

Supporting Information

ZIF-8 as a catalyst in ethylene oxide and propylene oxide reaction with CO₂ to cyclic organic carbonates

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The Cartesian coordinates of all the structures optimized at the B3LYP-D3-TZVP level are reported in the following.

ZIF-8

C, -1, 1.7807492197, 2.2695692681, 3.0705433552
H, 0, 1.9908149342, 3.0856794102, 3.7376551081
N, 0, 2.4471201558, 1.0614549755, 3.1447084445
C, 0, 1.9769893504, 0.2374889105, 2.1752726134
C, 0, 2.4392832373, -1.1570799524, 1.9552858762
H, 0, 3.1691480653, 0.8234994212, 3.8050797383
H, 0, 1.6459156156, -1.8651935954, 2.2041277611
H, 0, 3.3116031343, -1.3790254987, 2.5695543829
H, 0, 2.6884600984, -1.3118219909, 0.9053602357
C, 0, 0.9088016606, 2.1370354587, 2.0328126664
C, 0, 1.2350888795, -2.2416974966, -1.7422451938
C, -1, -1.6299702392, 3.0700525983, -2.3962767816
C, 0, -1.4167222035, -1.7243659051, 2.1088825544
C, 0, -0.6900350193, 2.1125034335, -2.1626298859
C, -1, 2.3062520596, -2.4188885734, -2.5892013356
H, 0, 0.2108435475, 2.8525178401, 1.6349673564
H, 0, 0.4426198754, -2.9142218023, -1.4566845682
H, 0, -1.7325942433, 3.8033036414, -3.1753800034
H, 0, -0.7562867286, -1.3388620614, 2.8701114632
H, 0, 0.1905484797, 1.8627119902, -2.7279337069
H, 0, 2.5769650133, -3.2875203874, -3.1678411135
N, -1, 1.0395525097, 0.8770286533, 1.488792421
N, -1, 1.3070776634, -0.9532845007, -1.2320676357
N, 0, -2.5515457925, 2.9392369636, -1.375016375
N, -1, -1.3170950488, -1.3196337611, 0.7875929678
N, -1, -1.0285642891, 1.4178294031, -1.0187886751
N, 0, 3.0561165453, -1.2644607565, -2.6192233691
C, 0, 2.4319826606, -0.4230336623, -1.8049729534
C, 0, -2.1632030467, 1.9301723983, -0.5566330145
C, 0, 2.943532245, 0.9437528412, -1.4803213246
C, 0, -2.9321398808, 1.490009747, 0.6374257262
Zn, 0, -0.0041294349, -0.1205811772, -0.0492197397
H, 0, -3.3908962738, 3.484163904, -1.2629770294
H, 0, -3.698697075, 2.222967436, 0.8902053678
H, 0, -2.2760651917, 1.3556523886, 1.496226655
H, 0, -3.4083670759, 0.5244469051, 0.4616770246
H, 0, 3.5379756674, 0.9490834343, -0.5596713636
H, 0, 2.1357698467, 1.6650752424, -1.3381000918
H, 0, 3.586902294, 1.2910537813, -2.2875982111
H, 0, -3.0988622953, -0.9102702257, -1.5438751799
H, 0, -3.2328954318, -2.6664407127, -1.641630305
H, 0, -1.6722768558, -1.8731968849, -1.9105305615
C, -1, -2.4540828754, -2.6292290877, 2.1952656839
H, 0, -2.8221670399, -3.1595647726, 3.059297793
N, 0, -3.0133008962, -2.7935200522, 0.9514571429
C, 0, -2.3104375385, -2.00503129, 0.1449249051
C, 0, -2.5877732937, -1.8525919613, -1.3155948988

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C, -1, 6.3438389628, 9.4554276469, 10.4572344996
H, 0, 5.6736293224, 9.0514794884, 9.7148151069
N, 0, 6.6576392567, 8.7668789139, 11.6027766755
C, 0, 7.4944492076, 9.5555283017, 12.2666831006
C, 0, 8.1172084131, 9.1836352433, 13.5731298226
H, 0, 9.1885538443, 9.3955584263, 13.5886611746
H, 0, 7.9734785996, 8.1177147007, 13.738998398
H, 0, 7.6694483117, 9.717451755, 14.4185934746
C, 0, 6.9985491903, 10.6704569513, 10.464370393
C, 0, 9.5436322476, 12.834708451, 15.2168793884
C, -1, 7.9397540511, 15.7449023865, 10.2274452533
C, 0, 11.3538682229, 10.27189358, 11.6977179172

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 H, 0, 10, 6645490639, 9, 4478875119, 11, 6221541924
 H, 0, 7, 5249494719, 15, 158104867, 12, 3118843182
 H, 0, 9, 1736151955, 13, 2929769005, 17, 367689636
 N, -1, 7, 7442773239, 10, 7421994175, 11, 6289780081
 N, -1, 8, 6482277024, 12, 5938279225, 14, 1942605112
 N, 0, 8, 6877280023, 15, 0614688689, 9, 2921852923
 N, -1, 10, 9188165621, 11, 5577734017, 11, 9868897169
 N, -1, 8, 7214455562, 13, 8450614861, 11, 1037853422
 N, 0, 7, 5176803533, 12, 9642159477, 16, 0222143977
 C, 0, 7, 4247700884, 12, 6714343316, 14, 7015888048
 C, 0, 9, 147594187, 13, 9130834331, 9, 8461652049
 C, 0, 6, 1422785102, 12, 4467425735, 13, 9839970313
 C, 0, 9, 9568692803, 12, 9117412178, 9, 1075423127
 Zn, 0, 9, 0516958496, 12, 0939468414, 12, 2119509403
 H, 0, 6, 7363460212, 13, 0625328499, 16, 6498145286
 H, 0, 8, 8690041899, 15, 3572300321, 8, 3468332775
 H, 0, 10, 3782159849, 13, 3513955088, 8, 2034290628
 H, 0, 9, 3477454411, 12, 0537978619, 8, 8193826984
 H, 0, 10, 7656831246, 12, 536340202, 9, 7318782212
 H, 0, 6, 0097461564, 11, 3900120304, 13, 7470568618
 H, 0, 6, 1311407928, 12, 9802414089, 13, 0343681225
 H, 0, 5, 2988657669, 12, 7848719404, 14, 5862664611
 H, 0, 11, 8383148292, 14, 3461979521, 11, 3512489947
 H, 0, 13, 053100842, 14, 0900449394, 12, 6023537616
 H, 0, 11, 3271413875, 14, 0764100755, 13, 0107393056
 C, -1, 12, 7251561683, 10, 3107375294, 11, 5734114719
 H, 0, 13, 4095998516, 9, 5053130314, 11, 3602826385
 N, 0, 13, 1626298865, 11, 5998150082, 11, 7792403134
 C, 0, 12, 0650238976, 12, 3053672227, 12, 0232635001
 C, 0, 12, 0660107178, 13, 7809331732, 12, 2618447968
 O, 0, 9, 4145692787, 8, 0725624072, 9, 855383733
 C, 0, 9, 3406369953, 8, 9033538818, 9, 0531998071
 O, 0, 9, 2963572189, 9, 7186555267, 8, 2243325346

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C, -1, 6, 3438571242, 9, 4553977767, 10, 4571669198
 H, 0, 5, 6570784897, 9, 0602016607, 9, 7256577559
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 C, 0, 7, 6130146029, 9, 4988336916, 12, 1903277318
 C, 0, 8, 2978400793, 9, 099617688, 13, 4575547855
 H, 0, 9, 3421246254, 9, 4169042477, 13, 480045559
 H, 0, 8, 2613251006, 8, 0159554454, 13, 554492951
 H, 0, 7, 8098377138, 9, 5276413621, 14, 3407265277
 C, 0, 6, 9214723601, 10, 7067641136, 10, 5158113575
 C, 0, 9, 5406765028, 12, 8837440226, 15, 2063011131
 C, -1, 7, 939708111, 15, 7450349909, 10, 2274361846
 C, 0, 11, 3495040803, 10, 2853155864, 11, 6456569307
 C, 0, 7, 935116792, 14, 954675679, 11, 3356315232
 C, -1, 8, 852396547, 13, 0722740011, 16, 3661953129
 H, 0, 6, 8391998184, 11, 5496671989, 9, 8482665024
 H, 0, 10, 599322951, 12, 9252177067, 15, 0214613775
 H, 0, 7, 463499625, 16, 6841118087, 10, 0114134355
 H, 0, 10, 6508886785, 9, 483220824, 11, 4777203825
 H, 0, 7, 4371183466, 15, 1065458013, 12, 2770072834
 H, 0, 9, 1735562265, 13, 3077187965, 17, 3644671685
 N, -1, 7, 7442335494, 10, 742222694, 11, 6290872941
 N, -1, 8, 6482144519, 12, 5938348063, 14, 1942143083
 N, 0, 8, 7448364047, 15, 0952540787, 9, 3159877576
 N, -1, 10, 9187959783, 11, 5577792504, 11, 9869107586
 N, -1, 8, 7214864822, 13, 8449482349, 11, 1036990622
 N, 0, 7, 5223763624, 12, 885190322, 16, 0398612926
 C, 0, 7, 4291979627, 12, 594296461, 14, 7187897851
 C, 0, 9, 2054920887, 13, 9465468709, 9, 8673002929
 C, 0, 6, 1499218362, 12, 3019559638, 14, 0199093658
 C, 0, 10, 088438811, 12, 9945954335, 9, 1511051065
 Zn, 0, 9, 0477211893, 12, 1009571772, 12, 2017243948
 H, 0, 6, 7449057264, 12, 9342364097, 16, 6778791429
 H, 0, 8, 9619074912, 15, 4104255764, 8, 3846394296
 H, 0, 10, 4223859575, 13, 4285221658, 8, 2081438647
 H, 0, 9, 5756077488, 12, 0557736771, 8, 9240632992
 H, 0, 10, 9596451758, 12, 7501956792, 9, 75724133
 H, 0, 6, 0820124705, 11, 2453829423, 13, 7580063522
 H, 0, 6, 0829379452, 12, 855789358, 13, 0842811211
 H, 0, 5, 2994407161, 12, 5692758006, 14, 6473913269
 H, 0, 12, 839342964, 14, 2682577813, 11, 9308936419
 H, 0, 12, 356527163, 13, 8472549702, 13, 5644421448
 C, 0, 11, 1198763412, 14, 1980210518, 12, 3520392059
 C, -1, 12, 725207756, 10, 3107082457, 11, 5733901595
 H, 0, 13, 4068621364, 9, 5106325578, 11, 331506903
 N, 0, 13, 1698828142, 11, 5800445351, 11, 8622544273
 C, 0, 12, 0722316362, 12, 2851375225, 12, 1081628364
 C, 0, 12, 0905530728, 13, 725596045, 12, 509123031
 C, 0, 10, 597699555, 9, 2605826997, 8, 2470214337
 C, 0, 9, 2725417137, 8, 9036755673, 8, 7552272957
 O, 0, 9, 4560114765, 10, 0881573178, 7, 9622116749
 H, 0, 11, 0019794356, 8, 734686068, 7, 3871695775
 H, 0, 11, 3230572729, 9, 6969396836, 8, 9263198995
 H, 0, 9, 0219713658, 9, 0835979964, 9, 7925741129
 H, 0, 8, 7025604846, 8, 1183147558, 8, 2702960212

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C, -1, 1, 117539, 3, 441426, 1, 273389
 H, 0, 1, 7063037141, 4, 0969102435, 1, 8953198818
 N, 0, 0, 6293481339, 3, 84241884, 0, 0528655264

C,0,-0.0244607948,2.7897008749,-0.4249319747
 C,0,-0.7787849878,2.7991974176,-1.7147347557
 H,0,-0.6416987183,1.8766056913,-2.2820180873
 H,0,-0.4363485685,3.6354116045,-2.3219095111
 H,0,-1.8553039117,2.9247878923,-1.5527221192
 C,0,0.7385182107,2.137105899,1.5084034072
 C,0,-3.4058259481,-0.5974388263,-1.4769300875
 C,-1,-0.782409,-2.301633,3.632708
 C,0,1.2196926571,-0.3203973623,-2.3534085806
 C,0,-1.4230615756,-1.6086131889,2.6516074836
 C,-1,-4.699599,-0.172675,-1.445064
 H,0,0.9551421709,1.4824252018,2.3372567801
 H,0,-2.9290030686,-1.2983574894,-2.1394616803
 H,0,-1.1278699357,-2.721412204,4.5599474871
 H,0,1.4233370848,0.7342905803,-2.2721133207
 H,0,-2.4573968677,-1.3208227586,2.5870139098
 H,0,-5.5529567729,-0.4198652908,-2.0500047235
 N,-1,0.001764,1.706597,0.4156
 N,-1,-2.694395,0.051117,-0.487467
 N,0,0.5252689839,-2.4127996245,3.2106171341
 N,-1,0.313673,-0.949704,-1.512649
 N,-1,-0.523371,-1.302307,1.651908
 N,0,-4.7599300537,0.7519731107,-0.4207574026
 C,0,-3.5310091472,0.8680902272,0.1408433029
 C,0,0.6591626544,-1.7976162102,2.0107494055
 C,0,-3.2228572894,1.7554945296,1.2921934956
 C,0,1.9474623706,-1.7025711464,1.2831950546
 Zn,0,-0.658028143,-0.0928321652,-0.0419701335
 H,0,-5.5747067531,1.2748919024,-0.143852331
 H,0,1.2731718051,-2.8682526639,3.7076592564
 H,0,2.6465836558,-2.4543910709,1.6509210017
 H,0,2.4158492156,-0.7221829193,1.407871559
 H,0,1.7934327972,-1.8565837868,0.2174240743
 H,0,-2.1859694212,2.0850509768,1.239643996
 H,0,-3.3622252263,1.2295233792,2.2404154577
 H,0,-3.8724710166,2.6312890047,1.2923472587
 H,0,-0.5990029928,-4.1658988261,-1.9348674154
 H,0,-1.4830954637,-2.9656402598,-0.9738596656
 H,0,-0.0115736396,-3.6886629176,-0.3422972772
 C,-1,1.723873,-1.268391,-3.21526
 H,0,2.4455958605,-1.1495161246,-4.0075729582
 N,0,1.1498980831,-2.4872525369,-2.9332236702
 C,0,0.3200837623,-2.2556100873,-1.9226631807
 C,0,-0.4893370203,-3.3209549319,-1.2568228284
 C,0,4.8364403484,0.7661968895,-0.0995249333
 C,0,3.7006507674,1.6824992054,0.0211072323
 O,0,4.0243284227,0.7752706442,1.0920747834
 H,0,5.829079426,1.1800039078,0.0693937386
 H,0,2.7763537957,1.4575425097,-0.4978752549
 H,0,3.8575084558,2.7308081363,0.2458082027
 C,0,4.7867518693,-0.4719637264,-0.947336968
 H,0,5.266862816,-0.2858660026,-1.9113323585
 H,0,5.3182632116,-1.2945079973,-0.4619728275
 H,0,3.7597486627,-0.7782664447,-1.1437688424

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C,-1,-2.632138,-1.572105,3.50563
 H,0,-2.7827223431,-2.2677957294,4.3159373904
 N,0,-3.2398316611,-0.3400973055,3.4857760053
 C,0,-2.8287793738,0.2337417354,2.3615215285
 C,0,-3.282884021,1.5823229399,1.9052985141
 H,0,-2.4545803362,2.1986221047,1.5491164863
 H,0,-3.7641208279,2.0940194647,2.7367954796
 H,0,-4.0101547909,1.511813044,1.0888584138
 C,0,-1.8609586501,-1.7165861559,2.3724180432
 C,0,-2.3337999119,1.7045594049,-2.2737919836
 C,-1,0.618247,-3.504888,-1.772449
 C,0,0.435888268,2.1590625543,1.5670281008
 C,0,-0.2637674344,-2.4674653306,-1.8089190368
 C,-1,-3.466537,1.729428,-3.028509
 H,0,-1.2601919509,-2.5459311655,2.0339861167
 H,0,-1.5007045475,2.3848259867,-2.2660640445
 H,0,0.7537705562,-4.3587449514,-2.4108645327
 H,0,-0.1816806177,1.9288102361,2.4197344777
 H,0,-1.0652766113,-2.2787510352,-2.5010824571
 H,0,-3.8112074989,2.4079036384,-3.7875018002
 N,-1,-1.980278,-0.552569,1.627867
 N,-1,-2.38492,0.621094,-1.419179
 N,0,1.443094777,-3.2496569149,-0.694131127
 N,-1,0.293262,1.476364,0.368822
 N,-1,0.018421,-1.599029,-0.77385
 N,0,-4.2122728509,0.6434624053,-2.6106539462
 C,0,-3.5333187799,-0.0083393154,-1.6345100802
 C,0,1.0525738687,-2.0973723571,-0.104691692
 C,0,-4.0166099572,-1.2391970127,-0.9569727302
 C,0,1.6354095637,-1.5456638586,1.1437282023
 Zn,0,-0.9996763557,0.0317275035,0.0213217145
 H,0,-5.1220654128,0.3834703209,-2.9551959125
 H,0,2.3007187071,-3.7305499201,-0.4674857258
 H,0,2.5691377466,-2.0421546869,1.3920749904
 H,0,0.9326949658,-1.6693482762,1.9705983859
 H,0,1.8085215917,-0.476181851,1.0378337155
 H,0,-3.6877243369,-1.2436863396,0.0818984663
 H,0,-3.6137115021,-2.1340177458,-1.4383309239
 H,0,-5.1048585217,-1.2974185467,-0.9863084149
 H,0,2.18849964,0.7516058944,-1.9111649927
 H,0,1.8154204691,2.3797340901,-2.4741195202
 H,0,0.5309540129,1.1736274856,-2.3046926528
 C,-1,1.440278,3.087448,1.40713
 H,0,1.8223987084,3.805948317,2.1143976636

N,0,1.9415088863,2.9902651483,0.1233433464
 C,0,1.228333622,2.0275319633,-0.4579040466
 C,0,1.4506163671,1.5563118998,-1.8600294509
 O,0,4.7142192671,-0.4661479713,1.0457369087
 C,0,4.5892235119,0.9773269768,1.088100544
 C,0,4.7790986045,1.3760256995,-0.3706044596
 O,0,4.4448105787,0.1508569809,-1.0733870926
 C,0,4.4926377661,-0.888133836,-0.217356111
 O,0,4.3381578832,-2.0351857015,-0.5292476069
 H,0,3.5950358109,1.237296827,1.4510280251
 H,0,5.3501835533,1.3667944588,1.7585122496
 H,0,5.81020244,1.6321659241,-0.6160823572
 H,0,4.0886340557,2.1605272594,-0.6699190483

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C,-1,-2.6321421385,-1.5721167061,3.5056284249
 H,0,-2.7769075933,-2.2647940535,4.319570268
 N,0,-3.2650739336,-0.3532869939,3.4698681095
 C,0,-2.8528190882,0.2211041253,2.3462405537
 C,0,-3.3284566812,1.5575262106,1.8762639298
 H,0,-2.5113643903,2.1786016855,1.5030161815
 H,0,-3.8078776464,2.0751446549,2.7052138052
 H,0,-4.0632191699,1.4673049337,1.0684478271
 C,0,-1.8447808136,-1.708350897,2.3823866092
 C,0,-2.3357272015,1.7068277586,-2.2704686858
 C,-1,0.6182431849,-3.5049483223,-1.7724863671
 C,0,0.4066265944,2.1902212475,1.5522072175
 C,0,-0.2763790629,-2.4776651405,-1.7965002229
 C,-1,-3.4665311228,1.7294414172,-3.028498767
 H,0,-1.2203353351,-2.5259810792,2.0583058894
 H,0,-1.5064205891,2.3916543159,-2.2565270144
 H,0,0.7487013775,-4.3628824664,-2.406450018
 H,0,-0.2487689181,1.9995165071,2.38628957
 H,0,-1.0969937928,-2.3046851937,-2.47010485
 H,0,-3.8119887326,2.409078063,-3.7861016464
 N,-1,-1.9802581434,-0.5525426172,1.6278679449
 N,-1,-2.3849442736,0.6210561635,-1.4192094558
 N,0,1.4644350393,-3.2330802047,-0.7136429892
 N,-1,0.2932509256,1.4763919079,0.3688164392
 N,-1,0.0184633211,-1.5988810558,-0.7737536441
 N,0,-4.2090888498,0.6394358078,-2.6158352031
 C,0,-3.5300181175,-0.0123062055,-1.6394505541
 C,0,1.0713882846,-2.0818453452,-0.1245291429
 C,0,-4.0103558321,-1.246864109,-0.9665240687
 C,0,1.6748449051,-1.4998918149,1.1007749328
 Zn,0,-0.997947465,0.0326703111,0.0215141361
 H,0,-5.1169982314,0.3770104204,-2.9634439056
 H,0,2.3499191612,-3.679098672,-0.5157507314
 H,0,2.5203145124,-2.0939463488,1.4368877644
 H,0,0.9327700686,-1.458972215,1.9000640992
 H,0,1.9923496913,-0.4764774134,0.9107475598
 H,0,-3.6690794687,-1.2610068057,0.0682154069
 H,0,-3.6180463993,-2.1395513994,-1.4603884544
 H,0,-5.0991969867,-1.2999281046,-0.9822660346
 H,0,1.9934686805,0.491148366,-1.824376912
 H,0,2.1856964914,2.1708237649,-2.3397416603
 H,0,0.6003343668,1.3943029085,-2.3964261959
 C,-1,1.4402532468,3.0873422128,1.4070974249
 H,0,1.818079052,3.8101417046,2.1121847057
 N,0,1.9928648482,2.9372515213,0.1501385135
 C,0,1.2741677798,1.9798360623,-0.4341389768
 C,0,1.5247782993,1.4780170694,-1.8205230686
 O,0,5.3533496315,-0.8946902585,0.9237612924
 C,0,5.3320475391,0.5648576558,0.9507171171
 C,0,4.7651371376,0.9128120324,-0.4343953409
 O,0,4.1989232147,-0.3409803633,-0.8903644725
 C,0,4.6273904441,-1.3506494708,-0.1105852336
 O,0,4.3709051485,-2.5076417674,-0.3038123191
 H,0,6.3694450003,0.8794766712,1.0524282202
 H,0,5.5365491171,1.2081075928,-1.1451926032
 H,0,3.974557996,1.6610256915,-0.3894199919
 C,0,4.4992544309,1.0598354266,2.1115527911
 H,0,4.881342662,0.6647764094,3.0529918252
 H,0,4.535594304,2.1497665256,2.1431175806
 H,0,3.4520347356,0.7804749748,2.0026679196

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C,-1,-1.788688,3.141271,0.146663
 H,0,-2.6450072255,3.7466081467,-0.1051280564
 N,0,-1.0155519931,3.4013898982,1.2523833429
 C,0,-0.0773211834,2.4600981559,1.2524172691
 C,0,1.0350011611,2.3997119827,2.2481812865
 H,0,1.2355694074,1.3806688089,2.5839878912
 H,0,0.7734265677,3.0071800326,3.1128723616
 H,0,1.9685254352,2.795620879,1.833155014
 C,0,-1.2891664778,2.033708045,-0.5064655482
 C,0,3.9788456066,-0.1706402691,0.4381444147
 C,-1,0.150973,-1.476037,-3.985801
 C,0,-0.112017519,-1.146468891,2.6028486158
 C,0,0.9337888411,-0.8118828443,-3.0917679251
 C,-1,5.104444,0.538275,0.145421
 H,0,-1.6238881039,1.5251013882,-1.3961231443
 H,0,3.8648037989,-1.0688059027,1.0193128553
 H,0,0.2267485717,-1.6094521919,-5.0495895129
 H,0,-0.5258675398,-0.1782186085,2.8282267829
 H,0,1.8416851606,-0.2607615853,-3.2613038258
 H,0,6.1363956267,0.3896460389,0.4067399682
 N,-1,-0.186862,1.585173,0.203054
 N,-1,2.888622,0.462711,-0.123955

N, 0, -0.8778014504, -2.0153028353, -3.2421810125
 N, -1, 0.584642, -1.377144, 1.427706
 N, -1, 0.391397, -0.942551, -1.830055
 N, 0, 4.6769958702, 1.6195616034, -0.6000305798
 C, 0, 3.3305075436, 1.5484347707, -0.7464904956
 C, 0, -0.7123165281, -1.6788827654, -1.9410379164
 C, 0, 2.5246018522, 2.5327507862, -1.5145022045
 C, 0, -1.633856913, -2.1065174481, -0.861296424
 Zn, 0, 0.8659117975, -0.0705215073, -0.003212048
 H, 0, 5.2608929442, 2.3559884532, -0.9615709173
 H, 0, -1.6550450572, -2.5464452468, -3.599262641
 H, 0, -2.4997132359, -2.6122206075, -1.2874909213
 H, 0, -2.000745162, -1.2572805616, -0.284969128
 H, 0, -1.1316452517, -2.7803192962, -0.1671063366
 H, 0, 1.5157933343, 2.5837037401, -1.1071842191
 H, 0, 2.4516825552, 2.2445889905, -2.5665930186
 H, 0, 2.9742012459, 3.5251005744, -1.4664990279
 H, 0, 1.0514395093, -3.7843627179, -0.3524000933
 H, 0, 2.2647699492, -4.2287289797, 0.8442535955
 H, 0, 2.4225892439, -2.7217142843, -0.0781256123
 C, -1, -0.122118, -2.319024, 3.325802
 H, 0, -0.557898158, -2.5181928804, 4.2920889517
 N, 0, 0.5582132547, -3.2877796078, 2.623178184
 C, 0, 0.9625729739, -2.6891864536, 1.5085181758
 C, 0, 1.7163230371, -3.3874635084, 0.4225837181
 C, 0, -3.6825824055, -0.6386711289, 2.305810176
 C, 0, -3.3233730123, 0.7313101757, 1.9357174666
 O, 0, -3.5262070491, -0.2704218288, 0.924333682
 H, 0, -4.703154785, -0.8617871598, 2.6014677706
 H, 0, -2.9141673038, -1.3064187796, 2.6811343154
 H, 0, -2.3017066819, 1.0736362805, 2.0360772593
 H, 0, -4.0782549555, 1.5092120571, 1.9519814493
 C, 0, -4.4346947012, 0.7383903319, -1.459256488
 O, 0, -3.8199410565, -0.032421618, -2.0757262236
 O, 0, -5.0698578795, 1.5277738235, -0.8979814087

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C, -1, 1.08381063, 3.422795723, 1.3500787269
 H, 0, 1.655052947, 4.07188263, 1.9948080803
 N, 0, 0.6457963604, 3.828715791, 0.1131351484
 C, 0, -0.0015781894, 2.7825933898, -0.3891585054
 C, 0, -0.7232405481, 2.8071953087, -1.6973409765
 H, 0, -0.6083250642, 1.8750689771, -2.2529159114
 H, 0, -0.3378326855, 3.6248438904, -2.3041857605
 H, 0, -1.797351385, 2.9744789811, -1.5590975932
 C, 0, 0.6834794495, 2.1210060497, 1.5694454888
 C, 0, -3.3957858978, -0.5900248319, -1.5093043835
 C, -1, -0.7879787435, -2.3819935881, 3.5768377055
 C, 0, 1.2433020436, -0.2643355535, -2.3443674961
 C, 0, -1.4264990173, -1.6654483724, 2.611274131
 C, -1, -4.692251768, -0.1737889434, -1.47698792
 H, 0, 0.8391740727, 1.4626816552, 2.408747746
 H, 0, -2.9112386607, -1.2754666444, -2.182301229
 H, 0, -1.1322139728, -2.8146936374, 4.4984903682
 H, 0, 1.4506667845, 0.786280858, -2.2292707501
 H, 0, -2.4597801523, -1.3723800008, 2.5534641377
 H, 0, -5.5406454886, -0.4148025587, -2.0913377197
 N, -1, -0.0147625928, 1.6986557785, 0.4495720806
 N, -1, -2.6939965835, 0.0437549356, -0.5035506395
 N, 0, 0.5193956047, -2.487334061, 3.1512031835
 N, -1, 0.3267705366, -0.9139482794, -1.5325202213
 N, -1, -0.5252147167, -1.3393921072, 1.6189643796
 N, 0, -4.764180471, 0.7310086279, -0.4358584616
 C, 0, -3.5391247975, 0.8436304082, 0.1349507533
 C, 0, 0.6555748343, -1.8477793197, 1.9659477242
 C, 0, -3.2427793927, 1.7106964896, 1.3047197909
 C, 0, 1.9351758077, -1.7665511754, 1.2218162676
 Zn, 0, -0.6569324645, -0.1005697166, -0.0453908546
 H, 0, -5.5838923809, 1.2431255108, -0.1534377091
 H, 0, 1.2744211164, -2.9274010642, 3.6512475486
 H, 0, 2.7041412613, -2.3441802525, 1.73417752
 H, 0, 2.2958173628, -0.7402844153, 1.1480182735
 H, 0, 1.8170431656, -2.1475880496, 0.208420985
 H, 0, -2.2125263703, 2.0608189241, 1.2554450372
 H, 0, -3.3668265005, 1.1606679366, 2.2413147697
 H, 0, -3.9094470458, 2.5732328903, 1.3279079098
 H, 0, -0.6393072034, -4.0908148177, -2.0794634029
 H, 0, -1.4721714904, -2.9218045546, -1.0371617986
 H, 0, -0.0091666223, -3.7160823008, -0.4768936693
 C, -1, 1.7484902379, -1.1865925191, -3.2335071118
 H, 0, 2.4757746495, -1.0466743368, -4.0173761628
 N, 0, 1.1653144259, -2.4102554212, -2.9949298792
 C, 0, 0.3289192224, -2.2055482069, -1.9834638161
 C, 0, -0.494319762, -3.2862456475, -1.3599862461
 C, 0, 4.8396865253, 0.9184285913, -0.1042523806
 C, 0, 3.6955004695, 1.8209860848, 0.0399307478
 O, 0, 3.9097790407, 0.755614975, 0.987368553
 H, 0, 5.8068771545, 1.2930526735, 0.225346284
 H, 0, 2.824106633, 1.6908235941, -0.5904208496
 H, 0, 3.8301171653, 2.817680495, 0.4418447866
 C, 0, 4.8764988354, -0.1857890086, -1.1194252582
 H, 0, 5.3987692248, 0.1489495145, -2.0193935834
 H, 0, 5.4106343362, -1.054082497, -0.7258288063
 H, 0, 3.8697873618, -0.4920665395, -1.4039824382
 C, 0, 3.4224507789, 1.2293579402, 3.6079769584
 O, 0, 3.9243819021, 2.2720646306, 3.5562775317
 O, 0, 2.9069780916, 0.1935928742, 3.7271442804



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