49.593217 (+6.567343) 0.7 ms ✓, 20 iters	-56.027092 (+0.133469) 25.0 ms ✓, 14 iters	-56.235375 (-0.074814) 22.0 ms ✓, 16 iters	-55.860412 (+0.300149) 23.2 ms ✓, 16 iters	-52.410917 (+3.749644) 2.2 ms ✓, 20 iters	-56.104316 (+0.056245) 5.0 ms ✓, 15 iters	-56.160049 (+0.000511) 9.8 ms ✓, 9 iters	-56.160558 (+0.000003) 19.7 ms ✓, 6 iters	-56.160561 (-0.000000) 46.6 ms ✓, 0 iters	-56.160561 (-0.000000) 98.8 ms ✓, 0 iters
ocs	-510.154449	-501.880272 (+8.274177) 1.0 ms X	-510.754073 (-0.599625) 34.6 ms X	-510.991359 (-0.836911) 65.0 ms X	-508.752433 (+1.402016) 66.6 ms X	-504.184155 (+5.970293) 5.4 ms X	-509.444962 (+0.709487) 12.6 ms X	-510.147709 (+0.006740) 24.4 ms X	-510.154433 (+0.000016) 49.7 ms ✓, 16 iters	-510.154451 (-0.000003) 134.1 ms ✓, 2 iters	-510.154449 (-0.000000) 292.0 ms ✓, 0 iters
oxadiazole	-260.395601	-235.030599 (+25.365002) 1.3 ms X	-261.744778 (-1.349177) 45.4 ms ✓, 66 iters	-262.635424 (-2.239823) 60.6 ms ✓, 49 iters	-258.217005 (+2.178596) 71.6 ms X	-248.781853 (+11.613748) 9.3 ms X	-259.988629 (+0.406971) 24.0 ms ✓, 59 iters	-260.397594 (-0.001993) 24.0 ms ✓, 59 iters	-260.395517 (+0.000084) 45.8 ms ✓, 22 iters	-260.395601 (-0.000000) 219.7 ms ✓, 2 iters	-260.395601 (-0.000000) 473.5 ms ✓, 2 iters
oxetane	-191.815955	-169.115682 (+22.700273) 1.3 ms X	-192.620085 (-0.804131) 37.3 ms ✓, 27 iters	-193.486136 (-1.670181) 47.7 ms ✓, 26 iters	-189.579528 (+2.236426) 42.0 ms ✓, 29 iters	-179.389310 (+12.426644) 7.3 ms X	-190.696429 (+1.119525) 17.5 ms ✓, 27 iters	-191.811370 (+0.004585) 35.9 ms ✓, 16 iters	-191.815914 (+0.000040) 71.5 ms ✓, 8 iters	-191.815955 (+0.000000) 173.9 ms ✓, 0 iters	-191.815955 (-0.000000) 356.0 ms ✓, 0 iters
oxirane	-152.783185	-136.595968 (+16.187217) 1.0 ms X	-153.403008 (-0.619823) 37.0 ms ✓, 32 iters	-153.963234 (-1.180049) 47.6 ms ✓, 32 iters	-150.987929 (+1.795256) 46.0 ms ✓, 36 iters	-143.018790 (+9.764395) 5.4 ms X	-152.567485 (+0.215700) 11.9 ms ✓, 27 iters	-152.780928 (+0.002257) 24.0 ms ✓, 14 iters	-152.783176 (-0.000009) 45.7 ms ✓, 6 iters	-152.783185 (-0.000000) 115.3 ms ✓, 1 iters	-152.783185 (-0.000000) 259.5 ms ✓, 1 iters
oxirene	-151.508448	-138.225334 (+13.283114) 0.8 ms X	-152.075810 (-0.567363) 37.6 ms ✓, 38 iters	-152.495823 (-0.987376) 46.0 ms ✓, 37 iters	-149.961386 (+1.547062) 49.4 ms X	-144.062566 (+7.445882) 4.5 ms X	-150.901379 (+0.607069) 11.4 ms ✓, 35 iters	-151.202148 (+0.306300) 22.0 ms ✓, 26 iters	-151.501585 (+0.006862) 46.5 ms ✓, 21 iters	-151.508444 (+0.000004) 116.4 ms ✓, 11 iters	-151.508448 (-0.000000) 232.4 ms ✓, 2 iters
p2	-681.355099	-677.284808 (+4.070291) 0.8 ms ✓, 10 iters	-681.421267 (-0.066168) 13.5 ms ✓, 8 iters	-681.545871 (-0.190772) 24.6 ms ✓, 8 iters	-680.823679 (+0.531421) 26.4 ms ✓, 8 iters	-677.892024 (+3.463075) 4.3 ms ✓, 15 iters	-679.835709 (+1.519390) 10.4 ms X	-680.879559 (+0.475541) 20.4 ms X	-681.071971 (+0.283129) 39.2 ms X	-681.353675 (+0.001424) 110.5 ms X	-681.355099 (+0.000000) 197.3 ms X
p4	-1362.670836	-1354.216692 (+8.454144) 1.4 ms ✓, 28 iters	-1363.803240 (-1.132404) 12.9 ms ✓, 12 iters	-1364.283588 (-1.612752) 27.1 ms ✓, 12 iters	-1361.331601 (+1.339235) 25.8 ms ✓, 30 iters	-1354.982389 (+7.688448) 12.6 ms X	-1360.061060 (+2.609776) 37.2 ms ✓, 30 iters	-1362.624455 (+0.046381) 68.5 ms ✓, 17 iters	-1362.670498 (+0.000338) 127.5 ms ✓, 13 iters	-1362.670838 (-0.000002) 314.1 ms ✓, 8 iters	-1362.670836 (-0.000000) 623.1 ms ✓, 3 iters
pf3	-638.940459	-618.707721 (+20.232738) 1.0 ms ✓, 31 iters	-639.521164 (-0.580705) 23.9 ms ✓, 20 iters	-639.533843 (-0.593384) 46.1 ms ✓, 20 iters	-638.463911 (+0.476548) 47.6 ms ✓, 20 iters	-629.431036 (+9.509423) 7.3 ms ✓, 24 iters	-637.974690 (+0.965770) 17.9 ms ✓, 19 iters	-638.924890 (+0.015569) 35.1 ms ✓, 13 iters	-638.940605 (-0.000146) 70.7 ms ✓, 7 iters	-638.940509 (-0.000050) 171.6 ms ✓, 12 iters	-638.940459 (-0.000000) 348.6 ms ✓, 1 iters
pf5	-837.699467	-809.093663 (+28.605804) 1.4 ms X	-839.222719 (-1.523252) 24.0 ms ✓, 18 iters	-839.163654 (-1.464187) 45.4 ms ✓, 18 iters	-836.793731 (+0.905736) 48.6 ms ✓, 21 iters	-820.049854 (+17.649613) 17.3 ms ✓, 26 iters	-836.135533 (+1.563934) 42.0 ms ✓, 20 iters	-837.687610 (+0.011858) 79.5 ms ✓, 20 iters	-837.701418 (-0.001950) 165.3 ms ✓, 14 iters	-837.699475 (-0.000008) 403.4 ms ✓, 5 iters	-837.699468 (-0.000000) 794.5 ms ✓, 1 iters
ph3	-342.395807	-338.455359 (+3.940448) 0.8 ms ✓, 11 iters	-342.170983 (+0.224824) 24.2 ms ✓, 9 iters	-342.355341 (+0.044066) 25.5 ms ✓, 10 iters	-342.181846 (+0.213961) 27.8 ms ✓, 9 iters	-339.032158 (+3.363649) 2.7 ms ✓, 11 iters	-341.790639 (+0.605168) 6.8 ms ✓, 9 iters	-342.392785 (+0.003022) 14.4 ms ✓, 7 iters	-342.395805 (+0.000002) 28.2 ms ✓, 4 iters	-342.395807 (-0.000000) 69.2 ms ✓, 0 iters	-342.395807 (-0.000000) 140.0 ms ✓, 0 iters
propane	-118.215867	-98.248261 (+19.967606) 1.2 ms ✓, 22 iters	-118.501286 (-0.285419) 28.0 ms ✓, 10 iters	-119.310639 (-1.094772) 22.7 ms ✓, 12 iters	-116.249918 (+1.687802) 25.8 ms ✓, 13 iters	-110.403350 (+7.812517) 6.8 ms ✓, 15 iters	-118.091830 (+0.124037) 17.0 ms ✓, 12 iters	-118.223398 (-0.007531) 33.6 ms ✓, 8 iters	-118.215994 (-0.000128) 65.0 ms ✓, 6 iters	-118.215867 (-0.000000) 163.4 ms ✓, 3 iters	-118.215868 (-0.000001) 329.7 ms ✓, 3 iters
propene	-117.027773	-98.346336 (+18.681436) 1.1 ms X	-117.398366 (-0.370593) 26.5 ms ✓, 16 iters	-118.083879 (-1.056106) 22.3 ms ✓, 11 iters	-115.339971 (+1.687802) 22.6 ms ✓, 20 iters	-111.271323 (+5.756450) 5.2 ms ✓, 23 iters	-116.835702 (-0.192071) 12.9 ms ✓, 17 iters	-117.043728 (-0.015955) 26.4 ms ✓, 15 iters	-117.027810 (-0.000037) 52.7 ms ✓, 6 iters	-117.027773 (-0.000000) 136.1 ms ✓, 1 iters	-117.027773 (-0.000000) 265.4 ms ✓, 4 iters
propyne	-115.822973	-97.624948 (+18.198025) 1.0 ms X	-116.262064 (-0.439091) 22.8 ms ✓, 54 iters	-116.805852 (-0.982879) 21.9 ms ✓, 47 iters	-114.349531 (+1.473442) 22.6 ms ✓, 66 iters	-111.598825 (+4.224148) 5.0 ms ✓, 61 iters	-115.639670 (+0.183303) 12.1 ms ✓, 48 iters	-115.821695 (+0.001278) 25.8 ms ✓, 43 iters	-115.823009 (-0.000036) 49.1 ms ✓, 21 iters	-115.822977 (-0.000004) 123.5 ms ✓, 4 iters	-115.822974 (-0.000000) 247.6 ms ✓, 3 iters
pyrrole	-208.729298	-182.612691 (+26.116608) 1.5 ms X	-210.309356 (-1.580058) 35.0 ms ✓, 28 iters	-211.465767 (-2.736469) 43.7 ms ✓, 26 iters	-206.675609 (+2.053689) 46.3 ms ✓, 26 iters	-194.465047 (+14.264251) 14.0 ms X	-207.413026 (+1.316272) 28.6 ms ✓, 21 iters	-208.626838 (+0.102460) 57.1 ms ✓, 25 iters	-208.729777 (-0.000479) 112.7 ms ✓, 11 iters	-208.729298 (+0.000000) 112.7 ms ✓, 0 iters	-208.729298 (-0.000000) 299.7 ms ✓, 2 iters
s2o	-869.607861	-859.779291 (+9.828571) 1.3 ms X	-870.392130 (-0.784269) 23.7 ms X	-870.538290 (-0.930428) 44.8 ms X	-869.136198 (+0.471664) 44.5 ms X	-862.707444 (+6.900418) 7.2 ms X	-868.359848 (+1.248014) 15.3 ms X	-869.560624 (+0.047237) 32.1 ms X	-869.602765 (+0.005096) 60.7 ms X	-869.607856 (+0.000005) 151.2 ms X	-869.607866 (-0.000005) 299.7 ms X
sf6	-993.517421	-960.394104 (+33.123317) 1.9 ms ✓, 31 iters	-995.976385 (-2.458964) 28.3 ms ✓, 17 iters	-995.857048 (-2.339627) 43.6 ms ✓, 17 iters	-992.137647 (+1.379773) 47.5 ms ✓, 17 iters	-973.190995 (+20.326426) 23.7 ms ✓, 22 iters	-991.558347 (+1.959074) 57.7 ms ✓, 16 iters	-993.502036 (+0.015385) 117.7 ms ✓, 11 iters	-993.517475 (-0.000054) 231.8 ms ✓, 11 iters	-993.517421 (-0.000000) 601.8 ms ✓, 0 iters	-993.517421 (-0.000000) 1185.1 ms ✓, 0 iters
si2h6	-581.214896	-573.682545 (+7.532351) 1.2 ms ✓, 9 iters	-580.839606 (+0.375290) 24.5 ms ✓, 8 iters	-581.249856 (-0.034960) 26.6 ms ✓, 8 iters	-580.593306 (+0.621590) 28.0 ms ✓, 9 iters	-574.684634 (+6.530262) 6.5 ms ✓, 11 iters	-580.060969 (+1.153927) 15.0 ms ✓, 9 iters	-581.208261 (+0.006636) 31.3 ms ✓, 7 iters	-581.214892 (+0.000004) 62.1 ms ✓, 4 iters	-581.214896 (-0.000000) 146.8 ms ✓, 2 iters	-581.214896 (-0.000000) 307.2 ms ✓, 2 iters
sif4	-686.719911	-664.361183 (+22.358728) 1.1 ms ✓, 25 iters	-687.287189 (-0.567278) 27.8 ms ✓, 19 iters	-687.200701 (-0.480791) 45.2 ms ✓, 19 iters	-686.167303 (+0.552608) 48.8 ms ✓, 19 iters	-675.473488 (+11.246422) 10.8 ms ✓, 21 iters	-685.588313 (+1.311597) 25.0 ms ✓, 19 iters	-686.700543 (+0.019368) 51.0 ms ✓, 14 iters	-686.720260 (-0.000349) 97.8 ms ✓, 11 iters	-686.719927 (-0.000016) 270.1 ms ✓, 8 iters	-686.719911 (-0.000000) 501.8 ms ✓, 0 iters

sih3f	-390.056215	-379.705256 (+10.350958) 1.1 ms ✗	-389.886235 (+0.169980) 34.5 ms ✓, 21 iters	-390.024924 (+0.031291) 44.7 ms ✓, 21 iters	-389.660750 (+0.395465) 45.9 ms ✓, 21 iters	-383.913066 (+6.143149) 3.9 ms ✗	-389.343013 (+0.713202) 10.1 ms ✓, 20 iters	-390.049846 (+0.006369) 20.3 ms ✓, 12 iters	-390.056212 (+0.000003) 41.0 ms ✓, 5 iters	-390.056215 (-0.000000) 97.4 ms ✓, 1 iters	-390.056216 (-0.000002) 199.5 ms ✓, 2 iters
sih4	-291.173681	-287.348370 (+3.825311) 0.9 ms ✓, 9 iters	-290.813459 (+0.360222) 28.2 ms ✓, 8 iters	-291.018438 (+0.155243) 27.6 ms ✓, 8 iters	-290.841126 (+0.332556) 26.6 ms ✓, 8 iters	-288.019494 (+3.154188) 3.2 ms ✓, 9 iters	-290.602121 (+0.571561) 7.8 ms ✓, 8 iters	-291.170057 (+0.003624) 14.0 ms ✓, 6 iters	-291.173680 (+0.000001) 29.6 ms ✓, 4 iters	-291.173681 (-0.000000) 72.8 ms ✓, 0 iters	-291.173681 (-0.000000) 140.1 ms ✓, 0 iters
silole	-443.732812	-422.162531 (+21.570281) 1.9 ms ✗	-444.780620 (-1.047809) 36.6 ms ✓, 25 iters	-445.831903 (-2.099092) 48.4 ms ✓, 24 iters	-441.870200 (+1.862611) 51.6 ms ✓, 27 iters	-430.370448 (+13.362364) 15.3 ms ✗	-442.939594 (+0.793217) 38.2 ms ✓, 20 iters	-443.726500 (+0.006312) 74.6 ms ✓, 13 iters	-443.732812 (-0.000001) 150.3 ms ✓, 13 iters	-443.732813 (-0.000001) 364.2 ms ✓, 2 iters	-443.732812 (-0.000000) 744.1 ms ✓, 1 iters
sio	-363.701534	-355.500350 (+8.201185) 0.7 ms ✗	-363.603889 (+0.097645) 27.2 ms ✗	-363.648111 (+0.053423) 48.8 ms ✗	-363.329473 (+0.372062) 46.4 ms ✗	-360.626351 (+3.075184) 4.1 ms ✗	-362.860500 (+0.841035) 8.3 ms ✗	-363.498603 (+0.202931) 16.1 ms ✗	-363.697313 (+0.004221) 31.9 ms ✗	-363.701597 (-0.000063) 79.4 ms ✗	-363.701583 (-0.000049) 157.9 ms ✗
so2	-546.906035	-536.792722 (+10.113133) 0.9 ms ✓, 38 iters	-547.868862 (-0.962827) 24.7 ms ✓, 36 iters	-548.001624 (-1.095589) 44.6 ms ✓, 36 iters	-546.346618 (+0.559417) 46.1 ms ✓, 36 iters	-539.623764 (+7.282271) 5.4 ms ✗	-545.836369 (+1.069666) 12.4 ms ✗	-546.642984 (+0.263051) 26.6 ms ✗	-546.654334 (+0.251701) 53.2 ms ✗	-546.900637 (+0.005398) 117.8 ms ✓, 27 iters	-546.906035 (+0.000000) 231.9 ms ✓, 9 iters
so3	-621.563457	-606.735588 (+14.827869) 1.0 ms ✗	-623.363160 (-1.799702) 23.9 ms ✓, 23 iters	-623.542813 (-1.979356) 42.6 ms ✓, 23 iters	-620.584831 (+0.978626) 49.4 ms ✓, 23 iters	-610.762847 (+10.800611) 7.0 ms ✗	-620.448515 (+1.114942) 19.1 ms ✗	-621.548446 (+0.015011) 32.5 ms ✗	-621.563775 (-0.000318) 70.4 ms ✗	-621.563457 (-0.000000) 167.6 ms ✓, 1 iters	-621.563457 (-0.000000) 344.4 ms ✓, 0 iters
t-butadiene	-154.863640	-128.300689 (+26.562951) 1.3 ms ✗	-155.553967 (-0.690327) 24.0 ms ✓, 17 iters	-156.396025 (-1.532385) 21.9 ms ✓, 17 iters	-152.913863 (+1.949777) 25.5 ms ✓, 21 iters	-146.496290 (+8.367350) 7.7 ms ✓, 27 iters	-153.471141 (+1.392498) 20.1 ms ✓, 21 iters	-154.860735 (+0.002905) 37.9 ms ✓, 12 iters	-154.864996 (-0.001356) 79.2 ms ✓, 12 iters	-154.863640 (-0.000000) 206.7 ms ✓, 1 iters	-154.863640 (-0.000000) 408.8 ms ✓, 1 iters
t-hcoh	-113.726427	-104.186515 (+9.539912) 0.7 ms ✗	-113.836421 (-0.109994) 38.4 ms ✓, 26 iters	-114.077597 (-0.351170) 41.5 ms ✓, 26 iters	-113.224039 (+0.502389) 45.3 ms ✓, 27 iters	-108.226450 (+5.499977) 2.8 ms ✗	-113.566979 (+0.159448) 7.3 ms ✓, 26 iters	-113.725872 (+0.000555) 14.2 ms ✓, 14 iters	-113.726419 (+0.000008) 28.0 ms ✓, 6 iters	-113.726427 (+0.000000) 72.6 ms ✓, 2 iters	-113.726427 (-0.000000) 135.7 ms ✓, 0 iters
t-hono	-204.520185	-191.404324 (+13.115860) 0.9 ms ✗	-204.914963 (-0.394778) 34.4 ms ✓, 162 iters	-205.206307 (-0.686122) 42.6 ms ✓, 157 iters	-203.634469 (+0.885716) 42.2 ms ✓, 177 iters	-198.233042 (+6.287143) 4.1 ms ✗	-204.218902 (+0.301283) 9.5 ms ✓, 91 iters	-204.515437 (+0.004747) 18.0 ms ✓, 87 iters	-204.520099 (+0.000086) 36.2 ms ✓, 27 iters	-204.520185 (+0.000000) 96.8 ms ✓, 1 iters	-204.520185 (-0.000000) 187.6 ms ✓, 0 iters
t-n2h2	-109.926845	-100.732559 (+9.194285) 0.7 ms ✓, 13 iters	-110.035862 (-0.109017) 23.5 ms ✓, 11 iters	-110.383433 (-0.456589) 22.3 ms ✓, 11 iters	-109.088083 (+0.838762) 22.1 ms ✓, 18 iters	-105.488365 (+4.438480) 2.8 ms ✓, 13 iters	-109.141889 (+0.784956) 6.6 ms ✓, 56 iters	-109.907981 (+0.018864) 13.2 ms ✓, 43 iters	-109.926996 (-0.000152) 26.3 ms ✓, 24 iters	-109.926845 (-0.000000) 69.1 ms ✓, 7 iters	-109.926845 (-0.000000) 131.3 ms ✓, 3 iters
tetrahedrane	-153.506597	-135.184126 (+18.322471) 1.2 ms ✗	-155.291386 (-1.784788) 26.4 ms ✓, 10 iters	-156.265900 (-2.759303) 22.3 ms ✓, 10 iters	-151.604887 (+1.901710) 23.0 ms ✓, 12 iters	-138.780502 (+14.726095) 7.2 ms ✓, 18 iters	-150.313459 (+3.193138) 17.8 ms ✓, 16 iters	-153.498955 (+0.007643) 37.2 ms ✓, 11 iters	-153.506555 (+0.000042) 67.8 ms ✓, 8 iters	-153.506602 (-0.000004) 170.3 ms ✓, 4 iters	-153.506614 (-0.000016) 344.4 ms ✓, 5 iters
thiophene	-551.184720	-530.051776 (+21.132945) 1.6 ms ✗	-552.683112 (-1.498391) 39.9 ms ✓, 20 iters	-553.662071 (-2.477351) 45.0 ms ✓, 24 iters	-549.083851 (+2.100869) 51.3 ms ✓, 25 iters	-537.640807 (+13.543913) 13.8 ms ✗	-550.389776 (+0.794944) 33.1 ms ✓, 20 iters	-551.177255 (+0.007466) 70.1 ms ✓, 15 iters	-551.184728 (-0.000007) 145.0 ms ✓, 10 iters	-551.184720 (-0.000000) 358.8 ms ✓, 2 iters	-551.184720 (-0.000000) 690.8 ms ✓, 1 iters
trans-c2f2c12	-1193.354865	-1157.194624 (+36.160241) 1.5 ms ✗	-1194.738826 (-1.383961) 35.8 ms ✓, 24 iters	-1195.227045 (-1.872180) 63.6 ms ✓, 24 iters	-1191.619061 (+1.735804) 70.7 ms ✓, 27 iters	-1181.868320 (+11.486545) 18.6 ms ✓, 24 iters	-1190.816052 (+2.538813) 49.0 ms ✓, 25 iters	-1193.596014 (-0.241149) 85.9 ms ✓, 17 iters	-1193.354616 (+0.000249) 182.8 ms ✓, 13 iters	-1193.354866 (-0.000001) 429.7 ms ✓, 5 iters	-1193.354868 (-0.000003) 874.2 ms ✓, 4 iters