

Cl atom and OH radical initiated kinetic and mechanistic study on the degradation of propyl butanoate under tropospheric conditions

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Table S1 Optimized Cartesian Coordinates for the reaction of PB with Cl atoms at the BHandHLYP/6-311+G(2d,2p) level of theory.

Table S1-1 Geometry of propyl butanoate (PB).

C	4.23897200	-0.59203300	-0.00010200
C	3.00904900	0.29872500	-0.00014700
H	5.14701500	-0.00249700	-0.00033300
H	4.26222100	-1.23218400	0.87493100
H	4.26201600	-1.23255700	-0.87486900
C	1.72297400	-0.50326900	0.00017300
H	3.02201200	0.95173500	0.86399400
H	3.02181400	0.95136700	-0.86457100
H	1.66923400	-1.15819700	-0.86383400
H	1.66944100	-1.15780500	0.86449300
C	0.48543500	0.34640400	0.00016300
O	0.46718600	1.53967100	0.00006400
O	-0.61582600	-0.40052600	0.00005100
C	-1.86092000	0.29651000	-0.00003700
C	-2.96803500	-0.72532200	0.00000600
H	-1.90681400	0.93412400	-0.87366700
H	-1.90686500	0.93426300	0.87348700
C	-4.33724800	-0.06745800	-0.00010200
H	-2.85965100	-1.36304100	-0.87007100
H	-2.85971700	-1.36289400	0.87019800
H	-4.47481000	0.55719900	0.87499300
H	-4.47473900	0.55705900	-0.87530900
H	-5.12340300	-0.81107300	-0.00007400

Table S1-2 Geometry of pre-reactive complex for reaction channel R1.

C	-2.82275600	-0.15736600	0.25408800
C	-1.48190500	-0.85638000	0.10524200
H	-3.63301600	-0.87685700	0.22213200
H	-2.88984500	0.37396500	1.19667500
H	-2.98004200	0.56253900	-0.54169200
C	-0.32251100	0.11861800	0.15150800
H	-1.35949600	-1.59465700	0.88814700
H	-1.45013800	-1.40506000	-0.82785700
H	-0.40724400	0.86602800	-0.63111600
H	-0.31298600	0.67372900	1.08410900
C	1.01853300	-0.53979000	0.00287200
O	1.19936600	-1.70945300	-0.14987400
O	2.00494100	0.35077300	0.06143600
C	3.33281500	-0.15580000	-0.07013700
C	4.28759300	1.00536100	0.03050300
H	3.42220300	-0.66405100	-1.02163900
H	3.50922500	-0.88582000	0.70934200
C	5.73218200	0.55407000	-0.10019900
H	4.04940300	1.72623400	-0.74342700
H	4.13637700	1.50524500	0.98056700
H	5.99695400	-0.15098900	0.67932100
H	5.90979900	0.07176800	-1.05449700
H	6.40846500	1.39552200	-0.02610000
Cl	-6.14693000	0.55644600	-0.14410100

Table S1-3 Geometry of pre-reactive complex for reaction channel R2.

C	2.92599500	-2.52033200	0.19785600
C	1.79856600	-1.56782300	0.55228800
H	3.35312800	-2.96286200	1.08875500
H	2.57531200	-3.32588200	-0.43708100
H	3.71973800	-2.00366000	-0.32861200
C	1.18287900	-0.92937900	-0.69319200
H	1.02745400	-2.09803500	1.10055400
H	2.16876900	-0.78388100	1.20141700
H	1.93888400	-0.37303900	-1.22952600
H	0.77781900	-1.69391600	-1.34226200
C	0.09250500	0.02432500	-0.32186200
O	0.25860700	1.17012600	0.00694700
O	-1.10611600	-0.52779600	-0.35279200
C	-2.21296900	0.29376700	0.03658500
C	-3.46596600	-0.53465800	-0.07116900
H	-2.24662800	1.15911500	-0.61182300
H	-2.04734600	0.64312000	1.04705500
C	-4.69681300	0.26608200	0.31857700
H	-3.56252000	-0.89795000	-1.08793100

H	-3.36946700	-1.40651600	0.56576000
H	-4.63012900	0.61976300	1.34087600
H	-4.82330100	1.13096000	-0.32213200
H	-5.59096400	-0.33752400	0.23696700
Cl	2.57318500	2.17645700	0.08413200

Table S1-4 Geometry of pre-reactive complex for reaction channel R3.

C	-4.37085700	0.02563800	-0.52499200
C	-3.17195400	-0.64549300	0.12173600
H	-5.29790500	-0.38375400	-0.14436300
H	-4.37740400	1.09241200	-0.33110200
H	-4.36723100	-0.11184100	-1.60062400
C	-1.86026900	-0.08725900	-0.39431000
H	-3.21214800	-0.52306100	1.19717000
H	-3.20136000	-1.71336300	-0.05716900
H	-1.77787600	-0.20826800	-1.46998200
H	-1.79298300	0.98035400	-0.21535000
C	-0.65539500	-0.73232100	0.22245900
O	-0.67428100	-1.60102200	1.03674600
O	0.48543000	-0.22331800	-0.26696800
C	1.70203200	-0.81961500	0.19999200
C	2.83609500	-0.32584800	-0.65994400
H	1.59972100	-1.89439100	0.14415000
H	1.84075300	-0.55312800	1.23979600
C	4.16224100	-0.92567700	-0.22378400
H	2.63124600	-0.58236900	-1.69319400
H	2.88205600	0.75520700	-0.60722100
H	4.39568200	-0.66184400	0.80118800
H	4.14824700	-2.00736900	-0.29126500
H	4.97042800	-0.56725100	-0.84749700
Cl	0.65989500	2.47275500	0.31001800

Table S1-5 Geometry of pre-reactive complex for reaction channel R4.

C	-4.57472600	-0.63312300	-0.00013900
C	-3.22745700	0.06756400	0.00026400
H	-5.38555700	0.08403400	0.00027900
H	-4.69221500	-1.26225100	-0.87550000
H	-4.69221100	-1.26326800	0.87449200
C	-2.07421500	-0.91577600	-0.00033200
H	-3.14453400	0.71535900	-0.86376500
H	-3.14450700	0.71432900	0.86506300
H	-2.11649700	-1.57168800	0.86353000
H	-2.11641900	-1.57054200	-0.86506900
C	-0.72262200	-0.26339400	0.00011900

O	-0.54457000	0.92164400	0.00064200
O	0.25107700	-1.15815700	-0.00012900
C	1.59682100	-0.67267700	0.00019800
C	2.51819600	-1.86444300	-0.00023800
H	1.74532200	-0.05344700	0.87453900
H	1.74545300	-0.05269900	-0.87358800
C	3.97709100	-1.44078900	0.00013900
H	2.30531500	-2.47517300	0.86981300
H	2.30553500	-2.47438400	-0.87089200
H	4.21521000	-0.84672500	-0.87441200
H	4.21502700	-0.84764700	0.87536400
H	4.62935600	-2.30411100	-0.00025000
Cl	1.26589000	2.90800800	-0.00022200

Table S1-6 Geometry of pre-reactive complex for reaction channel R5.

C	4.37082800	0.02577000	0.52492300
C	3.17194700	-0.64568000	-0.12151800
H	5.29789100	-0.38390300	0.14463300
H	4.37745000	1.09242700	0.33039900
H	4.36709100	-0.11106700	1.60063800
C	1.86024400	-0.08720200	0.39421100
H	3.21217000	-0.52378700	-1.19701100
H	3.20135700	-1.71346100	0.05791400
H	1.77771700	-0.20786500	1.46991200
H	1.79303600	0.98036000	0.21491800
C	0.65538400	-0.73236500	-0.22248400
O	0.67429700	-1.60118200	-1.03665000
O	-0.48543200	-0.22328500	0.26684500
C	-1.70205000	-0.81958400	-0.20006100
C	-2.83607100	-0.32583700	0.65994000
H	-1.59973900	-1.89436100	-0.14424100
H	-1.84082400	-0.55307700	-1.23985300
C	-4.16224100	-0.92566700	0.22385900
H	-2.63115500	-0.58236700	1.69317400
H	-2.88205300	0.75522300	0.60724000
H	-4.39573400	-0.66185700	-0.80110600
H	-4.14825800	-2.00735900	0.29136400
H	-4.97039300	-0.56721700	0.84760400
Cl	-0.65986600	2.47279100	-0.31002100

Table S1-7 Geometry of pre-reactive complex for reaction channel R6.

C	5.31567800	-1.03146700	-0.38135900
C	4.17832800	-0.35640000	0.36478200
H	6.22611600	-1.02088300	0.20432600

H	5.08087700	-2.06604200	-0.60604000
H	5.52300700	-0.53136600	-1.32098800
C	2.88992300	-0.35817100	-0.43353100
H	4.00995000	-0.85134800	1.31343900
H	4.44599400	0.66483100	0.60696200
H	3.01781800	0.14765900	-1.38546200
H	2.58324600	-1.36957600	-0.68096100
C	1.74332700	0.30030400	0.27673200
O	1.79525600	0.79621000	1.36085300
O	0.63374900	0.26787100	-0.45812400
C	-0.52868900	0.86308400	0.11541900
C	-1.66224500	0.71095000	-0.86554900
H	-0.32244300	1.90421600	0.32847900
H	-0.74733100	0.37330700	1.05562700
C	-2.94822400	1.31774900	-0.33148100
H	-1.38742600	1.18493700	-1.80093500
H	-1.80608100	-0.34211200	-1.07848000
H	-3.24597500	0.84787800	0.60042400
H	-2.83719100	2.37801500	-0.13531600
H	-3.75545700	1.20177500	-1.04349400
Cl	-5.30269000	-1.15942500	0.25003000

Table S1-8 Geometry of transition state for reaction channel R1.

C	-2.87236100	1.09163200	0.00022400
C	-1.76289700	0.09274400	0.00015500
H	-4.06352900	0.35029500	-0.00001800
H	-3.03055000	1.65854700	0.90383500
H	-3.03039700	1.65884200	-0.90323000
C	-0.40615300	0.78923500	0.00036400
H	-1.83389400	-0.54969200	0.86762800
H	-1.83377100	-0.54941900	-0.86753400
H	-0.29226700	1.43233700	-0.86526000
H	-0.29241600	1.43204800	0.86622800
C	0.73931000	-0.18548900	0.00033300
O	0.62768800	-1.37251400	0.00058400
O	1.90583000	0.44711400	0.00001200
C	3.07846800	-0.37120200	0.00001400
C	4.28036900	0.53670600	-0.00036300
H	3.05872000	-1.00924100	-0.87384700
H	3.05898200	-1.00886200	0.87415800
C	5.57711700	-0.25468400	-0.00037400
H	4.23571800	1.18141400	-0.87078900
H	4.23597000	1.18180500	0.86978500
H	5.65181900	-0.88940000	0.87497000
H	5.65154600	-0.88982100	-0.87543600

H	6.43298000	0.40723100	-0.00066600
Cl	-5.29530400	-0.42332500	-0.00039400

Table S1-9 Geometry of transition state for reaction channel R2.

C	3.56045400	-1.33113000	-0.49597200
C	2.33032600	-0.83120800	0.18863600
H	4.45628000	-0.96749400	-0.01259200
H	3.58163700	-2.41829700	-0.45922600
H	3.58647400	-1.03560600	-1.53705800
C	1.01842800	-1.07815900	-0.48491300
H	2.30227100	-0.94844300	1.26075400
H	2.46046600	0.51720200	0.15217300
H	0.96479800	-0.59049100	-1.44930400
H	0.91390100	-2.14566700	-0.68020700
C	-0.16485100	-0.67925500	0.35599300
O	-0.15187300	-0.61476300	1.54672600
O	-1.23255500	-0.44581000	-0.38922500
C	-2.43172500	-0.08662200	0.30395300
C	-3.50758800	0.15385700	-0.72223500
H	-2.23719500	0.79778900	0.89578800
H	-2.69561500	-0.88800400	0.98178700
C	-4.82252800	0.54454700	-0.06954800
H	-3.17981100	0.93400800	-1.39958600
H	-3.63688900	-0.74383200	-1.31623100
H	-5.18004000	-0.23346100	0.59510100
H	-4.71898000	1.45326200	0.51190900
H	-5.58708600	0.71680800	-0.81548500
Cl	2.59706600	1.99321400	-0.02607700

Table S1-10 Geometry of transition state for reaction channel R3.

C	3.80182600	-0.83486600	0.66739700
C	2.51543200	-1.25616900	-0.01985400
H	4.62986500	-1.44084500	0.32461800
H	4.03583300	0.20067000	0.45700800
H	3.73016300	-0.94957300	1.74273600
C	1.31452400	-0.49621600	0.44018000
H	2.59922400	-1.17386000	-1.09574400
H	2.31635700	-2.30909500	0.17559300
H	1.21154400	-0.34792000	1.50446500
H	1.51465600	0.75508300	0.08818000
C	0.02334000	-0.78160200	-0.24513600
O	-0.06604500	-1.41604800	-1.25237700
O	-0.99868300	-0.24165000	0.39644100
C	-2.28759600	-0.39727000	-0.20548400

C	-3.29128300	0.32854700	0.65094300
H	-2.51104000	-1.45363200	-0.27955900
H	-2.25024600	0.00532700	-1.20920600
C	-4.69386300	0.21960300	0.07764300
H	-3.26381500	-0.08300200	1.65351700
H	-2.99847900	1.36895100	0.73026500
H	-4.74780500	0.64881500	-0.91604100
H	-5.01357500	-0.81380200	0.00882900
H	-5.40623700	0.74343400	0.70104200
Cl	1.78688800	2.20111000	-0.30778500

Table S1-11 Geometry of transition state for reaction channel R4.

C	-4.71496000	0.08594900	-0.55718200
C	-3.47728000	0.06926500	0.32230800
H	-5.59851200	0.32173600	0.02167700
H	-4.62892400	0.82700600	-1.34378000
H	-4.87724700	-0.87677600	-1.02888100
C	-2.22465300	-0.25820800	-0.46612200
H	-3.35091800	1.02941600	0.80687900
H	-3.59671000	-0.65436600	1.11965000
H	-2.30361400	-1.22408900	-0.95520600
H	-2.06180100	0.45955700	-1.26442200
C	-0.98511800	-0.27381100	0.36821600
O	-0.90206700	-0.02529800	1.52365600
O	0.09293500	-0.62837400	-0.38425900
C	1.33033300	-0.59426300	0.20104600
C	2.33106800	-1.42808500	-0.52888700
H	1.29561100	-0.66511700	1.27768100
H	1.75073500	0.64768900	0.07016700
C	3.71543300	-1.35542100	0.09001700
H	1.96438100	-2.45246000	-0.51654900
H	2.35490100	-1.12167700	-1.56783000
H	4.10354100	-0.34598600	0.06269600
H	3.70164600	-1.68291300	1.12268800
H	4.40241900	-1.99306800	-0.44963300
Cl	2.20403600	2.08752100	-0.17921700

Table S1-12 Geometry of transition state for reaction channel R5.

C	4.69307700	0.92858200	0.37055400
C	3.63128300	0.01760900	-0.21993000
H	5.66126900	0.73589500	-0.07357400
H	4.45488600	1.97273700	0.20148800
H	4.78693900	0.78304600	1.44101600
C	2.26427900	0.26961200	0.38456900

H	3.57673200	0.15581800	-1.29275100
H	3.90379400	-1.01964900	-0.06728800
H	2.27643100	0.12362700	1.46012400
H	1.95074600	1.29780900	0.23434300
C	1.19021600	-0.61053700	-0.17856300
O	1.33422400	-1.43661400	-1.02554200
O	0.00764500	-0.36025800	0.39262800
C	-1.09147200	-1.10940100	-0.09337700
C	-2.31648800	-0.67599400	0.63206500
H	-0.91430000	-2.16849200	0.07810600
H	-1.19078600	-0.97134100	-1.16240900
C	-3.58687800	-1.38348000	0.29092700
H	-2.15875600	-0.46583000	1.67944800
H	-2.51614300	0.60991800	0.20801500
H	-3.74104800	-1.42967800	-0.77943400
H	-3.55425400	-2.40344500	0.66681200
H	-4.43982300	-0.89410300	0.73919100
Cl	-2.79616100	1.96648900	-0.31689700

Table S1-13 Geometry of transition state for reaction channel R6.

C	5.17932000	-0.23303900	-0.62338900
C	3.90568100	-0.51784300	0.15293800
H	6.01953900	-0.77065700	-0.20290400
H	5.08381400	-0.53162500	-1.66144100
H	5.42320100	0.82346300	-0.60744500
C	2.71259200	0.22437500	-0.41554500
H	3.69767900	-1.58071900	0.15092100
H	4.03412300	-0.24268900	1.19271100
H	2.88068800	1.29674100	-0.41563800
H	2.54261900	-0.04352300	-1.45370700
C	1.43660600	-0.03350300	0.32956900
O	1.31492400	-0.75351000	1.27153600
O	0.41998600	0.65523300	-0.19443600
C	-0.84995700	0.47279900	0.42039100
C	-1.81905400	1.39326300	-0.28065300
H	-0.77445800	0.70566500	1.47459700
H	-1.14866900	-0.56252600	0.32880600
C	-3.19193900	1.34267000	0.29836300
H	-1.45422400	2.41697500	-0.20144600
H	-1.84815400	1.16359500	-1.33918800
H	-3.70699100	0.07570000	-0.01005100
H	-3.28166100	1.30889800	1.37265200
H	-3.94543100	1.94050700	-0.18596500
Cl	-4.21416800	-1.24152500	-0.37345600

Table S1-14 Geometry of post-reactive complex for reaction channel R1.

C	-2.73540700	1.27708500	0.00000100
C	-1.65609400	0.25828300	-0.00000200
H	-4.59520000	0.12477200	0.00000800
H	-3.03576600	1.75162400	0.91623600
H	-3.03577500	1.75161800	-0.91623400
C	-0.26678700	0.89547600	-0.00001500
H	-1.74083200	-0.38422800	0.86756300
H	-1.74084400	-0.38423800	-0.86755800
H	-0.12879300	1.53407200	-0.86518000
H	-0.12877900	1.53408000	0.86514000
C	0.83758400	-0.12401500	-0.00002200
O	0.67998400	-1.30642900	-0.00002300
O	2.03081700	0.45919300	-0.00000200
C	3.16727500	-0.40713200	0.00000300
C	4.40652700	0.44933700	0.00001000
H	3.12172700	-1.04396000	-0.87388300
H	3.12171800	-1.04396200	0.87388700
C	5.66891400	-0.39578600	0.00001700
H	4.38905500	1.09563800	-0.87021200
H	4.38904500	1.09563700	0.87023200
H	5.71652700	-1.03338400	0.87519200
H	5.71653600	-1.03338500	-0.87515600
H	6.55209000	0.22929400	0.00002200
Cl	-5.69524600	-0.53736300	0.00001100

Table S1-15 Geometry of post-reactive complex for reaction channel R2.

C	3.41621700	-1.71108300	-0.41867500
C	2.20833400	-1.18965000	0.26500900
H	4.32096300	-1.45650500	0.11667900
H	3.38354000	-2.79886100	-0.49665700
H	3.50106300	-1.32990300	-1.43100700
C	0.90159500	-1.20567100	-0.43442300
H	2.19286300	-1.11101100	1.33598800
H	2.64237800	0.92812400	0.17904500
H	0.94547300	-0.68196300	-1.38508700
H	0.61178500	-2.22584300	-0.69640100
C	-0.22855000	-0.63051600	0.37577000
O	-0.16488900	-0.34189200	1.53113700
O	-1.32475000	-0.49824300	-0.35844700
C	-2.47904300	0.02584200	0.30215900
C	-3.59579900	0.10645500	-0.70545700
H	-2.23584400	0.99872200	0.70851400
H	-2.73279600	-0.62368000	1.12992000

C	-4.86760900	0.65941400	-0.08543300
H	-3.27990500	0.73248100	-1.53217000
H	-3.77700700	-0.88200000	-1.11227300
H	-5.21314400	0.03443400	0.72993600
H	-4.71283200	1.65769100	0.30717800
H	-5.66219600	0.71356200	-0.81783300
Cl	2.92952400	2.14335900	-0.13006100

Table S1-16 Geometry of post-reactive complex for reaction channel R3.

C	-4.19699100	0.06495100	0.64408100
C	-3.24496200	-0.56501300	-0.36959900
H	-5.20665000	-0.29136500	0.48604400
H	-3.90762900	-0.18563800	1.65670900
H	-4.20650900	1.14469200	0.55704200
C	-1.85860500	-0.07135600	-0.23690900
H	-3.24814200	-1.64263600	-0.28310700
H	-3.60021100	-0.33009800	-1.37234500
H	-1.66777700	0.98503200	-0.20920000
H	0.64415900	1.66251800	-0.06492200
C	-0.73712900	-0.96944800	-0.15630100
O	-0.81444100	-2.16879200	-0.16782300
O	0.44557900	-0.32699300	-0.06285900
C	1.60488900	-1.16261800	0.02329100
C	2.82467600	-0.28321200	0.11578500
H	1.63788400	-1.79901100	-0.85102100
H	1.50718700	-1.80043800	0.89176300
C	4.09563700	-1.11040400	0.20958700
H	2.86721600	0.36341000	-0.75346000
H	2.73729500	0.36088200	0.98357300
H	4.08584000	-1.75000000	1.08444200
H	4.21890400	-1.74360600	-0.66126400
H	4.96590100	-0.47147000	0.27822700
Cl	0.65872500	2.94391800	-0.07509600

Table S1-17 Geometry of post-reactive complex for reaction channel R4.

C	-4.70444700	0.25333200	-0.57351600
C	-3.47949500	0.12478400	0.31449000
H	-5.57790800	0.52157800	0.00667900
H	-4.56445700	1.01716600	-1.33019500
H	-4.92145800	-0.67840400	-1.08395500
C	-2.24083200	-0.24890100	-0.47534300
H	-3.29980100	1.05522900	0.83877500
H	-3.65181000	-0.62083100	1.08119800
H	-2.37846000	-1.18563400	-1.00640600

H	-2.02435600	0.49010800	-1.24074800
C	-1.01472600	-0.38509800	0.37081700
O	-0.94108400	-0.20890500	1.54237700
O	0.05065100	-0.74706600	-0.38448000
C	1.26829000	-0.87153700	0.21652900
C	2.29359300	-1.54705000	-0.60817700
H	1.25547000	-0.91247500	1.28908000
H	1.91820800	1.17530800	0.11914700
C	3.66110600	-1.54897400	0.05474400
H	1.97461100	-2.57252600	-0.79951100
H	2.34280500	-1.06846100	-1.58136900
H	4.02733000	-0.54137700	0.20498500
H	3.62728100	-2.03946500	1.02016200
H	4.37998700	-2.07568200	-0.55825700
Cl	2.31265200	2.37787600	-0.11882500

Table S1-18 Geometry of post-reactive complex for reaction channel R5.

C	4.58144200	1.01733600	0.37943300
C	3.57182900	0.04877300	-0.21098200
H	5.56108700	0.87247300	-0.05780500
H	4.29049800	2.04670100	0.20211600
H	4.67625400	0.88374800	1.45137800
C	2.18994800	0.23250500	0.38426500
H	3.51662100	0.17716100	-1.28499900
H	3.89690400	-0.97195300	-0.05014400
H	2.20381800	0.09368200	1.46069000
H	1.82519400	1.24250600	0.22595300
C	1.16583100	-0.70644100	-0.17942000
O	1.36082000	-1.52532300	-1.02379900
O	-0.02912100	-0.51723400	0.38525800
C	-1.08773400	-1.34181600	-0.08718200
C	-2.31735300	-0.99249000	0.65316700
H	-0.81387300	-2.38559600	0.05883400
H	-1.20907400	-1.20184000	-1.15559600
C	-3.62382700	-1.52975500	0.20490700
H	-2.19893700	-0.67552200	1.67422100
H	-2.43421900	1.13684600	0.12022200
H	-3.73951300	-1.45229500	-0.87040000
H	-3.72637800	-2.58552600	0.45824900
H	-4.44824200	-1.00973600	0.67409700
Cl	-2.64320900	2.34124400	-0.27433000

Table S1-19 Geometry of post-reactive complex for reaction channel R6.

C	5.16197400	-0.58445200	-0.64827000
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C	3.91758800	-0.57907100	0.22216200
H	5.99346700	-1.05092600	-0.13554200
H	4.99567000	-1.13031000	-1.57032800
H	5.46228500	0.42317700	-0.91367700
C	2.73797100	0.07093800	-0.47298800
H	3.65315600	-1.59182100	0.50039300
H	4.11540900	-0.05826400	1.15115200
H	2.96124100	1.09640200	-0.74992800
H	2.50322600	-0.43693900	-1.40329600
C	1.48803900	0.08789800	0.35631300
O	1.37531400	-0.36904800	1.45183300
O	0.48605800	0.68860600	-0.28762900
C	-0.76047400	0.74955900	0.39646100
C	-1.72454700	1.50516700	-0.48595600
H	-0.62219000	1.24763800	1.34716100
H	-1.10642500	-0.25580800	0.59656200
C	-3.05610400	1.67763700	0.14151800
H	-1.29554300	2.48235900	-0.71223100
H	-1.81736500	1.00027700	-1.44235300
H	-3.96573200	-0.30647000	-0.03359700
H	-3.15882400	1.70761300	1.21087900
H	-3.87668800	2.05117400	-0.44115900
Cl	-4.43055000	-1.48827300	-0.22194800

Table S1-20 Geometry of product for reaction channel R1.

C	-4.27710800	-0.60284800	0.00358400
C	-3.07083000	0.25736200	0.01400500
H	-4.24621500	-1.59792300	-0.39820000
H	-5.23661200	-0.19725200	0.25827000
C	-1.77913200	-0.53858000	0.01746300
H	-3.07041200	0.92066500	-0.85085600
H	-3.09058200	0.92366200	0.86975700
H	-1.71755500	-1.17984400	0.88980100
H	-1.72854700	-1.20236500	-0.83943100
C	-0.55094800	0.32386100	-0.00373100
O	-0.54680900	1.51707800	-0.02977100
O	0.55716600	-0.41114200	0.01060300
C	1.79563500	0.29850100	-0.00629000
C	2.91288500	-0.71191800	0.01404300
H	1.83565100	0.95497400	0.85343100
H	1.83347500	0.91750600	-0.89346600
C	4.27521300	-0.04006100	-0.00153800
H	2.81189200	-1.33191600	0.89764500
H	2.81024600	-1.36891100	-0.84224000
H	4.40522100	0.56764700	-0.88958800

H	4.40739200	0.60377300	0.86034100
H	5.06890800	-0.77541100	0.01266400

Table S1-21 Geometry of product for reaction channel R2.

C	4.31918600	-0.49044500	0.04399900
C	3.02642200	0.23189300	0.04518100
H	5.14691600	0.17269400	0.25496100
H	4.33407100	-1.28939800	0.78188900
H	4.51842400	-0.96312600	-0.91880400
C	1.75678500	-0.51975100	-0.06178500
H	2.98976500	1.30142800	-0.00051000
H	1.70716900	-1.09724000	-0.98724400
H	1.66247000	-1.26683700	0.72438500
C	0.52553000	0.34251100	-0.02386500
O	0.51341200	1.53477300	-0.01252800
O	-0.57715300	-0.40070700	-0.01509100
C	-1.82026200	0.30077200	0.00215300
C	-2.93063200	-0.71735500	0.00892900
H	-1.87283300	0.94298700	-0.86763200
H	-1.85368100	0.93368200	0.87957300
C	-4.29735300	-0.05456800	0.02705400
H	-2.83395800	-1.35091000	-0.86552200
H	-2.81514900	-1.35965200	0.87467300
H	-4.42319600	0.56595500	0.90679300
H	-4.44205700	0.57492600	-0.84337100
H	-5.08607200	-0.79538200	0.03175400

Table S1-22 Geometry of product for reaction channel R3.

C	3.86355500	-1.03105200	0.00018200
C	2.35442900	-0.85703100	-0.00020900
H	4.13247000	-2.07926300	0.00003100
H	4.30961700	-0.57400200	-0.87494200
H	4.30909700	-0.57439200	0.87578000
C	1.92879800	0.56138100	0.00000500
H	1.91714200	-1.35928200	-0.86045100
H	1.91670200	-1.35970400	0.85956100
H	2.65175800	1.35429600	0.00015700
C	0.55474700	0.99491500	-0.00000700
O	0.21716000	2.15144700	0.00010000
O	-0.31753700	-0.01927400	-0.00018000
C	-1.69763700	0.33383700	-0.00012700
C	-2.50545500	-0.93817400	0.00010300
H	-1.90754000	0.93843600	-0.87344600
H	-1.90737900	0.93864100	0.87308800
C	-3.99775100	-0.65426500	0.00009100

H	-2.23721400	-1.52669400	-0.87011300
H	-2.23715400	-1.52645400	0.87046800
H	-4.29096600	-0.08576000	0.87510100
H	-4.29102700	-0.08605500	-0.87509400
H	-4.56661000	-1.57481600	0.00026800

Table S1-23 Geometry of product for reaction channel R4.

C	4.16228600	-0.04593000	0.30730800
C	2.79233300	0.52028200	-0.02229400
H	4.92727700	0.71593300	0.22836800
H	4.19360100	-0.44050800	1.31687700
H	4.42913600	-0.85156300	-0.36766300
C	1.70136600	-0.52639000	0.08302900
H	2.56070800	1.34451300	0.64121300
H	2.79206500	0.93562900	-1.02268200
H	1.89266700	-1.36300200	-0.58149700
H	1.66107700	-0.95184000	1.08108500
C	0.33493800	0.00091100	-0.23810500
O	0.07372500	1.12294600	-0.53088500
O	-0.58003500	-0.98305500	-0.16095900
C	-1.91348200	-0.71171300	-0.36197600
C	-2.62695800	0.23151000	0.52979100
H	-2.41379000	-1.56222400	-0.78423400
C	-4.09789400	0.34004500	0.16284700
H	-2.53000800	-0.11155400	1.56187900
H	-2.15522500	1.20468700	0.48725600
H	-4.21964800	0.72348800	-0.84237400
H	-4.59003200	-0.62438300	0.21379900
H	-4.61287700	1.00939800	0.83913100

Table S1-24 Geometry of product for reaction channel R5.

C	4.19417200	-0.61492500	0.03703400
C	2.97056100	0.28421800	0.01502900
H	5.10618600	-0.03164400	0.04203700
H	4.20299300	-1.24742500	0.91782400
H	4.22270000	-1.26324600	-0.83175600
C	1.67915400	-0.50913800	0.00778600
H	2.97815400	0.94473900	0.87345700
H	2.99764400	0.92888700	-0.85499100
H	1.63111000	-1.17208100	-0.85039500
H	1.61038200	-1.15463800	0.87772300
C	0.44784600	0.34856400	-0.01549000
O	0.43605000	1.54174000	-0.02802400
O	-0.65802700	-0.39241900	-0.01966000

C	-1.89578800	0.31371800	-0.04541600
C	-2.99927200	-0.66482700	-0.05432900
H	-1.90881300	0.95678100	-0.92430900
H	-1.95168600	0.97261200	0.81516100
C	-4.39661500	-0.20143600	0.10638400
H	-2.79236200	-1.65024800	-0.42563300
H	-4.48703200	0.51913400	0.91331800
H	-4.76902800	0.29153200	-0.79287600
H	-5.06478600	-1.02602300	0.31591900

Table S1-25 Geometry of product for reaction channel R6.

C	-4.17125900	-0.59988000	0.02453400
C	-2.94435100	0.29485000	0.00826800
H	-5.08112100	-0.01325500	0.02853700
H	-4.19978500	-1.24578700	-0.84605100
H	-4.18493400	-1.23466000	0.90363400
C	-1.65563200	-0.50293800	0.00284200
H	-2.96643300	0.94178200	-0.86016400
H	-2.95212900	0.95333100	0.86829600
H	-1.59173200	-1.15098600	0.87124700
H	-1.60762800	-1.16383200	-0.85698900
C	-0.42146700	0.35079300	-0.01575400
O	-0.40594300	1.54362900	-0.03366800
O	0.68335500	-0.39272900	-0.00997400
C	1.92383700	0.30959600	-0.03214500
C	3.03266700	-0.71467400	-0.00731800
H	1.97382900	0.96677700	0.82619700
H	1.96869400	0.92334600	-0.92136100
C	4.37399800	-0.08667800	0.03752400
H	2.88407800	-1.35803600	0.86147800
H	2.94556400	-1.36381200	-0.87219200
H	4.52405300	0.85777400	0.52521000
H	5.24148700	-0.62625200	-0.28640000

Table S1-26 Geometry of HCl.

Cl	0.00000000	0.00000000	0.07050100
H	0.00000000	0.00000000	-1.19851300

Table S2 Optimized Cartesian Coordinates for the reaction of PB with OH radicals at the M062x/6-311+G(2d,2p) level of theory.

Table S2-1 Geometry of propyl butanoate (PB).

C	4.25490200	-0.56513900	-0.00015300
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C	3.00986800	0.31451600	-0.00009500
H	5.16293000	0.03583200	-0.00032700
H	4.27898800	-1.20845100	0.88065200
H	4.27877200	-1.20864000	-0.88082600
C	1.73606400	-0.51642000	0.00015600
H	3.00781300	0.97043600	0.87081900
H	3.00759400	0.97024400	-0.87115200
H	1.69241600	-1.17458800	-0.87102000
H	1.69261600	-1.17436100	0.87151300
C	0.48687100	0.32693300	0.00021400
O	0.45994500	1.52776100	0.00001900
O	-0.61904300	-0.43397800	0.00011600
C	-1.86087600	0.28195300	-0.00000600
C	-2.98546300	-0.72843400	-0.00001400
H	-1.89853500	0.92532300	-0.88049400
H	-1.89864600	0.92543200	0.88039700
C	-4.34241300	-0.03252700	-0.00013600
H	-2.88732000	-1.36992900	-0.87709200
H	-2.88742300	-1.36982000	0.87715600
H	-4.45779400	0.60001000	0.88072500
H	-4.45770500	0.59987300	-0.88110700
H	-5.15463700	-0.75691000	-0.00012100

Table S2-2 Geometry of pre-reactive complex for reaction channel R1.

C	3.80712000	1.47709800	-0.00000100
C	2.69814900	0.43204600	-0.00000100
H	4.78727800	1.00388100	0.00000000
H	3.74352400	2.11702400	-0.88118100
H	3.74352300	2.11702400	0.88117800
C	1.31922800	1.07445600	0.00000200
H	2.79517400	-0.21480400	-0.87368400
H	2.79517800	-0.21480800	0.87367900
H	1.18162200	1.72001700	0.87098100
H	1.18161900	1.72002200	-0.87097400
C	0.19463500	0.07434400	0.00000200
O	0.32585000	-1.12659400	0.00000400
O	-0.99986300	0.66460300	0.00000000
C	-2.13612200	-0.21542700	0.00000000
C	-3.38604100	0.63482400	-0.00000200
H	-2.08486400	-0.85588400	0.88133400
H	-2.08486200	-0.85588700	-0.88133300
C	-4.63530900	-0.24024100	0.00000000
H	-3.37518700	1.28278500	0.87745200
H	-3.37518700	1.28278200	-0.87745900
H	-4.66320900	-0.88199900	-0.88112100

H	-4.66320700	-0.88199700	0.88112100
H	-5.53797200	0.36745700	0.00000000
O	2.74036900	-2.65020000	-0.00000300
H	1.85577200	-2.23067800	0.00000400

Table S2-3 Geometry of pre-reactive complex for reaction channel R2.

C	-3.54830800	-1.58427700	0.19799200
C	-2.24403600	-0.88979400	0.56616200
H	-4.11055800	-1.86028900	1.08856600
H	-4.17231500	-0.92359900	-0.40427600
H	-3.35900700	-2.49166000	-0.37693500
C	-1.43945700	-0.51790400	-0.68729800
H	-2.45715900	0.01613300	1.13694700
H	-1.63618300	-1.53427900	1.20442400
H	-1.13558900	-1.41371100	-1.22546900
H	-2.05909900	0.10073200	-1.33706500
C	-0.22750200	0.28639500	-0.31162300
O	-0.26249700	1.44376800	0.04308100
O	0.90308600	-0.41334100	-0.36508500
C	2.09611800	0.28372600	0.03162000
C	3.25432400	-0.68185400	-0.07402000
H	1.96619200	0.65082400	1.05031000
H	2.22918800	1.14816500	-0.62012700
C	4.56126300	-0.01206500	0.33618300
H	3.05343500	-1.54564600	0.56131900
H	3.31943200	-1.04740000	-1.09971800
H	4.78183700	0.84339700	-0.30304000
H	4.51260100	0.34481800	1.36537400
H	5.39510500	-0.70734000	0.26280100
O	-3.01645000	2.09490800	0.10358200
H	-2.03540900	2.11181300	0.09017100

Table S2-4 Geometry of pre-reactive complex for reaction channel R3.

C	-3.54735600	-1.58442700	0.19815500
C	-2.24271500	-0.89025600	0.56568300
H	-4.10859500	-1.86156200	1.08901500
H	-4.17206100	-0.92306200	-0.40263500
H	-3.35857400	-2.49107900	-0.37808900
C	-1.43993000	-0.51636700	-0.68837000
H	-2.45534700	0.01477800	1.13810100
H	-1.63390300	-1.53553500	1.20221000
H	-1.13652700	-1.41138600	-1.22813200
H	-2.06065400	0.10306700	-1.33634100
C	-0.22760100	0.28759400	-0.31314400

O	-0.26189300	1.44542900	0.04011300
O	0.90241500	-0.41324300	-0.36462300
C	2.09571600	0.28359000	0.03167500
C	3.25356000	-0.68254600	-0.07272800
H	1.96570700	0.65188400	1.04991600
H	2.22942200	1.14724000	-0.62099100
C	4.56071300	-0.01247400	0.33638200
H	3.05257300	-1.54544200	0.56378600
H	3.31845100	-1.04944600	-1.09795800
H	4.78119200	0.84218800	-0.30394100
H	4.51233100	0.34566300	1.36514900
H	5.39445900	-0.70792600	0.26361900
O	-3.01644100	2.09270500	0.10674800
H	-2.03544000	2.11080700	0.09247100

Table S2-5 Geometry of pre-reactive complex for reaction channel R4.

C	4.50703100	-0.49872300	-0.00001400
C	3.18456900	0.25928600	-0.00001600
H	5.35287300	0.18654900	-0.00003400
H	4.59283700	-1.13640000	0.88072900
H	4.59282200	-1.13643300	-0.88073500
C	1.99584200	-0.68944700	0.00000700
H	3.12088300	0.91142500	0.87120900
H	3.12087000	0.91139800	-0.87126100
H	2.01303000	-1.34901800	-0.87088200
H	2.01305200	-1.34899500	0.87091500
C	0.67111300	0.02469600	0.00002000
O	0.54195200	1.22589100	0.00006900
O	-0.35441000	-0.82519400	-0.00002500
C	-1.66826800	-0.24048700	0.00000300
C	-2.68437700	-1.35933700	-0.00001200
H	-1.77389200	0.39108900	-0.88381800
H	-1.77387700	0.39105100	0.88385200
C	-4.10139400	-0.79487100	0.00001000
H	-2.52256800	-1.98641800	-0.87769700
H	-2.52255400	-1.98645200	0.87764600
H	-4.27522200	-0.17529700	0.87995800
H	-4.27524000	-0.17527200	-0.87991600
H	-4.83951700	-1.59436200	0.00000600
O	-1.85115900	2.78298000	-0.00004300
H	-0.94165200	2.42102300	0.00003500

Table S2-6 Geometry of pre-reactive complex for reaction channel R5.

C	4.35827200	0.50339600	-0.00006000
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C	3.17690900	-0.45923500	-0.00010100
H	5.30383500	-0.03608100	-0.00020300
H	4.33996500	1.14674000	-0.88076900
H	4.34009600	1.14650600	0.88082400
C	1.84828000	0.28147300	0.00012900
H	3.21822200	-1.11311500	-0.87147200
H	3.21837500	-1.11337900	0.87106400
H	1.75999500	0.93389200	0.87318400
H	1.75985000	0.93420500	-0.87267500
C	0.66288600	-0.64744600	0.00006300
O	0.70678800	-1.84422200	-0.00008500
O	-0.50008300	0.03985900	0.00018900
C	-1.70251200	-0.75108100	0.00007000
C	-2.88486300	0.19271000	0.00003900
H	-1.69730800	-1.39213900	0.88191900
H	-1.69719100	-1.39205100	-0.88184100
C	-4.19638700	-0.58599200	-0.00012500
H	-2.82977800	0.83913400	0.87845200
H	-2.82963900	0.83923600	-0.87829800
H	-4.27174800	-1.22343100	-0.88157900
H	-4.27189300	-1.22355000	0.88123100
H	-5.04974700	0.08875000	-0.00014700
O	-1.21663000	2.85274300	-0.00010900
H	-0.78915000	1.97529600	0.00025300

Table S2-7 Geometry of pre-reactive complex for reaction channel R6.

C	-4.50703300	-0.49872100	0.00002900
C	-3.18457200	0.25929000	0.00004300
H	-5.35287700	0.18655100	0.00008500
H	-4.59284900	-1.13636400	-0.88073700
H	-4.59281300	-1.13646400	0.88072700
C	-1.99584500	-0.68944200	-0.00002300
H	-3.12089500	0.91145800	-0.87116000
H	-3.12086600	0.91137200	0.87131000
H	-2.01301900	-1.34904000	0.87084600
H	-2.01306800	-1.34896500	-0.87095100
C	-0.67111600	0.02470000	-0.00004200
O	-0.54195400	1.22589600	-0.00012600
O	0.35440700	-0.82519200	0.00003500
C	1.66826500	-0.24048700	-0.00001900
C	2.68437400	-1.35933700	0.00003900
H	1.77389500	0.39112300	0.88378000
H	1.77387100	0.39101700	-0.88389100
C	4.10139200	-0.79487200	-0.00001500
H	2.52257100	-1.98638300	0.87775000

H	2.52254600	-1.98648800	-0.87759400
H	4.27521200	-0.17533100	-0.87998800
H	4.27524400	-0.17524000	0.87988700
H	4.83951300	-1.59436300	0.00001300
O	1.85118200	2.78296000	0.00008100
H	0.94166900	2.42101900	-0.00007200

Table S2-8 Geometry of transition state for reaction channel R1.

C	-3.50724600	-0.96002100	0.00454300
C	-2.33616300	-0.00061600	-0.00428800
H	-4.51373300	-0.36167300	-0.01654800
H	-3.55057700	-1.59396400	-0.88033500
H	-3.56240500	-1.56490400	0.90874000
C	-1.00586200	-0.74380100	0.00945000
H	-2.37521600	0.63950900	-0.88634800
H	-2.37847000	0.66123700	0.86173500
H	-0.91947500	-1.38561500	0.88906500
H	-0.91129600	-1.40467600	-0.85482500
C	0.17457600	0.19533500	0.00595300
O	0.10303800	1.39430500	0.00728700
O	1.33396700	-0.47638200	0.00201700
C	2.51820500	0.33376400	-0.00053000
C	3.71720000	-0.58718400	-0.00392400
H	2.50824000	0.97694400	0.88052400
H	2.50389600	0.97762600	-0.88103000
C	5.01555300	0.21312200	-0.00721400
H	3.67166400	-1.23407100	0.87333800
H	3.66703400	-1.23364000	-0.88125700
H	5.07811800	0.85239800	-0.88844800
H	5.08245700	0.85269100	0.87349600
H	5.88197200	-0.44529200	-0.00922100
O	-5.52315200	0.60493400	-0.02356000
H	-4.95060400	1.37698200	0.10121100

Table S2-9 Geometry of transition state for reaction channel R2.

C	-3.85175800	-1.22568200	-0.02234800
C	-2.66459800	-0.37395700	0.37674500
H	-4.77876000	-0.81788600	0.37557100
H	-3.94248400	-1.28101400	-1.10737000
H	-3.74025000	-2.24420600	0.35731500
C	-1.35099200	-0.86031400	-0.19526800
H	-2.85598000	0.69818900	-0.04919800
H	-2.59899600	-0.22528800	1.45436100
H	-1.12345400	-1.87583800	0.13811000

H	-1.40155600	-0.90405300	-1.28675200
C	-0.17934000	0.02071700	0.15753600
O	-0.25643900	1.12736900	0.62954100
O	0.98329300	-0.56868000	-0.12974000
C	2.16147300	0.21151200	0.12739600
C	3.36335300	-0.61550200	-0.26896600
H	2.18424900	0.47586200	1.18537500
H	2.10297700	1.13754300	-0.44618600
C	4.65752800	0.15201900	-0.02107300
H	3.35748800	-1.54560100	0.30095900
H	3.27652100	-0.88470500	-1.32251400
H	4.67945600	1.07851600	-0.59556800
H	4.76415700	0.41047600	1.03286600
H	5.52396700	-0.44019300	-0.30895100
O	-2.76962500	1.99074900	-0.56529200
H	-1.91916000	2.16993200	-0.12823600

Table S2-10 Geometry of transition state for reaction channel R3.

C	3.63291900	-1.46647700	-0.03049200
C	2.26704500	-1.04036500	-0.55501000
H	4.17501300	-2.04349400	-0.77771100
H	4.22680100	-0.58907200	0.22438500
H	3.53270500	-2.08170300	0.86426400
C	1.50114600	-0.22776700	0.47617100
H	2.37880900	-0.43670200	-1.45679600
H	1.67288300	-1.91773900	-0.82682600
H	1.33740500	-0.75830000	1.41239400
H	2.18447300	0.71070700	0.73365700
C	0.23741000	0.36542600	-0.07095500
O	0.20947900	1.31459000	-0.81483700
O	-0.85377700	-0.28760100	0.33153800
C	-2.10175000	0.20920500	-0.18073600
C	-3.21382900	-0.62150900	0.41731900
H	-2.08559300	0.14135300	-1.26938200
H	-2.19484300	1.26256300	0.08610600
C	-4.57417900	-0.15711400	-0.09194700
H	-3.05002000	-1.66986700	0.16413400
H	-3.16767700	-0.54388100	1.50447000
H	-4.75129100	0.88867000	0.16097400
H	-4.64067900	-0.25366900	-1.17607700
H	-5.37682500	-0.74715700	0.34601300
O	2.78488700	1.90518500	0.52813200
H	2.14154800	2.21250300	-0.13438500

Table S2-11 Geometry of transition state for reaction channel R4.

C	4.47538600	-0.45422600	-0.29344700
C	3.18782500	0.22069800	0.16369900
H	5.34693600	0.14482100	-0.03476000
H	4.59206900	-1.43333500	0.17334200
H	4.47821200	-0.60040100	-1.37435200
C	1.96366100	-0.60917200	-0.19091700
H	3.20696800	0.38621800	1.24113100
H	3.09280600	1.20676100	-0.29177500
H	1.89913900	-0.78340400	-1.26776600
H	2.00762800	-1.60010800	0.26777700
C	0.67504600	0.03619300	0.23857700
O	0.57975000	1.09301500	0.80568900
O	-0.38898600	-0.71549700	-0.09360200
C	-1.65748400	-0.20964600	0.27875600
C	-2.74134700	-1.12574300	-0.22341800
H	-1.80169600	0.83318300	-0.22219700
H	-1.69376500	-0.02095700	1.35269000
C	-4.11990200	-0.56381500	0.10594000
H	-2.62327800	-1.24850800	-1.30080200
H	-2.60633300	-2.11142300	0.22901700
H	-4.25237100	-0.45789600	1.18306500
H	-4.25248800	0.41917500	-0.34581200
H	-4.90472100	-1.21956800	-0.26532700
O	-1.72220400	2.16557700	-0.67216400
H	-0.93669400	2.37495900	-0.13875600

Table S2-12 Geometry of transition state for reaction channel R5.

C	4.45428500	0.63337100	0.23618800
C	3.28463200	-0.26652800	-0.14465500
H	5.40301800	0.19667400	-0.07127200
H	4.36658700	1.61156500	-0.23876800
H	4.49195000	0.79127600	1.31484800
C	1.95299400	0.33739500	0.27324400
H	3.27367800	-0.44141700	-1.22065700
H	3.39240900	-1.24737300	0.31905000
H	1.91736000	0.51308800	1.35123300
H	1.79984500	1.31432400	-0.19257800
C	0.77838000	-0.53421300	-0.08615700
O	0.84046300	-1.60122800	-0.62924700
O	-0.38806000	0.03299000	0.28393600
C	-1.56735500	-0.72508800	-0.02425000
C	-2.75238100	0.02627300	0.52004100
H	-1.47864600	-1.71733100	0.42245300
H	-1.63726800	-0.84769400	-1.10592200
C	-4.07963900	-0.59474300	0.13771700

H	-2.65444400	0.19072300	1.59332300
H	-2.70879700	1.09455300	0.05194000
H	-4.17719100	-0.66891900	-0.94517000
H	-4.16772100	-1.60114000	0.55344300
H	-4.91100700	-0.00325300	0.51459900
O	-2.20905700	2.25213400	-0.58791800
H	-1.28203600	2.08496000	-0.35345900

Table S2-13 Geometry of transition state for reaction channel R6.

C	-4.77148000	-0.14935100	-0.41089000
C	-3.46328200	0.45475600	0.08571700
H	-5.61973800	0.48591300	-0.16092000
H	-4.75710000	-0.27814900	-1.49404900
H	-4.94418600	-1.12944700	0.03628100
C	-2.27256500	-0.42847800	-0.25283400
H	-3.31025900	1.44178900	-0.35146800
H	-3.49936500	0.60589200	1.16484800
H	-2.37964500	-1.42386000	0.18520200
H	-2.18901600	-0.58622400	-1.33090700
C	-0.96441000	0.14508500	0.22647800
O	-0.83432400	1.18420100	0.81426000
O	0.06756300	-0.65629500	-0.08596500
C	1.35778400	-0.17818600	0.31049200
C	2.38363900	-1.20838800	-0.10775800
H	1.36355200	-0.02400200	1.39106600
H	1.54912400	0.78157600	-0.17002700
C	3.77768000	-0.78393700	0.30166900
H	2.13861500	-2.16821700	0.35477700
H	2.33342400	-1.34975800	-1.18782600
H	4.02602100	0.22136800	-0.24199500
H	3.87392400	-0.59021800	1.36939500
H	4.55693900	-1.46653300	-0.02909000
O	4.08847600	1.51696300	-0.78974400
H	3.99978900	2.01190900	0.03906300

Table S2-14 Geometry of post-reactive complex for reaction channel R1.

C	-3.43669000	-1.38725600	0.02423500
C	-2.35093000	-0.36868300	0.06338900
H	-4.98644600	0.40287700	0.00708300
H	-3.77694600	-1.78687500	-0.92012000
H	-3.72804500	-1.91194900	0.92239000
C	-0.95878400	-1.00403400	-0.02805700
H	-2.45749200	0.33865300	-0.76057500
H	-2.40064600	0.21257500	0.98567800

H	-0.79051100	-1.71093200	0.78596300
H	-0.84659500	-1.57329300	-0.95267700
C	0.13490600	0.03476300	0.01475100
O	-0.04390400	1.22093100	0.07775900
O	1.34811800	-0.53027000	-0.02950500
C	2.45745300	0.38005700	-0.00200900
C	3.73103800	-0.43454600	-0.02563600
H	2.38961000	0.99389400	0.89715600
H	2.38932800	1.04549000	-0.86397500
C	4.95728000	0.47210400	-0.01176300
H	3.74097900	-1.10124200	0.83778300
H	3.73345800	-1.06437000	-0.91634400
H	4.96870500	1.12784100	-0.88287500
H	4.96911600	1.10095700	0.87903800
H	5.87540500	-0.11203700	-0.02081000
O	-5.27883800	1.31492600	-0.08160300
H	-4.48857300	1.83927600	0.05961000

Table S2-15 Geometry of post-reactive complex for reaction channel R2.

C	-3.92669300	-1.12492900	-0.06728500
C	-2.61087800	-0.72106200	0.49363400
H	-4.74842700	-0.85739500	0.59426200
H	-4.09613800	-0.65144500	-1.03869000
H	-3.98417700	-2.20757300	-0.23679900
C	-1.39048300	-0.83519000	-0.34877200
H	-3.27933200	2.01539600	-0.24059600
H	-2.49420000	-0.54719700	1.55313000
H	-1.08284400	-1.87408100	-0.51284000
H	-1.58368600	-0.41640200	-1.34397000
C	-0.21300300	-0.07051900	0.20076300
O	-0.29350800	0.90313200	0.90898000
O	0.94989000	-0.57552500	-0.21127300
C	2.12406000	0.14163800	0.20244700
C	3.32764400	-0.55456200	-0.39057500
H	2.16120800	0.15613900	1.29238000
H	2.04398800	1.17327100	-0.14247000
C	4.61661400	0.16060000	-0.00010800
H	3.34629100	-1.58910400	-0.04498400
H	3.22114400	-0.58119200	-1.47588100
H	4.61248300	1.19308200	-0.35068100
H	4.74395700	0.17663700	1.08274100
H	5.48418600	-0.33489900	-0.43134900
O	-2.42080500	2.22335900	-0.61235400
H	-1.79262600	1.96117300	0.07230100

Table S2-16 Geometry of post-reactive complex for reaction channel R3.

C	-3.20828800	-0.85341700	-0.95580400
C	-2.63123600	-1.03402200	0.46147700
H	-4.26129700	-0.58580500	-0.89464800
H	-2.69037900	-0.04877700	-1.47445200
H	-3.10858900	-1.77031700	-1.53617900
C	-1.18159700	-1.33865800	0.41997300
H	-2.79966400	-0.10982600	1.01584300
H	-3.15919900	-1.83847200	0.97235300
H	-0.80795100	-2.35089500	0.46828500
H	-2.96303200	3.09238500	0.28673400
C	-0.21352200	-0.28490500	0.21752600
O	-0.48638700	0.89793200	0.10188000
O	1.04881400	-0.73982200	0.16802600
C	2.05988800	0.25510500	-0.03159600
C	3.40324700	-0.43867700	-0.03237500
H	1.99051600	0.99651200	0.76607900
H	1.87124500	0.76724600	-0.97675200
C	4.53373500	0.56409500	-0.23824300
H	3.53001600	-0.96538400	0.91446100
H	3.41371200	-1.19130500	-0.82202500
H	4.42559300	1.08598200	-1.18954100
H	4.54175300	1.31290400	0.55440700
H	5.50175700	0.06692100	-0.23814600
O	-3.05118600	2.15596400	0.10710900
H	-2.14777000	1.80910200	0.09171700

Table S2-17 Geometry of post-reactive complex for reaction channel R4.

C	4.25266200	-0.51518500	-0.46417200
C	3.01226400	-0.18814700	0.35888100
H	5.16249400	-0.27302800	0.08251100
H	4.28624800	-1.57566500	-0.71787900
H	4.26134900	0.05013300	-1.39679300
C	1.73547200	-0.51760400	-0.39857000
H	3.02458700	-0.73956500	1.29972900
H	3.00254300	0.86909400	0.62511900
H	1.67000200	0.05545600	-1.32769800
H	1.69568000	-1.57101300	-0.68516700
C	0.49725400	-0.19465400	0.38301100
O	0.45217400	0.35846000	1.44670900
O	-0.61910700	-0.58968600	-0.28607200
C	-1.83782000	-0.24119700	0.23297900
C	-3.00139700	-0.84061800	-0.46259500
H	-1.01788200	2.06603000	-0.65366500

H	-1.84911700	0.03497800	1.27766200
C	-4.31502600	-0.23587200	0.02382300
H	-2.88638900	-0.69888400	-1.53990600
H	-3.00942800	-1.92644400	-0.30089000
H	-4.43579600	-0.38279300	1.09719800
H	-4.34587900	0.83519800	-0.17371600
H	-5.16362900	-0.69905400	-0.47542200
O	-0.15091800	2.47748400	-0.59587600
H	0.08756900	2.38516100	0.33068600

Table S2-18 Geometry of post-reactive complex for reaction channel R5.

C	4.25206900	0.39219900	0.16420200
C	3.05479300	-0.49044000	-0.16847500
H	5.18202700	-0.06066000	-0.17597600
H	4.16016400	1.36957000	-0.31108400
H	4.33164700	0.55401000	1.24005900
C	1.75005500	0.14325300	0.28844500
H	3.00466100	-0.67163800	-1.24252800
H	3.16193000	-1.46985100	0.29871800
H	1.75542900	0.33161700	1.36526400
H	1.58928700	1.11759800	-0.18126400
C	0.55128500	-0.71270200	-0.01437700
O	0.56307100	-1.79749300	-0.52315600
O	-0.59532800	-0.09874500	0.36107500
C	-1.80969100	-0.80697200	0.06937300
C	-2.94842800	0.06520100	0.43980400
H	-1.79852200	-1.74923500	0.63042900
H	-1.83004100	-1.06898200	-0.99062600
C	-4.29489300	-0.19820600	-0.13182000
H	-2.85179200	0.64885700	1.34563800
H	-1.27253400	3.07437200	-0.75932700
H	-4.23935700	-0.37089800	-1.20833900
H	-4.75551000	-1.09237800	0.30679500
H	-4.97437000	0.63220900	0.04990400
O	-0.47715000	2.71678500	-0.36266800
H	-0.71890300	1.83703500	-0.05257300

Table S2-19 Geometry of post-reactive complex for reaction channel R6.

C	-4.64493600	0.22217400	-0.60359700
C	-3.40168500	0.25515700	0.27778900
H	-5.53237100	0.51596500	-0.04531500
H	-4.54211600	0.90182400	-1.45060400
H	-4.81626000	-0.77889700	-1.00174200
C	-2.15587600	-0.15442400	-0.49211000

H	-3.25362800	1.25389400	0.68886400
H	-3.52560500	-0.40767400	1.13445600
H	-2.25627600	-1.16190800	-0.90278300
H	-1.98643200	0.50054100	-1.35003800
C	-0.90925800	-0.12660800	0.35428800
O	-0.86266100	0.18472000	1.51337400
O	0.17018100	-0.49955000	-0.35141500
C	1.41056100	-0.47686600	0.36358600
C	2.49221000	-0.94097100	-0.59110300
H	1.33430800	-1.13542300	1.22998200
H	1.60406100	0.53619400	0.71389900
C	3.81452100	-1.04567200	0.08254200
H	2.19930700	-1.91589900	-1.00239000
H	2.54618900	-0.25333300	-1.43745000
H	3.95183600	1.30203200	0.00975200
H	3.87365400	-1.30018300	1.13164300
H	4.71653000	-1.13535100	-0.50369100
O	3.46581100	2.04624400	-0.35969000
H	3.86693200	2.83018000	0.01889700

Table S2-20 Geometry of product for reaction channel R1.

C	-4.29996000	-0.55846900	-0.00211100
C	-3.07831300	0.29060400	-0.00052600
H	-4.68748900	-0.96464500	-0.92405000
H	-4.73253100	-0.90783700	0.92279900
C	-1.79408800	-0.54797900	0.00263700
H	-3.05888600	0.94137900	-0.87559600
H	-3.06329500	0.94516400	0.87121800
H	-1.75188900	-1.20097400	0.87617500
H	-1.75133200	-1.20618400	-0.86701000
C	-0.55236200	0.30822300	0.00032400
O	-0.53828200	1.50926600	-0.00249400
O	0.55943000	-0.44243400	0.00196200
C	1.79606100	0.28379500	-0.00005600
C	2.92702300	-0.71987600	0.00107900
H	1.82951700	0.92848100	0.87932200
H	1.82851200	0.92532900	-0.88175700
C	4.28049500	-0.01720400	-0.00087400
H	2.83200600	-1.35992300	0.87926800
H	2.83105100	-1.36291900	-0.87481900
H	4.39260400	0.61409600	-0.88282000
H	4.39369200	0.61689700	0.87892200
H	5.09571900	-0.73808700	-0.00023200

Table S2-21 Geometry of product for reaction channel R2.

C	4.33300100	-0.46922100	-0.03552000
C	3.03057500	0.24572900	-0.04431500
H	5.16271300	0.20226500	-0.24469900
H	4.52902800	-0.94269700	0.93496300
H	4.35156900	-1.27398400	-0.77657400
C	1.76906300	-0.52947600	0.05086600
H	2.97783800	1.31991900	0.03386200
H	1.68416100	-1.27120100	-0.75157500
H	1.72118900	-1.12239900	0.97522300
C	0.52677900	0.32831900	0.01851500
O	0.50499200	1.52811200	0.01000300
O	-0.58021900	-0.42953900	0.01067700
C	-1.82077900	0.28908700	-0.00227900
C	-2.94583000	-0.72127200	-0.00747800
H	-1.85037200	0.92845400	-0.88561100
H	-1.86484500	0.93539300	0.87546700
C	-4.30327700	-0.02638700	-0.02070000
H	-2.83977200	-1.36535600	-0.88144300
H	-2.85362700	-1.35899500	0.87271000
H	-4.42638200	0.60890300	0.85689900
H	-4.41252700	0.60237900	-0.90479800
H	-5.11434100	-0.75193800	-0.02438500

Table S2-22 Geometry of product for reaction channel R3.

C	-3.86361900	-1.03668400	-0.02800400
C	-2.35107800	-0.85345700	0.02990900
H	-4.13116900	-2.09146300	-0.00390300
H	-4.34651400	-0.54672700	0.81738600
H	-4.27114600	-0.60618300	-0.94256200
C	-1.93867900	0.57255000	0.00806700
H	-1.94122600	-1.32664200	0.92919900
H	-1.86586300	-1.37712700	-0.80004300
H	-2.67047500	1.36770300	0.00493700
C	-0.55721600	1.00327900	0.00203300
O	-0.19975600	2.16155500	-0.00783700
O	0.30807100	-0.03443400	0.00877000
C	1.69267300	0.32476300	0.00142000
C	2.50567900	-0.95058700	-0.00212500
H	1.90841200	0.93486700	0.88030100
H	1.89945400	0.93403400	-0.88010200
C	3.99995500	-0.64672800	-0.00814500
H	2.24134600	-1.54181700	0.87595400
H	2.23434000	-1.54115500	-0.87853900
H	4.27809300	-0.06819800	-0.88968800
H	4.28541000	-0.06959200	0.87197200

H	4.58652600	-1.56349000	-0.01132300
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Table S2-23 Geometry of product for reaction channel R4.

C	4.15953400	0.02550800	0.33057500
C	2.78717800	-0.51946600	-0.04661800
H	4.93076700	-0.73394700	0.21246200
H	4.42945200	0.87688000	-0.29585900
H	4.17576700	0.36056800	1.36868600
C	1.70235000	0.53523800	0.10524200
H	2.79141600	-0.87985100	-1.07575100
H	2.53602900	-1.38067400	0.57286700
H	1.65808800	0.91305200	1.13008000
H	1.90148200	1.40648800	-0.52323900
C	0.33382000	0.01678900	-0.24656300
O	0.07040400	-1.10777600	-0.55949100
O	-0.58765500	1.01187400	-0.17197500
C	-1.92147300	0.71295700	-0.36740900
C	-2.60278200	-0.27330400	0.51200700
H	-2.45381400	1.57169900	-0.75179500
C	-4.09433400	-0.34029800	0.19763800
H	-2.14354500	-1.25481400	0.39481400
H	-2.45338800	0.01671000	1.56082400
H	-4.56783100	0.63293800	0.33095300
H	-4.25577800	-0.65556800	-0.83271800
H	-4.59639500	-1.05081500	0.85118200

Table S2-24 Geometry of product for reaction channel R5.

C	-4.21006800	-0.58917300	0.04176700
C	-2.97183000	0.29962200	0.01838500
H	-5.12240500	0.00515300	0.04688600
H	-4.23972300	-1.24101300	-0.83250300
H	-4.21900500	-1.22432600	0.92869100
C	-1.69209200	-0.52197500	0.00886600
H	-2.98554200	0.94791600	-0.85807400
H	-2.96352900	0.96265400	0.88380900
H	-1.63086500	-1.17090200	0.88582800
H	-1.65575900	-1.18821000	-0.85645800
C	-0.44946400	0.32987000	-0.01804900
O	-0.42929800	1.53063700	-0.03295200
O	0.66112300	-0.42487300	-0.02304500
C	1.89615200	0.29984000	-0.05480100
C	3.01514600	-0.66839900	-0.05330700
H	1.94434700	0.97206700	0.80675900
H	1.89896300	0.94083000	-0.94591500

C	4.40438800	-0.16913700	0.11925800
H	2.83266500	-1.64885200	-0.46918300
H	4.77029700	0.34221200	-0.78039400
H	4.46565700	0.55409400	0.93546200
H	5.09691300	-0.98161900	0.33036100

Table S2-25 Geometry of product for reaction channel R6.

C	-4.18617200	-0.57711600	0.02179400
C	-2.94586700	0.30903500	0.00990300
H	-5.09719800	0.01919800	0.02680600
H	-4.21333700	-1.22299500	-0.85697700
H	-4.20048100	-1.21816500	0.90440000
C	-1.66789900	-0.51535400	0.00150800
H	-2.95382700	0.96272600	-0.86255900
H	-2.94032100	0.96673500	0.87944000
H	-1.61262200	-1.17013300	0.87448700
H	-1.62916700	-1.17613000	-0.86796700
C	-0.42325500	0.33376700	-0.01486500
O	-0.40002500	1.53416200	-0.03071700
O	0.68698800	-0.42273400	-0.01033200
C	1.92389400	0.29857900	-0.03298300
C	3.04896200	-0.71543600	0.00002600
H	1.96427300	0.96500500	0.82958900
H	1.96391800	0.91389300	-0.93192100
C	4.37979700	-0.05403300	0.02865000
H	2.91028500	-1.35359100	0.88316200
H	2.96684800	-1.37929300	-0.86345500
H	4.49993700	0.91909800	0.48210300
H	5.26922300	-0.59442600	-0.25291800

Table S2-26 Geometry of H₂O.

O	0.00000000	0.00000000	0.11641900
H	0.00000000	0.76107600	-0.46567500
H	0.00000000	-0.76107600	-0.46567500

Table S2-27 Geometry of OH radical.

O	0.00000000	0.00000000	0.10787100
H	0.00000000	0.00000000	-0.86297200

Table S3 Vibrational frequencies (in cm^{-1}) for all the stationary points involved in the PB + Cl reaction at the BHandHLYP/6-311+G(2d,2p) level of theory.

Species	
PB	HCl
36.4	3029.4
62.6	
73.1	
91.0	
107.1	
197.9	
200.6	
244.6	
250.6	
304.9	
345.9	
374.8	
523.2	
614.1	
746.0	
781.5	
789.7	
923.4	
928.0	
931.7	
955.7	
990.7	
1061.8	
1088.4	
1097.9	
1176.8	
1178.9	
1197.8	
1236.5	
1275.7	
1306.4	
1327.9	
1374.0	
1381.1	
1390.3	
1402.7	
1471.8	
1477.3	
1478.1	
1498.6	

1522.6	
1551.0	
1553.1	
1558.5	
1559.5	
1565.7	
1569.5	
1581.3	
1873.8	
3112.9	
3119.0	
3125.0	
3126.8	
3140.0	
3145.9	
3146.5	
3151.0	
3159.8	
3176.0	
3183.0	
3185.1	
3189.5	
3195.1	

Pre-reactive complexes					
Pre1	Pre2	Pre3	Pre4	Pre5	Pre6
11.4	26.4	29.3	27.6	29.3	12.5
15.7	45.4	35.5	37.5	35.5	17.4
38.6	65.9	58.6	49.4	58.6	30.5
44.9	71.7	67.0	60.3	67.0	45.1
60.9	79.6	71.5	77.6	71.5	68.6
75.5	82.1	85.0	77.8	85.0	81.3
92.8	110.5	95.7	94.7	95.7	91.9
105.9	151.5	113.1	107.8	113.1	107.6
197.0	180.7	196.0	199.5	196.0	197.4
201.5	244.0	217.7	210.6	217.7	201.0
239.6	250.5	241.8	234.8	241.8	253.5
253.0	254.8	253.6	253.4	253.5	255.5
306.4	301.9	305.0	305.4	305.0	305.4
345.3	353.2	347.4	341.7	347.4	345.6
375.8	384.3	376.7	379.9	376.7	375.1
523.2	507.2	522.1	523.3	522.1	523.0
613.9	681.0	612.0	616.3	612.0	613.8
746.2	781.6	743.0	744.7	743.0	745.9

782.4	789.7	782.2	781.9	782.2	781.0
790.5	808.9	789.3	792.0	789.3	789.3
924.7	920.8	923.9	923.6	923.9	922.6
931.1	930.0	927.1	929.6	927.1	927.7
932.3	939.4	931.4	933.7	931.4	930.7
960.0	949.5	955.7	956.3	955.7	955.4
990.3	989.9	981.5	990.2	981.5	990.5
1061.8	1060.1	1050.9	1058.5	1050.9	1062.4
1086.7	1083.0	1088.2	1088.6	1088.2	1088.4
1097.5	1094.9	1093.3	1094.9	1093.3	1097.8
1176.8	1158.3	1176.9	1177.8	1176.9	1176.8
1180.6	1168.7	1178.6	1179.4	1178.6	1178.9
1197.4	1197.8	1195.8	1197.3	1195.8	1197.1
1236.2	1235.9	1232.0	1235.0	1232.0	1234.3
1277.1	1294.6	1248.3	1288.1	1248.3	1274.5
1306.7	1327.8	1309.1	1308.5	1309.1	1306.2
1327.1	1346.4	1330.0	1328.0	1330.0	1326.4
1374.3	1375.9	1377.2	1377.9	1377.2	1375.0
1381.0	1380.5	1382.9	1382.9	1382.9	1380.7
1390.6	1391.8	1389.9	1391.8	1389.9	1390.3
1403.3	1415.6	1399.9	1404.9	1399.9	1402.8
1471.7	1449.5	1471.6	1472.3	1471.6	1468.2
1473.3	1475.0	1476.7	1477.5	1476.7	1472.1
1477.2	1478.3	1477.8	1478.3	1477.8	1477.5
1498.5	1494.4	1493.9	1501.8	1493.9	1499.1
1522.6	1546.1	1522.1	1520.1	1522.1	1521.9
1550.9	1553.6	1551.2	1551.1	1551.2	1551.0
1552.5	1553.8	1553.1	1553.1	1553.1	1552.0
1553.3	1557.0	1558.9	1557.9	1558.9	1558.8
1558.5	1559.7	1559.2	1558.9	1559.2	1559.8
1565.9	1565.3	1564.4	1565.3	1564.4	1566.5
1569.7	1568.9	1569.5	1569.4	1569.5	1569.3
1581.6	1580.2	1579.4	1580.4	1579.4	1581.4
1873.8	1808.9	1882.4	1841.8	1882.4	1874.3
3108.6	3117.8	3114.1	3114.1	3114.1	3107.6
3118.9	3120.7	3119.5	3120.3	3119.5	3113.2
3126.1	3125.6	3128.7	3126.0	3128.7	3125.0
3127.5	3129.1	3130.9	3128.0	3130.9	3129.0
3140.5	3153.5	3140.9	3141.6	3140.9	3140.2
3147.0	3154.4	3151.8	3148.2	3151.8	3146.4
3148.2	3156.9	3154.1	3153.5	3154.1	3146.6
3151.6	3161.7	3157.6	3155.3	3157.6	3148.9
3159.0	3180.0	3164.1	3161.3	3164.1	3160.2
3165.7	3183.3	3180.1	3180.2	3180.1	3167.2
3176.1	3187.0	3184.4	3185.5	3184.4	3179.8

3187.3	3192.4	3187.2	3186.8	3187.2	3183.4
3189.8	3203.4	3191.3	3190.6	3191.3	3185.5
3196.2	3213.6	3205.8	3206.5	3205.8	3195.4

Transition states					
TS1	TS2	TS3	TS4	TS5	TS6
<i>i</i> 1025.6	<i>i</i> 922.9	<i>i</i> 1195.2	<i>i</i> 854.9	<i>i</i> 978.9	<i>i</i> 1021.7
16.6	18.5	27.3	33.8	25.7	26.2
42.4	42.9	53.3	44.2	33.0	30.7
58.0	67.3	70.5	62.3	46.5	44.6
68.5	77.7	75.1	76.5	78.5	73.6
77.5	85.8	92.4	94.7	93.8	88.0
96.5	125.2	95.9	107.4	115.6	100.9
106.5	149.6	131.5	124.0	148.4	145.1
192.7	189.1	197.4	196.8	188.6	196.5
198.2	203.2	207.7	212.1	197.3	204.1
238.3	225.6	238.9	246.6	210.2	252.1
277.4	240.0	252.8	250.3	249.2	308.6
340.8	307.1	308.2	309.9	309.7	343.9
357.1	342.1	343.1	356.9	342.0	375.2
430.2	375.8	374.9	383.4	376.3	436.4
510.4	467.7	424.8	440.8	470.8	488.7
525.8	515.6	519.5	537.3	527.7	528.7
614.8	619.0	665.9	599.9	610.9	612.8
742.6	750.3	750.0	742.5	747.7	746.7
784.4	790.3	768.5	777.7	780.6	770.0
790.7	796.6	790.2	782.1	786.3	781.7
866.8	910.0	901.0	912.5	903.6	885.4
910.5	930.5	930.1	923.6	924.0	918.8
931.3	932.4	931.0	929.5	928.6	924.8
940.5	955.7	953.7	957.1	956.4	948.5
989.7	991.8	980.1	975.9	987.2	980.6
991.8	1016.8	1014.3	1074.1	1010.8	1009.2
1036.6	1046.7	1062.5	1088.0	1054.1	1028.8
1082.4	1063.4	1086.3	1091.8	1085.8	1079.7
1090.4	1095.0	1097.2	1126.2	1095.9	1090.8
1106.9	1146.5	1119.0	1158.8	1155.1	1134.9
1171.9	1177.5	1195.6	1177.4	1177.9	1177.8
1192.4	1197.2	1199.0	1199.7	1181.0	1179.5
1197.1	1208.8	1218.2	1212.5	1206.5	1203.2
1236.2	1236.7	1236.0	1226.2	1233.1	1225.2
1279.3	1289.5	1280.2	1268.2	1268.4	1269.8
1308.9	1300.6	1327.9	1307.7	1307.3	1297.4
1327.9	1328.6	1332.8	1343.4	1324.4	1307.6

1375.2	1376.1	1376.4	1377.6	1375.8	1363.2
1376.7	1379.0	1385.6	1383.2	1381.9	1382.4
1378.9	1399.3	1401.6	1392.3	1399.4	1393.3
1398.1	1466.6	1473.1	1465.0	1470.8	1404.3
1460.1	1477.1	1477.4	1478.3	1473.8	1473.6
1477.6	1479.2	1481.1	1482.5	1478.0	1478.1
1497.0	1499.9	1501.3	1485.2	1495.6	1500.8
1521.6	1505.5	1523.4	1518.6	1521.4	1521.3
1529.2	1536.1	1553.4	1534.1	1536.5	1522.2
1553.4	1548.5	1558.7	1551.8	1547.7	1530.6
1557.6	1553.6	1558.8	1558.8	1551.1	1550.8
1558.6	1559.2	1564.5	1559.5	1552.7	1558.9
1566.1	1566.1	1565.4	1566.7	1558.3	1569.2
1581.4	1581.1	1580.2	1569.9	1569.6	1580.1
1877.2	1877.7	1855.9	1912.6	1881.6	1881.3
3120.0	3086.2	3084.4	3097.3	3099.3	3081.3
3128.0	3096.6	3119.8	3115.8	3106.7	3113.8
3136.0	3120.0	3125.1	3125.9	3114.4	3125.4
3149.8	3129.0	3130.3	3129.3	3127.0	3141.1
3152.8	3151.3	3150.3	3141.2	3140.7	3147.5
3156.8	3154.6	3155.7	3149.0	3148.7	3151.6
3165.5	3168.4	3168.6	3159.2	3161.9	3160.4
3178.2	3179.2	3178.8	3162.9	3171.5	3160.8
3184.5	3183.0	3190.3	3187.5	3174.9	3185.0
3191.3	3191.1	3192.2	3187.7	3185.2	3186.4
3198.9	3202.0	3199.5	3192.8	3186.3	3191.0
3199.3	3206.5	3200.9	3204.9	3205.4	3203.1
3273.8	3228.2	3221.1	3219.0	3218.8	3282.3

Post-reactive complexes					
Post1	Post2	Post3	Post4	Post5	Post6
11.7	14.5	16.1	20.2	15.1	15.3
18.1	22.9	28.4	30.0	20.3	21.9
41.9	46.5	45.4	45.7	35.9	37.3
60.6	69.2	52.7	61.5	59.6	57.4
60.7	72.6	81.3	66.7	69.7	83.3
75.3	84.8	83.7	86.0	90.1	90.8
106.6	95.8	104.6	95.7	92.0	97.1
107.6	113.5	122.6	122.6	101.4	125.1
193.2	170.0	193.6	185.9	156.9	194.7
199.3	192.7	210.2	215.1	178.2	202.0
207.7	206.6	241.6	245.3	207.6	228.0
237.8	243.4	269.1	248.1	250.6	253.0
306.2	307.6	316.5	308.9	308.3	307.0

341.7	342.8	360.0	350.5	342.0	344.9
366.4	368.8	381.3	378.4	366.3	373.5
385.0	395.6	429.8	415.7	378.0	388.4
395.4	436.8	488.4	429.9	405.2	404.6
523.1	514.6	535.7	528.3	523.9	526.9
613.2	531.6	605.6	598.3	563.9	613.3
660.4	618.4	718.5	639.7	612.3	621.0
754.1	748.5	784.8	745.4	746.4	746.6
777.4	790.6	794.7	780.6	781.4	781.8
790.5	930.0	824.0	825.2	923.8	803.5
908.9	930.2	929.4	922.5	927.4	918.1
931.6	945.5	933.7	930.6	954.3	924.8
940.2	960.1	962.7	961.8	957.4	948.7
991.4	992.4	995.5	978.3	990.5	985.5
1028.5	1056.3	1053.8	1081.4	1073.0	1074.1
1080.4	1060.9	1091.7	1088.9	1080.8	1077.9
1101.4	1095.5	1097.2	1129.7	1090.8	1090.9
1104.5	1144.5	1125.9	1152.5	1160.5	1126.2
1165.1	1193.3	1198.2	1176.5	1177.9	1177.9
1197.0	1199.0	1207.0	1201.2	1180.0	1179.3
1236.2	1236.3	1235.4	1210.9	1205.0	1193.2
1270.3	1251.8	1256.1	1252.9	1268.7	1272.0
1298.1	1281.4	1328.1	1307.4	1299.8	1277.9
1327.4	1328.0	1331.5	1322.9	1307.7	1307.8
1366.0	1375.2	1378.2	1372.9	1378.5	1359.9
1375.0	1379.1	1389.2	1382.9	1382.4	1382.3
1378.8	1399.0	1402.1	1392.9	1400.8	1390.0
1396.9	1466.7	1470.2	1469.2	1470.1	1401.2
1454.3	1478.8	1477.7	1477.9	1475.1	1473.4
1477.6	1483.0	1485.0	1481.9	1478.4	1477.8
1495.8	1498.4	1526.8	1486.9	1500.5	1499.2
1519.6	1505.0	1539.2	1519.6	1521.5	1522.1
1528.7	1538.0	1553.9	1537.8	1536.4	1525.3
1553.1	1540.8	1556.9	1551.3	1540.9	1532.8
1553.5	1553.6	1559.3	1558.2	1551.0	1551.2
1558.7	1559.7	1563.4	1559.9	1554.7	1558.9
1566.1	1565.7	1565.9	1564.9	1558.4	1569.6
1581.6	1581.1	1581.6	1569.8	1569.4	1578.6
1874.6	1877.1	1777.9	1898.9	1879.0	1879.1
2788.7	2754.7	2857.7	2726.6	2781.8	2789.7
3119.6	3053.0	3075.2	3057.9	3062.0	3059.6
3127.8	3057.4	3120.7	3114.8	3080.2	3114.1
3135.7	3119.9	3123.8	3125.1	3114.1	3125.6
3144.1	3128.1	3126.9	3126.4	3126.4	3131.3
3148.9	3129.3	3152.3	3129.2	3140.8	3140.8

3152.4	3134.5	3153.4	3141.1	3142.0	3147.4
3163.5	3149.7	3177.5	3147.6	3147.1	3151.3
3177.5	3153.2	3179.5	3161.6	3148.2	3161.1
3186.6	3178.3	3193.1	3186.3	3161.6	3184.6
3190.5	3191.0	3193.3	3186.8	3184.5	3186.2
3198.2	3191.4	3197.8	3188.2	3186.3	3196.7
3216.3	3199.7	3201.7	3198.1	3192.2	3222.5
3317.5	3276.6	3283.4	3287.0	3256.0	3325.3

Products					
P1	P2	P3	P4	P5	P6
39.1	26.7	25.4	42.6	34.0	35.2
63.8	60.3	65.6	49.1	50.3	62.6
73.5	67.6	72.6	51.0	67.6	70.4
92.5	85.0	86.0	101.6	90.2	92.2
103.3	93.6	134.0	117.3	92.6	101.8
126.1	110.1	191.0	162.5	120.8	125.3
198.1	189.6	194.7	237.4	175.8	199.3
203.3	203.5	237.3	252.5	202.5	203.5
243.3	244.0	255.3	269.4	250.4	250.3
308.4	308.8	307.1	292.6	308.6	308.2
346.6	316.0	347.6	338.0	341.5	345.8
380.5	346.7	416.7	388.3	376.4	375.8
493.6	381.2	531.7	522.7	399.7	489.5
524.5	523.4	543.7	559.3	524.7	532.3
612.1	608.0	718.5	607.5	613.4	613.5
747.3	745.5	751.8	756.0	746.1	746.2
788.8	789.4	789.8	780.4	781.7	781.3
796.8	929.5	819.1	825.2	924.2	793.9
917.3	930.8	929.0	913.4	928.0	919.5
930.4	952.1	930.8	922.8	958.4	925.0
950.0	962.8	957.7	945.3	963.3	947.4
993.6	992.1	998.9	969.8	991.7	984.9
1039.3	1038.3	1077.3	1070.8	1059.7	1067.8
1066.9	1063.2	1092.8	1088.7	1074.0	1076.6
1097.1	1097.2	1104.7	1121.9	1090.1	1090.2
1123.8	1144.3	1137.6	1149.6	1159.7	1127.0
1166.7	1196.2	1188.1	1175.7	1177.1	1176.9
1197.5	1202.9	1197.7	1195.9	1179.9	1179.1
1226.7	1236.2	1236.1	1199.5	1205.2	1195.2
1236.6	1248.6	1320.8	1262.8	1275.9	1274.3
1276.1	1274.9	1327.7	1306.5	1296.5	1278.3
1328.0	1328.0	1336.9	1325.4	1306.5	1306.5
1357.5	1374.3	1367.9	1377.8	1377.9	1358.1

1374.4	1375.8	1374.4	1381.5	1381.2	1381.2
1388.1	1397.6	1401.2	1400.1	1401.7	1386.6
1400.5	1466.8	1471.2	1470.0	1470.3	1400.2
1470.9	1477.7	1476.5	1475.2	1474.9	1471.0
1477.9	1483.8	1478.5	1477.1	1478.5	1477.5
1498.4	1498.8	1498.4	1484.0	1501.9	1496.2
1522.1	1506.0	1519.0	1521.3	1522.5	1522.4
1526.8	1533.2	1553.0	1542.7	1534.2	1525.1
1534.8	1542.9	1558.1	1550.9	1542.0	1536.8
1553.1	1553.1	1558.4	1557.5	1551.0	1551.0
1559.4	1559.5	1562.2	1558.8	1556.0	1558.5
1565.8	1565.8	1565.7	1563.4	1558.5	1569.5
1581.2	1581.1	1581.5	1569.5	1569.6	1577.6
1873.2	1877.9	1769.0	1890.3	1874.2	1875.4
3066.7	3053.7	3090.9	3044.3	3053.5	3051.7
3119.3	3056.5	3103.6	3114.0	3074.7	3113.3
3127.4	3097.1	3118.9	3122.5	3113.3	3125.3
3130.7	3102.4	3122.7	3125.2	3125.6	3135.6
3137.2	3119.4	3125.9	3140.5	3126.3	3140.4
3146.9	3127.2	3144.0	3147.0	3131.8	3146.9
3151.6	3147.0	3149.9	3160.8	3140.4	3152.7
3167.2	3151.5	3175.2	3163.7	3147.1	3160.2
3176.6	3176.7	3182.2	3184.5	3160.3	3183.6
3190.0	3189.3	3188.8	3185.6	3183.5	3185.5
3196.2	3190.0	3190.8	3185.9	3185.5	3198.7
3231.4	3196.3	3193.1	3193.8	3186.9	3234.8
3334.2	3306.1	3293.3	3279.7	3281.5	3339.7

Table S4 Vibrational frequencies (in cm^{-1}) for all the stationary points involved in the PB + OH reaction at the M062x/6-311+G(2d,2p) level of theory.

Species		
PB	OH	H ₂ O
19.4	3767.2	1637.1
45.3		3894.5
77.1		3997.3
88.4		
106.5		
196.2		
197.0		
205.6		
274.6		
299.5		
342.3		
372.1		

512.6		
596.8		
727.3		
754.3		
757.5		
890.3		
897.0		
907.1		
933.6		
969.4		
1050.7		
1071.2		
1081.0		
1136.7		
1150.5		
1164.3		
1189.7		
1239.4		
1262.2		
1281.2		
1331.1		
1337.1		
1337.5		
1353.8		
1415.6		
1421.5		
1427.9		
1451.7		
1471.5		
1497.2		
1502.5		
1505.4		
1512.1		
1517.1		
1520.3		
1528.2		
1840.7		
3044.9		
3058.3		
3062.9		
3066.6		
3087.7		
3088.5		
3089.2		
3097.1		

3112.8		
3116.0		
3126.4		
3135.5		
3137.7		
3141.6		

Pre-reactive complexes					
Pre1	Pre2	Pre3	Pre4	Pre5	Pre6
25.4	27.6	27.6	32.0	29.0	32.0
46.8	54.1	54.3	43.2	39.8	43.1
75.1	66.4	66.5	58.5	41.1	58.5
77.0	76.3	76.5	72.6	66.7	72.6
102.0	86.2	86.4	89.4	89.7	89.4
102.4	131.8	131.9	95.3	90.1	95.3
120.8	153.7	153.7	108.1	115.9	108.1
159.2	158.2	158.3	155.2	153.3	155.2
195.6	189.6	189.7	202.3	193.9	202.3
205.4	229.9	230.0	216.9	200.4	216.9
230.5	251.5	251.4	231.6	244.1	231.6
271.9	276.4	275.6	249.5	261.7	249.5
300.9	295.9	295.9	300.2	299.0	300.2
348.3	347.5	347.5	344.7	344.2	344.7
380.8	383.4	383.4	383.0	370.2	383.0
472.8	498.4	498.5	478.5	400.5	478.5
515.3	561.4	561.2	514.6	470.5	514.6
544.4	616.2	616.3	538.4	517.2	538.4
587.4	667.1	667.1	596.0	585.8	596.0
728.7	757.9	757.9	727.4	728.8	727.4
768.8	762.3	762.4	754.6	758.1	754.6
772.7	788.7	788.8	772.8	764.2	772.8
892.5	892.5	892.5	891.1	896.9	891.1
907.3	894.0	893.9	909.1	907.0	909.1
910.1	913.4	913.4	911.3	909.3	911.3
937.2	926.2	926.2	935.2	936.4	935.2
978.0	970.0	970.0	973.6	969.1	973.6
1046.2	1050.8	1050.7	1044.3	1043.3	1044.3
1071.9	1067.7	1067.7	1069.1	1071.6	1069.1
1077.0	1078.9	1078.9	1075.7	1076.5	1075.7
1131.3	1123.6	1123.6	1135.1	1133.7	1135.1
1146.6	1135.4	1135.5	1147.6	1150.1	1147.6
1167.3	1165.1	1165.1	1167.5	1164.8	1167.5
1196.0	1190.2	1190.3	1190.2	1191.2	1190.2
1245.9	1251.5	1251.5	1250.8	1217.9	1250.8

1261.2	1283.0	1283.0	1260.7	1262.5	1260.7
1286.4	1300.2	1300.3	1281.9	1285.9	1281.9
1332.3	1328.3	1328.3	1332.4	1335.1	1332.4
1333.2	1330.1	1330.1	1335.9	1338.9	1335.9
1342.2	1339.4	1339.4	1339.9	1341.8	1339.9
1359.3	1375.0	1375.0	1356.4	1351.6	1356.4
1416.7	1395.9	1395.8	1419.1	1418.9	1419.1
1423.0	1420.2	1420.2	1423.7	1421.2	1423.7
1428.0	1425.1	1425.1	1424.9	1432.6	1424.9
1449.0	1443.8	1443.8	1453.6	1448.6	1453.6
1463.0	1497.8	1497.9	1467.7	1467.2	1467.7
1502.9	1500.6	1500.6	1500.2	1499.2	1500.2
1505.4	1505.9	1505.8	1502.3	1502.1	1502.3
1507.7	1509.5	1509.5	1509.3	1511.4	1509.3
1516.0	1512.8	1512.8	1511.1	1514.0	1511.1
1517.5	1514.8	1514.6	1516.8	1514.8	1516.8
1521.3	1523.5	1523.5	1517.5	1518.1	1517.5
1531.1	1524.8	1524.9	1533.3	1531.4	1533.3
1807.8	1794.0	1794.1	1809.7	1858.3	1809.7
3048.9	3056.5	3056.4	3065.3	3050.7	3065.3
3050.6	3058.7	3058.5	3068.5	3058.0	3068.5
3062.6	3064.7	3064.8	3069.6	3062.2	3069.6
3070.0	3068.1	3068.2	3071.2	3065.0	3071.2
3076.4	3078.3	3078.4	3080.7	3082.7	3080.7
3080.3	3097.1	3097.1	3087.8	3085.2	3087.8
3091.5	3098.3	3098.7	3098.3	3092.9	3098.3
3096.2	3103.5	3103.6	3101.0	3102.0	3101.0
3111.3	3119.9	3119.9	3116.6	3114.4	3116.6
3120.4	3130.6	3130.4	3121.1	3124.1	3121.1
3126.1	3133.2	3133.2	3137.7	3134.7	3137.7
3131.3	3136.3	3136.3	3140.8	3136.9	3140.8
3146.2	3146.2	3145.9	3143.5	3143.9	3143.5
3151.1	3156.7	3157.0	3150.7	3150.3	3150.7
3619.1	3583.8	3584.1	3646.3	3669.6	3646.3

Transition states					
TS1	TS2	TS3	TS4	TS5	TS6
<i>i</i> 900.9	<i>i</i> 866.6	<i>i</i> 1218.4	<i>i</i> 876.8	<i>i</i> 845.1	<i>i</i> 859.1
25.5	28.9	21.4	45.5	39.7	33.3
56.2	63.6	49.6	62.1	46.2	49.0
59.2	80.6	64.8	79.8	70.7	70.7
77.2	94.5	74.7	91.9	81.4	83.1
91.6	99.6	105.9	109.1	105.5	98.5
103.1	126.1	118.9	126.9	125.9	105.5

109.5	158.9	143.1	140.1	131.7	134.7
186.3	198.5	179.3	200.1	197.4	157.4
194.3	209.6	216.7	221.8	198.0	199.5
196.2	241.4	239.3	259.8	218.0	201.5
246.3	251.8	267.0	277.1	242.8	263.0
290.6	299.5	272.3	300.1	294.9	302.2
334.2	341.8	341.0	337.9	303.7	338.1
360.5	375.3	368.7	372.1	343.1	343.3
363.5	460.8	421.7	397.7	370.3	372.1
511.8	511.5	466.7	514.3	508.1	512.8
589.9	590.9	641.8	591.6	592.1	598.4
698.8	684.2	719.6	656.7	660.3	726.8
734.7	734.6	762.6	728.0	727.7	748.1
755.7	761.4	787.8	758.4	752.8	763.9
764.4	765.5	818.1	789.8	761.4	822.2
886.0	898.1	900.3	893.7	897.4	869.0
901.7	907.2	908.7	903.4	907.0	900.4
919.7	920.0	919.6	920.9	922.0	916.4
962.4	950.7	935.2	953.8	942.9	938.0
983.0	973.5	982.2	974.3	969.6	967.1
1031.3	1048.6	1003.1	1004.2	1036.3	1051.6
1064.5	1072.9	1048.6	1059.2	1064.3	1069.2
1076.9	1078.1	1069.8	1070.3	1070.5	1070.3
1091.1	1093.3	1079.7	1114.1	1107.2	1115.8
1127.3	1148.5	1131.2	1134.7	1135.2	1137.0
1165.6	1151.6	1157.1	1157.1	1148.9	1149.9
1194.3	1165.6	1166.0	1167.4	1173.4	1175.6
1229.6	1194.1	1191.3	1182.2	1184.3	1215.9
1244.8	1246.9	1202.7	1251.2	1225.0	1236.6
1270.4	1261.4	1260.3	1259.8	1262.6	1262.2
1286.6	1286.2	1282.9	1278.1	1284.8	1274.3
1322.6	1320.5	1306.4	1323.3	1324.8	1310.7
1333.7	1330.6	1329.7	1334.5	1338.5	1337.5
1336.1	1341.6	1338.8	1344.0	1345.9	1341.1
1343.6	1356.9	1357.7	1357.8	1361.8	1345.0
1358.7	1409.1	1395.4	1415.5	1415.2	1353.8
1414.2	1419.1	1418.2	1426.6	1417.8	1417.7
1420.9	1425.3	1423.6	1427.2	1425.4	1427.4
1426.3	1443.7	1446.8	1437.6	1437.8	1436.1
1449.6	1456.4	1491.1	1467.7	1472.8	1447.6
1466.9	1457.2	1502.2	1499.2	1498.6	1474.0
1479.5	1500.6	1506.3	1501.7	1499.4	1475.7
1501.9	1502.0	1508.5	1504.4	1504.1	1496.1
1509.3	1507.8	1514.0	1512.9	1508.5	1505.0
1513.9	1512.5	1515.2	1515.0	1516.5	1512.3

1516.1	1515.0	1526.8	1520.0	1521.3	1522.1
1532.1	1529.2	1528.2	1521.9	1563.6	1534.9
1840.4	1818.8	1810.4	1830.3	1849.6	1842.0
3060.0	3050.1	3054.4	3056.8	3052.1	3049.3
3060.9	3056.2	3056.5	3059.7	3052.9	3056.8
3073.4	3058.5	3057.5	3062.5	3062.0	3064.6
3077.8	3067.2	3066.7	3067.6	3081.9	3074.7
3089.6	3086.6	3081.8	3079.6	3084.8	3082.4
3093.2	3089.2	3092.4	3088.8	3094.6	3084.6
3093.8	3100.6	3099.7	3093.9	3097.7	3097.3
3104.2	3103.6	3122.3	3109.8	3110.1	3103.8
3120.9	3117.8	3122.5	3110.8	3118.3	3112.4
3125.6	3123.2	3127.7	3132.1	3129.6	3133.1
3143.5	3139.5	3134.5	3133.0	3132.2	3134.4
3144.1	3148.7	3136.2	3145.4	3132.8	3138.1
3157.9	3151.4	3145.7	3146.8	3141.1	3156.4
3786.6	3743.4	3748.5	3776.0	3780.3	3800.9

Post-reactive complexes					
Post1	Post2	Post3	Post4	Post5	Post6
20.3	21.4	24.0	30.3	22.3	28.4
27.9	55.4	42.9	34.7	41.7	38.9
43.2	69.2	72.5	51.8	54.7	52.4
67.8	71.1	81.5	62.3	66.3	77.5
82.2	89.6	99.7	95.1	75.0	90.4
88.2	107.9	102.9	105.2	83.0	94.7
112.0	130.5	137.1	120.2	94.9	110.2
124.5	138.4	168.1	151.3	128.2	140.7
143.2	155.0	180.7	162.1	141.3	157.9
193.7	193.6	190.3	190.7	173.4	163.4
207.5	214.9	218.4	216.6	186.3	198.2
234.7	235.5	225.3	248.0	217.3	205.2
236.1	239.6	278.9	267.6	243.1	215.7
259.3	274.8	299.4	302.7	287.7	253.6
301.3	298.5	363.3	347.2	305.1	295.0
323.4	326.3	388.3	354.2	347.8	308.0
340.4	354.1	391.8	380.1	372.5	345.3
365.0	379.1	524.3	424.9	473.8	371.9
510.5	498.5	561.2	515.6	506.1	511.8
579.5	553.3	577.4	575.8	511.4	548.8
586.4	613.1	692.2	608.6	591.0	592.3
729.2	742.8	757.5	727.9	728.0	726.4
753.6	761.0	767.8	753.3	762.5	754.5
765.3	894.6	822.2	791.9	896.8	772.7

880.0	906.9	893.4	890.6	905.6	891.6
901.2	919.6	906.5	909.8	929.7	897.7
921.4	938.2	932.7	938.7	935.5	924.7
970.2	975.4	974.0	961.0	965.5	967.0
1015.9	1007.1	1032.3	1061.8	1027.3	1040.0
1062.8	1051.8	1057.9	1069.5	1055.7	1064.7
1088.0	1080.2	1080.0	1084.5	1072.0	1069.3
1091.1	1124.2	1113.7	1126.5	1136.8	1107.2
1119.3	1163.7	1160.2	1132.8	1138.8	1133.9
1167.5	1167.1	1164.9	1172.6	1149.5	1148.1
1194.1	1190.8	1192.8	1181.4	1177.1	1162.1
1225.3	1210.3	1248.8	1225.4	1214.1	1236.0
1249.0	1256.4	1283.4	1261.6	1265.1	1237.9
1284.5	1279.9	1302.1	1273.5	1268.3	1258.9
1317.4	1323.9	1326.0	1324.7	1334.2	1316.6
1329.3	1335.8	1337.1	1334.6	1339.7	1331.4
1332.6	1360.4	1340.1	1345.3	1351.2	1341.4
1346.7	1414.6	1408.1	1419.4	1418.5	1351.3
1398.2	1422.4	1417.8	1421.4	1423.8	1417.4
1429.0	1432.0	1427.1	1425.8	1430.9	1422.6
1441.4	1450.2	1481.0	1442.8	1454.7	1446.9
1465.6	1455.1	1493.8	1460.8	1474.2	1470.1
1479.3	1484.7	1500.9	1486.6	1484.6	1474.0
1502.7	1500.1	1502.2	1499.8	1493.0	1479.4
1504.9	1501.7	1506.9	1510.5	1504.1	1500.4
1515.0	1511.1	1514.5	1513.3	1505.6	1511.0
1517.0	1512.4	1516.2	1514.6	1508.1	1517.9
1529.6	1525.8	1531.3	1516.8	1521.0	1524.3
1647.7	1655.6	1671.9	1655.4	1649.0	1631.2
1836.7	1810.8	1722.9	1838.5	1852.2	1841.3
3059.0	3000.1	3050.3	2998.7	3001.1	3006.8
3068.2	3020.4	3060.8	3057.7	3025.6	3063.5
3071.2	3053.7	3062.3	3060.6	3053.5	3069.3
3074.5	3057.7	3076.2	3061.3	3060.4	3079.7
3084.1	3065.0	3078.8	3070.1	3072.4	3087.3
3095.9	3067.5	3094.4	3079.3	3078.0	3093.0
3108.0	3078.0	3115.1	3096.5	3094.6	3097.8
3116.0	3100.3	3126.8	3112.4	3104.7	3115.0
3126.9	3120.2	3127.8	3126.9	3110.4	3136.2
3142.4	3129.0	3131.4	3132.8	3128.2	3139.2
3146.0	3134.9	3138.8	3136.5	3129.0	3141.3
3170.6	3135.9	3162.1	3145.2	3133.2	3164.7
3277.0	3219.1	3223.8	3250.4	3190.9	3268.0
3854.7	3799.1	3754.0	3853.7	3836.3	3832.6
3966.4	3956.8	3971.9	3941.4	3971.9	3960.9

Products					
P1	P2	P3	P4	P5	P6
23.9	32.4	45.0	33.4	36.3	44.2
39.5	61.7	79.8	47.1	56.9	73.5
61.5	76.4	87.5	65.1	75.6	89.1
80.8	84.5	95.0	109.6	89.0	93.1
91.9	92.9	138.9	118.8	101.4	111.5
107.1	120.9	190.1	162.4	127.9	197.4
196.2	187.6	194.2	229.5	179.3	201.7
198.0	200.3	262.3	261.8	203.2	243.0
239.6	239.3	264.4	267.2	280.8	273.5
298.3	303.3	301.7	285.4	303.2	302.9
333.7	305.7	347.9	334.2	341.6	345.1
360.9	343.0	409.8	382.5	373.5	372.5
477.3	376.4	516.5	499.1	433.5	491.4
519.0	512.2	521.0	545.3	513.7	522.4
589.8	584.8	700.1	585.0	595.6	595.2
727.2	724.5	725.6	737.4	726.6	727.6
750.8	762.1	774.0	755.7	759.5	754.8
762.4	897.3	786.6	796.9	895.7	761.9
878.1	908.8	910.8	888.7	909.3	892.1
899.0	914.3	911.8	894.7	932.5	901.7
918.2	939.3	937.8	924.9	938.7	927.3
968.8	971.9	977.6	948.3	971.0	967.1
1014.1	1000.0	1062.1	1054.6	1021.4	1032.6
1061.5	1048.7	1065.9	1070.3	1063.8	1065.6
1088.8	1079.2	1073.7	1084.4	1070.6	1071.7
1091.5	1119.6	1121.9	1123.4	1134.5	1108.4
1120.3	1163.3	1156.6	1131.0	1137.6	1136.4
1164.2	1174.0	1167.1	1162.2	1151.7	1150.8
1192.6	1192.4	1194.8	1167.3	1177.0	1163.4
1224.7	1201.9	1275.7	1227.4	1238.4	1230.5
1248.0	1233.4	1286.3	1259.0	1261.7	1237.9
1282.9	1283.0	1289.1	1279.0	1262.3	1262.2
1315.6	1327.8	1327.7	1327.2	1334.0	1315.8
1327.6	1330.7	1331.5	1335.1	1337.5	1335.4
1329.1	1345.7	1356.2	1350.4	1357.1	1337.5
1341.9	1414.1	1423.0	1418.7	1416.0	1353.3
1398.4	1422.0	1427.7	1419.4	1424.1	1420.4
1422.3	1432.7	1429.9	1428.0	1429.6	1428.0
1443.0	1448.6	1450.7	1434.7	1459.8	1448.2
1465.9	1455.2	1465.8	1467.3	1470.7	1470.8
1478.2	1483.9	1504.8	1491.4	1487.8	1480.2

1498.9	1495.4	1512.3	1501.4	1491.3	1483.7
1502.2	1502.2	1513.7	1509.6	1502.4	1502.5
1511.7	1511.6	1514.0	1514.4	1505.2	1517.0
1514.6	1514.6	1515.1	1515.2	1516.5	1520.2
1529.3	1529.4	1529.6	1519.1	1520.3	1525.5
1839.3	1845.5	1747.2	1852.5	1840.3	1842.7
3069.4	3001.1	3026.5	2992.6	2996.7	2991.4
3072.9	3007.6	3060.1	3058.6	3025.2	3063.3
3074.2	3042.2	3066.2	3059.7	3064.0	3066.0
3082.1	3058.5	3069.8	3060.1	3065.9	3070.4
3084.2	3069.4	3075.2	3082.5	3068.4	3088.4
3103.8	3072.9	3085.8	3090.7	3071.9	3089.9
3107.2	3082.2	3107.0	3109.9	3088.2	3096.7
3123.4	3103.8	3125.2	3112.0	3096.1	3116.4
3127.6	3123.4	3134.7	3130.5	3116.1	3137.8
3140.0	3140.0	3143.5	3133.6	3128.5	3138.2
3148.4	3144.4	3143.7	3137.3	3137.7	3141.5
3175.4	3148.5	3146.6	3142.9	3141.9	3184.7
3278.1	3242.4	3209.8	3207.3	3217.4	3288.3

Figure S1 Intrinsic Reaction Coordinate (IRC) scans for the various channels for the reaction of PB with Cl atoms at the BHandHLYP/6-311+G(2d,2p) level of theory.

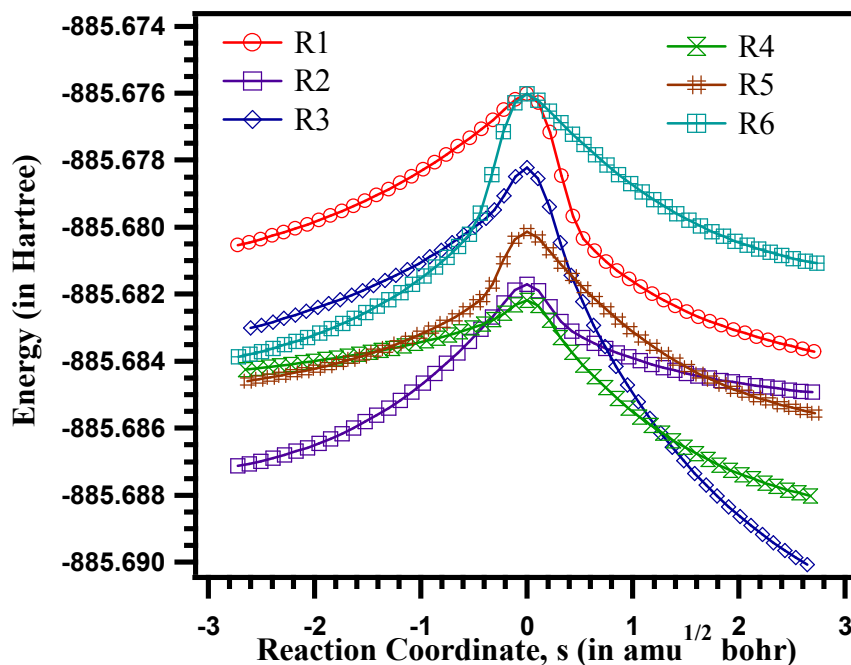


Figure S2 Intrinsic Reaction Coordinate (IRC) scans for the various channels for the reaction of PB with OH radicals at the M062x/6-311+G(2d,2p) level of theory.

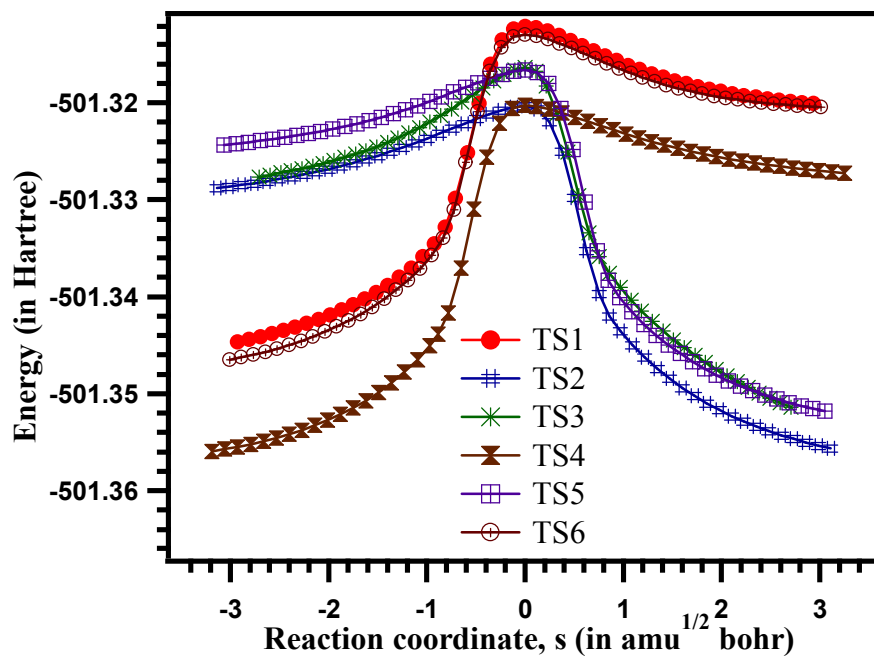


Figure S3 Bond length plots for the various channels for the reaction of PB with Cl atoms at the BHandHLYP/6-311+G(2d,2p) level of theory. (The dashed and the solid lines depict the breaking and the forming bonds along the reaction coordinate).

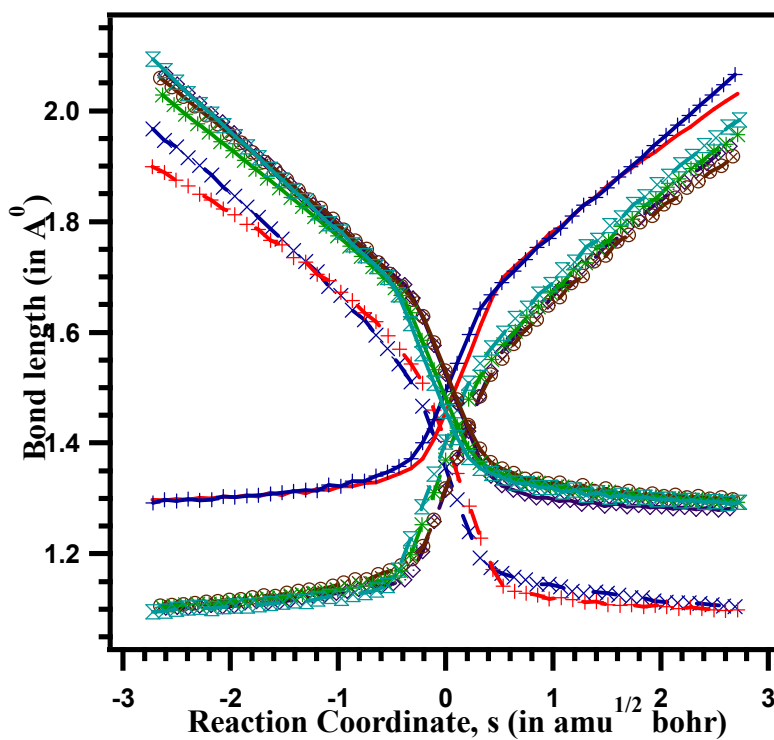


Figure S4 Bond length plots for the various channels for the reaction of PB with OH radicals at the M062x/6-311+G(2d,2p) level of theory. (The dashed and the solid lines depict the breaking and the forming bonds along the reaction coordinate).

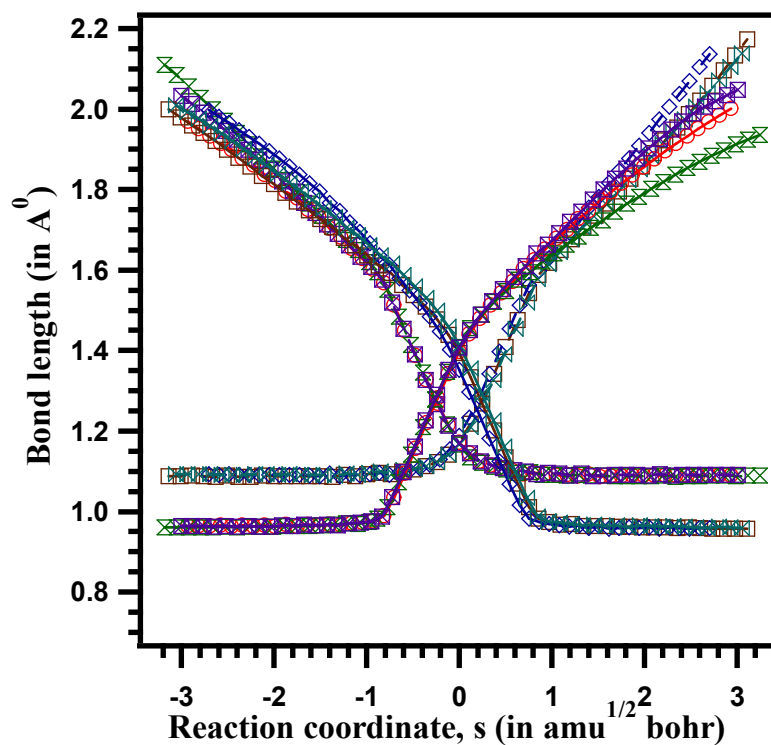


Table S5 $\langle S^2 \rangle$ values for all the geometries involved in the reaction of PB with Cl atoms calculated at the BHandHLYP/6-311+G(2d,2p) level of theory.

Species	$\langle S^2 \rangle$
R1	0.7538
Cl	1.0000
RC1	0.7539
RC2	0.7553
RC3	0.7543
RC4	0.7543
RC5	0.7543
RC6	0.7539
TS1	0.7623
TS2	0.7622
TS3	0.7649
TS4	0.7618
TS5	0.7622
TS6	0.7623
P1	0.7554
P2	0.756
P3	0.7638
P4	0.7552

P5	0.7558
P6	0.7553
HCl	1.0000
PC1	0.7552
PC2	0.7557
PC3	0.7627
PC4	0.7551
PC5	0.7555
PC6	0.7553

Table S6 $\langle S^2 \rangle$ values for all the geometries involved in the reaction of PB with OH radicals calculated at the M062x/6-311+G(2d,2p) level of theory.

Species	$\langle S^2 \rangle$
R1	0.7529
OH	1.0000
RC1	0.7529
RC2	0.7529
RC3	0.7529
RC4	0.7529
RC5	0.7529
RC6	0.7529
TS1	0.7584
TS2	0.7584
TS3	0.7588
TS4	0.7584
TS5	0.7583
TS6	0.7584
P1	0.7552
P2	0.7552
P3	0.7594
P4	0.7545
P5	0.7551
P6	0.7551
H ₂ O	1.0000
PC1	0.7551
PC2	0.7552
PC3	0.7574
PC4	0.7543
PC5	0.755
PC6	0.755

Table S7 T1 diagnostic values for all the geometries involved in the reaction of PB with Cl atoms evaluated at the CCSD(T)//BHandHLYP/6-311+G(2d,2p) level of theory.

Species	T1Diag
R1	0.012
Cl	0.006

RC1	0.014
RC2	0.015
RC3	0.013
RC4	0.013
RC5	0.015
RC6	0.012
TS1	0.013
TS2	0.014
TS3	0.014
TS4	0.014
TS5	0.013
TS6	0.013
P1	0.013
P2	0.013
P3	0.015
P4	0.014
P5	0.013
P6	0.013
HCl	0.006
PC1	0.013
PC2	0.013
PC3	0.014
PC4	0.014
PC5	0.013
PC6	0.013

Table S8 T1 diagnostic values for all the geometries involved in the reaction of PB with OH radicals evaluated at the CCSD(T)//M026x/6-311+G(2d,2p) level of theory.

Species	T1Diag
R1	0.013
OH	0.010
RC1	0.020
RC2	0.019
RC3	0.019
RC4	0.017
RC5	0.016
RC6	0.017
TS1	0.017
TS2	0.017
TS3	0.017
TS4	0.017
TS5	0.017
TS6	0.016
P1	0.013

P2	0.013
P3	0.015
P4	0.014
P5	0.013
P6	0.013
H ₂ O	0.010
PC1	0.020
PC2	0.019
PC3	0.019
PC4	0.017
PC5	0.016
PC6	0.017

Table S9 Equilibrium constants (K_{eq} , in units of $\text{cm}^3 \text{ molecule}^{-1}$) for the H-abstraction channels involved in the reaction of PB with Cl atoms.

T (in K)	R1	R2	R3	R4	R5	R6
200	3.8×10^{-23}	4.8×10^{-21}	1.1×10^{-22}	3.8×10^{-21}	1.1×10^{-22}	3.1×10^{-23}
225	4.0×10^{-23}	1.9×10^{-21}	7.2×10^{-23}	1.8×10^{-21}	7.2×10^{-23}	3.3×10^{-23}
250	4.3×10^{-23}	9.1×10^{-22}	5.2×10^{-23}	9.9×10^{-22}	5.2×10^{-23}	3.6×10^{-23}
272	4.5×10^{-23}	5.4×10^{-22}	4.1×10^{-23}	6.5×10^{-22}	4.1×10^{-23}	3.8×10^{-23}
275	4.6×10^{-23}	5.1×10^{-22}	4.0×10^{-23}	6.2×10^{-22}	4.0×10^{-23}	3.8×10^{-23}
298	4.9×10^{-23}	3.2×10^{-22}	3.3×10^{-23}	4.4×10^{-22}	3.4×10^{-23}	4.1×10^{-23}
325	5.2×10^{-23}	2.1×10^{-22}	2.8×10^{-23}	3.1×10^{-22}	2.8×10^{-23}	4.4×10^{-23}
350	5.5×10^{-23}	1.5×10^{-22}	2.5×10^{-23}	2.4×10^{-22}	2.5×10^{-23}	4.7×10^{-23}
375	5.9×10^{-23}	1.1×10^{-22}	2.2×10^{-23}	1.9×10^{-22}	2.2×10^{-23}	5.0×10^{-23}
400	6.3×10^{-23}	8.9×10^{-22}	2.1×10^{-23}	1.6×10^{-22}	2.1×10^{-23}	5.4×10^{-23}

Table S10 Equilibrium constants (K_{eq} , in units of $\text{cm}^3 \text{ molecule}^{-1}$) for the H-abstraction channels involved in the reaction of PB with OH radicals.

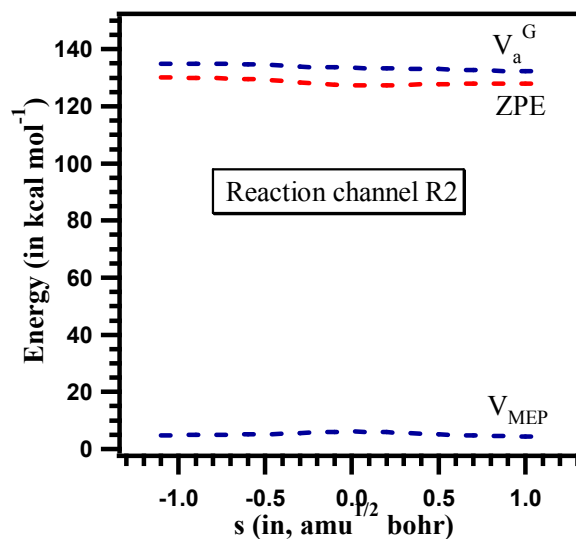
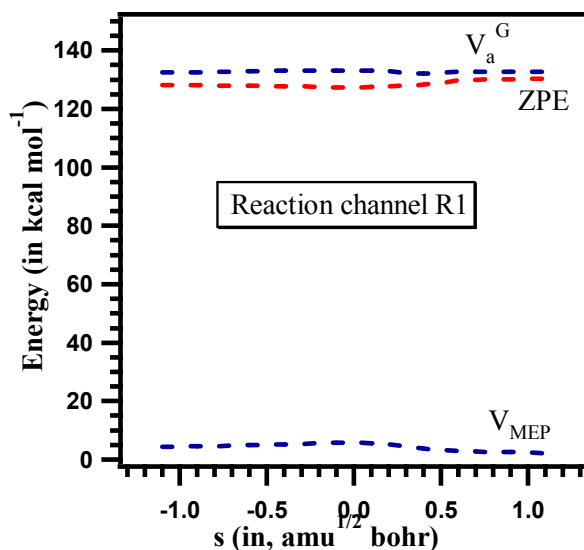
T (in K)	R1	R2	R3	R4	R5	R6
200	2.5×10^{-18}	3.2×10^{-19}	3.2×10^{-19}	2.6×10^{-18}	2.3×10^{-20}	2.6×10^{-18}
225	4.2×10^{-19}	6.2×10^{-20}	6.2×10^{-20}	4.6×10^{-19}	7.3×10^{-21}	4.6×10^{-19}
250	1.0×10^{-19}	1.7×10^{-20}	1.7×10^{-20}	1.2×10^{-19}	3.1×10^{-21}	1.2×10^{-19}
272	3.7×10^{-20}	6.7×10^{-21}	6.7×10^{-21}	4.3×10^{-20}	1.6×10^{-21}	4.3×10^{-20}
275	3.3×10^{-20}	6.0×10^{-21}	5.9×10^{-21}	3.8×10^{-20}	1.5×10^{-21}	3.8×10^{-20}
298	1.4×10^{-20}	2.7×10^{-21}	2.7×10^{-21}	1.7×10^{-20}	9.5×10^{-22}	1.7×10^{-20}
325	6.0×10^{-21}	1.2×10^{-21}	1.2×10^{-21}	7.3×10^{-21}	5.5×10^{-22}	7.3×10^{-21}
350	3.1×10^{-21}	6.8×10^{-22}	6.7×10^{-22}	3.9×10^{-21}	3.7×10^{-22}	3.9×10^{-21}
375	1.8×10^{-21}	4.1×10^{-22}	4.0×10^{-22}	2.3×10^{-21}	2.7×10^{-22}	2.3×10^{-21}
400	1.1×10^{-21}	2.6×10^{-22}	2.6×10^{-22}	1.4×10^{-21}	2.1×10^{-22}	1.4×10^{-21}

Table S11 Bimolecular rate coefficients ($k_{\text{PB+Cl}}$, in $\text{cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$) for the H-abstraction channels involved in the reaction of PB with Cl atoms.

T (in K)	$k_{\text{PB+Cl}}$
200	3.01×10^{-10}
225	2.43×10^{-10}
250	2.10×10^{-10}
272	1.92×10^{-10}
275	1.91×10^{-10}
298	1.80×10^{-10}
325	1.34×10^{-10}
350	1.37×10^{-10}
375	1.41×10^{-10}
400	1.47×10^{-10}

Table S12 Bimolecular rate coefficients ($k_{\text{PB+OH}}$, in $\text{cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$) for the H-abstraction channels involved in the reaction of PB with OH radicals.

T (in K)	$k_{\text{PB+Cl}}$
200	6.67×10^{-11}
225	1.80×10^{-11}
250	2.49×10^{-11}
272	1.34×10^{-11}
275	1.26×10^{-11}
298	8.03×10^{-12}
325	5.75×10^{-12}
350	6.54×10^{-12}
375	5.64×10^{-12}
400	5.12×10^{-12}



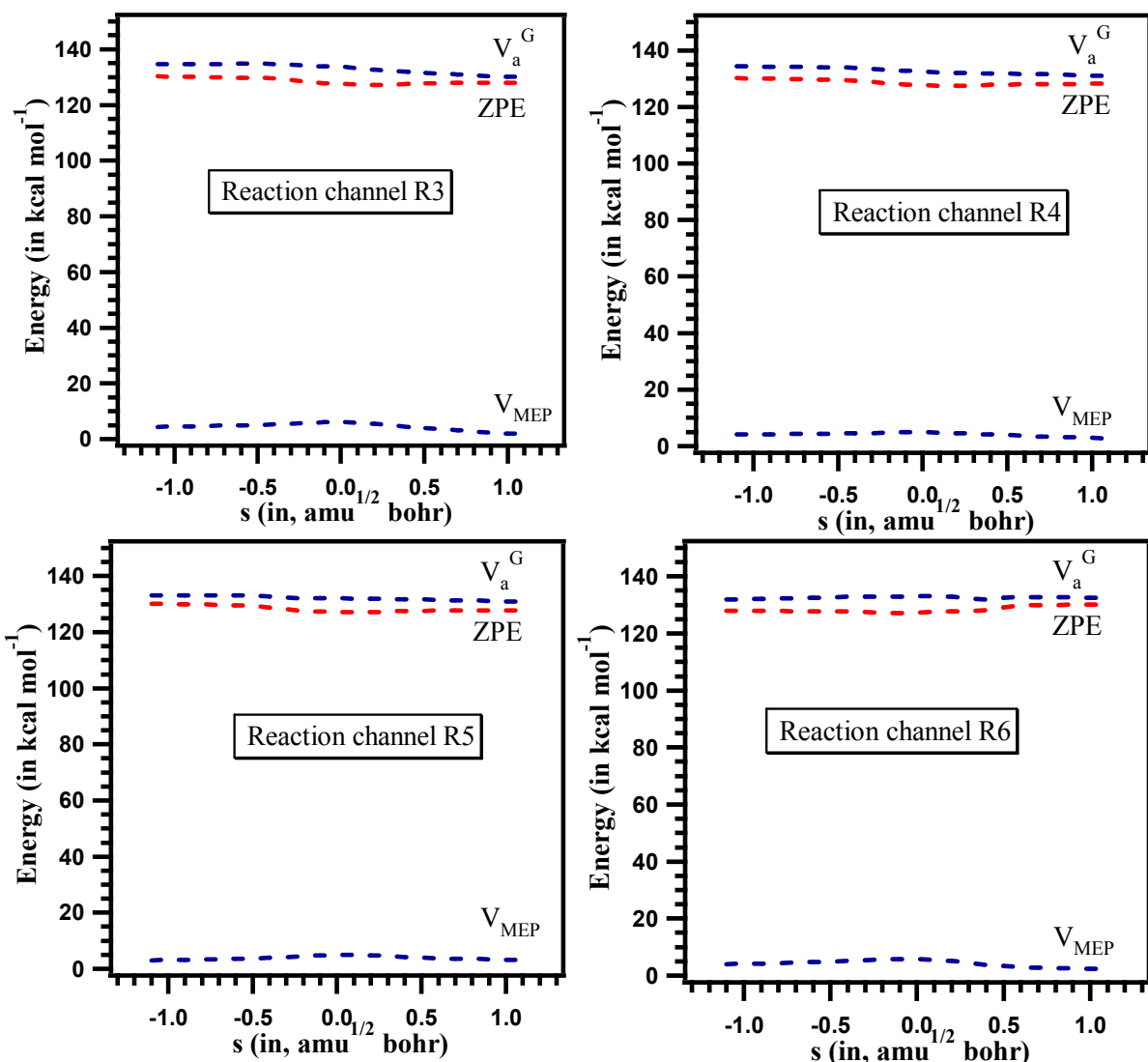
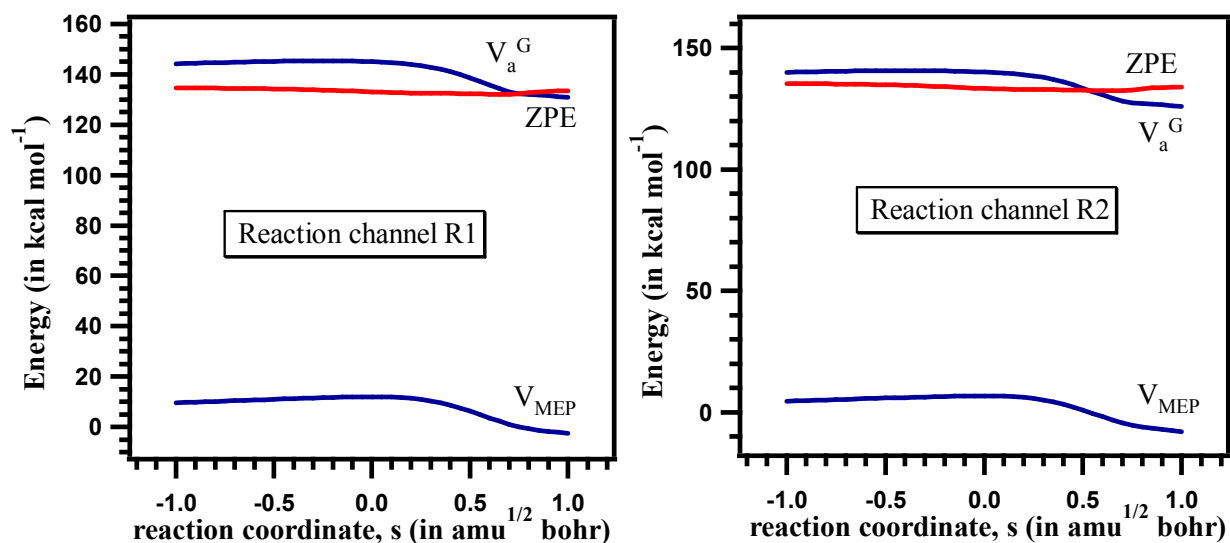


Figure S5 Classical potential energy curve (V_{MEP}), ground-state vibrational adiabatic energy curve (V_a^G), and zero-point energy curve (ZPE) as functions of $s(\text{amu})^{1/2}\text{bohr}$ for the H-abstraction channels involved in the reaction of PB with Cl atoms.



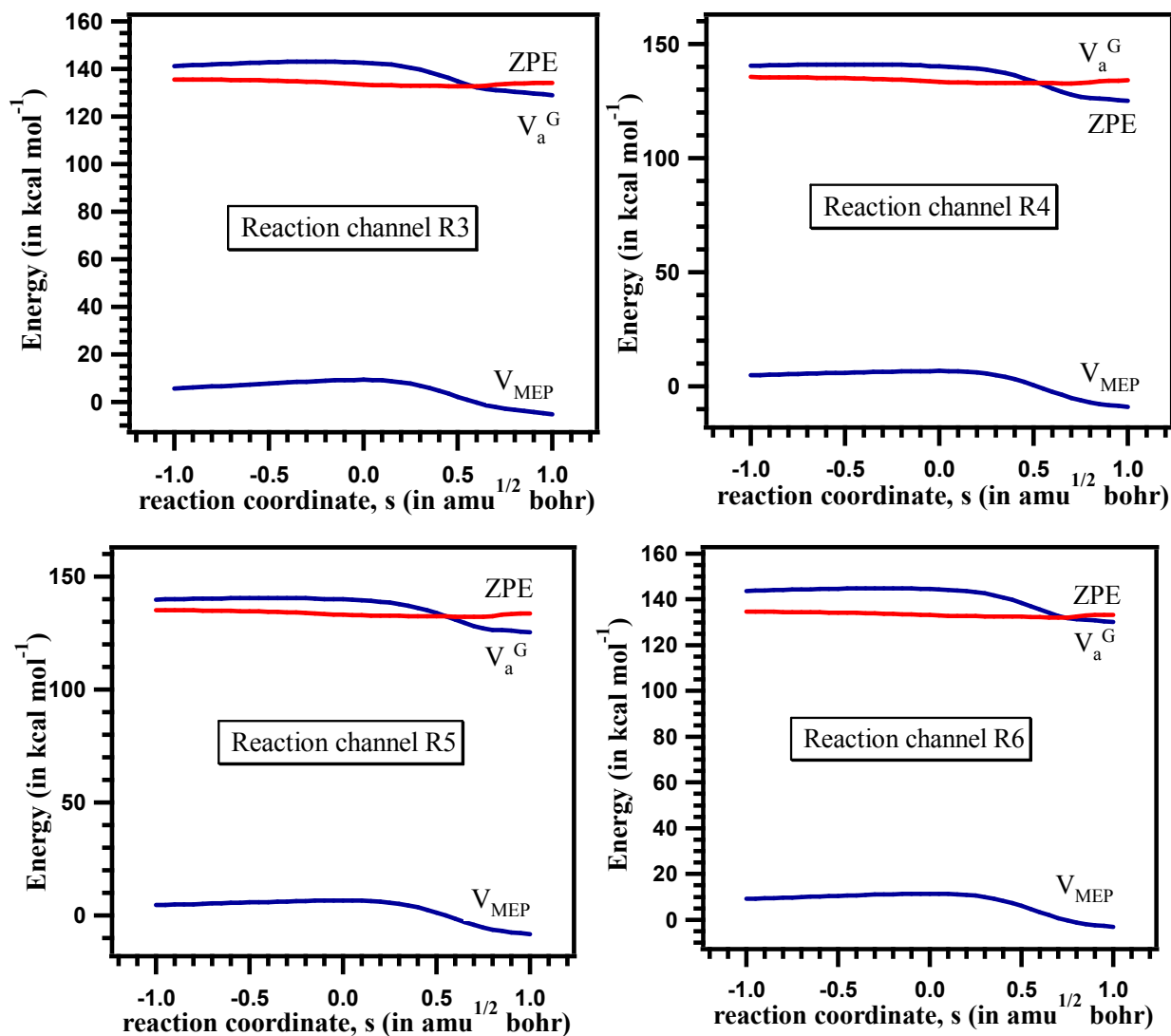


Figure S6 Classical potential energy curve (V_{MEP}), ground-state vibrational adiabatic energy curve (V_a^G), and zero-point energy curve (ZPE) as functions of $s(\text{amu})^{1/2}\text{bohr}$ for the H-abstraction channels involved in the reaction of PB with OH radicals.

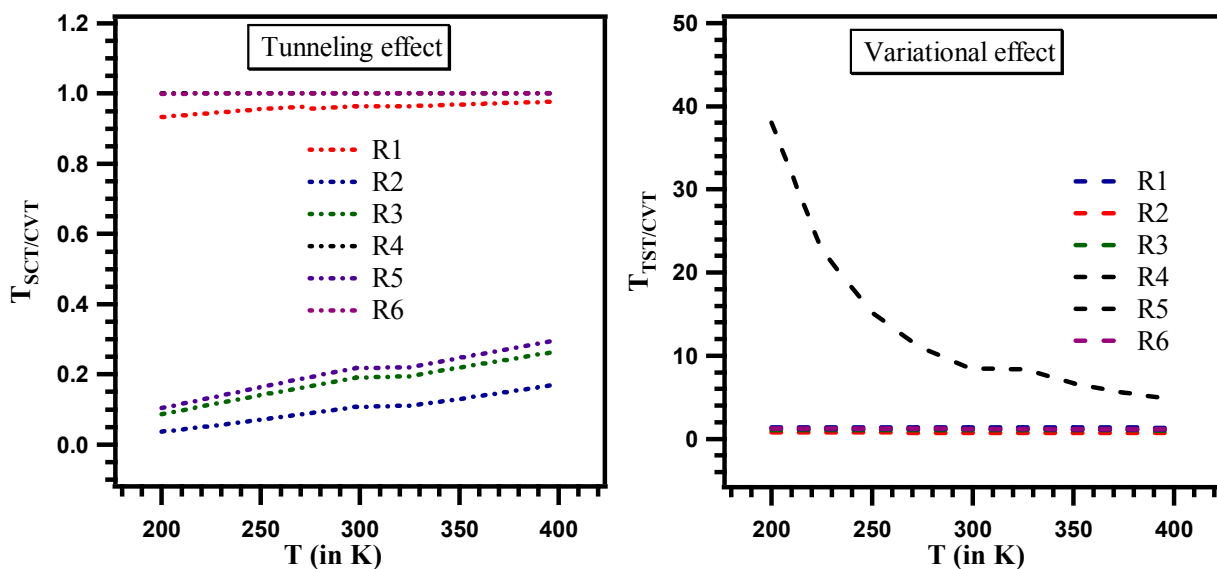


Figure S7 Canonical variational transmission coefficients $\Gamma^{\text{CVT}}(T)$ and small-curvature tunneling transmission coefficients $\kappa^{\text{SCT}}(T)$ for the PB + Cl reaction in the temperature range of 200-400 K.

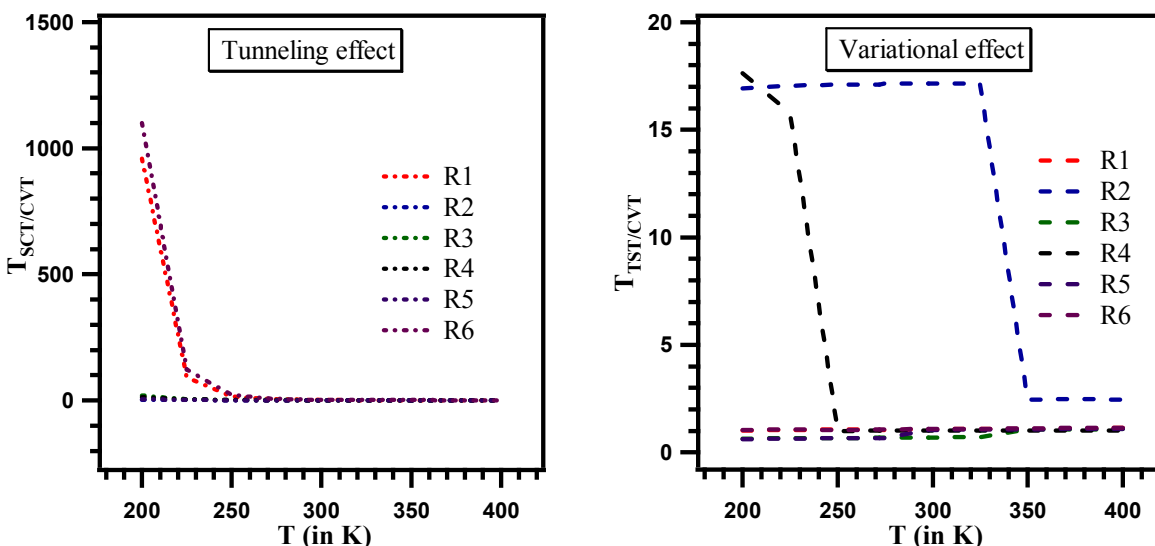


Figure S8 Canonical variational transmission coefficients $\Gamma^{\text{CVT}}(T)$ and small-curvature tunneling transmission coefficients $\kappa^{\text{SCT}}(T)$ for the PB + OH reaction in the temperature range of 200-400 K.

Table S13 Percentage contribution of various H-abstraction channels to the total rate coefficient for the reaction of PB with Cl atoms over the temperature range of 200-400 K obtained at the CCSD(T)//BHandHLYP/6-311+G(2d,2p) level of theory.

T(K)	R1	R2	R3	R4	R5	R6
200	0.1	26.2	0.1	11.1	8.9	0.1
225	0.2	25.1	0.1	11.6	9.5	0.2
250	0.3	23.8	0.2	12.0	9.9	0.3
272	0.4	22.8	0.3	12.1	10.3	0.3
275	0.4	22.8	0.3	12.1	10.3	0.4
298	0.5	21.9	0.3	12.1	10.5	0.4
325	0.7	19.7	0.4	11.8	11.9	0.7
350	0.9	19.2	0.5	11.8	11.9	0.8
375	1.0	18.7	0.5	11.6	11.8	0.9
400	1.2	18.1	0.6	11.5	11.8	1.0

Table S14 Percentage contribution of various H-abstraction channels to the total rate coefficient for the reaction of PB with OH radicals over the temperature range of 200-400 K obtained at the CCSD(T)//M062x/6-311+G(2d,2p) level of theory.

T(K)	R1	R2	R3	R4	R5	R6
200	2.3	21.8	21.5	41.5	7.5	5.4
225	1.8	22.8	23.2	35.7	12.2	4.2
250	0.4	6.8	7.9	78.5	5.3	0.9

275	0.4	7.4	10.4	73.2	7.8	0.8
298	0.5	7.7	13.5	70.4	7.1	0.9
325	0.6	7.6	17.3	65.5	8.5	0.6
350	0.6	37.6	10.1	44.1	7.2	0.5
375	0.9	36.1	11.8	42.3	8.3	0.6
400	1.2	34.8	13.6	40.4	9.4	0.7