Theoretical Study of the Ring-Opening of Epoxides Catalyzed by Boronic Acids and Pyridinic Bases

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Table S1 - Cartesian coordinates for the transition state of propylene oxide's ring-opening, when catalyzed by $-CH_3$ substituted 2,6-phenylboronic acid and pyridine, at the M06-2X/6-31+G(d,p).

C	-2.25290900	-1.30826600	1.46196900
C	-1.60815800	-0.10697300	0.95030300
H	-1.96215900	-2.26273500	1.03879300
H	-2.73673200	-1.27815800	2.42930100
H	-2.04467400	0.83531700	1.29606000
O	-0.64551500	-0.62702000	1.85934300
C	-1.19821200	-0.05986000	-0.50218000
H	-2.05416000	0.22133900	-1.12471700
H	-0.41047800	0.68598000	-0.64955900
H	-0.82929200	-1.03574700	-0.83396300
C	3.48867300	-1.67931700	-1.57485000
C	3.53431200	-1.37723700	-0.19915400
C	4.77013800	-1.38418300	0.47447000
C	5.94027200	-1.69960600	-0.22522200
C	5.89260200	-1.99417700	-1.58605000
C	4.67166200	-1.98031300	-2.25771900
H	6.89055200	-1.71336200	0.30300000
H	6.80572800	-2.23538200	-2.12292700
H	4.63365100	-2.20595400	-3.32063300
B	2.19446900	-1.03781000	0.57035700
O	2.01151300	0.24418500	1.04498900
H	1.14372400	0.33187600	1.48010500
O	1.23995000	-1.99566600	0.74146100
H	0.42857800	-1.58322100	1.17998400
C	4.84699900	-1.04714500	1.94507100
H	4.77437500	0.03419900	2.10512700
H	4.03335200	-1.51570500	2.50822800
H	5.79460000	-1.38395800	2.37326300
C	2.17321900	-1.68382200	-2.31869500
H	1.57506600	-2.56415800	-2.05999800
H	1.57260500	-0.80004800	-2.07690200
H	2.33733700	-1.69538400	-3.39921800
N	-4.08769600	-1.44126900	0.52769100
C	-4.17048900	-1.96996700	-0.69710100
C	-5.11914900	-0.74688100	1.01665400
C	-5.30962700	-1.83833900	-1.48446000
C	-6.29741700	-0.56816900	0.29975000
C	-6.39234200	-1.12527600	-0.97379400
H	-3.29611500	-2.51308600	-1.04860500
H	-4.99020600	-0.32560100	2.01097000
H	-7.11509500	-0.00310400	0.73299900
H	-7.29704300	-1.00352000	-1.56117700
H	-5.34108400	-2.28362700	-2.47255500

Table S2 - Cartesian coordinates for the transition state of propylene oxide's ring-opening, when catalyzed by -CF_3 substituted 2,6-phenylboronic acid and pyridine, at the M06-2X/6-31+G(d,p).

C	-2.26078400	-1.31487100	1.37585800
C	-1.64670300	-0.10720900	0.84261400
H	-2.00410100	-2.26279100	0.91730600
H	-2.68150300	-1.29999300	2.37263200
H	-2.05612800	0.83145100	1.22769000
O	-0.63334500	-0.64487300	1.68550400
C	-1.31170100	-0.04160300	-0.62706200
H	-2.19432700	0.25451200	-1.20331100
H	-0.52586100	0.70065500	-0.80053700
H	-0.96564400	-1.01508500	-0.98829000
C	3.72197400	-1.65681000	-1.60984300
C	3.59214200	-1.36774300	-0.24387300
C	4.77088200	-1.43515300	0.51194300
C	6.00468200	-1.76347900	-0.04879800
C	6.08972900	-2.04355500	-1.40795100
C	4.94273100	-1.99181200	-2.19321800
H	6.89383000	-1.80212900	0.57213400
H	7.04425800	-2.30093900	-1.85349100
H	4.99919300	-2.20903000	-3.25478700
B	2.18430100	-0.98899100	0.41367900
O	2.01468000	0.31065500	0.82026400
H	1.13817800	0.43572200	1.22613400
O	1.23157900	-1.93980100	0.54368100
H	0.40263400	-1.52122400	0.97271300
N	-4.16252700	-1.42958400	0.57012900
C	-4.34287200	-1.93229900	-0.65505400
C	-5.16118500	-0.77261600	1.16695400
C	-5.55057100	-1.80928400	-1.33399500
C	-6.40225300	-0.60355600	0.56203100
C	-6.59775700	-1.13243900	-0.71200300
H	-3.49226800	-2.44635100	-1.09678800
H	-4.95305200	-0.37409800	2.15740800
H	-7.19009900	-0.06841100	1.08004100
H	-7.55325300	-1.01684100	-1.21376900
H	-5.66077500	-2.23369200	-2.32558800
C	2.49855800	-1.63875400	-2.48523600
C	4.72665400	-1.11578900	1.98158400
F	1.63440300	-0.66526700	-2.13058100
F	1.80746000	-2.79744800	-2.42660700
F	2.79489300	-1.44158600	-3.78106100
F	3.55904400	-1.48574900	2.54746700
F	4.86419500	0.20502300	2.22582900
F	5.70173900	-1.73092800	2.67232600

Table S3 - Cartesian coordinates for the transition state of propylene oxide's ring-opening, when catalyzed by -H substituted 2,6-phenylboronic acid and pyridine, at the M06-2X/6-31+G(d,p).

C	-2.34985600	-1.68905300	1.24546000
C	-1.60104000	-0.48129400	0.92827800
H	-2.20003400	-2.56176000	0.62071600
H	-2.76679600	-1.80771800	2.23667700
H	-1.90420500	0.41204100	1.48358000
O	-0.65571500	-1.27289200	1.63615300
C	-1.26737000	-0.18588800	-0.51367100
H	-2.11394500	0.30300000	-1.00687600
H	-0.40484100	0.48593600	-0.57138700
H	-1.03169200	-1.10922500	-1.05234900
C	3.94549900	-2.53350100	-1.07880800
C	3.64488200	-1.45594300	-0.23169600
C	4.64238600	-0.49484700	-0.00689700
C	5.89757100	-0.60332900	-0.60541200
C	6.17603600	-1.68355000	-1.44445800
C	5.19769800	-2.65042500	-1.68169500
H	6.65677600	0.15106800	-0.42090500
H	7.15280000	-1.77271500	-1.91115700
H	5.41290500	-3.49206500	-2.33359400
B	2.22804000	-1.33219800	0.44049000
O	1.98368600	-0.25587900	1.26555100
H	1.07623500	-0.29680800	1.62062500
O	1.27275900	-2.27741600	0.20193200
H	0.43047900	-2.02534400	0.68809700
N	-4.23743800	-1.43560800	0.45944500
C	-4.45745100	-1.70810600	-0.83021000
C	-5.14019000	-0.73175100	1.14830300
C	-5.61352700	-1.29803400	-1.48607100
C	-6.32446200	-0.28351700	0.57252200
C	-6.56330700	-0.57363800	-0.76912000
H	-3.68122600	-2.27017100	-1.34434200
H	-4.90077900	-0.52466600	2.18880100
H	-7.03544700	0.28182100	1.16450500
H	-7.47627800	-0.23712300	-1.25040400
H	-5.75907200	-1.54081500	-2.53271400
H	4.43315400	0.35004500	0.64464800
H	3.18915900	-3.29140700	-1.26768200

Table S4 - Cartesian coordinates for the transition state of propylene oxide's ring-opening, when catalyzed by -NH_2 substituted 2,6-phenylboronic acid and pyridine, at the M06-2X/6-31+G(d,p).

C	-2.33113700	-1.73497000	1.13194700
C	-1.69459800	-0.45016500	1.38597000
H	-2.00709700	-2.30301000	0.26747000
H	-2.84539100	-2.23880200	1.93911900
H	-2.16481100	0.15305700	2.16896800
O	-0.75565200	-1.38356900	1.90536900
C	-1.21785800	0.37723900	0.21755700
H	-2.05003900	0.94315300	-0.21355800
H	-0.45670000	1.09073500	0.54845400
H	-0.78822900	-0.26499100	-0.55805500
C	3.72355500	-2.62169600	-1.14148000
C	3.50924500	-1.60849300	-0.16161900
C	4.58192600	-0.70088500	0.07566600
C	5.78538200	-0.79192900	-0.64638000
C	5.94493000	-1.78394000	-1.60411000
C	4.93225000	-2.69942000	-1.85614800
H	6.57888500	-0.07818900	-0.44383800
H	6.87451100	-1.84442800	-2.16409500
H	5.05922000	-3.48133700	-2.59946000
B	2.13297400	-1.47756400	0.58396200
O	1.96106200	-0.52003700	1.57033600
H	1.05213800	-0.54913400	1.92272500
O	1.06798900	-2.28541200	0.27204200
H	0.27429900	-2.02108500	0.82746500
N	-4.14187200	-1.36215700	0.20261400
C	-4.17634100	-1.14776200	-1.11606700
C	-5.22617900	-1.10840600	0.94086500
C	-5.31706700	-0.67991300	-1.76009800
C	-6.41021600	-0.64166700	0.37950300
C	-6.45380600	-0.42440600	-0.99591600
H	-3.26097800	-1.36024500	-1.66398400
H	-5.13526100	-1.28868000	2.00962000
H	-7.27117600	-0.45004700	1.01012500
H	-7.36121600	-0.05796700	-1.46555800
H	-5.30780600	-0.51984400	-2.83233800
N	4.51278800	0.28087600	1.05429300
H	3.59059800	0.55225600	1.36500100
H	5.15567700	1.05082200	0.92467200
N	2.77825800	-3.60445600	-1.39706500
H	2.87972700	-4.06638500	-2.29108000
H	1.82497200	-3.39770300	-1.13257100

Table S5 - Cartesian coordinates for the transition state of propylene oxide's ring-opening, when catalyzed by $-CH_3$ substituted 2,6-phenylboronic acid and DMAP, at the M06-2X/6-31+G(d,p).

C	-2.32259200	-1.66215700	2.05375500
C	-1.74995200	-0.53831500	1.32735800
H	-2.06977900	-2.66532900	1.73238600
H	-2.70948000	-1.50717200	3.05190900
H	-2.14808900	0.44323400	1.60464600
O	-0.68447300	-0.95169900	2.17380500
C	-1.52864800	-0.67058200	-0.16017300
H	-2.46220000	-0.45534800	-0.69237900
H	-0.76962100	0.04307600	-0.49701600
H	-1.20321900	-1.68354400	-0.41915200
C	3.10940000	-1.57371600	-1.72317500
C	3.27424900	-1.24989700	-0.36192500
C	4.57086700	-1.07291600	0.15881900
C	5.68165300	-1.22994600	-0.67692100
C	5.51502200	-1.54437000	-2.02400600
C	4.23320300	-1.71149200	-2.54465300
H	6.68057100	-1.10158700	-0.26717400
H	6.38258200	-1.65729400	-2.66820400
H	4.09969300	-1.95067800	-3.59693200
B	2.00333100	-1.07471600	0.56437700
O	1.72393800	0.18120800	1.06025300
H	0.91222100	0.16715700	1.59980400
O	1.20321900	-2.14098400	0.85163000
H	0.40734000	-1.82779000	1.38602100
C	4.77555600	-0.70594000	1.60978300
H	4.54708100	0.35088500	1.78469800
H	4.12851500	-1.29360100	2.26917000
H	5.81177600	-0.87760000	1.91215800
C	1.72923000	-1.77681200	-2.30475500
H	1.30398700	-2.73495200	-1.98664000
H	1.03736400	-0.99089800	-1.98288300
H	1.76279800	-1.77182600	-3.39721000
N	-4.20887000	-1.89227500	1.23495700
C	-4.29423400	-2.67875300	0.15063900
C	-5.03796300	-0.83755500	1.29020100
C	-5.18688200	-2.47540900	-0.88281000
C	-5.97051600	-0.53800500	0.31667600
C	-6.06383400	-1.36168200	-0.83507600
H	-3.60144400	-3.51686900	0.11014500
H	-4.94219700	-0.19874700	2.16572400
H	-6.60528400	0.32943500	0.44664000
H	-5.18942700	-3.16706700	-1.71550900
N	-6.92868800	-1.08754100	-1.84209000
C	-7.90996000	-0.02307700	-1.68210400
H	-7.41984300	0.94318800	-1.52925900
H	-8.50951400	0.03933000	-2.58866100
H	-8.57744200	-0.21417300	-0.83291300
C	-7.07043600	-2.02614100	-2.94621500
H	-6.11547400	-2.16981800	-3.46005100
H	-7.43669800	-3.00195900	-2.60407100
H	-7.78195700	-1.61935500	-3.66274800