Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Proton Transfer Mechanism along the PO_4 Anion Chain in the $[Zn(HPO_4)(H_2PO_4)]^{2-}$ Coordination Polymer

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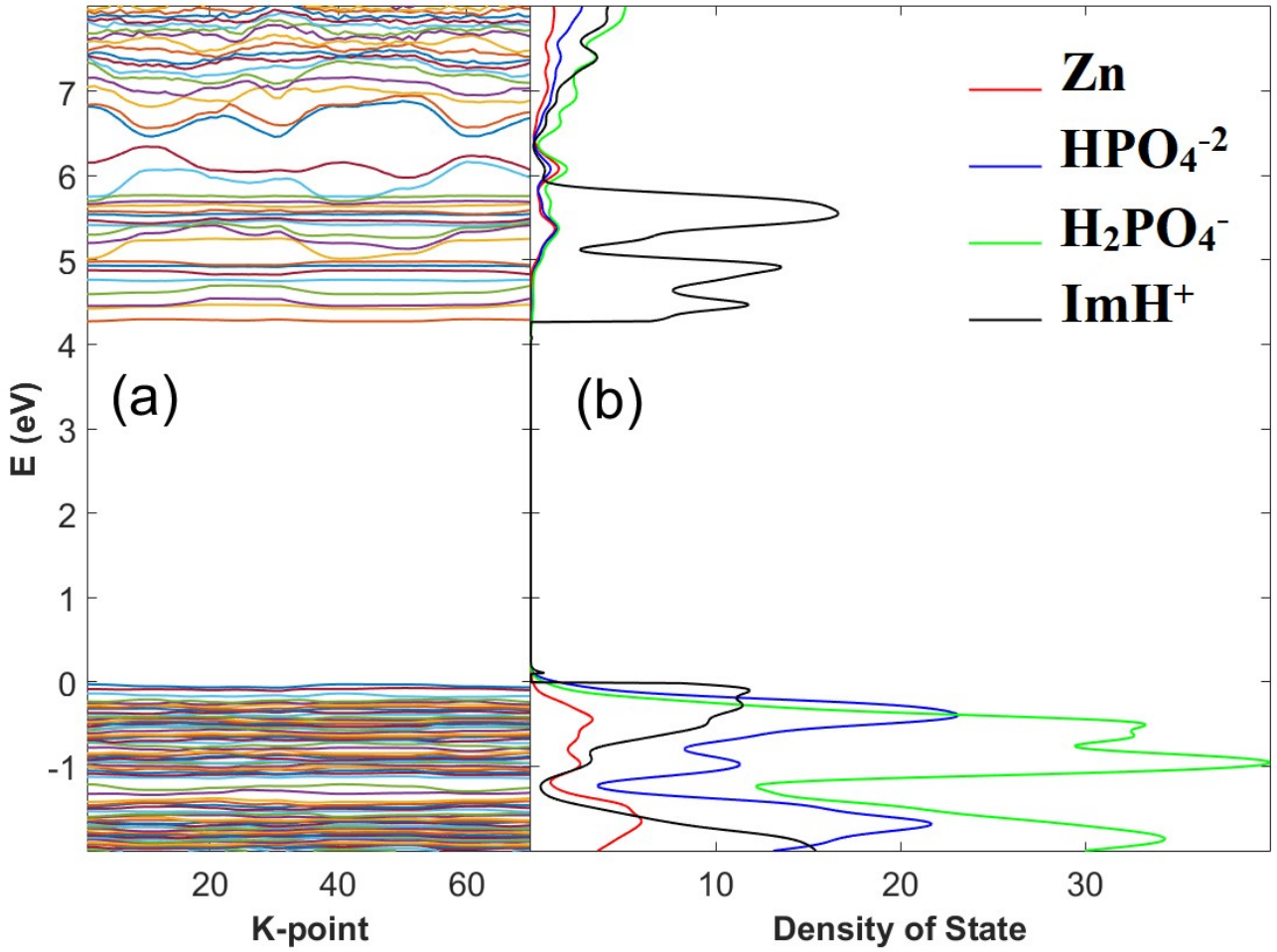

Figure s1: (a) Band structure of Zn coordination polymers (CPs), (b) PDOS of Zn^{2+}, HPO_4^{2-}, $H_2PO_4^-$, and ImH^+ given by PBE calculations

Position of atoms in initial structure for $M^{(1)}$ case:

Zn	16.27948000	7.04311800	5.08939900
Zn	25.35612700	7.04309700	5.08939900
Zn	20.66713400	3.48896900	5.10362600
P	22.23775200	6.12046700	5.68317900
P	23.73219600	9.11868200	3.63849700
P	18.58441700	8.17278600	6.73955000
P	17.68282000	4.23333500	4.41870600
O	22.24850200	4.79566800	4.86906600
O	17.08590900	7.87907600	6.66200900
O	26.39583800	6.87162800	6.80595600
O	21.45592000	5.78282600	7.01937300
O	19.50009200	7.25440000	7.46499800
O	23.68175400	6.55053300	6.01576400
O	14.75139200	5.80628500	5.58858100
O	21.51834400	7.27261500	4.94327000
O	18.73250200	9.64728200	7.33001100
O	19.03947300	8.28518300	5.18738800
O	23.84891200	10.34766100	2.67688100
O	25.13026500	8.65405200	4.02147700
O	16.73540700	8.52616800	3.73544100
O	22.87810000	9.56629300	4.86469100
O	22.93237100	8.00784600	2.88366300
O	17.24040400	5.65935300	4.10358800
O	24.99561200	5.33930200	3.97129600
O	21.12765700	3.11311900	7.07445000
O	16.35167800	3.67284400	5.23471000
O	18.86616300	4.19899000	5.40373200
O	17.92017900	3.30141200	3.25146400
O	20.16039700	2.31674800	3.58505300
H	20.65797000	6.39221900	7.25507700
H	17.91093600	10.14322100	7.39564100
H	19.90434900	7.84991800	4.99815200
H	22.24210400	8.88531300	5.19641400
H	22.21307600	7.58560500	3.43325300
H	16.23520500	2.72037000	5.16656100
H	17.66737600	8.70511000	3.97462800
H	16.69835100	8.29962300	2.80106400
H	20.63340300	1.84534500	2.89958900
H	19.19487900	2.62325200	3.29382400
H	21.33210100	4.01550600	7.40082800
H	20.44346600	2.73515200	7.63485400
H	25.80202500	6.62363900	7.52652000
H	27.25541500	7.13670200	7.14299500
H	25.22558000	5.09634300	3.07120500
H	24.12626400	4.95026700	4.21236600
H	15.09367600	4.88942900	5.48039000
H	14.18715300	5.86497400	6.36313000
H	24.72663500	10.71659800	2.53115700

Position of atoms in transition state (ts) structure for $M^{(1)}$ case:

Zn	16.27949200	7.04310300	5.08939900
Zn	25.35611800	7.04308500	5.08939900
Zn	20.66713100	3.48899600	5.10362600
P	22.23286600	6.10795600	5.62723500
P	23.86002700	9.38007500	4.01375900
P	18.62976800	8.23788500	6.58442700
P	17.66578900	4.22297300	4.46449200
O	22.26203300	4.76596100	4.85146200
O	17.14979600	7.87039600	6.63272600
O	27.14583100	7.07739100	6.03936100
O	21.42033900	5.81241500	6.94894300
O	19.58506700	7.43188800	7.40087300
O	23.65868500	6.58000500	5.94450400
O	14.77575000	5.81999000	5.69560600
O	21.48888200	7.24027000	4.85845800
O	18.77966000	9.80078100	6.89973600
O	19.01401300	8.22220500	5.02305700
O	24.01340700	10.63981200	3.08617000
O	25.25165600	8.83690000	4.33323200
O	16.63692100	8.47187000	3.65489400
O	23.17399100	9.86800400	5.35357500
O	22.93848600	8.37999100	3.31871500
O	17.18690800	5.62371800	4.09766100
O	25.02783800	5.32856300	3.97715500
O	21.13698200	3.13318700	7.07865100
O	16.37898200	3.68051700	5.36124900
O	18.88845300	4.25687000	5.40165900
O	17.87027900	3.23332700	3.33862400
O	20.11882000	2.26737800	3.64147500
H	20.66086900	6.46959700	7.19243400
H	18.52921600	10.06766200	7.78993800
H	19.87791400	7.78832400	4.82969100
H	22.34443500	9.44629700	5.61743800
H	22.19015000	7.81126200	3.95197800
H	16.25765300	2.72752700	5.31101900
H	17.56659200	8.70608500	3.83884900
H	16.57679200	8.18039900	2.73948500
H	20.57532900	1.78108700	2.95515800
H	19.14343700	2.56705400	3.36698700
H	21.31633800	4.04065300	7.40168000
H	20.48140700	2.72748800	7.65311700
H	27.50743900	6.42989700	6.65190700
H	27.63917900	7.90206600	6.10388600
H	25.30343600	5.05386100	3.09930300
H	24.15192600	4.94029300	4.19099100
H	15.11840900	4.90142800	5.60946800
H	14.25189500	5.90876400	6.49522000
H	24.87781300	11.06221600	3.05471800

Position of atoms in final structure for $M^{(1)}$ case:

Zn	16.27950600	7.04308900	5.08939900

Zn	25.35614100	7.04310000	5.08939900
Zn	20.66709400	3.48899600	5.10362600
P	22.32058900	6.02931700	5.73412300
P	24.57364100	9.26946300	3.51996700
P	18.60422000	8.19337500	6.73349700
P	17.69184900	4.24846800	4.40807600
O	22.25275300	4.75665400	4.87372300
O	17.11426700	7.87957000	6.65258800
O	26.57082400	6.35186700	6.56394400
O	21.42549300	5.78147300	6.99240700
O	19.53846400	7.26781900	7.43057200
O	23.74608800	6.42904800	6.09283500
O	14.75967200	5.80492200	5.59505800
O	21.61139100	7.25337900	4.97828800
O	18.74492700	9.64571000	7.37112900
O	19.05117200	8.34963600	5.18254700
O	25.07276500	9.55883300	2.04904900
O	25.72121100	8.85497000	4.45868800
O	16.70622700	8.54745600	3.75047900
O	24.03494900	10.69370400	3.98355700
O	23.53744700	8.17853900	3.45824500
O	17.24643900	5.67505600	4.09559500
O	24.82812700	5.72776000	3.55296300
O	21.09230800	3.09519600	7.08283700
O	16.36297400	3.68424400	5.22775600
O	18.87532600	4.22306700	5.39437900
O	17.92858300	3.31644400	3.24325800
O	20.16851900	2.31389700	3.58327100
H	20.62403100	6.43699900	7.21081100
H	17.92595400	10.14642700	7.43574200
H	19.93092900	7.97363900	4.98450100
H	24.08459300	10.89062100	4.92461700
H	22.21048500	7.72108400	4.33725600
H	16.23874600	2.73433300	5.13900900
H	17.63737300	8.74811600	3.96813300
H	16.64934600	8.34483900	2.81149200
H	20.65441700	1.86137000	2.89357100
H	19.21266200	2.62151200	3.28396300
H	21.24892700	3.99025500	7.44468500
H	20.43586000	2.65240700	7.62832100
H	26.10632100	5.96568700	7.31481400
H	27.49264000	6.51450400	6.78026500
H	24.33755900	6.28283200	2.92496300
H	24.20893300	5.04286800	3.85756300
H	15.10309900	4.88789900	5.48709400
H	14.17178400	5.86037200	6.35179000
H	25.62623700	10.33505800	1.91241000

Position of atoms in initial structure for $M^{(2)}$ case:

Zn	16.27965800	7.04302300	5.08944600
Zn	25.35603000	7.04309700	5.08938300
Zn	20.66705200	3.48895900	5.10362100

P	22.28871400	6.07804800	5.62995800
P	24.42662300	9.62863600	3.49758600
P	18.58420100	8.21701700	6.74493900
P	17.62738900	4.19706900	4.98319200
O	21.84406300	4.99353200	4.66037700
O	17.10135200	8.13973700	6.43775500
O	26.96695300	7.67343700	6.16035700
O	21.64546200	5.69572000	7.06407400
O	19.50325000	8.60102900	5.62039900
O	23.79076500	6.13963100	5.80199200
O	14.73152300	6.02292100	5.93876700
O	21.75348500	7.50533900	5.26031400
O	19.08783700	6.76262000	7.28365900
O	18.75882300	9.12923300	8.02497300
O	22.86205700	9.61862100	3.77242400
O	25.10742000	8.90425800	4.67016900
O	15.90141100	8.41321400	3.62423400
O	24.60882600	8.47569900	2.29483900
O	24.91278800	10.91995800	3.01705600
O	17.18486900	5.51858300	4.36325800
O	25.74639300	6.32624700	3.22851400
O	21.56532800	2.98942000	6.88030200
O	16.46402200	3.96709200	6.12854400
O	18.97227400	4.39313000	5.74415000
O	17.66174800	2.98465000	4.09631500
O	19.95620700	2.08531800	3.91183700
H	20.86817900	6.20858400	7.36629300
H	18.88158900	5.96554300	6.74323400
H	19.48723300	9.75782000	7.99181300
H	24.52419400	8.86638100	1.41855700
H	20.79251900	7.87789300	5.36241300
H	16.41606600	3.06255700	6.45526900
H	16.25323600	9.30375000	3.73141200
H	15.81258600	8.20950000	2.68832500
H	20.31444400	1.63860400	3.14351900
H	18.94623600	2.29216300	3.83387400
H	21.71722500	3.81004800	7.38283500
H	21.47742400	2.23321500	7.46434900
H	27.73901700	7.36330600	6.63729200
H	26.99739400	8.62985900	6.01500900
H	25.42861100	7.04240500	2.62189700
H	25.51452600	5.46228000	2.88098100
H	15.05203000	5.11584400	6.11511200
H	14.15983000	6.32638500	6.64835700
H	22.51941600	8.89347800	4.31869000

Position of atoms in transition state structure for $M^{(2)}$ case:

Zn	16.27965100	7.04303300	5.08945200
Zn	25.35610300	7.04306700	5.08940900
Zn	20.66706700	3.48900400	5.10361100
P	22.30977600	6.09414800	5.66129100
P	24.42658900	9.62865000	3.49757100

P	18.58420000	8.21701600	6.74492900
P	17.62734300	4.19703100	4.98319400
O	21.83804600	5.00831900	4.65929100
O	17.10694600	8.26783500	6.34762800
O	27.00890800	7.64311900	6.18461600
O	21.71006300	5.64005600	7.14884500
O	19.58520400	8.59993200	5.63216700
O	23.83796500	6.07815300	5.83825100
O	14.76724400	6.02330200	6.04575300
O	21.75514900	7.52601100	5.36285600
O	19.01347600	6.73524400	7.29333800
O	18.72795100	9.14240800	8.04296300
O	22.83706300	9.53056800	3.74283000
O	25.14366800	8.93863300	4.70083400
O	15.66667700	8.34839700	3.61118200
O	24.70195500	8.45547900	2.27138000
O	24.85750400	10.95756900	3.00191800
O	17.17732900	5.52084100	4.32084900
O	25.80436200	6.32238500	3.21411600
O	21.56352200	2.97142800	6.89816700
O	16.41657700	3.94307200	6.12569600
O	18.96134600	4.43165700	5.79317200
O	17.68211800	2.96140000	4.09647500
O	20.00341000	2.07269700	3.86106900
H	20.90653500	6.13652000	7.43080800
H	18.89781000	5.93283400	6.68901400
H	19.56708600	9.63219700	8.10324900
H	24.70357700	8.88020400	1.39635300
H	20.63410800	8.01531300	5.49011600
H	16.29509500	2.99654900	6.31670000
H	15.92701700	9.28353600	3.65097800
H	15.50721100	8.09921700	2.68671400
H	20.37697800	1.82892100	3.00117700
H	18.98374100	2.28475400	3.79493900
H	21.72626900	3.84839200	7.33827900
H	21.26956700	2.31667300	7.54950800
H	27.90413700	7.29563900	6.31578500
H	27.04434300	8.60023400	5.98784600
H	25.47248100	7.08083500	2.62478800
H	25.43646400	5.48434800	2.89259800
H	15.12769200	5.10520600	6.19328100
H	14.32236600	6.33921900	6.84791000
H	22.53165200	8.80425800	4.33993800

Position of atoms in final structure for $M^{(2)}$ case:

Zn	16.27978800	7.04300000	5.08952000
Zn	25.35608100	7.04305400	5.08940400
Zn	20.66709700	3.48902500	5.10361800
P	22.47686800	5.92805400	5.71869500
P	24.42659300	9.62864900	3.49757400
P	18.58412000	8.21701900	6.74488200
P	17.62727300	4.19705300	4.98316700

O	22.07767100	4.79439900	4.77424200
O	17.49284300	8.44466700	5.72691400
O	27.07819200	7.66174000	5.99477900
O	21.83723300	5.39682600	7.14816200
O	20.00068100	8.68276300	6.35960100
O	23.99211600	5.98142600	5.93342800
O	15.25918400	6.19249500	6.62829300
O	21.87434500	7.29384500	5.42972900
O	18.62471200	6.69325500	7.16266000
O	18.18547800	8.99865200	8.05209900
O	22.87017800	9.37855000	3.72537700
O	25.16154000	8.91375300	4.64680500
O	15.27710000	8.31145200	3.85733800
O	24.78114300	8.60851400	2.22327600
O	24.75193300	11.00335800	3.12380500
O	17.00702400	5.43814500	4.34609800
O	25.55667800	6.31312600	3.18924600
O	21.32097700	2.78241500	6.91199000
O	16.63311000	3.94542600	6.27752300
O	19.02278300	4.55040300	5.58627300
O	17.66505000	2.93326900	4.17902100
O	19.99152300	2.11813600	3.83293900
H	21.86857000	6.03736000	7.86595700
H	18.92794800	5.95060700	6.56773300
H	18.90112700	9.27757200	8.63302700
H	24.78602400	9.07571600	1.38176700
H	20.74220300	8.08767000	5.94278500
H	16.55183400	3.01823300	6.52321600
H	15.61704000	9.21158500	3.80282400
H	14.69709100	8.12750000	3.11346700
H	20.34618300	1.80959300	2.99748100
H	18.98346900	2.27293400	3.79907400
H	21.64960400	3.56338600	7.39416600
H	21.76196900	1.97824600	7.19178100
H	27.88155400	7.34924900	6.41421000
H	27.11404400	8.61057500	5.80735600
H	25.35570700	7.06152900	2.57449700
H	25.13310400	5.50621500	2.88673200
H	15.57120100	5.26763800	6.73615900
H	15.02397000	6.57832800	7.47537700
H	22.58954500	8.66371000	4.32453200

Position of atoms in initial structure for $M^{(3)}$ case:

Zn	16.27951500	7.04308300	5.08940700
Zn	25.35625100	7.04312100	5.08938000
Zn	21.70955400	7.04845500	13.40945700
Zn	20.66713100	3.48897700	5.10365000
P	22.39500900	5.72756700	5.48835700
P	18.54316000	6.28931200	13.96478500
P	24.01317900	8.44466600	2.46970700
P	20.36664500	8.45007900	10.78972900

P	18.72953700	7.81239300	6.97308300
P	17.52716200	4.17866800	4.47142800
O	22.21529300	4.57818400	4.50705000
O	18.82306200	4.84812300	13.25779000
O	17.26883400	7.44985200	6.77936300
O	25.90042400	7.55900600	6.97186300
O	22.38417400	7.20367700	15.30178800
O	21.43709100	5.36399500	6.67262500
O	17.69044800	5.89759200	15.25824700
O	19.66731900	6.80568200	7.62485800
O	23.84625500	6.00704800	5.88663000
O	19.95803700	6.68106700	14.40000400
O	14.74426100	5.91995800	5.81438100
O	21.80627700	7.11300300	4.90400700
O	17.78371200	7.20579100	13.07746400
O	18.83293700	9.18355000	7.71697700
O	19.23460800	8.07791700	5.44517800
O	22.88789500	7.53435100	1.80488800
O	20.70976100	9.26535200	9.59333600
O	24.02312000	8.15662400	3.99228600
O	21.37303400	8.32970300	11.95781900
O	16.91826500	8.74896600	4.16379400
O	25.32456300	8.17578000	1.81003800
O	18.94547000	8.86149400	11.32259000
O	23.51939200	9.95090400	2.33696000
O	20.22998900	6.87206300	10.34318500
O	17.10337100	5.59778700	4.09266500
O	26.65481800	6.97003700	3.59875600
O	21.43970100	5.38107000	12.23653400
O	20.31163200	2.39520700	6.81784000
O	16.23845800	3.68877800	5.40710000
O	18.77629200	4.16983700	5.39212800
O	17.67097000	3.16496100	3.36505700
O	20.05765400	2.32677800	3.55647500
H	20.70028300	6.00235100	7.07151300
H	16.91958000	6.45919300	15.39067600
H	19.56116700	9.31655500	8.39430500
H	20.14698900	7.81122800	5.23262500
H	22.53767900	7.73107100	4.64850300
H	18.48281500	8.29236900	11.98278400
H	23.70480000	10.37857600	1.49349800
H	19.95017900	6.75024900	9.41050800
H	15.97758900	2.78662900	5.19498900
H	26.41038700	8.28654500	7.33812400
H	25.23594000	7.25592000	7.60406500
H	26.27576100	7.42987400	2.76163200
H	27.41206000	6.41807900	3.39612600
H	19.07598000	2.55949700	3.35106500
H	20.53992100	2.15354800	2.74580100
H	19.45854900	2.78857900	7.05907000
H	20.26308000	1.43874500	6.89416000
H	15.05378200	4.99227600	5.69455600

H	14.46173600	6.04060400	6.72568600
H	17.87813000	8.74336700	4.36219700
H	16.57951300	9.64233700	4.26350400
H	20.71467700	4.84651000	12.60362900
H	21.10442500	5.74125300	11.38196400
H	23.03113100	7.72037700	15.78698100
H	21.56772100	7.07912700	15.81203000
H	18.05115800	4.44892000	12.84384100
H	22.03980700	7.45386500	2.25600400

Position of atoms in transition state structure for $M^{(3)}$ case:

Zn	16.27945300	7.04308600	5.08937900
Zn	25.35623100	7.04311600	5.08939000
Zn	21.70958500	7.04843700	13.40948700
Zn	20.66715000	3.48896500	5.10365100
P	22.39503200	5.72754400	5.48837800
P	18.54313900	6.28930900	13.96477800
P	24.01318600	8.44468400	2.46967800
P	20.36666000	8.45010700	10.78972800
P	18.76641400	7.84017400	7.01004900
P	17.52716900	4.17867800	4.47143100
O	22.18620500	4.65678200	4.39642600
O	18.82946700	4.82563400	13.31563700
O	17.30318400	7.50251800	6.78161800
O	25.90384900	7.36098600	7.01609400
O	22.42497500	7.24240000	15.27520500
O	21.44716500	5.32434900	6.62162400
O	17.67444600	5.94387900	15.25641000
O	19.59558100	6.66557900	7.68696000
O	23.87618500	5.96931900	5.85175000
O	19.95862900	6.70201800	14.38764800
O	14.74569900	5.92110300	5.79713100
O	21.84650600	7.17442800	4.98041000
O	17.80864600	7.18659000	13.03401900
O	19.02302800	9.07846400	7.84429400
O	19.34208500	8.00500400	5.51301300
O	22.55049100	8.01469800	1.99641500
O	20.69323300	9.31023900	9.58312500
O	24.12070500	8.23837100	3.99552300
O	21.40276100	8.35308100	11.91634000
O	17.04033900	8.67872500	4.12594800
O	25.09427800	7.72068300	1.72336700
O	18.95646500	8.86542800	11.31709800
O	23.97869400	10.01242300	2.24697700
O	20.25607400	6.90333700	10.30719200
O	17.13868100	5.61352300	4.11418200
O	26.57439900	6.74799700	3.54703300
O	21.43592200	5.39023200	12.23806700
O	20.24548000	2.21986600	6.68944100
O	16.19663700	3.69463300	5.36100300
O	18.74227300	4.11212600	5.42624900
O	17.66826500	3.19094700	3.34167100

O	20.06202300	2.34367900	3.52497700
H	20.28801100	6.09004200	7.18675500
H	16.92575400	6.53438700	15.39181400
H	19.90650400	9.26825100	8.70969800
H	20.27998400	7.78239700	5.31380900
H	22.54006700	7.76584800	4.61997000
H	18.47640700	8.28187500	11.96234400
H	23.96909400	10.30985900	1.33103600
H	19.94025800	6.74168800	9.38726200
H	15.91692400	2.80929600	5.10658600
H	26.34164200	8.06409000	7.50179500
H	25.19931800	6.95543400	7.54128100
H	26.13079800	7.09401500	2.69147500
H	27.26370500	6.10840200	3.36171400
H	19.08454700	2.57755000	3.32376400
H	20.55495000	2.26038700	2.70620200
H	19.38078300	2.60662800	6.90218400
H	20.14939800	1.26984600	6.57786800
H	15.05612500	4.99147200	5.67087900
H	14.42667600	6.03075500	6.69719900
H	17.99983400	8.59418100	4.30656700
H	16.78763400	9.60018400	4.22543600
H	20.71468500	4.84582300	12.59943800
H	21.12805100	5.71731800	11.36465800
H	23.13569800	7.69254800	15.73734400
H	21.64457300	7.12875200	15.83893600
H	18.05411400	4.36908900	12.97293100
H	22.40966700	7.07092600	1.85852000

Position of atoms in final structure for $M^{(3)}$ case:

Zn	16.27953300	7.04310300	5.08943600
Zn	25.35614900	7.04310500	5.08937900
Zn	21.70955000	7.04846400	13.40944400
Zn	20.66715600	3.48896800	5.10364400
P	22.39506600	5.72753400	5.48842300
P	18.54315300	6.28930300	13.96478900
P	24.01322800	8.44471400	2.46964500
P	20.36663500	8.45006900	10.78970900
P	18.72341100	7.81659600	6.99284700
P	17.52713500	4.17866700	4.47143100
O	22.18600400	4.66961300	4.38187900
O	18.82547000	4.82068700	13.32714000
O	17.25092900	7.49369300	6.78054100
O	25.91722800	7.30152700	7.02156700
O	22.45610200	7.22013200	15.26129100
O	21.45526500	5.30219500	6.61786500
O	17.66625600	5.96102200	15.25292400
O	19.51124900	6.59460600	7.67504700
O	23.87824500	5.96951400	5.85249800
O	19.96051300	6.70092800	14.38483100
O	14.72902600	5.91535300	5.76818200

O	21.84496100	7.17885400	4.99515500
O	17.82174000	7.18392200	13.01936500
O	19.04382100	9.02992700	7.81175700
O	19.29016200	7.91457300	5.48130600
O	22.55043200	8.00634200	2.00457800
O	20.74023000	9.41918500	9.65425700
O	24.12709900	8.24549900	3.99640700
O	21.39665200	8.34499000	11.91204900
O	17.03492200	8.66609500	4.09499100
O	25.09593700	7.72360300	1.72279300
O	18.94927800	8.84280100	11.29531900
O	23.97011200	10.01108800	2.23769700
O	20.30145500	6.95576300	10.20584600
O	17.13321300	5.60916900	4.10824300
O	26.57664700	6.75162300	3.54676400
O	21.41853300	5.40931000	12.20946800
O	20.22365600	2.20313100	6.67458400
O	16.19705000	3.68818100	5.35802900
O	18.74139200	4.11536000	5.42787200
O	17.67425200	3.18686000	3.34444200
O	20.06249900	2.34181500	3.52681600
H	20.19326100	6.03785500	7.17299600
H	16.92143400	6.55751100	15.38435800
H	20.08661400	9.39767700	8.85311100
H	20.23919300	7.73477400	5.29982200
H	22.53482500	7.77439900	4.63670700
H	18.46151900	8.25373500	11.93640000
H	23.95884100	10.30247500	1.31987400
H	19.94493400	6.79876900	9.28906000
H	15.91953100	2.80422500	5.09658000
H	26.36148800	7.97990800	7.53520900
H	25.20672800	6.87984800	7.52628700
H	26.13202600	7.09844800	2.69242900
H	27.25866300	6.10483700	3.35951200
H	19.08294700	2.57929900	3.32749300
H	20.55532400	2.27065300	2.70676700
H	19.36311600	2.60420700	6.87975100
H	20.10365800	1.26075200	6.52569200
H	15.04444700	4.98810200	5.64214000
H	14.41616200	6.02169800	6.67086300
H	17.99399600	8.55446700	4.26358500
H	16.80598000	9.58919200	4.23104500
H	20.69066900	4.86219400	12.55360000
H	21.15004600	5.71880300	11.31978300
H	23.20279300	7.61781700	15.71499400
H	21.69750500	7.10217000	15.85229200
H	18.04772500	4.35079000	13.00825400
H	22.40258300	7.05893800	1.90212000

Position of atoms in initial structure for $R^{(1)}$ case:

Zn	16.27955200	7.04306500	5.08944200
Zn	25.35591100	7.04317100	5.08933000

Zn	20.66712600	3.48902400	5.10364800
P	22.78072400	5.87426200	6.15117900
P	24.42454500	9.62750100	3.49668100
P	19.07580100	7.77076200	6.80622200
P	17.54677600	4.12449300	5.25218100
O	22.18951800	4.91884000	5.11941200
O	17.63364200	7.68983400	6.35518700
O	27.06780900	6.31530000	5.90218500
O	22.14052900	5.49773500	7.57808500
O	20.07923800	8.27230900	5.79620700
O	24.29830000	5.84248100	6.27929500
O	14.88345700	6.26645300	6.36273400
O	22.43611700	7.36834400	5.81794500
O	19.55758100	6.34330300	7.35288300
O	19.11543700	8.67984400	8.11722800
O	25.28060800	10.51121000	2.47753500
O	25.40566400	8.86827700	4.40281300
O	15.95119000	8.34213400	3.62197300
O	23.69667000	10.67426400	4.46701000
O	23.44641800	8.80347200	2.72076300
O	17.06280000	5.34351800	4.47071100
O	24.30007100	6.35354400	3.42864400
O	21.47063900	2.86290700	6.92361200
O	16.48039900	4.11902200	6.52419600
O	18.95269400	4.36407800	5.89415200
O	17.49273600	2.77525600	4.59551500
O	19.75464300	1.64733000	4.86359500
H	21.24721300	5.87980300	7.73242700
H	19.22244500	5.54163600	6.82259600
H	22.83249900	10.97191000	4.16619200
H	21.48871600	7.73757400	5.75331600
H	16.41789000	3.26311300	6.95973000
H	16.73319000	8.57337800	2.99777300
H	15.26975900	9.01525700	3.57768400
H	20.00517100	0.85486800	4.38689600
H	18.78355900	1.88516000	4.71039000
H	21.83004000	3.58257200	7.46900700
H	20.99359200	2.23195600	7.46788100
H	26.92596800	5.65302900	6.58757600
H	27.98896700	6.58323700	5.86485900
H	23.87774700	7.11819600	2.96827300
H	23.65479500	5.64433300	3.55622800
H	15.21903800	5.35775800	6.53323100
H	14.70650100	6.69217200	7.20649200
H	19.83154200	9.32183700	8.13548900
N	20.18952700	4.16210400	3.15359300
N	19.47634200	5.75568900	1.84003500
N	19.72253300	9.08312400	0.75378700
N	18.09106800	8.84449800	2.19765900
C	18.91148600	4.59287100	1.37417900
C	19.36102700	3.61137000	2.20240600
C	20.22740500	5.46059100	2.91337100

C	20.32257300	8.99056300	1.99160100
C	18.38268400	8.99958300	0.92329200
C	19.29152100	8.84320700	2.87807700
H	20.20014900	9.23668000	-0.12123200
H	21.39840400	9.01231500	2.12557800
H	19.35119000	8.72700500	3.95190900
H	17.67676900	9.05671700	0.10969800
H	18.24839100	4.57045100	0.52729600
H	19.31800700	6.68762000	1.48851100
H	20.76319400	6.19324600	3.49748000
H	19.11565400	2.56339400	2.20002200
H	26.00654300	11.00603200	2.87169900

Position of atoms in transition state structure for $R^{(1)}$ case:

Zn	16.27955700	7.04304900	5.08945300
Zn	25.35580000	7.04319500	5.08933300
Zn	20.66706900	3.48906300	5.10361200
P	22.80201800	5.85019800	6.16085900
P	24.41890800	9.61702600	3.62705400
P	19.13871600	7.68644200	6.76064900
P	17.51909500	4.10723600	5.24773000
O	22.05998300	4.95553800	5.19368800
O	17.67806400	7.61214800	6.35935700
O	26.98387100	6.61449700	6.25565400
O	22.28387600	5.49644600	7.64446100
O	20.11344400	8.13129500	5.70098200
O	24.32431200	5.72315000	6.13366700
O	14.91061200	6.29314800	6.40974900
O	22.54751400	7.37274800	5.88252400
O	19.61326000	6.27903100	7.36565000
O	19.23987300	8.64778400	8.03483900
O	25.13599100	9.08391200	2.23233000
O	25.22451900	8.93128500	4.72576600
O	15.96627400	8.34750700	3.62683700
O	24.87259200	11.15495300	3.66420300
O	22.96352700	9.41610800	3.50151100
O	17.03392000	5.32721200	4.46541300
O	25.40929200	6.52203700	3.09998000
O	21.46521400	2.84999400	6.93737500
O	16.45108000	4.10690800	6.52092300
O	18.92560400	4.33138700	5.88693000
O	17.45317400	2.75696200	4.59156900
O	19.73295300	1.65662800	4.86544900
H	21.38074900	5.84406900	7.81525600
H	19.26265800	5.48055800	6.84751900
H	24.15264300	11.77861200	3.52674600
H	21.61992100	7.73631700	5.71167500
H	16.37428600	3.24656700	6.94492900
H	16.75215800	8.56110800	2.99353000
H	15.32046700	9.05627200	3.61300200
H	19.97277200	0.85723200	4.39530800
H	18.76116800	1.90100300	4.71045400

H	21.86608900	3.55017200	7.47729600
H	20.96914900	2.24201800	7.49078600
H	26.76332600	5.99995800	6.96489300
H	27.73326700	7.16242900	6.50190300
H	25.34124600	7.29221300	2.49870100
H	25.04472600	5.73040400	2.69797600
H	15.23442100	5.37485400	6.55639500
H	14.82155800	6.72082400	7.26671500
H	19.92645100	9.31761400	7.96287500
N	20.18952300	4.16206700	3.15358100
N	19.27551800	5.78208700	2.00379000
N	19.69988600	9.29218900	0.78260500
N	18.09107100	8.84449600	2.19765400
C	18.78787800	4.61173500	1.47299200
C	19.36448100	3.61457100	2.19692000
C	20.10038500	5.47494700	3.01732400
C	20.29589300	9.20529700	2.02054200
C	18.37470900	9.07504800	0.93102100
C	19.28106700	8.93209000	2.89169300
H	20.16656900	9.50273500	-0.08556600
H	21.35370900	9.33870700	2.20001100
H	19.35256600	8.77632900	3.95953000
H	17.67173100	9.09465100	0.11328500
H	18.08194800	4.59435600	0.66134700
H	18.97542700	6.71858500	1.77555300
H	20.58981200	6.20811700	3.64116100
H	19.21567800	2.55135700	2.11552000
H	25.91624700	9.58855500	1.97725500

Position of atoms in final structure for $R^{(1)}$ case:

Zn	16.27955600	7.04307300	5.08942500
Zn	25.35575600	7.04306500	5.08905500
Zn	20.66721200	3.48903600	5.10373000
P	22.87111700	5.81892400	6.02872600
P	24.44336400	9.62420200	3.53673100
P	19.18861600	7.71913300	6.74183600
P	17.51572700	4.10750600	5.26655700
O	22.21534700	4.83467200	5.07655800
O	17.76872500	7.69202700	6.20213600
O	27.26995400	7.04313900	5.79579200
O	22.19840100	5.64204000	7.47078000
O	20.27167000	8.11893000	5.77997300
O	24.38170900	5.69850200	6.17118900
O	14.95134000	6.31803300	6.45391900
O	22.68515100	7.30678900	5.52582000
O	19.54706100	6.29211800	7.38218300
O	19.19726800	8.68002200	8.01741500
O	24.42942500	8.62594000	2.22691300
O	25.35886500	8.89063900	4.51283200
O	15.89517000	8.22771000	3.53238800
O	25.27389900	10.84217600	2.87426500
O	23.08458500	10.02067200	3.95927400

O	17.00662600	5.31267800	4.47877800
O	24.76311600	6.18888900	3.29890000
O	21.40372300	2.94665600	6.99284400
O	16.47900500	4.12540900	6.56642400
O	18.93323500	4.35843800	5.87514800
O	17.44741300	2.74694100	4.63631600
O	19.73911100	1.65901100	4.88861300
H	21.26757700	5.95642600	7.57072700
H	19.20506800	5.49825700	6.84686200
H	25.01385300	11.71093700	3.19635800
H	21.78210600	7.74765600	5.55073400
H	16.40706100	3.27067600	7.00262200
H	16.64170300	8.46079000	2.88363000
H	15.12114900	8.76810200	3.36429600
H	19.98655500	0.84550200	4.44756600
H	18.76504700	1.88677800	4.73810200
H	21.82442100	3.65938500	7.49855700
H	20.88065100	2.38995000	7.57464900
H	27.66757300	6.43866100	6.42782700
H	27.78457200	7.85331300	5.72689400
H	24.54969600	6.86559100	2.62960900
H	24.08260700	5.50558600	3.33098100
H	15.27578100	5.40311800	6.62174000
H	14.80662100	6.75693300	7.29690700
H	19.90475700	9.33226700	8.00878700
N	20.18956200	4.16214200	3.15359800
N	19.23167800	5.78902800	2.04459400
N	19.92254700	9.77445200	1.43780800
N	18.09106400	8.84449900	2.19766900
C	18.74398900	4.62009700	1.51182100
C	19.34614200	3.61927600	2.21040100
C	20.08400800	5.47602500	3.03349700
C	20.19666300	9.42365700	2.74133600
C	18.65186900	9.41610400	1.15077500
C	19.04411000	8.85213800	3.19517300
H	20.55433600	10.24773600	0.81149700
H	21.14862500	9.62303200	3.22074100
H	18.85019100	8.46009900	4.17688700
H	18.18698800	9.58921400	0.19313500
H	18.02082800	4.60568000	0.7154220
H	18.91654900	6.72595000	1.83043000
H	20.57964100	6.20908600	3.65330000
H	19.20676700	2.55562800	2.11797500
H	24.53976300	9.07940600	1.38578300

Position of atoms in initial structure for $R^{(2)}$ case:

Zn	16.27955000	7.04307000	5.08944200
Zn	25.35594300	7.04315700	5.08935000
Zn	20.66711400	3.48901400	5.10364500
P	22.38188200	6.03436800	5.79535400
P	24.42452600	9.62752200	3.49666500
P	18.58345400	8.21481400	6.74841000

P	17.64931600	4.17661800	4.57791600
O	22.11374600	4.88934200	4.84924600
O	17.13256600	7.74957000	6.76364700
O	27.19192400	6.60544600	5.80155900
O	21.56709100	5.74540500	7.13148000
O	19.08986100	7.64922800	5.33094800
O	23.85051700	6.29302700	6.10397100
O	14.79861400	5.85374200	5.83290200
O	21.75498600	7.40351400	5.24775500
O	19.48442900	7.27258700	7.77201900
O	18.93335600	9.62880300	6.99224400
O	24.83333500	11.15165000	3.33260400
O	25.35023100	8.94509900	4.51738000
O	16.49874600	8.64797000	3.86771700
O	23.00482400	9.64925700	4.32385300
O	24.22935100	8.95491200	2.18909800
O	17.20272000	5.58536300	4.17368400
O	24.64322700	6.42840800	3.25141600
O	21.28289300	3.00337200	7.01076700
O	16.35421500	3.67847600	5.48895300
O	18.87998100	4.20103800	5.52034200
O	17.83760400	3.18371900	3.46257300
O	20.35260800	2.48475500	3.39814200
H	20.77102700	6.30286500	7.34852100
H	19.60494300	7.70867000	8.62366200
H	22.25048400	10.05841700	3.87081700
H	20.04802200	7.65327500	5.16911500
H	16.18679600	2.73482700	5.40096800
H	17.41273700	8.81622800	3.52171700
H	16.07828700	9.49896800	4.01558100
H	20.75080100	2.96077700	2.63825800
H	19.35985600	2.53395900	3.27015900
H	21.41697200	3.85343000	7.46635400
H	20.78292700	2.41112600	7.57915500
H	27.43672400	5.86024200	6.35850800
H	27.95617600	7.17154500	5.65242400
H	24.53647000	7.15964200	2.60218000
H	23.88809900	5.82587100	3.16955900
H	15.13515000	4.93387700	5.72962800
H	14.48393900	5.97539100	6.73294500
H	22.32849900	8.18311500	5.07594400
N	20.99597000	4.72782700	1.86953500
N	20.29461600	6.72461000	2.48847100
N	20.28598200	10.90795200	1.81055900
N	18.97748000	9.56698200	2.95968600
C	21.57882500	6.89709900	2.03458700
C	21.99159000	5.64693200	1.64923000
C	19.98766900	5.41415300	2.36167200
C	20.46936800	11.23304400	3.13742500
C	19.38074900	9.91066900	1.75352400
C	19.65284600	10.38707500	3.84085600
H	20.74459000	11.33797800	1.02147600

H	21.09142200	12.05902100	3.44397400
H	19.48489300	10.33540500	4.91117400
H	19.05676100	9.46119600	0.82723400
H	22.07315100	7.85721000	1.99596700
H	19.67599900	7.43364700	2.86562600
H	19.00754200	5.02394700	2.58800600
H	22.92113000	5.36230100	1.17716000
H	25.25621500	11.55945500	4.09618700

Position of atoms in transition state structure for $R^{(2)}$ case:

Zn	16.27955000	7.04307000	5.08944200
Zn	25.35594300	7.04315700	5.08935000
Zn	20.66711400	3.48901400	5.10364500
P	22.38188200	6.03436800	5.79535400
P	24.42452600	9.62752200	3.49666500
P	18.58345400	8.21481400	6.74841000
P	17.64931600	4.17661800	4.57791600
O	22.10170800	4.84530500	4.91500900
O	17.13256600	7.74957000	6.76364700
O	26.92956000	6.29569500	6.10599500
O	21.55062100	5.87672400	7.14851200
O	19.33382500	7.20462600	5.74881300
O	23.85296800	6.26081800	6.12220500
O	14.71516000	5.86913000	5.60556100
O	21.84402100	7.36868300	5.09126300
O	19.34391700	7.75139200	8.10245000
O	18.82717000	9.63664700	6.38568500
O	24.88916700	11.12844800	3.28274800
O	25.34570000	8.93492300	4.51636200
O	16.87878800	8.77523100	4.13124900
O	23.02920500	9.71281100	4.34676800
O	24.19328100	8.92700700	2.20725000
O	17.26689700	5.61240800	4.19499000
O	24.73716200	6.41720100	3.23080500
O	21.08928600	3.08719900	7.10348400
O	16.30066000	3.71620800	5.43283300
O	18.84541200	4.10729500	5.55432700
O	17.82993700	3.20744700	3.43900800
O	20.29961000	2.32893600	3.50741100
H	20.74033000	6.41096200	7.27231000
H	19.17359800	8.27934100	8.88865700
H	22.27144000	10.11975400	3.89434700
H	20.07127800	7.58451200	5.24794800
H	16.14005600	2.76849900	5.38380000
H	17.62425900	8.72941100	3.50032700
H	17.13139800	9.44917100	4.78356700
H	20.74703100	2.67475800	2.70889300
H	19.31511100	2.43355100	3.35373200
H	21.31186800	3.93932800	7.51487900
H	20.34072500	2.71629300	7.58272300
H	26.78359800	5.69684300	6.84593400
H	27.86814700	6.47870300	6.00465300

H	24.61654600	7.16621300	2.60307300
H	23.99552600	5.80260200	3.11917700
H	15.06096100	4.94651300	5.56012900
H	14.15845700	5.97740400	6.38030400
H	22.39532300	8.17939200	5.04197500
N	21.15075900	4.41585500	1.87175000
N	20.50602100	6.44360200	2.44724800
N	20.62535500	10.58281600	1.53018100
N	19.43946100	9.28122200	2.85014000
C	21.79540900	6.57014100	1.99894100
C	22.17414200	5.30056900	1.63890600
C	20.15966900	5.14257900	2.34305900
C	20.65358900	11.17100600	2.77418500
C	19.88401900	9.46113600	1.62216900
C	19.91486000	10.35014500	3.58517200
H	21.09160800	10.91849900	0.70080100
H	21.14297900	12.11517900	2.95122800
H	19.67691700	10.44995000	4.63774400
H	19.70640200	8.80541900	0.78289300
H	22.30651700	7.52226800	1.95191200
H	19.92851300	7.18250200	2.83206200
H	19.16583400	4.78183800	2.56540700
H	23.09930400	4.97763400	1.18306700
H	25.33174100	11.54409000	4.03086900

Position of atoms in final structure for $R^{(2)}$ case:

Zn	16.27946500	7.04326900	5.08942800
Zn	25.35599700	7.04315600	5.08936300
Zn	20.66718900	3.48893800	5.10370600
P	22.38191600	6.03437700	5.79528600
P	24.42449600	9.62752100	3.49668600
P	18.58342900	8.21493800	6.74839000
P	17.64926600	4.17661000	4.57793700
O	22.07306300	4.85735100	4.89817600
O	17.13259200	7.74932700	6.76363400
O	26.97053200	6.40121000	6.12563600
O	21.68463200	5.77919600	7.20811200
O	19.40030100	6.79842400	6.83865600
O	23.86622600	6.25680200	6.05832200
O	14.73429900	5.85918700	5.65829800
O	21.73199600	7.32793600	5.16446200
O	18.96074700	8.88308400	8.14027300
O	19.01289700	9.07923400	5.62160000
O	24.87554600	11.13694300	3.30883300
O	25.27020200	8.96710200	4.59816300
O	16.87025000	8.64801500	3.98175700
O	22.94320600	9.67987700	4.18259000
O	24.34389500	8.91379400	2.19248800
O	17.21817500	5.58945800	4.17288600
O	24.90342700	6.43176500	3.18129400
O	21.27481400	3.04329000	7.02894700
O	16.36715300	3.69604400	5.50542800

O	18.88674200	4.31084700	5.53092300
O	17.87229500	3.15256600	3.51159800
O	20.37091900	2.31911200	3.50906300
H	20.83219400	6.28329400	7.30786900
H	18.50722300	8.51503200	8.90571200
H	22.21880500	9.83998800	3.55786700
H	19.03907300	6.03421400	6.33502200
H	16.22431200	2.74421300	5.47960600
H	17.35423700	8.54847400	3.14037300
H	17.50301100	9.14230800	4.54567400
H	20.81677900	2.73189100	2.73302700
H	19.39725500	2.36337700	3.33307100
H	21.50630700	3.88387900	7.46509200
H	20.84940200	2.45279000	7.65506300
H	26.86636500	5.81636700	6.88297200
H	27.88871600	6.67276100	6.03833500
H	24.79113900	7.20650700	2.57850200
H	24.14612900	5.83985700	3.05804900
H	15.06499400	4.93511900	5.63307000
H	14.14870500	5.98732900	6.40818600
H	22.17672200	8.19476800	5.18798500
N	21.21630300	4.38989100	1.92866200
N	20.65878200	6.47460300	2.37131800
N	20.37509200	10.13590700	0.73921700
N	19.08089300	9.11300000	2.19644400
C	21.95457700	6.51605900	1.93027700
C	22.28115800	5.21068800	1.65474200
C	20.25571900	5.18934600	2.34548500
C	20.66439500	10.69274700	1.96285600
C	19.41903000	9.20131000	0.92826300
C	19.85433400	10.04639900	2.85819300
H	20.80371400	10.37961000	-0.14035400
H	21.36308500	11.50771300	2.06761400
H	19.76481800	10.17592900	3.92747600
H	19.01396800	8.60782500	0.12313600
H	22.50109200	7.44362700	1.82353700
H	20.10043500	7.26157700	2.68198900
H	19.24688200	4.88760800	2.58591100
H	23.19675200	4.81824300	1.23635100
H	25.17137000	11.59062000	4.10543400