Global picture of isomerization and dissociation of CN_2O_2: New metastable isomers.

Supporting Information.

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SI1: Cartesian coordinates, energies (HF), energies with zero-point energy correction (E_{zpec})(HF+ZPE) and smallest frequency (lf) of the isomers of $^1CN_2O_2$ at the B3LYP/aug-cc-VTZ level.

SI2: Cartesian coordinates, energies (HF), energies with zero-point energy correction (E_{zpec})(HF+ZPE) and smallest frequency (lf) of the transition states of $^1CN_2O_2$ at the B3LYP/aug-cc-VTZ level.

SI3: The IRC confirm of transition states 1-ts01/14, 2-ts01/14, 1-ts22/29, 2-ts22/29, 1-ts25/29, 2-ts25/29, 1-ts28/29, 2-ts28/29. (Noted that the "//" means the discontinuous energy)

SI1:

01 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.072501778 HF+ZPE=-298.054147 lf=120.0782
8 -2.166826 -0.003648 0.000000
7 -1.119213 -0.493360 0.000000
7 0.000000 0.553149 0.000000
8 2.278077 -0.156687 0.000000
6 1.157414 0.144027 0.000000

02 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.065341171 HF+ZPE=-298.047306 lf=95.1638
7 0.000000 0.931494 0.000000
8 1.966842 -0.421507 0.000000
6 0.994788 0.210837 0.000000
8 -1.470065 -0.835214 0.000000
7 -1.420421 0.324042 0.000000

03 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.049396586 HF+ZPE=-298.030635 lf=276.6370
6 -0.534937 -0.032698 0.000067
7 0.657328 -0.979894 0.000072
7 1.403273 -0.020476 -0.000110
8 0.292131 1.057316 0.000058
8 -1.693954 -0.157469 -0.000075

04 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.039840635 HF+ZPE=-298.021708 lf=120.5559
7 -1.037046 1.610317 0.000000
6 0.000000 1.075395 0.000000
8 -0.592205 -1.420885 0.000000
8 1.047065 0.385385 0.000000
7 0.517206 -1.348655 0.000000

05 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.037975646 HF+ZPE=-298.020094 lf=121.7157
7 2.353684 0.071703 0.000000
8 0.000000 0.680064 0.000000
6 1.228584 0.359751 0.000000
7 -1.023863 -0.721695 0.000000
8 -2.085032 -0.381134 0.000000

06 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.005791548 HF+ZPE=-297.986086 lf=215.6319
8 1.093548 1.030483 0.000000
7 0.000000 0.502609 0.000000
8 -1.093481 1.030624 0.000000
6 -0.000078 -0.920507 0.000000
7 -0.000009 -2.069154 0.000000

07 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.005889393 HF+ZPE=-297.988805 lf=71.5431
6 -1.364550 0.142004 -0.000248
7 2.324796 0.039963 0.000318
7 -2.373611 -0.467215 0.000322
8 -0.301929 0.761724 0.000042
8 1.368055 -0.494382 -0.000416

08 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.967663913 HF+ZPE=-297.949907 lf=104.3865
8 -2.247148 0.260428 0.000000
7 -1.254931 -0.406528 0.000000
6 0.000000 0.252170 0.000000
7 1.152121 -0.004322 0.000000
8 2.337107 -0.090062 0.000000

09 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.959364084 HF+ZPE=-297.941090 lf=64.6694
8 1.089695 0.988878 0.000000
7 0.000000 0.487730 0.000000
8 -1.089531 0.989233 0.000000
7 -0.000230 -0.937451 0.000000
6 0.000049 -2.112807 0.000000

10 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.953131681 HF+ZPE=-297.936069 lf=130.4942
6 1.738635 -0.803588 0.000387
7 1.068348 0.165906 -0.000124
8 0.165014 1.075728 -0.000496
8 -1.212432 -0.848013 -0.000557
7 -1.361559 0.262639 0.000995

11 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.948273684 HF+ZPE=-297.931664 lf=141.1014
8 -2.037352 -0.382261 0.000000
7 -0.959494 -0.696286 0.000000
6 2.379870 0.022490 0.000000
8 0.000000 0.683518 0.000000
7 1.248008 0.332715 0.000000

12 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.933060451 HF+ZPE=-297.914470 lf=429.4162
7 -1.246621 -0.000049 -0.637584
6 -0.011728 -0.000002 0.000000
7 -1.246553 0.000049 0.637715
8 1.095161 0.774642 -0.000117
8 1.095163 -0.774640 0.000003

13 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.937341303 HF+ZPE=-297.919846 lf=185.9622
6 -0.622782 0.037812 -0.000053
7 0.755938 -1.009625 0.000146
7 0.277785 1.069923 0.000176
8 -1.770746 -0.171895 -0.000029
8 1.333324 0.090775 -0.000214

14 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.931467607 HF+ZPE=-297.913821 lf=184.0221
7 -0.521146 -0.784415 -0.413099
6 0.614648 0.000000 -0.036935
7 -0.521146 0.784415 -0.413099
8 1.760385 0.000000 0.202987
8 -1.309365 0.000000 0.547637

15 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.929918107 HF+ZPE=-297.913592 lf=141.5036
6 -0.422414 -0.174196 0.000207
7 -1.556905 -0.690400 -0.000057
7 0.984721 -0.652918 -0.000040
8 1.723126 0.285186 -0.000030
8 -0.905655 1.020864 -0.000040

16 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.926212733 HF+ZPE=-297.910153 lf=13.7200
7 -0.974852 1.093403 0.013884
6 -0.400858 -0.021644 0.004224
8 -1.512272 -0.658564 -0.020725
7 0.973718 -0.600719 0.038142
8 1.813909 0.243699 -0.027965

17 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.918888036 HF+ZPE=-297.900834 lf=193.0501
7 1.980467 -0.551480 0.000000
6 1.003762 0.070401 0.000000
7 0.000000 0.964057 0.000000
8 -1.309841 -0.845508 0.000000
8 -1.175890 0.431702 0.000000

18 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.915163341 HF+ZPE=-297.897324 lf=209.4187
8 2.098051 -0.024289 0.000079
8 0.876699 -0.370227 -0.000098
7 -2.350412 -0.217169 0.000028
7 0.006339 0.598989 -0.000015
6 -1.231582 0.080564 0.000009

uL1 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.919330796 HF+ZPE=-297.904759 lf=33.8809
8 -2.216961 0.313904 0.000000
7 -1.092422 0.782490 0.000000
6 0.000000 1.277140 0.000000
8 1.167652 -1.033381 0.000000
7 2.291632 -1.054922 0.000000

19 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.910346541 HF+ZPE=-297.894352 lf=77.1073
6 -2.342937 -0.556529 0.000211
7 -1.364566 0.106871 0.000010
7 2.270780 -0.005067 0.000413
8 -0.308521 0.795635 -0.000206
8 1.272787 -0.467317 -0.000323

20 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.906540979 HF+ZPE=-297.889980 lf=189.5118
8 -2.176970 0.133798 0.000000
8 -0.923326 -0.296750 0.000000
6 0.000000 0.596036 0.000000
7 1.220532 -0.075782 0.000000
7 2.322664 -0.248875 0.000000

u21 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.902350696 HF+ZPE=-297.885358 lf=396.7731
7 0.970217 -0.880398 0.520816
6 0.000000 0.000000 0.090317
8 0.000000 1.240249 -0.489583
7 -0.970217 0.880398 0.520816
8 0.000000 -1.240249 -0.489583

22 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.893289468 HF+ZPE=-297.875816 lf=232.8269
7 -2.106038 0.000084 -0.217823
6 -0.993678 -0.000180 0.077718
7 0.271374 -0.000178 0.630878
8 1.175163 0.727876 -0.209739
8 1.175426 -0.727659 -0.209973

23 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.882926170 HF+ZPE=-297.864732 lf=238.5044
8 -0.343259 -1.744755 0.000000
7 0.184382 -0.669635 0.000000
6 1.301284 0.175893 0.000000
7 0.000000 0.694512 0.000000
8 -0.794038 1.591068 0.000000

24 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.873416902 HF+ZPE=-297.856555 lf=206.0971
7 -1.211271 0.822404 0.000001
6 -0.294151 -0.196465 0.000000
7 -1.622578 -0.410647 0.000000
8 0.844504 -0.633322 -0.000001
8 1.855727 0.420384 0.000000

25 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.870978947 HF+ZPE=-297.853936 lf=129.0789
6 -2.001952 0.520954 0.000042
7 -0.993696 -0.096108 -0.000009
7 -0.011132 -0.961039 -0.000048
8 1.231829 0.909333 -0.000039
8 1.148859 -0.375045 0.000058

26 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.861648094 HF+ZPE=-297.847845 lf=50.7912
6 1.632979 -0.169836 0.678462
7 1.605002 -0.225983 -0.580783
7 -2.158599 0.177029 -0.018619
8 -1.246102 -0.441614 0.033319
8 0.505765 0.611826 -0.017689

u27 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.879478100 HF+ZPE=-297.863123 lf=91.2402
8 2.283239 -0.335381 0.000000
7 1.105455 -0.139003 0.000000
6 0.000000 0.269811 0.000000
8 -1.25443 -0.242975 0.000000
7 -2.281228 0.568715 0.000000

28 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.863803183 HF+ZPE=-297.847086 lf=174.2561
6 -2.388616 -0.208578 0.000080
7 -0.039327 0.587038 0.000014
7 -1.230723 0.026063 -0.000086
8 0.839085 -0.374710 -0.000070
8 2.063671 -0.005320 0.000072

29 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.846540623 HF+ZPE=-297.830208 lf=160.5204
8 1.145340 0.730445 -0.193432
7 0.221171 -0.000425 0.611077
7 -0.995709 0.000266 0.007944
6 -2.151553 -0.000271 -0.205917
8 1.146045 -0.730103 -0.193773

30 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.757647978 HF+ZPE=-297.742400 lf=246.2720
8 1.103001 0.168564 0.000000
7 -0.154415 -0.033528 0.961763
7 -0.154415 -0.033528 -0.961763
8 -0.716965 -0.934979 0.000000
6 -0.154415 1.100120 0.000000

31 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.755956337 HF+ZPE=-297.740295 lf=203.2050
7 -0.890819 1.356886 0.000000
8 0.000000 0.521474 0.000000
8 1.429307 0.659597 0.000000
6 -0.228589 -0.862672 0.000000
7 -0.546741 -1.967248 0.000000

32 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.728250502 HF+ZPE=-297.712826 lf=211.6066
7 -0.157224 -0.931074 -0.166518
7 -0.755965 0.327886 -0.649716
8 1.130478 -0.342599 0.025869
8 0.395018 0.967394 0.135526
6 -0.968608 -0.129341 0.737079

SI2:

ts01/02 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.063512338 HF+ZPE=-298.045519 lf=-116.1548
6 -1.066868 0.137985 -0.062047
7 -0.048902 0.785411 -0.232512
7 1.310465 0.281197 0.389022
8 -2.073261 -0.430985 0.089957
8 1.769544 -0.605786 -0.180367

ts03/P1 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.049334023 HF+ZPE=-298.031282 lf=-275.6900
6 -0.534004 -0.020093 -0.000006
7 0.682499 -0.968540 0.000000
7 1.423097 -0.022617 0.000018
8 -1.686409 -0.198231 -0.000023
8 0.244517 1.080563 0.000012

ts02/03 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.035543461 HF+ZPE=-298.017494 lf=-404.3511
6 -0.659407 0.090092 -0.000001
7 0.357571 1.038724 0.000000
7 1.323550 0.190639 0.000002
8 0.798861 -0.983173 0.000001
8 -1.775286 -0.160089 -0.000002

ts04/05 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.028851978 HF+ZPE=-298.011543 lf=-169.2136
6 -1.169158 0.122232 -0.044630
7 -2.052265 -0.628077 0.074592
7 1.297502 0.110251 0.486512
8 1.734302 -0.556428 -0.283571
8 -0.197016 0.917851 -0.173923

ts02/P2 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.025168809 HF+ZPE=-298.008457 lf=-624.9939
6 -0.942918 -0.214849 0.000000
7 0.174870 0.931820 0.000004
7 1.256388 0.399354 0.000004
8 -2.077682 -0.222856 -0.000010
8 1.532520 -0.780784 0.000003

ts01/05 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.024406601 HF+ZPE=-298.007081 lf=-170.6490
6 1.091594 0.105988 -0.063389
7 1.438591 -1.024602 -0.031190
7 -0.982999 -0.125971 0.483561
8 0.520878 1.197999 -0.043518
8 -1.738216 -0.270738 -0.304765

ts01/07 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-298.002545964 HF+ZPE=-297.985744 lf=-101.6237
6 -1.208714 0.106079 -0.040739
7 -1.659912 -0.992020 -0.040620
7 2.081581 -0.227533 -0.261070
8 -0.615979 1.169481 -0.022502
8 1.153554 -0.181932 0.317035

ts01/P2 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.991116127 HF+ZPE=-297.975001 lf=-856.7800
6 -1.301007 0.373199 0.000001
7 0.061074 -0.345328 -0.000001
7 1.114672 0.229317 0.000000
8 -2.343250 -0.122477 0.000000
8 2.290227 -0.055912 -0.000001

ts01/P4 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.963802112 HF+ZPE=-297.949902 lf=-498.0321
6 0.807538 -1.225656 0.000000
7 0.000000 0.537031 0.000000
7 -1.215308 0.407212 0.000000
8 1.863158 -1.616246 0.000000
8 -1.405417 1.709275 0.000000

ts13/P3 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.937039517 HF+ZPE=-297.920068 lf=-218.6171
6 -0.694429 0.059180 0.000000
7 0.937126 -0.998979 0.000001
7 0.192539 1.056481 0.000000
8 -1.808677 -0.253667 0.000000
8 1.341042 0.158968 -0.000001

ts10/11 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.936179356 HF+ZPE=-297.920225 lf=-199.0282
6 2.047850 -0.705669 0.079379
7 1.176308 0.073757 -0.039456
7 -1.236287 0.098637 0.496055
8 0.209125 0.922921 -0.169151
8 -1.692531 -0.544514 -0.289907

ts08/08 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.952309424 HF+ZPE=-297.935651 lf=-537.7799
6 0.000000 0.206928 0.000000
7 -1.178705 -0.256475 0.000000
7 1.178703 -0.256480 0.000000
8 -2.311079 0.146827 0.000000
8 2.311081 0.146813 0.000000

ts04/10 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.934232959 HF+ZPE=-297.917268 lf=-328.0466
6 -1.059671 0.911414 0.000048
7 -1.168658 -0.329901 0.000032
7 1.105193 -0.258872 -0.000039
8 0.784535 0.902094 -0.000011
8 0.065750 -1.070478 -0.000018

ts06/09 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.932387881 HF+ZPE=-297.915282 lf=-388.0885
6 -1.420092 0.000000 0.639053
7 0.516037 0.000000 0.014285
7 -1.415975 0.000000 -0.551225
8 0.926257 1.092049 -0.004734
8 0.926257 -1.092049 -0.004734

ts01/15 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.928984492 HF+ZPE=-297.913552 lf=-339.8578
6 -0.493437 -0.156337 0.000000
7 0.959614 -0.713865 -0.000001
7 -1.621634 -0.670519 0.000002
8 -0.718011 1.100502 0.000001
8 1.667356 0.228087 -0.000002

ts15/16 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.924330267 HF+ZPE=-297.908406 lf=-112.0067
6 0.401572 -0.113132 0.081250
7 1.361434 -0.875424 -0.171020
7 -1.005424 -0.196162 0.511801
8 1.158764 0.926771 -0.002270
8 -1.771453 0.095716 -0.356850

1-uts13/P1 mol=C1N2O2
UB3LYP/Aug-CC-pVTZ HF=-297.915947053 HF+ZPE=-297.900473 lf=-2473.3602
6 0.070806 -0.000003 -0.000006
7 -1.217208 0.018546 -0.623742
7 -1.217202 -0.018556 0.623745
8 1.038491 0.897724 0.011279
8 1.038513 -0.897713 -0.011278

ts08/11 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.923403730 HF+ZPE=-297.907297 lf=-199.8132
6 0.968809 1.318208 -0.020093
7 -0.972684 -0.019794 0.467989
7 1.075431 0.127440 -0.072645
8 -1.771796 0.022060 -0.292374
8 0.955286 -1.104906 -0.038484

ts05/06 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.918057692 HF+ZPE=-297.901678 lf=-838.8739
6 0.900884 -0.050043 0.052422
7 1.993422 -0.438928 -0.061554
7 -0.619745 -0.145626 0.178570
8 -0.195520 1.105851 -0.046807
8 -1.682111 -0.556834 -0.094898

ts13/16 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.917821035 HF+ZPE=-297.901095 lf=-282.0750
6 -0.489968 -0.076475 0.000000
7 0.848256 -0.795386 0.000000
7 -0.371359 1.219376 0.000000
8 -1.651025 -0.449128 0.000001
8 1.601216 0.135493 -0.000001

ts08/L1 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.897764731 HF+ZPE=-297.882507 lf=-451.8427
6 0.469943 1.282350 -0.067891
7 -1.698039 -0.315797 -0.544927
7 1.093414 0.259647 -0.019664
8 1.714312 -0.791187 0.021850
8 -1.537722 -0.121445 0.523085

ts11/19 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.908043745 HF+ZPE=-297.892366 lf=-112.4880
6 -2.660199 0.162603 0.000151
7 -1.496962 -0.055474 -0.000075
7 2.165442 -0.409492 0.000331
8 -0.262072 -0.284959 -0.000272
8 1.672301 0.569853 -0.000065

ts20/P1 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.905210996 HF+ZPE=-297.890666 lf=-437.9595
6 0.100559 0.607290 0.000002
7 -1.287352 -0.088593 0.000001
7 -2.392693 -0.059909 -0.000002
8 2.226276 0.021350 -0.000001
8 0.918343 -0.346879 0.000000

ts12/14 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.904532393 HF+ZPE=-297.888037 lf=-699.2463
6 0.594962 0.015426 -0.030763
7 -0.572611 -0.852507 0.232423
7 -0.289743 1.052239 0.162439
8 1.769484 -0.136045 -0.092787
8 -1.461146 -0.050289 -0.229645

ts01/09 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.903362669 HF+ZPE=-297.886567 lf=-357.0558
6 1.493758 -0.050176 0.000097
7 0.554277 -1.007178 -0.000051
7 -0.426091 -0.057950 -0.000057
8 0.356360 1.060894 -0.000037
8 -1.588841 -0.091275 0.000058

ts08/15 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.899031925 HF+ZPE=-297.884127 lf=-621.3045
6 0.200870 -0.146615 0.000000
7 1.345067 -0.659236 0.000000
7 -1.089209 -0.406431 0.000000
8 -2.025292 0.356408 -0.000001
8 1.650764 0.686012 0.000000

ts06/P8 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.888882686 HF+ZPE=-297.874044 lf=-504.5034
6 1.748148 -0.026810 0.599316
7 1.534257 0.013601 -0.550835
7 -0.996097 0.002319 0.190525
8 -0.880001 1.112977 -0.058713
8 -0.902000 -1.106800 -0.075502

ts08/16 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.886323936 HF+ZPE=-297.871989 lf=-622.5602
6 0.170384 0.265371 0.348584
7 -0.930235 -0.325087 -0.095948
7 1.278853 0.690249 -0.161362
8 1.636921 -0.578460 -0.004639
8 -2.069749 0.059916 -0.031653

ts14/P4 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.885120831 HF+ZPE=-297.870283 lf=-442.5590
6 -0.825601 -0.107017 0.117543
7 0.365093 -0.000951 0.711796
7 1.119649 0.804020 -0.237175
8 -1.909185 0.028215 -0.221963
8 1.229237 -0.650637 -0.281488

2-ts13/P1 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.883024341 HF+ZPE=-297.867780 lf=-859.8223
6 0.140795 0.000000 -0.414002
7 -1.387594 0.000000 -0.508004
7 -1.282594 0.000001 0.674472
8 1.115409 0.774879 0.082420
8 1.115409 -0.774879 0.082421

2-ts01/14 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.881398620 HF+ZPE=-297.866700 lf=-1781.1276
6 -0.637634 0.119277 0.045969
7 0.295267 1.033757 -0.264502
7 0.788548 -0.034853 0.720486
8 -1.708976 -0.341827 -0.044168
8 1.238864 -0.621672 -0.389295

ts14/P1 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.877920855 HF+ZPE=-297.863369 lf=-685.1719
6 -0.554643 -0.067173 -0.118664
7 1.094614 -0.305680 0.695875
7 0.581829 -0.672336 -0.593234
8 -1.679490 -0.016262 0.179082
8 0.628584 0.922405 -0.179895

ts17/P3 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.873948238 HF+ZPE=-297.858264 lf=-692.9048
6 0.000000 0.648461 0.000000
7 0.074723 1.849739 0.000000
7 -1.026111 -0.407897 0.000000
8 1.021071 -0.423571 0.000000
8 -0.188606 -1.324386 0.000000

ts08/17 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.870823472 HF+ZPE=-297.853795 lf=-530.9772
6 1.103739 0.530203 0.000015
7 -0.103403 1.156510 -0.000012
7 1.016970 -0.734658 0.000026
8 -0.567748 -1.002424 0.000000
8 -1.059428 0.235651 -0.000023

ts02/25 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.869600587 HF+ZPE=-297.852860 lf=-130.0548
6 1.647022 0.723292 0.000115
7 1.042197 -0.305731 -0.000148
7 -0.021002 -1.060265 0.000033
8 -1.016915 0.965243 -0.000059
8 -1.111897 -0.312466 0.000072

ts12/24 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.861974755 HF+ZPE=-297.845785 lf=-391.9038
6 -0.214591 -0.224178 -0.062687
7 -1.513953 -0.351053 0.320465
7 -1.120330 0.748773 -0.273994
8 0.890811 -0.754343 -0.198495
8 1.575130 0.574472 0.204848

ts16/21mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.861484026 HF+ZPE=-297.846176 lf=-547.2271
6 -0.099478 0.034324 0.097007
7 -1.130993 0.842952 0.009569
7 1.114357 -0.069437 0.709933
8 1.233798 0.042164 -0.622014
8 -1.144633 -0.744733 -0.080305

ts11/26 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.860744529 HF+ZPE=-297.847035 lf=-101.7827
6 1.600429 0.760176 0.039076
7 1.841936 -0.479872 0.091435
7 -2.015603 0.055837 -0.420421
8 0.439884 -0.174720 -0.285744
8 -1.488246 -0.024381 0.544299

ts17/18 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.855906182 HF+ZPE=-297.839490 lf=-887.5290
6 -1.233593 -0.028984 0.049256
7 -2.346115 0.304003 -0.109092
7 -0.046550 -0.431328 0.290897
8 1.909580 0.539744 0.063589
8 1.109196 -0.406596 -0.259610

ts18/22 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.850964806 HF+ZPE=-297.835564 lf=-778.4202
6 1.113764 -0.008791 0.086273
7 2.210784 -0.178759 -0.251049
7 -0.106238 0.142667 0.635270
8 -0.990623 0.619319 -0.292372
8 -1.686178 -0.581146 -0.108526

ts17/22 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF= -297.877579740 HF+ZPE=-297.830701 lf= -559.3959
6 0.977325 -0.058895 -0.042876
7 2.075873 0.262570 0.149792
7 -0.146944 -0.713877 -0.384906
8 -1.205952 0.882247 -0.129250
8 -1.214855 -0.443181 0.367132

uts27/P8 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.846079862 HF+ZPE= -297.8629161 lf=-959.1036
8 2.290145 -0.139411 0.000000
7 1.117550 0.064250 0.000000
6 0.000000 0.470989 0.000000
8 -1.210836 -0.369061 0.000000
7 -2.351046 0.113156 0.000000

1-ts28/29 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.810247166 HF+ZPE=-297.795646 lf=-598.3633
6 2.247956 -0.218176 -0.256813
7 1.121195 0.011879 0.034309
7 -0.059648 0.108428 0.610117
8 -0.942929 0.630239 -0.260026
8 -1.671891 -0.571876 -0.111237

1-ts25/29 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.796588790 HF+ZPE=-297.782175 lf=-971.2675
6 -2.128378 0.301438 -0.137623
7 -0.988077 -0.002594 -0.010247
7 0.067262 -0.683007 0.390020
8 1.252971 0.862042 0.112818
8 1.149026 -0.488220 -0.341903

1-ts22/29 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.791281322 HF+ZPE=-297.777762 lf=-424.4545
6 -1.539256 -0.599226 -0.019574
7 0.262995 -0.106831 0.612027
7 -1.426604 0.576862 -0.182275
8 1.094118 0.752137 -0.080202
8 1.078482 -0.713994 -0.281151

ts08/P6 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.781338945 HF+ZPE=-297.766969 lf=-778.5120
6 -0.999593 0.242620 0.000038
7 -0.297616 1.255152 -0.220240
7 -0.840595 -0.979136 0.220004
8 0.734342 -0.782951 -0.376652
8 1.011288 0.359471 0.376830

ts02/29 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.777641172 HF+ZPE=-297.763470 lf=-738.9161
6 -1.107217 0.815190 -0.134707
7 -1.133040 -0.468904 -0.112742
7 0.037258 -0.835605 0.399935
8 0.714055 0.915469 0.208014
8 1.075167 -0.385415 -0.358278

ts13/30 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.757535564 HF+ZPE=-297.742716 lf=-300.5317
8 1.161870 -0.097422 -0.153391
6 -0.660486 0.177894 0.865476
8 -0.916337 -0.037521 -0.655212
7 0.242555 0.955492 -0.001725
7 0.042966 -0.953752 0.184005

2-ts22/29 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.755788917 HF+ZPE=-297.741011 lf=-518.5003
6 -1.094747 0.000000 0.734034
7 -0.026850 0.000000 -0.269953
7 -1.612424 0.000000 -0.396561
8 1.127713 -0.747388 0.016337
8 1.127713 0.747388 0.016337

2-ts28/29 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.753486655 HF+ZPE=-297.738615 lf=-375.4141
6 -1.300487 0.743628 -0.372625
7 -0.258165 -0.128103 -0.147028
7 -1.359734 -0.380301 0.470832
8 1.498120 0.569521 0.275884
8 0.892907 -0.682388 -0.279744

ts31/P3 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.747815640 HF+ZPE=-297.733389 lf=-532.8609
6 0.848545 -0.033177 0.000009
7 -1.479352 -0.937469 0.000012
7 1.949716 -0.395005 -0.000016
8 -0.594263 -0.154990 0.000006
8 -0.453714 1.345787 -0.000009

2-ts25/29 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.745814787 HF+ZPE=-297.731033 lf=-535.1757
6 1.564087 -0.296278 0.505574
7 1.117959 0.651466 -0.417524
7 0.280628 -0.241780 -0.022976
8 -0.886024 -0.698201 -0.271375
8 -1.510805 0.561934 0.277631

ts08/32 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.720511267 HF+ZPE=-297.706773 lf=-623.4711
6 1.232417 -0.099846 0.538706
7 0.595782 0.702451 -0.471325
7 0.349714 -0.860861 -0.247097
8 -0.997369 -0.619233 0.029691
8 -0.754253 0.832726 0.194898

ts32/P8 mol=C1N2O2
RB3LYP/Aug-CC-pVTZ HF=-297.717750453 HF+ZPE=-297.704528 lf=-792.6588
6 -1.090827 -0.005415 0.653622
7 -0.459935 -0.724321 -0.416682
7 -0.468138 0.718679 -0.418092
8 0.820184 -0.866986 0.119874
8 0.810000 0.875983 0.120337

1-uts01/14 mol=C1N2O2
UB3LYP/Aug-CC-pVTZ HF=-297.902779905 HF+ZPE=-297.887675 lf=-1439.1000
6 0.647033 0.064980 -0.000901
7 -0.278770 1.028687 0.112953
7 -0.637025 -0.505093 0.581521
8 -1.454251 -0.259006 -0.442443
8 1.770297 -0.247873 -0.164546

uts17/P6 mol=C1N2O2
UB3LYP/Aug-CC-pVTZ HF=-297.885312317 HF+ZPE=-297.870679 lf=-462.7865
6 -1.118095 0.195735 0.000003
7 -1.837438 -0.747398 -0.000011
7 -0.302439 1.170189 0.000018
8 1.378205 -0.861029 -0.000014
8 1.332759 0.344285 0.000005

uts18/P6 mol=C1N2O2
UB3LYP/Aug-CC-pVTZ HF=-297.884208476 HF+ZPE=-297.869776 lf=-462.2105
6 1.317115 0.151066 0.000002
7 2.358246 -0.414278 -0.000026
7 0.233158 0.823950 0.000034
8 -2.194735 -0.032783 0.000006
8 -1.060580 -0.438980 -0.000015

uts06/22 mol=C1N2O2
UB3LYP/Aug-CC-pVTZ HF=-297.866569226 HF+ZPE=-297.852706 lf=-1058.8269
6 0.980648 -0.000001 0.055565
7 2.111980 0.000011 -0.156795
7 -0.326828 -0.000019 0.498646
8 -1.148757 0.883027 -0.170391
8 -1.148737 -0.883020 -0.170403

uts28/P10 mol=C1N2O2
UB3LYP/Aug-CC-pVTZ HF=-297.861631095 HF+ZPE=-297.847991 lf=-450.4911
6 -2.342056 -0.450784 0.000018
7 -1.297606 0.143416 0.000004
7 -0.225639 0.783905 -0.000011
8 0.973316 -0.461480 0.000002
8 2.116066 -0.011838 -0.000010

uts23/P8 mol=C1N2O2
UB3LYP/Aug-CC-pVTZ HF=-297.854418296 HF+ZPE=-297.839435 lf=-881.6966
6 0.350291 1.384058 0.000001
7 0.700831 0.124941 0.000000
7 -0.874252 0.327420 0.000000
8 1.459441 -0.805821 0.000000
8 -1.570416 -0.628038 0.000000

uts09/29 mol=C1N2O2
UB3LYP/Aug-CC-pVTZ HF=-297.818693674 HF+ZPE=-297.805620 lf=-1033.2850
6 2.149913 0.010223 -0.134341
7 0.980847 -0.003105 -0.012822
7 -0.294759 -0.013451 0.495032
8 -1.111845 0.894858 -0.156149
8 -1.100916 -0.888038 -0.165029

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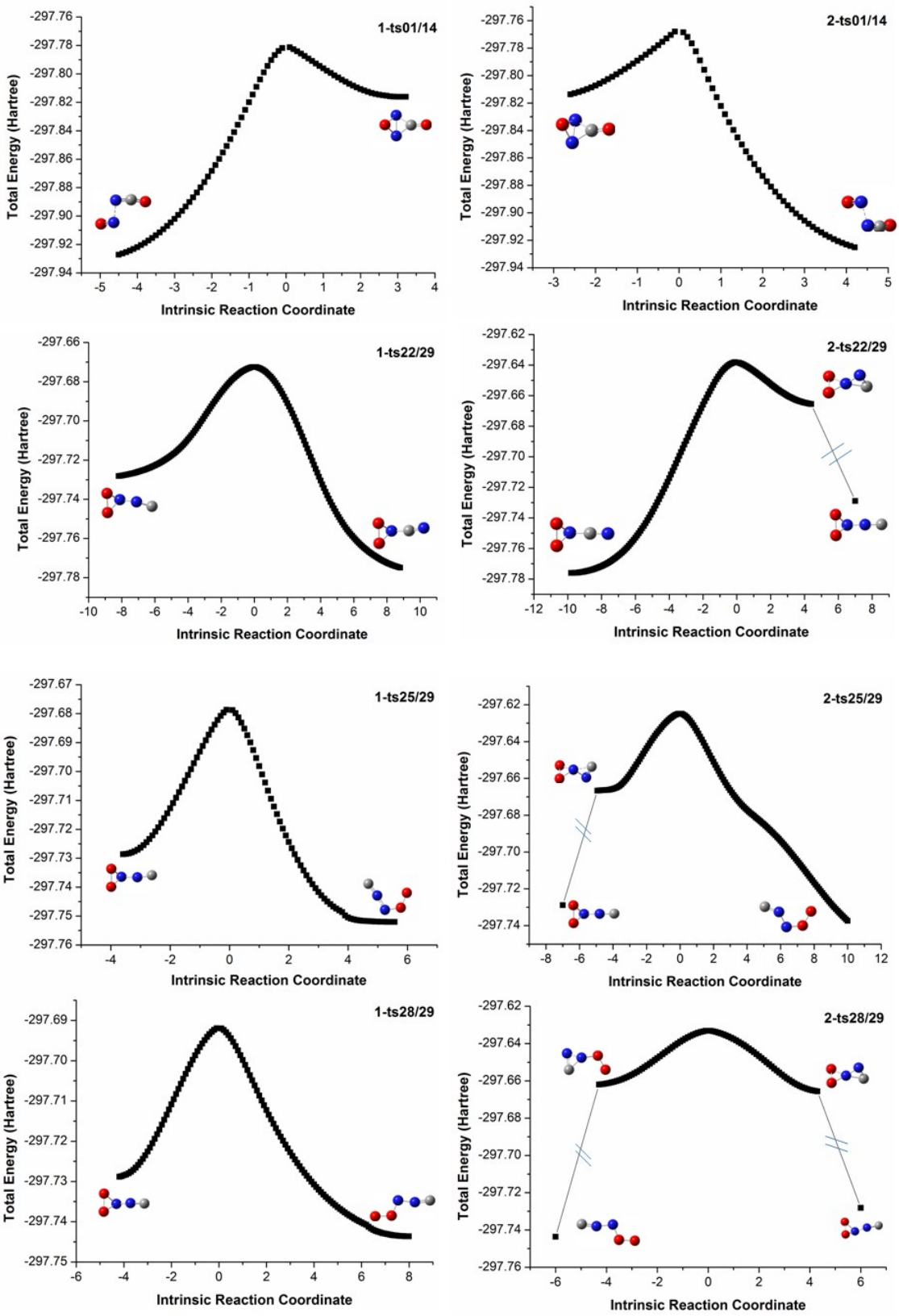
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Total Energy (Hartree)
Intrinsic Reaction Coordinate