

Supporting Information

**Theoretical investigation of a C₂N Monolayer as
Bifunctional Electrocatalyst for Rechargeable
Non-aqueous Li-Air Batteries**

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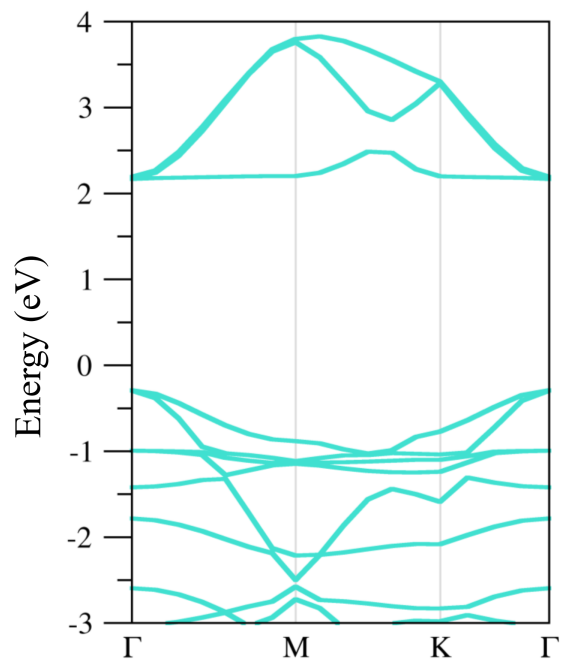


Figure S1: The Electronic band structure of C_2N monolayer using HSE06 functional. The Fermi level is set to zero.

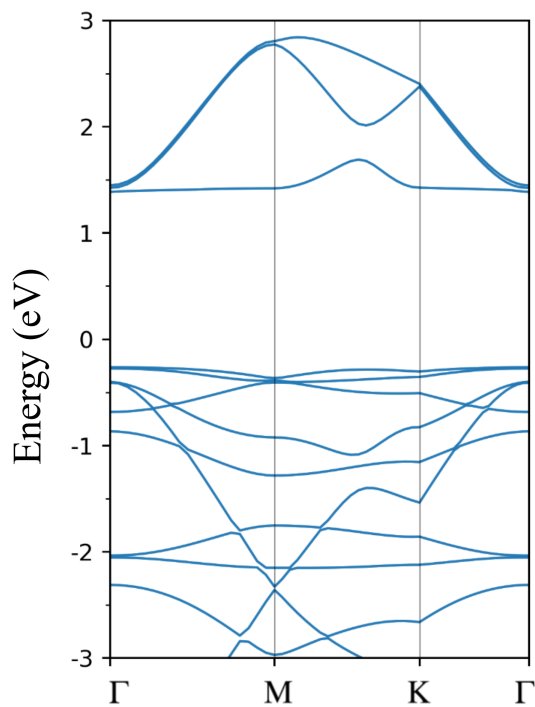


Figure S2: The Electronic band structure of C_2N monolayer using spin-orbit coupling, respectively. The Fermi level is set to zero.

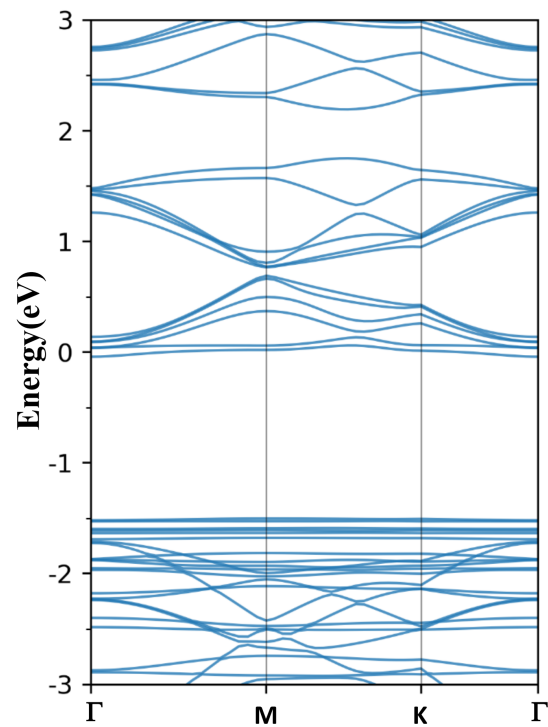


Figure S3: The Electronic band structure of C₂N monolayer after the adsorption of Li atom. The Fermi level is set to zero.

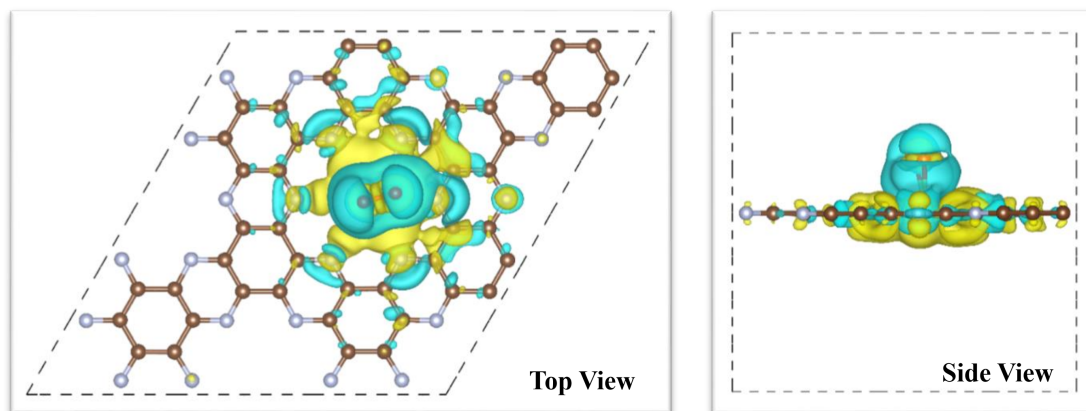


Figure S4: Charge density difference plot of LiO₂ adsorbed C₂N monolayer.

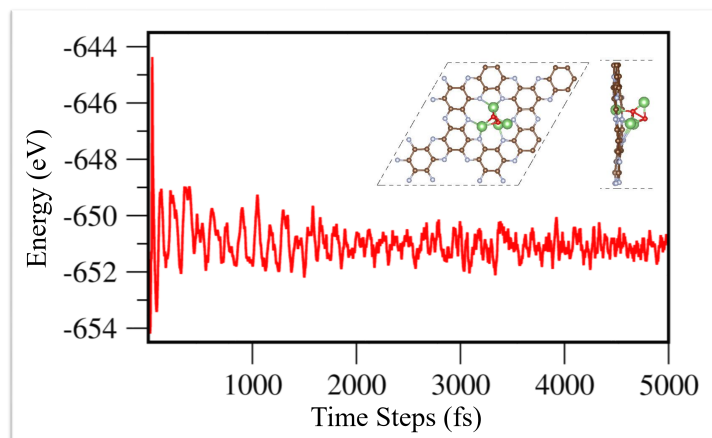


Figure S5: Total potential energy fluctuation during AIMD simulation at 300K of Li_4O_2 adsorbed C_2N monolayer.

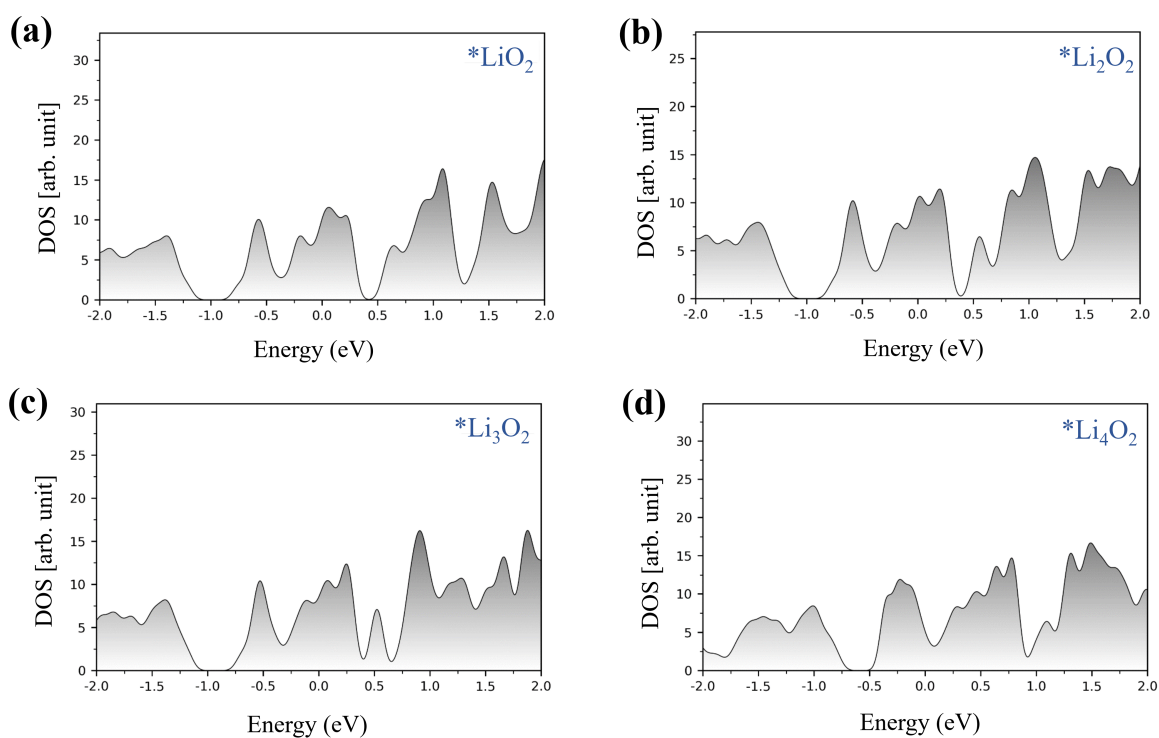


Figure S6: Density of states (DOS) of LiO_2 , Li_2O_2 , Li_3O_2 and Li_4O_2 adsorbed C_2N monolayer, respectively. The Fermi level is set to zero.

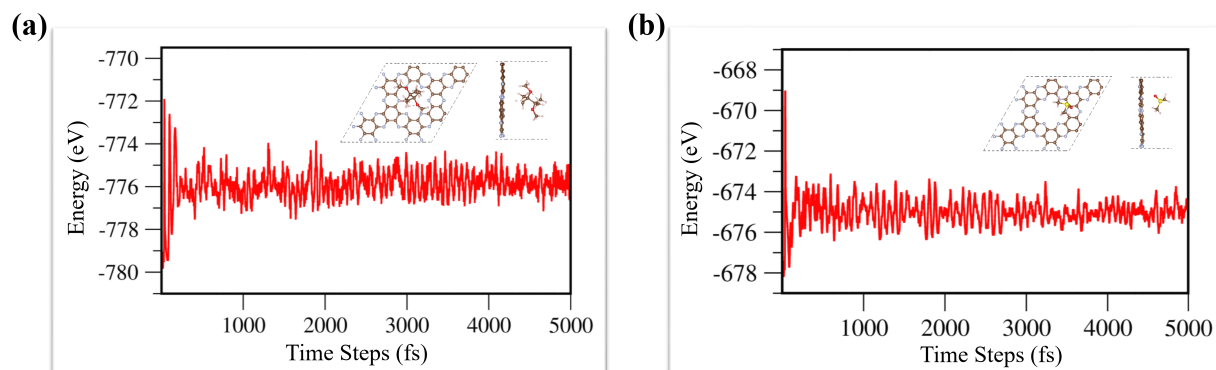


Figure S7: Total potential energy fluctuation during AIMD simulation at 300K of (a) DMDMB and (b) DMSO adsorbed C₂N monolayer.

Table S1: The Calculated Energy, zero point energy (ZPE), -TS, and Gibbs free energy (G) of a single lithium atom, oxygen molecule, C₂N monolayer and *Li_xO_{2y} species.

System	Energy (eV)	ZPE (eV)	-TS (eV)	G (eV)
Li	-2.00	0.03	-0.37	-2.34
O ₂	-8.77	0.10	-0.68	-9.35
C ₂ N	-627.82	11.14	-2.17	-618.85
C ₂ N – LiO ₂	-642.20	11.27	-2.26	-633.19
C ₂ N – Li ₂ O ₂	-646.53	11.33	-2.35	637.55
C ₂ N – Li ₃ O ₂	-650.70	11.38	-2.34	-641.66
C ₂ N – Li ₄ O ₂	-654.64	11.40	-2.41	-645.65
C ₂ N – Li ₂ O ₄	-656.95	-	-	-
C ₂ N – Li ₃ O ₄	-660.60	-	-	-
C ₂ N – Li ₄ O ₄	-665.03	-	-	-

Reaction free energy



$$\Delta G_1 = G_{*LiO_2} - G^* - G_{Li} - G_{O_2} \quad (5)$$

$$\Delta G_2 = G_{*Li_2O_2} - G^*_{Li_2O_2} - G_{Li} \quad (6)$$

$$\Delta G_3 = G^*_{Li_3O_2} - G^*_{Li_2O_2} - G_{Li} \quad (7)$$

$$\Delta G_4 = G^*_{Li_4O_2} - G^*_{Li_3O_2} - G_{Li} \quad (8)$$

Optimized Structures (VASP format):

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0.0000000000000000 0.0000000000000000 15.0000000000000000

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C N Li O

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0.9613091695373479 0.8720820794658376 0.4995499712060045
0.3729095371105477 0.4598557678216317 0.4933484794993903
0.3730910816982347 0.9594761556571760 0.4977219328190533
0.8722928975199811 0.4602678609198874 0.4962907449380060
0.8730134590764709 0.9604229584064690 0.4992386121702234
0.1193831277268060 0.2066490746381958 0.4986736217193105
0.1197715869662364 0.7067324887315304 0.4984402391599996
0.6194976234255439 0.2069687070564425 0.4962941870554595
0.6205989873132157 0.7066397237315267 0.4934467400521320
0.1191855595590561 0.2926730104465901 0.4991260698230663
0.1199868007941852 0.7923850426113804 0.4984845500288473
0.0399270268508381 0.2047653934786806 0.4976211253315562
0.0404148205802370 0.7048098730269036 0.4990661644673591
0.5402514822696435 0.2048630907716881 0.4975665668403058
0.5410968645850648 0.7036527593394224 0.4937883085661939
0.2057144099460727 0.0389653389432048 0.4983242255597065
0.2057904295926402 0.5392832034119742 0.4980512950574300
0.7057251783034695 0.0395079983414857 0.4982931099106882
0.7044985814195321 0.5400298986563199 0.4912263750754767
0.3749893943772659 0.0390125717023836 0.4984952215161982
0.3751657897377597 0.5391039839223799 0.4914287194328700
0.8748630127367474 0.0397921778831946 0.4984500482909466
0.8749424451815164 0.5394531135600454 0.4968634309766150

0.3748423798289411 0.2046293702762055 0.4989363252916243
0.3756305585051635 0.7041228799500151 0.4941511253597035
0.8744510775004103 0.2052825664075105 0.4967164449573050
0.8750672294269559 0.7047404954017208 0.4981101406572183
0.2055838868791686 0.3738776839462378 0.4990490653658257
0.2062120509607638 0.8734394308863499 0.4980674214536818
0.7050425781181809 0.3748117897495593 0.4925200416234449
0.7056779815317357 0.8741619696806165 0.4973784432702960
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C2N-Li2O2

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16.6399993895999998 0.0000000000000000 0.0000000000000000
8.3199996947999999 14.4106621904000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000

C N O Li

48 24 2 2

Direct

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0.7909711585777158 0.8714962921537875 0.5046386360278579
0.3748324472756557 0.2838274834064338 0.4980409262615495
0.3777847631697908 0.7832630522309535 0.5158208005597509
0.8739306747137116 0.2865785803880646 0.5073369792065561

0.8767862425192687 0.7857057421484969 0.5040009190405721
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0.9629314643327936 0.3710267819753073 0.5057092756720170
0.9650757396971354 0.8715482798043527 0.5046144350618086
0.3746919662357887 0.4566056385242306 0.4950183629983933
0.3759491428112440 0.9581293344875523 0.5112881923066461
0.8753740810105753 0.4593366172038080 0.5079850784778708
0.8768022362663856 0.9597830993620367 0.5042033175351761
0.1213251426574463 0.2047255573685555 0.5065818450869638
0.1233800409701759 0.7053051886948409 0.5023881131976141
0.6220752343238817 0.2056500453087226 0.4992500137613375
0.6249354984865333 0.7070047478081601 0.5187788005062739
0.1215334301306520 0.2906488080041517 0.5036767344235509
0.1238783661587496 0.7907720260834062 0.5056701565097966
0.6218226564679973 0.2915465304030860 0.4981271125860792
0.6234689207613369 0.7929233359382153 0.5121924577253820
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0.2123454437134717 0.7897253844919749 0.5083056853963472
0.7088032497214031 0.2927659052995470 0.5019642401612309
0.7116304187547128 0.7924770377788896 0.5083183130534846
0.2954755805626487 0.2047536191524554 0.5028257868397306
0.2981780692108270 0.7036656859780388 0.5070098028417312
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0.7976142850907487 0.7065158222552578 0.5072874169610002
0.2955477272057285 0.1166916321955817 0.5065208965687227
0.2970872101852204 0.6165094317746025 0.5008667916339629

0.7959846415014974 0.1185209893056337 0.5033550376784156
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0.7909192604181079 0.9595725743487352 0.5035489538605779
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0.4648058137456241 0.7845785365156240 0.5192348789814990
0.9625097050624145 0.2855045465844857 0.5070977725587137
0.9647989953328373 0.7856378039254225 0.5031880219245084
0.0426873385476995 0.3723235737792726 0.5034331640309356
0.0449081076752588 0.8727066642385531 0.5063265053508383
0.5413010462089529 0.3725712992830592 0.4947951520575050
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0.0414375083277454 0.2036121403830441 0.5077595921363975
0.0436672719494821 0.7039538451665435 0.5015866441968412
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0.5455999849141064 0.7039593627841522 0.5255266782842819
0.2085288840763364 0.0365808094291286 0.5111116656063623
0.2078875933977616 0.5379528754165549 0.4979283761950320
0.7091940699230308 0.0383510818044419 0.5019993298156805
0.7088316238887467 0.5403000027737916 0.5205178586757900
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0.3778561000942054 0.5359695789974954 0.4971699432677790
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0.8789574762803711 0.7042453872339616 0.5049119331638225
0.2074811618140141 0.3719564527510809 0.4988430477481322
0.2104459239378914 0.8709715600732753 0.5107962370652867
0.7062552832476187 0.3748436807825263 0.5044065792358068
0.7095241027092658 0.8738291288824500 0.5066250552769045
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C2N-Li3O2

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16.6399993895999998 0.0000000000000000 0.0000000000000000
8.3199996947999999 14.4106621904000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000

C N O Li

48 24 2 3

Direct

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0.7889422136911176 0.3714752719856770 0.5250473972107433

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0.3747391547022006 0.2854364148715542 0.4967102133209189
0.3754613371144860 0.7852706181427468 0.5039971794716458
0.8744686810860474 0.2858044022301767 0.5158928440280779
0.8751990342061906 0.7852937568704301 0.4984220640044298
0.4622912634317063 0.3713904828660873 0.5036043561305374
0.4630920727330249 0.8710814519978991 0.5041348558544950
0.9627252318937931 0.3712772295653654 0.5135910316012525
0.9630134450403169 0.8713198233014262 0.4943414085252184
0.3751429126019397 0.4586768778257345 0.4987226490917523
0.3749693650614811 0.9591481832658193 0.5012981385838677
0.8746248990094662 0.4592441684851547 0.5183400121429660
0.8751798219769756 0.9592259707553457 0.4961588167225887
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0.1212358382108552 0.2921013560128198 0.5049314308037973
0.1214968665331449 0.7920057445175205 0.4931912301535771
0.6226328370630307 0.2901752929249923 0.5101338816390301
0.6222228777058146 0.7922371561035566 0.5071654729122131
0.2093239258729225 0.2921095699767824 0.5003760327035709
0.2092482350532264 0.7921534527931411 0.4950430741100494
0.7102614981345536 0.2899881919380033 0.5162578594505931
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0.7961165075942642 0.7061046593037321 0.5069729199133964
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0.4625802271416882 0.7855817597015397 0.5099288027872654
0.9626405915189198 0.2855750807989204 0.5128633445767965
0.9629834299665353 0.7853768643827329 0.4949365073107658
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0.5429222233231215 0.7044615628694173 0.5200954722405466
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0.7078344092249574 0.5399003686934886 0.5318851856240282
0.3768859713809636 0.0385966996196066 0.4997828597633743
0.3762878793883478 0.5391568323034304 0.4968257418128172
0.8773075568349930 0.0385576103032266 0.4992254578091904
0.8772349989880350 0.5383203822784481 0.5141854337369457
0.3767543853091533 0.2040095295041414 0.4969384804880463
0.3765437608899898 0.7036641277381337 0.5002866378971528
0.8770391390199319 0.2042154086996731 0.5099604922554344
0.8774551437869518 0.7038393736979001 0.5033277798809983
0.2074314847790709 0.3734701845293478 0.4985681926117011
0.2078867464095617 0.8733830963234988 0.4963853664120876
0.7075527153249240 0.3719552550609007 0.5279451555054546
0.7078557149455003 0.8733897151108447 0.4996768893498996
0.5960938396620868 0.5081184006985164 0.6920603456745898
0.5141227727498238 0.5502468004810298 0.6347566311079750
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C2N-Li4O2

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8.3199996947999999 14.4106621904000001 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.0000000000000000

C N O Li

48 24 2 4

Direct

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0.7882794760572821 0.8708057143321583 0.4968524193717059
0.3744945057138097 0.2848890973862326 0.5001632272560295
0.3747685193056161 0.7847389282656531 0.5019815456983656
0.8743918402384890 0.2849229113990104 0.5147387240803843
0.8743132222528064 0.7848919960865202 0.4967492617235137
0.4616983700748623 0.3711679713452253 0.5094143263489807
0.4624705564384473 0.8700842992872072 0.5022202231466156
0.9624570200063639 0.3705154283089176 0.5113367171295407
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0.2952749141362510 0.1170382147704049 0.4983330435778680
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0.2071533105339782 0.3726712582742420 0.5007256449332018
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0.7069128392503675 0.8727957329877549 0.4989120026988660
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0.4812611622523376 0.5716517406062791 0.7520484176983314

C2N-DMDMB

1.0000000000000000

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8.3199996947999999 14.4106621904000001 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.0000000000000000

C N O H

56 24 2 18

Direct

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