Supporting Information for

Chemical reaction mechanism of ZnO grown by DEZn and N_2O in MOCVD

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Geometries Optimized at B3LYP-D3BJ/6-311++G(d,p)

Structure: IM1 **-2122.571337 Hartree**

0 1

Zn	**0.646241**	**-0.547827**	**-0.123600**
C	**2.388175**	**0.347149**	**-0.338001**
C	**2.576242**	**1.599155**	**0.538504**
H	**2.499785**	**0.612542**	**-1.396212**
H	**3.180860**	**-0.380611**	**-0.128680**
H	**3.552854**	**2.070353**	**0.374638**
H	**1.813858**	**2.355670**	**0.331967**
H	**2.511017**	**1.361619**	**1.605062**
C	**-1.072315**	**-1.494576**	**0.099525**
C	**-0.968310**	**-3.026949**	**0.209103**
H	**-1.721385**	**-1.229796**	**-0.744921**
H	**-1.570645**	**-1.096071**	**0.992467**
H	**-1.950456**	**-3.498915**	**0.331168**
H	**-0.510052**	**-3.466641**	**-0.682113**
H	**-0.357910**	**-3.3312820**	**1.064897**
N	**-3.196399**	**1.604708**	**0.105349**
N	**-2.090788**	**1.741300**	**-0.040541**
O	**-0.920950**	**1.883401**	**-0.193591**

Structure: TS1 **-2122.509485 Hartree**

0 1

Zn	**0.378679**	**0.066259**	**-0.070689**
C	**-0.428322**	**1.931252**	**-0.621740**
C	**-0.804108**	**2.769545**	**0.585126**
H	**-1.198405**	**1.891272**	**-1.384197**
H	**0.521587**	**2.236922**	**-1.082654**
H	**-0.954625**	**3.819776**	**0.298751**
H	**-1.733123**	**2.412612**	**1.032262**
H	**-0.031090**	**2.759984**	**1.359654**
C	**1.882679**	**-1.127300**	**0.378878**
C	**3.270883**	**-0.666090**	**-0.096317**
H	**1.648096**	**-2.112775**	**-0.041251**
H	**1.883156**	**-1.261006**	**1.466820**
H	**4.056277**	**-1.377883**	**0.184268**
H	**3.311821**	**-0.555527**	**-1.184153**
H	**3.545603**	**0.301533**	**0.334359**
N	**-2.350973**	**-2.486816**	**0.038304**
N	**-2.375863**	**-1.373107**	**0.072191**
O	**-1.606074**	**-0.065956**	**-0.139044**

Structure: IM2 **-2122.680996 Hartree**

0 1

Zn	**-0.349686**	**0.172464**	**-0.078615**
C	**1.285075**	**-2.203562**	**-0.301448**
C	**0.187485**	**-2.997202**	**0.402772**
H	**2.260338**	**-2.495759**	**0.110318**
H	**1.298554**	**-2.472695**	**-1.368587**
H	**0.344491**	**-4.075351**	**0.294146**
H	**0.167477**	**-2.759495**	**1.470486**
H	**-0.796359**	**-2.761642**	**-0.021695**
C	**-1.922307**	**1.318218**	**0.023446**
C	**-3.268953**	**0.575987**	**0.030804**
H	**-1.874389**	**2.013155**	**-0.821299**
H	**-1.818466**	**1.929008**	**0.926308**
H	**-4.110477**	**1.275259**	**0.093291**
H	**-3.411158**	**-0.018756**	**-0.876014**
H	**-3.353229**	**-0.106592**	**0.881195**
N	**1.947305**	**2.101035**	**0.123761**
N	**3.028674**	**2.270602**	**0.155948**
O	**1.158018**	**-0.807894**	**-0.152637**

Structure: IM3 **-2013.117045 Hartree**

0 1

Zn	**-0.324744**	**-0.501682**	**-0.014313**
C	**2.535573**	**-0.055012**	**0.181237**
C	**2.315380**	**1.435756**	**-0.061502**
H	**3.391211**	**-0.394764**	**-0.417210**
H	**2.802922**	**-0.215268**	**1.236638**
H	**3.211262**	**2.015024**	**0.1849170**
H	**2.065356**	**1.620465**	**-1.110382**
H	**1.494704**	**1.813703**	**0.560705**
C	**-2.257095**	**-0.266302**	**0.069586**
C	**-2.724877**	**1.197401**	**-0.002073**
H	**-2.607288**	**-0.733568**	**0.995366**
H	**-2.693300**	**-0.846159**	**-0.750189**
H	**-3.817225**	**1.268384**	**0.048512**
H	**-2.324678**	**1.794346**	**0.822287**
H	**-2.412665**	**1.680056**	**-0.932334**
O	**1.427267**	**-0.852851**	**-0.166550**

Structure: IM4 **-2197.847108 Hartree**

0 1

Zn	**0.606187**	**-0.361106**	**-0.336092**
C	**-2.053600**	**-1.530783**	**-0.234753**
C	**-1.611585**	**-2.625328**	**0.732622**
H	**-2.143144**	**-1.953379**	**-1.247081**
H	**-3.054642**	**-1.180038**	**0.049744**
H	**-2.323525**	**-3.457119**	**0.740965**
H	**-0.632981**	**-3.027428**	**0.444455**
H	**-1.532976**	**-2.228483**	**1.748652**
C	**2.549559**	**-0.244202**	**-0.433592**
C	**3.219294**	**0.243586**	**0.862562**
H	**2.786952**	**0.432459**	**-1.261080**
H	**2.938872**	**-1.226368**	**-0.719033**
H	**4.306597**	**0.317795**	**0.745715**
H	**2.857485**	**1.231759**	**1.159478**
H	**3.030303**	**-0.435613**	**1.698761**
O	**-1.197503**	**-0.411147**	**-0.237787**
N	**-1.324788**	**2.299260**	**0.145956**
N	**-2.433731**	**2.409968**	**0.264346**
O	**-0.143861**	**2.203067**	**0.023919**

Structure: TS2 **-2197.776224 Hartree**

0 1

Zn	**0.256649**	**-0.525686**	**-0.377204**
C	**-2.585098**	**-0.952302**	**-0.161835**
C	**-2.589547**	**-0.361339**	**1.245321**
H	**-3.260148**	**-1.817578**	**-0.191343**
H	**-2.989289**	**-0.211442**	**-0.868491**
H	**-3.599746**	**-0.068811**	**1.549920**
H	**-2.209578**	**-1.089650**	**1.967396**
H	**-1.957505**	**0.533474**	**1.294956**
C	**2.323637**	**-0.691381**	**-0.290699**
C	**2.859273**	**-0.735969**	**1.125527**
H	**2.829004**	**0.019741**	**-0.933865**
H	**2.296031**	**-1.675278**	**-0.779308**
H	**3.904264**	**-1.075129**	**1.125634**
H	**2.831576**	**0.252957**	**1.584420**
H	**2.299967**	**-1.425298**	**1.763814**
O	**-1.312250**	**-1.393260**	**-0.581928**
N	**0.136558**	**2.603555**	**-0.037527**
N	**-0.874960**	**3.063714**	**-0.068565**
O	**0.971648**	**1.281095**	**-0.163603**

Structure: IM5 **-2197.941368 Hartree**

0 1

Zn	**0.173182**	**-0.246149**	**-0.423874**
C	**-2.539812**	**-1.014553**	**-0.259222**
C	**-2.533977**	**-1.163249**	**1.258273**
H	**-3.211734**	**-1.762299**	**-0.697641**
H	**-2.942644**	**-0.026859**	**-0.530609**
H	**-3.542427**	**-1.052454**	**1.669865**
H	**-2.148799**	**-2.145289**	**1.544319**
H	**-1.899864**	**-0.398350**	**1.723056**
C	**2.953857**	**0.220132**	**0.006863**
C	**3.037855**	**-1.069341**	**0.815650**
H	**3.551982**	**0.997603**	**0.497838**
H	**3.392057**	**0.058925**	**-0.988665**
H	**4.074671**	**-1.405024**	**0.918362**
H	**2.623013**	**-0.923009**	**1.816871**
H	**2.478382**	**-1.875515**	**0.324257**
O	**-1.266026**	**-1.218750**	**-0.841466**
N	**-1.197014**	**3.246503**	**0.342367**
N	**-1.096263**	**2.182297**	**0.105831**
O	**1.637938**	**0.728400**	**-0.112059**

Structure: IM6 **-2088.376208 Hartree**

0 1

Zn	**0.000000**	**-0.634729**	**0.000001**
C	**-2.749599**	**0.096076**	**-0.119588**
C	**-2.371621**	**1.572281**	**-0.080173**
H	**-3.635740**	**-0.070518**	**0.504565**
H	**-3.021122**	**-0.187818**	**-1.146366**
H	**-3.197124**	**2.201108**	**-0.428425**
H	**-2.113767**	**1.875882**	**0.938184**
H	**-1.509438**	**1.771641**	**-0.729161**
C	**2.749599**	**0.096076**	**0.119586**
C	**2.371621**	**1.572281**	**0.080173**
H	**3.635739**	**-0.070517**	**-0.504569**
H	**3.021124**	**-0.187820**	**1.146363**
H	**3.197125**	**2.201107**	**0.428425**
H	**2.113765**	**1.875884**	**-0.938182**
H	**1.509440**	**1.771640**	**0.729164**
O	**-1.735829**	**-0.759937**	**0.376608**
O	**1.735828**	**-0.759937**	**-0.376609**

Structure: TS3 **-2088.374458 Hartree**

0 1

Zn	**-0.131815**	**-0.544841**	**-0.026218**
C	**2.608692**	**0.103094**	**0.550107**
C	**3.473798**	**1.012446**	**-0.310610**
H	**3.232676**	**-0.669726**	**1.018252**
H	**2.160244**	**0.686505**	**1.366395**
H	**3.928054**	**0.440241**	**-1.122910**
H	**2.873337**	**1.812949**	**-0.751578**
H	**4.272492**	**1.465861**	**0.285578**
O	**1.627574**	**-0.541850**	**-0.252446**
O	**-1.887222**	**-0.768784**	**0.163050**
C	**-2.882658**	**0.159995**	**-0.228999**
H	**-3.057560**	**0.098472**	**-1.312516**
H	**-3.811879**	**-0.148732**	**0.264660**
C	**-2.557677**	**1.598518**	**0.156101**
H	**-3.371099**	**2.275844**	**-0.122635**
H	**-2.396142**	**1.680379**	**1.234481**
H	**-1.651410**	**1.944177**	**-0.357617**

Structure: IM7 **-2088.375154 Hartree**

0 1

Zn	**-0.142579**	**-0.429297**	**0.007229**
C	**2.512829**	**0.566299**	**0.390570**
C	**3.903222**	**0.366336**	**-0.191734**
H	**2.527970**	**0.341077**	**1.466638**
H	**2.217269**	**1.620123**	**0.284362**
H	**4.217833**	**-0.673397**	**-0.074580**
H	**3.906756**	**0.606893**	**-1.257555**
H	**4.629722**	**1.010297**	**0.314269**
O	**1.603497**	**-0.287328**	**-0.293530**
O	**-1.857881**	**-0.808338**	**0.293504**
C	**-2.961159**	**-0.058953**	**-0.183883**
H	**-3.161893**	**-0.303693**	**-1.236586**
H	**-3.835115**	**-0.383034**	**0.393787**
C	**-2.784407**	**1.447532**	**-0.033575**
H	**-3.675826**	**1.985837**	**-0.370796**
H	**-2.598772**	**1.710240**	**1.011535**
H	**-1.938404**	**1.802614**	**-0.636013**

Structure: TS4 **-2088.279394 Hartree**

0 1

Zn	**-0.164757**	**-0.376177**	**0.005865**
C	**2.969071**	**0.640036**	**0.593429**
C	**3.911503**	**0.187210**	**-0.384842**
H	**2.931411**	**0.159432**	**1.565996**
H	**2.667318**	**1.682541**	**0.606883**
H	**2.576082**	**-0.339169**	**-0.849984**
H	**4.312165**	**0.913907**	**-1.083540**
H	**4.578498**	**-0.624512**	**-0.114606**
O	**1.612493**	**-0.095908**	**-0.208797**
O	**-1.869172**	**-0.813280**	**0.317056**
C	**-3.014529**	**-0.140224**	**-0.173077**
H	**-3.210511**	**-0.429221**	**-1.215476**
H	**-3.866020**	**-0.491649**	**0.422286**
C	**-2.918533**	**1.377903**	**-0.072766**
H	**-3.841261**	**1.855469**	**-0.417367**
H	**-2.738406**	**1.683787**	**0.961499**
H	**-2.098191**	**1.758682**	**-0.694180**

Structure: IM8 **-2088.358796 Hartree**

0 1

Zn	**-0.281490**	**0.265032**	**0.357964**
C	**3.918124**	**-0.807322**	**0.220789**
C	**4.019220**	**-0.284734**	**-0.998658**
H	**3.506198**	**-1.797808**	**0.384193**
H	**4.248601**	**-0.267497**	**1.101744**
H	**1.984509**	**0.741831**	**-0.021599**
H	**4.436020**	**0.703263**	**-1.162796**
H	**3.692777**	**-0.826498**	**-1.880116**
O	**1.189685**	**1.249805**	**0.180850**
O	**-1.774773**	**-0.633979**	**0.720261**
C	**-2.820457**	**-0.908237**	**-0.194761**
H	**-2.548004**	**-1.750696**	**-0.846860**
H	**-3.683072**	**-1.230554**	**0.400857**
C	**-3.213162**	**0.292539**	**-1.047411**
H	**-4.052465**	**0.050597**	**-1.707210**
H	**-3.504917**	**1.134566**	**-0.413944**
H	**-2.376571**	**0.611748**	**-1.681825**

Structure: IM9 **-2009.734049 Hartree**

0 1

Zn	**-0.752913**	**-0.143408**	**-0.012708**
H	**-2.953324**	**0.341243**	**0.715546**
O	**-2.379747**	**0.584796**	**-0.016330**
O	**0.829526**	**-0.929019**	**-0.214417**
C	**2.074061**	**-0.413133**	**0.225786**
H	**2.203089**	**-0.594185**	**1.302360**
H	**2.851400**	**-0.987726**	**-0.291768**
C	**2.256378**	**1.070432**	**-0.070561**
H	**3.245951**	**1.416889**	**0.243779**
H	**2.147853**	**1.264912**	**-1.140975**
H	**1.511544**	**1.671085**	**0.466948**

Structure: TS5 **-2009.732378 Hartree**

0 1

Zn	**0.874690**	**0.046372**	**-0.065166**
C	**-1.936050**	**0.445700**	**0.397009**
C	**-3.008180**	**-0.555824**	**-0.006806**
H	**-2.335970**	**1.466111**	**0.331461**
H	**-1.654359**	**0.280821**	**1.446161**
H	**-3.298959**	**-0.396180**	**-1.047709**
H	**-2.636845**	**-1.579589**	**0.090744**
H	**-3.896528**	**-0.447168**	**0.623986**
O	**-0.820640**	**0.347854**	**-0.481179**
O	**2.578502**	**-0.396497**	**0.207722**
H	**3.184455**	**0.334735**	**0.356763**

Structure: IM10 **-2009.733083 Hartree**

0 1

Zn	**0.905035**	**-0.058567**	**-0.012876**
C	**-1.889829**	**0.564184**	**-0.004890**
C	**-3.220137**	**-0.171777**	**0.014097**
H	**-1.836749**	**1.207263**	**-0.895016**
H	**-1.818515**	**1.220259**	**0.874230**
H	**-3.312435**	**-0.812681**	**-0.865959**
H	**-3.293585**	**-0.800351**	**0.904699**
H	**-4.053265**	**0.538373**	**0.018099**
O	**-0.837981**	**-0.394595**	**-0.008819**
O	**2.671021**	**0.127383**	**0.132396**
H	**3.158993**	**0.187401**	**-0.693624**

Structure: TS6 **-2009.637454 Hartree**

0 1

Zn	**-0.945176**	**-0.056523**	**0.025163**
C	**2.316882**	**0.750670**	**0.002908**
C	**3.173139**	**-0.393416**	**-0.054506**
H	**2.226199**	**1.310993**	**0.927666**
H	**2.146669**	**1.342112**	**-0.890877**
H	**1.786331**	**-0.955587**	**-0.005280**
H	**3.651215**	**-0.627802**	**-0.999616**
H	**3.731614**	**-0.659929**	**0.836440**
O	**0.855681**	**-0.216429**	**0.055114**
O	**-2.716490**	**0.101983**	**-0.173293**
H	**-3.240400**	**0.057930**	**0.631780**

Structure: IM11 **-2009.716829 Hartree**

0 1

Zn	**1.083114**	**0.140042**	**0.005299**
C	**-3.430079**	**-0.039121**	**-0.562309**
C	**-3.088354**	**-0.806099**	**0.469912**
H	**-3.335131**	**-0.385338**	**-1.586084**
H	**-3.822861**	**0.962445**	**-0.422961**
H	**-1.179430**	**0.749437**	**0.097047**
H	**-3.188549**	**-0.462021**	**1.493780**
H	**-2.701958**	**-1.810475**	**0.330508**
O	**-0.331607**	**1.194616**	**0.215723**
O	**2.557227**	**-0.860142**	**-0.045742**
H	**3.040159**	**-0.859788**	**-0.876744**

Structure: P **-1931.092015 Hartree**

0 1

Zn	**-0.000001**	**0.000013**	**0.012744**
H	**-2.259220**	**0.523894**	**0.482487**
O	**-1.775358**	**-0.083351**	**-0.084195**
O	**1.775349**	**0.083233**	**-0.084287**
H	**2.259313**	**-0.523334**	**0.483047**