

Density Functional Theory Study of the Mechanism of Zinc Carbenoid Promoted Cyclopropanation of Allenamides†

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1. Cartesian coordinates and energies of computed structures of Figure 2

1

C,0,-3.5318969194,-0.2809668573,0.0445369663
H,0,-4.0240465495,-0.4839247406,0.9962595039
H,0,-4.0908952216,-0.5440818499,-0.8541459938
C,0,-2.3460197646,0.2586062983,-0.0156015195
C,0,-1.1621871376,0.8187247083,-0.0821855396
H,0,-1.023531465,1.8982500961,-0.1218490677
N,0,0.0379264509,0.1075368402,-0.1115866418
C,0,0.1418829995,-1.3165179328,0.0883114511
C,0,1.2618370752,0.7376891335,0.0111668051
O,0,1.4725265169,1.9197982159,0.0332766615
O,0,2.2194345496,-0.2182985564,0.1105138551
C,0,1.646737697,-1.5066502391,-0.1006950185
H,0,1.8884472772,-1.8346482382,-1.1192632225
H,0,2.0899011022,-2.2069691754,0.6115209752
H,0,-0.2106919806,-1.597257173,1.0926430026
H,0,-0.4539616302,-1.8699755296,-0.6468542174

Sum of electronic and thermal Free Energies=
-437.634740 (Hartree/Particle)

No imaginary frequency.

M-RC-T

C,0,-4.9792599272,-1.8159103121,-1.193405327
H,0,-5.7563436115,-2.3935081011,-0.6925791495
H,0,-5.2293225633,-1.4092284418,-2.1731416221
C,0,-3.8074144622,-1.6308513507,-0.6538666943
C,0,-2.6250498592,-1.4676669065,-0.1137114833
H,0,-1.7992507451,-2.1575224618,-0.2760793909
N,0,-2.3039773751,-0.3903967677,0.7239937218
C,0,-3.1597229236,0.7651183291,0.8883749801
C,0,-1.017956805,-0.1059394633,1.0644248541
O,0,-0.0374832822,-0.8071639366,0.8710015135
O,0,-0.9581821456,1.0804183612,1.6821740102
C,0,-2.2563451072,1.6870071267,1.7133896492
H,0,-2.1704338722,2.6894482962,1.2855317487
H,0,-2.568821854,1.7635111709,2.7595586676
H,0,3.0845570594,-1.5389205175,1.3741301417
C,0,3.0357777051,-1.346684078,0.2989827364
H,0,2.7988019898,-2.2911277068,-0.1983437839
Zn,0,1.7903942224,0.0822642226,-0.1419967388
Cl,0,4.7279808423,-0.9063759121,-0.2220363277
C,0,1.0291398697,1.7361247566,-0.874713269
H,0,1.629433034,2.1742998717,-1.6752004142
H,0,0.8575618703,2.5058979975,-0.1170333607
Cl,0,-0.6155814191,1.4273423917,-1.6311826348
H,0,-3.4101754076,1.1821637636,-0.0976235408
H,0,-4.0908822327,0.4988116685,1.4011127053

Sum of electronic and thermal Free Energies=
-1663.667199 (Hartree/Particle)

No imaginary frequency.

M-TS-T1

C,0,-1.8830127003,0.3501262678,3.4412584144
H,0,-2.562258383,-0.2168059484,4.0787524005
H,0,-1.5352695505,1.3079989189,3.8277832773
C,0,-1.5001813072,-0.106552735,2.2831872947
C,0,-1.1488810594,-0.6580269757,1.1253773736
H,0,-0.3216334385,-1.3679726949,1.049147184
N,0,-1.9383302758,-0.5304704214,-0.0265467022
C,0,-3.2660769598,0.0550706509,-0.0283995763
C,0,-1.3775913063,-0.4335741113,-1.2872986752
O,0,-0.2142255969,-0.5732725362,-1.5852292738
O,0,-2.3440602581,-0.1324904763,-2.1685473151
C,0,-3.6120834023,-0.0981590496,-1.504433951
H,0,-4.1910655617,0.7320917688,-1.9128482198
H,0,-4.1346293931,-1.0410499878,-1.7045139566
H,0,-3.9431723751,-0.4946101858,0.6329917105
H,0,-3.2352055441,1.1062014014,0.2985397973
H,0,-0.7011093614,1.773838946,0.6394390549
C,0,0.1419524168,1.1709298096,0.9902762528
H,0,0.4360107742,1.4753234109,2.0012081204
Zn,0,1.5252649717,0.3666282916,-0.2220311887
Cl,0,1.6664891366,2.7018864111,-0.2699345413
C,0,2.7043801026,-1.1595500907,-0.4964978559
H,0,2.7255377963,-1.5113579175,-1.5301313354
H,0,3.7282586749,-1.0565560712,-0.133419275
Cl,0,1.9832766004,-2.5508006752,0.4735269861

Sum of electronic and thermal Free Energies=
-1663.622528 (Hartree/Particle)

One imaginary frequency -350.75.

M-TS-T2

C,0,-0.1968334487,3.9080647495,-1.2082915899
H,0,0.7435844054,3.9429063299,-1.7580625094
H,0,-0.8918065219,4.7307262903,-1.3791963262
C,0,-0.4853135689,2.9456015683,-0.3768150818
C,0,-0.9391435268,2.0744039592,0.5189234694
H,0,-0.7241323171,2.1854430193,1.5830482413
N,0,-1.7448948068,0.994786477,0.2385682667
C,0,-2.0881305209,0.5212765559,-1.0856215646
C,0,-1.9632377333,0.0100648998,1.2033186921
O,0,-1.6037280495,0.0482204152,2.3491427915
O,0,-2.6445246135,-0.9934808667,0.6294085802
C,0,-2.9799527448,-0.6663993914,-0.7257972174
H,0,-4.0448729356,-0.4106971064,-0.7614119538
H,0,-2.7800852182,-1.5464314476,-1.3405194059
H,0,-2.6089411994,1.2912064441,-1.6646894667
H,0,-1.18156144,0.2126117874,-1.6304438577
H,0,1.5046697409,1.7776142647,-1.0380022301
C,0,1.3262862868,1.4368289849,-0.0153230561
H,0,1.7303571224,2.1444251522,0.7108562645
Zn,0,1.2735075382,-0.5071179716,0.3077507003
Cl,0,3.4787759309,0.170314539,-0.0048051952

C,0,0.4904251014,-2.284209318,0.3858708892
H,0,1.2224980902,-3.0785106854,0.5415712413
H,0,-0.3356508578,-2.4144635146,1.08815158
Cl,0,-0.2132967129,-2.5915741347,-1.2849362619

Sum of electronic and thermal Free Energies=
-1663.623374 (Hartree/Particle)
One imaginary frequency -282.43.

M-TS-T3

C,0,0.2127609757,0.413391041,2.9422109338
H,0,1.2826000091,0.2391120639,2.8255607185
H,0,-0.0918807198,1.0672572274,3.7585667905
C,0,-0.6660207504,-0.135235496,2.1480399632
C,0,-1.7470848695,-0.5691953062,1.5078844937
H,0,-2.2457658428,-1.5029252608,1.7713867269
N,0,-2.3069109133,0.0668483887,0.4217757997
C,0,-1.796280625,1.2730694476,-0.1955612851
C,0,-3.1837569356,-0.6081362041,-0.4279684051
O,0,-3.6222221201,-1.7122949145,-0.2635827874
O,0,-3.4483092019,0.1949807231,-1.4753660895
C,0,-2.8522069357,1.4814186073,-1.2786933564
H,0,-3.6341510181,2.179239594,-0.9569809995
H,0,-2.4392998174,1.8200669972,-2.2308725854
H,0,-1.735564154,2.1019871317,0.5173960516
H,0,-0.7863087785,1.1074384781,-0.6003769694
H,0,0.7311874198,-2.1173098689,1.4802139619
C,0,0.4835084856,-1.5061230754,0.6100288647
H,0,-0.3213311471,-1.968397558,0.0314642823
Zn,0,1.762573303,-0.2874101512,-0.2264281967
Cl,0,2.2227379022,-2.5375884835,-0.7402244913
C,0,2.6013957136,1.3863665993,-0.7356066731
H,0,3.5951419552,1.514509648,-0.2999320312
H,0,2.6896044451,1.5139885963,-1.8168178351
Cl,0,1.6067276201,2.7992657748,-0.1370778819

Sum of electronic and thermal Free Energies=
-1663.623168 (Hartree/Particle)
One imaginary frequency -330.08.

M-PC-T

C,0,-2.2832847416,0.043139563,3.4786958001
H,0,-3.1070913764,-0.6656338871,3.5349752547
H,0,-2.19242961,0.7673639715,4.2847834794
C,0,-1.422491846,0.0164410439,2.478091827
C,0,-1.0567773857,-0.5848821034,1.2021807617
H,0,-0.52426532,-1.5370043759,1.1939499648
N,0,-1.9199058066,-0.4374179467,0.0641250681
C,0,-3.1070689049,0.3934378397,0.0065902727
C,0,-1.4722978394,-0.7106031119,-1.1812671516
O,0,-0.3767160644,-1.1912345692,-1.4695101769
O,0,-2.3877733919,-0.3926123301,-2.0958653211
C,0,-3.547569267,0.1363168432,-1.4362265457
H,0,-3.8536801351,1.0410902803,-1.9650134886
H,0,-4.3456896409,-0.6115509998,-1.5013541048

H,0,-3.8540194291,0.0824344391,0.7440768092
H,0,-2.854552664,1.4487184154,0.1871772316
H,0,-0.4216440814,1.5842670497,1.3020174279
C,0,-0.28688914,0.6126475447,1.7802593502
H,0,0.7296032601,0.4050673418,2.1197295911
Zn,0,1.2440253963,0.1599248896,-1.1230581347
Cl,0,0.1725841134,2.009130077,-1.4874281836
C,0,2.7869474075,-0.9115829858,-0.615823956
H,0,2.9741739818,-1.7163559541,-1.3302170913
H,0,3.7077231919,-0.3443282714,-0.4712556447
Cl,0,2.4399122934,-1.7294377632,0.9772519605

Sum of electronic and thermal Free Energies=
-1663.734247 (Hartree/Particle)
No imaginary frequency.

M-RC-B1

C,0,-1.4885579793,1.3320918946,2.1049261301
H,0,-2.1728000977,1.8493472556,1.4319100555
H,0,-1.8037441338,1.2016943056,3.1374620065
C,0,-0.3241197298,0.8755891807,1.6736804293
C,0,0.5790480137,0.7505399221,0.5308604347
H,0,0.3375380269,-0.0047129652,-0.2208761403
N,0,1.187043534,1.9032026301,-0.0570392762
C,0,0.9397048395,3.2808525327,0.3217191119
C,0,1.9351294682,1.8183823959,-1.175863669
O,0,2.3118862353,0.7904733497,-1.7368473647
O,0,2.2194635982,3.0310018925,-1.6505661561
C,0,1.4797753843,4.0150078348,-0.9097554009
H,0,2.1570285871,4.8367279414,-0.6689917804
H,0,0.6744158223,4.3820860734,-1.5551597155
H,0,-0.1315623549,3.4518137872,0.4744419273
H,0,1.4743828719,3.5375823286,1.2461761966
H,0,1.7357249554,0.7916113804,2.4513760328
C,0,0.963554816,0.2346355816,1.9192849695
H,0,1.0238564888,-0.8480637344,2.044469402
Zn,0,2.7307249887,-1.0540960007,-0.7640380167
Cl,0,4.2226879971,-0.4822046023,0.6659611105
C,0,1.5275939074,-2.3620974507,-1.5876937372
H,0,1.0871937349,-1.9942372007,-2.5180764754
H,0,1.970556724,-3.3423166646,-1.7717158628
Cl,0,0.1024551816,-2.7035819505,-0.4724920486
Zn,0,-2.180765735,-0.8131640534,-0.2677048179
C,0,-2.7830667212,-1.8494786134,1.2601310432
H,0,-3.2030141802,-2.8245373044,1.0000402311
H,0,-1.9896263393,-2.0006639992,1.9987339707
Cl,0,-4.1064251635,-0.9225238326,2.1022748682
C,0,-1.851486607,0.2748619521,-1.8589937387
H,0,-0.8664296433,0.1006536566,-2.3052834443
H,0,-2.6012146389,0.1116151427,-2.6376102869
Cl,0,-1.9237608514,2.0642673338,-1.4891089884

Sum of electronic and thermal Free Energies=
-2889.758534 (Hartree/Particle)
No imaginary frequency.

M-TS-B1

C,0,2.423030728,3.3979466345,0.7870002464
H,0,3.0815609874,3.6165027621,-0.0514932616
H,0,2.6251770007,3.9314293682,1.7133135512
C,0,1.5187862682,2.4153234784,0.7314675529
C,0,0.9151621988,1.3605398323,-0.0704757332
H,0,0.1515655303,1.6348833398,-0.8027972249
N,0,1.6853025278,0.2328473845,-0.4999624311
C,0,2.9624219583,-0.1819540856,0.0504644819
C,0,1.0791065373,-0.8124908569,-1.115945344
O,0,-0.0944364768,-0.8617666873,-1.4744908695
O,0,1.9413603564,-1.8108457917,-1.3016746275
C,0,3.2323180612,-1.4124404554,-0.8140779041
H,0,3.660330588,-2.251573068,-0.2633606036
H,0,3.864942924,-1.1793631024,-1.6779267387
H,0,3.7254395425,0.5946495635,-0.0652979382
H,0,2.8671171574,-0.432169316,1.1179034914
H,0,0.8774184523,0.8460501921,2.1360166848
C,0,0.5325960908,1.5752243375,1.4013723458
H,0,-0.4745738355,1.9567809814,1.5821341694
Zn,0,-1.5302971914,-0.7696881488,0.1354429338
Cl,0,-0.3433910191,-1.8083616878,1.6142452356
C,0,-3.0283292202,0.2884199141,-0.515343541
H,0,-3.285848202,0.0379347293,-1.546740144
H,0,-3.9272503289,0.2345043165,0.1004556962
Cl,0,-2.543024632,2.0503429821,-0.5381079311
Zn,0,1.5507736942,6.4250593204,-0.1754650599
C,0,0.6355372654,4.7015188014,0.1135470874
H,0,0.3114631989,4.0975980624,-0.7374677419
H,0,0.0230087072,4.5088310345,0.9965925418
Cl,0,-0.7421239915,6.5897441281,-0.5501305494
C,0,3.1212707831,7.5565438066,-0.2639399219
H,0,3.2767404827,8.0190396809,-1.240880444
H,0,3.1485227976,8.3411160845,0.495084344
Cl,0,4.5863480787,6.5036623449,0.0399417568

Sum of electronic and thermal Free Energies=
-2889.717859 (Hartree/Particle)

One imaginary frequency -326.46.

M-PC-B1

C,0,-1.7133075462,0.6318846447,1.2869486209
H,0,-2.0108142887,1.5608658088,0.7964520335
H,0,-1.8501604192,0.6062493859,2.3663733702
C,0,-0.5753465226,-0.1116554848,0.7115749166
C,0,0.5605648389,0.1359309008,-0.1855806968
H,0,0.6423399177,-0.4857129238,-1.0767529919
N,0,1.0822441639,1.4546002414,-0.4081572406
C,0,0.7098079746,2.6663067369,0.2982827097
C,0,2.2942032672,1.6061632921,-0.9908950783
O,0,2.9864732871,0.7081707842,-1.4683572891
O,0,2.6665165424,2.8849102084,-0.9932819146
C,0,1.634256788,3.6742656167,-0.3873601939
H,0,2.1042633107,4.3771488009,0.3032013107
H,0,1.1213883634,4.2296254326,-1.1805712608

H,0,-0.3460073687,2.9139057439,0.1527713892
H,0,0.9138614276,2.5701348117,1.3755530351
H,0,1.2560428752,0.0023842896,1.9351782559
C,0,0.757992356,-0.569765948,1.1535907345
H,0,0.9949527305,-1.6329674909,1.1226614063
Zn,0,3.860826578,-0.583679044,-0.0068737473
Cl,0,4.0065843245,0.8471602364,1.6154102998
C,0,4.0078057251,-2.3475037085,-0.8153950877
H,0,4.5121506449,-2.3118717555,-1.783591709
H,0,4.4962429401,-3.0957723073,-0.1890157401
Cl,0,2.3299264949,-2.9816828259,-1.1492073768
Zn,0,-4.3719045688,0.5307109693,0.5968619219
C,0,-1.9188956865,-0.6929858709,0.5379551928
H,0,-2.3206679945,-0.6651386799,-0.4772326802
H,0,-2.1953484795,-1.5578151088,1.1374123064
Cl,0,-4.9815981418,-0.3844002398,2.4044822662
C,0,-4.3845278575,1.4921784151,-1.0944923969
H,0,-4.9370410809,0.9306132187,-1.8518607038
H,0,-4.8634187957,2.4677142982,-0.9805827854
Cl,0,-2.7410617999,1.8002915515,-1.7873818766

Sum of electronic and thermal Free Energies=
-2889.820043 (Hartree/Particle)

No imaginary frequency.

M-IM-T

C,0,2.1313492121,3.058822608,1.6705415105
H,0,3.2058609721,3.1677583549,1.5343683415
H,0,1.6932266094,3.5252351185,2.5499923654
C,0,1.3929622266,2.3953925183,0.8017655125
C,0,1.3759172677,1.6057489893,-0.4335470296
H,0,1.4966367249,2.1047326996,-1.3997124808
N,0,1.9192560546,0.2825968262,-0.3683859242
C,0,3.3422090687,0.0501680667,-0.2020685191
C,0,1.3591055836,-0.7353523834,-1.0724684309
O,0,0.2461834681,-0.7540876412,-1.5770063391
O,0,2.1978284636,-1.7810087834,-1.1272901323
C,0,3.4072628617,-1.4596042384,-0.4259653651
H,0,3.413959378,-2.0212905303,0.5151194301
H,0,4.2525525589,-1.7726802631,-1.0432434913
H,0,3.9139150997,0.6093565905,-0.9581722365
H,0,3.6779430625,0.3525398048,0.7956941367
H,0,-0.3284094143,1.0270586875,0.8832489639
C,0,0.1059705081,1.87748625,0.3590207405
H,0,-0.6214064997,2.5531337728,-0.0874240186
H,0,-2.3032223204,-2.2528778111,-2.9945480501
C,0,-1.9921264821,-1.4535377176,-3.6728609264
H,0,-2.5014164799,-0.537510058,-3.3607784154
Zn,0,-0.0565873782,-1.2468715743,-3.7299874139
Cl,0,-2.6694061737,-1.8810705462,-5.3113786324
C,0,1.7899170908,-1.1554667883,-4.3915322351
H,0,1.8636597534,-1.056057604,-5.4767162419
H,0,2.3998389894,-2.0102995289,-4.0862056522
Cl,0,2.6656555045,0.317825041,-3.7263443464

Sum of electronic and thermal Free Energies=
-1702.919627 (Hartree/Particle)
No imaginary frequency.

M-RC-B1'

C,0,0.1752709443,1.5492945493,2.2750469121
H,0,-0.547413596,1.8041879555,1.4999494048
H,0,0.173197594,2.1752846463,3.1648283552
C,0,1.0265690981,0.5479283908,2.1586749409
C,0,1.57433385,-0.5579326172,1.3575798168
H,0,1.0096944584,-1.4929080438,1.3099855455
N,0,2.3555837514,-0.3005793342,0.17566986
C,0,3.8049556898,-0.386755309,0.1268476639
C,0,1.8318683359,-0.5869042825,-1.0520169146
O,0,0.6693464011,-0.8300656121,-1.3156969859
O,0,2.8061883374,-0.5996013817,-1.9780066627
C,0,4.0319659398,-0.184962832,-1.3676083442
H,0,4.8452665274,-0.7870035258,-1.7776698708
H,0,4.2020379496,0.8699001448,-1.613981688
H,0,4.2866884776,0.3946872884,0.7237484261
H,0,4.1567416582,-1.3662139143,0.4854577172
H,0,3.126823858,0.3110644754,2.7349304342
C,0,2.1570606723,-0.1876120086,2.7132660378
H,0,2.0070116316,-0.8980065157,3.5249665066
Zn,0,-1.2919220466,-0.0483764077,-0.3759598126
C,0,-1.9276077533,-1.6432458053,0.5466374175
H,0,-1.3184672794,-2.5206555747,0.3086847759
H,0,-1.975516432,-1.5402651768,1.6348631863
Cl,0,-3.6198165169,-2.041485089,-0.0008081541
C,0,-1.0390576872,1.7230101284,-1.1580061539
H,0,-0.0067767494,2.0720009104,-1.0405594902
H,0,-1.2785014545,1.74873457,-2.2245605381
Cl,0,-2.0889396597,2.9907053711,-0.3713093855

Sum of electronic and thermal Free Energies=
-1702.910253 (Hartree/Particle)
No imaginary frequency.

M-TS-B1'

C,0,-1.5829968564,1.3590632523,0.7233968598
H,0,-1.9864063039,1.839276764,-0.1662863004
H,0,-2.169671475,1.4593797657,1.6346777862
C,0,-0.3673233051,0.8046645976,0.7296852924
C,0,0.8802425131,0.5644334274,0.0186028935
H,0,0.972423936,-0.3078061828,-0.6301154459
N,0,1.6476499879,1.6495726383,-0.4927034035
C,0,1.7086853414,2.9718898399,0.0855757456
C,0,2.7523586379,1.4003724383,-1.2836326132
O,0,3.0869712963,0.3466201891,-1.7538200035
O,0,3.417687148,2.56914282,-1.464403819
C,0,2.6640908938,3.639239893,-0.9003887019
H,0,3.3535727372,4.3456877704,-0.4322602499
H,0,2.118506688,4.1491917906,-1.7044825529
H,0,0.7254333313,3.4558484704,0.1133308526
H,0,2.1156210462,2.954319313,1.1098327911

H,0,1.2109895817,0.9159853932,2.2488447225
C,0,0.7423461861,0.2599852947,1.5147821555
H,0,0.7527690509,-0.7943869393,1.7905070759
Zn,0,-4.2039546402,-0.4724476786,-0.0305488875
C,0,-2.2829776923,-0.809946865,0.2152473305
H,0,-1.6232503065,-0.9710066792,-0.6396577711
H,0,-1.887241214,-1.2608774938,1.127026606
Cl,0,-3.6378291696,-2.7357188327,-0.2918303834
C,0,-5.7851021644,0.6420450015,-0.1101183693
H,0,-6.2787286994,0.6454329167,-1.084122291
H,0,-6.5311016701,0.4089985253,0.6525649137
Cl,0,-5.255446879,2.3644585702,0.201962767

Sum of electronic and thermal Free Energies=
-1702.866646 (Hartree/Particle)
One imaginary frequency -323.56.

M-PC-B1'

C,0,-0.0990230038,-0.2672945457,0.7449601667
H,0,0.028624343,0.1576141398,-0.2552876193
H,0,-0.6124961329,0.3743984279,1.4629785762
C,0,1.0377096859,-1.082851903,1.2277297695
C,0,2.4572425816,-1.0892695185,0.8409730335
H,0,2.9267786262,-2.0187010048,0.5243241313
N,0,2.9851946355,0.0179041172,0.1075030246
C,0,2.8915347259,1.4046193573,0.5032047956
C,0,3.9967727309,-0.1655920894,-0.8080638466
O,0,4.4584373107,-1.2074228664,-1.1931953033
O,0,4.4152356396,1.057303606,-1.2335616865
C,0,3.5479390983,2.0577747618,-0.7069753598
H,0,4.1397958963,2.9432530371,-0.4634577726
H,0,2.8010448334,2.3206985922,-1.4685143895
H,0,1.8532913722,1.7327816946,0.6395674605
H,0,3.4470367151,1.5966493729,1.4358083885
H,0,2.1672729121,0.0280291862,2.7709220889
C,0,2.0545401343,-0.9459213407,2.2964348493
H,0,2.2505126858,-1.7914284177,2.9524706683
Zn,0,-2.5345478565,0.2677681881,-0.6795719629
C,0,-0.2103049259,-1.7789264384,0.8941528993
H,0,-0.2555436863,-2.3698286762,-0.0180917359
H,0,-0.8372816256,-2.1484637588,1.7032756135
Cl,0,-3.1383277127,-1.6882391287,-1.159700949
C,0,-2.2527932899,2.1636911836,-0.4101384358
H,0,-3.0359216137,2.7567729514,-0.8871309664
H,0,-2.209778834,2.430490897,0.6486802997
Cl,0,-0.6840712455,2.6861441753,-1.1519597375

Sum of electronic and thermal Free Energies=
-1702.968339 (Hartree/Particle)
No imaginary frequency.

M-TS-T1cis

C,0,-2.0278070281,0.6291349328,3.5548330168
H,0,-2.817338549,0.2604630644,4.20884891
H,0,-1.5536035946,1.5678181259,3.8397761621

C,0,-1.703418451,-0.0119567308,2.4692944559
C,0,-1.3957971609,-0.7965072098,1.4429283666
H,0,-0.6524365196,-1.5864202244,1.5698739071
N,0,-1.940561066,-0.7562263312,0.1668204593
C,0,-1.8060965858,-1.8244070325,-0.8090501308
C,0,-2.7998111683,0.2373608451,-0.2842560847
O,0,-3.1896916341,1.1891532926,0.3334777589
O,0,-3.124661328,-0.0423201812,-1.5663978701
C,0,-2.2949411971,-1.0976724327,-2.0562150819
H,0,-2.8866800239,-1.7230112459,-2.7276724415
H,0,-1.4627563356,-0.6534879893,-2.6182943785
H,0,-0.7687486464,-2.1721816058,-0.8897586336
H,0,-2.4464064056,-2.6770689797,-0.542782746
H,0,-0.6774211892,1.8261998158,1.1404366973
C,0,0.1313864261,1.125035872,1.3616271171
H,0,0.4921737816,1.2195578659,2.3879452663
Zn,0,1.3025005055,0.4534521388,-0.0539930233
Cl,0,1.883727284,2.6424684419,0.480649365
C,0,2.0396892729,-0.8878425247,-1.2521118923
H,0,1.5748828743,-0.9403995632,-2.2400083852
H,0,3.1181456849,-0.7900209188,-1.3919938197
Cl,0,1.7899877839,-2.5392718154,-0.4909480247

Sum of electronic and thermal Free Energies=
-1663.618478 (Hartree/Particle)
One imaginary frequency -272.53.

M-TS-T2cis

C,0,0.0126902105,0.428554816,-0.1001688766
H,0,-0.0133938423,0.4483142507,0.9890798809
H,0,0.9728066297,0.6320334006,-0.5734359925
C,0,-1.0395976474,0.1453658312,-0.8118211062
C,0,-2.0629146464,-0.0360452014,-1.6393232223
H,0,-2.6195212639,0.8341676231,-1.9911686849
N,0,-2.4670745776,-1.2295197181,-2.2177256824
C,0,-3.5568012473,-1.3223808547,-3.1714121865
C,0,-2.1813192085,-2.477749518,-1.6655799758
O,0,-1.4789736362,-2.6922351099,-0.7167116897
O,0,-2.8425200054,-3.4106569657,-2.3753273062
C,0,-3.4972254386,-2.8127610771,-3.4952430974
H,0,-4.4854120986,-3.2652302253,-3.6001970767
H,0,-2.9002432892,-3.0127527704,-4.3934211315
H,0,-4.5160812163,-1.0442835525,-2.70735644
H,0,-3.379296248,-0.6931017065,-4.0500007896
H,0,-2.2829790709,-0.7388533246,1.0586047729

C,0,-2.9561312036,0.0036017209,0.6245582248
H,0,-2.6644666618,1.0278239064,0.8594524801
Zn,0,-4.8352680586,-0.5073677287,0.3697131479
Cl,0,-4.4575016406,-0.0245789713,2.6134999935
C,0,-6.4597799016,-1.1257805836,-0.5051522304
H,0,-7.272988721,-1.2934577645,0.2039529208
H,0,-6.8336257926,-0.4894294494,-1.3114723228
Cl,0,-6.119447659,-2.7572006309,-1.2627592243

Sum of electronic and thermal Free Energies=
-1663.616516 (Hartree/Particle)
One imaginary frequency -265.66.

M-TS-T3cis

C,0,0.110709157,0.0353159048,-0.2326391132
H,0,0.2230567694,-0.0315110023,0.8475730403
H,0,1.0246614305,0.0770260061,-0.8224615477
C,0,-1.0563130112,0.0173187697,-0.822469944
C,0,-1.9844386172,0.1632438812,-1.7708737783
H,0,-2.3171988677,1.1614850404,-2.0598115946
N,0,-2.7025456835,-0.8553359042,-2.3903865692
C,0,-3.4680483045,-0.6416190231,-3.6047458293
C,0,-2.6207315253,-2.2047058567,-2.0737880606
O,0,-2.003012083,-2.7116725231,-1.1738324976
O,0,-3.3809129993,-2.8923584348,-2.9478162195
C,0,-4.1562993884,-1.9981236792,-3.7457596017
H,0,-5.1794251618,-1.9829325912,-3.3525875842
H,0,-4.1724487875,-2.3723943462,-4.7713809823
H,0,-4.1814106358,0.182715562,-3.4905822676
H,0,-2.8036389199,-0.4142094671,-4.4496091297
H,0,-2.5404552233,0.7650490207,1.0789296882
C,0,-2.6526753073,-0.227386014,0.6345822197
H,0,-3.5453212392,-0.2687322089,0.0090294535
Zn,0,-1.9841418018,-1.9335960764,1.356601423
Cl,0,-3.9717065281,-1.1297119669,2.477269322
C,0,-0.7999958224,-3.3930098347,1.8340547681
H,0,-0.7717909073,-3.6214255001,2.9011223779
H,0,-1.0393297973,-4.3049764935,1.282125423
Cl,0,0.9166664687,-2.9680472628,1.3647911512

Sum of electronic and thermal Free Energies=
-1663.615427 (Hartree/Particle)
One imaginary frequency -469.73.

2. Cartesian coordinates and energies of computed structures of Figure 3

M-RC-O

C,0,0.0918169888,-1.4987224028,-1.6096112327
H,0,-0.6844668986,-2.1126074357,-1.1432332483
H,0,0.1717730359,-1.5580133934,-2.6958159708
C,0,0.885259197,-0.733846001,-0.9047760685
C,0,1.6863069777,0.0392722318,-0.2057807772
H,0,1.4565294955,1.0846231888,0.0105077148
N,0,2.9014227356,-0.3725630782,0.32880333
C,0,3.5341782373,-1.6397666798,0.052481869
C,0,3.7787172713,0.5312993652,0.9077942087
O,0,3.5757576958,1.6939666966,1.1240895503
O,0,4.9269559956,-0.1238862333,1.1923697152
C,0,4.7742913986,-1.520516827,0.9396920317
H,0,5.6865106577,-1.8887801194,0.4648373052
H,0,4.6380719526,-2.0354208923,1.8982095494
H,0,2.8886788566,-2.4807127938,0.331785653
H,0,3.7725391648,-1.7321211727,-1.0178658156
H,0,-0.5065599235,2.3252417786,-1.2506544965
C,0,-1.5057204452,1.8954000124,-1.1357365133
H,0,-1.8720639402,1.6244892731,-2.1297379912
Zn,0,-1.5852401636,0.4169838474,0.1166777021
Cl,0,-2.5824347765,3.2297166079,-0.5273448713
C,0,-1.881481577,-0.9915301926,1.4235888445
H,0,-0.9561977003,-1.4184268046,1.8197824068
H,0,-2.5185495369,-0.7022286668,2.2621353763
Cl,0,-2.7513436988,-2.3559173082,0.5742877287

Sum of electronic and thermal Free Energies=
-1663.656898 (Hartree/Particle)
No imaginary frequency.

M-TS-O1

C,0,0.0882449787,-1.1105041737,0.0905285394
H,0,-0.3640288137,-1.4595353375,1.0203718135
H,0,-0.3647224632,-1.5000525293,-0.8225427729
C,0,1.1928810665,-0.3899937063,0.0769476259
C,0,2.2727598587,0.3558353227,0.0736495704
H,0,2.2296464517,1.4460659119,0.0503974054
N,0,3.5673025158,-0.1418402117,0.1005568018
C,0,3.9167683802,-1.5375122065,-0.0160446934
C,0,4.6652749785,0.6867719231,-0.0876084707
O,0,4.6553969273,1.8822605026,-0.1816002772
O,0,5.7683265408,-0.0918056553,-0.1522675285
C,0,5.4355135245,-1.4488418314,0.1396833126
H,0,5.9824966496,-2.0957100847,-0.5498496772
H,0,5.7517005546,-1.6723968845,1.1653887241
H,0,3.4425322739,-2.1364012652,0.7701901784
H,0,3.6011693565,-1.9387609866,-0.9908614212
H,0,-0.4651413255,1.3509845662,0.9676247374
C,0,-0.9285051772,0.9777449559,0.0519908284
H,0,-0.4222263422,1.35037355,-0.8409320208
Zn,0,-2.8233076702,0.4429496206,-0.0013653648
Cl,0,-2.5780542626,2.7646971026,0.0141653412
C,0,-4.2393629425,-0.8783873464,-0.0518232468

H,0,-4.8892971754,-0.8686250723,0.8255838572
H,0,-4.8659266668,-0.8263151705,-0.9445956779
Cl,0,-3.4468872181,-2.527591994,-0.0810275845

Sum of electronic and thermal Free Energies=
-1663.618622(Hartree/Particle)
One imaginary frequency -314.48.

M-TS-O2

C,0,0.0438967888,-1.0758913773,-0.0202005715
H,0,-0.5011291177,-1.400504523,0.8673472079
H,0,-0.5082489118,-1.1407144227,-0.9588798046
C,0,1.21453219,-0.4695881305,0.0636640128
C,0,2.3001913917,0.2568927585,0.1802725778
H,0,2.200790786,1.330999534,0.3543062718
N,0,3.6297951994,-0.1371148138,0.1136979126
C,0,4.1369682739,-1.4103304865,-0.3488911005
C,0,4.6280976035,0.8352774956,0.1106604608
O,0,4.4811072386,2.0114587328,0.2939405598
O,0,5.8066151701,0.2304850065,-0.1431733746
C,0,5.6381968566,-1.1863279554,-0.1731432829
H,0,6.2355240339,-1.5915603081,-0.9927685736
H,0,6.0020006287,-1.6011415668,0.7742295844
H,0,3.7718453474,-2.2497401147,0.2526196748
H,0,3.8513001003,-1.58673199,-1.3975463085
H,0,1.7947480634,-2.7499598034,-1.0846565967
C,0,1.1804633937,-3.0654032312,-0.2414321426
H,0,1.698905365,-2.969659316,0.713257538
Zn,0,-0.266664496,-4.3761675999,-0.4730559431
Cl,0,1.8847172369,-5.3535227534,-0.4928430191
C,0,-2.107899153,-4.9526783856,-0.6158902697
H,0,-2.3662093821,-5.3835866673,-1.5854488327
H,0,-2.4156733174,-5.6510570435,0.1651322831
Cl,0,-3.1487795798,-3.4644412084,-0.4174639239

Sum of electronic and thermal Free Energies=
-1663.615832 (Hartree/Particle)
One imaginary frequency -330.78.

M-PC-O

C,0,0.0877013431,-0.2971818587,-0.608080451
H,0,-0.24775375,-1.2437669774,-0.1732928731
H,0,0.0939510297,-0.2562596715,-1.6985994921
C,0,1.0718121218,0.4798151042,0.1373733062
C,0,2.3086731183,0.6297448651,0.5867465075
H,0,2.6029374759,1.4733039333,1.2076046927
N,0,3.3562031709,-0.2417448466,0.3256612338
C,0,3.2939818796,-1.3692608021,-0.573722912
C,0,4.661673491,0.0666124907,0.6762217194
O,0,5.0381406281,1.0181797992,1.3029986195
O,0,5.4710397227,-0.9005021837,0.1826756869
C,0,4.6929597503,-1.9553909232,-0.3781501591

H,0,5.163931716,-2.276782349,-1.3102705112
H,0,4.6859733902,-2.7969945164,0.3251984455
H,0,2.5012622865,-2.0696729503,-0.2878095011
H,0,3.1046411833,-1.0371833039,-1.6055438426
H,0,-0.8503838727,0.940987096,1.0647097469
C,0,-0.278528686,1.0170957664,0.1352031958
H,0,-0.5010488656,1.8850945183,-0.4870558832
Zn,0,-2.6186074425,-0.1048560006,-0.6364808028
Cl,0,-2.719639788,0.9021177028,-2.5023927339
C,0,-3.1475238645,-1.1321404002,0.9281768554
H,0,-3.9120780814,-0.5974977867,1.4971534117
H,0,-3.5631568418,-2.0973198943,0.6285763444
Cl,0,-1.797254115,-1.4816388116,2.0761313963

Sum of electronic and thermal Free Energies=
-1663.721839 (Hartree/Particle)

No imaginary frequency.

M-RC-B2

C,0,-3.6500412087,-0.5729645011,-2.1989015931
H,0,-4.4207982468,-1.338053689,-2.1062377588
H,0,-3.0917862557,-0.6140216926,-3.1339604126
C,0,-2.9731501775,-0.0980557617,-0.9920190201
C,0,-2.1095491866,-0.2875396654,-0.0091517345
H,0,-1.9220723264,0.4561077095,0.7634661985
N,0,-1.349167628,-1.4530607952,0.1506889938
C,0,-1.2999283142,-2.5218853759,-0.8252316438
C,0,-0.2465876849,-1.4813142117,0.9541473134
O,0,0.1015051837,-0.6179431127,1.7439836752
O,0,0.427700656,-2.6218262548,0.7727522756
C,0,-0.2454951842,-3.4342463431,-0.1971181565
H,0,0.4977355923,-3.7909254672,-0.9139481389
H,0,-0.6869983781,-4.2906616502,0.3244353302
H,0,-2.2756644485,-3.0064096351,-0.9364878574
H,0,-0.9886077642,-2.1227911892,-1.8008812655
H,0,-4.9058202082,0.9457049532,-1.1208337602
C,0,-3.9420884073,0.7991671208,-1.6070324752
H,0,-3.5769259322,1.6719094766,-2.1468742729
H,0,-0.7095613314,2.8457489392,1.7024009497
C,0,0.2461073622,2.5284918109,2.1307804401
H,0,0.0510814003,2.1304611879,3.1304683194
Zn,0,1.2082141977,1.2429179089,1.0329895415
Cl,0,1.226908957,4.0477925439,2.3589218614
C,0,2.3699273147,0.3264478188,-0.2453569751
H,0,3.1302207013,0.9417531959,-0.7299505174
H,0,2.8500003702,-0.56425038,0.169385125
Cl,0,1.3079889475,-0.2914889406,-1.6161294416

Sum of electronic and thermal Free Energies=
-1702.926335 (Hartree/Particle)

No imaginary frequency.

M-TS-B2

C,0,-0.2441337338,-0.3828054714,0.2952555509
H,0,-0.4138741364,0.4894109645,0.9258929414

H,0,-0.4514747127,-1.3329545454,0.7884007591
C,0,0.805142148,-0.3225004205,-0.7216092819
C,0,2.094386684,-0.1052875263,-1.0240041423
H,0,2.4287384829,0.036908783,-2.0511551465
N,0,3.1165061318,-0.0028635695,-0.109545072
C,0,2.9985833869,-0.212747588,1.3199329194
C,0,4.4453314631,-0.1231452373,-0.5213217008
O,0,4.8347757848,-0.2063545226,-1.655316798
O,0,5.2245211464,-0.1530055042,0.5718803075
C,0,4.439121946,0.0505576489,1.7524416825
H,0,4.790181433,-0.6478501409,2.5144713113
H,0,4.5874669781,1.0833546316,2.0888948161
H,0,2.2833988467,0.4819605788,1.7717704974
H,0,2.6834475744,-1.2457502827,1.5351422623
H,0,-0.9657352507,0.681176306,-1.5521502082
C,0,-0.5756226658,-0.268033215,-1.1875627392
H,0,-1.0033286865,-1.1435296972,-1.6762606132
H,0,0.7904512111,-2.739915336,-0.7778701534
C,0,1.673319559,-2.4731297486,-1.3639719955
H,0,1.4012023037,-2.2510961116,-2.3974248912
Zn,0,3.413161208,-3.2591860634,-0.8862787522
Cl,0,2.0681207375,-4.8417624699,-1.9646352923
C,0,5.1113496223,-3.457088804,0.0377100474
H,0,5.5850413378,-4.4268437143,-0.1241983892
H,0,5.8405386032,-2.665477787,-0.148085317
Cl,0,4.7401276273,-3.388911767,1.8366317875

Sum of electronic and thermal Free Energies=
-1702.885581 (Hartree/Particle)

One imaginary frequency -273.96.

M-PC-B2

C,0,-3.3870411985,0.0923606494,-1.6179450476
H,0,-3.8456024238,-0.8925262315,-1.5555273591
H,0,-3.188442317,0.4331667317,-2.6316924035
C,0,-2.4580366221,0.5250922809,-0.5501022169
C,0,-1.5804169342,-0.058224487,0.4733406641
H,0,-1.7440212627,0.2209920183,1.514911754
N,0,-1.0754698481,-1.3960795859,0.3339142272
C,0,-1.4179780219,-2.3424972757,-0.7088232277
C,0,0.051745246,-1.7817018754,0.9782287081
O,0,0.6907040579,-1.1254872294,1.7943090705
O,0,0.3878410328,-3.0296776678,0.644852442
C,0,-0.5734284101,-3.54658837,-0.2817523289
H,0,-0.0329769417,-4.012217766,-1.109001497
H,0,-1.1685570007,-4.307762861,0.2350061918
H,0,-2.4884403433,-2.5719931269,-0.7126842625
H,0,-1.1420409076,-1.9585584016,-1.7022653816
H,0,-4.5320341806,0.8067000904,0.1621451092
C,0,-3.8090194763,1.1171052568,-0.5886439816
H,0,-3.8989347258,2.1529281202,-0.9071093386
H,0,-0.3671701846,0.7382278631,-1.2336870955
C,0,-1.078421564,1.0441456597,-0.4653354392
H,0,-0.9215460223,2.0334085961,-0.0352016266
Zn,0,1.3031720489,0.8691264215,1.4252156249
Cl,0,0.3421804957,2.0371812195,2.9541668326

C,0,2.5221391755,0.7155044806,-0.1020869112
H,0,2.577302245,1.6204308011,-0.7115652882
H,0,3.5356873996,0.4507201581,0.2079536168
Cl,0,2.0072956842,-0.615405469,-1.2471958356

Sum of electronic and thermal Free Energies=
-1702.992655 (Hartree/Particle)
No imaginary frequency.

M-RC-B3

C,0,-0.0579444311,1.4183122041,2.6496730832
H,0,-0.768882119,1.9607748751,3.2728439658
H,0,0.648088563,2.0605234859,2.120735061
C,0,-0.4877035635,0.1692095499,2.0257017116
C,0,-1.2824662645,-0.4796426924,1.178049107
H,0,-1.334174762,-1.5672698953,1.1415646383
N,0,-2.1292004629,0.130891904,0.2647655221
C,0,-2.2207704479,1.5582382111,0.0445878568
C,0,-2.7107921854,-0.5859492217,-0.7708312982
O,0,-2.6644372765,-1.7755543213,-0.9398137885
O,0,-3.346487629,0.2822380576,-1.5843681313
C,0,-3.302690175,1.6007469114,-1.0356716467
H,0,-3.0814004498,2.3029947532,-1.8425874819
H,0,-4.2898983833,1.834397998,-0.619321811
H,0,-2.5167060696,2.0840314062,0.9590302787
H,0,-1.2524957401,1.960956791,-0.2882095183
H,0,0.0502977277,-0.2902823913,4.1134721745
C,0,0.4305887615,0.0666889143,3.1570848369
H,0,1.4760762395,-0.1897302317,2.9748278425
H,0,0.4902666364,-3.0934971244,0.3072667511
C,0,0.6547103007,-2.4599147747,-0.5696343758
H,0,-0.2684126149,-2.4518649193,-1.1560680661
Zn,0,1.3263187463,-0.6991910478,-0.1081172902
Cl,0,1.9309004566,-3.2878760852,-1.5718071692
C,0,2.3592592699,0.9450006095,0.0762374184
H,0,2.5772714093,1.2425649092,1.10605111
H,0,3.305175176,0.9045594722,-0.4690529326
Cl,0,1.4248422878,2.3293646526,-0.665164848

Sum of electronic and thermal Free Energies=
-1702.918166 (Hartree/Particle)
No imaginary frequency.

M-TS-B3

C,0,-3.3416312855,0.3382700379,-1.4908307376
H,0,-3.9102560201,-0.4961272738,-1.9001439191
H,0,-2.7744370813,0.8916426356,-2.2415469872
C,0,-2.8067297766,0.2222964921,-0.1343961232
C,0,-2.0998692853,-0.4988581975,0.7466061863
H,0,-2.1479513961,-0.3240909636,1.8210048148
N,0,-1.2213177117,-1.5025605008,0.3989654227
C,0,-0.8992581922,-1.9074384334,-0.9548385545
C,0,-0.251861645,-1.9441387843,1.2992041245
O,0,-0.144405919,-1.615530506,2.4482632524
O,0,0.5633388401,-2.8001533371,0.6532073482

C,0,0.0764961896,-3.0463445479,-0.6683133295
H,0,0.9278567162,-3.0700063338,-1.3515334835
H,0,-0.4201426214,-4.0238089542,-0.6777332295
H,0,-1.7880454588,-2.2370118201,-1.5028091776
H,0,-0.4421940613,-1.08214167,-1.5213069205
H,0,-4.9192020703,0.8151813472,0.0452786472
C,0,-3.9428757405,1.1174711463,-0.3302844384
H,0,-3.7727586521,2.1943391696,-0.3152375365
H,0,-1.5869773915,2.3187850088,0.7115564786
C,0,-0.8835525217,1.6794485349,0.176397315
H,0,-0.2588262243,1.1218390693,0.8802322496
Zn,0,-0.2489725995,2.0349825598,-1.633934302
Cl,0,0.7285652046,3.4658324323,-0.0398272793
C,0,0.0279316529,1.8182193298,-3.5422474423
H,0,-0.5193921082,2.5386736066,-4.1543296444
H,0,1.0822862234,1.8669450394,-3.8227245549
Cl,0,-0.5554838142,0.1663882931,-4.0749689192

Sum of electronic and thermal Free Energies=
-1702.884876 (Hartree/Particle)
One imaginary frequency -305.73.

M-PC-B3

C,0,0.0159118604,0.7294043248,2.2700531787
H,0,-0.8246134084,1.3306976345,2.6134714116
H,0,0.9117066689,1.3081086387,2.0435591516
C,0,-0.2968428477,-0.4771157579,1.4749882972
C,0,-1.4529598116,-0.9207828521,0.6997077545
H,0,-1.9379359559,-1.8580398846,0.9675639323
N,0,-2.4136556335,0.0089037574,0.198754071
C,0,-2.1080511587,1.2009487929,-0.5612808153
C,0,-3.6987529209,-0.4209523095,-0.0661564679
O,0,-4.1959694699,-1.4725629404,0.2381623801
O,0,-4.3494103424,0.5607864485,-0.7426669961
C,0,-3.5206949654,1.7174771229,-0.8107612493
H,0,-3.6481205587,2.1848871614,-1.7901202771
H,0,-3.8342804049,2.4245966274,-0.031839655
H,0,-1.4910649924,1.9115366918,-0.0001128
H,0,-1.5815824817,0.9580765706,-1.4988231994
H,0,-0.5324208514,-0.9823334884,3.6088886375
C,0,0.1847612725,-0.6547369149,2.8597256348
H,0,1.1976149998,-1.0248563034,3.0178524738
H,0,0.3369972623,-2.0317425857,-0.0215293587
C,0,-0.053339889,-1.0213195644,0.0948453484
H,0,0.1737176789,-0.3240976697,-0.7164818712
Zn,0,2.5850305525,-0.499550457,0.4395379675
Cl,0,3.0485934875,-2.4482716297,1.1241285678
C,0,2.8070163101,1.3405861122,-0.1388941373
H,0,2.9357384439,2.008439015,0.7170447935
H,0,3.6991647519,1.4185483357,-0.7652367566
Cl,0,1.4356444039,1.9958341238,-1.1127870163

Sum of electronic and thermal Free Energies=
-1702.968405 (Hartree/Particle)
No imaginary frequency.

3. Cartesian coordinates and energies of computed structures of Figure 4

M-RC-C

C,0,0.6607665404,-0.828619469,3.0932013504
H,0,0.4963647628,-1.3791743761,4.0167892416
H,0,1.3363266927,0.0255131092,3.1252866484
C,0,0.0834618351,-1.1685969114,1.9792788943
C,0,-0.4579878375,-1.5171822571,0.8363866345
H,0,0.0588049264,-2.2073247788,0.1628187228
N,0,-1.7214007883,-1.0053808369,0.4199716067
C,0,-2.9645771344,-1.7400176044,0.593809848
C,0,-1.8033249181,-0.200113289,-0.6854420243
O,0,-0.8893725534,0.382401463,-1.2353021055
O,0,-3.0754232543,-0.1372501512,-1.1084921382
C,0,-3.9148479224,-0.8307174454,-0.177885011
H,0,-4.3896063725,-0.0893563608,0.4756953206
H,0,-4.6849867526,-1.3643285976,-0.7384309287
H,0,-2.8915790436,-2.7484084019,0.1586472368
H,0,-3.2322118351,-1.8341096244,1.6507089852
H,0,1.2088456213,2.4962113792,1.7759640871
C,0,0.4936658717,2.1597963732,1.0207371428
H,0,-0.4324907596,1.8737006974,1.5301638196
Zn,0,1.1349418136,0.8121796797,-0.2456710515
Cl,0,0.0814667218,3.6388100523,0.0286877842
C,0,2.2828020272,-0.3349912392,-1.3389172185
H,0,3.1604122447,0.1577717828,-1.7632382965
H,0,1.7370249858,-0.823880366,-2.150743313
Cl,0,2.9445291283,-1.6921458276,-0.2965122357

Sum of electronic and thermal Free Energies=
-1663.659853 (Hartree/Particle)
No imaginary frequency.

M-TS-C1

C,0,0.875142335,0.0543730824,2.8782055953
H,0,0.6425838677,-0.5284818858,3.7664023042
H,0,1.7547456705,0.6898465262,2.9036102577
C,0,0.0874699086,-0.0742781632,1.8087099499
C,0,-0.6328609748,-1.0257747559,1.1424985732
H,0,-0.304752096,-2.0659101684,1.144285269
N,0,-1.8305905246,-0.7241897994,0.4300660934
C,0,-3.1438269567,-1.2643764123,0.7445910941
C,0,-1.7808757019,-0.344907667,-0.8690845083
O,0,-0.7738373248,0.0078301386,-1.4787021614
O,0,-2.9884118406,-0.3856164689,-1.4343286936
C,0,-3.9585576834,-0.7147634329,-0.4260509714
H,0,-4.4932431335,0.2044413721,-0.1613159232
H,0,-4.6637895493,-1.4307100099,-0.8527083317
H,0,-3.114775122,-2.3638056572,0.766894166
H,0,-3.502217467,-0.9077399905,1.7151128448
H,0,0.7879964,2.2942799043,1.7637839135
C,0,0.0849759412,1.8461318701,1.0602162646
H,0,-0.938461457,1.9934668686,1.4095322885
Zn,0,0.9065308823,0.2858748683,-0.2428915027

Cl,0,0.173893731,2.923752889,-0.4723770805
C,0,2.6828405562,-0.302051852,-0.80093544
H,0,3.4821223445,0.409363676,-0.5847446408
H,0,2.7330256392,-0.5708582112,-1.8580658887
Cl,0,3.0897065554,-1.8199457209,0.128794528

Sum of electronic and thermal Free Energies=
-1663.609276 (Hartree/Particle)
One imaginary frequency -368.26.

M-IM-C

C,0,0.5618481519,-0.5400961098,3.157000854
H,0,0.7730511037,-1.6008491084,3.2754568724
H,0,0.8270566828,0.1117777605,3.9860254977
C,0,0.0308740543,-0.0617769943,2.0252801167
C,0,-0.2135562751,-0.8899156751,0.8147779054
H,0,-0.0695380377,-1.9543439705,1.0522640996
N,0,-1.5468146868,-0.6846580242,0.2737993471
C,0,-2.783040155,-1.1377802234,0.882479885
C,0,-1.7399128807,-0.4034469751,-1.0378618479
O,0,-0.8653450763,-0.1533570564,-1.8588230382
O,0,-3.0450878517,-0.4344637457,-1.3440349511
C,0,-3.7963596219,-0.6169765826,-0.1342626727
H,0,-4.2090577474,0.3560061093,0.1591680077
H,0,-4.617399348,-1.3061340744,-0.3420032852
H,0,-2.792193968,-2.234620895,0.9781362611
H,0,-2.9215331678,-0.7076456083,1.8819276042
H,0,-0.0648007899,1.9286592968,2.8525403389
C,0,-0.3148521996,1.387609934,1.9378439111
H,0,-1.3693890984,1.5487996098,1.6904606641
Zn,0,1.0223158995,-0.3437738532,-0.6884953577
Cl,0,0.596464212,2.2251556122,0.58843918
C,0,2.6404715537,-0.1726348989,-1.7587593784
H,0,3.2057231771,0.7409111099,-1.5582790584
H,0,2.4549895814,-0.234056012,-2.8337503138
Cl,0,3.7622074879,-1.5588916254,-1.3571026418

Sum of electronic and thermal Free Energies=
-1663.719753 (Hartree/Particle)
No imaginary frequency.

M-TS-C2

C,0,-0.5000163364,1.985157685,2.9846257412
H,0,-0.6300251974,1.210560357,3.7358492676
H,0,-0.3021707191,2.9976182476,3.3276365003
C,0,-0.5519777391,1.6830115314,1.6700395881
C,0,-0.4544902713,0.3691528357,1.0093807766
H,0,-0.0107737852,-0.4355354844,1.6178517216
N,0,-1.580593257,-0.0074811932,0.2247003981
C,0,-2.8540016753,-0.4505284501,0.7777904417

C,0,-1.4414826705,-0.4646092781,-1.0550021749
O,0,-0.430987432,-0.399012079,-1.7373314761
O,0,-2.5943711803,-0.9761522623,-1.4973001121
C,0,-3.6132392175,-0.7726903896,-0.5061129557
H,0,-4.2445254019,0.0609760494,-0.835262974
H,0,-4.2176247453,-1.6799092582,-0.4472106682
H,0,-2.7008271874,-1.3331602129,1.416667599
H,0,-3.3294904507,0.3365619668,1.3736235714
H,0,0.3305555577,3.4522446401,0.6834055575
C,0,-0.2861145776,2.5589283186,0.5953411802
H,0,-0.750649047,2.3876326319,-0.3734520356
Zn,0,1.2733627249,0.1377345334,-0.4353983167
Cl,0,1.9987851016,2.1763268303,-1.0544175069
C,0,2.1420451412,-1.6100701516,-0.0833314044
H,0,3.0423968785,-1.571310127,0.5331551255
H,0,2.376245583,-2.133054581,-1.0140733647
Cl,0,0.9825799041,-2.7116331599,0.8094865202

Sum of electronic and thermal Free Energies=
-1663.654758 (Hartree/Particle)
One imaginary frequency -368.03.

M-TS-C3

C,0,-1.1693521091,2.0845708379,-1.617490536
H,0,-2.024181536,1.4106202037,-1.7303527755
H,0,-1.3245903729,3.143765658,-1.795471303
C,0,0.0575007441,1.5982925521,-1.178552136
C,0,0.4009518397,0.2185561493,-1.061644217
H,0,0.0702121025,-0.4191779221,-1.8872049023
N,0,1.7297495095,-0.0569689073,-0.5951021753
C,0,2.9262185999,-0.0008178382,-1.4207846928
C,0,1.924647753,-0.9292723624,0.434891088
O,0,1.0676294519,-1.3611655555,1.1916032513
O,0,3.2140091767,-1.2834778673,0.5191688197
C,0,3.9673273744,-0.5250482354,-0.4371306172
H,0,4.4770027758,0.2874592257,0.0944299679
H,0,4.7138678261,-1.1841719285,-0.8849155768
H,0,2.8155831654,-0.6387929544,-2.3111847316
H,0,3.1384278927,1.0218831213,-1.7546871245
H,0,0.3217833214,3.6644093777,-0.5542515622
C,0,0.5570584685,2.6234241233,-0.3568669014
H,0,1.1616555289,2.396104999,0.5160237958
Zn,0,-0.8269609418,-0.4094734963,0.6550268293
Cl,0,-0.756190568,1.4337266086,1.9990089749
C,0,-2.4194598524,-1.5116866055,0.2580235729
H,0,-3.279604858,-1.3198407811,0.9028577464
H,0,-2.2497473035,-2.589875726,0.2150515252
Cl,0,-2.9960009891,-1.0622316765,-1.4393753198

Sum of electronic and thermal Free Energies=
-1663.667333 (Hartree/Particle)
One imaginary frequency -351.64.

M-PC-C

C,0,0.6712328805,-3.1787355064,2.5369537205
H,0,1.4368990312,-2.8274234014,3.2262207097
H,0,0.3232076096,-4.201582918,2.6602812623
C,0,0.1815146502,-2.3929386376,1.5973154726
C,0,0.2463934518,-1.0621822331,0.9791592791
H,0,-0.1695787356,-0.203909267,1.5185011443
N,0,1.4024800263,-0.7726929544,0.1860582781
C,0,2.7136638812,-0.5817157814,0.7792973821
C,0,1.3311690677,-0.1056294691,-0.9952055106
O,0,0.3301541184,0.1212809271,-1.6647748955
O,0,2.550882503,0.2573251479,-1.3998827621
C,0,3.5221014699,-0.2394847367,-0.467253936
H,0,3.9948223222,-1.125052449,-0.9079151505
H,0,4.2744917981,0.5361268581,-0.3128628127
H,0,2.6896114747,0.2419854557,1.5094010099
H,0,3.0575432329,-1.4935605794,1.2784458712
H,0,-1.7697470259,-1.9956722655,0.6340070318
C,0,-0.7031029281,-2.1495701108,0.4726825764
H,0,-0.4658269699,-2.5805911054,-0.4997434851
Zn,0,-1.5239220647,0.8288459643,-0.9681612152
Cl,0,-2.9731751682,-0.5606443225,-1.7304322201
C,0,-1.1276481686,2.4620209582,0.0405139161
H,0,-1.7860438323,2.6065588587,0.900058352
H,0,-1.1949909827,3.3520895345,-0.5898888387
Cl,0,0.5706233582,2.4748410333,0.7153988204

Sum of electronic and thermal Free Energies=
-1663.733877 (Hartree/Particle)
No imaginary frequency.

4. Cartesian coordinates and energies of computed structures of Figures 5 and 6

D-RC1

C,0,-6.2321260543,-1.944764217,-1.0081146336
H,0,-6.9526416446,-1.7481768142,-1.8019596591
H,0,-6.5233513098,-2.6739382939,-0.2524575912
C,0,-5.0748557875,-1.3474104413,-0.967410082
C,0,-3.9055794972,-0.7568467955,-0.9492620615
H,0,-3.0308086087,-1.1726957151,-1.4484758135
N,0,-3.6695895137,0.4656402813,-0.3035241034
C,0,-4.6581257597,1.1613843337,0.4964921363
C,0,-2.4222614665,0.8875013183,0.0242771991
O,0,-1.3592993224,0.3984846436,-0.3397449473
O,0,-2.4869163601,1.9695922453,0.802651572
C,0,-3.8545856411,2.396002497,0.8897437597
H,0,-4.0399376177,2.7440918064,1.9069106262
H,0,-3.9901490807,3.2200221945,0.1789271112
H,0,-5.5499306725,1.3966998382,-0.0931208796
H,0,-4.9511032463,0.5398078354,1.3558819223
Zn,0,0.5093107335,1.787702007,0.0073893457
C,0,6.2333634007,1.9413887767,-1.0118965366
H,0,6.9545122705,1.7421063705,-1.8044961899
H,0,6.5239034515,2.6732977534,-0.2586266569
C,0,5.0761965204,1.3439183537,-0.9699111446
C,0,3.9069914937,0.7532455381,-0.9506520769
H,0,3.0325676696,1.167208408,-1.4520302757
N,0,3.6706971842,-0.4670479409,-0.3008829218
C,0,4.6587721014,-1.1600767012,0.5020068973
C,0,2.4231755427,-0.887691522,0.0278039184
O,0,1.3604592412,-0.3997873307,-0.3384323476
O,0,2.4873502229,-1.967066681,0.8099337495
C,0,3.8549724607,-2.3932986479,0.8990875491
H,0,4.0398157815,-2.7379902256,1.9174979028
H,0,3.9907428828,-3.2197412466,0.1911288701
H,0,5.5508856997,-1.39746634,-0.0863011048
H,0,4.9513283005,-0.5355955013,1.3594395032
Zn,0,-0.5080180086,-1.7878256886,0.0137472874
C,0,-0.7324834647,-1.7641920643,1.965379559
H,0,-0.0017044309,-1.1151293507,2.4595008574
H,0,-0.6767299902,-2.7496056641,2.4346927656
C,0,-0.4197091154,-2.4217140387,-1.8435910381
H,0,-1.1836026056,-3.1309207125,-2.1730824359
H,0,-0.4038290512,-1.5774257873,-2.5419826429
C,0,0.7330799566,1.7711096746,1.9591936209
H,0,0.0017247204,1.1243410152,2.4554888629
H,0,0.6778667497,2.758264734,2.4248910822
C,0,0.420514761,2.4150621223,-1.8521596765
H,0,1.184385494,3.1230557804,-2.1843082631
H,0,0.4046131029,1.5682409373,-2.5474767879
Cl,0,1.1775331389,-3.2923299061,-2.104132171
Cl,0,-2.3779247929,-1.1061243099,2.4612813064
Cl,0,-1.1767077478,3.2847156147,-2.1157226284
Cl,0,2.3779626458,1.1138252357,2.4581201175

Sum of electronic and thermal Free Energies=
-3327.344463 (Hartree/Particle)
No imaginary frequency.

D-TS1

C,0,4.574419606,2.1188698869,1.8288536014
H,0,4.1771784508,2.5630931399,2.7404585866
H,0,5.6231420625,2.3174918276,1.6064174236
C,0,3.8436809787,1.3963913383,1.0237609393
C,0,3.3377223881,0.6407604776,0.0513503026
H,0,2.865087928,1.0641696158,-0.8413401992
N,0,3.4054968705,-0.7377177571,0.0735151168
C,0,4.0900231195,-1.5195010008,1.0824902294
C,0,2.5989013723,-1.5287965328,-0.7150689207
O,0,1.7608459054,-1.1394492474,-1.4998172544
O,0,2.8942933561,-2.8115749254,-0.4966078343
C,0,3.8612328453,-2.9397485519,0.5530562019
H,0,4.7662270036,-3.382849803,0.1259586065
H,0,3.4443865299,-3.6087020558,1.3103829031
H,0,1.3875279438,0.5184359946,1.8901986579
C,0,1.5193052119,1.519663211,1.456544914
H,0,1.9469881814,2.2134878578,2.1842884278
Zn,0,0.3329243957,2.1897863334,0.0245410908
Cl,0,-0.8309755139,2.4579942583,2.0878130049
H,0,3.6301276291,-1.3548384907,2.0674395719
C,0,0.2191243005,2.9715962857,-1.7601968998
H,0,-0.7470295448,2.8095577313,-2.2434360043
H,0,0.4873332879,4.026513292,-1.8492125105
Cl,0,1.4379544314,2.0657084546,-2.8022227861
H,0,5.148822552,-1.2445246172,1.1393651631
C,0,-4.2487770986,-1.5610931219,3.7415185055
H,0,-4.4535850116,-0.9557045687,4.6244208491
H,0,-4.7651240591,-2.5187860626,3.6754746901
C,0,-3.4212315834,-1.1642650534,2.8162077147
C,0,-2.5742010285,-0.7653717785,1.8999133924
H,0,-1.5058990454,-0.9810742884,1.944539207
N,0,-2.9618892202,0.0136939333,0.7985305892
C,0,-4.2042935303,0.762268894,0.7580901769
C,0,-2.0744117458,0.5189557795,-0.08713651
O,0,-0.8859139823,0.2107949232,-0.2018945482
O,0,-2.6515129675,1.4410498099,-0.8575685127
C,0,-4.061015465,1.4668328754,-0.586893044
H,0,-4.5576475264,0.922798948,-1.3984811716
H,0,-4.3866205723,2.5082170136,-0.5770747905
H,0,-4.2350489681,1.453370928,1.6131359565
H,0,-5.071706721,0.0960587687,0.8038619041
Zn,0,-0.4226572421,-1.8267583492,-1.2618361525
C,0,-1.2089932612,-1.2005458335,-2.9417448617
H,0,-0.9815330242,-0.1425085917,-3.1149846297
H,0,-0.97744813,-1.7629129384,-3.8484002638
C,0,-0.2330479214,-3.0119414067,0.3101813573
H,0,0.3083825316,-3.9369495946,0.0932256464

H,0,-1.1902169649,-3.2835882987,0.7656745819
Cl,0,0.7148334364,-2.2465253602,1.7004001414
Cl,0,-3.0451981906,-1.29697235,-2.7731515599

Sum of electronic and thermal Free Energies=
-3327.299052 (Hartree/Particle)
One imaginary frequency -254.39.

D-TS2

C,0,-5.6406371414,0.3151595258,2.58416568
H,0,-5.9634410495,-0.2555496254,3.4549130201
H,0,-6.34044633,1.0552087584,2.1968494653
C,0,-4.4727166273,0.1284106962,2.0381317262
C,0,-3.2879179224,-0.0619899532,1.5116388776
H,0,-2.4025015396,0.4851523517,1.8336834662
N,0,-3.0381842857,-0.9990751508,0.5025419283
C,0,-4.033178518,-1.8790700071,-0.0728648245
C,0,-1.8987309555,-1.0212772546,-0.2187621414
O,0,-0.9172609505,-0.2897121517,-0.0666634579
O,0,-1.9440579197,-1.9750367247,-1.1451307807
C,0,-3.1460434628,-2.7437518772,-0.9674535292
H,0,-3.5706599275,-2.9362503034,-1.9542851544
H,0,-2.8629493616,-3.6856406126,-0.4846241559
H,0,-4.5427867289,-2.452517449,0.7084398316
H,0,-4.7760502669,-1.2923953574,-0.6319535921
Zn,0,0.9628048227,-1.5596903862,0.109421487
C,0,3.567876641,0.6241985502,3.6056549966
H,0,4.2515116357,1.3676282087,4.0161919464
H,0,3.3891261987,-0.2630335793,4.212128192
C,0,2.9910347503,0.809259364,2.4508003176
C,0,2.4805026287,1.1900204977,1.2841301166
H,0,1.5723047288,1.7939222005,1.2328479174
N,0,3.0773342326,0.9642587135,0.0596103371
C,0,4.2840653446,0.1840296042,-0.1424654742
C,0,2.4133638234,1.1741932213,-1.1338627178
O,0,1.3062865543,1.6418959449,-1.2799074417
O,0,3.1944010562,0.7791962314,-2.1408002709
C,0,4.4761616394,0.3558705757,-1.6473515417
H,0,4.7319425521,-0.5786141622,-2.1509389802
H,0,5.2045073471,1.1368140403,-1.8913149283
H,0,5.1152398972,0.5842255541,0.4472827022
H,0,4.1091004507,-0.8658208049,0.1378309565
Zn,0,-0.9633252365,1.9880600916,-0.8067137434
C,0,-1.6679996299,1.4538172479,-2.5523255032
H,0,-1.1298732704,0.5918045523,-2.9601061551
H,0,-1.7286847955,2.2241902151,-3.3234715259
C,0,-0.8507030268,2.8594871775,0.94971419
H,0,-1.7643680267,3.3884555136,1.2353702334
H,0,-0.6154563894,2.1582647482,1.7609885796
C,0,1.4122559168,-2.0953861851,-1.7153386661
H,0,1.3727481249,-1.2824264216,-2.4467021895
H,0,0.773149103,-2.9072259009,-2.0702602801
C,0,1.3964010284,-0.8594784445,1.9078084245
H,0,2.0820064496,-1.4026175128,2.5634190551
H,0,0.6445469872,-0.3148524562,2.4863902661
Cl,0,0.4748902137,4.1209183251,0.9952790928

Cl,0,-3.4034578473,0.8737636645,-2.3182362126
Cl,0,-0.1478196552,-2.8656856893,1.7837962537
Cl,0,3.1246297375,-2.7615745645,-1.8067937933

Sum of electronic and thermal Free Energies=
-3327.305388 (Hartree/Particle)
One imaginary frequency -289.07.

D-PC1

C,0,6.0763750791,1.791318207,1.7446291811
H,0,6.5137539902,2.0304848367,2.7112794282
H,0,6.7606629751,1.6669006805,0.9071425659
C,0,4.7716164119,1.6690554567,1.5909824037
C,0,3.6872562034,1.3724281603,0.6440846804
H,0,3.4004352642,2.1122596211,-0.1101054918
N,0,3.5507747953,0.0066863922,0.2310887066
C,0,4.5195248356,-0.6690652323,-0.6121873544
C,0,2.3558076468,-0.6092684304,0.1484435805
O,0,1.2700646083,-0.2026377695,0.5590059421
O,0,2.4790666767,-1.8144288924,-0.4220320693
C,0,3.8618620522,-2.0412669049,-0.7450429376
H,0,3.9095833678,-2.4582834291,-1.7528639887
H,0,4.2619287692,-2.7668009978,-0.0280622132
H,0,3.06675665,0.846967838,2.7245903608
C,0,3.416572675,1.6788049283,2.1119508576
H,0,2.9099249502,2.6206339272,2.3199113548
Zn,0,0.2238442071,1.7430820901,0.0533558733
Cl,0,0.2944007459,3.1106931621,1.7409058143
H,0,5.5003829535,-0.7091788709,-0.1271099264
C,0,0.3122604199,1.6739117969,-1.9153944049
H,0,-0.5048956417,1.0794440409,-2.3379497907
H,0,0.2956960266,2.6601616239,-2.3843385138
Cl,0,1.8505269184,0.8854000536,-2.543303611
H,0,4.6156333938,-0.1489152387,-1.5770727027
C,0,-5.6414301213,-2.6219398197,2.1217628606
H,0,-6.4048686969,-2.4596050735,2.8824394585
H,0,-5.7482716647,-3.5113056743,1.501578637
C,0,-4.6424355139,-1.8000196129,1.9666832726
C,0,-3.6376370424,-0.9674363378,1.8466139001
H,0,-2.7086832876,-1.0696638112,2.4128840404
N,0,-3.6880238665,0.1687101447,1.019668365
C,0,-4.8576128195,0.5836136728,0.2714943177
C,0,-2.5775829601,0.7500975846,0.5125592519
O,0,-1.4137303671,0.4432041983,0.7612209491
O,0,-2.8975644864,1.7495321729,-0.3065429861
C,0,-4.3289640299,1.8595521649,-0.3846487435
H,0,-4.6002946351,1.9528829091,-1.4381132119
H,0,-4.6262373543,2.7646839359,0.1548992752
H,0,-5.7072169578,0.7604653249,0.9391533012
H,0,-5.1331122913,-0.1941434841,-0.4557108427
Zn,0,-0.5077385965,-1.7327907029,0.4498537819
C,0,-0.8842386736,-1.7897768972,-1.4843672505
H,0,-0.2317535867,-1.1245601093,-2.0601340965
H,0,-0.8116702215,-2.7897394114,-1.9197940708
C,0,-0.2672151182,-2.4548924065,2.2623850975
H,0,0.7140433254,-2.9296711211,2.3678920833

H,0,-1.0187785474,-3.1902024334,2.5656389656
Cl,0,-0.3141498035,-1.1453281718,3.5327365605
Cl,0,-2.5998776577,-1.2455030905,-1.8769166606

Sum of electronic and thermal Free Energies=
-3327.415069 (Hartree/Particle)
No imaginary frequency.

D-RC-B1

C,0,-4.692674754,-1.459244145,-1.4545634129
H,0,-5.2438403234,-1.3905384248,-2.390204905
H,0,-5.1978004271,-1.8941532117,-0.5925781819
C,0,-3.436997709,-1.047320552,-1.3670968999
C,0,-2.2645541766,-0.908950384,-0.4923647842
H,0,-2.2403162387,-0.1195524472,0.2717560143
N,0,-1.552943174,-2.0958178309,-0.1321932214
C,0,-2.1106772919,-3.1561176255,0.6935007809
C,0,-0.2083613025,-2.0737761899,-0.0016278949
O,0,0.5635029849,-1.1902322476,-0.3678453277
O,0,0.2316931593,-3.1996859899,0.5705789541
C,0,-0.8916594658,-4.0644791189,0.8251359241
H,0,-0.7673825576,-4.4958126328,1.8199807977
H,0,-0.8799571758,-4.8624398751,0.0743812482
H,0,-1.636973219,-1.1134000455,-2.6228747782
C,0,-2.2332670027,-0.4889332284,-1.9573327278
H,0,-2.1445207738,0.5803681157,-2.1535451279
Zn,0,0.5495678645,1.0463362083,0.1486376567
Cl,0,-0.1208889941,2.2147861989,-1.5641725076
H,0,-2.9586971187,-3.6375795756,0.1963313756
C,0,0.4042110184,0.9544390488,2.1080459592
H,0,1.3772582474,0.7553788055,2.5697214464
H,0,-0.0067697459,1.8630246775,2.5538156863
Cl,0,-0.7025300009,-0.3936145894,2.6815067448
H,0,-2.4496349164,-2.7537447593,1.6576162512
C,0,7.9025051559,0.0413146544,-1.4479798676
H,0,8.5358276229,0.5527502059,-2.1726231656
H,0,8.389612369,-0.681430991,-0.7943104469
C,0,6.6225318012,0.2731318073,-1.3737655069
C,0,5.3345848086,0.5123270298,-1.3357415183
H,0,4.6089698058,-0.0295660805,-1.9474034404
N,0,4.7764640802,1.5337121471,-0.5457417102
C,0,5.5475313679,2.4714647442,0.2470925117
C,0,3.4910198884,1.5170717592,-0.1295426811
O,0,2.6356186065,0.6852755017,-0.4289589901
O,0,3.2346980921,2.5572841119,0.6608616902
C,0,4.4266265348,3.3499946993,0.8019232998
H,0,4.5436462384,3.5928726607,1.8595928241
H,0,4.2879856836,4.2699232825,0.2243976218
H,0,6.258468657,3.0202102357,-0.3788336417
H,0,6.1029803244,1.9335271787,1.0291341495
Zn,0,2.8738110059,-1.6784110703,-0.0885840251
C,0,3.0555961536,-1.5470023848,1.8674469831
H,0,2.1098307213,-1.2917697977,2.3582554242
H,0,3.4413126972,-2.4557437531,2.3367420966
C,0,3.1386398106,-2.4298729524,-1.8817363082
H,0,2.5125802281,-3.3173429121,-2.0223869226

H,0,4.1694276917,-2.7188240722,-2.108340144
Cl,0,2.6462068491,-1.2703342054,-3.2011735652
Cl,0,4.2395240848,-0.2318553279,2.3746108813
Zn,0,-4.7295968427,1.0962947525,0.2752960751
C,0,-3.8841300725,2.3763445254,-0.910670818
H,0,-2.8142368232,2.548812741,-0.7520454775
H,0,-4.0419444927,2.1556771269,-1.9706225967
Cl,0,-4.7359879393,3.9574824124,-0.5814995846
C,0,-5.7528699472,0.123275691,1.6182501595
H,0,-6.7435219378,-0.1736892277,1.2626166398
H,0,-5.8821088449,0.7008953595,2.5367134974
Cl,0,-4.9217132852,-1.4202500331,2.1200474863

Sum of electronic and thermal Free Energies=
-4553.434502 (Hartree/Particle)
No imaginary frequency.

D-TS-B1

C,0,6.1957203017,0.2944874168,-1.9597487601
H,0,6.5620631624,0.650402126,-2.9205016833
H,0,6.9131963515,0.2901273985,-1.1409011248
C,0,4.9019551876,0.030055378,-1.7620393063
C,0,3.877328202,-0.3282740985,-0.7715670419
H,0,3.8083813125,-1.3579673292,-0.4019135872
N,0,3.5333809542,0.6812023223,0.1818583517
C,0,4.4231212501,1.0805842346,1.2581864607
C,0,2.2494359159,0.9393402858,0.520566128
O,0,1.2324000059,0.554549754,-0.0493616049
O,0,2.196756024,1.7527671727,1.5804390241
C,0,3.5340701695,2.0814378434,1.9939968634
H,0,3.5824854558,1.9981720477,3.0812478113
H,0,3.7357963655,3.1155473293,1.6944916042
H,0,2.98283949,0.8575102663,-2.4464036821
C,0,3.5328008153,-0.0596403921,-2.2305298248
H,0,3.1913700993,-0.9203896596,-2.8070175077
Zn,0,0.5417313824,-1.5838702632,-0.4550507437
Cl,0,0.7615493821,-2.012639396,-2.5776262889
H,0,5.3385729414,1.5342993638,0.8640260838
C,0,0.7992978806,-2.3818291533,1.3267056183
H,0,-0.0564022445,-2.2034841612,1.9864256576
H,0,0.9856341435,-3.4573273344,1.291723562
Cl,0,2.2490839155,-1.6859416856,2.218996409
H,0,4.691948834,0.2126775195,1.8785552696
C,0,-6.1436714261,2.0150279511,-0.6565636864
H,0,-6.8847382635,2.0281804525,-1.455567911
H,0,-6.4054281684,2.5354297831,0.2641228823
C,0,-4.9948332733,1.4172185181,-0.7983161899
C,0,-3.8387909981,0.8264381404,-0.9763987798
H,0,-2.9703586082,1.3316091318,-1.4050895919
N,0,-3.6281518148,-0.5322172075,-0.6839004134
C,0,-4.6572113788,-1.443885069,-0.2265035127
C,0,-2.4025360451,-1.0468633845,-0.4504108453
O,0,-1.3316157213,-0.4460503429,-0.5284895841
O,0,-2.4791553191,-2.3374501695,-0.1354980678
C,0,-3.8586611355,-2.7462715033,-0.1362547023
H,0,-4.0410574012,-3.3063993407,0.7828618456

H,0,-4.0143025928,-3.3975292823,-1.0022781392
H,0,-5.4824939227,-1.4928071358,-0.9444688413
H,0,-5.0522645507,-1.1093652174,0.7434135599
Zn,0,-0.8041382346,1.5194943526,0.7290712203
C,0,-1.0177447054,0.6407151516,2.4762439944
H,0,-0.2386986002,-0.1011603659,2.6803458195
H,0,-1.0469884053,1.3366692905,3.3185961743
C,0,-0.8565050298,2.9934089661,-0.5668264132
H,0,-0.0197448443,3.6836002949,-0.416814165
H,0,-1.7749801076,3.5873493414,-0.5297200587
Cl,0,-0.7102346062,2.4141199656,-2.290412706
Cl,0,-2.6099296122,-0.277926202,2.5860246921
Zn,0,8.2955248733,-2.1570231932,-2.6246517221
C,0,6.3422079458,-1.9625313309,-2.4860858242
H,0,5.8067554347,-2.3611556623,-1.6215724458
H,0,5.6950710998,-1.8943278344,-3.3624355841
Cl,0,7.1779569874,-4.1445316552,-3.1332526557
C,0,10.1244487398,-1.533424035,-2.4852175586
H,0,10.6410190226,-1.4544361343,-3.4441027044
H,0,10.7432782632,-2.1282482662,-1.8101727783
Cl,0,10.0880053504,0.1571640871,-1.7863752251

Sum of electronic and thermal Free Energies=
-4553.397506 (Hartree/Particle)
One imaginary frequency -314.63.

D-PC-B1

C,0,-4.3748080487,-0.4313193397,-1.3452186312
H,0,-4.5163894346,-0.4110636216,-2.4243339976
H,0,-4.6107835764,-1.3771469592,-0.8531429131
C,0,-3.2869324807,0.3816581741,-0.77778659
C,0,-2.1205967004,0.1542191126,0.1036895716
H,0,-2.0585796901,0.712107203,1.0433902879
N,0,-1.5671443977,-1.1657925277,0.1633179437
C,0,-2.1996337835,-2.2282428216,0.930914872
C,0,-0.2315601456,-1.3793363464,0.1148964552
O,0,0.6480557811,-0.598785912,-0.2401471235
O,0,0.0618926593,-2.6354876558,0.472312851
C,0,-1.1494769583,-3.3287095634,0.811767066
H,0,-0.9776030021,-3.8767420636,1.7402290931
H,0,-1.3741931971,-4.0346979661,0.0046964192
H,0,-1.443545351,0.4028546243,-1.9977510308
C,0,-1.9834781877,0.9125332358,-1.2013377159
H,0,-1.7795984898,1.9783133853,-1.1318759673
Zn,0,1.1904657281,1.435966812,0.6096474141
Cl,0,0.7537028309,2.9695739585,-0.869964008
H,0,-3.1648466225,-2.5163920024,0.5031249393
C,0,1.154257303,1.0696659375,2.5461091586
H,0,2.1348075713,0.7450504591,2.9097178417
H,0,0.8412543645,1.9325713819,3.1381737327
Cl,0,-0.0005669012,-0.2735450154,3.0349969361
H,0,-2.3622010766,-1.9028678599,1.9700905225
C,0,7.9586182183,-0.5357287543,-2.2528362498
H,0,8.5613575158,0.0084653465,-2.9797336148
H,0,8.3908301952,-1.4478498298,-1.8425389498
C,0,6.7735221562,-0.124686915,-1.9003790328

C,0,5.5760355761,0.2982785136,-1.5775745284
H,0,4.6739022052,0.0175604159,-2.1255013516
N,0,5.3470497416,1.2011236436,-0.5258027596
C,0,6.3866436023,1.8034172491,0.2827378801
C,0,4.1416934377,1.3437816976,0.0658159568
O,0,3.0998409098,0.7730886258,-0.25157822
O,0,4.2050298109,2.2228937743,1.0647555246
C,0,5.549200973,2.7205213131,1.1763041729
H,0,5.8345701949,2.6802539182,2.2293301553
H,0,5.5521322677,3.7598695077,0.8326001837
H,0,7.1031588192,2.3459046483,-0.3429804233
H,0,6.9256999506,1.0258991231,0.8428922534
Zn,0,2.8171411827,-1.6079010875,-0.3225938847
C,0,3.2334403912,-1.8393856709,1.5862095208
H,0,2.4687398206,-1.4092996503,2.2412780403
H,0,3.376852451,-2.8826309714,1.8795070107
C,0,2.7323536542,-2.0804214908,-2.2251835657
H,0,1.923657083,-2.795377355,-2.4102897749
H,0,3.6516474056,-2.5186718361,-2.6253143965
Cl,0,2.3652878722,-0.6413761239,-3.2832999111
Cl,0,4.8085590019,-1.010450696,2.0577603313
Zn,0,-7.0258286991,-0.3132416766,-0.8979531501
C,0,-4.6578192487,0.8798666324,-0.5780446495
H,0,-5.0567525592,0.8065080987,0.4362112576
H,0,-4.9843875858,1.7366733715,-1.1650906929
Cl,0,-7.5094263762,0.5656486379,-2.7661246469
C,0,-7.2529390558,-1.2431744672,0.7977286457
H,0,-7.7411335644,-2.2093218983,0.6498018429
H,0,-7.8694747136,-0.6541159728,1.48119914
Cl,0,-5.7055388281,-1.5807507506,1.6762367562

Sum of electronic and thermal Free Energies=
-4553.500370 (Hartree/Particle)
No imaginary frequency.

D-RC2

C,0,5.1425809778,1.9263240456,1.9278914561
H,0,5.4934462323,2.6005967212,2.7093072718
H,0,5.9075105109,1.3799719703,1.3745185485
C,0,3.8725806121,1.7926873162,1.6633972974
C,0,2.5791083567,1.6932080791,1.4534629841
H,0,1.9527820271,0.9773392891,1.9871201342
N,0,1.8767865728,2.4877082115,0.5440885328
C,0,2.5042072308,3.4354327327,-0.3624144027
C,0,0.6320856883,2.1600609668,0.1045361863
O,0,-0.109977083,1.2945957889,0.5487688637
O,0,0.2847529294,2.9493267201,-0.9164051085
C,0,1.2711714537,3.9826168217,-1.0719655964
H,0,1.4161447068,4.1561973603,-2.1391651388
H,0,0.8800520979,4.8891897271,-0.5956842763
H,0,3.0562780956,4.201650732,0.1909600642
H,0,3.1983857197,2.9073090066,-1.0322608767
Zn,0,-2.3223106653,1.6623255891,-0.274413542
C,0,-7.7505502774,-0.478411237,0.0661442692
H,0,-8.4718761779,-0.8366498609,0.8005497678
H,0,-8.1546895834,-0.0800972215,-0.8641595078

C,0,-6.4677554507,-0.5142545801,0.2914949899
C,0,-5.1815660263,-0.538079915,0.5390221029
H,0,-4.6600191255,0.2867477934,1.0238360216
N,0,-4.3569494345,-1.6270784214,0.2221960223
C,0,-4.8053829501,-2.7989196535,-0.5038245154
C,0,-3.0070342913,-1.5204884116,0.1525393447
O,0,-2.321928931,-0.5689302,0.5105563816
O,0,-2.4768644502,-2.6368975578,-0.3506634356
C,0,-3.5162823572,-3.6139375568,-0.513040478
H,0,-3.3358476772,-4.1510701503,-1.4454204357
H,0,-3.4577256968,-4.3053401701,0.335445182
H,0,-5.6268253385,-3.2979842606,0.0201132163
H,0,-5.146646058,-2.5089507395,-1.508885429
Zn,0,-0.0368769821,-1.1513397842,0.7446600248
C,0,0.4836918261,-1.3174593487,-1.1421147669
H,0,-0.2862048015,-0.9457459203,-1.8264666796
H,0,0.7649281452,-2.3279639796,-1.4465174187
C,0,-0.2928825433,-1.3510009706,2.6778186425
H,0,0.5843351807,-1.5899758328,3.2850863821
H,0,-0.7859932713,-0.4711835208,3.1048455863
C,0,-2.1736245433,1.2200109984,-2.1841889921
H,0,-1.1619148121,0.9049637332,-2.4633956462
H,0,-2.4596010868,2.0410130275,-2.8469374651
C,0,-2.8312080079,2.589222915,1.38066761
H,0,-3.8562567585,2.9651157204,1.4391355482
H,0,-2.6430700682,1.960319437,2.257420443
Cl,0,-1.4511407829,-2.7463964135,2.9620031931
Cl,0,1.9704171241,-0.2890501911,-1.5564735866
Cl,0,-1.7710901347,4.0701641822,1.6148268883
Cl,0,-3.2673701573,-0.1755070276,-2.6716440767
H,0,3.9404096107,-2.0708203662,2.4040286556
C,0,3.2263586384,-1.80134534,1.6211225888
H,0,2.4029921267,-1.2557737942,2.0930026756
Zn,0,4.0542272646,-0.8771180068,0.1116755339
Cl,0,2.5037612743,-3.3725449865,1.0369745093
C,0,5.4043821469,-0.3614909892,-1.2108450343
H,0,6.4323858794,-0.4508523752,-0.8485618442
H,0,5.3123404543,-0.9708214911,-2.1147057517
Cl,0,5.2372086405,1.3667773888,-1.773850914

Sum of electronic and thermal Free Energies=
-4553.375082 (Hartree/Particle)

No imaginary frequency.

D-TS3

C,0,0.0160569283,-0.2155275033,0.0093874929
H,0,-0.068888281,-0.2855789754,1.0927489231
H,0,1.0189241582,-0.210682705,-0.4145798889
C,0,-1.0440035833,-0.1463296941,-0.7490055606
C,0,-2.2755887765,-0.0637522069,-1.2533922099
H,0,-2.8310646709,-0.938084073,-1.5953717935
N,0,-2.9179095873,1.1415008146,-1.4469676651
C,0,-2.6725161077,2.3635592558,-0.698687585
C,0,-3.9072738327,1.2996410295,-2.3803967933
O,0,-4.2712392727,0.4532510186,-3.1802159691
O,0,-4.4275649669,2.5170705161,-2.286663897
C,0,-3.6326031978,3.3301424926,-1.4018656746

H,0,-3.0943925147,4.0621654152,-2.0141499126
H,0,-4.3126497883,3.8429165627,-0.7192959135
H,0,-2.909340797,2.205736758,0.3604557619
H,0,-1.6288593808,2.688938843,-0.7950410258
Zn,0,-6.4844076824,0.6757968508,-3.9533223042
C,0,-10.4181310932,-1.7847728324,-7.4654401394
H,0,-10.7965664537,-2.7627315236,-7.7626120026
H,0,-11.0983325856,-0.940894791,-7.5776480996
C,0,-9.2149339762,-1.6308310449,-6.9899458104
C,0,-8.009117469,-1.4931496647,-6.4967290832
H,0,-7.7968307323,-1.5760435179,-5.4311196558
N,0,-6.8788184443,-1.2471257268,-7.2897223885
C,0,-6.9276946717,-1.0256808756,-8.7219192485
C,0,-5.7218960025,-0.7595093561,-6.780085856
O,0,-5.4303937958,-0.6262447537,-5.5963520169
O,0,-4.8739935563,-0.4482827498,-7.7626202776
C,0,-5.4403152108,-0.8610194592,-9.0165499921
H,0,-5.2153416245,-0.094153737,-9.7592607655
H,0,-4.9671275921,-1.8083951509,-9.2992264351
H,0,-7.3780102059,-1.8795891406,-9.2379277504
H,0,-7.5188960818,-0.1239190168,-8.9408143257
Zn,0,-3.0834636219,-0.35623507,-5.331377653
C,0,-2.8143491241,1.4658858194,-6.00041933
H,0,-3.7414738585,1.9339240068,-6.3462739157
H,0,-2.0750247698,1.516455627,-6.8032973121
C,0,-2.8892763459,-2.2492901,-4.8680606584
H,0,-1.866736192,-2.5824975261,-4.6700109992
H,0,-3.5326709985,-2.536552898,-4.0290000104
C,0,-6.4361328482,2.3526634673,-4.9750685567
H,0,-5.418729493,2.7507207798,-5.053338492
H,0,-7.0773783405,3.1453595317,-4.5823434562
C,0,-7.0240806513,-0.7533005624,-2.7158340279
H,0,-8.0939072844,-0.9495488898,-2.6090150625
H,0,-6.5204662894,-1.6947075438,-2.9623390695
Cl,0,-3.4601634082,-3.2662098966,-6.2833697392
Cl,0,-2.169503375,2.6284202823,-4.7195368617
Cl,0,-6.4484226285,-0.3325407522,-1.0218130522
Cl,0,-6.9959287867,2.1124165479,-6.7108352795
H,0,0.145484798,-0.9436433633,-2.6794583688
C,0,-0.4974894298,-0.0961283136,-2.937435914
H,0,-1.399118692,-0.4838338612,-3.4215655916
Zn,0,0.1551056375,1.66888276,-3.5610754972
Cl,0,0.5464866388,0.0506881167,-5.2280814645
C,0,0.8943049896,3.4601848667,-3.3183981253
H,0,1.912206924,3.4978700748,-2.9244421966
H,0,0.856319173,4.0461487418,-4.2397846873
Cl,0,-0.119041568,4.4115351131,-2.112500347

Sum of electronic and thermal Free Energies=
-4553.339507 (Hartree/Particle)

One imaginary frequency -351.26.

D-PC2

C,0,4.8902979701,0.035646253,2.0368458299
H,0,5.6301359837,0.7058791832,1.6009030949
H,0,5.2134369927,-0.9706705103,2.3025526891

C,0,3.6498536077,0.434270491,2.269501391
C,0,2.632586384,1.4748259125,2.0650560021
H,0,2.5718865815,2.3075108257,2.772765248
N,0,2.3050185646,1.8579826476,0.7233431316
C,0,2.9364601485,3.0434547904,0.1632307603
C,0,1.100825241,1.6565022283,0.1343450534
O,0,0.2148959687,0.8762215979,0.4657040938
O,0,0.9692354503,2.4451091846,-0.9408459709
C,0,2.1926547977,3.1635095321,-1.1586866119
H,0,2.7324332806,2.671648387,-1.9773897993
H,0,1.9421037289,4.1888197264,-1.4371081417
H,0,2.763763055,3.9050936729,0.8276253749
H,0,4.0131441554,2.8895577122,0.0306921019
Zn,0,-1.8565368111,1.8102257587,-0.2262201463
C,0,-7.6376722685,0.6763520995,0.3604293719
H,0,-8.3624748486,0.2846616493,1.0741995448
H,0,-8.0215494766,1.3455325539,-0.4092632988
C,0,-6.3734129521,0.3687763755,0.4290928817
C,0,-5.1023914396,0.0657282206,0.5245213593
H,0,-4.4026464381,0.6499902221,1.1212742842
N,0,-4.5252580652,-1.0459212816,-0.1034852159
C,0,-5.2395396706,-1.9395286825,-0.9924309066
C,0,-3.1877090567,-1.1596871218,-0.2958320167
O,0,-2.3126156446,-0.4352407488,0.1630468647
O,0,-2.916477655,-2.2192057715,-1.0619841208
C,0,-4.1329477434,-2.9423391383,-1.3042306588
H,0,-4.1238810487,-3.2857865219,-2.3399258705
H,0,-4.1509051385,-3.8019409171,-0.6242192538
H,0,-6.1011853648,-2.3910578717,-0.4903840799
H,0,-5.5895108131,-1.3890273279,-1.8785194436
Zn,0,-0.1604557303,-1.5128407093,0.3360180457
C,0,0.3477216003,-1.6000075843,-1.5647593523
H,0,-0.3981688894,-1.1370873806,-2.2189648006
H,0,0.5602385939,-2.6081677807,-1.9293287415
C,0,-0.6064710505,-1.9780582696,2.1859172946
H,0,0.149073627,-2.5662018914,2.7130164615
H,0,-0.8491350273,-1.090899324,2.7807270248
C,0,-1.8864026131,1.6408566551,-2.1826553909
H,0,-1.0245662901,1.0718936306,-2.546234896
H,0,-1.9056259511,2.5939781559,-2.7170896996
C,0,-2.016913946,2.6045062894,1.5678799578
H,0,-2.8856369733,3.2390266646,1.7601232143
H,0,-1.966052096,1.837118417,2.3476170298
Cl,0,-2.1258408901,-3.0096949814,2.2110774724
Cl,0,1.8998515264,-0.6526682012,-1.9534958392
Cl,0,-0.5662086275,3.6959981764,1.8844996803
Cl,0,-3.366700058,0.7338679537,-2.7884423768
H,0,1.9655289956,0.0869413268,3.6614966129
C,0,2.2758189299,0.1072249344,2.6176988472
H,0,1.7535982758,-0.6130745277,1.9884093101
Zn,0,3.8110034924,-1.4367522304,-0.3919935661
Cl,0,2.7251591472,-2.8755080892,0.7868504779
C,0,5.3672584104,-0.7151327822,-1.3179685124
H,0,6.2995126259,-0.8521246182,-0.7650924215
H,0,5.4813258291,-1.15405274,-2.3123461973
Cl,0,5.1981626132,1.0776337752,-1.5875171768

Sum of electronic and thermal Free Energies=
-4553.440680 (Hartree/Particle)

No imaginary frequency.

D-RC-B2

C,0,-4.6413421327,1.2923101382,0.7825465338
H,0,-4.5035335211,0.504661843,0.0399794462
H,0,-5.6536081504,1.4375364979,1.1544042452
C,0,-3.6339819535,2.046205608,1.1849807543
C,0,-2.2295342977,2.4179726638,1.0166519586
H,0,-1.4613066302,1.8471391136,1.539378611
N,0,-1.7361001265,2.9005500299,-0.2444400245
C,0,-2.5593391887,3.567065225,-1.2402127722
C,0,-0.7086852096,2.2710067012,-0.8553329242
O,0,0.0387300216,1.4317901382,-0.3539867758
O,0,-0.6109730775,2.6364410722,-2.1349391153
C,0,-1.5550847599,3.6876168411,-2.3815316222
H,0,-1.012244472,4.6397837207,-2.3545379069
H,0,-1.9885255545,3.5344387451,-3.3712148662
H,0,-3.4292446467,2.9438772701,-1.4967594118
H,0,-2.9109841181,4.5437678416,-0.8924770587
Zn,0,1.0089383736,-0.025219419,-1.7602231539
C,0,3.5228798591,-5.1679192684,-1.4911947928
H,0,3.6249121815,-6.1119657695,-0.9560124078
H,0,3.8036629804,-5.1687910904,-2.5439613315
C,0,3.080239329,-4.0916265969,-0.9050312914
C,0,2.6183425482,-3.0266035629,-0.2966581515
H,0,1.5551678003,-2.7910252453,-0.2389562509
N,0,3.4437333091,-2.1190905885,0.3847779074
C,0,4.8778592369,-2.2708321072,0.5300099456
C,0,3.0850417277,-0.8321420488,0.6102407659
O,0,1.9898798823,-0.3243306558,0.3867183365
O,0,4.0991234319,-0.1505081843,1.1417015142
C,0,5.1857239961,-1.054171808,1.3970837417
H,0,6.1160087298,-0.5468315179,1.1365977797
H,0,5.1745603859,-1.2926718066,2.467007401
H,0,5.1249576867,-3.2212051497,1.0137708891
H,0,5.3633508248,-2.2350041102,-0.4565529122
Zn,0,1.6567306642,1.7091412344,1.4825233752
C,0,2.7481800022,3.0014939621,0.488492557
H,0,3.2934053894,2.5552089086,-0.3494408749
H,0,3.4667212002,3.542240517,1.1093166643
C,0,0.8189546148,0.9060155856,3.0693041732
H,0,0.4939845572,1.6056584462,3.8443475031
H,0,-0.0023217522,0.2166790468,2.8540693515
C,0,2.5215575081,0.9059475516,-2.6022258774
H,0,2.6523021508,1.930498094,-2.2402860847
H,0,2.4707609549,0.9385576653,-3.693355818
C,0,-0.4705053416,-1.3433480185,-1.8210887143
H,0,-0.4339344431,-2.046391794,-2.6571513856
H,0,-0.5620579562,-1.9177790454,-0.8916987615
Cl,0,2.0996421442,-0.1362915322,3.8735206457
Cl,0,1.6843493947,4.311771941,-0.2433486825
Cl,0,-2.1124653332,-0.5037268431,-2.0233139024
Cl,0,4.1073747982,0.0441976497,-2.2401636763
H,0,-2.9728108452,3.2203539654,2.9573425585

C,0,-3.1620413668,3.2451677258,1.884970788
H,0,-3.5058912744,4.2140164549,1.5211077213
Zn,0,-3.1241063748,-1.8395515542,0.2367880288
C,0,-1.7576961797,-1.1459913241,1.4391444768
H,0,-1.1878290011,-0.326063106,0.9894387342
H,0,-2.1371305879,-0.8263267939,2.4144046035
Cl,0,-0.5399500336,-2.4706471859,1.7746721545
C,0,-4.5462283724,-2.7632562951,-0.7218993305
H,0,-5.1344991147,-3.4512041202,-0.1104872537
H,0,-4.1666916088,-3.3060735609,-1.5916644011
Cl,0,-5.723667259,-1.5343230953,-1.3779516335

Sum of electronic and thermal Free Energies=
-4592.619360 (Hartree/Particle)
No imaginary frequency.

D-TS-B2

C,0,2.6884341077,3.0571080393,0.2126836923
H,0,1.9443622083,3.1305090923,-0.5794193557
H,0,3.263255912,3.957722809,0.4209335263
C,0,2.98000601,1.8728269675,0.7622912985
C,0,2.7177692964,0.4470448772,0.637161023
H,0,1.9874627579,-0.0031704069,1.3129322514
N,0,2.6647081938,-0.1551063685,-0.6644024157
C,0,3.6990704642,-0.0705801596,-1.6764769549
C,0,1.4441775587,-0.2467584904,-1.2507600115
O,0,0.3623082835,-0.1280846479,-0.681447794
O,0,1.5602918493,-0.4514922946,-2.5639413126
C,0,2.9481220799,-0.6586719508,-2.8712236234
H,0,3.112337799,-1.7378937964,-2.9640774509
H,0,3.1657827249,-0.1654228334,-3.819870766
H,0,4.0070469398,0.9746546214,-1.8421678037
H,0,4.5789680577,-0.6640717054,-1.4078282926
Zn,0,-1.6763920006,0.2168835047,-1.7427137321
C,0,-7.4746527342,0.4956687639,-0.9721225401
H,0,-8.2424991939,0.8589341931,-0.2891992031
H,0,-7.7669862466,0.3646209983,-2.0135713458
C,0,-6.2627584228,0.2412907995,-0.5673340855
C,0,-5.0445330268,0.0072256428,-0.1462851973
H,0,-4.2697225586,0.7719334732,-0.1300000322
N,0,-4.6341525263,-1.2360039027,0.3574998486
C,0,-5.4884450434,-2.4056977224,0.4227074331
C,0,-3.3331826973,-1.602341697,0.4420341277
O,0,-2.3516150591,-0.8929811614,0.2398695389
O,0,-3.2324640476,-2.8799734383,0.8122033079
C,0,-4.5437700414,-3.3839738609,1.1113453647
H,0,-4.6090402103,-4.4058049882,0.7343612385
H,0,-4.6631122147,-3.378671272,2.2010619625
H,0,-6.3954400648,-2.1993914346,0.9995860698
H,0,-5.7735147076,-2.7199230409,-0.5926662601
Zn,0,-0.3758779516,-1.7049523061,1.1045600099
C,0,-0.1060544373,-3.3156066958,0.0189035188
H,0,-0.8042249517,-3.3695080474,-0.8227459831
H,0,-0.1924758852,-4.2461933464,0.585759893
C,0,-0.518127801,-0.4883299015,2.6355087804
H,0,0.3034888733,-0.4290270397,3.3549426513

H,0,-0.8037428491,0.5285011692,2.3419129536
C,0,-1.7536224767,-1.356158574,-2.9144576241
H,0,-0.9518172438,-2.0718709853,-2.7026943515
H,0,-1.7424859695,-1.1415438786,-3.9855648637
C,0,-1.9447573784,2.0169274456,-0.9970812298
H,0,-2.8572198275,2.5414601459,-1.2945510306
H,0,-1.9002434636,2.001941014,0.1000739392
Cl,0,-1.9551719961,-1.1186006867,3.5963859666
Cl,0,1.5700182633,-3.3732723991,-0.7321797623
Cl,0,-0.5921746328,3.1640352504,-1.5051561956
Cl,0,-3.3211949643,-2.2832547105,-2.6395936846
H,0,4.0392430688,0.7556718643,2.3947386235
C,0,3.9737660536,0.9561039553,1.326175838
H,0,4.9352451465,0.9195739476,0.8112085768
Zn,0,-0.0229960325,4.5915714439,0.9300687333
C,0,0.8904820113,2.9656196073,1.609993537
H,0,0.5510603841,2.0119037709,1.1949585788
H,0,1.3439168511,2.8469619843,2.5983918512
Cl,0,-1.3899188028,3.3969468208,2.4405754245
C,0,0.013452685,6.340474621,0.0823656715
H,0,0.0989898443,7.1948312408,0.7567054172
H,0,-0.8246132651,6.5091564651,-0.5975216413
Cl,0,1.5186797004,6.3787658645,-0.9678409543

Sum of electronic and thermal Free Energies=
-4592.579928 (Hartree/Particle)
One imaginary frequency -349.11.

D-PC-B2

C,0,-3.5489843433,0.6429916133,0.998219397
H,0,-2.8864471767,0.1497009807,0.2821623935
H,0,-4.6135588306,0.5671003461,0.78327423
C,0,-3.0249409129,1.9049063129,1.553068874
C,0,-2.0480863364,2.8790585118,1.0283784293
H,0,-1.1935328766,3.1900226981,1.6354987495
N,0,-1.8010363889,2.8456428206,-0.3831668327
C,0,-1.9807578642,3.9813265716,-1.2704539954
C,0,-0.9161500787,1.9786658552,-0.9193209084
O,0,-0.3575638388,1.0343749712,-0.3588366088
O,0,-0.7076020567,2.250830749,-2.2118991398
C,0,-1.5170623098,3.3748869959,-2.5931107622
H,0,-0.9012748573,4.0477244508,-3.1932934235
H,0,-2.3516861506,3.0009315385,-3.1962703968
H,0,-3.0257168115,4.305829335,-1.3008840057
H,0,-1.3546818607,4.8252273577,-0.9470266405
Zn,0,0.8969570438,-0.3370735142,-1.76243869
C,0,4.5421566567,-4.9306112796,-1.8134360565
H,0,4.7296824638,-5.8841678758,-1.3198932895
H,0,4.9237618054,-4.8203051567,-2.8281072295
C,0,3.8842972674,-3.9724321401,-1.2245606296
C,0,3.204465389,-3.0273945099,-0.623703264
H,0,2.1202016915,-2.9522852152,-0.6879122639
N,0,3.8018063536,-2.0446088638,0.1784652439
C,0,5.232382324,-1.9342448026,0.3866861773
C,0,3.193172153,-0.8714636507,0.4795896699
O,0,2.0233741273,-0.5696794459,0.2624852985

O,0,4.0457168217,-0.0498182502,1.092681903
C,0,5.2666493921,-0.7574990068,1.3548245629
H,0,6.0994034501,-0.0711543406,1.1947102961
H,0,5.2430053013,-1.0823935507,2.4018272879
H,0,5.6401672166,-2.8568266075,0.8118189688
H,0,5.7351538231,-1.7275133405,-0.569897182
Zn,0,1.2046303393,1.231745083,1.5101961132
C,0,2.2561273077,2.7088403059,0.74525878
H,0,2.879359198,2.3713412414,-0.0896110306
H,0,2.9100664544,3.1978160493,1.4721092387
C,0,0.4459061006,0.0009986262,2.8314022469
H,0,-0.1246205497,0.4331738486,3.657377261
H,0,-0.1504284794,-0.7873590984,2.3552387476
C,0,2.1991795084,0.8643218772,-2.6126351529
H,0,2.1839952176,1.8740911597,-2.1907870651
H,0,2.0878072102,0.9520805948,-3.6963280053
C,0,-0.2911599995,-1.8971376428,-1.5548228046
H,0,-0.095775983,-2.7699935808,-2.1836052079
H,0,-0.3289275512,-2.2154932101,-0.5055532229
Cl,0,1.8511503704,-0.8755119234,3.6339458797
Cl,0,1.2360837943,4.0743007254,0.0528384749
Cl,0,-2.0449145825,-1.4565557556,-1.9493465037
Cl,0,3.9209011535,0.2608859116,-2.3674704379
H,0,-3.4721161027,3.9127405526,2.3888421216
C,0,-3.4280652937,3.3181009111,1.479139562
H,0,-4.1444676153,3.6045081704,0.7099806143
Zn,0,-3.4414605561,-2.2183463467,0.0996036851
C,0,-3.0751409628,0.7272701867,2.4351946515
H,0,-2.1470137652,0.2142156402,2.6793310273
H,0,-3.8306779129,0.7064195051,3.2173076712
Cl,0,-1.9106140836,-2.7894203452,1.4910762636
C,0,-5.2666493395,-2.1135415741,-0.5762499108
H,0,-5.9958291324,-1.9364857075,0.2181460876
H,0,-5.5520128008,-3.024698051,-1.1075026586
Cl,0,-5.4572005308,-0.752733711,-1.762773589

Sum of electronic and thermal Free Energies=
-4592.695923 (Hartree/Particle)
No imaginary frequency.

D-RC-O

C,0,-4.8929548203,2.2215743416,-0.3673680671
H,0,-5.5076749845,2.6598654974,-1.153529971
H,0,-5.4047828972,2.0092862432,0.573487519
C,0,-3.622819422,1.9711820096,-0.5391283653
C,0,-2.3490459384,1.7390853245,-0.7490769544
H,0,-1.9827220856,0.8062447982,-1.177465522
N,0,-1.3408960398,2.6587579142,-0.439281555
C,0,-1.5883564402,3.8960324131,0.2756833391
C,0,-0.0403762521,2.2802972942,-0.2817506397
O,0,0.4654836162,1.2147813983,-0.5991509015
O,0,0.6607502265,3.2761632784,0.2672361286
C,0,-0.1685994075,4.4430880703,0.3579922737
H,0,0.0591327725,4.9527564739,1.2953102429
H,0,0.0746474323,5.0928936663,-0.4909821835
H,0,-2.2705251199,4.5473030078,-0.2795896505

H,0,-2.0261621552,3.6743227427,1.2609916782
Zn,0,2.8755146645,1.4340339298,-0.4463514289
C,0,7.7704287981,-1.600632243,-1.404480213
H,0,8.2082037278,-2.2766389464,-2.1390005877
H,0,8.4652030654,-1.0245547656,-0.7938867096
C,0,6.4802803293,-1.4781451783,-1.2693345778
C,0,5.1810828498,-1.351624807,-1.1580605254
H,0,4.6088876627,-0.6272159338,-1.7371640099
N,0,4.4021562301,-2.1404921493,-0.2995867218
C,0,4.9535226849,-3.0908431817,0.646435722
C,0,3.143766884,-1.7906825021,0.0671363482
O,0,2.4593906586,-0.8932725681,-0.4117534007
O,0,2.7032824091,-2.5906101289,1.0392468884
C,0,3.6658532606,-3.6325535858,1.2582064825
H,0,3.7273906433,-3.8183253133,2.3315296792
H,0,3.3067877887,-4.530448886,0.74186968
H,0,5.5456250932,-3.8574485971,0.1366477357
H,0,5.5936331949,-2.5661130006,1.3712828587
Zn,0,0.1690596638,-1.073070479,0.1763170806
C,0,0.2247763523,-0.5915339771,2.0829674758
H,0,1.2448579933,-0.3720994199,2.4174829403
H,0,-0.1909370942,-1.3602578274,2.7398176154
C,0,-0.2102740351,-1.9363396436,-1.5449610621
H,0,-1.2523402571,-2.1918933099,-1.758826117
H,0,0.1859180864,-1.3479854958,-2.3797456977
C,0,3.1800520247,1.5968232983,1.4857930727
H,0,2.2523921678,1.4895013239,2.058849455
H,0,3.6522162369,2.5366139867,1.7831476764
C,0,2.9798563158,1.7150343497,-2.3854721594
H,0,3.9766899561,1.8436515447,-2.8159671555
H,0,2.4710982122,0.9052684555,-2.9198953474
Cl,0,0.6803819216,-3.5399572458,-1.6081975191
Cl,0,-0.7428965407,0.9275912019,2.4831385152
Cl,0,2.0665923916,3.2428018574,-2.8350673764
Cl,0,4.304840217,0.2877795682,2.1220074154
H,0,-2.8599529681,-1.2919297149,-0.5521076884
C,0,-3.1810768828,-1.2641818395,0.493706984
H,0,-2.5391076634,-0.5690771052,1.0457287085
Zn,0,-5.0512288238,-0.8145185787,0.6969663284
Cl,0,-2.8773288784,-2.922371079,1.1697456915
C,0,-6.9490501213,-0.4858518785,0.9532586977
H,0,-7.503838237,-1.3848835691,1.2326851063
H,0,-7.1730128989,0.2919867279,1.6885683576
Cl,0,-7.6461225685,0.0791672327,-0.6312415889

Sum of electronic and thermal Free Energies=
-4553.361343 (Hartree/Particle)
No imaginary frequency.

D-TS-O

C,0,4.6233421153,1.4275015566,-0.4038044778
H,0,5.4276835958,1.5737391699,0.3183643808
H,0,4.9298934074,1.3940032635,-1.4498189896
C,0,3.3522578718,1.4476559972,-0.0527486346
C,0,2.0978212176,1.386713868,0.3215498083
H,0,1.6205512855,0.4353193884,0.5664140601

N,0,1.2503520824,2.4851289152,0.4478229943
C,0,1.5856991678,3.8382923655,0.051390394
C,0,-0.1046375295,2.322213188,0.4845681323
O,0,-0.6985162136,1.2599853214,0.5909969749
O,0,-0.7129407016,3.501414946,0.4052660125
C,0,0.2715034054,4.5470228328,0.3786634829
H,0,-0.0326732916,5.2769684743,-0.3733790469
H,0,0.287968586,5.0165953743,1.3681385086
H,0,2.4334538714,4.2229974543,0.6276593501
H,0,1.8388504588,3.8651289571,-1.0188273458
Zn,0,-2.950434874,1.291626964,1.2075141302
C,0,-7.4694921916,-1.9940732605,2.2706257633
H,0,-7.7858452211,-2.8878003777,2.8082311272
H,0,-8.2320804569,-1.2385383818,2.0835814064
C,0,-6.2379990756,-1.8289728164,1.8785641155
C,0,-4.9911956699,-1.6686838641,1.5088483355
H,0,-4.2461225206,-1.1989454869,2.150228275
N,0,-4.494990437,-2.1049414033,0.2710989594
C,0,-5.3160421498,-2.7206850177,-0.7524658322
C,0,-3.355783697,-1.611677715,-0.2744268722
O,0,-2.5353572931,-0.8793720513,0.2686949487
O,0,-3.2088092436,-2.0524509051,-1.524293157
C,0,-4.2585070441,-2.9869080282,-1.8191885195
H,0,-4.6010614236,-2.802121806,-2.838560003
H,0,-3.8383534128,-3.9964135061,-1.7443712736
H,0,-5.7924865114,-3.6328268696,-0.378963705
H,0,-6.098207594,-2.0188648691,-1.0781293332
Zn,0,-0.5272507079,-0.6519436002,-0.9267196189
C,0,-1.0779017804,0.4014771174,-2.4898389608
H,0,-2.1216473658,0.72941985,-2.4279609358
H,0,-0.9378759644,-0.1060412139,-3.4472913743
C,0,0.3937010109,-1.9436556133,0.2306679667
H,0,1.4468309514,-2.1658057652,0.0289535598
H,0,0.2904190692,-1.6765023147,1.2890329425
C,0,-3.7706113724,2.0897113276,-0.388787254
H,0,-3.016215687,2.3599957034,-1.1361974866
H,0,-4.3730598167,2.9781905938,-0.1842469716
C,0,-2.5010348359,0.928936277,3.0835554447
H,0,-3.3264943723,0.856898909,3.7964145811
H,0,-1.8772608584,0.0334675615,3.1799586305
Cl,0,-0.4721597311,-3.5493722461,0.0500558631
Cl,0,-0.0898134561,1.9501786848,-2.638410922
Cl,0,-1.4607945308,2.3143509361,3.6960530637
Cl,0,-4.9184104599,0.9370211415,-1.2455812446
H,0,3.8910284061,-0.8259580082,0.8463959726
C,0,4.3033340867,-0.8410053204,-0.165554147
H,0,3.5199708318,-0.9235573081,-0.9234879993
Zn,0,6.1258914709,-1.5387594113,-0.4822713579
Cl,0,4.6275274652,-3.2680164464,-0.0918549339
C,0,8.0121082191,-1.2705576733,-0.8375818221
H,0,8.6707059407,-1.6702800591,-0.0636881608
H,0,8.3439800824,-1.6557341169,-1.8039267541
Cl,0,8.3099358917,0.5347381865,-0.8790700508

Sum of electronic and thermal Free Energies=
-4553.326141 (Hartree/Particle)
One imaginary frequency -328.66.

D-PC-O

C,0,-4.6666735843,0.4460153557,-0.1537616731
H,0,-5.2095031298,1.2005982187,-0.7315710993
H,0,-4.7551745824,0.5468341771,0.9301560959
C,0,-3.3846488872,-0.0186025653,-0.6887874726
C,0,-2.1110625617,0.2534289936,-0.9125181558
H,0,-1.4235145693,-0.458320208,-1.3660774767
N,0,-1.5250628541,1.4885514386,-0.6106179764
C,0,-2.2327017594,2.6307530928,-0.0608769827
C,0,-0.191481366,1.6169745502,-0.3874150161
O,0,0.6633139674,0.7535851639,-0.5498089975
O,0,0.0979808147,2.8462204797,0.0360987771
C,0,-1.0944458188,3.6451961507,0.0021111874
H,0,-1.1098677062,4.2704368764,0.8963241038
H,0,-1.0501353419,4.2758808718,-0.8933532772
H,0,-3.0521868952,2.9460487284,-0.7144736058
H,0,-2.6451667382,2.3860484144,0.9288701997
Zn,0,2.8984310147,1.4455684452,-0.6020105196
C,0,8.2405538056,-0.7834684799,-1.373583356
H,0,8.7741936841,-1.4720160251,-2.0286892454
H,0,8.8341345841,-0.0066688005,-0.8921876892
C,0,6.9549012148,-0.8761601805,-1.1830604614
C,0,5.6589585071,-0.9687966274,-1.0149888865
H,0,4.9445373188,-0.4517895907,-1.655113573
N,0,5.067950529,-1.747398868,-0.0093039782
C,0,5.8154699114,-2.434832055,1.024543312
C,0,3.7782997339,-1.5821930163,0.3768631668
O,0,2.9248169551,-0.9017430034,-0.1802036791
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H,0,-6.716930036,1.8587590638,2.3246224958
Cl,0,-6.3564129311,3.439509466,0.5887032371

Sum of electronic and thermal Free Energies=
-4553.428116 (Hartree/Particle)
No imaginary frequency.

D-RC-B3

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C,0,-4.277231417,-2.9353458944,-0.7088672685
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H,0,6.0831243615,-0.7943205571,-0.8433881356
H,0,5.2009497747,-1.5541445355,-2.1692012098
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Sum of electronic and thermal Free Energies=
-4592.635219 (Hartree/Particle)
No imaginary frequency.

D-TS-B3

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C,0,-1.0434589663,0.8807990641,-0.3058630609
C,0,-1.481736401,2.0752487026,-0.733875691
H,0,-2.452726487,2.2142626871,-1.2091270996
N,0,-0.7284009898,3.229640807,-0.6246401215
C,0,0.2621639167,3.5101352724,0.4045090058
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Sum of electronic and thermal Free Energies=
-4592.602192 (Hartree/Particle)

One imaginary frequency -290.03.

D-PC-B3

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H,0,2.2587471601,2.3709695141,2.6412721982
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C,0,2.8956048765,2.9607387503,0.0009353154
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C,0,2.2842967129,0.1415447045,2.5447886364
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Sum of electronic and thermal Free Energies=
-4592.699197 (Hartree/Particle)

No imaginary frequency.

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Complete List of Authors for References with more than 10 Authors

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6. Comparison of different polarized continuum models

Table S1. Free energies and enthalpies of mono-cyclopropanation of **1** from **SM1** (kcal/mol)

ΔG_{DCE} (ΔH_{DCE})	SM1	M-RC-T	M-TS-T1	M-TS-T2	M-TS-T3	M-PC-T
IEFPCM	0.0 (0.0)	3.3 (-8.7)	27.3 (14.2)	26.1 (12.1)	26.2 (13.8)	-46.6 (-59.6)
CPCM	0.0 (0.0)	3.7 (-8.3)	27.5 (14.4)	26.0 (12.0)	26.0 (13.6)	-47.1 (-60.0)

Table S2. Free energies and enthalpies of mono-cyclopropanation of **1** from **SM2** (kcal/mol)

ΔG_{DCE} (ΔH_{DCE})	SM2	D-RC1	D-TS1	D-TS2	D-PC1
IEFPCM	0.0 (0.0)	7.2 (-31.9)	34.2 (-7.3)	29.5 (-10.4)	-45.6 (-84.4)
CPCM	0.0 (0.0)	7.8 (-31.3)	34.6 (-7.0)	29.9 (-10.0)	-46.0 (-84.8)

As showed in Tables S1 and S2, the relative free energies and enthalpies with CPCM are similar to those with IEFPCM.

7. Explicit solvent effects

Table S3. Explicit solvent effects on mono-cyclopropanation of **1** in monomeric form (kcal/mol)

ΔG_{DCE} (ΔH_{DCE})	SM1	M-RC-T	M-TS-T1	M-TS-T2	M-PC-T
IEFPCM	0.0 (0.0)	3.3 (-8.7)	27.3 (14.2)	26.1 (12.1)	-46.6 (-59.6)
Explicit Solvent	0.0 (0.0)	9.7 (-12.8)	36.6 (10.2)	33.0 (8.0)	-37.6 (-62.9)

Table S4. Explicit solvent effects on mono-cyclopropanation of **1** in dimeric form (kcal/mol)

ΔG_{DCE} (ΔH_{DCE})	SM2	D-RC1	D-TS1	D-TS2	D-PC1
IEFPCM	0.0 (0.0)	7.2 (-31.9)	34.2 (-7.3)	29.5 (-10.4)	-45.6 (-84.4)
Explicit Solvent	0.0 (0.0)	13.9 (-35.9)	39.3 (-12.7)	39.1 (-14.0)	-35.6 (-85.2)

From the statistics in Tables S3 and S4 for the selected reaction pathways, direct solvent molecules involved in the reaction would lower the relative enthalpies but the entropy would increase significantly. The energy barriers from RC to TS are similar between IEFPCM solvation and explicit solvent involving system. This indicates the PCM solvation is more appropriate than the direct involvement of solvent molecules for the reaction in this paper.

8. PES scan of alpha-unsubstituted allenamide **1** with frozen dihedral angle coordinates

A relaxed PES scan of an alpha-unsubstituted molecule **1** along the dihedral angle D (C1, N, C2, C3) was done in which D (O1, C1, O2, C5) and D (O1, C1, N, C6) were frozen. As showed in Figure S1, energy profile is smooth since the structure of the oxazolidinone ring was nearly fixed. In contrast, the scan profile showed in Figure 1 in the article indicates some delay effect of some coordinates when changing D (C1, N, C2, C3).

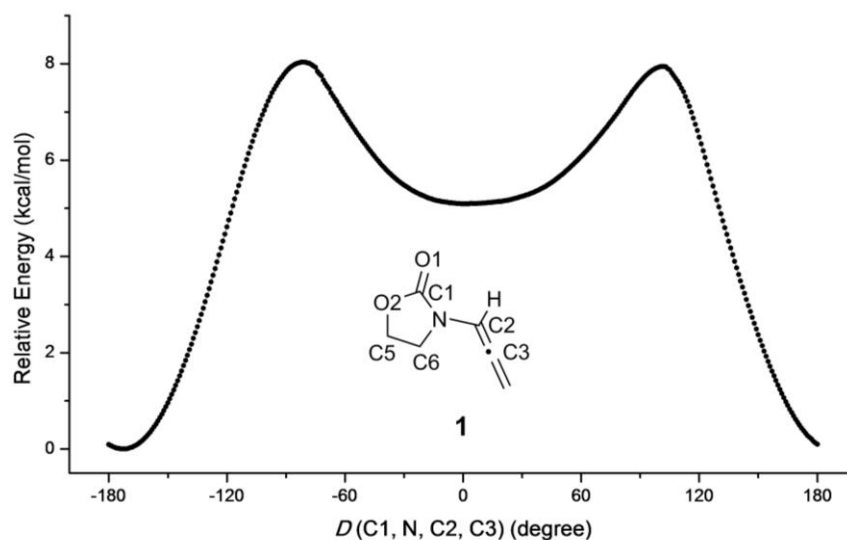


Figure S1. Scan profile of alpha-substituted allenamide **4**.

9. PES scan of alpha-substituted allenamide **4**

To exploit the influence of alpha-substituent over the energy of allenamides, a relaxed PES scan of an alpha-substituted molecule **4** was done. As shown in Figure S1, the relative energy of the molecule with the dihedral angle $D(C1, N, C2, C3)$ around 0° is about 2.0 kcal/mol while it is about 3.4 kcal/mol with $D(C1, N, C2, C3)$ around 180° . In fact, the scan profile seems to fluctuate dramatically due to the effects from both the oxazolidinone ring and the alpha-phenyl group.

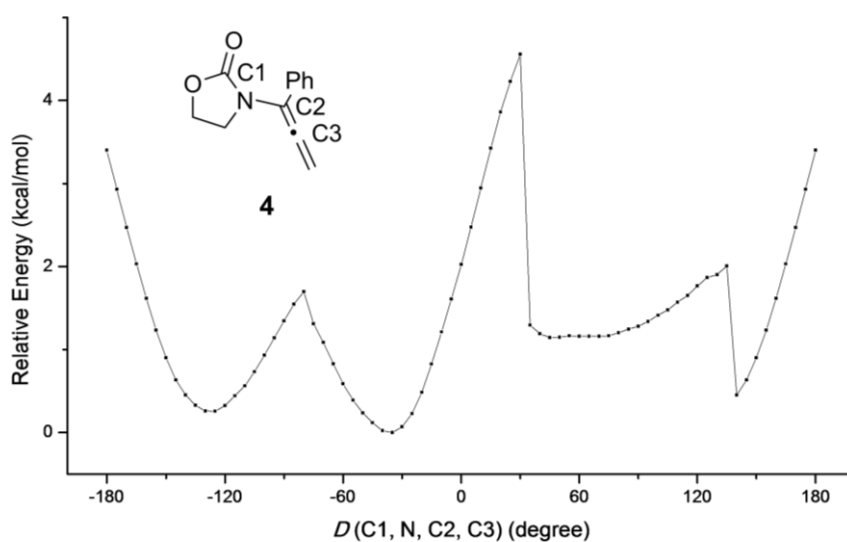


Figure S2. Scan profile of alpha-substituted allenamide **4**.

10. Cartesian coordinates and energies of computed structures of the model reaction with allenamine



M-TS-T1-mod

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H,0,-2.8673325971,0.077007014,3.9866905824
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C,0,-1.6327457511,-0.0338597816,2.2911932592
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H,0,-0.602053415,-1.578033952,1.3198963235
N,0,-2.0434118164,-0.8021360043,0.0380730193
C,0,-3.0451533093,0.2172250433,-0.1735867554
C,0,-1.309984914,-1.2005069392,-1.1458224609
H,0,-3.6901029872,0.2966548769,0.7060955531
H,0,-2.5925162184,1.2061471233,-0.3634803876
H,0,-0.5619286272,1.9535532336,1.0455247329
C,0,0.2442829358,1.2857867981,1.3476868139
H,0,0.4520083601,1.343553478,2.4159473725
Zn,0,1.5291001377,0.5139912509,0.1185821943
Cl,0,1.9357781441,2.8004985417,0.7489653156
C,0,2.5245854002,-0.7249753263,-0.9895833318
H,0,2.275363839,-0.6752350482,-2.0525224334
H,0,3.6068670171,-0.6227532546,-0.8869294281
Cl,0,2.1281566122,-2.4299524363,-0.4547445832
H,0,-3.6596125878,-0.0521567572,-1.0385626182
H,0,-0.5640066874,-1.9613782198,-0.8936215443
H,0,-1.9989417415,-1.6138553293,-1.8909975844
H,0,-0.7837833279,-0.3454208178,-1.6091015571

Sum of electronic and thermal Free Energies=
-1476.324748 (Hartree/Particle)
One imaginary frequency -315.38.

M-TS-T2-mod

C,0,-0.2301124831,3.7781236748,-1.1387438936
H,0,0.7537601813,3.9563371214,-1.5757472751
H,0,-1.0034433213,4.5018644047,-1.4036592182
C,0,-0.4719380093,2.7649693535,-0.3429592598
C,0,-1.1412611343,1.9761117773,0.5126672775
H,0,-1.1076184384,2.2267392923,1.5764914965
N,0,-1.7318797431,0.7845313516,0.2354604107
C,0,-1.9766422813,0.4150040593,-1.1437356987
C,0,-2.5483738652,0.1315373231,1.2394667485
H,0,-2.8853864448,0.8916716014,-1.5409146903
H,0,-1.1277812443,0.7289582858,-1.7618739756
H,0,1.7530123549,1.9468024826,-1.0202673495
C,0,1.5219791978,1.4879978567,-0.0596957176
H,0,1.7692443856,2.1405306066,0.77618606
Zn,0,1.2858700128,-0.4239491942,0.120480945
Cl,0,3.5901663755,0.3836282559,0.0266320122
C,0,0.9700658248,-2.3354778115,0.1812228808
H,0,1.4893054033,-2.829006158,-0.6444914482
H,0,1.3308493828,-2.78252321,1.1111356248
Cl,0,-0.7796589657,-2.8324513553,0.031161303
H,0,-2.0803021225,-0.6733277085,-1.2084909644

H,0,-2.2051053056,0.4187680339,2.2377479498
H,0,-3.6103566171,0.403074592,1.1421548256
H,0,-2.4471728326,-0.9543632754,1.1391776465

Sum of electronic and thermal Free Energies=
-1476.325725 (Hartree/Particle)
One imaginary frequency -376.09.

M-TS-T3-mod

C,0,0.1685098799,0.4172050829,2.9089879375
H,0,1.2399019329,0.2196688912,2.8356197621
H,0,-0.1386413598,1.1088170056,3.6946142784
C,0,-0.6974913361,-0.1393105506,2.1005397683
C,0,-1.8373894854,-0.5148907716,1.5097336622
H,0,-2.3223355315,-1.435785696,1.8419807532
N,0,-2.4562761036,0.1093441871,0.4598585132
C,0,-1.8229821156,1.2745675521,-0.1170189814
C,0,-3.2326928544,-0.6964718611,-0.4588186156
H,0,-1.4269803323,1.9164134328,0.6740867156
H,0,-0.988237972,1.0024413538,-0.7871610835
H,0,0.7224737073,-2.1305538984,1.4407937546
C,0,0.5237755095,-1.5188705423,0.5610179743
H,0,-0.3136295217,-1.9074636034,-0.0197818951
Zn,0,1.7607428255,-0.224395801,-0.1668057507
Cl,0,2.1199499336,-2.5696232337,-0.7643945958
C,0,2.729032228,1.3661878428,-0.6892999496
H,0,3.754584969,1.3843782606,-0.3136459319
H,0,2.7620637328,1.5145113113,-1.7711075013
Cl,0,1.9018179311,2.8360534534,0.0073084888
H,0,-2.5591561845,1.839083957,-0.6983716928
H,0,-2.6120668333,-1.1311212663,-1.2608013148
H,0,-3.7223998133,-1.513122006,0.0807894251
H,0,-4.009283366,-0.0806680601,-0.9256316308

Sum of electronic and thermal Free Energies=
-1476.323869 (Hartree/Particle)
One imaginary frequency -372.90.

M-TS-O1-mod

C,0,0.1370150494,-1.213627808,-0.0411401036
H,0,-0.3204316704,-1.6849285108,0.8320668857
H,0,-0.305534575,-1.4925678112,-0.9996360271
C,0,1.2238616304,-0.46991596,0.0433835477
C,0,2.2756533092,0.3089098325,0.2039635248
H,0,2.1181903255,1.386167745,0.3014811047
N,0,3.5978138898,-0.0904747984,0.3028257738
C,0,3.8664997876,-1.4875501801,0.0509889789
C,0,4.5897175831,0.8274106841,-0.2183111128
H,0,3.1973189306,-2.1058067542,0.658833302
H,0,3.7171170932,-1.7600991196,-1.0085167775
H,0,-0.4500164281,1.1408322167,1.1058606421

C,0,-0.932103956,0.8804889282,0.1623930277
H,0,-0.4268453933,1.3253668765,-0.6960663077
Zn,0,-2.8108683796,0.3407201057,0.0837174994
Cl,0,-2.5203314132,2.6785988593,0.3253520384
C,0,-4.3124529442,-0.8724603208,-0.0576130314
H,0,-4.959607821,-0.8822467515,0.8219860164
H,0,-4.934505879,-0.7088718799,-0.940141649
Cl,0,-3.6360059021,-2.563964926,-0.2143043175
H,0,4.9005956875,-1.7150907397,0.3286874488
H,0,5.5710571382,0.5817625674,0.2022733429
H,0,4.6672711325,0.7952274233,-1.3184053949
H,0,4.340807385,1.8516014216,0.0788943982

Sum of electronic and thermal Free Energies=
-1476.316999 (Hartree/Particle)
One imaginary frequency -310.54.

M-TS-O2-mod

C,0,-1.0650505886,-1.4618863311,-0.1297873891
H,0,-0.4899671281,-1.5875201428,-1.0498481436
H,0,-0.5784900639,-1.8346189419,0.7738552184
C,0,-2.1649591469,-0.7295767042,-0.0785076788
C,0,-3.14505396,0.1505622181,-0.0314512122
H,0,-2.833934474,1.1851584163,0.1393805874
N,0,-4.508668858,0.001324136,-0.20377619
C,0,-5.0362016143,-1.3392215682,-0.2862632966
C,0,-5.3518704899,0.9465773394,0.5001804976
H,0,-4.5108609722,-1.9040525464,-1.0627324015
H,0,-4.9454418443,-1.8906950577,0.6665930147
H,0,-2.9317376677,-3.2841496618,0.3558608751
C,0,-2.2500643323,-3.4072456619,-0.4864968109
H,0,-2.6934454979,-3.0638498944,-1.4223118127
Zn,0,-0.82695158,-4.7568047673,-0.474751963
Cl,0,-2.9587428266,-5.6907785723,-0.8672197343
C,0,0.9905859724,-5.411425887,-0.3406948649
H,0,1.1679598299,-6.050360047,0.5270546825
H,0,1.3383203551,-5.9377937016,-1.2320419609
Cl,0,2.0842432377,-3.9603327637,-0.1417389549
H,0,-6.0955971812,-1.2951548818,-0.5574253129
H,0,-6.3406327637,0.97449304,0.02949332
H,0,-5.4834630598,0.6929204941,1.5654970468
H,0,-4.9194786156,1.9504750573,0.4370197038

Sum of electronic and thermal Free Energies=
-1476.313963 (Hartree/Particle)
One imaginary frequency -315.34.