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

Electronic Supporting Information for

DFT Mechanistic Studies of Boron-Silicon Exchange Reactions Between Silyl-Substituted Arenes and Boron Bromides

Christopher S. Qiu, Nicholas P. Qiu, Christopher Flinn, and Yuming Zhao*

Department of Chemistry, Memorial University of Newfoundland

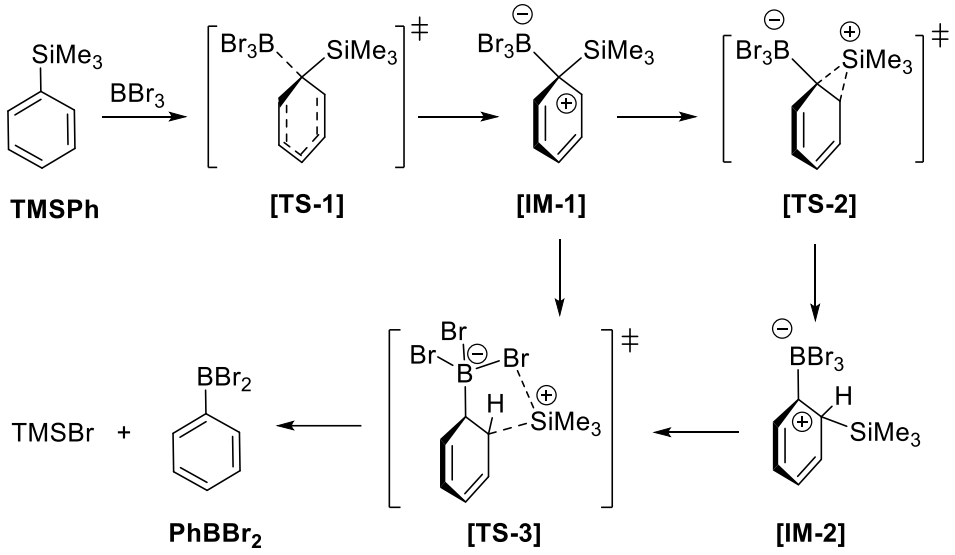
Core Science Facility 45 Arctic Avenue, St. John's, NL

Canada A1C 5S7

Phone: 1 (709) 864 8747; Fax: 1 (709) 864 3702; Email: yuming@mun.ca

1. Cartesian Coordinates for the stationary points investigated (all calculated at the M06-2X/Def2-SVP level)

1.1 Stationary points for the exchange reaction of TMSPh and BBr_3



Gas Phase	In Solvent (DCM)
BBr_3 Coordinates (x,y,z): B 0.00000000 0.00000000 0.00000000 Br 0.00000000 1.90009800 0.00000000 Br 1.64553300 -0.95004900 0.00000000 Br -1.64553300 -0.95004900 0.00000000 E(RM062X): -7746.588695 Hartree Dipole Moment: 0.000000 Debye	**BBr_3** Coordinates (x,y,z): B 0.00000000 0.00000000 0.00000000 Br 0.00000000 1.90009800 0.00000000 Br -1.64553300 -0.95004900 0.00000000 Br 1.64553300 -0.95004900 0.00000000 E(RM062X): -7746.589622 Hartree Dipole Moment: 0.000000 Debye
IM-1 Coordinates (x,y,z): C 1.25293000 1.03728400 -1.16660100 C 2.60311000 2.66604600 -0.01825800 C 1.10463200 1.26224800 1.24300900 C 2.05097500 2.27428400 1.20711400 C 0.65975300 0.60561200 0.05541900 C 2.22282900 2.03639600 -1.20297400 H 3.33762300 3.47338800 -0.04675300	**IM-1 (Do not exist)**

H 0.64433500 0.96835700 2.18970400 H 2.65162700 2.34855800 -2.15578900 H 0.88970700 0.58719400 -2.09474400 H 2.35311700 2.77464700 2.12780600 Si 2.09979200 -1.07664100 0.07339700 C 3.70208600 -0.46412600 0.82057100 H 4.13200000 0.39345900 0.28665000 H 4.41276500 -1.30221700 0.72862200 H 3.60380600 -0.21277400 1.88455900 C 1.32133600 -2.36178500 1.16651100 H 2.05313300 -3.18696500 1.20364900 H 0.37443700 -2.73534300 0.75770000 H 1.14448900 -1.99293900 2.18438900 C 2.44742100 -1.69556500 -1.65574800 H 3.08225800 -0.99092400 -2.21083100 H 1.53066400 -1.89708700 -2.22201500 H 3.00001600 -2.64315100 -1.54470600 B -0.89871400 0.04079900 0.00147600 Br -1.13118600 -1.40068600 -1.41653100 Br -1.98202200 1.67324900 -0.51979100 Br -1.52404700 -0.64049300 1.79868000 E(RM062X): -8386.963193 Hartree Dipole Moment: 10.377517 Debye	
IM-2 Coordinates (x,y,z): C 2.39839900 1.51757700 -1.37055300 C 1.36838000 0.55560500 -1.10511700 H 1.19045300 -0.24340400 -1.83869000 C 2.45529200 2.69153100 -0.65625300 H 3.24559000 3.41911200 -0.84205800 C 1.45697900 2.95130200 0.30585900 H 1.49834700 3.87958900 0.87968000 C 0.29146700 0.87654500 -0.22502000 C 0.40715300 2.07223900 0.51347100 H -0.38415300 2.32268200 1.22243300 Si 2.56237100 -0.70955600 0.16751300 C 2.72514800 0.10611100 1.82929600 H 3.44909200 -0.48897600 2.40948700 H 1.76265400 0.10304600 2.35966200 H 3.10854600 1.13294700 1.75909400	**IM-2** Coordinates (x,y,z): C 2.42292100 1.46429000 -1.37466300 C 1.37054500 0.53493200 -1.12139300 H 1.20904300 -0.27987000 -1.83806300 C 2.50904700 2.63971100 -0.65211800 H 3.32267800 3.34224200 -0.83100200 C 1.51895000 2.92123800 0.30088900 H 1.57942900 3.84411300 0.88069100 C 0.30744400 0.87065000 -0.23119200 C 0.44380000 2.06031800 0.50032800 H -0.33571600 2.33473900 1.21358900 Si 2.64751200 -0.71078500 0.17688800 C 2.74546300 0.10859700 1.83798700 H 3.45816400 -0.49053100 2.42821000 H 1.77211100 0.09974500 2.34655200 H 3.13034400 1.13530200 1.78329400

C 4.20046100 -0.81522200 -0.73948900 H 4.78271800 -1.62756000 -0.27592200 H 4.78558000 0.11126500 -0.66545200 H 4.06754100 -1.07310900 -1.80064000 C 1.78275600 -2.39370300 0.19404000 H 2.49998700 -3.03217300 0.73840400 H 1.64919300 -2.79834300 -0.81788800 H 0.81794100 -2.41500600 0.71468700 H 3.14766500 1.29486900 -2.13149900 B -1.05410700 -0.01284600 -0.06341500 Br -1.06543200 -0.71533100 1.85917900 Br -1.13454800 -1.53718200 -1.39317300 Br -2.62116300 1.22511800 -0.35791400 E(RM062X): -8386.965714 Hartree Dipole Moment: 10.937621 Debye	C 4.28505800 -0.80832800 -0.71081000 H 4.86441200 -1.60655200 -0.21978300 H 4.85530500 0.12738100 -0.64273000 H 4.16258900 -1.08658200 -1.76734600 C 1.82124600 -2.37312700 0.16927000 H 2.51388000 -3.03658200 0.71448800 H 1.70035700 -2.75986500 -0.85137700 H 0.85049500 -2.37666700 0.67858500 H 3.16647700 1.22944600 -2.13694800 B -1.04668200 0.00289600 -0.06231600 Br -1.11616500 -0.71904300 1.85398500 Br -1.18012100 -1.52902600 -1.38943400 Br -2.63594800 1.24665500 -0.35691600 E(RM062X): -8386.983702 Hartree Dipole Moment: 14.935577 Debye
Ph-BBr_2 Coordinates (x,y,z): C -3.90054300 0.00037000 -0.00002600 C -3.20332500 1.20905300 -0.00012900 C -1.81212000 1.20714200 -0.00005800 C -1.08648100 0.00015400 0.00005700 C -1.81230000 -1.20670800 0.00010500 C -3.20350900 -1.20841300 0.00010400 H -4.99194900 0.00045100 -0.00004100 H -3.74686500 2.15471800 -0.00039200 H -1.27362100 2.15622100 -0.00011600 H -1.27392000 -2.15586400 0.00013100 H -3.74718300 -2.15400000 0.00032200 B 0.46422000 0.00000000 0.00006400 Br 1.46849900 -1.63418600 -0.00005100 Br 1.46927600 1.63386800 0.00003500 E(RM062X): -5404.062804 Hartree Dipole Moment: 2.467000 Debye	**Ph-BBr_2** Coordinates (x,y,z): C 3.90243000 -0.00003800 -0.00019400 C 3.20525700 -1.20978600 -0.00041300 C 1.81363500 -1.20819700 -0.00065500 C 1.08772200 -0.00006400 -0.00067200 C 1.81361300 1.20807700 -0.00043200 C 3.20523200 1.20969700 -0.00020600 H 4.99373900 -0.00002600 -0.00001500 H 3.74906900 -2.15518900 -0.00037200 H 1.27858200 -2.15925000 -0.00084700 H 1.27852600 2.15911700 -0.00041800 H 3.74902400 2.15511200 -0.00006500 B -0.45947900 -0.00002000 -0.00094700 Br -1.47019400 1.63397100 0.00040400 Br -1.47034500 -1.63390800 0.00022100 E(RM062X): -5404.065326 Hartree Dipole Moment: 3.070700 Debye
TMS-Br Coordinates (x,y,z): Si 0.00000000 0.00000000 -0.83327400	**TMS-Br** Coordinates (x,y,z): Si 0.00000000 0.00000000 -0.85273000

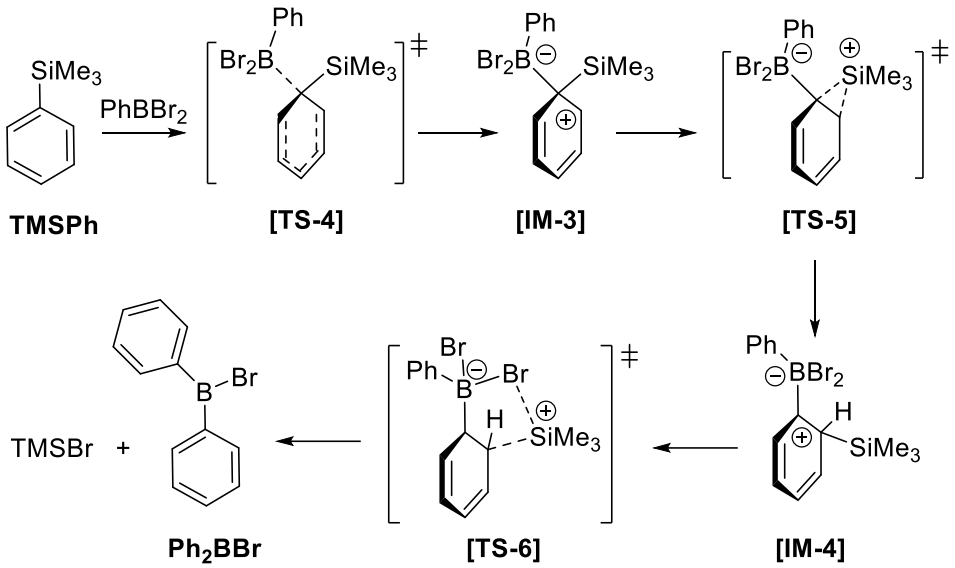
Br 0.00000000 0.00000000 1.42799900 C 0.00000000 1.78875900 -1.38088900 H 0.00000000 1.85162300 -2.48012500 H 0.89051700 2.31063700 -1.00295500 H -0.89051700 2.31063700 -1.00295500 C -1.54911000 -0.89437900 -1.38088900 H -1.60355200 -0.92581100 -2.48012500 H -2.44632900 -0.38410800 -1.00295500 H -1.55581200 -1.92652900 -1.00295500 C 1.54911000 -0.89437900 -1.38088900 H 1.60355200 -0.92581100 -2.48012500 H 1.55581200 -1.92652900 -1.00295500 H 2.44632900 -0.38410800 -1.00295500 E(RM062X): -2982.936192 Hartree Dipole Moment: 2.556700 Debye	Br 0.00000000 0.00000000 1.43184200 C 0.00000000 1.79276100 -1.37600500 H 0.00000000 1.85677500 -2.47513600 H 0.89296300 2.30963200 -0.99712600 H -0.89296300 2.30963200 -0.99712600 C -1.55257700 -0.89638100 -1.37600500 H -1.60801400 -0.92838800 -2.47513600 H -2.44668100 -0.38148700 -0.99712600 H -1.55371800 -1.92814400 -0.99712600 C 1.55257700 -0.89638100 -1.37600500 H 1.60801400 -0.92838800 -2.47513600 H 1.55371800 -1.92814400 -0.99712600 H 2.44668100 -0.38148700 -0.99712600 E(RM062X): -2982.939356 Hartree Dipole Moment: 3.477500 Debye
TMS-Ph Coordinates (x,y,z): C 0.03317000 3.24349600 0.00000000 C 0.03363800 2.54319200 -1.20572900 C 0.03363800 1.14846100 -1.20114000 C 0.03149000 0.42227900 0.00000000 C 0.03363800 1.14846100 1.20114000 C 0.03363800 2.54319200 1.20572900 H 0.03503400 4.33483100 0.00000000 H 0.03673300 3.08556700 -2.15285300 H 0.03937800 0.61845100 -2.15764500 H 0.03937800 0.61845100 2.15764500 H 0.03673300 3.08556700 2.15285300 Si -0.01835100 -1.46697500 0.00000000 C 0.84741200 -2.11224500 1.54267300 H 0.87614500 -3.21237500 1.53262400 H 0.32335100 -1.80332800 2.45958700 H 1.88232900 -1.74356100 1.60005000 C -1.81486200 -2.03276800 0.00000000 H -1.88791700 -3.13095300 0.00000000 H -2.34056100 -1.65334000 -0.88892100 H -2.34056100 -1.65334000 0.88892100 C 0.84741200 -2.11224500 -1.54267300 H 0.87614500 -3.21237500 -1.53262400 H 1.88232900 -1.74356100 -1.60005000	**TMS-Ph** Coordinates (x,y,z): C -0.03240800 3.24558800 0.00000000 C -0.03262500 2.54461400 1.20644400 C -0.03262500 1.14882900 1.20183300 C -0.03088300 0.42197300 0.00000000 C -0.03262500 1.14882900 -1.20183300 C -0.03262500 2.54461400 -1.20644400 H -0.03432100 4.33700400 0.00000000 H -0.03533700 3.08698700 2.15368500 H -0.03714400 0.61939400 2.15870800 H -0.03714400 0.61939400 -2.15870800 H -0.03533700 3.08698700 -2.15368500 Si 0.01706000 -1.47062100 0.00000000 C -0.84835800 -2.11169800 -1.54331300 H -0.87424400 -3.21196300 -1.53138700 H -0.32400700 -1.79991800 -2.45916800 H -1.88418900 -1.74463000 -1.59795800 C 1.81453700 -2.03246300 0.00000000 H 1.88342600 -3.13096600 0.00000000 H 2.33885000 -1.65431300 0.89052100 H 2.33885000 -1.65431300 -0.89052100 C -0.84835800 -2.11169800 1.54331300 H -0.87424400 -3.21196300 1.53138700 H -1.88418900 -1.74463000 1.59795800

H 0.32335100 -1.80332800 -2.45958700 E(RM062X): -640.380710 Hartree Dipole Moment: 0.178275 Debye	H -0.32400700 -1.79991800 2.45916800 E(RM062X): -640.383471 Hartree Dipole Moment: 0.318899 Debye
TS-1 Coordinates (x,y,z): C -0.39957000 1.63015300 1.25290300 C 0.40286300 3.53740600 0.03401600 C -0.48346500 1.65696300 -1.16602000 C 0.06812900 2.92729900 -1.17772100 C -0.71473200 0.93917400 0.04471800 C 0.16161000 2.89524700 1.25317000 H 0.86262600 4.52789000 0.02953100 H -0.70679500 1.16273800 -2.11481000 H 0.42448700 3.38301600 2.19194500 H -0.57025000 1.12202100 2.20557200 H 0.26320600 3.43597000 -2.12190500 Si -2.44087300 -0.00028700 0.04477100 C -3.55598700 1.20392800 0.97154800 H -3.27608700 1.27967100 2.03287300 H -4.60233000 0.86492500 0.92268100 H -3.50011700 2.21019500 0.52932600 C -3.05028300 -0.10547400 -1.72913000 H -4.03277000 -0.60286000 -1.72162700 H -2.38007500 -0.68973300 -2.37346000 H -3.18523200 0.89541200 -2.16517200 C -2.53504900 -1.67014000 0.88096300 H -2.29894800 -1.61356100 1.95158800 H -1.87287600 -2.41325500 0.41844000 H -3.57852100 -2.00955100 0.77355100 B 0.73917900 -0.44734600 -0.01027000 Br 0.69266600 -1.40045800 1.72897200 Br 2.44666400 0.51683100 -0.27016300 Br 0.27692400 -1.61350100 -1.55368500 E(RM062X): -8386.957432 Hartree Dipole Moment: 6.089226 Debye Imaginary Frequency: 173.24i cm^{-1}	**TS-1** Coordinates (x,y,z): C -0.41062500 1.63857300 1.25652400 C 0.57252100 3.47269800 0.05080800 C -0.49968700 1.69372200 -1.16054500 C 0.17724700 2.90388600 -1.16328000 C -0.79965500 0.99982600 0.04516300 C 0.27544500 2.84313500 1.26407700 H 1.11795800 4.41829700 0.05265200 H -0.78939700 1.24604900 -2.11458000 H 0.58111800 3.29734200 2.20686600 H -0.64240700 1.15448500 2.20912400 H 0.41002100 3.40249400 -2.10447000 Si -2.50219600 0.05811500 0.04477000 C -3.64208000 1.25305300 0.94949700 H -3.35289700 1.36000000 2.00574400 H -4.67862400 0.88375100 0.91548100 H -3.61371500 2.24845700 0.48119400 C -3.09726900 -0.09728500 -1.73066200 H -4.07809700 -0.59763200 -1.71874500 H -2.42005300 -0.69093800 -2.35942400 H -3.23079200 0.89341200 -2.18993700 C -2.57590300 -1.60048700 0.91435000 H -2.31766400 -1.51887400 1.97891600 H -1.92556200 -2.35510100 0.45277000 H -3.62056000 -1.94365200 0.83921900 B 0.78471700 -0.48989600 -0.01491400 Br 0.69650700 -1.41048200 1.72467500 Br 2.46714000 0.48352900 -0.28149800 Br 0.25543600 -1.61033100 -1.55068000 E(RM062X): -8386.964549 Hartree Dipole Moment: 6.267293 Debye Imaginary Frequency: 251.67i cm^{-1}
TS-2	**TS-2 (Do not exist)**

Coordinates (x,y,z): C 0.54820700 0.69092100 0.05559400 C 1.91701100 2.46048400 1.05464200 C 2.32344700 1.82057200 -1.23997200 C 2.61172900 2.63305200 -0.15742200 C 1.30610900 0.85049900 -1.13330600 C 0.92283300 1.50528300 1.16443000 H 2.15368300 3.09843800 1.90977700 H 2.86090700 1.93665400 -2.18410400 H 3.38129100 3.40467300 -0.23840900 H 0.99377400 0.29208000 -2.02135100 H 0.35617600 1.39779700 2.09344800 B -0.95002100 0.03063000 -0.00549000 Br -1.02061700 -1.55812900 -1.28489800 Br -1.62249300 -0.51057800 1.82129600 Br -2.08095000 1.54123400 -0.74493300 Si 2.23332000 -0.95965700 0.13596800 C 2.64312100 -1.82082100 -1.47438100 H 3.22124200 -2.72909200 -1.22143100 H 3.26204600 -1.18709800 -2.13022000 H 1.73178300 -2.13027400 -2.00911100 C 3.77834700 -0.22564800 0.89428900 H 4.33192600 0.44917000 0.22494200 H 4.42549000 -1.09971500 1.10101400 H 3.59053700 0.28490900 1.85097700 C 1.40372600 -2.08059100 1.36796200 H 2.13590700 -2.88844400 1.56150500 H 0.47447400 -2.52328600 0.98076900 H 1.17928400 -1.56472800 2.31380300 E(RM062X): -8386.962694 Hartree Dipole Moment: 10.744727 Debye Imaginary Frequency: 39.42i cm^{-1}	Coordinates (x,y,z): N/A E(RM062X): N/A Dipole Moment: N/A Imaginary Frequency: N/A
TS-3 Coordinates (x,y,z): C 0.35114200 1.02493500 0.10014400 C 1.59020300 2.80599600 1.22226400 C 2.04354900 2.33970000 -1.10452400 C 2.28988100 3.08839900 0.04035300 C 1.08519500 1.32031500 -1.07394500	**TS-3** Coordinates (x,y,z): C -0.37490200 2.00282400 1.11737300 C -2.05424100 3.27068400 -0.08317200 C -0.99529600 1.35871700 -1.11453100 C -1.90875200 2.41493700 -1.17273900 C -0.19724100 1.13255300 0.02699100

C 0.64088800 1.79337200 1.25153400 H 1.78427500 3.39543300 2.12197900 H 2.57717000 2.55922800 -2.03271700 H 3.02587000 3.89633300 0.02143800 H 0.07777200 1.59630100 2.16776400 B -0.96695300 0.09539800 0.01489800 Br -2.43220100 1.06386500 -0.93864900 Br -1.57948500 -0.59455000 1.80399800 C 2.90789100 -1.46142000 -1.57889900 H 2.43688800 -2.37011900 -1.98375800 H 3.98908200 -1.63883900 -1.43200800 H 2.79426200 -0.65229600 -2.31708900 C 3.36691900 0.03090700 1.05432700 H 3.72106400 0.94123500 0.55148300 H 4.23447700 -0.64629700 1.18789400 H 2.98142500 0.28826500 2.05253400 C 1.60446000 -2.38407100 1.20853800 H 0.73600500 -2.06477100 1.80957700 H 2.43763800 -2.62710800 1.89260700 H 1.30780400 -3.27214800 0.63015200 H 0.83653700 0.78855000 -1.99700200 Br -0.37829300 -1.55096600 -1.16626300 Si 2.16164100 -1.01155500 0.07613500 E(RM062X): -8386.950134 Hartree Dipole Moment: 8.981821 Debye Imaginary Frequency: 127.65i cm^{-1}	C -1.28617700 3.05723000 1.06431400 H -2.76368300 4.09867400 -0.12362500 H -1.39567900 3.72108700 1.92374000 H 0.22694400 1.85987200 2.01660900 H -2.50174300 2.56993500 -2.07601800 Si -2.61440900 -1.02044200 0.15328900 C -3.63107500 0.39095100 0.75015300 H -3.04972100 1.08227500 1.37607200 H -4.40924600 -0.06581900 1.38653200 H -4.10957300 0.93968500 -0.06873400 C -3.06062900 -1.68137700 -1.50620600 H -4.14696000 -1.87157800 -1.48576300 H -2.51981700 -2.60493300 -1.74073300 H -2.86778900 -0.92946300 -2.28428300 C -1.87443900 -2.04661200 1.48711400 H -1.05154700 -1.49925500 1.97321800 H -1.48714100 -2.99549700 1.09811800 H -2.66125900 -2.22413800 2.23807500 B 0.98645800 0.04752100 -0.01061400 Br 1.59240100 -0.55239900 1.83796100 Br 2.57815000 0.81353300 -1.02074000 Br 0.33124500 -1.63702100 -1.03858100 H -0.85966600 0.72431000 -1.99435300 E(RM062X): -8386.965897 Hartree Dipole Moment: 15.807672 Debye Imaginary Frequency: 91.25i cm^{-1}

1.2 Stationary points for the exchange reaction of TMSPh and $PhBBr_2$



Gas Phase	In Solvent (DCM)
IM-3	**IM-3**
Coordinates (x,y,z):	Coordinates (x,y,z):
C -0.61250100 1.53129500 1.25951400	C -0.73881300 1.47958700 1.26806400
C -0.52619500 3.61376300 0.05958200	C -1.06230900 3.52612100 0.03814200
C -0.42499200 1.54164400 -1.15551100	C -0.63427100 1.47754300 -1.15212400
C -0.44403400 2.92865400 -1.15746200	C -0.90701000 2.84139800 -1.16933700
C -0.52101100 0.77928900 0.04951200	C -0.54265600 0.73623100 0.06464100
C -0.61607700 2.91926600 1.26849400	C -0.98744800 2.84492300 1.25732200
H -0.51568000 4.70574000 0.06406500	H -1.24940400 4.60131300 0.02950500
H -0.30940400 0.99207600 -2.09462800	H -0.45463000 0.94839000 -2.09228600
H -0.67712400 3.46434800 2.21096100	H -1.11995500 3.38501600 2.19509300
H -0.66240700 0.97561600 2.20021100	H -0.66782900 0.94786700 2.22008000
H -0.36229700 3.48084300 -2.09411000	H -0.97163100 3.37550100 -2.11749600
Si -2.56891900 0.26292400 -0.18842300	Si -2.64323700 0.09076800 -0.18017600
C -3.56673300 1.72231100 0.44154000	C -3.75875100 1.45211900 0.44180700
H -3.51528300 1.82674800 1.53380200	H -3.68363300 1.59836900 1.52690900
H -4.61757200 1.54487400 0.16117800	H -4.78302300 1.11974400 0.20483800
H -3.25503900 2.67084300 -0.01915000	H -3.59498900 2.41121100 -0.06709100
C -2.96679800 0.06401600 -2.00634700	C -3.01886600 -0.21950600 -1.98293700
H -3.99085600 -0.34015700 -2.06251700	H -4.00105400 -0.71948700 -2.00927700
H -2.29328100 -0.63132100 -2.51973800	H -2.28469900 -0.86954400 -2.47147400
H -2.95701400 1.03785500 -2.51662000	H -3.10077600 0.72904800 -2.53169500
C -2.93224700 -1.25450300 0.82248600	C -2.78865000 -1.42647400 0.88425800
H -2.73616800 -1.09993900 1.89090000	H -2.57772500 -1.20964500 1.93903600

H -2.35360100 -2.12232800 0.48295600 H -4.00815200 -1.45269500 0.68000300 B 0.45106300 -0.61952000 0.08987900 Br 0.25658400 -1.56563400 1.89043700 Br -0.07305500 -1.91593800 -1.40582700 C 1.95600800 -0.05793100 -0.09460800 C 4.50926900 1.13203100 -0.39101400 C 2.56084900 0.65549500 0.95435700 C 2.67345900 -0.15892700 -1.29468600 C 3.93360700 0.42528700 -1.44324000 C 3.81541100 1.24334900 0.81485500 H 2.04349800 0.73413300 1.91474900 H 2.24497700 -0.71543100 -2.13014300 H 4.46923800 0.32009300 -2.38877100 H 4.25908800 1.78352300 1.65346800 H 5.49503000 1.58659900 -0.50429900 E(RM062X): -6044.427216 Hartree Dipole Moment: 8.994317 Debye	H -2.13221300 -2.23681800 0.54567600 H -3.84010300 -1.74530800 0.78769300 B 0.52834400 -0.53681300 0.08472100 Br 0.47271600 -1.52708900 1.89582400 Br 0.10000100 -1.91141700 -1.39174500 C 1.99565200 0.11342500 -0.12038200 C 4.48497100 1.43636400 -0.43222700 C 2.54711500 0.89916100 0.90836800 C 2.73173000 0.01667800 -1.30995600 C 3.96046700 0.66505200 -1.46653600 C 3.76943100 1.55121600 0.76190200 H 2.01130400 0.99157200 1.85738300 H 2.34231100 -0.58311200 -2.13447400 H 4.50956100 0.56262800 -2.40470100 H 4.16883900 2.14875400 1.58373600 H 5.44460600 1.94248700 -0.55138400 E(RM062X): -6044.442194 Hartree Dipole Moment: 12.385355 Debye
IM-4 Coordinates (x,y,z): C 0.33764400 1.42132400 -1.55240200 C 1.57523200 3.27470600 -0.55548500 C 1.12807900 1.25820300 0.72347700 C 1.68275700 2.57349200 0.62091100 C 0.34662800 0.70468600 -0.33001000 C 0.92032500 2.67213300 -1.65350100 H 1.99450600 4.27682300 -0.64888800 H 0.85156800 3.21904100 -2.59640900 H -0.20373500 0.99470300 -2.39921900 H 2.20518500 2.99912600 1.48047800 C 2.56807400 -1.53216900 -0.76658700 H 1.87975600 -2.22146900 -0.26362000 H 3.55977300 -2.00869800 -0.85379300 H 2.18178400 -1.33100900 -1.77455300 C 3.98773000 1.14316800 -0.81346500 H 4.85341900 0.52768400 -1.10721900 H 4.34959900 2.01274600 -0.25043300 H 3.50211000 1.49244600 -1.73562200 C 3.48224300 -0.25031300 1.92286300 H 2.75956600 -0.86056600 2.48262800	**IM-4** Coordinates (x,y,z): C 0.37012400 1.42862100 -1.54108100 C 1.68334700 3.22920000 -0.54682500 C 1.17192400 1.22099000 0.72382300 C 1.77364600 2.51240400 0.62632800 C 0.36669900 0.70358700 -0.33108200 C 1.00110600 2.66171100 -1.64045500 H 2.14361500 4.21317300 -0.63513800 H 0.94811900 3.21439300 -2.58052000 H -0.19098900 1.03778100 -2.39218900 H 2.32275200 2.90939000 1.48261800 C 2.56498800 -1.55115500 -0.74906200 H 1.85248500 -2.20738900 -0.23659500 H 3.53241500 -2.07310000 -0.84322500 H 2.18571000 -1.32726000 -1.75498500 C 4.06218300 1.09003400 -0.82538700 H 4.91863200 0.45944100 -1.11404900 H 4.43327300 1.96060100 -0.27038800 H 3.57180200 1.43062600 -1.74815000 C 3.53592500 -0.28837700 1.93306400 H 2.80657600 -0.89243900 2.49053700

H 3.65665600 0.69409400 2.45726400 H 4.43548800 -0.79940900 1.86895800 B -0.71031600 -0.50732500 -0.07951200 Br -0.78572800 -1.72676900 -1.71677700 C -2.11658600 0.23925800 0.20707100 C -4.47378500 1.72997200 0.69263000 C -3.08312100 0.42335500 -0.79336400 C -2.36550000 0.83164100 1.45706600 C -3.52502100 1.56433200 1.70167600 C -4.24803400 1.15408700 -0.55572700 H -2.92942800 -0.03089100 -1.77394500 H -1.64480700 0.69512300 2.26716300 H -3.69298500 2.00227300 2.68751500 H -4.98664200 1.26784000 -1.35159700 H -5.38598500 2.29874400 0.88144300 H 1.01320200 0.81208100 1.71670100 Si 2.86242500 0.03286500 0.18509800 Br -0.13488300 -1.62212900 1.57073200 E(RM062X): -6044.426373 Dipole Moment: 9.854012 Debye	H 3.71744900 0.65459400 2.46664700 H 4.48373800 -0.84656100 1.87816200 B -0.72874400 -0.47024400 -0.08464400 Br -0.84078300 -1.71211200 -1.72182800 C -2.13281300 0.28050400 0.20186600 C -4.48319600 1.78533400 0.69904300 C -3.10247600 0.47426600 -0.79438200 C -2.37442600 0.87482100 1.45353000 C -3.52983500 1.61376200 1.70414300 C -4.26370900 1.21154300 -0.55215800 H -2.95280900 0.03002000 -1.78022500 H -1.64660500 0.74367100 2.25820800 H -3.68889400 2.05547000 2.68981600 H -5.00190000 1.33494200 -1.34708400 H -5.39089100 2.35997300 0.89176400 H 1.06272700 0.77206400 1.71582900 Si 2.94274700 0.00338400 0.19214700 Br -0.20272800 -1.63100200 1.56165400 E(RM062X): -6044.442878 Hartree Dipole Moment: 13.241858 Debye
Ph_2-BBr Coordinates (x,y,z): C 1.37846700 -0.32187800 -0.02726500 C 3.85239700 -1.66582000 -0.13153900 C 1.49087000 -1.59444600 -0.61992800 C 2.54507900 0.26188900 0.50030000 C 3.76523200 -0.40590800 0.46314600 C 2.71541600 -2.25634100 -0.68183700 H 0.60700300 -2.06409600 -1.05681800 H 2.48777300 1.25600900 0.94819300 H 4.65476800 0.05924700 0.89053900 H 2.78322400 -3.23492400 -1.15943400 H 4.81122000 -2.18574400 -0.17107300 B 0.00005100 0.40545100 -0.00012000 C -1.37838500 -0.32192000 0.02704100 C -3.85228600 -1.66593400 0.13164700 C -2.54498500 0.26160700 -0.50080500 C -1.49078800 -1.59430000 0.62008800 C -2.71532600 -2.25620900 0.68221500 C -3.76510000 -0.40623900 -0.46350600	**Ph_2-BBr** Coordinates (x,y,z): C 1.37984200 -0.32357500 -0.02701900 C 3.85738600 -1.66272900 -0.13224000 C 1.49435600 -1.59675600 -0.61964400 C 2.54579100 0.26248800 0.50185100 C 3.76789400 -0.40268600 0.46381700 C 2.72081300 -2.25615700 -0.68205200 H 0.61237400 -2.07040600 -1.05577200 H 2.48854800 1.25464500 0.95426200 H 4.65637200 0.06347400 0.89223900 H 2.79011600 -3.23498500 -1.15875800 H 4.81719700 -2.18066300 -0.17207300 B 0.00001500 0.39810900 0.00003200 C -1.37981900 -0.32357500 0.02708500 C -3.85741100 -1.66267800 0.13215100 C -2.54570600 0.26246800 -0.50193900 C -1.49442300 -1.59671700 0.61978400 C -2.72089200 -2.25609100 0.68211500 C -3.76783300 -0.40268400 -0.46398000

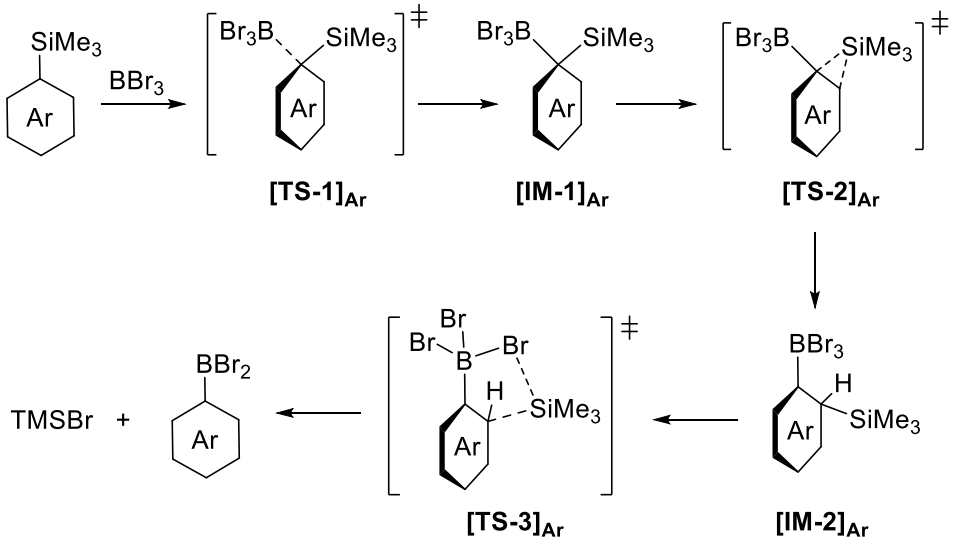
H -2.48772900 1.25558600 -0.94902600 H -0.60693100 -2.06378800 1.05717800 H -2.78307500 -3.23462800 1.16015400 H -4.65462300 0.05873200 -0.89111500 H -4.81112000 -2.18583200 0.17130600 Br -0.00012300 2.34586200 0.00009600 E(RM062X): -3061.527814 Hartree Dipole Moment: 2.126800 Debye	H -2.48841600 1.25458300 -0.95443300 H -0.61249300 -2.07036500 1.05602400 H -2.79024900 -3.23488700 1.15887800 H -4.65625500 0.06346800 -0.89253200 H -4.81723400 -2.18059300 0.17192300 Br -0.00000100 2.34563800 0.00001400 E(RM062X): -3061.531968 Hartree Dipole Moment: 2.785500 Debye
TS-4 Coordinates (x,y,z): C -0.33491300 1.62893600 1.23601000 C 0.60227900 3.50501900 0.06737300 C -0.10614800 1.57761100 -1.17469800 C 0.44203200 2.84885600 -1.15828800 C -0.51744100 0.90457600 0.01823100 C 0.20656600 2.90360400 1.26619300 H 1.05106200 4.50051500 0.08812000 H -0.20201200 1.03845100 -2.12191700 H 0.34132300 3.42684600 2.21315700 H -0.61862600 1.13750700 2.17110100 H 0.76919000 3.32465000 -2.08286600 Si -2.51672900 0.63496600 -0.19093700 C -3.24577800 2.23428100 0.48433400 H -3.14347500 2.30424200 1.57690100 H -4.31851300 2.27821400 0.23898100 H -2.75864900 3.11291300 0.03387300 C -2.93392600 0.56772400 -2.01747200 H -4.01705500 0.38170000 -2.09713400 H -2.40798800 -0.23343500 -2.55016800 H -2.72155300 1.53186500 -2.50252100 C -3.19215500 -0.81680100 0.76149000 H -3.00831300 -0.72642600 1.83976200 H -2.77430900 -1.77086700 0.41652600 H -4.28125700 -0.81396000 0.58754500 B 0.29096400 -0.69668800 0.08892200 Br -0.10225000 -1.56423400 1.87969200 Br -0.40737300 -1.87794100 -1.41027100 C 1.85683100 -0.34573600 -0.07226000 C 4.55085000 0.48216400 -0.35208200 C 2.56923700 0.21038700 1.00287700	**TS-4** Coordinates (x,y,z): C -0.24184000 1.64745600 1.24907300 C 1.26989900 3.13683000 0.12122500 C -0.07044100 1.61542500 -1.16533000 C 0.87836600 2.62552000 -1.11860600 C -0.64789600 1.05591700 0.01345000 C 0.70147400 2.65792800 1.30847200 H 2.02822200 3.92105200 0.16593700 H -0.35690500 1.19889000 -2.13490800 H 1.00832900 3.07299800 2.26876100 H -0.67177800 1.26542700 2.17892500 H 1.32499600 3.00722000 -2.03680300 Si -2.58778700 0.78959800 -0.14434300 C -3.28530900 2.35784300 0.63018300 H -3.08774100 2.39553800 1.71177400 H -4.37535600 2.39739400 0.48060500 H -2.84028200 3.25104600 0.16569500 C -3.04846600 0.79342800 -1.96461500 H -4.14073500 0.67069500 -2.03392000 H -2.57554800 -0.01878600 -2.53137400 H -2.78776500 1.75491900 -2.43139600 C -3.30862000 -0.69045700 0.74441200 H -3.12126600 -0.64728400 1.82572600 H -2.92472200 -1.64396900 0.35990700 H -4.39771100 -0.65180300 0.57908100 B 0.26217100 -0.69378400 0.06555500 Br -0.22010100 -1.55792200 1.82212200 Br -0.51446500 -1.76284500 -1.45866600 C 1.82569300 -0.39325800 -0.07723500 C 4.57462700 0.24199300 -0.32500700 C 2.59817700 -0.03266700 1.03862800

C 2.54142200 -0.48400800 -1.28916500 C 3.86912500 -0.07760900 -1.43023900 C 3.89423500 0.62165700 0.87046400 H 2.07893300 0.30699900 1.97518700 H 2.02915100 -0.92736900 -2.14511800 H 4.37468200 -0.20697900 -2.38914600 H 4.42013900 1.04359900 1.72907000 H 5.59017800 0.79761400 -0.45919900 E(RM062X): -6044.426812 Hartree Dipole Moment: 7.827221 Debye Imaginary Frequency: 42.21i cm^{-1}	C 2.47733400 -0.42988600 -1.32204800 C 3.83036800 -0.11921700 -1.44879900 C 3.95276300 0.28284500 0.92183800 H 2.13064100 -0.00131300 2.02513500 H 1.91393900 -0.70845100 -2.21498300 H 4.30650900 -0.16220500 -2.43001000 H 4.52382000 0.55770300 1.81047100 H 5.63457400 0.48411400 -0.42039100 E(RM062X): -6044.437230 Hartree Dipole Moment: 8.058845 Debye Imaginary Frequency: 129.84i cm^{-1}
TS-5 Coordinates (x,y,z): C 0.43458500 0.70953800 0.24363200 C 0.99461900 2.68943900 1.57453800 C 1.35769700 2.74985400 -0.81032600 C 1.38777100 3.38636800 0.41525300 C 0.89714500 1.41641500 -0.89547200 C 0.54850400 1.38345600 1.49513400 H 1.02922500 3.19246800 2.54257100 H 1.67109800 3.27013100 -1.71682800 H 1.71977600 4.42307600 0.48913600 H 0.75458100 0.95641800 -1.87712700 H 0.21706600 0.85513500 2.39181100 B -0.63035300 -0.53393600 0.07747400 Br -0.10288500 -1.70103200 -1.54709100 Br -0.64223600 -1.70648300 1.75288500 Si 2.69782400 0.06401200 -0.16600600 C 3.22554000 -0.18623400 -1.94049700 H 4.18229100 -0.73333300 -1.92018800 H 3.38360800 0.77103600 -2.45603100 H 2.49256900 -0.78985900 -2.49041800 C 3.83603100 1.27847300 0.68474500 H 3.98846100 2.20922100 0.12552000 H 4.80357700 0.75061500 0.73708800 H 3.53203400 1.51483200 1.71204000 C 2.63462000 -1.51736200 0.80467200 H 3.66720400 -1.90655100 0.77671100 H 1.95588800 -2.25631800 0.36278900 H 2.33958700 -1.35000700 1.84805700	**TS-5** Coordinates (x,y,z): C 0.47749200 0.71694800 0.18534200 C 1.08436200 2.74058600 1.43041600 C 1.35031100 2.72041200 -0.97054600 C 1.42953700 3.39643300 0.23574900 C 0.88265000 1.39248000 -0.99564900 C 0.63503200 1.43128100 1.40823100 H 1.16483100 3.27060700 2.38054300 H 1.63388200 3.20949800 -1.90324200 H 1.77010500 4.43237000 0.26240500 H 0.72319800 0.89992500 -1.95841200 H 0.35009700 0.93661600 2.33899300 B -0.61737900 -0.50202500 0.08766300 Br -0.14638800 -1.79594700 -1.46022700 Br -0.66357700 -1.60640400 1.83021500 Si 2.72629700 0.03328100 -0.17759300 C 3.18787400 -0.30226600 -1.95283200 H 4.14025600 -0.85675200 -1.92607600 H 3.34311200 0.63181300 -2.50945500 H 2.43926300 -0.92066600 -2.46253800 C 3.87078900 1.28490800 0.59095500 H 3.97289000 2.20885000 0.00982900 H 4.84857100 0.77293400 0.58868500 H 3.61936000 1.52436700 1.63136900 C 2.64826600 -1.50100700 0.86659300 H 3.67414300 -1.90648100 0.84300900 H 1.95484100 -2.25034300 0.46805000 H 2.37649000 -1.27290400 1.90488600

C -2.06137500 0.18031400 -0.16340800 C -4.46011900 1.63495100 -0.55888100 C -2.47713100 0.57475400 -1.44550700 C -2.88535100 0.54186000 0.91443200 C -4.06793000 1.25637200 0.72382700 C -3.65818400 1.28873500 -1.64526600 H -1.87397000 0.29741000 -2.31295700 H -2.60429100 0.24071700 1.92579500 H -4.69035500 1.51198000 1.58358100 H -3.95749600 1.56888100 -2.65715700 H -5.38792500 2.18910600 -0.71174200 E(RM062X): -6044.425680 Hartree Dipole Moment: 9.823736 Debye Imaginary Frequency: 61.60i cm^{-1}	C -2.05218900 0.20298400 -0.16350700 C -4.46888700 1.63266800 -0.56623900 C -2.59585200 0.37823000 -1.44581000 C -2.75600100 0.77669200 0.91016200 C -3.94517200 1.47906800 0.71832800 C -3.78741500 1.07849000 -1.64839100 H -2.08357700 -0.05178900 -2.30879600 H -2.36935600 0.66019400 1.92547900 H -4.46795700 1.90555000 1.57671800 H -4.18550900 1.18767800 -2.65917100 H -5.40189900 2.17756900 -0.72069100 E(RM062X): -6044.441716 Hartree Dipole Moment: 12.884793 Debye Imaginary Frequency: 47.74i cm^{-1}
TS-6 Coordinates (x,y,z): C -0.47244500 1.53545400 1.67709200 C -1.47050600 3.50353600 0.67338600 C -0.73205000 1.67174300 -0.71532900 C -1.31092500 2.94337200 -0.58527900 C -0.27669600 0.94338500 0.40950000 C -1.05458000 2.78932700 1.80657300 H -1.91454200 4.49419100 0.78377800 H -1.17951500 3.22890000 2.79801000 H -0.12836400 0.99874700 2.56322200 H -1.62300700 3.49087200 -1.47660100 C -2.76023700 -1.77085000 0.67252200 H -2.60614000 -2.67724800 0.07412300 H -3.74407900 -1.79361500 1.16663200 H -1.97700700 -1.74317500 1.44465200 C -3.69571800 1.07864700 0.44140600 H -4.67557200 0.58879400 0.58401100 H -3.84344600 1.97213500 -0.17565900 H -3.32412500 1.37328400 1.43058100 C -3.21209300 -0.33353500 -2.18277900 H -2.98370900 -1.31447500 -2.61764100 H -2.70827600 0.43764500 -2.78147500 H -4.29658300 -0.14465400 -2.22682700 B 0.69375400 -0.34039400 0.21187200 Br 0.72021700 -1.54077100 1.85575600	**TS-6** Coordinates (x,y,z): C -0.64893500 1.74375000 1.48026200 C -1.85395500 3.46340800 0.27037700 C -0.89341500 1.58411900 -0.90639800 C -1.61624500 2.78319300 -0.91953400 C -0.37556000 1.04105100 0.29073600 C -1.37248600 2.93432100 1.47275300 H -2.41424100 4.39968400 0.26786700 H -1.55889500 3.46067300 2.41066800 H -0.26276800 1.35571900 2.42463900 H -1.98618600 3.18327700 -1.86538400 C -2.64363200 -1.92965500 0.81873100 H -2.35836600 -2.86685400 0.32660300 H -3.59098200 -2.04871500 1.36811300 H -1.85444500 -1.65654100 1.53575000 C -3.90055400 0.81355100 0.25410800 H -4.84698100 0.32917100 0.55474500 H -4.11742300 1.58067800 -0.49750300 H -3.46095000 1.27599300 1.14755400 C -3.17981400 -0.89913700 -2.20957700 H -2.77075900 -1.86653100 -2.52228500 H -2.74269600 -0.10075200 -2.82487500 H -4.27219600 -0.88022400 -2.35789700 B 0.69840700 -0.15832900 0.23126500 Br 0.82336300 -1.17632500 2.02880200

C 2.16704700 0.09643800 -0.25554400 C 4.71300800 1.08746400 -1.00016000 C 3.16345300 0.34806300 0.70133300 C 2.48657000 0.36087400 -1.59684700 C 3.74020300 0.84556500 -1.96844700 C 4.41801600 0.83680700 0.33874200 H 2.95620400 0.14477100 1.75396200 H 1.74659200 0.16783700 -2.37688800 H 3.95939600 1.02941800 -3.02196700 H 5.17167700 1.01646700 1.10773900 H 5.69637700 1.46330600 -1.28798200 H -0.53421000 1.28029100 -1.71603900 Si -2.67944200 -0.25001100 -0.39452700 Br -0.26783200 -1.44291800 -1.34314500 E(RM062X): -6044.413649 Hartree Dipole Moment: 7.744616 Debye Imaginary Frequency: 129.28i cm^{-1}	C 2.17172000 0.27903500 -0.22825000 C 4.78236900 1.04968100 -1.00211400 C 2.51561100 1.62904100 -0.38935900 C 3.17737000 -0.67560900 -0.46426900 C 4.46249900 -0.30291200 -0.84713800 C 3.80545900 2.01421100 -0.77003100 H 1.76459500 2.40352100 -0.21297800 H 2.93996900 -1.73624000 -0.34278700 H 5.22173400 -1.06690600 -1.02573800 H 4.04405100 3.07332400 -0.88545300 H 5.78941600 1.34576300 -1.30141500 H -0.66567000 1.09309600 -1.85619200 Si -2.88605900 -0.57820500 -0.41296900 Br -0.03842000 -1.55395800 -1.19508700 E(RM062X): -6044.428655 Hartree Dipole Moment: 12.522731 Debye Imaginary Frequency: 126.59i cm^{-1}

1.3 Stationary points for the exchange reaction of TMSAr (Ar = tolyl) andBBr_3



Gas Phase	In Solvent (DCM)
$[IM\text{-}1]_{tolyl}$ Coordinates (x,y,z):	**$[IM\text{-}1]_{tolyl}$** Coordinates (x,y,z):

C -1.36877200 -0.39717900 -1.16520800 C -3.25226800 -1.36587200 0.00675900 C -1.32671700 -0.57767500 1.24789400 C -2.57737000 -1.16465200 1.22461000 C -0.66461600 -0.15058900 0.05330500 C -2.63504600 -0.96145500 -1.18665000 H -0.79741300 -0.44925700 2.19574900 H -3.14042900 -1.13165100 -2.13898700 H -0.86347800 -0.14587900 -2.10220100 H -3.04460600 -1.49101600 2.15582900 Si -1.24679100 1.92383500 0.06192700 C -2.96732500 2.02329400 0.80155300 H -3.69083200 1.37874900 0.28284100 H -3.30225200 3.06591700 0.67648300 H -2.98090800 1.78375700 1.87306700 C -0.02722700 2.83879100 1.12672100 H -0.37095100 3.88710500 1.13179900 H 0.98960800 2.79294700 0.71708500 H -0.00695500 2.46331600 2.15740100 C -1.33575200 2.59488100 -1.68243500 H -2.19936900 2.18167700 -2.22245100 H -0.41877200 2.41096100 -2.25398500 H -1.47608500 3.68476400 -1.59501300 B 0.99343800 -0.29941700 0.00121500 Br 1.80940900 0.87332000 -1.44500300 Br 1.29769400 -2.25095800 -0.46630500 Br 1.84642700 0.10284900 1.78922700 C -4.61894700 -1.98258800 -0.00579500 H -4.69703900 -2.78128100 0.74358900 H -5.37337900 -1.22029200 0.24695100 H -4.86856200 -2.39053500 -0.99286200 E(RM062X): -8426.233579 Hartree Dipole Moment: 10.872120 Debye	C -1.35042800 -0.44087900 -1.16558700 C -3.21349500 -1.46249300 -0.00152200 C -1.29423500 -0.66002800 1.24510000 C -2.53468400 -1.26762200 1.21651300 C -0.64428600 -0.20417800 0.05410700 C -2.60725700 -1.02734700 -1.19009900 H -0.77556100 -0.53386600 2.19828800 H -3.11642800 -1.17977700 -2.14306200 H -0.86517100 -0.16344500 -2.10519000 H -2.99443900 -1.60846300 2.14580700 Si -1.40134900 1.86622800 0.06735500 C -3.12053400 1.85286800 0.79415800 H -3.81689900 1.20612300 0.24375100 H -3.48486600 2.88925600 0.70061900 H -3.12882800 1.57693700 1.85636600 C -0.21788900 2.79681800 1.15981300 H -0.60749200 3.82821900 1.18990000 H 0.80074500 2.81135000 0.75319400 H -0.19317400 2.39590500 2.18094700 C -1.47203400 2.54587200 -1.67081100 H -2.29327100 2.08805500 -2.23936100 H -0.53030100 2.42414600 -2.21809300 H -1.67939800 3.62395700 -1.57147900 B 0.99742600 -0.25577200 0.00181800 Br 1.78197900 0.95298500 -1.43728000 Br 1.44716300 -2.20012400 -0.47618500 Br 1.86432200 0.16890200 1.78703200 C -4.57209900 -2.09189100 -0.01938700 H -4.66580100 -2.85230200 0.76621100 H -5.33421200 -1.32017500 0.17595600 H -4.79270900 -2.54267100 -0.99447200 E(RM062X): -8426.250690 Hartree Dipole Moment: 14.401074 Debye
[IM-2]$_{tolyl}$ Coordinates (x,y,z): C 2.58191900 0.86159200 -1.13768200 C 1.32891700 0.17565500 -0.99978500 H 0.99238100 -0.47666500 -1.81791500 C 2.92218300 1.90855100 -0.30810800 C 1.95968700 2.31085400 0.65149500	**[IM-2]$_{tolyl}$** Coordinates (x,y,z): C 2.56329000 0.86367200 -1.15753200 C 1.31134700 0.19173200 -1.02641700 H 1.00259400 -0.49557500 -1.82366000 C 2.91183500 1.91410000 -0.32170900 C 1.95160100 2.32553500 0.62387100

H 2.20825800 3.13608700 1.32484800 C 0.32786300 0.67032600 -0.11502000 C 0.71265900 1.72150000 0.74400200 H -0.01812600 2.09942600 1.46148700 Si 2.10181500 -1.45520700 0.16837400 C 2.39708700 -0.86414800 1.90633100 H 2.91445100 -1.67920200 2.43811900 H 1.44485200 -0.66129200 2.41604700 H 3.03714500 0.02757100 1.94625000 C 3.70002800 -1.90017300 -0.70790600 H 4.03625100 -2.87196900 -0.31261700 H 4.49606400 -1.16377300 -0.53252200 H 3.55492800 -2.02035600 -1.79178100 C 0.92565400 -2.88429600 0.02380800 H 1.43672600 -3.72850000 0.51807200 H 0.73486000 -3.15266600 -1.02362300 H -0.03383400 -2.70480100 0.52333100 H 3.28400400 0.52383600 -1.90260600 B -1.20419300 0.14657700 -0.07178000 Br -1.48814800 -0.69207700 1.77466900 Br -1.60477200 -1.18496600 -1.54310100 Br -2.38867700 1.76776100 -0.28471100 C 4.24390000 2.61867000 -0.40733000 H 4.85416100 2.21352300 -1.22438500 H 4.09670900 3.69299200 -0.58871000 H 4.81324900 2.51948000 0.52883500 E(RM062X): -8426.233866 Hartree Dipole Moment: 11.402322 Debye	H 2.19753100 3.15079700 1.29703600 C 0.31650000 0.67845500 -0.13125000 C 0.69679700 1.73518500 0.71071600 H -0.02595600 2.12438200 1.43050900 Si 2.22707300 -1.40727800 0.17935600 C 2.44965900 -0.77605400 1.91028000 H 2.96313600 -1.58228900 2.45957200 H 1.48394300 -0.58102000 2.39549700 H 3.08103100 0.12099700 1.95806200 C 3.83660600 -1.81201700 -0.67424200 H 4.19746200 -2.75974400 -0.24358500 H 4.60154600 -1.04149600 -0.50943300 H 3.70123600 -1.96581900 -1.75432800 C 1.04911700 -2.83366500 0.01485700 H 1.55472300 -3.67973900 0.51031400 H 0.87720000 -3.09838300 -1.03691200 H 0.08599600 -2.65690900 0.50779100 H 3.26259800 0.52742900 -1.92510700 B -1.20395500 0.13623600 -0.06961000 Br -1.51487900 -0.71268900 1.77100800 Br -1.62584100 -1.20594800 -1.53487000 Br -2.45856100 1.73047000 -0.27679400 C 4.25187700 2.58831800 -0.40650400 H 4.80410600 2.26385700 -1.29702200 H 4.13882200 3.68043000 -0.44138100 H 4.85783700 2.34809200 0.48022300 E(RM062X): -8426.252106 Hartree Dipole Moment: 15.574825 Debye
P-Tolyl-BBr_2 Coordinates (x,y,z): C 3.55903100 0.00000200 -0.01033100 C 2.84015700 -1.20246900 -0.01112000 C 1.45097700 -1.20350300 -0.00630800 C 0.71961800 0.00000400 -0.00309000 C 1.45097900 1.20351100 -0.00630000 C 2.84015800 1.20247500 -0.01111200 H 3.38180300 -2.15079800 -0.01806300 H 0.91709400 -2.15532400 -0.00804600 H 0.91709800 2.15533300 -0.00803400 H 3.38180600 2.15080300 -0.01804600	**P-Tolyl-BBr_2** Coordinates (x,y,z): C 3.56127800 0.00000100 -0.01017300 C 2.84198300 -1.20357900 -0.01086600 C 1.45269600 -1.20459000 -0.00598100 C 0.72074400 0.00000300 -0.00283600 C 1.45269800 1.20459500 -0.00597100 C 2.84198400 1.20358200 -0.01085500 H 3.38361400 -2.15173300 -0.01773700 H 0.92150800 -2.15799200 -0.00753900 H 0.92151200 2.15799800 -0.00752200 H 3.38361800 2.15173500 -0.01771600

B -0.82705100 0.00000100 -0.00054100 Br -1.83392100 1.63476800 0.00182500 Br -1.83390600 -1.63477400 0.00182900 C 5.06288000 0.00000400 0.01803100 H 5.42530400 0.00008700 1.05794600 H 5.47165000 -0.89192300 -0.47471200 H 5.47164700 0.89185800 -0.47484900 E(RM062X): -5443.330701 Hartree Dipole Moment: 3.185019 Debye	B -0.82245600 0.00000100 -0.00043500 Br -1.83543500 1.63486000 0.00174500 Br -1.83542500 -1.63486300 0.00174900 C 5.06430700 0.00000300 0.01685500 H 5.42458900 0.00008400 1.05747000 H 5.47170800 -0.89329900 -0.47398800 H 5.47170500 0.89323400 -0.47412200 E(RM062X): -5443.333466 Hartree Dipole Moment: 3.961802 Debye
TMS-Toluene Coordinates (x,y,z): C -2.82236900 0.00000000 0.01211400 C -2.10150300 -1.19900600 0.00389300 C -0.70807600 -1.19734200 -0.01709500 C 0.02316000 0.00000000 -0.02663200 C -0.70807600 1.19734300 -0.01709500 C -2.10150300 1.19900700 0.00389300 H -2.64198900 -2.14877300 0.01371000 H -0.18333900 -2.15684400 -0.02658300 H -0.18333800 2.15684500 -0.02658300 H -2.64198900 2.14877300 0.01371000 Si 1.91078400 0.00000000 -0.00169100 C 2.54531400 1.54269300 -0.87607900 H 3.64511500 1.53480600 -0.91630000 H 2.23995100 2.45951400 -0.34971200 H 2.16542700 1.59829400 -1.90702900 C 2.50579400 -0.00000200 1.78580600 H 3.60501400 -0.00000200 1.84174700 H 2.13447300 -0.88887300 2.31738100 H 2.13447300 0.88886900 2.31738300 C 2.54531400 -1.54269200 -0.87608100 H 3.64511500 -1.53480500 -0.91630200 H 2.16542700 -1.59829000 -1.90703100 H 2.23995100 -2.45951300 -0.34971600 C -4.32852200 0.00000000 -0.00059800 H -4.70969500 -0.00001900 -1.03375100 H -4.73138800 -0.89073800 0.50001400 H -4.73138800 0.89075500 0.49998300	**TMS-Toluene** Coordinates (x,y,z): C -2.82462500 0.00000000 0.01209800 C -2.10283900 -1.19969500 0.00421200 C -0.70834500 -1.19794600 -0.01659200 C 0.02376200 0.00000000 -0.02644800 C -0.70834500 1.19794700 -0.01659200 C -2.10283900 1.19969500 0.00421200 H -2.64322300 -2.14956000 0.01433800 H -0.18411500 -2.15782800 -0.02486300 H -0.18411400 2.15782800 -0.02486400 H -2.64322300 2.14956100 0.01433800 Si 1.91434500 0.00000000 -0.00251000 C 2.54541600 1.54326500 -0.87629300 H 3.64538200 1.53342900 -0.91366300 H 2.23732100 2.45914500 -0.34970700 H 2.16727600 1.59637300 -1.90823300 C 2.50559000 -0.00000200 1.78607600 H 3.60505700 -0.00000200 1.83808400 H 2.13557400 -0.89042800 2.31640000 H 2.13557400 0.89042400 2.31640100 C 2.54541600 -1.54326400 -0.87629500 H 3.64538200 -1.53342800 -0.91366600 H 2.16727600 -1.59637000 -1.90823600 H 2.23732000 -2.45914500 -0.34971100 C -4.33075800 0.00000000 -0.00025800 H -4.71103900 -0.00001800 -1.03369000 H -4.73294400 -0.89178200 0.49876300 H -4.73294400 0.89179800 0.49873300

E(RM062X): -679.647470 Hartree Dipole Moment: 0.303921 Debye	E(RM062X): -679.650289 Hartree Dipole Moment: 0.287066 Debye
[TS-1]$_{tolyl}$ Coordinates (x,y,z): C 0.89337900 1.21578200 1.24560500 C 2.95688500 1.53680300 0.02684100 C 0.86728600 1.30525800 -1.16549400 C 2.23412500 1.50978500 -1.17635300 C 0.13599000 1.10587600 0.04193400 C 2.26093700 1.40955300 1.24127400 H 0.33291300 1.24481700 -2.11691300 H 2.81221400 1.44747700 2.18251500 H 0.37829000 1.09878900 2.20277700 H 2.76397200 1.61964900 -2.12423700 Si -1.62529500 1.94497600 0.04623000 C -1.31642100 3.55565300 0.97684700 H -1.07895900 3.37046100 2.03517200 H -2.21140000 4.19570000 0.93980600 H -0.47775900 4.11107200 0.53038300 C -2.07781200 2.37570400 -1.72672000 H -3.05647800 2.88030400 -1.71934700 H -2.15984000 1.48806300 -2.36831000 H -1.34708700 3.06935800 -2.16853600 C -3.03264000 1.03744400 0.88261000 H -2.84426100 0.87371500 1.95191600 H -3.24692800 0.06684700 0.41666100 H -3.92205200 1.68111100 0.78319800 B -0.12460400 -0.94571500 -0.01216900 Br -0.92626700 -1.44109600 1.72752800 Br 1.65515800 -1.75788600 -0.26772600 Br -1.33807500 -1.22506100 -1.55520300 C 4.45113400 1.65056300 0.01544500 H 4.82527600 2.13933900 0.92419800 H 4.88659500 0.63899600 -0.02316400 H 4.80689000 2.20019300 -0.86539800 E(RM062X): -8426.228130 Hartree Dipole Moment: 5.954476 Debye Imaginary Frequency: 198.89i cm^{-1}	**[TS-1]$_{tolyl}$** Coordinates (x,y,z): C 0.71208000 1.35324300 1.24646000 C 2.75466300 1.82892200 0.03595800 C 0.68291200 1.46425000 -1.16246500 C 2.03525900 1.75838500 -1.16817800 C -0.03219100 1.21579600 0.04169400 C 2.06674300 1.63643400 1.24600400 H 0.15468800 1.39629000 -2.11701800 H 2.61061700 1.70751500 2.18977000 H 0.20444100 1.20978000 2.20442700 H 2.55490600 1.92096200 -2.11428400 Si -1.88353000 1.78160600 0.04888700 C -1.82931000 3.43379200 0.95248300 H -1.53891500 3.30382900 2.00588600 H -2.82083000 3.91163300 0.92904300 H -1.10615500 4.11373300 0.47744200 C -2.42290900 2.09512200 -1.72434500 H -3.46585400 2.44777700 -1.70993200 H -2.37721500 1.19354900 -2.35038000 H -1.80903800 2.88029400 -2.19021100 C -3.12034800 0.67672000 0.92478900 H -2.87559100 0.54906800 1.98816700 H -3.20693500 -0.31628900 0.46422400 H -4.09710600 1.18238800 0.85556700 B 0.00782100 -1.01329900 -0.01705900 Br -0.71412500 -1.56843500 1.72506800 Br 1.87685600 -1.52822000 -0.28507700 Br -1.16989200 -1.38553900 -1.54951200 C 4.23480900 2.06629600 0.02848900 H 4.56517100 2.56794800 0.94691700 H 4.75778100 1.09805600 -0.02886400 H 4.54069500 2.66048900 -0.84197200 E(RM062X): -8426.234724 Hartree Dipole Moment: 6.176169 Debye Imaginary Frequency: 242.43i cm^{-1}
[TS-2]$_{tolyl}$	**[TS-2]$_{tolyl}$**

Coordinates (x,y,z): C -0.50302600 -0.44058700 0.08277400 C -2.31001000 -1.74823300 1.08158900 C -2.60406600 -0.89332700 -1.14126300 C -3.10379200 -1.63714100 -0.08692500 C -1.32924800 -0.28362000 -1.05670000 C -1.06509500 -1.16251500 1.17485500 H -2.69427800 -2.32935000 1.92396200 H -3.19022800 -0.77675200 -2.05553900 H -0.89133200 0.17383900 -1.94808200 H -0.45594300 -1.29371700 2.07151600 B 1.10985700 -0.21697300 -0.01177700 Br 1.57826400 1.30697900 -1.28931200 Br 1.94523600 0.10700100 1.79850200 Br 1.76860300 -1.97014300 -0.78477200 Si -1.71118600 1.66602200 0.15279700 C -1.87203900 2.66382400 -1.41782900 H -2.18397400 3.68123700 -1.13092000 H -2.63272600 2.24330400 -2.08981900 H -0.91000400 2.73112100 -1.94195100 C -3.38618600 1.38259700 0.93384500 H -4.14971400 1.05881000 0.21570700 H -3.68160900 2.36936300 1.32855900 H -3.36019700 0.68357500 1.77943700 C -0.56683000 2.44269100 1.39327700 H -1.02650100 3.41662200 1.63483300 H 0.44109100 2.60985000 0.99521400 H -0.48680000 1.84604300 2.31087600 C -4.45478500 -2.29101900 -0.14403400 H -4.38874500 -3.34745700 0.15179200 H -5.14979600 -1.79845900 0.55366800 H -4.88506100 -2.23782000 -1.15170400 E(RM062X): -8426.232165 Hartree Dipole Moment: 11.312745 Debye Imaginary Frequency: 52.97i cm^{-1}	Coordinates (x,y,z): C -0.51584300 -0.43158600 0.08119000 C -2.31608000 -1.74431300 1.08743400 C -2.59406700 -0.93586600 -1.15661400 C -3.09813600 -1.66416600 -0.08883900 C -1.32829000 -0.31693000 -1.07437100 C -1.07696100 -1.14143600 1.17869900 H -2.70321400 -2.30663700 1.94038200 H -3.17443600 -0.83840400 -2.07622400 H -0.90293400 0.14134300 -1.97064300 H -0.48637800 -1.24688000 2.09057000 B 1.08952600 -0.20094200 -0.00772600 Br 1.59332000 1.30076800 -1.29617400 Br 1.94550400 0.13764000 1.79999800 Br 1.81407300 -1.96351100 -0.75772000 Si -1.76905100 1.67103600 0.14814900 C -1.90629700 2.62696300 -1.44538100 H -2.23648300 3.64286000 -1.17380500 H -2.65237900 2.18431200 -2.11881600 H -0.93910600 2.70178400 -1.95820100 C -3.43101700 1.34689300 0.92033500 H -4.17590700 0.98070900 0.20362300 H -3.75531400 2.33903500 1.27819500 H -3.38885200 0.67763300 1.78864600 C -0.61871400 2.45764700 1.37697800 H -1.08140700 3.43273000 1.60632800 H 0.38717900 2.62819600 0.97629100 H -0.54701400 1.87104800 2.30168100 C -4.44550200 -2.32226500 -0.14525600 H -4.38859300 -3.35663000 0.22041900 H -5.15486700 -1.78489800 0.50299200 H -4.84716400 -2.32705100 -1.16557900 E(RM062X): -8426.249933 Hartree Dipole Moment: 14.944349 Debye Imaginary Frequency: 43.19i cm^{-1}
$[TS\text{-}3]_{tolyl}$ Coordinates (x,y,z): C -1.39687800 -0.54271100 -1.09072700	**$[TS\text{-}3]_{tolyl}$** Coordinates (x,y,z): C -1.36359400 -0.64068100 -1.13231900

C -3.26962600 -1.64580100 -0.00694700	C -3.17035000 -1.87878300 -0.07325700
C -1.16620600 -1.31815300 1.17563200	C -1.04979000 -1.52840200 1.07224300
C -2.46317800 -1.79331100 1.14197300	C -2.33212100 -2.05542700 1.04385300
C -0.58338700 -0.67348700 0.05463400	C -0.52226600 -0.80108200 -0.01738100
C -2.71846700 -1.00975400 -1.11442600	C -2.66352200 -1.16336300 -1.15675100
H -0.55875300 -1.45599800 2.07218000	H -0.42776100 -1.68593200 1.95586400
H -0.96684400 -0.12526600 -2.00372100	H -0.98735800 -0.12872600 -2.02086100
H -2.87696700 -2.29826600 2.01845500	H -2.70396300 -2.61707100 1.90446100
B 1.00922100 -0.42385500 -0.00274600	B 1.02283000 -0.36633700 -0.03341200
Br 1.26799900 1.24117600 -1.26226400	Br 1.30513900 1.21962000 -1.33315300
Br 1.93603300 -1.99757000 -0.80974300	Br 2.17505100 -1.92077500 -0.65822900
Br 1.77608000 0.03928100 1.80892600	Br 1.65403400 0.22955100 1.82152300
Si -1.22233800 1.96685500 0.08977200	Si -1.55830800 2.13524200 0.14574200
C -2.55725100 1.53798400 1.31856600	C -2.62400100 1.36688000 1.43012500
H -3.27337900 0.78706100 0.96676100	H -3.20531400 0.51936700 1.04703200
H -2.12940900 1.22080400 2.27870400	H -2.03191800 1.06187800 2.30271200
H -3.09738200 2.48834600 1.47688700	H -3.32134100 2.16548800 1.74073400
C -1.95280500 2.56370800 -1.51976500	C -2.24964800 2.45932500 -1.53057900
H -1.19847600 2.66428900 -2.30887600	H -1.45295600 2.48241700 -2.28543800
H -2.76477600 1.90958500 -1.86208400	H -3.02264000 1.73382400 -1.80927900
H -2.37608800 3.56088200 -1.30931200	H -2.69941900 3.46612200 -1.47655900
C -0.05159300 3.14166200 0.93719800	C -0.28014000 3.28894800 0.79479600
H 0.50453900 3.73698700 0.20275500	H 0.23284800 3.82372800 -0.01255200
H -0.65894200 3.79627300 1.58402600	H -0.82367100 4.00153200 1.43945800
H 0.66884800 2.59756100 1.56337700	H 0.45397500 2.75379300 1.41277100
H -3.31282300 -0.89756900 -2.02425400	H -3.28365800 -1.02043800 -2.04503800
C -4.68151100 -2.16162300 -0.01038700	C -4.56619100 -2.43957600 -0.07672000
H -4.70823600 -3.22196200 0.27903600	H -4.55942400 -3.50669200 0.18700100
H -5.29866700 -1.61108800 0.71614400	H -5.19344500 -1.92541300 0.66728300
H -5.14454500 -2.06044800 -0.99983900	H -5.03985800 -2.32645600 -1.05991500
E(RM062X): -8426.218846 Hartree	E(RM062X): -8426.234153 Hartree
Dipole Moment: 9.368729 Debye	Dipole Moment: 15.627926 Debye
Imaginary Frequency: 134.56i cm^{-1}	Imaginary Frequency: 90.92i cm^{-1}

1.4 Stationary points for the exchange reaction of TMSAr (Ar = 1-anthryl) andBBr_3

Gas Phase	In Solvent (DCM)
1-Anthryl-BBr_2	**1-Anthryl-BBr_2**
Coordinates (x,y,z):	Coordinates (x,y,z):

C 0.46096700 3.35263800 0.52371600 C -0.89179900 3.17904300 0.54236400 C -1.47225200 1.89577100 0.28630800 C -0.61141500 0.76735300 0.03538100 C 0.82803900 0.96588400 0.06702500 C 1.31495400 2.24205500 0.27225400 H -3.49802500 2.60457400 0.44868000 H 0.89838000 4.33472300 0.70583300 H -1.56019500 4.01994000 0.73942500 C -2.86113600 1.73794000 0.25516900 C -1.21049500 -0.45693000 -0.27787200 C -2.60203000 -0.61660900 -0.31478800 C -3.45216300 0.50424200 -0.03267900 H -0.59270400 -1.32344400 -0.51182300 H 2.39337000 2.40991600 0.27065600 B 1.89097000 -0.16471900 0.01890400 Br 3.57163900 0.11067400 -0.86911100 Br 1.68028500 -1.83559800 0.94008200 C -4.56638400 -2.01018100 -0.65648800 H -5.01606500 -2.97491300 -0.89537900 C -5.41175000 -0.89399200 -0.37232900 H -6.49476400 -1.02211800 -0.39893400 C -4.87227000 0.32390400 -0.07112200 H -5.51328600 1.18098700 0.14466900 C -3.20739100 -1.87561900 -0.62981300 H -2.55814900 -2.72674500 -0.84438200 E(RM062X): -5710.991612 Hartree Dipole Moment: 2.445344 Debye	C 0.46104300 3.35451900 0.52115600 C -0.89215200 3.17936100 0.54400600 C -1.47185300 1.89498000 0.28655600 C -0.61089500 0.76781300 0.02838700 C 0.82875500 0.96810300 0.05865700 C 1.31572400 2.24473000 0.26590200 H -3.49867100 2.60098300 0.45982400 H 0.89848900 4.33623200 0.70434200 H -1.56054100 4.01905700 0.74536900 C -2.86131500 1.73620300 0.26047500 C -1.20823300 -0.45633200 -0.29046000 C -2.60062000 -0.61745400 -0.32261700 C -3.45097100 0.50150700 -0.03038700 H -0.59060600 -1.32027800 -0.53558500 H 2.39381300 2.41516200 0.26719000 B 1.88933600 -0.16182600 0.01653300 Br 3.57196800 0.10163000 -0.87542800 Br 1.67836300 -1.82595500 0.95496100 C -4.56564600 -2.01102900 -0.66407300 H -5.01607700 -2.97444700 -0.90702800 C -5.41132400 -0.89702900 -0.36880200 H -6.49424400 -1.02682500 -0.39100100 C -4.87192300 0.32058600 -0.06279400 H -5.51242800 1.17595100 0.16099700 C -3.20573400 -1.87597400 -0.64322800 H -2.55711400 -2.72522400 -0.86709200 E(RM062X): -5710.996608 Hartree Dipole Moment: 3.041633 Debye
1-TMS-anthracene Coordinates (x,y,z): C 1.48748400 3.05972700 0.00015400 C 0.12496000 3.04129900 0.00002300 C -0.58600100 1.79784300 0.00001600 C 0.15968000 0.56405200 0.00014300 C 1.60882900 0.60449600 0.00021800 C 2.22276500 1.83460700 0.00025100 C -1.98409500 1.76821200 -0.00009200 C -0.56119400 -0.63699700 0.00019100 C -1.96113400 -0.67062100 0.00010300	**1-TMS-anthracene** Coordinates (x,y,z): C -1.48649400 3.06082000 -0.00025300 C -0.12324600 3.04304900 -0.00032000 C 0.58702300 1.79818400 -0.00020100 C -0.15935900 0.56375700 -0.00002000 C -1.60928600 0.60372600 0.00000900 C -2.22235800 1.83500800 -0.00008900 C 1.98592200 1.76934800 -0.00024400 C 0.56127100 -0.63833200 0.00014700 C 1.96197500 -0.67136800 0.00011600

C -2.69408400 0.56347600 -0.00005300	C 2.69532600 0.56335700 -0.00009500
C -4.12564300 0.51653900 -0.00015400	C 4.12779400 0.51718100 -0.00013400
H -4.67781500 1.45854800 -0.00028700	H 4.67999600 1.45917600 -0.00029600
C -4.78567500 -0.67909000 -0.00009600	C 4.78743400 -0.67951200 0.00003100
C -4.05682700 -1.90813200 0.00007600	C 4.05804700 -1.90928500 0.00024700
C -2.69101400 -1.90321700 0.00017200	C 2.69146800 -1.90521800 0.00028800
H -2.53493300 2.71223600 -0.00019100	H 2.53683200 2.71325800 -0.00038800
H 2.02700700 4.00805800 0.00018800	H -2.02658100 4.00885900 -0.00033300
H -0.44977400 3.96984900 -0.00006500	H 0.45163900 3.97150000 -0.00045600
H 3.31316000 1.89852400 0.00034800	H -3.31263500 1.90056700 -0.00006100
H -0.02979800 -1.59009800 0.00032200	H 0.03093600 -1.59202100 0.00032000
H -5.87635300 -0.70308300 -0.00018300	H 5.87812900 -0.70423200 0.00000000
H -4.60097600 -2.85365800 0.00013300	H 4.60277600 -2.85451100 0.00037900
H -2.13089100 -2.84069300 0.00030100	H 2.13139900 -2.84271400 0.00045300
Si 2.69310300 -0.95260800 -0.00004600	Si -2.69788100 -0.95464700 0.00008400
C 4.50049900 -0.42221400 0.00006700	C -4.50169200 -0.41792400 0.00008500
H 5.14271200 -1.31605300 -0.00021600	H -5.14324200 -1.31226300 0.00010100
H 4.75173100 0.17080800 -0.89197800	H -4.74987000 0.17544100 0.89275700
H 4.75184800 0.17037400 0.89236200	H -4.74986000 0.17539900 -0.89261900
C 2.38699900 -1.98115600 1.55035100	C -2.38773500 -1.98062000 -1.55059900
H 2.59179000 -1.37921700 2.44839500	H -2.58375800 -1.37614100 -2.44903300
H 1.35509700 -2.35091600 1.62572900	H -1.35931300 -2.36196200 -1.61667300
H 3.06133000 -2.85129400 1.56368100	H -3.07160300 -2.84333600 -1.56532700
C 2.38689000 -1.98026600 -1.55101700	C -2.38772900 -1.98060200 1.55077200
H 1.35472900 -2.34919900 -1.62688000	H -1.35927700 -2.36185200 1.61692500
H 2.59247000 -1.37813000 -2.44874100	H -2.58387500 -1.37614800 2.44919700
H 3.06059700 -2.85089200 -1.56438700	H -3.07152500 -2.84337800 1.56544500
E(RM062X): -947.315866 Hartree	E(RM062X): -947.320849 Hartree
Dipole Moment: 0.137227 Debye	Dipole Moment: 0.267701 Debye
[IM-1]$_{1\text{-anthryl}}$	**[IM-1]$_{1\text{-anthryl}}$**
Coordinates (x,y,z):	Coordinates (x,y,z):
C 3.87368000 0.28453200 -0.47620100	C 3.87279300 0.25175800 -0.49349200
H 3.83950200 1.94926500 -1.84809000	H 3.83917500 1.89927100 -1.88780400
C 3.23913100 1.26818300 -1.24023300	C 3.23975100 1.22856300 -1.26823700
C 1.66252000 -0.48994400 0.27151900	C 1.66159000 -0.49455500 0.28227800
C 1.84522700 1.38799800 -1.25517300	C 1.84625600 1.35788300 -1.27487500
C 3.06027500 -0.62093700 0.28363200	C 3.05959000 -0.63485200 0.28870200
C 1.02583100 0.50841400 -0.46127200	C 1.02537700 0.49379700 -0.46393500
C 1.22324800 2.35962000 -2.09789500	C 1.23123100 2.32894200 -2.12212500
H 1.06912800 -1.19547400 0.85262500	H 1.07335600 -1.18253000 0.88827800

C -0.13632900 2.50752700 -2.13395300 H 1.86487700 2.98797500 -2.72080300 H -0.60559100 3.24933400 -2.77961600 C -0.94267300 1.67953000 -1.31931900 B -1.44973300 -0.64455700 -0.20547200 Br -1.41131300 -1.42622300 1.68739400 Br -3.39624200 -0.21010700 -0.60803000 Br -0.81029800 -2.04352300 -1.51784200 Si -0.67346100 2.05593400 1.21942700 H -2.02768600 1.79684000 -1.37775400 C -0.44347300 0.68061000 -0.45848000 C -0.10882800 3.78041800 0.73927200 H -0.05412700 4.35845500 1.67633500 H -0.80280700 4.29196000 0.05918800 H 0.89457400 3.78193700 0.29028900 C 0.51852900 1.44767500 2.52322100 H 0.29565500 2.02998400 3.43297300 H 1.55596700 1.65137900 2.22319100 H 0.40062700 0.38322800 2.75357600 C -2.45465000 2.09258700 1.75740000 H -2.49432400 2.78057400 2.61863000 H -2.81313600 1.10410900 2.06978300 H -3.11970700 2.47419100 0.97188100 C 5.87351800 -0.85220300 0.30065000 H 6.95873700 -0.96043500 0.32104900 C 5.06511100 -1.75732900 1.05352900 H 5.54568600 -2.54354300 1.63723900 C 5.29706400 0.13814600 -0.44277000 H 5.90906100 0.82974900 -1.02484000 C 3.70276100 -1.64751300 1.04468400 H 3.07988200 -2.33884300 1.61477100 E(RM062X): -8693.901218 Hartree Dipole Moment: 10.314946 Debye	C -0.12865600 2.49216900 -2.15048100 H 1.87524600 2.94702000 -2.75182700 H -0.59370900 3.23808100 -2.79362600 C -0.93654500 1.67848100 -1.32865700 B -1.44768900 -0.61866100 -0.19141000 Br -1.42763400 -1.41735600 1.69626600 Br -3.40607200 -0.20159000 -0.59926000 Br -0.84305400 -2.06162900 -1.50450500 Si -0.62792400 2.10313400 1.21800800 H -2.01832800 1.81774100 -1.38396300 C -0.44283600 0.68333000 -0.45516000 C -0.03468600 3.79905700 0.70148100 H 0.02444000 4.38822000 1.63130900 H -0.72136700 4.30624100 0.01141500 H 0.97053200 3.77509500 0.25780600 C 0.54265400 1.46469500 2.52378700 H 0.33376400 2.06450700 3.42526900 H 1.58452500 1.64013100 2.22194900 H 0.39995600 0.40616300 2.76661900 C -2.41372800 2.15689400 1.74034200 H -2.45033800 2.85531300 2.59274000 H -2.78626300 1.17819400 2.06580800 H -3.06448200 2.54337300 0.94498900 C 5.87325000 -0.87984600 0.29029700 H 6.95789300 -0.99353900 0.30616900 C 5.06496800 -1.76479600 1.06762200 H 5.54609200 -2.54003200 1.66548100 C 5.29620700 0.09930100 -0.46861400 H 5.90641300 0.77745600 -1.06785200 C 3.70219700 -1.64863000 1.06697800 H 3.08260800 -2.32426600 1.65918700 E(RM062X): -8693.918190 Hartree Dipole Moment: 13.827475 Debye
[IM-2]$_{1\text{-anthryl}}$ Coordinates (x,y,z): C -0.30389600 2.55801600 -1.74782400 C 1.04529700 2.58562200 -1.73878100 C 1.78712200 1.58530200 -1.01155300 C 1.09099400 0.48270200 -0.37968100 C -0.35511300 0.39947600 -0.46156500	**[IM-2]$_{1\text{-anthryl}}$** Coordinates (x,y,z): C -0.28375100 2.55718600 -1.77062500 C 1.06855100 2.56130800 -1.76630300 C 1.79421900 1.55404200 -1.03864400 C 1.08297600 0.47340100 -0.38588400 C -0.36440800 0.41673100 -0.46449100

C -1.02229700 1.52269000 -1.01443900 H 3.68474300 2.49592800 -1.42894400 H -0.88290800 3.31404500 -2.28114600 H 1.60007000 3.35685500 -2.27601500 C 3.17356600 1.65826500 -0.94918800 C 1.85954800 -0.51471100 0.23222000 H 1.36850500 -1.37625700 0.67984700 H -2.06816000 1.36097200 -1.29355300 Si -1.46290000 2.50061400 0.81499400 C -0.02599200 3.65128700 1.14980400 H -0.18425300 4.09114900 2.14725200 H 0.93017300 3.10718200 1.17406700 H 0.05055000 4.46230800 0.41471900 C -1.74623000 1.43562400 2.31139000 H -2.05027400 2.12895800 3.11377500 H -2.53589700 0.68811300 2.16721700 H -0.83102100 0.91682100 2.62601200 C -3.01713200 3.39206600 0.27965300 H -3.81149800 2.66170200 0.06774000 H -3.35606100 4.04359500 1.10006000 H -2.85340300 4.01582900 -0.61009000 B -1.22527700 -0.95800700 -0.15495300 Br -0.65056900 -2.15707900 -1.68214200 Br -0.90963500 -1.85314600 1.63876700 Br -3.24117100 -0.62432100 -0.28907300 C 3.25839100 -0.44078100 0.29469500 C 3.93541900 0.67353200 -0.29771600 C 5.35936800 0.73380800 -0.22063800 H 5.87546000 1.58254100 -0.67298700 C 6.06173900 -0.25877600 0.40804700 H 7.15016000 -0.20452400 0.46142500 C 5.38951700 -1.37062900 0.99553400 H 5.97136400 -2.15004500 1.48862700 C 4.02619800 -1.45998100 0.93974600 H 3.49855500 -2.30567900 1.38428400 E(RM062X): -8693.902948 Hartree Dipole Moment: 9.658985 Debye	C -1.01134300 1.53032900 -1.04414300 H 3.70497600 2.42782200 -1.48119500 H -0.85167900 3.32368100 -2.29942200 H 1.63262600 3.32449700 -2.30475000 C 3.18458100 1.60488600 -0.98678100 C 1.84038000 -0.52183700 0.24636900 H 1.34333000 -1.36514900 0.72019000 H -2.07041700 1.41436300 -1.28861800 Si -1.37842300 2.57570100 0.82236200 C 0.14238400 3.59445100 1.16849000 H -0.01154600 4.05090600 2.15940200 H 1.04982800 2.97577800 1.22416500 H 0.29358200 4.39150700 0.43034500 C -1.77672600 1.50710800 2.28815800 H -2.09077100 2.21145400 3.07681900 H -2.59225100 0.79806600 2.10145300 H -0.89596800 0.95594400 2.64181700 C -2.85502000 3.55887400 0.24568900 H -3.69720800 2.89037600 0.01677400 H -3.15737600 4.22510400 1.06899700 H -2.62890800 4.17562100 -0.63431000 B -1.24162300 -0.93167300 -0.15138600 Br -0.66709900 -2.21785000 -1.62745600 Br -0.97452800 -1.80801800 1.66780000 Br -3.25883300 -0.61360800 -0.33399200 C 3.23973000 -0.47018400 0.29937800 C 3.93212900 0.62058400 -0.32241100 C 5.35916600 0.66055400 -0.25632800 H 5.88407100 1.49164700 -0.73044800 C 6.04967200 -0.32863300 0.38967100 H 7.13900800 -0.29152800 0.43585200 C 5.36212300 -1.41699100 1.00729300 H 5.93561100 -2.19345100 1.51477500 C 3.99745200 -1.48707700 0.96343100 H 3.46252200 -2.31481400 1.43248600 E(RM062X): -8693.918425 Hartree Dipole Moment: 13.326419 Debye
[TS-1]$_{1\text{-anthryl}}$ Coordinates (x,y,z): C 0.48186500 -0.89544400 2.93984800	**[TS-1]$_{1\text{-anthryl}}$** Coordinates (x,y,z): C 0.51433500 -0.90422400 2.89235200

C -0.85130100 -1.17999900 2.78769100	C -0.81111400 -1.21600500 2.74828400
C -1.62847600 -0.60344400 1.73837800	C -1.61187100 -0.62010100 1.72278700
C -0.98854200 0.26773200 0.78676400	C -1.00587200 0.31188000 0.80637000
C 0.45075100 0.55443300 0.91797800	C 0.41477100 0.64899100 0.95512500
C 1.09532000 -0.00823400 2.03454100	C 1.09498600 0.04527600 2.02028900
H -3.44582600 -1.57943400 2.35519600	H -3.39624800 -1.67673600 2.29990700
H 1.06261500 -1.34040600 3.74708200	H 1.11713000 -1.36302300 3.67540800
H -1.35032000 -1.86142800 3.48138100	H -1.28630400 -1.93320300 3.42158100
C -2.98579500 -0.91060800 1.62377400	C -2.95867600 -0.96490800 1.59610600
C -1.76120000 0.76314100 -0.25810700	C -1.79694900 0.82912000 -0.21610200
C -3.12802700 0.45670900 -0.38482700	C -3.15307800 0.48256300 -0.35617700
C -3.76157100 -0.39227400 0.58085300	C -3.75312800 -0.42875100 0.57417900
H -1.29935200 1.37930700 -1.02638600	H -1.36049500 1.50218100 -0.95155000
H 2.14758800 0.23625300 2.20119500	H 2.13666300 0.32329700 2.20163600
Si 1.03869200 2.39986600 0.66352300	Si 1.02905300 2.46573300 0.64492600
C 0.64771600 3.17841000 2.33712200	C 0.66008400 3.30174900 2.29267400
H 0.85067100 4.26022600 2.31732700	H 0.90867500 4.37297300 2.24216100
H -0.41407700 3.03687500 2.59185100	H -0.40831000 3.20938200 2.54158700
H 1.25314900 2.73344700 3.14112200	H 1.24335000 2.85016600 3.10907600
C 0.09947600 3.39724900 -0.62431200	C 0.12909600 3.44842300 -0.68241600
H -0.96070200 3.51456300 -0.36034300	H -0.92411200 3.61963500 -0.41938700
H 0.55608800 4.40024500 -0.62359900	H 0.62609100 4.43105600 -0.72226400
H 0.18294200 2.98900500 -1.63963700	H 0.18593200 3.00046200 -1.68299000
C 2.87728100 2.53415900 0.33086800	C 2.87456200 2.53623600 0.31373900
H 3.14393500 2.12905300 -0.65496200	H 3.13291000 2.11413200 -0.66741000
H 3.13197800 3.60600700 0.35257700	H 3.16170200 3.59978900 0.32248700
H 3.49180500 2.02322400 1.08490100	H 3.46925900 2.01888600 1.07979600
B 1.38361600 -0.66747000 -0.44927300	B 1.41487100 -0.71916100 -0.47294500
Br 3.32344400 -0.83949000 -0.04359000	Br 3.33909800 -0.87492800 -0.05486000
Br 0.44099900 -2.39824400 -0.33245500	Br 0.43941800 -2.41246300 -0.30844500
Br 1.08575800 0.26001200 -2.18178400	Br 1.06897700 0.23878400 -2.16257300
C -3.91121700 0.96923500 -1.46477400	C -3.95763900 1.01650900 -1.41096700
H -3.42530900 1.60928800 -2.20347800	H -3.49841800 1.70761200 -2.12039200
C -5.23948300 0.66122600 -1.57059000	C -5.27561800 0.66769300 -1.52687300
H -5.82718100 1.05718800 -2.39995500	H -5.88084300 1.08063200 -2.33511300
C -5.87010800 -0.17978600 -0.60559400	C -5.87293500 -0.23676600 -0.59782600
H -6.93048400 -0.41328300 -0.70953400	H -6.92540100 -0.50090200 -0.70895300
C -5.15287500 -0.69257400 0.43840300	C -5.13447700 -0.77021600 0.42198200
H -5.62722200 -1.34020200 1.17823000	H -5.58377900 -1.46434500 1.13474700
E(RM062X): -8693.894724 Hartree	E(RM062X): -8693.903972 Hartree
Dipole Moment: 6.327252 Debye	Dipole Moment: 6.628809 Debye
Imaginary Frequency: 184.22i cm^{-1}	Imaginary Frequency: 228.96i cm^{-1}

[TS-2]$_{1\text{-anthryl}}$	**[TS-2]$_{1\text{-anthryl}}$**
Coordinates (x,y,z):	Coordinates (x,y,z):
C -0.39150600 0.54257600 0.42474800	C -0.39160000 0.54343600 0.42439000
C 1.86449000 1.32062200 1.24019300	C 1.86460500 1.31927600 1.24138100
C -0.13357200 2.52002400 1.93769700	C -0.13300700 2.51967800 1.93876300
C 1.21127500 2.33674200 2.01756600	C 1.21179400 2.33548100 2.01881700
C -0.92097600 1.62934600 1.13724800	C -0.92056200 1.62969100 1.13810200
C 1.07567300 0.42888600 0.42130400	C 1.07561700 0.42840600 0.42175300
H -0.63596900 3.30630100 2.50442100	H -0.63499400 3.30605600 2.50570200
H -2.00954100 1.69872100 1.21939300	H -2.00913000 1.70010600 1.21935200
B -1.43821900 -0.72719100 0.18330100	B -1.43910000 -0.72599800 0.18341400
Br -3.33800100 -0.03771700 -0.16289200	Br -3.33841900 -0.03537300 -0.16325900
Br -1.06978400 -2.06538000 -1.29697500	Br -1.07115800 -2.06483100 -1.29637700
Br -1.34770500 -1.66988700 1.97400900	Br -1.34964200 -1.66845400 1.97429000
Si -0.68832900 2.22041500 -1.13449000	Si -0.68548100 2.21784400 -1.13626400
C -2.17287200 3.35266500 -0.99719900	C -2.16833900 3.35239100 -0.99923400
H -2.24486700 3.91867000 -1.94411800	H -2.23903500 3.91852400 -1.94618500
H -2.06456800 4.07418900 -0.17112800	H -2.05918700 4.07379400 -0.17316500
H -3.10237400 2.77794400 -0.86449100	H -3.09886000 2.77924300 -0.86690800
C 0.89962200 3.21353200 -1.17529600	C 0.90363200 3.20913700 -1.17680200
H 1.06895800 3.82333400 -0.27493300	H 1.07372800 3.81837400 -0.27618600
H 0.79150300 3.90439000 -2.03273200	H 0.79629500 3.90057500 -2.03387000
H 1.78367600 2.58180200 -1.35684500	H 1.78693800 2.57644700 -1.35866300
C -0.76876500 1.11633100 -2.63451600	C -0.76765100 1.11415300 -2.63646700
H -0.77159700 1.80032900 -3.50482300	H -0.76975400 1.79831800 -3.50664000
H -1.67597000 0.49440600 -2.65971000	H -1.67573100 0.49349400 -2.66150400
H 0.11251700 0.45933400 -2.70634600	H 0.11267600 0.45593600 -2.70857700
H 1.82689000 2.97723200 2.65582100	H 1.82766700 2.97540400 2.65740000
C 1.74901000 -0.51008600 -0.35402200	C 1.74884800 -0.51039400 -0.35388500
H 1.18348600 -1.19074800 -0.98763100	H 1.18329700 -1.19065100 -0.98793300
C 3.14979000 -0.61810600 -0.34329500	C 3.14963700 -0.61871800 -0.34301900
C 3.92744800 0.26304500 0.47437000	C 3.92739500 0.26153100 0.47554500
C 3.25465100 1.21870700 1.25192200	C 3.25473500 1.21676100 1.25363000
H 3.83432300 1.90682700 1.87443200	H 3.83443000 1.90422300 1.87683900
C 3.81640600 -1.60511700 -1.13251500	C 3.81632800 -1.60498300 -1.13314400
H 3.20878200 -2.28063700 -1.74012700	H 3.20881300 -2.27978100 -1.74165900
C 5.18000200 -1.70514700 -1.11151600	C 5.17992000 -1.70511900 -1.11209300
H 5.68346300 -2.46709200 -1.71067700	H 5.68340000 -2.46641200 -1.71207300
C 5.95634100 -0.81977800 -0.30571000	C 5.95630000 -0.82078100 -0.30517100
H 7.04473000 -0.91391500 -0.30675000	H 7.04467300 -0.91510700 -0.30608000
C 5.35140700 0.13602400 0.46446600	C 5.35134700 0.13426600 0.46588200
H 5.94584400 0.81189400 1.08492300	H 5.94570300 0.80940800 1.08720600

E(RM062X): -8693.899753 Hartree Dipole Moment: 10.429629 Debye Imaginary Frequency: 12.09i cm^{-1}	E(RM062X): -8693.916006 Hartree Dipole Moment: 13.372505 Debye Imaginary Frequency: No imaginary freq
[TS-3]$_{1\text{-anthryl}}$ Coordinates (x,y,z): C -0.22417700 2.54963800 -1.95719500 C 1.10079200 2.72330300 -1.72279100 C 1.85288300 1.71926300 -1.02046200 C 1.18749300 0.52374800 -0.55976800 C -0.25157900 0.37657000 -0.75298900 C -0.90150800 1.38583500 -1.45673400 H 3.70413800 2.79990600 -1.17288200 H -0.78775900 3.28272500 -2.53643600 H 1.62804800 3.60634000 -2.08991700 C 3.22189400 1.88392700 -0.82304300 C 1.97468900 -0.47679500 0.01674300 C 3.35836700 -0.32231000 0.20086400 C 3.99905800 0.89068500 -0.20954400 H 1.52380100 -1.41718200 0.32613600 H -1.93273700 1.23385600 -1.77244400 Si -1.99517100 2.00944300 0.85620700 C -0.35640500 2.52006800 1.56912300 H -0.57451300 3.24650400 2.37019400 H 0.13893000 1.64674500 2.01827900 H 0.31265500 2.98672000 0.83612400 C -3.09422900 1.33892700 2.20343500 H -2.73802700 0.38030600 2.59803100 H -3.06490500 2.09120800 3.01183400 H -4.12478500 1.22368500 1.84538200 C -2.92468400 3.28126000 -0.14275100 H -3.69970900 2.79996800 -0.75550000 H -3.43065900 3.93920300 0.58333600 H -2.27257800 3.88982200 -0.77956700 B -1.05171500 -0.94743400 -0.27160700 Br -0.59401900 -2.51555800 -1.41829900 Br -0.73799700 -1.35123800 1.71194200 Br -3.09745600 -0.54735700 -0.41606700 C 5.40550800 1.03493500 -0.00156400 H 5.89029100 1.96118000 -0.31612200 C 6.12846800 0.02863200 0.57771900	**[TS-3]$_{1\text{-anthryl}}$** Coordinates (x,y,z): C -0.20145500 2.46060300 -2.10156400 C 1.12236600 2.65074300 -1.85613000 C 1.86595900 1.67455300 -1.11121800 C 1.19749700 0.49553100 -0.61264000 C -0.23986100 0.34195400 -0.81849400 C -0.87569800 1.31383400 -1.57077400 H 3.71707500 2.75675800 -1.28174900 H -0.76311500 3.17621900 -2.70418800 H 1.64889400 3.52657700 -2.24049100 C 3.23503600 1.85313700 -0.90101400 C 1.98301000 -0.47111400 0.02652500 C 3.36180400 -0.30238600 0.22616400 C 4.00561200 0.89313100 -0.23350100 H 1.53247100 -1.39682600 0.37790700 H -1.92635800 1.18666200 -1.83148600 Si -2.08873700 2.23329600 0.96605200 C -0.37447700 2.58872200 1.53103200 H -0.46654000 3.34380400 2.33103200 H 0.08583500 1.68469300 1.95372800 H 0.24851500 2.99400900 0.72331900 C -3.21558600 1.43928000 2.18810300 H -2.80515200 0.50293700 2.58395100 H -3.29408600 2.16897300 3.01435800 H -4.21010100 1.26685500 1.75980400 C -2.92944200 3.34606900 -0.24033200 H -3.66610300 2.78945300 -0.83620800 H -3.48114300 4.08196400 0.36981000 H -2.22768800 3.87451300 -0.89468800 B -1.05232600 -0.94390600 -0.27685500 Br -0.52563900 -2.61468800 -1.29809400 Br -0.76458100 -1.24938600 1.74503900 Br -3.09302600 -0.66816900 -0.48530900 C 5.41078100 1.05377400 -0.01237400 H 5.89526500 1.96633900 -0.36522100 C 6.12937100 0.08084800 0.62551200

H 7.20205900 0.14674700 0.73201500 C 5.49274600 -1.18236200 0.98253900 H 6.08801500 -1.97303700 1.44094800 C 4.14858900 -1.35340700 0.79818800 H 3.65280600 -2.27586700 1.10593100 E(RM062X): -8693.887967 Hartree Dipole Moment: 8.111416 Debye Imaginary Frequency: 126.57i cm^{-1}	H 7.20012300 0.21033900 0.78987200 C 5.49046200 -1.11313000 1.08053800 H 6.08224000 -1.87754500 1.58596900 C 4.14989000 -1.29960200 0.88587600 H 3.65581000 -2.20948900 1.23230200 E(RM062X): -8693.903099 Hartree Dipole Moment: 14.063299 Debye Imaginary Frequency: -100.94i cm^{-1}

1.5 Stationary points for the exchange reaction of TMSAr (Ar = 2-anthryl) andBBr_3

Gas Phase	In Solvent (DCM)
2-Anthryl-BBr_2 Coordinates (x,y,z): C -6.42331100 -0.13008300 -0.00009900 C -5.43710200 -1.07512800 -0.00007400 C -4.05665600 -0.69449200 -0.00001700 C -3.72906200 0.70626200 0.00000900 C -4.79348900 1.66511200 -0.00001500 C -6.09764000 1.26113100 -0.00006700 C -3.02532500 -1.64261000 0.00001400 C -2.38457200 1.09096200 0.00005100 C -1.35579100 0.14171900 0.00007400 C -1.68298300 -1.25787700 0.00006200 C -0.60815400 -2.20727600 0.00010600 H -0.85381400 -3.27103400 0.00011800 C 0.69117200 -1.79878400 0.00012400 C 1.04091700 -0.39896700 0.00011500 C 0.01844500 0.52797700 0.00010800 H -3.27768300 -2.70564600 -0.00000100 H -7.47106800 -0.43394700 -0.00014400 H -5.68428700 -2.13848100 -0.00009900 H -4.53792700 2.72654200 0.00000800 H -6.90064700 1.99931700 -0.00008600 H -2.13058500 2.15381000 0.00006600 H 1.49114100 -2.54020800 0.00015300 H 0.24817900 1.59595400 0.00010100 B 2.51808200 0.06381700 0.00007900	**2-Anthryl-BBr_2** Coordinates (x,y,z): C -6.42411300 -0.12983000 -0.00020200 C -5.43804700 -1.07627700 -0.00019400 C -4.05726100 -0.69446800 -0.00023500 C -3.72947100 0.70692100 -0.00028500 C -4.79364100 1.66720700 -0.00029400 C -6.09825800 1.26207700 -0.00025300 C -3.02630500 -1.64448700 -0.00022800 C -2.38469200 1.09333500 -0.00032500 C -1.35676600 0.14212900 -0.00031500 C -1.68404300 -1.25810500 -0.00026700 C -0.60924600 -2.20893700 -0.00026100 H -0.85498500 -3.27256200 -0.00022900 C 0.69039700 -1.79995300 -0.00030200 C 1.04005100 -0.39921400 -0.00034900 C 0.01748800 0.52918100 -0.00034600 H -3.27885700 -2.70733400 -0.00019000 H -7.47211500 -0.43290000 -0.00017000 H -5.68528800 -2.13958800 -0.00015600 H -4.53787900 2.72849800 -0.00033300 H -6.90184400 1.99967100 -0.00025900 H -2.13085100 2.15604500 -0.00036200 H 1.48834200 -2.54365000 -0.00030300 H 0.24372600 1.59788500 -0.00037800 B 2.51461400 0.06302200 -0.00040100

Br 3.95847600 -1.20336200 -0.00007900 Br 3.00117000 1.92241700 -0.00000200 E(RM062X): -5710.998906 Hartree Dipole Moment: 3.338921 Debye	Br 3.95930800 -1.20354200 0.00040000 Br 3.00298100 1.92243700 0.00038600 E(RM062X): -5711.003552 Hartree Dipole Moment: 4.113243 Debye
2-TMS-anthracene Coordinates (x,y,z): C 5.22113300 -1.26240700 0.00001900 C 3.92604500 -1.69539300 0.00002100 C 2.83896100 -0.76232600 0.00000800 C 3.13651600 0.64455500 -0.00001000 C 4.50852600 1.05662400 -0.00001100 C 5.51684300 0.13555300 0.00000300 C 1.50252900 -1.17761200 0.00001300 C 2.08281700 1.56616600 -0.00002400 C 0.74858300 1.14927400 -0.00002200 C 0.45059300 -0.25635500 0.00000100 C -0.92283300 -0.66966200 0.00001600 H -1.12121500 -1.74564300 0.00003000 C -1.95771000 0.23136400 0.00000200 C -1.63561700 1.63508300 -0.00003300 C -0.34468000 2.07624700 -0.00004600 H 1.27572400 -2.24683100 0.00003000 H 6.04004400 -1.98317800 0.00003000 H 3.69528200 -2.76266100 0.00003400 H 4.73059400 2.12572900 -0.00002400 H 6.55752200 0.46290600 0.00000200 H 2.30887100 2.63542500 -0.00003700 H -2.44667500 2.36920000 -0.00006200 H -0.12050300 3.14520500 -0.00007800 Si -3.76316200 -0.32018200 0.00003600 C -3.84252900 -2.19980500 0.00019100 H -3.35447900 -2.62113900 0.89190000 H -4.89028000 -2.53592400 0.00014800 H -3.35441500 -2.62113500 -0.89149100 C -4.60858100 0.36536000 1.53717000 H -4.54866100 1.46371300 1.56585300 H -5.67272900 0.08514100 1.55767300 H -4.13300200 -0.02224600 2.45014400 C -4.60852700 0.36487500 -1.53734700 H -5.67273000 0.08483800 -1.55762800	**2-TMS-anthracene** Coordinates (x,y,z): C 5.22279900 1.26250300 -0.00006100 C 3.92727900 1.69681600 -0.00007900 C 2.83980400 0.76282100 -0.00003700 C 3.13733700 -0.64493000 0.00002400 C 4.50988100 -1.05840200 0.00004100 C 5.51846100 -0.13640900 0.00000000 C 1.50299600 1.17980400 -0.00005500 C 2.08356100 -1.56765800 0.00006500 C 0.74896700 -1.14904700 0.00004700 C 0.45089400 0.25740300 -0.00001400 C -0.92322500 0.67180300 -0.00003300 H -1.12085900 1.74791900 -0.00008200 C -1.95836400 -0.23004400 0.00000600 C -1.63607700 -1.63471400 0.00006700 C -0.34455500 -2.07694600 0.00008700 H 1.27664200 2.24907600 -0.00010100 H 6.04227100 1.98269500 -0.00009300 H 3.69681600 2.76413700 -0.00012600 H 4.73170300 -2.12760200 0.00008800 H 6.55928700 -0.46339900 0.00001300 H 2.30933800 -2.63693700 0.00011200 H -2.44686300 -2.36909800 0.00009900 H -0.12054700 -3.14592800 0.00013400 Si -3.76751200 0.32164800 -0.00001800 C -3.84473700 2.19984500 -0.00016300 H -3.35649000 2.62026000 -0.89228500 H -4.89383100 2.53198200 -0.00015400 H -3.35646100 2.62033600 0.89190800 C -4.60726100 -0.36786700 -1.53765900 H -4.54529100 -1.46631800 -1.56380300 H -5.67150000 -0.08765300 -1.55518200 H -4.13280000 0.02269900 -2.45024000 C -4.60722500 -0.36752200 1.53779900 H -5.67151200 -0.08747900 1.55516500

H -4.54839900 1.46320000 -1.56657500 H -4.13309600 -0.02328900 -2.45016300 E(RM062X): -947.317161 Hartree Dipole Moment: 0.266550 Debye	H -4.54506800 -1.46595300 1.56432900 H -4.13288100 0.02344600 2.45026900 E(RM062X): -947.322302 Hartree Dipole Moment: 0.417935 Debye
[IM-1]$_{2\text{-anthryl}}$ Coordinates (x,y,z): C -0.51650900 -0.03599700 0.57454200 C -2.19214700 -0.03281300 -1.23354900 C 0.18444800 0.17565900 -1.74543400 C -1.10436300 0.11980100 -2.16698100 C 0.54181100 0.10360400 -0.32836800 C -1.88338300 -0.11005000 0.16795500 H 1.00561200 0.26334900 -2.46032900 H -0.28065000 -0.15087600 1.63818800 H -1.33957800 0.16442100 -3.23221400 C -2.90794300 -0.26210600 1.10346400 C -4.24798800 -0.34035600 0.70080100 C -4.56055400 -0.25642700 -0.69936700 C -3.52211200 -0.10380000 -1.63508800 H -3.76729000 -0.04523100 -2.69788700 H -2.65922500 -0.32454400 2.16580600 C -5.93018600 -0.33481800 -1.09968700 C -5.31257600 -0.50015600 1.64251100 H -5.06576100 -0.56601900 2.70374900 C -6.61028100 -0.57059300 1.22016300 H -7.41691200 -0.69333500 1.94375900 C -6.92132200 -0.48667000 -0.16957000 H -6.16855400 -0.27323700 -2.16299600 H -7.96285700 -0.54658100 -0.48838800 Si 0.48899100 2.26647500 0.14404800 C 1.11461700 3.06219300 -1.42673100 H 2.04922700 2.61838700 -1.78674300 H 0.34910200 3.01872100 -2.21301600 H 1.30159700 4.12048300 -1.17888500 C 1.56124700 2.58419800 1.62798300 H 1.17475400 2.11065200 2.53911300 H 2.59142400 2.24300700 1.46521700 H 1.55909000 3.67888900 1.76538400 C -1.25659300 2.89087900 0.42578700 H -1.93766000 2.61400100 -0.39178200	**[IM-1]$_{2\text{-anthryl}}$** Coordinates (x,y,z): C -0.52196400 -0.05747200 0.58010100 C -2.19401100 -0.01443700 -1.22998200 C 0.18037700 0.22885300 -1.73369100 C -1.10826000 0.17213300 -2.15827600 C 0.53717300 0.12109000 -0.31911500 C -1.88498300 -0.12505200 0.17044700 H 0.99421300 0.35507200 -2.45083500 H -0.29691600 -0.19376900 1.64277400 H -1.34336200 0.25271900 -3.22109900 C -2.90985000 -0.30071200 1.10422800 C -4.24796400 -0.37294900 0.69621300 C -4.55996500 -0.25892200 -0.70322500 C -3.52276000 -0.08107600 -1.63632800 H -3.76753000 0.00492900 -2.69704600 H -2.66316500 -0.38241800 2.16531900 C -5.92918800 -0.33072000 -1.10736700 C -5.31295600 -0.55402700 1.63500500 H -5.06603100 -0.64055800 2.69454900 C -6.61020800 -0.61677100 1.20884700 H -7.41813300 -0.75470400 1.92822900 C -6.92033900 -0.50377600 -0.18002800 H -6.16628300 -0.24565300 -2.16920500 H -7.96186100 -0.55742500 -0.49995000 Si 0.45269400 2.30232100 0.17650700 C 1.11461400 3.11535400 -1.36706200 H 2.06648500 2.69481100 -1.70842300 H 0.37188900 3.06822700 -2.17450300 H 1.27248300 4.17319800 -1.09805300 C 1.50701000 2.57230200 1.68260100 H 1.10234700 2.07527400 2.57330400 H 2.54234600 2.24523900 1.52608300 H 1.49722800 3.66236800 1.85002000 C -1.30282800 2.88211000 0.44035800 H -1.96385500 2.61043300 -0.39476200

H -1.69036600 2.55104600 1.37563800 H -1.18875800 3.99108600 0.44915600 B 2.02616600 -0.53019600 0.04407400 Br 1.96194300 -2.38148800 -0.78008700 Br 3.54923200 0.52352200 -0.78951700 Br 2.31319900 -0.69258200 2.04327800 E(RM062X): -8693.903794 Hartree Dipole Moment: 11.886533 Debye	H -1.74045600 2.51981400 1.37955400 H -1.24621800 3.98237800 0.48158000 B 2.01203900 -0.51022000 0.03427900 Br 1.98230400 -2.37590900 -0.81322900 Br 3.55370800 0.53529400 -0.78540100 Br 2.33557500 -0.72529600 2.02816200 E(RM062X): -8693.921610 Hartree Dipole Moment: 15.497538 Debye
[IM-2]$_{2\text{-anthryl}}$ Coordinates (x,y,z): C -0.36451900 0.24777100 -0.36580900 C -2.06463700 -0.89023000 1.04655600 C 0.33102900 -1.04386400 1.58611000 C -0.97464300 -1.29629000 1.89416200 C 0.68173000 -0.34796700 0.37992100 C -1.76054000 -0.13564700 -0.13246300 H 1.13773700 -1.41678000 2.21866400 H -0.10377400 0.57133400 -1.38017300 H -1.21753000 -1.85731000 2.80051900 B 2.20205000 -0.39555300 -0.16899700 Br 2.55650400 0.99522000 -1.60664500 Br 2.18993300 -2.25717600 -0.98624500 Br 3.56060800 -0.25667600 1.30944900 C -2.78406800 0.24106300 -0.98580600 C -4.12554100 -0.09362300 -0.70668100 C -4.43396500 -0.82857000 0.48532700 C -3.38523700 -1.21569000 1.33805000 H -3.61280100 -1.78645600 2.24155900 H -2.55320100 0.79699900 -1.89784600 Si -0.22430200 2.14330200 0.58150900 C -1.60352500 2.17206300 1.84779500 H -2.59596500 2.01576700 1.40356400 H -1.44547800 1.42571600 2.63968100 H -1.58174600 3.16670000 2.32187600 C -0.57512000 3.25009400 -0.88233600 H 0.22001200 3.14729300 -1.63417000 H -1.54708200 3.02205700 -1.34144900 H -0.59547800 4.29537500 -0.53665300 C 1.37855500 2.55216800 1.43540900	**[IM-2]$_{2\text{-anthryl}}$** Coordinates (x,y,z): C -0.38085800 0.21009200 -0.39405800 C -2.07769500 -0.87832100 1.05607200 C 0.31353400 -0.98761600 1.61105900 C -0.99355700 -1.25036300 1.91977600 C 0.66250900 -0.32744800 0.38942800 C -1.77351800 -0.15760400 -0.14543500 H 1.11270600 -1.32860500 2.26996700 H -0.12793000 0.53473800 -1.40899500 H -1.23486600 -1.78486000 2.84177200 B 2.18615800 -0.38936800 -0.15296800 Br 2.56202000 0.96811600 -1.62230500 Br 2.27905200 -2.27188300 -0.94509100 Br 3.55524900 -0.20284400 1.32652700 C -2.79724900 0.19662800 -1.01157600 C -4.13662000 -0.13021500 -0.72053900 C -4.44552200 -0.83270700 0.49296000 C -3.40024000 -1.19677500 1.35754100 H -3.62778900 -1.73820700 2.27848100 H -2.56846400 0.72686800 -1.93895600 Si -0.26659700 2.16092600 0.55557000 C -1.63976100 2.17217400 1.81842800 H -2.62797500 1.99285200 1.37444000 H -1.46534400 1.44664700 2.62550000 H -1.63029400 3.17871900 2.26747100 C -0.62333500 3.20630900 -0.94581900 H 0.17728300 3.10174200 -1.69096600 H -1.58830000 2.94773500 -1.40230600 H -0.66482100 4.25780200 -0.62111000 C 1.33954300 2.59328800 1.39032100

H 2.23940800 2.55713800 0.75557300 H 1.25012900 3.56314100 1.85692500 H 1.59454000 1.85781300 2.25902100 C -5.79613100 -1.15543600 0.76515500 H -6.02341100 -1.71588000 1.67398300 C -6.48688700 -0.05144000 -1.27774400 H -7.29413500 0.24023100 -1.95097400 C -6.79381000 -0.77707600 -0.09098900 H -7.83118000 -1.03171900 0.12934100 C -5.19271300 0.27915300 -1.57783300 H -4.95649600 0.83338600 -2.48808700 E(RM062X): -8693.912595 Hartree Dipole Moment: 11.353024 Debye	H 2.19887500 2.58805400 0.70937000 H 1.20181900 3.61586600 1.77915000 H 1.55008900 1.92608500 2.23710300 C -5.80936100 -1.15019900 0.78332600 H -6.03664700 -1.68331000 1.70826700 C -6.49804100 -0.10085400 -1.29163200 H -7.30614700 0.17349600 -1.97106900 C -6.80569400 -0.79406500 -0.08372800 H -7.84371800 -1.04005200 0.14322800 C -5.20423200 0.22070400 -1.60243300 H -4.96757700 0.75154500 -2.52620800 E(RM062X): -8693.929102 Hartree Dipole Moment: 15.258345 Debye
[TS-1]$_{2\text{-anthryl}}$ Coordinates (x,y,z): C 0.32134500 0.91162000 0.52821500 C 1.96937900 0.56216900 -1.26207400 C -0.39004800 0.84259000 -1.79047400 C 0.88670800 0.65701700 -2.20666300 C -0.74469100 0.94906800 -0.37636700 C 1.66846900 0.69634500 0.13784000 H -1.19659100 0.88049000 -2.52586400 H 0.11505800 1.00385400 1.59926600 H 1.11676100 0.56224800 -3.26940500 Si -2.10491200 2.28095800 0.05647800 C -1.68586400 3.68516700 -1.12938300 H -1.87540300 3.40440300 -2.17577900 H -0.62788400 3.97414400 -1.03990400 H -2.30476800 4.56625900 -0.89927300 C -3.89967900 1.80936000 -0.18418700 H -4.49769200 2.69212700 0.09565700 H -4.20208300 0.96393300 0.44739500 H -4.12356100 1.55784800 -1.22933000 C -1.80820700 2.89444000 1.80910100 H -0.80533000 3.33547700 1.91264500 H -1.92887800 2.10133500 2.55938700 H -2.54425800 3.68326500 2.02918900 B -1.47944200 -0.89296800 0.08452900 Br -2.20621500 -0.75471600 1.93060800 Br -0.00927000 -2.20528000 -0.07840000	**[TS-1]$_{2\text{-anthryl}}$** Coordinates (x,y,z): C 0.27428800 1.01256900 0.53201900 C 1.92417000 0.63927200 -1.25625100 C -0.43210300 0.95450700 -1.78846800 C 0.84338200 0.74476300 -2.20277600 C -0.78026000 1.07342200 -0.37717500 C 1.62324600 0.77983000 0.14300100 H -1.23335000 1.01923600 -2.52840200 H 0.07411900 1.12626100 1.60198900 H 1.07444300 0.64916500 -3.26539200 Si -2.22550000 2.28122600 0.08124600 C -1.90507300 3.75591600 -1.04545000 H -2.04421300 3.49290200 -2.10447500 H -0.87903800 4.13128600 -0.91507700 H -2.60542600 4.56971100 -0.80185100 C -3.97617200 1.67816200 -0.21198800 H -4.64667000 2.50851500 0.06267000 H -4.23206800 0.80411900 0.40153800 H -4.15238200 1.42873000 -1.26729600 C -2.00817800 2.83489700 1.86425100 H -1.03595200 3.32964500 2.00810900 H -2.09313300 2.00705900 2.58160500 H -2.79655800 3.56771800 2.09618100 B -1.42416200 -0.97872100 0.09285500 Br -2.15655600 -0.86099000 1.91886400 Br 0.13133000 -2.16196200 -0.09469000

Br -2.87600600 -1.19720000 -1.28694900 C 2.68937500 0.59249700 1.08867200 C 4.01469600 0.36702100 0.70162200 C 4.31851900 0.23803500 -0.69801100 C 3.28667400 0.33772900 -1.64729700 H 3.52649100 0.23003200 -2.70737600 H 2.44367500 0.68190700 2.14956100 C 5.67562000 0.00548200 -1.08185300 C 5.07416300 0.25598000 1.65738300 H 4.83223800 0.35176400 2.71751500 C 6.35871100 0.03264600 1.25002800 H 7.16100100 -0.05219000 1.98381000 C 6.66122600 -0.09341600 -0.13902400 H 5.90852800 -0.09359500 -2.14352600 H 7.69251800 -0.27250200 -0.44654800 E(RM062X): -8693.897099 Hartree Dipole Moment: 6.838246 Debye Imaginary Frequency: 169.43i cm^{-1}	Br -2.77322300 -1.28381400 -1.30807500 C 2.64320800 0.67164600 1.09326100 C 3.96715900 0.43103000 0.70453800 C 4.27019700 0.29211700 -0.69442400 C 3.23878100 0.39947300 -1.64415100 H 3.47644600 0.28815400 -2.70435200 H 2.40213900 0.77279400 2.15405200 C 5.62502300 0.04452700 -1.07930000 C 5.02626900 0.31638700 1.66093800 H 4.78613500 0.42206600 2.72049600 C 6.30906600 0.07869300 1.25298300 H 7.11138900 -0.00819100 1.98660700 C 6.61056600 -0.05837100 -0.13578700 H 5.85591200 -0.06109800 -2.14082100 H 7.64034400 -0.24785500 -0.44207700 E(RM062X): -8693.906015 Hartree Dipole Moment: 6.916707 Debye Imaginary Frequency: 234.39i cm^{-1}
[TS-2]$_{2\text{-anthryl}}$ Coordinates (x,y,z): C 0.49575000 -0.57286700 0.39614200 C 2.19549400 0.46421500 -1.05836200 C -0.17840200 0.91494000 -1.38626100 C 1.14199800 1.08311600 -1.77358300 C -0.54723900 0.03061100 -0.30496100 C 1.85817200 -0.37243600 0.06777400 H -0.98384400 1.35418600 -1.98207000 H 0.24586400 -1.25806700 1.21165800 H 1.38365800 1.72594000 -2.62272200 B -2.05526900 -0.56582000 -0.11047000 Br -2.59739200 -0.46868600 1.86093100 Br -1.95163800 -2.50840500 -0.67861900 Br -3.42284600 0.38461900 -1.26690200 C 2.89323100 -0.98627700 0.79796500 C 4.22958800 -0.80047500 0.45527900 C 4.56562600 0.03854800 -0.67225600 C 3.54733700 0.64907100 -1.39980400 H 3.80042000 1.28227400 -2.25344200 H 2.63620700 -1.62500000 1.64599500 Si -0.35423300 2.33965900 0.54963300	**[TS-2]$_{2\text{-anthryl}}$** Coordinates (x,y,z): C 0.49256800 -0.55253000 0.41524900 C 2.19798400 0.42095600 -1.07685600 C -0.17171900 0.88663200 -1.41277500 C 1.14550700 1.03072000 -1.80744600 C -0.54400900 0.03712400 -0.30216400 C 1.85911400 -0.37241700 0.07886800 H -0.96532300 1.33698900 -2.01373100 H 0.24931400 -1.20698700 1.25740100 H 1.38980200 1.64931900 -2.67312000 B -2.04916900 -0.53983800 -0.10019000 Br -2.62882900 -0.44413500 1.85998600 Br -1.99150400 -2.51256400 -0.65592500 Br -3.43444500 0.38599400 -1.26607400 C 2.88861000 -0.96729900 0.82920100 C 4.22663500 -0.80454700 0.47308900 C 4.56423500 -0.01037900 -0.68522200 C 3.54720100 0.58414900 -1.43159000 H 3.80118000 1.18775400 -2.30573500 H 2.63170400 -1.57003300 1.70309100 Si -0.28261600 2.39219700 0.55028200

C 0.78029500 3.63306100 -0.19041500 H 1.82321200 3.28960500 -0.22699800 H 0.46253900 3.93801900 -1.19639500 H 0.73232800 4.51422100 0.47142000 C 0.29712500 1.84911300 2.22239300 H 0.24614100 2.75075100 2.85604800 H -0.31730600 1.05754600 2.66981600 H 1.34616300 1.52752900 2.16397000 C -2.10969400 2.92794200 0.51769700 H -2.08499700 3.85879900 1.11221000 H -2.45810500 3.16323300 -0.49543600 H -2.80599400 2.21998600 0.98221200 C 5.95033700 0.21587000 -1.00929200 H 6.20105300 0.84855900 -1.86268000 C 6.92777200 -0.39408600 -0.28169800 H 7.97616900 -0.25341300 -0.54791500 C 6.59469400 -1.22685500 0.83619500 H 7.39497400 -1.70588300 1.40162900 C 5.29408600 -1.42335800 1.19156200 H 5.03578500 -2.05869600 2.04060900 E(RM062X): -8693.888452 Hartree Dipole Moment: 12.630899 Debye Imaginary Frequency: 144.94i cm^{-1}	C 0.91382200 3.59466500 -0.21763600 H 1.93636400 3.19473100 -0.24178500 H 0.60918200 3.89304300 -1.22885200 H 0.90696700 4.48510700 0.43328900 C 0.29962600 1.88253100 2.23843000 H 0.26723400 2.79577300 2.85652500 H -0.35200700 1.12082300 2.68317600 H 1.33716500 1.52282400 2.20969900 C -2.03214300 2.98594900 0.44670100 H -2.01561800 3.93747300 1.00701800 H -2.34538100 3.19224100 -0.58416600 H -2.74642800 2.30402200 0.92195400 C 5.94798700 0.14489800 -1.03525100 H 6.19912300 0.74511100 -1.91156100 C 6.92442900 -0.44649200 -0.28884100 H 7.97292200 -0.32360800 -0.56333700 C 6.58965100 -1.23475300 0.86013500 H 7.38909900 -1.69784700 1.43989400 C 5.28813800 -1.40835400 1.22866400 H 5.02857100 -2.00870500 2.10235100 E(RM062X): -8693.908461 Hartree Dipole Moment: 16.449246 Debye Imaginary Frequency: 144.08i cm^{-1}
[TS-3]$_{2\text{-anthryl}}$ Coordinates (x,y,z): C 0.59492000 -0.54539300 0.52245400 C 2.26743300 0.02275800 -1.20489000 C -0.11611800 0.18904900 -1.67506100 C 1.17589100 0.32228300 -2.08760100 C -0.45202900 -0.25274900 -0.33310700 C 1.96271700 -0.41653000 0.13006200 H -0.93700800 0.38554100 -2.36920200 H 0.37645600 -0.92275600 1.52504200 H 1.40271800 0.64199800 -3.10696800 B -1.96785800 -0.70104700 -0.02239100 Br -2.30291300 -1.18770900 1.90159900 Br -2.52538900 -2.16954400 -1.26026300 Br -3.11301700 1.01239200 -0.47174700 C 3.00687300 -0.70838400 1.01384900 C 4.34574700 -0.57486100 0.62875400	**[TS-3]$_{2\text{-anthryl}}$** Coordinates (x,y,z): C 0.57649600 -0.64533400 0.50567100 C 2.26135800 -0.09797000 -1.22189200 C -0.12216600 0.05556400 -1.69864000 C 1.17144400 0.19004900 -2.11052300 C -0.45937800 -0.38146100 -0.36015600 C 1.95131800 -0.51929600 0.11672500 H -0.93585600 0.26231200 -2.39841900 H 0.36480600 -0.98850400 1.52121300 H 1.39943000 0.51305700 -3.12862200 B -1.99558700 -0.68146400 -0.01640900 Br -2.33618300 -1.09376400 1.94405500 Br -2.65918900 -2.22737300 -1.16204100 Br -3.11311000 1.00036700 -0.51743900 C 2.99382400 -0.78580900 1.00964200 C 4.33466200 -0.64743800 0.62698600

C 4.65023000 -0.12948200 -0.70446200	C 4.64368400 -0.22349300 -0.71222700
C 3.60212900 0.15795700 -1.59004400	C 3.59714300 0.04148000 -1.60668600
H 3.83664000 0.49287800 -2.60333300	H 3.83169200 0.36467400 -2.62382800
H 2.77024400 -1.04820600 2.02522400	H 2.75802500 -1.10790700 2.02696000
Si -0.70546000 2.37326200 0.38437600	Si -0.49628800 2.73352700 0.38797700
C -1.14376500 3.49405000 -1.04136300	C -1.06198800 3.61148000 -1.12826000
H -0.47965700 4.37216200 -1.01215400	H -0.45760500 4.52820400 -1.22236800
H -0.98810300 2.97816900 -1.99845300	H -0.86803200 2.98625000 -2.01188800
H -2.19347900 3.80833500 -0.98543900	H -2.12881000 3.85802500 -1.08289400
C 1.12656300 2.54233800 0.69324000	C 1.32901700 2.61391300 0.56605000
H 1.22654800 3.61343400 0.94933900	H 1.62830100 3.65286900 0.80124800
H 1.48423100 1.95111400 1.54488000	H 1.64108100 1.96667600 1.39422600
H 1.76124600 2.34883900 -0.18041400	H 1.83694500 2.32261300 -0.36216600
C -1.60309300 2.48287100 2.00619900	C -1.45533500 2.64266800 1.95172200
H -1.00985700 3.10889900 2.69096000	H -0.91721800 3.23571400 2.70821800
H -2.60730300 2.90199500 1.86564500	H -2.47889700 3.01187900 1.81905200
H -1.71549100 1.48141700 2.44843300	H -1.49680400 1.59730500 2.29811300
C 5.42552400 -0.86872900 1.52260100	C 5.41294900 -0.91622900 1.53147000
H 5.18798300 -1.20939400 2.53221600	H 5.17327200 -1.24006000 2.54620300
C 6.72288100 -0.72780700 1.12025200	C 6.71202000 -0.77182500 1.13250700
H 7.53800000 -0.95513800 1.80844200	H 7.52538900 -0.97974400 1.82910800
C 7.02538800 -0.28479100 -0.20351400	C 7.01906300 -0.34995500 -0.19801400
H 8.06792600 -0.18000700 -0.50715000	H 8.06252600 -0.24192600 -0.49746600
C 6.02338100 0.00411900 -1.08617300	C 6.01846800 -0.08501300 -1.09068100
H 6.25274700 0.34023200 -2.09916800	H 6.24914000 0.23549700 -2.10860300
E(RM062X): -8693.887477 Hartree	E(RM062X): -8693.905421 Hartree
Dipole Moment: 9.893951 Debye	Dipole Moment: 16.259457 Debye
Imaginary Frequency: 137.58i cm^{-1}	Imaginary Frequency: 80.52i cm^{-1}

1.6 Stationary points for the exchange reaction of TMSAr (Ar = 1-naphthyl) andBBr_3

Gas Phase	In Solvent (DCM)
1-Naphthyl-BBr_2	**1Naphthyl-BBr_2**
Coordinates (x,y,z):	Coordinates (x,y,z):
C 1.50697900 2.68139000 -0.83527200	C 1.50943500 2.67757700 -0.84762500
C 2.70870400 2.04992200 -0.64355200	C 2.71096500 2.04491700 -0.65321900
C 2.76110000 0.72126800 -0.14010800	C 2.76114400 0.71823600 -0.14170100
C 1.54723300 0.02420200 0.14140100	C 1.54619900 0.02477300 0.14585500

C 0.28867500 0.68503700 -0.10138700 C 0.30304900 1.99899400 -0.54889000 H 4.92564300 0.63953900 -0.12783100 H 1.47121000 3.70539900 -1.20842000 H 3.64802300 2.56263000 -0.86168500 C 4.01090400 0.08917800 0.10134800 C 1.64807000 -1.27965600 0.70190000 C 2.87088400 -1.86396500 0.93259500 C 4.06899600 -1.17944600 0.62118800 H 0.74233900 -1.82308300 0.96651100 H 2.91698800 -2.86403500 1.36595100 H 5.03243600 -1.65623700 0.80591500 H -0.64251700 2.51997900 -0.70902500 B -1.10919800 0.01201900 -0.01740600 Br -2.62330500 0.98777000 0.64688600 Br -1.45771500 -1.75079400 -0.69030600 E(RM062X): -5557.526952 Hartree Dipole Moment: 2.308663 Debye	C 0.28867700 0.68695600 -0.10065200 C 0.30396900 1.99868700 -0.55657800 H 4.92628300 0.63188300 -0.13184700 H 1.47467000 3.69907600 -1.22737700 H 3.65076500 2.55479300 -0.87538100 C 4.01076700 0.08490000 0.10197100 C 1.64387000 -1.27577200 0.71562300 C 2.86643500 -1.86183000 0.94794900 C 4.06611100 -1.18152800 0.62962300 H 0.73748900 -1.81434000 0.98892100 H 2.91156600 -2.85873800 1.38870900 H 5.02852200 -1.65968400 0.81618700 H -0.63991800 2.52084300 -0.72348700 B -1.10693300 0.01424000 -0.01704900 Br -2.62240600 0.98421800 0.65734400 Br -1.45759800 -1.74554700 -0.70300000 E(RM062X): -5557.530849 Hartree Dipole Moment: 2.848557 Debye
1-TMS-napthalene Coordinates (x,y,z): C -0.83213600 2.72542300 -0.00014100 C -2.03549200 2.07046900 -0.00002300 C -2.08192000 0.64919800 -0.00006500 C -0.86084100 -0.09141700 -0.00027400 C 0.39861400 0.60381200 -0.00039100 C 0.37789100 1.98625200 -0.00029100 H -4.24602600 0.54452500 0.00021500 H -0.79748600 3.81599600 -0.00005600 H -2.97555100 2.62638300 0.00010300 C -3.32450300 -0.04162400 0.00009600 C -0.95143300 -1.51322900 -0.00034200 C -2.16574500 -2.15673700 -0.00018600 C -3.37020600 -1.41354300 0.00003500 H -0.03687100 -2.10693500 -0.00053900 H -2.20281700 -3.24711100 -0.00022400 H -4.32954200 -1.93286600 0.00012400 H 1.31705000 2.54390300 -0.00034100 Si 2.07903600 -0.27906400 0.00008900 C 2.28316400 -1.33299300 -1.55016700 H 3.28197200 -1.79594700 -1.56113400	**1-TMS-naphthalene** Coordinates (x,y,z): C -0.83274800 2.72648100 -0.00006000 C -2.03715900 2.07173200 -0.00006400 C -2.08281700 0.64956300 -0.00013900 C -0.86082100 -0.09146200 -0.00015800 C 0.39959000 0.60364700 -0.00005700 C 0.37799600 1.98678400 -0.00007700 H -4.24812500 0.54468500 -0.00019400 H -0.79771300 3.81708200 -0.00003000 H -2.97715300 2.62776100 -0.00005200 C -3.32644900 -0.04129500 -0.00023400 C -0.95120600 -1.51415100 -0.00042200 C -2.16631700 -2.15778400 -0.00052300 C -3.37153200 -1.41406800 -0.00040100 H -0.03740300 -2.10921500 -0.00058700 H -2.20334600 -3.24815900 -0.00071600 H -4.33070800 -1.93379400 -0.00048800 H 1.31658500 2.54542000 -0.00003800 Si 2.08367600 -0.27965600 0.00026900 C 2.28111600 -1.33355400 -1.55023200 H 3.28061200 -1.79516100 -1.55875900

H 1.53676900 -2.13558700 -1.62691100 H 2.19058300 -0.70433700 -2.44847500 C 2.28192500 -1.33143400 1.55153500 H 1.53417900 -2.13272900 1.62889700 H 3.27998700 -1.79592200 1.56357100 H 2.18980100 -0.70151100 2.44901000 C 3.43934200 1.02415900 -0.00042300 H 4.42120900 0.52682400 -0.00037600 H 3.38899800 1.66578300 -0.89279900 H 3.38928600 1.66642000 0.89150700 E(RM062X): -793.851323 Hartree Dipole Moment: 0.117663 Debye	H 1.53530300 -2.13729100 -1.62277400 H 2.18949800 -0.70425900 -2.44842000 C 2.28094100 -1.33178100 1.55200500 H 1.53425700 -2.13458600 1.62587400 H 3.27993200 -1.79446600 1.56077000 H 2.19031000 -0.70121300 2.44940100 C 3.43962000 1.02567800 -0.00055900 H 4.42036500 0.52600700 -0.00055800 H 3.38722200 1.66641400 -0.89350600 H 3.38762200 1.66722700 0.89182400 E(RM062X): -793.855179 Hartree Dipole Moment: 0.256633 Debye
[IM-1]$_{1\text{-naphthyl}}$ Coordinates (x,y,z): H 4.95134600 -2.27891100 1.02805000 C 4.03969200 -1.77327200 0.70798500 H 4.92319800 -0.92559000 -1.05691400 C 4.02704600 -1.02333700 -0.44127000 C 1.69031500 -1.27255800 1.08744000 C 2.83670100 -0.36997000 -0.86021500 C 2.85399600 -1.90475800 1.46603000 C 1.64809300 -0.46565900 -0.07693200 C 2.81450100 0.34438100 -2.08880600 H 2.85574000 -2.52528800 2.36327300 H 0.78711800 -1.39785400 1.68235700 C 1.68023200 0.98604200 -2.52253400 H 3.72763600 0.37086500 -2.68882800 H 1.66835100 1.52887200 -3.46744400 C 0.51982200 0.93521500 -1.73053300 B -1.08812300 -0.36870300 -0.10664200 Br -1.58450000 -0.29963900 1.87763800 Br -2.57526000 0.59812200 -1.10218300 Br -1.03859600 -2.29591900 -0.71713800 Si 0.72844700 2.11474400 0.58202400 H -0.38106500 1.43496100 -2.09364000 C 0.43178800 0.24504200 -0.49790300 C 2.07076700 3.13226900 -0.24428500 H 2.31010200 3.94949200 0.45578900 H 1.75254100 3.57678700 -1.19644600 H 2.99354200 2.55850900 -0.40960100	**[IM-1]$_{1\text{-naphthyl}}$** Coordinates (x,y,z): H 4.90439500 -2.38842700 1.00579800 C 4.00170600 -1.86475200 0.69003100 H 4.89486600 -1.02526400 -1.07444900 C 3.99929800 -1.10973100 -0.45660800 C 1.66521200 -1.31545300 1.08075900 C 2.82100800 -0.42973700 -0.86842800 C 2.81732300 -1.97304500 1.45380200 C 1.63234800 -0.50561300 -0.08161100 C 2.81573200 0.29584000 -2.09062200 H 2.81251500 -2.59106100 2.35271700 H 0.76835200 -1.41895000 1.68829600 C 1.69544400 0.96908800 -2.51641600 H 3.72906400 0.31074600 -2.68969900 H 1.69705000 1.52805300 -3.45143800 C 0.53528800 0.93481400 -1.72620800 B -1.08319300 -0.33259600 -0.10326400 Br -1.59753800 -0.27551800 1.87934500 Br -2.57597000 0.65268000 -1.09109500 Br -1.11651500 -2.27921600 -0.72136000 Si 0.82441100 2.12176200 0.58746400 H -0.34679800 1.46607400 -2.08842400 C 0.43241900 0.23553400 -0.49760700 C 2.19255300 3.08135800 -0.24767700 H 2.44460700 3.89766000 0.44918400 H 1.88766900 3.52232000 -1.20527800 H 3.10015700 2.48048500 -0.39785000

C 1.36902800 1.65054700 2.27409900	C 1.42927700 1.61406900 2.27770800
H 1.36197300 2.58128600 2.86573200	H 1.45707900 2.54284700 2.87170300
H 2.40391600 1.28622400 2.20989100	H 2.44962300 1.21118400 2.21380200
H 0.74521400 0.90941000 2.78559700	H 0.77741600 0.89454700 2.78476900
C -0.87462000 3.05938500 0.59717600	C -0.76271300 3.09322900 0.59327400
H -0.67220600 3.98334800 1.16460200	H -0.54169100 4.01237600 1.16077800
H -1.67932400 2.50232400 1.09237200	H -1.58170000 2.55783000 1.08832400
H -1.20745000 3.33296900 -0.41248700	H -1.07694900 3.37618900 -0.41995400
E(RM062X): -8540.435228 Hartree	E(RM062X): -8540.451479 Hartree
Dipole Moment: 10.247305 Debye	Dipole Moment: 13.708184 Debye
[IM-2]$_{1\text{-naphthyl}}$	**[IM-2]$_{1\text{-naphthyl}}$**
Coordinates (x,y,z):	Coordinates (x,y,z):
C 2.02242600 1.34025200 -1.77996500	C 2.14803500 1.09114700 -1.86192000
C 3.04941900 0.49712300 -1.51564800	C 3.05773100 0.11359700 -1.60944500
C 2.86504900 -0.59398300 -0.60358800	C 2.72379700 -0.96374000 -0.73208300
C 1.57804400 -0.86265200 -0.03410000	C 1.40776700 -1.06676100 -0.17383900
C 0.45570800 -0.01442700 -0.36524500	C 0.41338300 -0.07652800 -0.49850300
C 0.74298700 1.14850000 -1.12866800	C 0.84644100 1.05288400 -1.23678400
H 4.93251700 -1.21154400 -0.73346600	H 4.69724700 -1.84101900 -0.85913500
H 2.14361600 2.18480200 -2.46080500	H 2.38841000 1.92747300 -2.51822100
H 4.02556500 0.62819200 -1.98569500	H 4.04777400 0.13473700 -2.06716900
C 3.95844900 -1.43579500 -0.29540700	C 3.70306400 -1.93923200 -0.42064600
C 1.44213300 -2.01918200 0.78317200	C 1.13926600 -2.17507400 0.68305500
C 2.52400700 -2.82287400 1.06385500	C 2.11225300 -3.10055200 0.97713300
C 3.79464200 -2.52585800 0.52997900	C 3.40619000 -2.98573500 0.42031600
H 0.46697400 -2.27043600 1.19235400	H 0.15291900 -2.28704400 1.12447200
H 2.39295500 -3.70011700 1.69794900	H 1.88270800 -3.93163300 1.64457100
H 4.64518100 -3.16995000 0.75888200	H 4.16745900 -3.73005600 0.65807900
H -0.12100800 1.65325800 -1.57246800	H 0.07487300 1.71644000 -1.64423100
Si 0.91427700 2.52040400 0.49384100	Si 1.31720500 2.37928400 0.43022400
C 2.71242900 2.51303600 1.00799400	C 2.21564700 1.38884000 1.72099100
H 2.79263700 3.12600800 1.91973600	H 2.57186600 2.10769300 2.47653800
H 3.05690000 1.49866200 1.25918200	H 1.54690200 0.66603300 2.20863100
H 3.37768600 2.93101000 0.24205400	H 3.09010200 0.86344000 1.31239700
C -0.14659700 2.20509100 1.98462900	C -0.26943300 3.16059900 0.99844100
H 0.00785000 3.07833900 2.64115600	H 0.03801200 3.91226200 1.74528000
H -1.21407400 2.12074200 1.74738000	H -0.77648800 3.67793300 0.17303600
H 0.16115600 1.30063500 2.52539700	H -0.96553300 2.45719400 1.46863000
C 0.40422900 4.07220600 -0.41532800	C 2.39004600 3.68125600 -0.37098100
H -0.65006200 3.99640100 -0.71914600	H 1.91865600 4.10574700 -1.26888100
H 0.50558200 4.93147100 0.26581400	H 2.50215300 4.49355900 0.36519200

H 1.02341600 4.26215500 -1.30286900 B -1.11304200 -0.41585100 -0.10135100 Br -1.36005900 -1.98520300 -1.35719200 Br -1.59711500 -0.91866500 1.80331300 Br -2.39137200 1.08744900 -0.65390900 E(RM062X): -8540.435586 Hartree Dipole Moment: 10.012001 Debye	H 3.38776800 3.30191500 -0.62682500 B -1.16247000 -0.26559800 -0.12124100 Br -1.79384000 -2.03243000 -0.91814200 Br -1.42220500 -0.25858900 1.91223500 Br -2.35876800 1.18699400 -0.90791300 E(RM062X): -8540.454790 Hartree Dipole Moment: 13.723623 Debye
[TS-1]$_{1\text{-naphthyl}}$ Coordinates (x,y,z): C -1.10239400 -0.36592700 2.75735600 C -2.33578500 -0.64894800 2.21313800 C -2.67617000 -0.25905300 0.89125000 C -1.70674900 0.41007800 0.08793600 C -0.37620900 0.68966500 0.63076700 C -0.16448100 0.32225700 1.97876100 H -4.67767600 -1.07940600 1.00836500 H -0.85659600 -0.66788300 3.77497900 H -3.08462600 -1.18480200 2.80202100 C -3.95898300 -0.56433700 0.36802800 C -2.06805000 0.72316100 -1.24394900 C -3.31859600 0.41053400 -1.73465700 C -4.28038900 -0.23092400 -0.92496700 H -1.33478100 1.18407200 -1.90026800 H -3.56300500 0.65440000 -2.76961300 H -5.26368900 -0.47092600 -1.33061200 H 0.79919400 0.56364200 2.43426900 Si 0.37756100 2.46768200 0.30775500 C -0.46352300 3.50279300 1.64225700 H -0.20202000 4.56600300 1.52762700 H -1.55857800 3.41270500 1.57101400 H -0.16072000 3.18511800 2.65129500 C -0.06010500 3.25714300 -1.34040900 H -1.14203400 3.41480300 -1.44845500 H 0.42280300 4.24778900 -1.33795900 H 0.31815500 2.69931800 -2.20658700 C 2.23267200 2.53049200 0.55418400 H 2.76802300 1.97262000 -0.22612500 H 2.52741300 3.59072500 0.49541900	**[TS-1]$_{1\text{-naphthyl}}$** Coordinates (x,y,z): C -1.01969900 -0.44994600 2.73333900 C -2.25801900 -0.73942900 2.20854700 C -2.64134500 -0.28346700 0.91679300 C -1.71802300 0.47284200 0.13607800 C -0.39662600 0.77927000 0.67229900 C -0.12547800 0.32510000 1.97695900 H -4.60747700 -1.18632900 1.01912000 H -0.73573000 -0.80231700 3.72455400 H -2.97478300 -1.33092900 2.78316900 C -3.92192400 -0.60646800 0.39842700 C -2.12017900 0.85544500 -1.16697800 C -3.36695000 0.52243300 -1.65484700 C -4.28305100 -0.20814700 -0.86690300 H -1.42411700 1.39634700 -1.80325200 H -3.64600800 0.82360800 -2.66561200 H -5.26532900 -0.46167600 -1.26691400 H 0.83357800 0.58450200 2.43322600 Si 0.41511800 2.51638000 0.34298000 C -0.36034000 3.58138700 1.69013500 H -0.02838000 4.62610100 1.58884900 H -1.45840700 3.56162200 1.61335600 H -0.07979500 3.22596700 2.69285600 C 0.01578200 3.33669800 -1.30096600 H -1.05546100 3.56210800 -1.39624900 H 0.55910300 4.29536500 -1.29973100 H 0.34608100 2.76230400 -2.17628100 C 2.27619300 2.48581100 0.57559000 H 2.78229300 1.92775600 -0.22426800 H 2.61911800 3.53227600 0.54209100

H 2.55238500 2.14126200 1.53050800 B 0.85248000 -0.72923000 -0.18000600 Br 2.54539800 -0.85300600 0.85730400 Br -0.17874300 -2.41402100 -0.11583600 Br 1.19277500 -0.09847100 -2.03468500 E(RM062X): -8540.428512 Hartree Dipole Moment: 6.246763 Debye Imaginary Frequency: 177.63i cm^{-1}	H 2.58158500 2.05945700 1.54139800 B 0.86526700 -0.78867900 -0.21620400 Br 2.55654700 -0.94092900 0.79324400 Br -0.22581500 -2.41915600 -0.14741300 Br 1.12451700 -0.07680800 -2.03834200 E(RM062X): -8540.436850 Hartree Dipole Moment: 6.554649 Debye Imaginary Frequency: 240.69i cm^{-1}
[TS-2]$_{1\text{-naphthyl}}$ Coordinates (x,y,z): C -0.43935800 0.13418600 -0.37628400 C -2.82468700 -0.49170800 -0.80273000 C -1.76955100 1.17948700 -2.21465700 C -2.84773100 0.39625200 -1.92113600 C -0.58116500 1.04136000 -1.44475700 C -1.64357300 -0.61654500 -0.00734000 H -1.78600000 1.87999700 -3.05182400 H 0.31581600 1.56489600 -1.78705800 B 1.12086700 -0.37836000 -0.10187600 Br 2.44646300 1.16374000 -0.37757100 Br 1.59787000 -1.19376200 1.69108100 Br 1.35609600 -1.76606400 -1.56005300 Si -0.88041500 2.14450100 0.64573400 C -0.18940600 3.71149900 -0.11166700 H -0.31322000 4.51888300 0.63353400 H -0.73438800 3.99975700 -1.02541200 H 0.88308800 3.61096500 -0.33864100 C -2.74058400 2.27223400 0.82298400 H -3.26755600 2.43517000 -0.12945200 H -2.91409500 3.16215500 1.45722400 H -3.17698600 1.39970100 1.33437200 C -0.11304200 1.74563900 2.29586700 H -0.36466800 2.59770200 2.95585900 H 0.98063500 1.64132400 2.23947400 H -0.53312400 0.82504300 2.73067200 H -3.76003400 0.45227500 -2.52192200 C -1.69967500 -1.46942600 1.12186200 H -0.81616200 -1.58155400 1.74659300 C -2.85106600 -2.16440300 1.43352800	**[TS-2]$_{1\text{-naphthyl}}$** Coordinates (x,y,z): C -0.44016900 0.15082700 -0.37898400 C -2.82283000 -0.48464500 -0.81497500 C -1.74678300 1.14727400 -2.26020300 C -2.83215400 0.37618300 -1.95302000 C -0.56691600 1.02014400 -1.48181800 C -1.64926800 -0.59328300 -0.00628200 H -1.75474800 1.82510200 -3.11602600 H 0.33313300 1.53966900 -1.82261400 B 1.11752400 -0.37784400 -0.09962400 Br 2.45676300 1.14946500 -0.38769900 Br 1.58454300 -1.18318800 1.70074700 Br 1.34590300 -1.78333000 -1.54192100 Si -0.86298200 2.12699800 0.64707600 C -0.17549000 3.68429400 -0.13410500 H -0.30086300 4.50017600 0.60168600 H -0.72385400 3.96050700 -1.04964800 H 0.89682900 3.58588500 -0.36227300 C -2.72383500 2.26362500 0.81444200 H -3.24628900 2.40228700 -0.14476800 H -2.90000200 3.17106600 1.42282100 H -3.16390900 1.40512000 1.34644900 C -0.09728100 1.76206100 2.30605300 H -0.35014100 2.62727100 2.94820800 H 0.99663200 1.65775700 2.25178100 H -0.51659500 0.85008900 2.75911100 H -3.73991700 0.42270700 -2.56172800 C -1.72030700 -1.41637900 1.14393000 H -0.84316500 -1.51815500 1.77956400 C -2.87835300 -2.09669000 1.46296700

H -2.86193900 -2.81753200 2.30933400 C -4.00530400 -2.05143000 0.63240800 H -4.90531400 -2.61590500 0.88625200 C -3.98878700 -1.22493600 -0.46860800 H -4.87599200 -1.11437000 -1.09771400 E(RM062X): -8540.432871 Hartree Dipole Moment: 10.477120 Debye Imaginary Frequency: 2.35i cm^{-1}	H -2.89991200 -2.72680500 2.35540400 C -4.02566200 -1.99942900 0.64932000 H -4.93099100 -2.55167500 0.91083300 C -3.99423800 -1.20360400 -0.47320900 H -4.87466900 -1.10517700 -1.11385900 E(RM062X): -8540.448758 Hartree Dipole Moment: 13.404551 Debye Imaginary Frequency: No imaginary freq
[TS-3]$_{1\text{-naphthyl}}$ Coordinates (x,y,z): C 1.32624100 2.09213200 -1.94181700 C 2.60096500 1.96476300 -1.48053300 C 2.94179800 0.89707500 -0.59216700 C 1.94289500 -0.03686600 -0.17983300 C 0.56991800 0.13712100 -0.61557700 C 0.31146900 1.19158700 -1.49508400 H 5.02051200 1.48316300 -0.46869500 H 1.07006000 2.86963400 -2.66332700 H 3.38885600 2.64847300 -1.80346600 C 4.27885200 0.74787100 -0.15052000 C 2.36146200 -1.13848900 0.61525800 C 3.67319700 -1.27109000 1.01571500 C 4.64012300 -0.31340200 0.64688300 H 1.64195000 -1.90207400 0.89918300 H 3.96496200 -2.13075500 1.62015600 H 5.67354300 -0.42539200 0.97820200 H -0.66176800 1.25015000 -1.98076700 Si -0.93566300 2.34538400 0.50923500 C 0.63799800 2.53559800 1.47701400 H 0.48358500 3.38972700 2.15813600 H 0.80929700 1.63411100 2.08317200 H 1.51606600 2.73256000 0.85047500 C -2.37635200 2.09539700 1.66221000 H -2.33892800 1.13070800 2.18110200 H -2.29818100 2.90662600 2.40827700 H -3.32761200 2.18171000 1.12275600 C -1.34645600 3.66938200 -0.73754400 H -2.09247200 3.30287900 -1.45657700 H -1.80488600 4.49830100 -0.17289700	**[TS-3]$_{1\text{-naphthyl}}$** Coordinates (x,y,z): C 1.33902200 2.01138000 -2.04882000 C 2.61216800 1.92028600 -1.56266100 C 2.95025900 0.89259200 -0.63268900 C 1.95347500 -0.03600200 -0.19901200 C 0.58746100 0.10714200 -0.66274900 C 0.33540200 1.11432400 -1.58763000 H 5.02073300 1.51083600 -0.49751100 H 1.08144900 2.76665200 -2.79321600 H 3.39289200 2.60845600 -1.89286100 C 4.28415500 0.77930400 -0.15930000 C 2.37501600 -1.09027700 0.66124800 C 3.67890000 -1.18692900 1.09292600 C 4.64483500 -0.23620800 0.69330800 H 1.65972800 -1.84618500 0.97487300 H 3.96918300 -2.01014600 1.74732400 H 5.67278400 -0.31921400 1.04905100 H -0.65528700 1.19274000 -2.03566400 Si -1.01839300 2.59580800 0.57893800 C 0.59718900 2.60014200 1.45608200 H 0.55992800 3.45123500 2.15836900 H 0.72307000 1.67297000 2.03241000 H 1.43936900 2.74066800 0.76644300 C -2.50919200 2.19428300 1.58186100 H -2.42069800 1.22568100 2.08765600 H -2.55240400 2.99062300 2.34714200 H -3.42046100 2.22448400 0.97283000 C -1.32723700 3.74011500 -0.83297800 H -2.03034700 3.29468500 -1.55081400 H -1.81762200 4.62640400 -0.39456800

H -0.46726500 4.04495300 -1.27324000 B -0.60694200 -0.89192900 -0.18957100 Br -0.38034500 -2.65581500 -1.09681100 Br -0.72078200 -1.10129500 1.84520100 Br -2.43648500 -0.05480400 -0.74861700 E(RM062X): -8540.421330 Hartree Dipole Moment: 8.566954 Debye Imaginary Frequency: 129.43i cm^{-1}	H -0.40653800 4.04820100 -1.34023700 B -0.59134800 -0.89444100 -0.19796000 Br -0.31280900 -2.75219100 -0.96366100 Br -0.73613300 -1.00712800 1.85931500 Br -2.44049400 -0.20948500 -0.82548400 E(RM062X): -8540.436506 Hartree Dipole Moment: 14.542209 Debye Imaginary Frequency: 98.74i cm^{-1}

1.7 Stationary points for the exchange reaction of TMSAr (Ar = 2-naphthyl) andBBr_3

Gas Phase	In Solvent (DCM)
2-Naphthyl-BBr_2 Coordinates (x,y,z): C 0.99525800 0.70878400 0.00025800 C 2.83645800 -0.90669100 -0.00021700 C 0.52760600 -1.66306800 -0.00056900 C 1.86689700 -1.94879700 -0.00052000 C 0.05540100 -0.31165200 -0.00013300 C 2.38834500 0.44608400 0.00018800 H -0.19824300 -2.47728800 -0.00081400 H 0.66811800 1.75103200 0.00057100 H 2.21053200 -2.98510500 -0.00079800 B -1.45952500 0.01117200 -0.00008700 Br -2.10948800 1.81753400 -0.00029100 Br -2.77785800 -1.38212100 0.00035100 C 3.34834800 1.49634300 0.00054100 C 4.23263400 -1.16745300 -0.00029400 C 5.13657000 -0.13251300 0.00002300 H 6.20688900 -0.34424300 -0.00005900 H 4.57470900 -2.20415700 -0.00060000 C 4.69161800 1.21415900 0.00045000 H 2.99539200 2.52957000 0.00090800 H 5.42253500 2.02370100 0.00073800 E(RM062X): -5557.534401 Hartree Dipole Moment: 2.930052 Debye	**2-Naphthyl-BBr_2** Coordinates (x,y,z): C -0.99614000 0.71006400 -0.00031100 C -2.83765400 -0.90659100 0.00001300 C -0.52870300 -1.66444700 -0.00022900 C -1.86842100 -1.95042100 -0.00004900 C -0.05648500 -0.31201100 -0.00038300 C -2.38945300 0.44697000 -0.00011700 H 0.19459000 -2.48101000 -0.00027700 H -0.67262600 1.75331800 -0.00039500 H -2.21260700 -2.98644500 0.00006000 B 1.45544900 0.01038500 -0.00062300 Br 2.11124000 1.81736900 0.00008900 Br 2.77895800 -1.38214800 0.00010600 C -3.34878200 1.49894000 -0.00006300 C -4.23400900 -1.16865500 0.00018800 C -5.13764300 -0.13217900 0.00022600 H -6.20805600 -0.34326800 0.00034800 H -4.57607700 -2.20519400 0.00028500 C -4.69255800 1.21525800 0.00010400 H -2.99612800 2.53221000 -0.00015900 H -5.42414700 2.02417700 0.00014200 E(RM062X): -5557.537966 Hartree Dipole Moment: 3.637367 Debye

2-TMS-naphthalene	**2-TMS-naphthalene**
Coordinates (x,y,z):	Coordinates (x,y,z):
C 0.29152200 1.55335900 0.00002800 C -1.04643800 1.85599000 0.00001700 C -2.02489500 0.82310200 0.00000900 C -1.58728700 -0.53199000 0.00002400 C -0.19008000 -0.80528900 0.00003300 C 0.75364100 0.20148200 0.00004000 H -3.74937200 2.13896700 -0.00003600 H 1.01881900 2.37073000 0.00002200 H -1.38125800 2.89572200 0.00000800 C -3.41936200 1.09798100 -0.00001900 C -2.55949600 -1.56940000 0.00001800 H 0.11910000 -1.85489800 0.00003000 C -3.90110800 -1.27476800 -0.00000100 C -4.33580700 0.07460600 -0.00002300 H -2.21889000 -2.60708800 0.00003200 H -4.63836000 -2.07894900 -0.00000300 H -5.40395300 0.29687100 -0.00004500 Si 2.60703000 -0.16088100 -0.00001300 C 3.37769100 0.60821900 -1.53688700 H 3.20361400 1.69436900 -1.56516200 H 4.46521300 0.44019700 -1.55736100 H 2.94489200 0.17371400 -2.45003100 C 3.37764100 0.60735800 1.53733700 H 2.94465700 0.17239800 2.45018000 H 4.46514200 0.43925100 1.55791300 H 3.20362300 1.69350500 1.56618600 C 2.88002900 -2.02235900 -0.00052300 H 2.43763600 -2.49133200 -0.89229200 H 3.95677000 -2.24904000 -0.00057000 H 2.43762600 -2.49183000 0.89098300	C -0.29174600 -1.55428700 0.00002800 C 1.04707700 -1.85759700 0.00005600 C 2.02565400 -0.82359000 0.00003300 C 1.58760800 0.53224200 -0.00002200 C 0.18958200 0.80610400 -0.00005200 C -0.75429500 -0.20152000 -0.00002500 H 3.75108300 -2.14007100 0.00010600 H -1.01873700 -2.37187900 0.00004500 H 1.38198400 -2.89735300 0.00009600 C 3.42094100 -1.09913100 0.00006300 C 2.55984300 1.57095400 -0.00004500 H -0.11903900 1.85581400 -0.00009700 C 3.90219600 1.27561700 -0.00001300 C 4.33736800 -0.07460200 0.00004200 H 2.21921600 2.60869400 -0.00008700 H 4.63971800 2.07962000 -0.00002900 H 5.40566900 -0.29633000 0.00006700 Si -2.61099800 0.16212600 -0.00002000 C -3.37705900 -0.60923200 -1.53726600 H -3.20278000 -1.69557100 -1.56280700 H -4.46439900 -0.43942500 -1.55470000 H -2.94505700 -0.17271800 -2.45011200 C -3.37688100 -0.60845800 1.53770000 H -2.94470000 -0.17152700 2.45026200 H -4.46420900 -0.43858700 1.55523600 H -3.20264200 -1.69479200 1.56373500 C -2.87926900 2.02285600 -0.00046200 H -2.43586200 2.49026900 -0.89264700 H -3.95656900 2.24725400 -0.00048700 H -2.43582300 2.49070000 0.89147800
E(RM062X): -793.852760 Hartree Dipole Moment: 0.227731 Debye	E(RM062X): -793.856758 Hartree Dipole Moment: 0.380138 Debye
[IM-1]$_{2\text{-naphthalene}}$	**[IM-1]$_{2\text{-naphthalene}}$**
Coordinates (x,y,z):	Coordinates (x,y,z):
C 1.20720200 -0.23108000 0.75795100 C 2.99868400 -0.45576000 -0.89144800	C 1.20402700 -0.26463700 0.75950600 C 2.99260400 -0.48926000 -0.89368700

C 0.72833300 0.03702600 -1.60736700 C 2.03887400 -0.18687300 -1.91623400 C 0.24961500 0.03786200 -0.23617000 C 2.57144600 -0.47308200 0.46836700 H -0.00948100 0.21135100 -2.39433900 H 0.87052100 -0.28755400 1.79846400 H 2.36973400 -0.18854000 -2.95654800 Si 0.45582300 2.19410600 0.08338900 C 2.23636600 2.62380600 0.48277000 H 2.54769300 2.28474500 1.47991200 H 2.30131300 3.72401700 0.45555600 H 2.94395200 2.22976700 -0.26054200 C 0.03330800 3.00399500 -1.54738000 H -0.05554400 4.08384600 -1.34229800 H -0.91632700 2.65136900 -1.96497100 H 0.84227600 2.85548300 -2.27567300 C -0.67594200 2.68738900 1.47226300 H -0.40569700 2.21575600 2.42525200 H -1.72334100 2.44910500 1.24789400 H -0.56502100 3.78077700 1.56924300 B -1.32149700 -0.43919200 0.01528100 Br -1.80743200 -0.46075100 1.98127500 Br -1.36882800 -2.33209600 -0.71005600 Br -2.64673400 0.70685000 -1.01285700 C 3.51220900 -0.73346100 1.50018100 C 4.36425100 -0.69708200 -1.17868000 C 5.25602400 -0.94511800 -0.15901000 H 6.30546000 -1.13193100 -0.39198800 H 4.69752100 -0.68591700 -2.21773800 C 4.83087100 -0.96533200 1.19192000 H 3.16662700 -0.74935200 2.53562500 H 5.55362400 -1.16831100 1.98262400 E(RM062X): -8540.437754 Hartree Dipole Moment: 11.187246 Debye	C 0.72937000 0.04423400 -1.60392600 C 2.03774400 -0.19331200 -1.91496600 C 0.24987400 0.02976900 -0.23335400 C 2.56428600 -0.51664600 0.46695600 H 0.00374700 0.24882600 -2.39442900 H 0.87686700 -0.32752700 1.80185400 H 2.37037800 -0.17514900 -2.95426600 Si 0.54115100 2.21113200 0.09376600 C 2.33156100 2.57388200 0.47787800 H 2.64015500 2.21035300 1.46675800 H 2.41569500 3.67312200 0.46717000 H 3.01822600 2.17833400 -0.28339000 C 0.09781200 3.02925800 -1.52371600 H 0.05639600 4.11009600 -1.30911500 H -0.87410500 2.71505100 -1.91932000 H 0.88137100 2.85363900 -2.27308100 C -0.57480700 2.69105200 1.50013400 H -0.30026400 2.19658400 2.44044200 H -1.63004300 2.48770500 1.27985600 H -0.43628900 3.77900700 1.61707800 B -1.31570400 -0.40965900 0.01200400 Br -1.83592700 -0.44735500 1.97475300 Br -1.43607600 -2.32120300 -0.71656900 Br -2.64249500 0.74555700 -1.01166600 C 3.50257400 -0.79467800 1.49776900 C 4.35482600 -0.74176900 -1.18584400 C 5.24340200 -1.00878600 -0.16759700 H 6.29124600 -1.20231900 -0.40149500 H 4.68784000 -0.72064600 -2.22450200 C 4.81816900 -1.03673300 1.18417300 H 3.15944500 -0.81233200 2.53372300 H 5.54053900 -1.25153000 1.97193900 E(RM062X): -8540.454856 Hartree Dipole Moment: 14.708278 Debye
[IM-2]$_{2\text{-naphthalene}}$ Coordinates (x,y,z): C 0.89134100 -1.32313400 0.22181300 C 2.94307400 -0.42068400 -0.80391400 C 0.76375700 0.64571600 -1.15315900 C 2.14134700 0.55773600 -1.42377300	**[IM-2]$_{2\text{-naphthalene}}$** Coordinates (x,y,z): C 0.60813700 -1.48681500 0.25413100 C 2.71537800 -0.71094600 -0.74932800 C 0.58877000 0.49590700 -1.06384000 C 1.98113900 0.43355400 -1.24382500

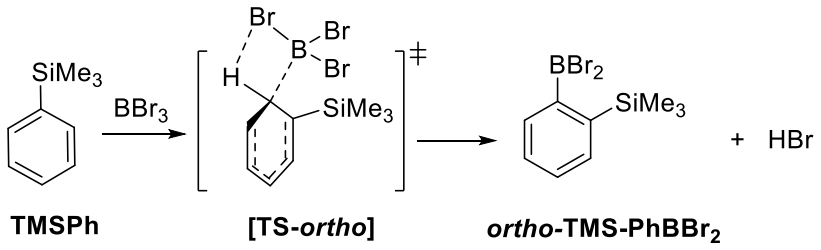
C 0.09519300 -0.34966100 -0.35051900	C -0.12556000 -0.44123600 -0.27857500
C 2.29730400 -1.37683400 0.03956900	C 2.00704300 -1.65995200 0.03544300
H 0.13911200 1.30464800 -1.76842400	H 0.03647000 1.31393300 -1.53521500
H 0.41611300 -2.09821200 0.82883300	H 0.09786300 -2.23562800 0.86544600
H 2.60247900 1.25135300 -2.12994400	H 2.43396800 1.04613100 -2.03279200
B -1.50674800 -0.36792500 -0.10699300	B -1.70265600 -0.21615600 -0.05429100
Br -1.81700900 0.12203500 1.86579600	Br -1.93638700 1.51999700 1.03009900
Br -2.20452900 -2.22819400 -0.45656900	Br -2.58466500 -1.74307400 0.94404100
Br -2.46469100 0.96492400 -1.30551300	Br -2.61106100 0.02724400 -1.86886100
C 3.09787800 -2.36907400 0.67211300	C 2.70404300 -2.77403400 0.57156400
C 4.45561300 -2.39911700 0.47384000	C 4.04667200 -2.93907300 0.31925900
C 5.09285000 -1.44844500 -0.37007400	C 4.74081800 -2.00276800 -0.48195700
C 4.35284600 -0.48128300 -0.99866900	C 4.09038200 -0.90587600 -1.00700400
H 6.17243500 -1.49643100 -0.51592700	H 5.80106000 -2.15362500 -0.68876700
H 4.82870800 0.25192200 -1.65333200	H 4.62672500 -0.18713600 -1.62900000
H 2.61036700 -3.10214500 1.31659400	H 2.15579000 -3.49531500 1.17982400
H 5.05857500 -3.16366000 0.96592900	H 4.57996700 -3.79669500 0.73029800
Si 1.29576200 2.21049600 0.31185500	Si 2.30230200 1.93150200 0.30485500
C 2.64546800 3.30076100 -0.40040900	C 4.13140800 2.22713600 0.09839400
H 3.62662900 2.80632000 -0.40836400	H 4.73103300 1.37172900 0.43585700
H 2.40501100 3.64538500 -1.41679500	H 4.39998900 2.48182300 -0.93617600
H 2.71749300 4.19462600 0.24006400	H 4.37648200 3.09332000 0.73431500
C 1.81959100 1.37809200 1.88605500	C 1.86633500 1.19106100 1.94925600
H 2.03701500 2.18904600 2.60108300	H 2.18402200 1.92693400 2.70628800
H 1.00596300 0.76323900 2.29549500	H 0.78560400 1.02981600 2.06050800
H 2.73060100 0.77538700 1.76993200	H 2.41033100 0.25552800 2.13938800
C -0.28884400 3.17501000 0.39554900	C 1.30295000 3.41456800 -0.20637200
H -0.07560600 4.03980200 1.04689400	H 1.65162000 4.27322800 0.38857300
H -0.59572800 3.54698000 -0.59149700	H 1.45743500 3.65445100 -1.26847000
H -1.11259200 2.59318500 0.82792300	H 0.23156100 3.26627600 -0.01421600
E(RM062X): -8540.435980 Hartree	E(RM062X): -8540.459939 Hartree
Dipole Moment: 12.852290 Debye	Dipole Moment: 18.175247 Debye
[TS-1]$_{2\text{-naphthalene}}$	**[TS-1]$_{2\text{-naphthalene}}$**
Coordinates (x,y,z):	Coordinates (x,y,z):
C 1.01471600 0.90413100 0.69736500	C 0.94196900 1.03944600 0.69853600
C 2.80843100 0.52759500 -0.91249300	C 2.74361300 0.66537800 -0.90813800
C 0.52123500 0.80660900 -1.67253000	C 0.45435800 0.93674500 -1.67211800
C 1.83837300 0.60912600 -1.95890500	C 1.77371600 0.73876900 -1.95611700
C 0.03599100 0.93162600 -0.31114400	C -0.02713500 1.06745400 -0.31312800
C 2.38350200 0.68484600 0.43982800	C 2.31513900 0.82460400 0.44262400

H -0.20760500 0.83443000 -2.48574100 H 0.70268100 1.00411400 1.74165300 H 2.17223100 0.49445500 -2.99163200 Si -1.33587800 2.29756600 -0.02710300 C -0.76353100 3.68614400 -1.16618000 H -0.84621100 3.40239300 -2.22570400 H 0.28488300 3.95297300 -0.96468500 H -1.38376800 4.58190900 -1.00756400 C -3.10549400 1.86449200 -0.45208500 H -3.70769500 2.76227300 -0.23606700 H -3.49106500 1.02883400 0.14612400 H -3.22664100 1.61489600 -1.51441100 C -1.20838200 2.91122200 1.74515900 H -0.21257200 3.33147500 1.95133700 H -1.42389100 2.12448900 2.48059800 H -1.94646200 3.71644800 1.88437000 B -0.78954600 -0.88071700 0.05133400 Br -1.68326200 -0.72684100 1.82177100 Br 0.66573600 -2.22039500 0.03322900 Br -2.06002500 -1.16717100 -1.44290000 C 3.33270800 0.59160700 1.49427400 C 4.65644000 0.35873000 1.21486200 C 5.07853000 0.20702400 -0.12935600 C 4.17967400 0.28769300 -1.16935600 H 6.13275600 0.01974600 -0.33988800 H 4.51167700 0.16284300 -2.20131200 H 2.98697200 0.70156300 2.52380100 H 5.38585900 0.28398200 2.02179100 E(RM062X): -8540.431391 Hartree Dipole Moment: 6.441428 Debye Imaginary Frequency: 170.21i cm^{-1}	H -0.26897000 0.97705600 -2.49032400 H 0.63513400 1.15754600 1.74240400 H 2.10975400 0.62723400 -2.98863700 Si -1.51792100 2.27359100 -0.01171600 C -1.09176300 3.74350400 -1.10889400 H -1.12017000 3.47116600 -2.17438900 H -0.08602600 4.12491900 -0.87704100 H -1.81683800 4.55559400 -0.94534300 C -3.22884900 1.66454400 -0.47618000 H -3.92385800 2.49452400 -0.26948900 H -3.54369600 0.79013100 0.10868500 H -3.29905400 1.41557200 -1.54379900 C -1.48215700 2.83651300 1.78084300 H -0.53583000 3.34628400 2.01569900 H -1.62453300 2.01013700 2.49067400 H -2.29987500 3.55841400 1.93084500 B -0.71892800 -0.97323400 0.05939300 Br -1.61727600 -0.85951800 1.81139700 Br 0.85376000 -2.14815800 0.02565900 Br -1.93504000 -1.29586300 -1.45561800 C 3.26420600 0.74159900 1.49780000 C 4.58995200 0.51214300 1.21902500 C 5.01547600 0.35626000 -0.12384900 C 4.11640600 0.43056000 -1.16500700 H 6.07078800 0.17351900 -0.33210700 H 4.44948200 0.30622600 -2.19672900 H 2.91985300 0.85968500 2.52691000 H 5.31923800 0.44666200 2.02698000 E(RM062X): -8540.439330 Hartree Dipole Moment: 6.590742 Debye Imaginary Frequency: 245.10i cm^{-1}
[TS-2]$_{2\text{-naphthalene}}$ Coordinates (x,y,z): C 0.60386000 1.07097000 -1.39372100 C 2.88025000 0.44841400 -1.86497000 C 1.64176500 -0.64900600 -0.01651000 C 2.83897300 -0.48011400 -0.77874200 C 0.44139500 0.10977800 -0.37651000 C 1.80551500 1.23664900 -2.14561100 H 3.80247300 0.52654800 -2.44760000	**[TS-2]$_{2\text{-naphthalene}}$** Coordinates (x,y,z): C 0.60386000 1.07097000 -1.39372100 C 2.88025000 0.44841300 -1.86497000 C 1.64176500 -0.64900600 -0.01651000 C 2.83897300 -0.48011500 -0.77874200 C 0.44139500 0.10977800 -0.37651000 C 1.80551500 1.23664900 -2.14561100 H 3.80247300 0.52654700 -2.44760000

H 1.83036100 1.96827900 -2.95563300 Si 0.87514500 2.18079500 0.64133200 C 0.00001000 1.80771400 2.24294000 H 0.24025800 2.65549700 2.91301800 H 0.35856900 0.87575000 2.70637600 H -1.09153700 1.74117900 2.12204400 C 2.72442700 2.23142000 0.92859000 H 3.09255300 1.32375300 1.43385400 H 2.89325600 3.09004000 1.60568100 H 3.31428000 2.40172400 0.01559800 C 0.25411600 3.76542600 -0.14046400 H 0.37481400 4.57595800 0.60146800 H -0.81523100 3.68447000 -0.39355700 H 0.82698500 4.03409300 -1.04283800 C 1.67827000 -1.55818600 1.06813700 H 0.78069400 -1.71712100 1.66237400 H 2.82864300 -2.93680200 2.23065000 C 2.83256100 -2.24755900 1.38330800 H 4.91146200 -2.63451800 0.87954000 C 4.00639400 -2.07943300 0.62280400 C 4.00336400 -1.21162700 -0.44594700 H 4.90339700 -1.06470500 -1.04860600 B -1.11914700 -0.38803900 -0.10503500 Br -1.62781000 -1.15140000 1.70382700 Br -2.43691200 1.15437500 -0.44651400 Br -1.33195100 -1.81379000 -1.52855400 H -0.28910300 1.59675700 -1.74220900 E(RM062X): -8540.433270 Hartree Dipole Moment: 10.445851 Debye Imaginary Frequency: 23.27i cm^{-1}	H 1.83036100 1.96827900 -2.95563300 Si 0.87514500 2.18079500 0.64133200 C 0.00001000 1.80771400 2.24294000 H 0.24025900 2.65549700 2.91301800 H 0.35856900 0.87575000 2.70637600 H -1.09153700 1.74117900 2.12204400 C 2.72442700 2.23141900 0.92859000 H 3.09255300 1.32375200 1.43385400 H 2.89325700 3.09003900 1.60568100 H 3.31428000 2.40172300 0.01559800 C 0.25411700 3.76542600 -0.14046400 H 0.37481500 4.57595800 0.60146800 H -0.81523000 3.68447000 -0.39355700 H 0.82698600 4.03409300 -1.04283800 C 1.67827000 -1.55818600 1.06813700 H 0.78069400 -1.71712100 1.66237400 H 2.82864200 -2.93680300 2.23065000 C 2.83256000 -2.24756000 1.38330800 H 4.91146100 -2.63451900 0.87954000 C 4.00639300 -2.07943400 0.62280400 C 4.00336400 -1.21162800 -0.44594700 H 4.90339700 -1.06470600 -1.04860600 B -1.11914700 -0.38803900 -0.10503500 Br -1.62781000 -1.15140000 1.70382700 Br -2.43691200 1.15437600 -0.44651400 Br -1.33195100 -1.81379000 -1.52855400 H -0.28910300 1.59675700 -1.74220900 E(RM062X): -8540.448953 Hartree Dipole Moment: 13.382750 Debye Imaginary Frequency: 9.11i cm^{-1}
[TS-3]$_{2\text{-naphthalene}}$ Coordinates (x,y,z): C 1.24126700 -0.73598200 0.72472400 C 3.07146500 -0.48978700 -0.89134300 C 0.77434400 -0.05285800 -1.54789700 C 2.10655900 -0.11322600 -1.86721800 C 0.29568900 -0.36684400 -0.22576400 C 2.62637400 -0.79848700 0.42806100 H 0.03864500 0.19859400 -2.31594000 H 0.90699900 -1.01523600 1.72740500	**[TS-3]$_{2\text{-naphthalene}}$** Coordinates (x,y,z): C 1.19846600 -0.85904700 0.70386600 C 3.04663100 -0.66431500 -0.90410300 C 0.75508100 -0.20974300 -1.57479900 C 2.08820500 -0.28842400 -1.88859200 C 0.26792400 -0.50285600 -0.25581400 C 2.58944500 -0.94839000 0.41479100 H 0.03472300 0.06265400 -2.35036900 H 0.86857400 -1.09892100 1.71757900

H 2.44357700 0.11223400 -2.88133800 B -1.28393400 -0.60383500 -0.00541100 Br -1.81314600 -0.86193400 1.91826400 Br -1.92576800 -2.11079000 -1.15254100 Br -2.17422700 1.17939300 -0.69984100 C 3.58436100 -1.15999400 1.41561000 C 4.92167300 -1.20466900 1.10794800 C 5.36303000 -0.89456600 -0.20388400 C 4.46068400 -0.54756900 -1.18069100 H 6.42813600 -0.93689100 -0.43627300 H 4.79909800 -0.31202700 -2.19159200 H 3.23429000 -1.40198700 2.42111400 H 5.65085100 -1.48299700 1.86983200 Si 0.32053500 2.32488300 0.20852500 C 0.11740100 3.37231000 -1.32266000 H 0.87723200 4.16933500 -1.30335200 H 0.27269600 2.77238300 -2.22917200 H -0.88846700 3.80860700 -1.36584100 C 2.13141700 2.30559100 0.65976000 H 2.33600600 3.37618800 0.84669100 H 2.34553600 1.75117500 1.58152600 H 2.80802900 1.97190600 -0.13592500 C -0.66123300 2.68320200 1.74398000 H -0.04283700 3.30059100 2.41425400 H -1.59853400 3.19643300 1.49539400 H -0.91731100 1.74634600 2.26129300 E(RM062X): -8540.422695 Hartree Dipole Moment: 9.579682 Debye Imaginary Frequency: 132.49i cm^{-1}	H 2.43227500 -0.06850600 -2.90168300 B -1.31595500 -0.56371800 -0.01024500 Br -1.83668000 -0.70445700 1.95044900 Br -2.10770500 -2.13311200 -1.03405700 Br -2.16196600 1.17969600 -0.76915400 C 3.53903400 -1.29887900 1.41350500 C 4.87952200 -1.35935700 1.11417200 C 5.33295600 -1.07593400 -0.19922400 C 4.43718100 -0.73749000 -1.18638700 H 6.39920800 -1.12921400 -0.42386500 H 4.78184700 -0.51838100 -2.19903800 H 3.18367400 -1.51762200 2.42265700 H 5.60130100 -1.62835000 1.88664700 Si 0.59348000 2.62823800 0.21390900 C 0.33835300 3.40691800 -1.43466600 H 1.06574400 4.23151400 -1.51465700 H 0.56170600 2.68244900 -2.23067700 H -0.68293100 3.78485100 -1.55644800 C 2.34646500 2.27689300 0.64009400 H 2.75746400 3.28379600 0.84464500 H 2.45466400 1.66900800 1.54621200 H 2.91981700 1.84098000 -0.18740700 C -0.51980200 2.87710500 1.65402300 H 0.02601500 3.49069900 2.38875700 H -1.45905400 3.36039200 1.36101800 H -0.74848500 1.90458500 2.11860000 E(RM062X): -8540.439599 Hartree Dipole Moment: 16.078557 Debye Imaginary Frequency: 79.32i cm^{-1}

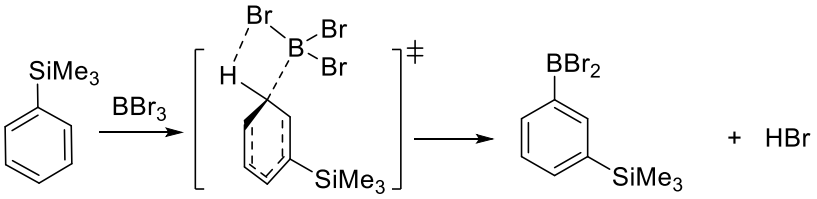
1.8 Stationary points for the electrophilic aromatic substitution reactions of TMSPh and BBr_3



Gas Phase	In Solvent (DCM)

***Ortho*-TMS-PhBBr$_2$**	***Ortho*-TMS-PhBBr$_2$**
Coordinates (x,y,z):	Coordinates (x,y,z):
C -1.42188500 0.80645400 0.00000000	C -1.42316200 0.80733900 0.00000000
C -0.57588300 3.52467500 0.00000000	C -0.57315800 3.52635600 0.00000000
C -0.02480600 1.12690700 0.00000000	C -0.02499600 1.12677000 0.00000000
C -2.32889700 1.87809100 0.00000000	C -2.32891600 1.88047900 0.00000000
C -1.92856900 3.21490700 0.00000000	C -1.92685900 3.21763100 0.00000000
C 0.35075400 2.48832900 0.00000000	C 0.35250100 2.48856700 0.00000000
H -3.39992100 1.67678900 0.00000000	H -3.40047100 1.68184400 0.00000000
H -2.68027300 4.00637900 0.00000000	H -2.67764100 4.00980700 0.00000000
H 1.40839700 2.74850000 0.00000000	H 1.40977900 2.75035100 0.00000000
H -0.23728500 4.56147800 0.00000000	H -0.23353700 4.56273000 0.00000000
Si -2.28505600 -0.91299300 0.00000000	Si -2.29000500 -0.91172000 0.00000000
C -1.92856900 -1.86117300 1.59933400	C -1.92685900 -1.85837300 1.59907000
H -1.77275100 -2.93190200 1.39995700	H -1.76967500 -2.92848700 1.39704200
H -2.79023700 -1.76335800 2.27655200	H -2.78953300 -1.76144600 2.27525800
H -1.03971100 -1.48712400 2.12356200	H -1.03851600 -1.48069900 2.12206600
C -1.92856900 -1.86117300 -1.59933400	C -1.92685900 -1.85837300 -1.59907000
H -1.03971100 -1.48712400 -2.12356200	H -1.03851600 -1.48069900 -2.12206600
H -2.79023700 -1.76335800 -2.27655200	H -2.78953300 -1.76144600 -2.27525800
H -1.77275100 -2.93190200 -1.39995700	H -1.76967500 -2.92848700 -1.39704200
C -4.15361300 -0.62822100 0.00000000	C -4.15628100 -0.62611300 0.00000000
H -4.63551600 -1.61915100 0.00000000	H -4.63648100 -1.61790900 0.00000000
H -4.50381200 -0.09167700 -0.89431600	H -4.50356000 -0.08858100 -0.89480200
H -4.50381200 -0.09167700 0.89431600	H -4.50356000 -0.08858100 0.89480200
B 1.15925600 0.10881000 0.00000000	B 1.15545600 0.10761800 0.00000000
Br 0.98913000 -1.80236100 0.00000000	Br 0.98916600 -1.80466000 0.00000000
Br 2.99922300 0.69605200 0.00000000	Br 3.00029700 0.69414300 0.00000000
E(RM062X): -5812.461181 Hartree Dipole Moment: 2.252459 Debye	E(RM062X): -5812.463860 Hartree Dipole Moment: 2.895259 Debye
[TS-1-*ortho*]	**[TS-1-*ortho*]**
Coordinates (x,y,z):	Coordinates (x,y,z):
C 0.35068900 3.63013000 0.00630200	C 0.34248400 3.62744900 -0.06300500
C 2.27366300 2.17819100 -0.16563600	C 2.27155500 2.17661400 -0.21717500
C 1.72302200 3.46017100 -0.15391700	C 1.71627600 3.45797600 -0.21700400
C -0.45386600 2.50634300 0.09842500	C -0.45932000 2.50314000 0.03106700
H -1.53039200 2.63355000 0.20957800	H -1.53563800 2.63393300 0.13900800
H -0.08970500 4.62655300 0.04879800	H -0.09936700 4.62312600 -0.02725200

H 3.35800900 2.09671000 -0.25181600 Br -1.00520400 -0.83905800 1.96656900 H -0.24989300 0.51179200 1.16674900 C 1.49994700 1.01399700 -0.05653000 C 0.07584900 1.19020300 0.03002100 B -1.03682600 -0.02211300 -0.23315800 Br -2.90129600 0.52952100 -0.48381900 Br -0.48330300 -1.44601300 -1.44779700 H 2.37758800 4.32860100 -0.24929600 Si 2.62673600 -0.56827600 -0.01228100 C 3.11931500 -0.97384700 -1.78203300 H 2.27398000 -1.32190800 -2.38807400 H 3.88961900 -1.76055800 -1.76980700 H 3.55125000 -0.08566700 -2.26719600 C 2.04318100 -2.07222800 0.94708400 H 1.91298400 -1.83193600 2.01192700 H 2.85664900 -2.81198900 0.86613500 H 1.11875800 -2.53067600 0.58043400 C 4.19872600 -0.02284600 0.89168000 H 3.96959800 0.46940800 1.84888800 H 4.83817600 0.64849100 0.30093300 H 4.79316100 -0.92235900 1.11475000 E(RM062X): -8386.911690 Hartree Dipole Moment: 5.117519 Debye Imaginary Frequency: 720.36i cm^{-1}	H 3.35647300 2.10202600 -0.29750200 Br -1.01064300 -0.73839700 2.03555700 H -0.23710700 0.56024300 1.14910200 C 1.50273900 1.01076400 -0.10314200 C 0.07381700 1.18380500 -0.02369200 B -1.02373500 -0.01220500 -0.28349600 Br -2.89807800 0.50265300 -0.53974600 Br -0.48597500 -1.52089800 -1.39003000 H 2.36936500 4.32681400 -0.31514400 Si 2.63638300 -0.56613400 -0.01867900 C 3.09965300 -1.05637000 -1.77492600 H 2.25249700 -1.44328300 -2.35422900 H 3.87837700 -1.83365500 -1.72983500 H 3.51865400 -0.18797400 -2.30532500 C 2.05036800 -2.01640900 1.02158400 H 1.93664000 -1.71397500 2.07263900 H 2.85852800 -2.76446400 0.97136500 H 1.11810200 -2.48729400 0.69266500 C 4.22365600 0.00590300 0.83388500 H 4.01261600 0.53161700 1.77728700 H 4.84935900 0.65458500 0.20459900 H 4.81778500 -0.88956200 1.07374100 E(RM062X): -8386.917307 Hartree Dipole Moment: 7.044446 Debye Imaginary Frequency: 815.95i cm^{-1}

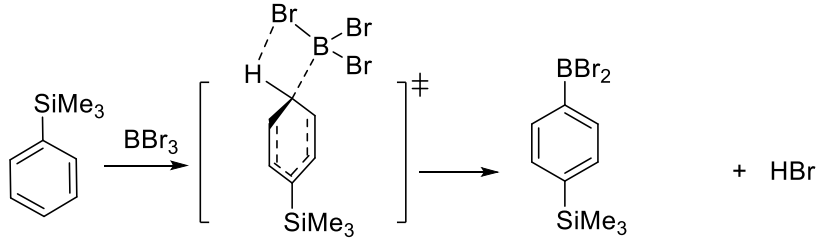


TMSPh **[TS-*meta*]** ***meta*-TMS-PhBBr$_2$**

Gas Phase	In Solvent (DCM)
HBr Coordinates (x,y,z): Br 0.00000000 0.00000000 0.03945900 H 0.00000000 0.00000000 -1.38107500	**HBr** Coordinates (x,y,z): Br 0.00000000 0.00000000 0.03952800 H 0.00000000 0.00000000 -1.38346700

E(RM062X): -2574.480598 Hartree Dipole Moment: 1.128900 Debye	E(RM062X): -2574.482976 Hartree Dipole Moment: 1.350500 Debye
***meta*-TMS-PhBBr$_2$** Coordinates (x,y,z): C -2.02198300 0.69921000 -0.00000200 C 0.40511500 2.13487200 -0.00001000 C -0.78695100 0.03785300 -0.00001200 C -2.00647500 2.10177100 0.00000400 C -0.80624400 2.81565700 0.00000000 C 0.44064800 0.72647500 -0.00001600 H -2.94953900 2.65509100 0.00001100 H -0.81882400 3.90660800 0.00000400 H 1.34077000 2.69650000 -0.00001300 Si -3.63080500 -0.29992100 0.00000200 C -3.66785300 -1.38256800 1.53858300 H -4.57935100 -1.99883900 1.56237500 H -3.64387300 -0.76875900 2.45102000 H -2.80145200 -2.06038600 1.56471000 C -3.66787000 -1.38255700 -1.53858600 H -2.80146800 -2.06037400 -1.56472700 H -3.64389900 -0.76874100 -2.45101800 H -4.57936700 -1.99882700 -1.56237300 C -5.09071500 0.88652700 0.00001500 H -6.03632900 0.32391000 0.00001700 H -5.08483500 1.53126000 -0.89183000 H -5.08482500 1.53125300 0.89186400 B 1.78852800 -0.03794600 -0.00002800 Br 1.86086300 -1.95607700 0.00000100 Br 3.46916100 0.88844100 0.00000600 H -0.76524700 -1.05626700 -0.00001700 E(RM062X): -5812.475386 Hartree Dipole Moment: 2.747739 Debye	***meta*-TMS-PhBBr$_2$** Coordinates (x,y,z): C -2.02357400 0.69829100 0.00000200 C 0.40447500 2.13632200 0.00000800 C -0.78820600 0.03703800 0.00001100 C -2.00793900 2.10163700 -0.00000400 C -0.80747700 2.81673000 -0.00000100 C 0.43985800 0.72702400 0.00001500 H -2.95042900 2.65568100 -0.00001100 H -0.82074200 3.90757900 -0.00000700 H 1.33845500 2.70078100 0.00000900 Si -3.63595500 -0.30117600 -0.00000200 C -3.66635400 -1.38315900 1.53893000 H -4.57684300 -2.00114800 1.55876800 H -3.64730700 -0.76743100 2.45036100 H -2.79724300 -2.05772800 1.56360000 C -3.66633900 -1.38317000 -1.53892500 H -2.79722800 -2.05773900 -1.56358200 H -3.64728500 -0.76745000 -2.45036100 H -4.57682800 -2.00116100 -1.55876800 C -5.09273900 0.88611300 -0.00001300 H -6.03675000 0.32071600 -0.00001600 H -5.08436200 1.53006600 -0.89237500 H -5.08437000 1.53007300 0.89234400 B 1.78577300 -0.03593100 0.00002500 Br 1.86298900 -1.95631700 -0.00000100 Br 3.47053800 0.88889000 -0.00000500 H -0.76824000 -1.05712800 0.00001600 E(RM062X): -5812.478147 Hartree Dipole Moment: 3.420801 Debye
[TS-1-*meta*] Coordinates (x,y,z): C 1.21640400 2.83073000 -0.10819900 C 2.40244000 0.68496200 -0.02390600 C 2.40030500 2.08945200 -0.10175300	**[TS-1-*meta*]** Coordinates (x,y,z): C 1.21026300 2.81568900 -0.23152500 C 2.40085400 0.67197600 -0.08389900 C 2.39566400 2.07568700 -0.18940500

C -0.00577900 2.17631200 -0.05359900 H -0.93686900 2.74569000 -0.05897000 H 1.25077900 3.91944400 -0.16053400 Br -1.99623200 -0.34576500 2.00269500 H -0.66029100 0.44250000 1.14211700 C 1.16338800 0.04755900 0.03425200 H 1.11359800 -1.04206100 0.10658400 C -0.06169800 0.76261500 0.00460700 B -1.50881600 -0.04693400 -0.21495800 Br -2.94963500 1.05525000 -0.95111300 Br -1.32131700 -1.83620500 -0.99098700 H 3.35205100 2.62797300 -0.15349100 Si 4.03179300 -0.29268300 -0.01199400 C 5.02734100 0.23582800 1.49338700 H 5.23876300 1.31553600 1.47365100 H 5.99132100 -0.29399600 1.52657500 H 4.48282200 0.01332300 2.42275500 C 3.62502600 -2.12365900 0.06230800 H 4.55074000 -2.71807900 0.04729000 H 3.01218700 -2.43472600 -0.79722700 H 3.07914700 -2.37873900 0.98308400 C 4.97477300 0.12147300 -1.58523500 H 5.18934200 1.19863600 -1.65234200 H 4.39759600 -0.16607700 -2.47621100 H 5.93601900 -0.41363800 -1.61259300 E(RM062X): -8386.919782 Hartree Dipole Moment: 6.395934 Debye Imaginary Frequency: 512.67i cm^{-1}	C -0.01020100 2.16077300 -0.18433400 H -0.93922400 2.73292600 -0.21136100 H 1.24450300 3.90283700 -0.30459100 Br -1.93081700 -0.17713600 2.05806100 H -0.59531700 0.52006200 1.11671800 C 1.16415100 0.03180500 -0.03451500 H 1.12034600 -1.05625400 0.06100200 C -0.06681000 0.74430500 -0.09004100 B -1.48923000 -0.05315100 -0.26516600 Br -2.97222500 0.98123700 -1.01628200 Br -1.36915400 -1.91316100 -0.86636800 H 3.34571300 2.61721200 -0.23421000 Si 4.03818000 -0.29763600 -0.02130300 C 5.00760600 0.28805800 1.47816500 H 5.21393600 1.36737100 1.42167900 H 5.97224800 -0.23830400 1.53788100 H 4.45035300 0.09201100 2.40600500 C 3.63535600 -2.12592900 0.10941800 H 4.56675900 -2.71113300 0.13481500 H 3.04400600 -2.46955100 -0.75275200 H 3.07222700 -2.34847700 1.02825300 C 4.99094900 0.07157800 -1.59822000 H 5.19411300 1.14839600 -1.69719200 H 4.42516600 -0.25484100 -2.48317500 H 5.95665400 -0.45615400 -1.59222900 E(RM062X): -8386.926687 Hartree Dipole Moment: 8.352316 Imaginary Frequency: 707.48i cm^{-1}



TMSPh **[TS-*para*]** ***para*-TMS-PhBBr$_2$**

Gas Phase	In Solvent (DCM)
***para*-TMS-PhBBr$_2$** Coordinates (x,y,z):	***para*-TMS-PhBBr$_2$** Coordinates (x,y,z):

C 0.32916600 -2.29610000 0.00000000 C -0.05990500 0.52354600 0.00000000 C 1.41950700 -1.41353500 0.00000000 C -0.96112000 -1.73950000 0.00000000 C -1.15474400 -0.36310300 0.00000000 C 1.23182100 -0.03397800 0.00000000 H -1.83841100 -2.39326400 0.00000000 H -2.16995800 0.03776300 0.00000000 Si 0.55418600 -4.17861400 0.00000000 C 2.39078800 -4.58061000 0.00000000 H 2.54061600 -5.67067700 0.00000000 H 2.89057300 -4.17317700 0.89168200 H 2.89057300 -4.17317700 -0.89168200 C -0.27064900 -4.87824600 -1.53987400 H 0.19340600 -4.47355900 -2.45127600 H -1.34125200 -4.62587900 -1.56484700 H -0.18128300 -5.97482900 -1.56637700 C -0.27064900 -4.87824600 1.53987400 H -0.18128300 -5.97482900 1.56637700 H -1.34125200 -4.62587900 1.56484700 H 0.19340600 -4.47355900 2.45127600 B -0.27064900 2.05882600 0.00000000 Br 1.21166400 3.27759400 0.00000000 Br -2.02669900 2.83288000 0.00000000 H 2.43917600 -1.80634300 0.00000000 H 2.10126800 0.62590200 0.00000000 E(RM062X): -5812.475241 Hartree Dipole Moment: 3.079578 Debye	C 0.33060400 -2.29745600 0.00000000 C -0.05997200 0.52274200 0.00000000 C 1.42131600 -1.41407500 0.00000000 C -0.96089100 -1.74159300 0.00000000 C -1.15524500 -0.36485300 0.00000000 C 1.23308200 -0.03429100 0.00000000 H -1.83794700 -2.39535100 0.00000000 H -2.17178400 0.03278400 0.00000000 Si 0.55716800 -4.18356000 0.00000000 C 2.39330000 -4.58049600 0.00000000 H 2.54034900 -5.67098000 0.00000000 H 2.89084000 -4.17176300 0.89234700 H 2.89084000 -4.17176300 -0.89234700 C -0.27092300 -4.87648500 -1.54031100 H 0.19536000 -4.47232600 -2.45097000 H -1.34124000 -4.62217500 -1.56082900 H -0.18101900 -5.97313300 -1.56412100 C -0.27092300 -4.87648500 1.54031100 H -0.18101900 -5.97313300 1.56412100 H -1.34124000 -4.62217500 1.56082900 H 0.19536000 -4.47232600 2.45097000 B -0.27092300 2.05524900 0.00000000 Br 1.21051100 3.27944500 0.00000000 Br -2.02798700 2.83386600 0.00000000 H 2.44133400 -1.80569200 0.00000000 H 2.10398200 0.62373700 0.00000000 E(RM062X): -5812.478115 Hartree Dipole Moment: 3.807316 Debye
[TS-1-*para*] Coordinates (x,y,z): C -2.04545400 -1.18211300 0.03458500 C -2.03237900 1.22969100 0.02787700 C -2.76175900 0.02917700 0.01386200 C -0.65975500 -1.19850200 0.05463200 H -0.12117200 -2.14782800 0.07479300 H -2.58189900 -2.13495300 0.03278000 H -2.55702000 2.18754700 0.02094900 Br 2.36554600 0.00338900 1.98201600 H 0.78900900 0.01288800 1.16489400	**[TS-1-*para*]** Coordinates (x,y,z): C -2.04004900 -1.18231700 -0.03774200 C -2.02715500 1.23282900 -0.04850200 C -2.75596700 0.03063900 -0.04662200 C -0.65538300 -1.19927200 -0.03852500 H -0.12230200 -2.15174500 -0.02100500 H -2.57562600 -2.13522400 -0.03033200 H -2.55152800 2.19051000 -0.04967100 Br 2.22634100 -0.00335100 2.04156300 H 0.69003300 0.01531400 1.14599000

C -0.64417100 1.22677300 0.04757000 H -0.09407500 2.16965800 0.06240000 C 0.08102900 0.01052100 0.04724700 Si -4.66528000 0.00443200 -0.02808300 C -5.26555200 -0.92090200 1.49393000 H -6.36450000 -0.97884200 1.50045500 H -4.94424900 -0.41469800 2.41592800 H -4.87440900 -1.94886300 1.51635600 C -5.29635800 1.77288100 -0.02745900 H -6.39637800 1.77976500 -0.05148800 H -4.93980000 2.32851700 -0.90771200 H -4.97875200 2.31433000 0.87625500 C -5.19401600 -0.89496900 -1.59141100 H -6.29139900 -0.95218200 -1.65088900 H -4.80123100 -1.92232000 -1.61232200 H -4.82908600 -0.37367400 -2.48839700 B 1.73357700 -0.00054700 -0.21577600 Br 2.41427500 -1.66712900 -0.98667100 Br 2.43565000 1.65191100 -0.99782900 E(RM062X): -8386.919334 Hartree Dipole Moment: 7.078320 Debye Imaginary Frequency: 508.33i cm^{-1}	C -0.64009200 1.23133200 -0.04976700 H -0.09587700 2.17768000 -0.04133200 C 0.09011800 0.01243700 -0.04709100 Si -4.66516400 0.00588800 -0.04318600 C -5.21355500 -0.90129800 1.50768300 H -6.31185000 -0.96146900 1.54209900 H -4.86866100 -0.37825200 2.41160700 H -4.81597000 -1.92676000 1.52876900 C -5.28978700 1.77437800 -0.05140100 H -6.39009400 1.77880200 -0.05028500 H -4.95081700 2.31548200 -0.94746200 H -4.94912800 2.32424600 0.83867800 C -5.21962000 -0.91910600 -1.58111600 H -6.31799800 -0.98111500 -1.60925500 H -4.82068000 -1.94418300 -1.59287800 H -4.87989800 -0.40555600 -2.49237600 B 1.71419500 0.00054000 -0.26895300 Br 2.47656900 -1.66130300 -0.96936300 Br 2.50310800 1.65092300 -0.96719000 E(RM062X): -8386.926394 Hartree Dipole Moment: 9.119408 Debye Imaginary Frequency: 704.21i cm^{-1}

2. Results of IRC calculations on for selected transition states

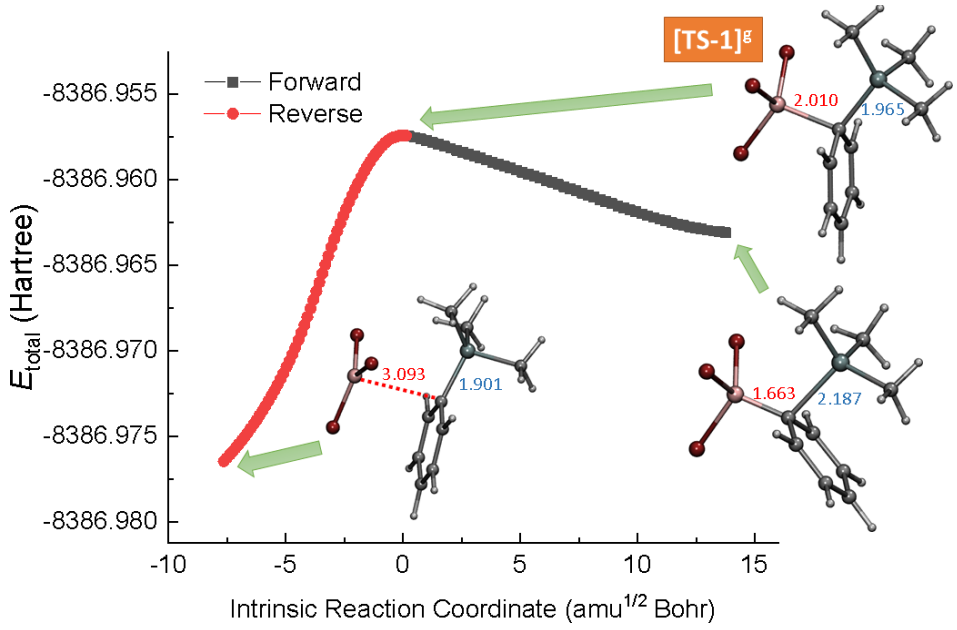


Figure S-1 IRC plot for the transition state **[TS-1]^{g}** involved in the *ipso* attack of BBr_3 on TMSPh occurring in the gas phase. The ending structure of the forward direction was further optimized, yielding a geometry consistent with **[IM-1]^{g}**. Selected bond distances are highlighted in Å.

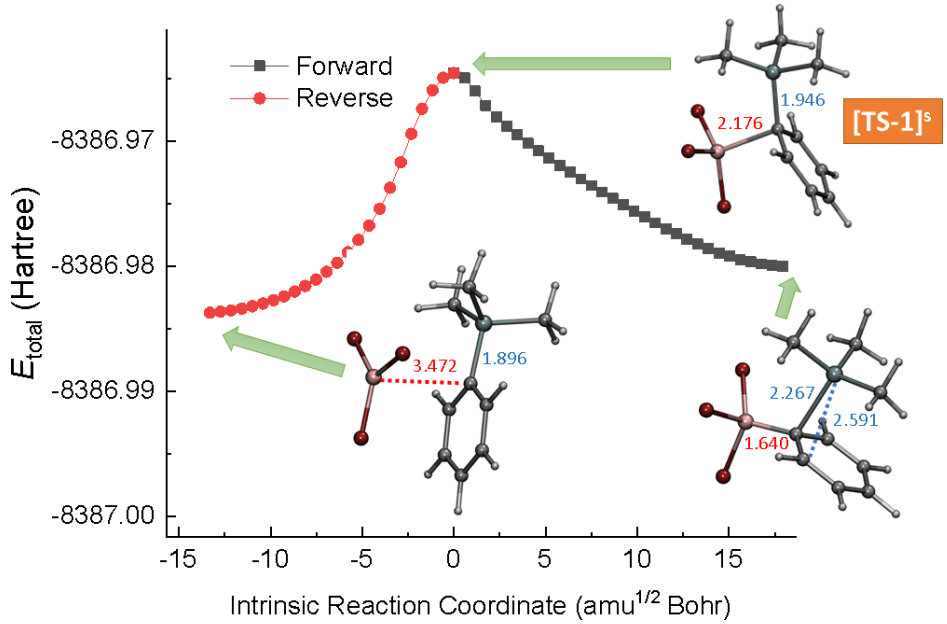


Figure S-2 IRC plot for the transition state **[TS-1]^{s}** involved in the *ipso* attack of BBr_3 on TMSPh occurring in CH_2Cl_2. The ending structure of the forward direction was further optimized, yielding a geometry consistent with **[IM-2]^{s}**. Selected bond distances are highlighted in Å.

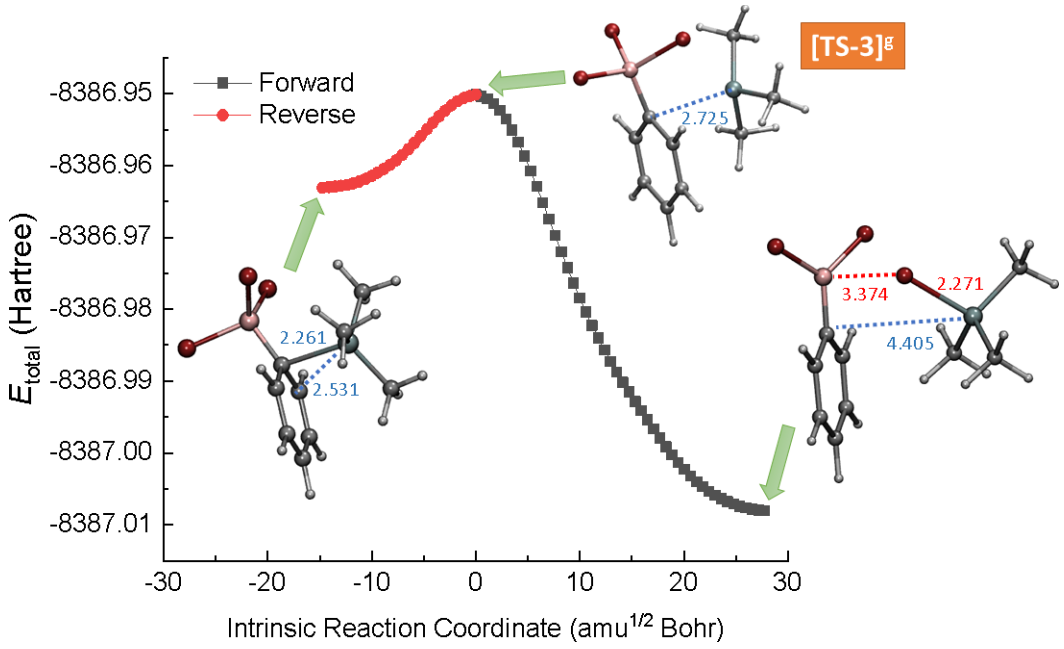


Figure S-3 IRC plot for the transition state **[TS-3]^{g}** involved in the elimination of TMSBr occurring in the gas phase. The ending structure of the reverse direction was further optimized, yielding a geometry consistent with **[IM-1]^{g}**. Selected bond distances are highlighted in Å.

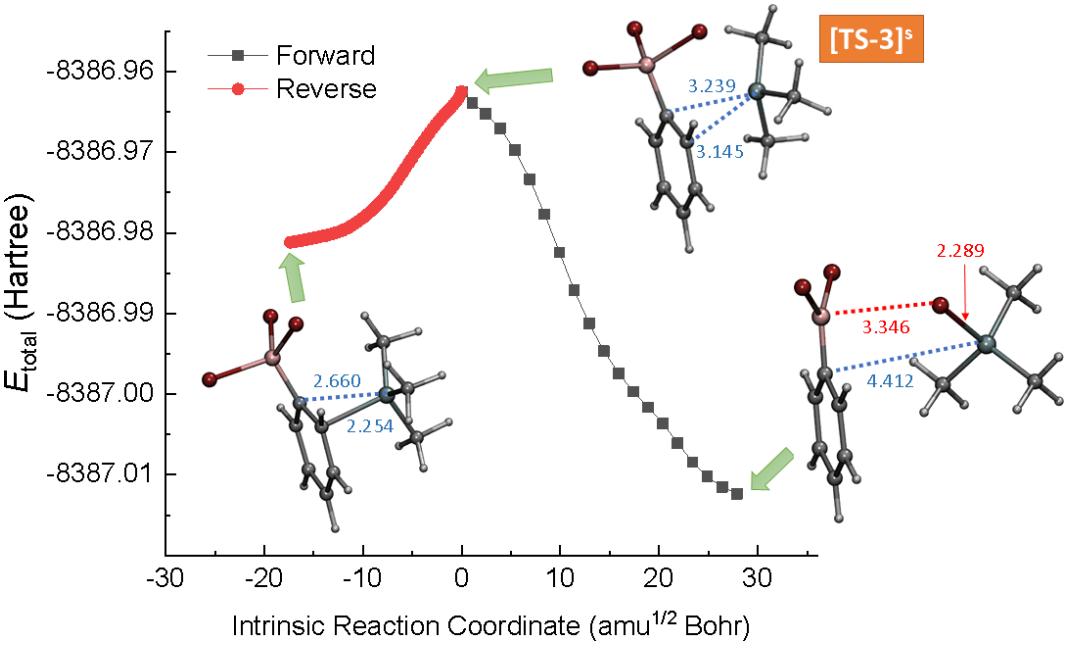


Figure S-4 IRC plot for the transition state **[TS-3]^{s}** involved in the elimination of TMSBr occurring in CH_2Cl_2. The ending structure of the reverse direction was further optimized, yielding a geometry consistent with **[IM-2]^{s}**. Selected bond distances are highlighted in Å.

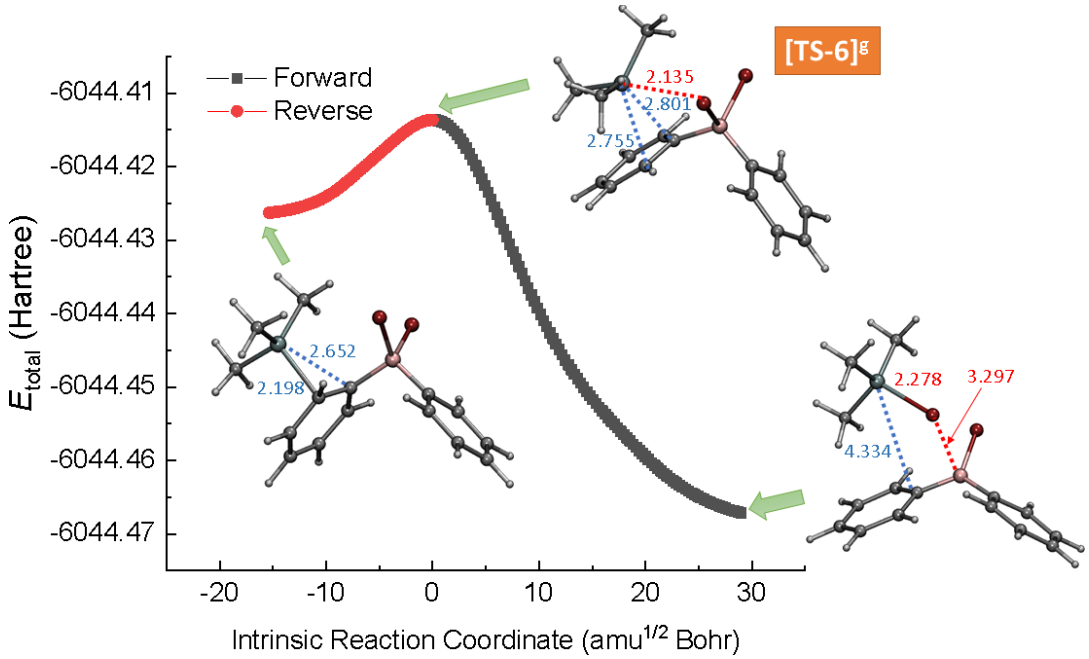


Figure S-5 IRC plot for the transition state **[TS-6]^{g}** involved in the elimination of TMSBr occurring in the gas phase. The ending structure of the reverse direction was further optimized, yielding a geometry consistent with **[IM-4]^{g}**. Selected bond distances are highlighted in Å.

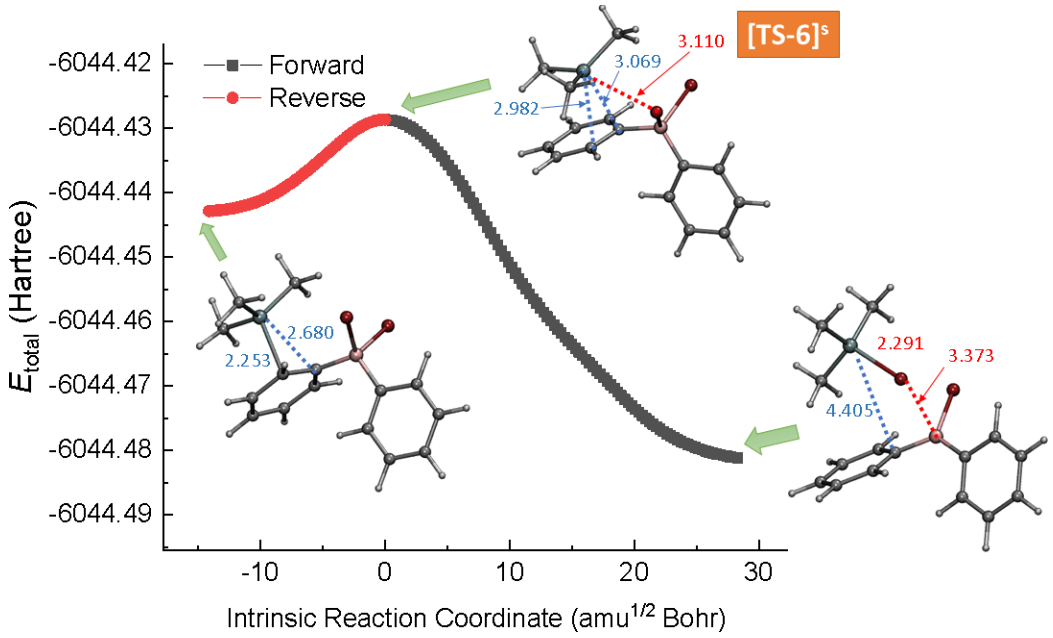


Figure S-6 IRC plot for the transition state **[TS-6]^{s}** involved in the elimination of TMSBr occurring in CH_2Cl_2. The ending structure of the reverse direction was further optimized, yielding a geometry consistent with **[IM-4]^{s}**. Selected bond distances are highlighted in Å.

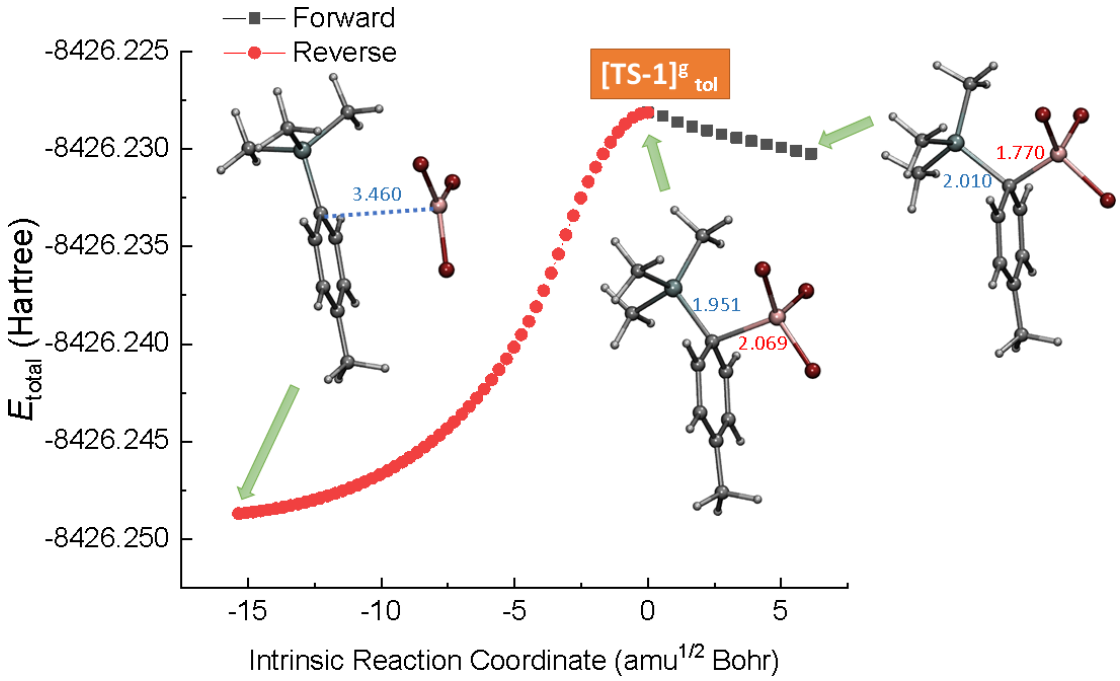


Figure S-7 IRC plot for the transition state **[TS-1]$^{g}_{tol}$** involved in the *ipso* attack of BBr_3 on *p*-trimethylsilyltoluene occurring in the gas phase. Selected bond distances are highlighted in Å.

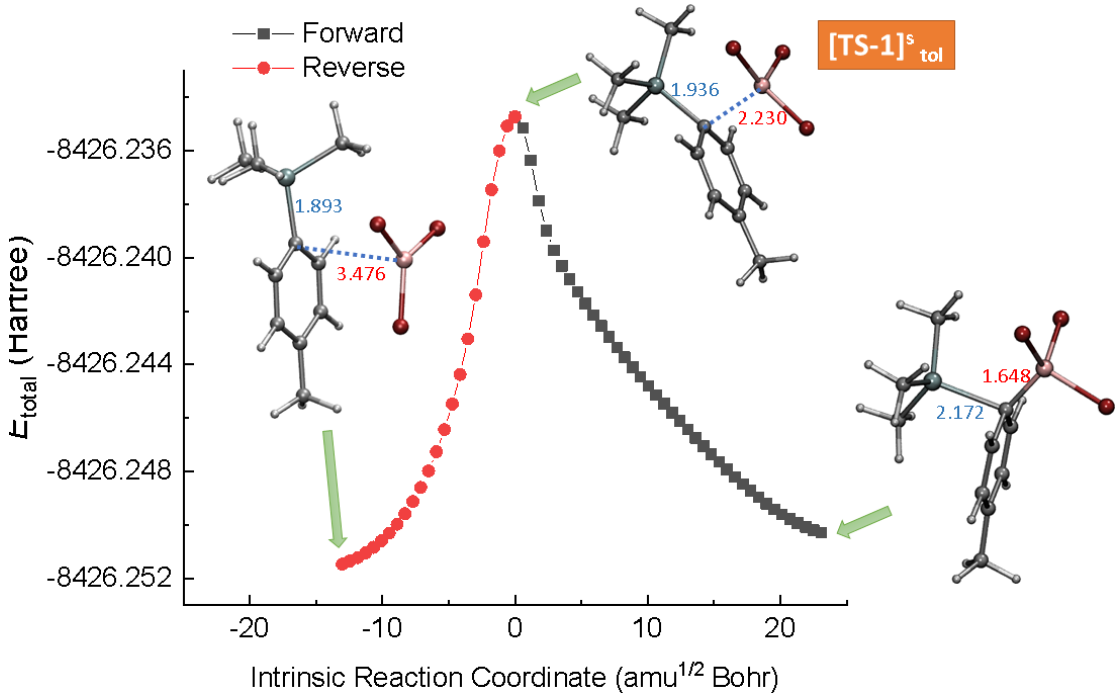


Figure S-8 IRC plot for the transition state **[TS-1]$^{s}_{tol}$** involved in the *ipso* attack of BBr_3 on *p*-trimethylsilyltoluene occurring in CH_2Cl_2. Selected bond distances are highlighted in Å.

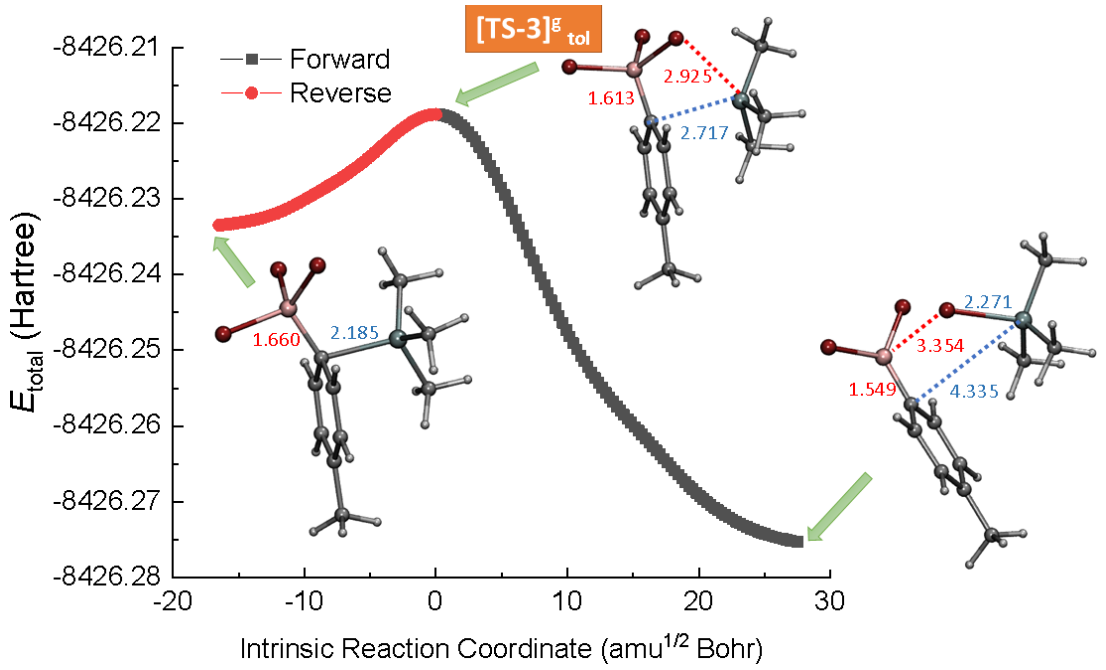


Figure S-9 IRC plot for the transition state **[TS-3]$^{g}_{tol}$** involved in the elimination of TMSBr occurring in the gas phase. Selected bond distances are highlighted in Å.

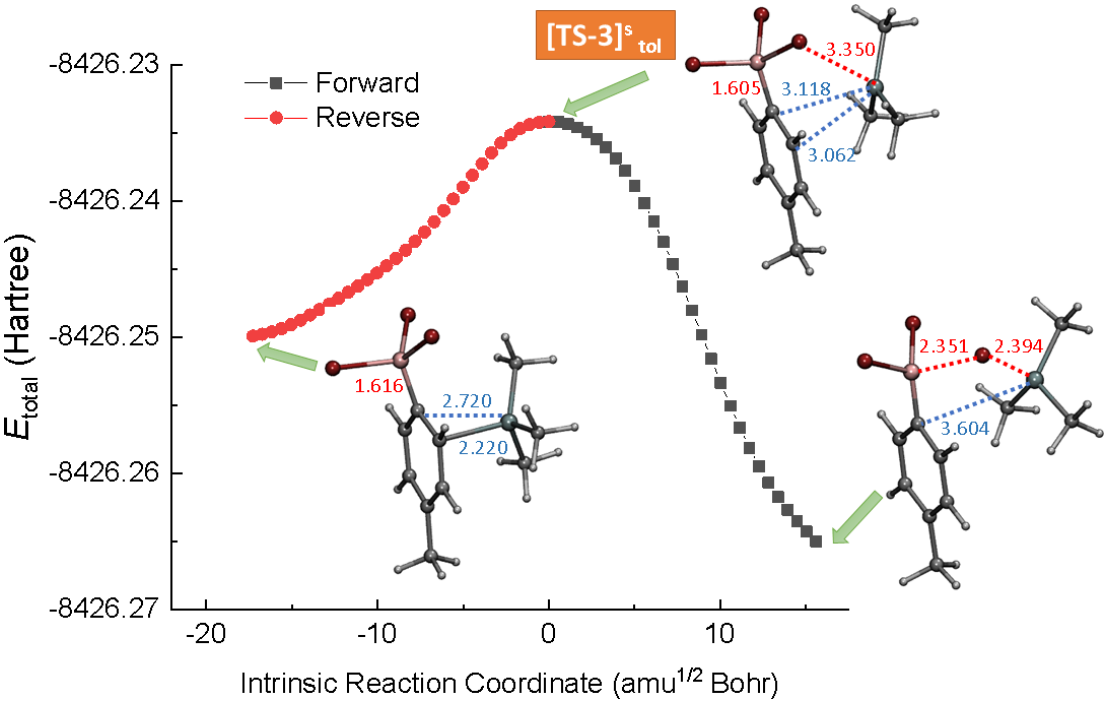


Figure S-10 IRC plot for the transition state **[TS-3]$^{s}_{tol}$** involved in the elimination of TMSBr occurring in CH_2Cl_2. Selected bond distances are highlighted in Å.

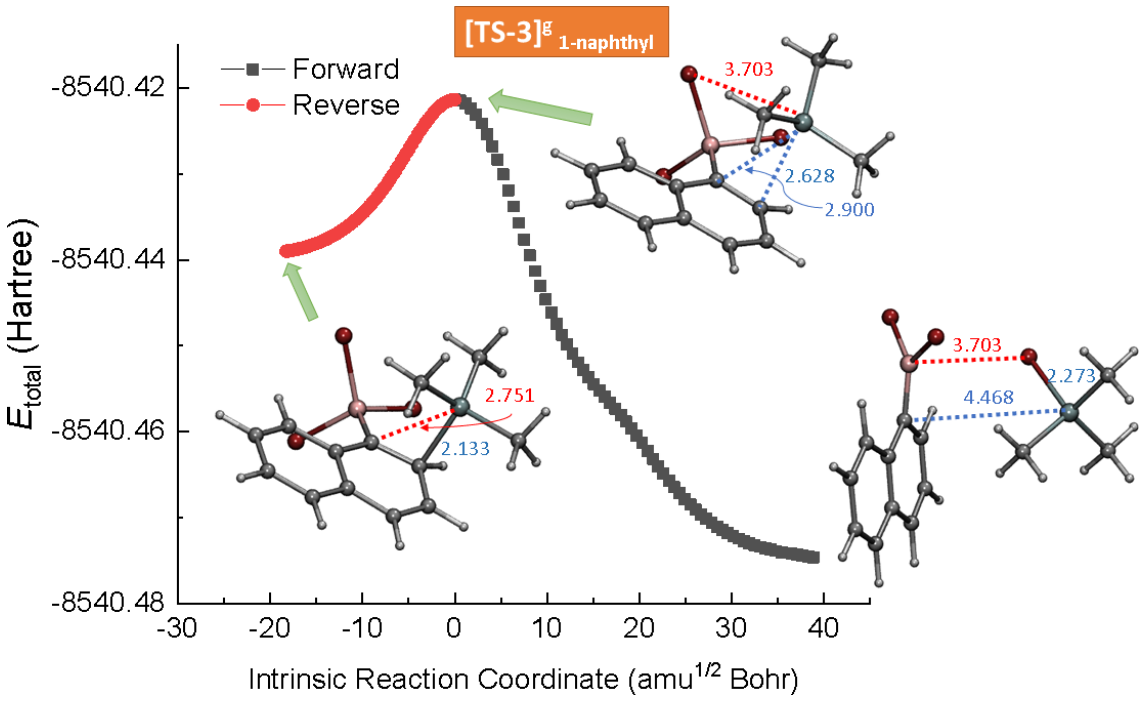


Figure S-11 IRC plot for the transition state **[TS-3]$^{g}_{1\text{-naphthyl}}$** involved in the elimination of TMSBr occurring in the gas phase. Selected bond distances are highlighted in Å.

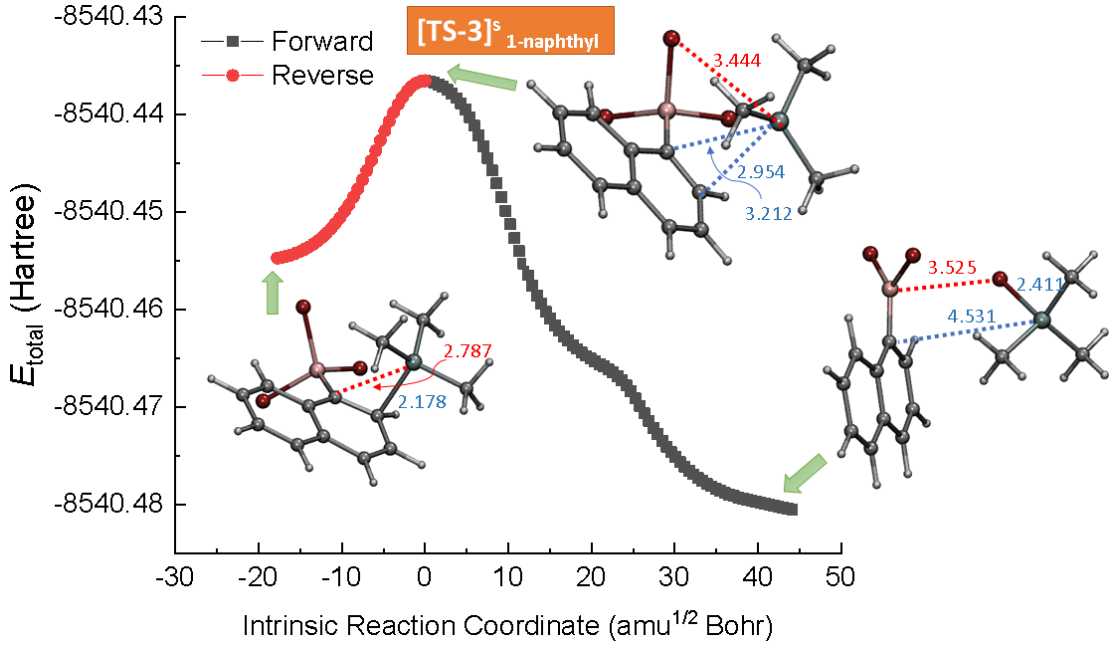


Figure S-12 IRC plot for the transition state **[TS-3]$^{s}_{1\text{-naphthyl}}$** involved in the elimination of TMSBr occurring in CH_2Cl_2. Selected bond distances are highlighted in Å.

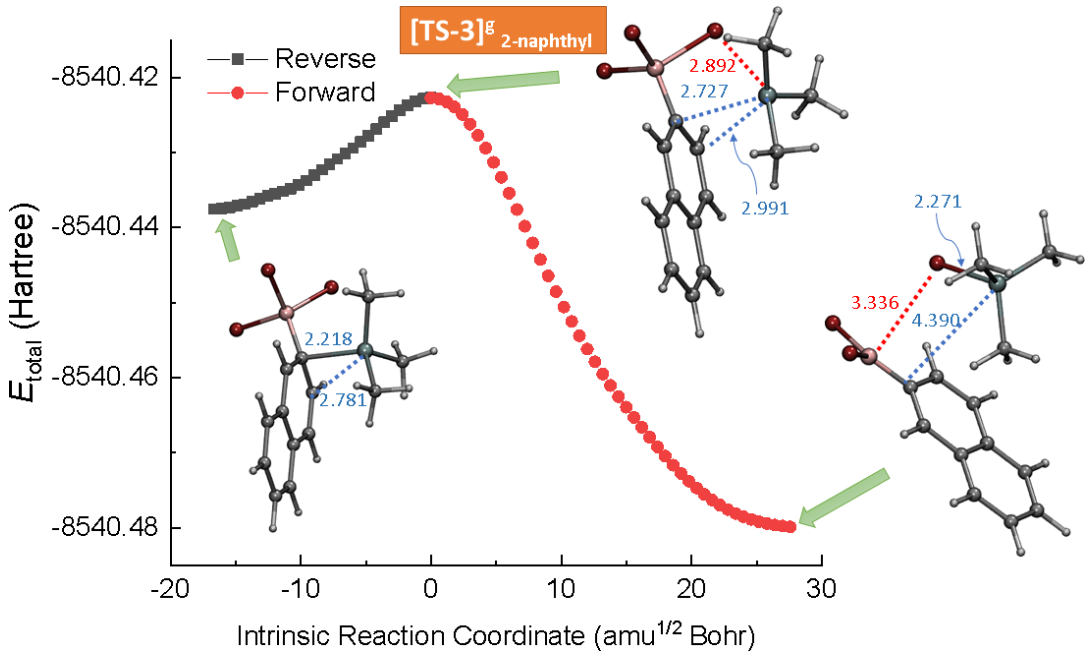


Figure S-13 IRC plot for the transition state **[TS-3]$^{g}_{2\text{-naphthyl}}$** involved in the elimination of TMSBr occurring in the gas phase. Selected bond distances are highlighted in Å.

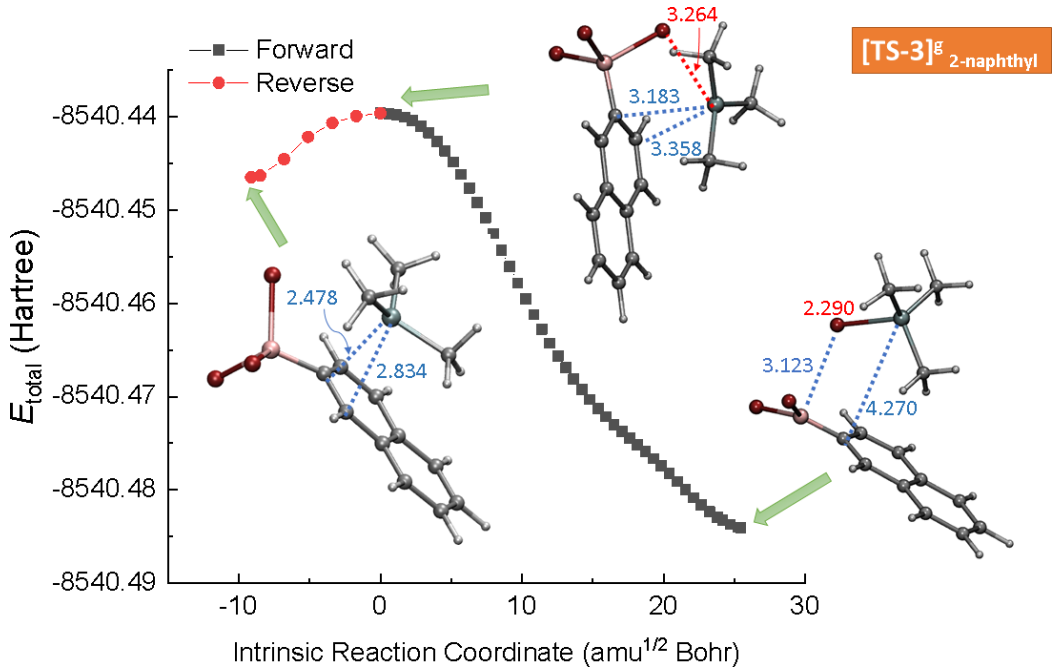


Figure S-14 IRC plot for the transition state **[TS-3]$^{s}_{2\text{-naphthyl}}$** involved in the elimination of TMSBr occurring in CH_2Cl_2. Selected bond distances are highlighted in Å.

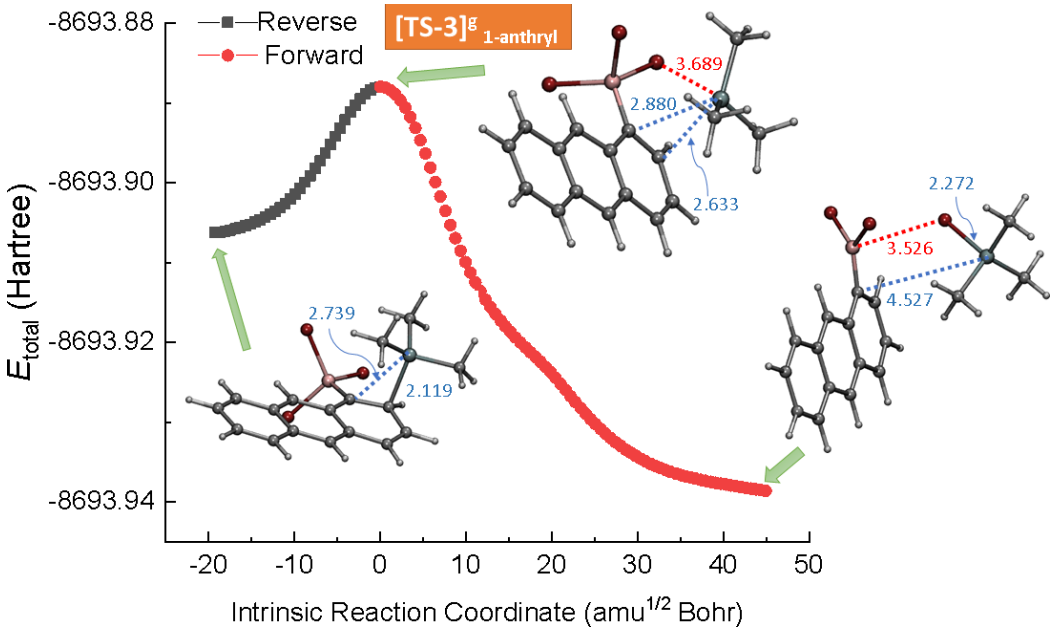


Figure S-15 IRC plot for the transition state **[TS-3]$^{g}_{1\text{-anthryl}}$** involved in the elimination of TMSBr occurring in the gas phase. Selected bond distances are highlighted in Å.

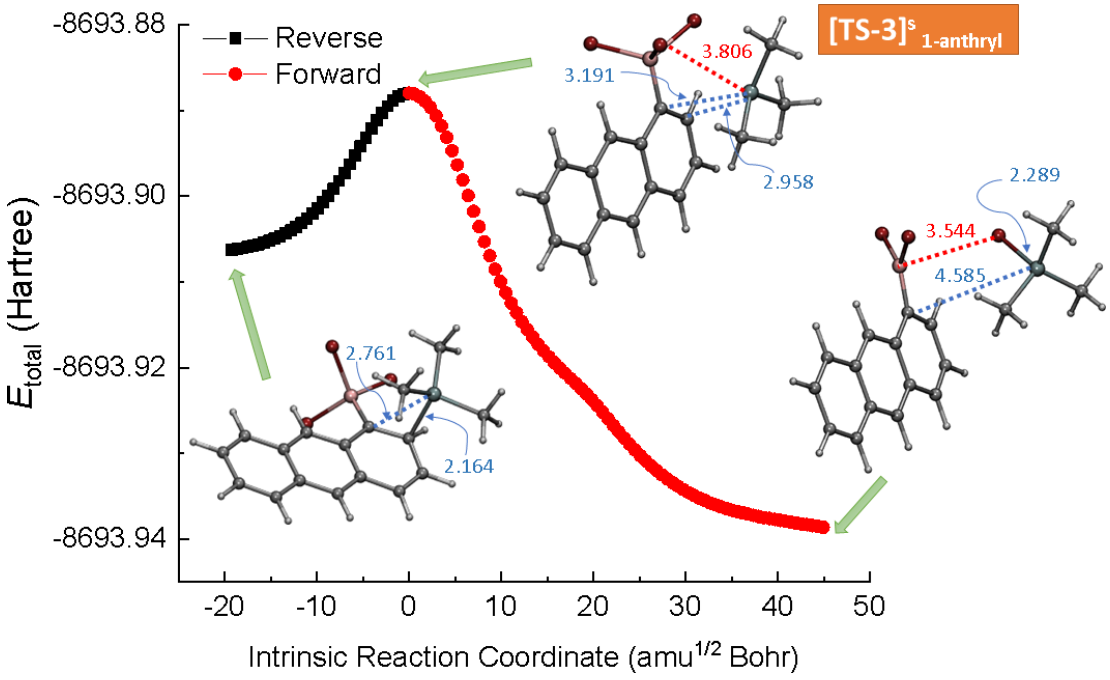


Figure S-16 IRC plot for the transition state **[TS-3]$^{s}_{1\text{-anthryl}}$** involved in the elimination of TMSBr occurring in CH_2Cl_2. Selected bond distances are highlighted in Å.

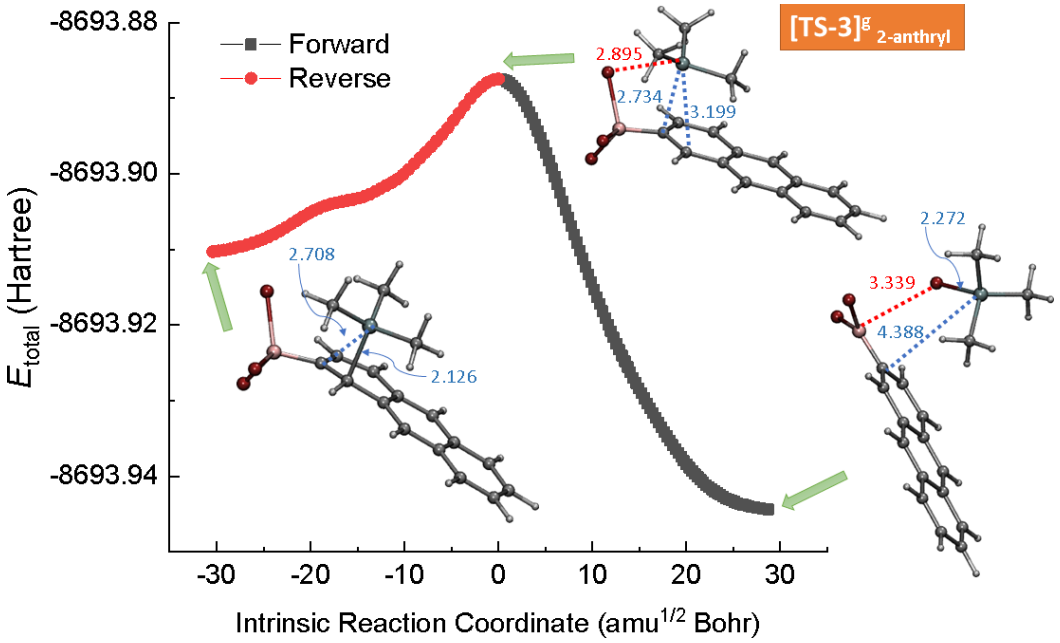


Figure S-17 IRC plot for the transition state **[TS-3]$^{g}_{2\text{-anthryl}}$** involved in the elimination of TMSBr occurring in the gas phase. Selected bond distances are highlighted in Å.

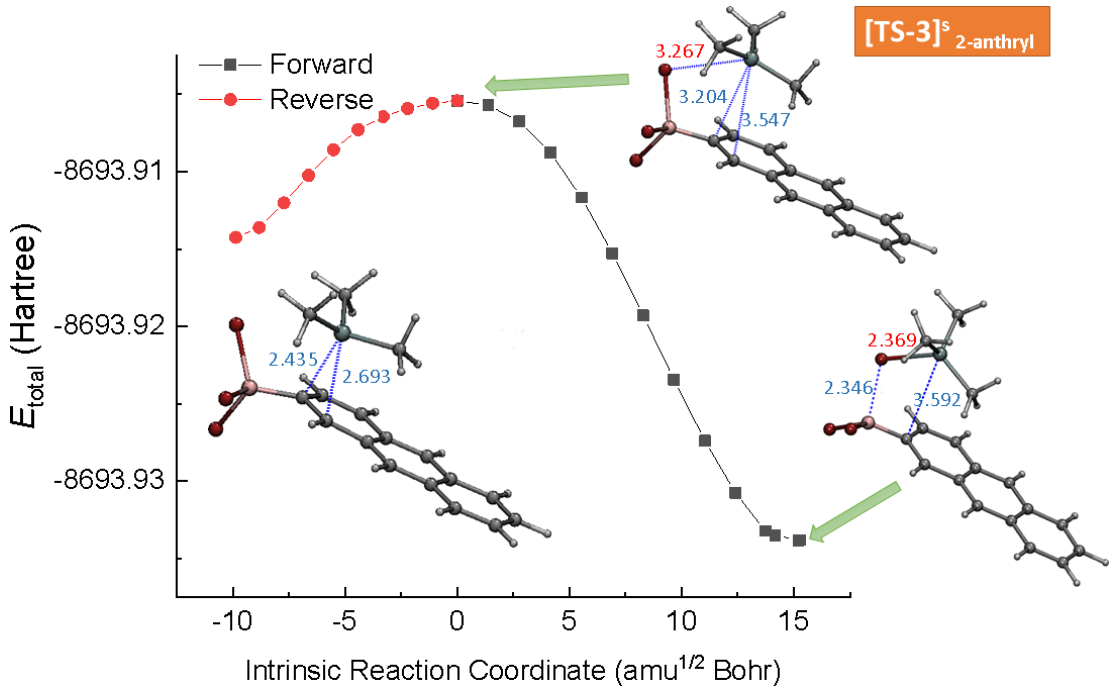


Figure S-18 IRC plot for the transition state **[TS-3]$^{s}_{2\text{-anthryl}}$** involved in the elimination of TMSBr occurring in CH_2Cl_2. Selected bond distances are highlighted in Å.

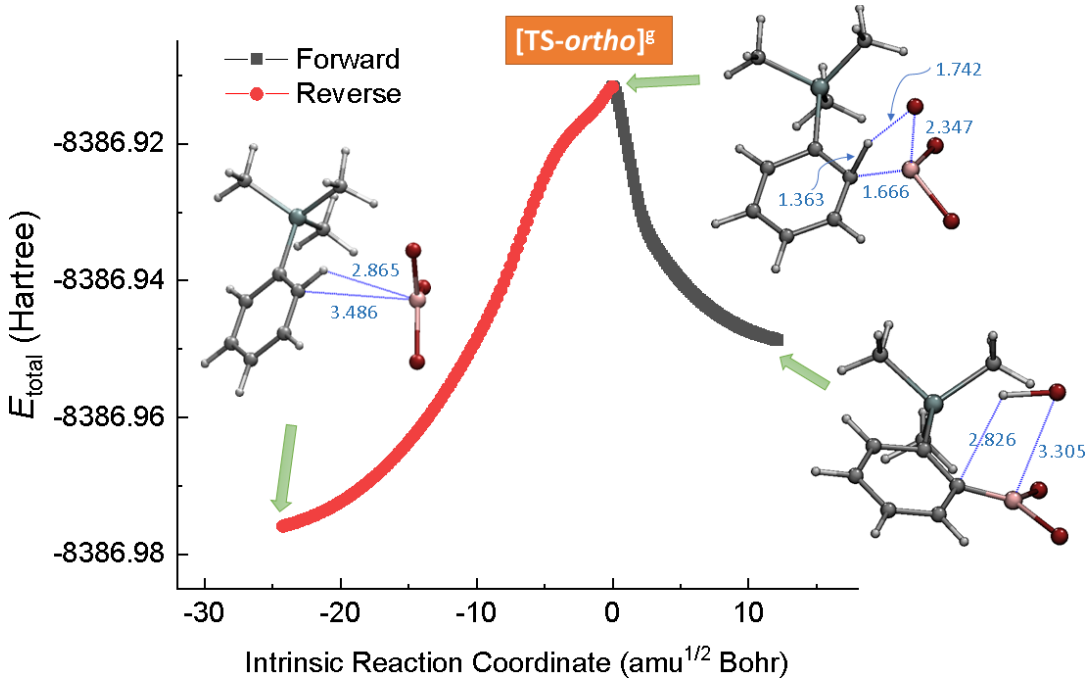


Figure S-17 IRC plot for the transition state **[TS-*ortho*]^{g}** involved in the electrophilic aromatic substitution of TMSPh and BBr_3 in the gas phase. Selected bond distances are highlighted in Å.

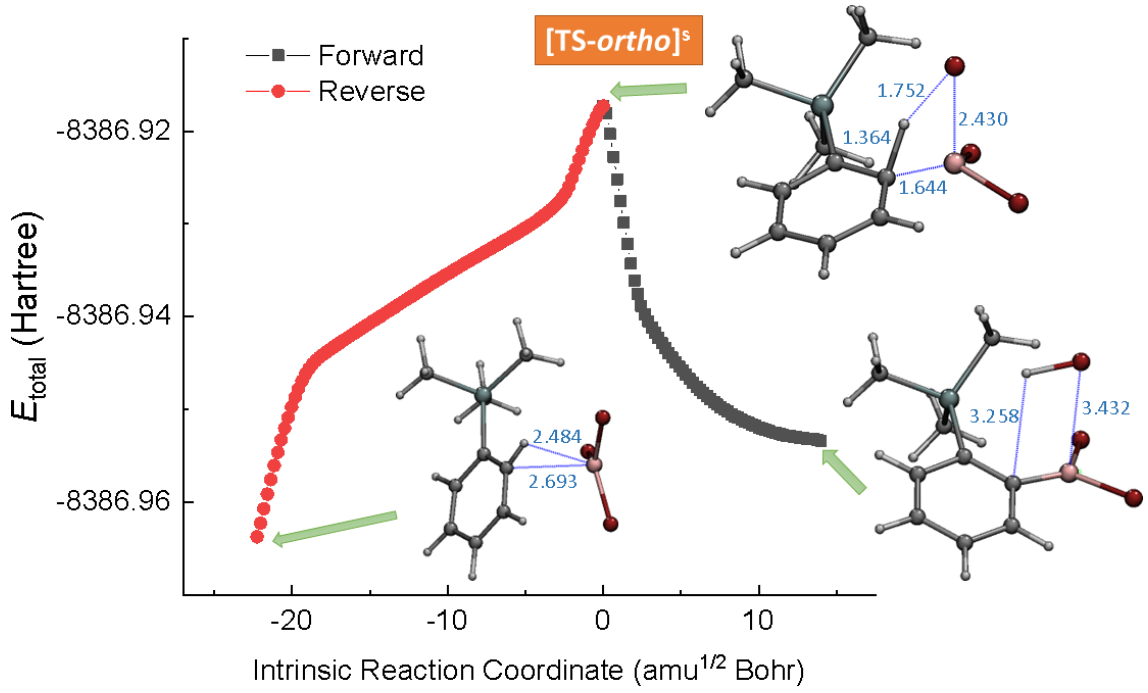


Figure S-18 IRC plot for the transition state **[TS-*ortho*]^{s}** involved in the electrophilic aromatic substitution of TMSPh and BBr_3 in CH_2Cl_2. Selected bond distances are highlighted in Å.

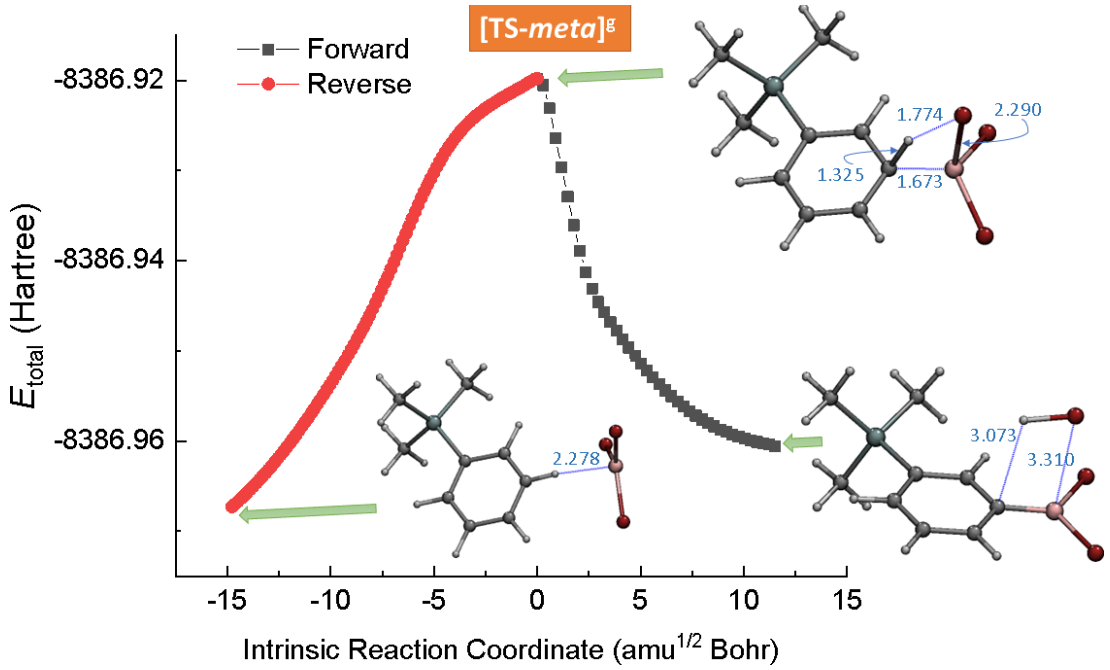


Figure S-19 IRC plot for the transition state **[TS-*meta*]^{g}** involved in the electrophilic aromatic substitution of TMSPh and BBr_3 in the gas phase. Selected bond distances are highlighted in Å.

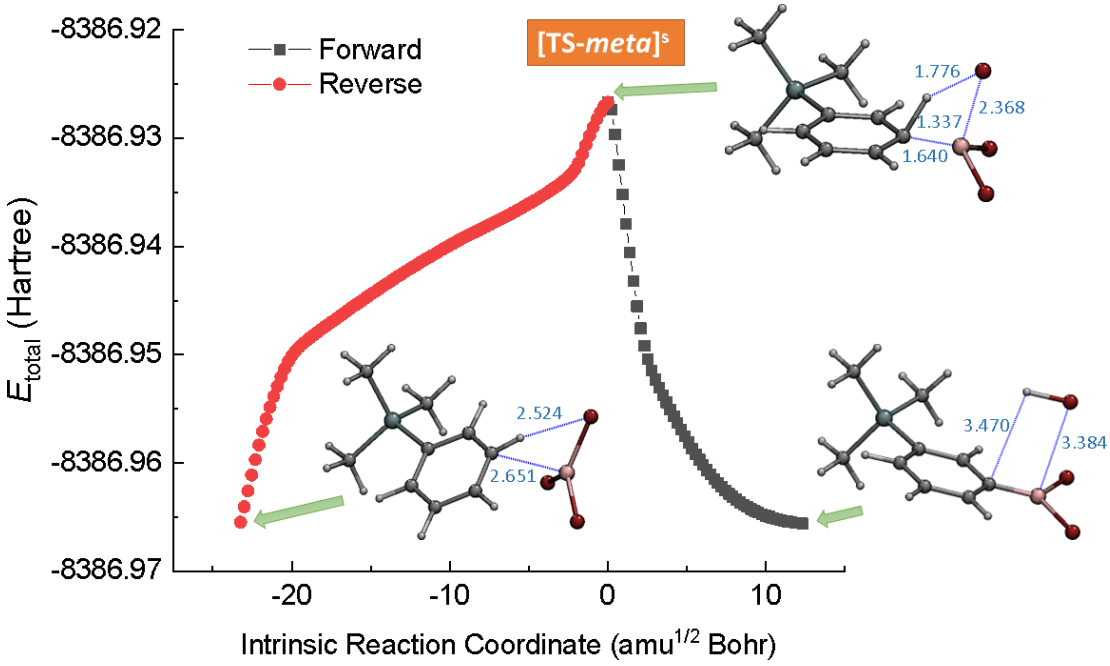


Figure S-20 IRC plot for the transition state **[TS-*meta*]^{s}** involved in the electrophilic aromatic substitution of TMSPh and BBr_3 in CH_2Cl_2. Selected bond distances are highlighted in Å.

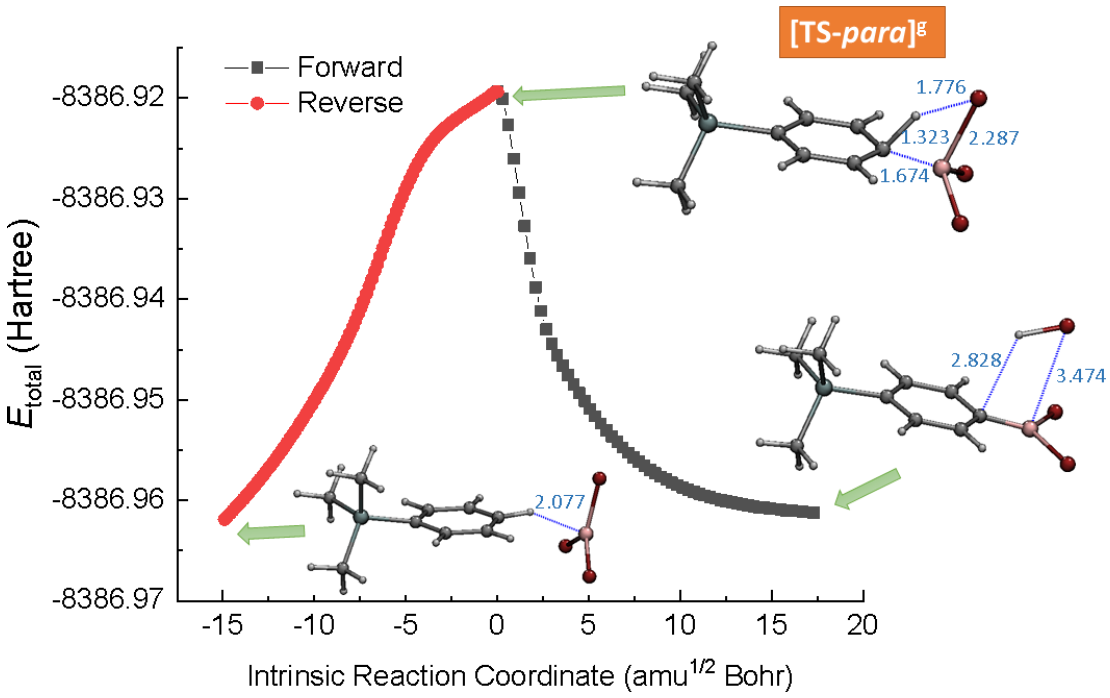


Figure S-21 IRC plot for the transition state **[TS-*para*]^{g}** involved in the electrophilic aromatic substitution of TMSPh and BBr_3 in the gas phase. Selected bond distances are highlighted in Å.

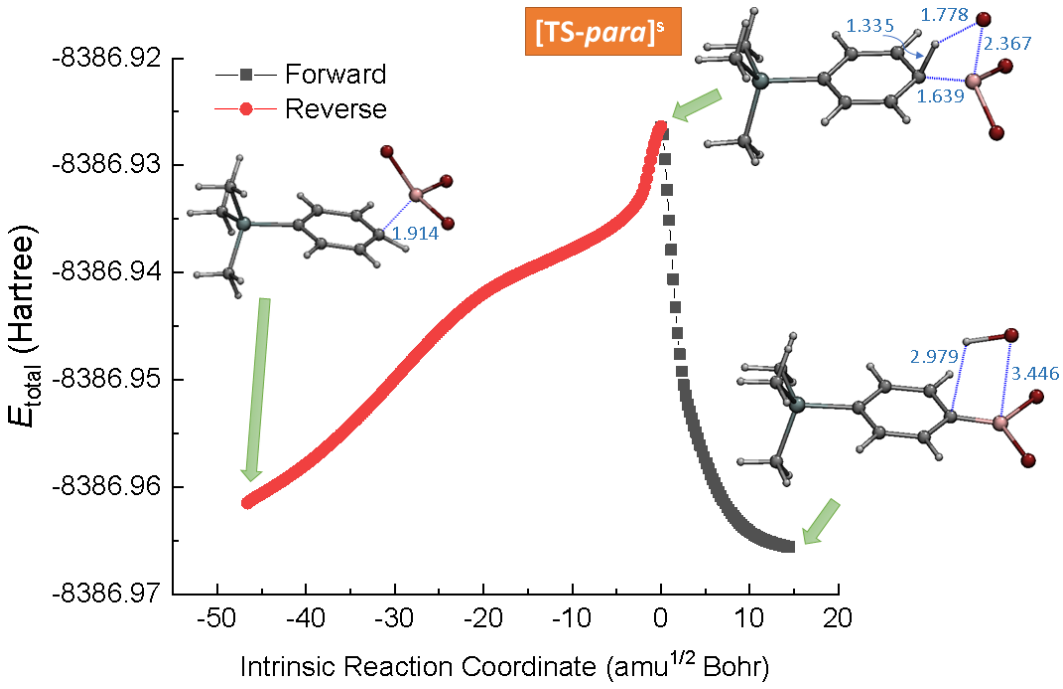


Figure S-22 IRC plot for the transition state **[TS-*para*]^{s}** involved in the electrophilic aromatic substitution of TMSPh and BBr_3 in CH_2Cl_2. Selected bond distances are highlighted in Å.

3. Assessments of Different Computational Methods

The first elementary step of the reaction between TMSPh and BBr_3 in the gas phase was calculated using a range of DFT methods and basis sets, in order to assess their performances in the computational analysis of the boron-silicon exchange reactions. In the following Tables, the Gibbs activation barrier ($\Delta G^{\ddagger}_1$) and Gibbs energy change (ΔG^{0}_1) calculated at various levels of theory are listed. We also used the data obtained at the MP2/def2-SVP level as references for accuracy assessment.

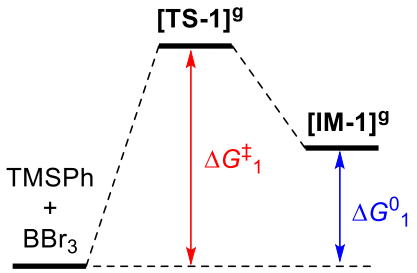


Table S-1 Comparison of the performances of various basis sets with M06-2X functional

Basis Set	$\Delta G^{\ddagger}_1$ (kcal mol^{-1})	ΔG^{0}_1 (kcal mol^{-1})
6-31G(d)	13.351	10.182
6-31+G(d,p)	7.573	3.077
Def2-SVP	**21.084**	**17.835**
Def2-SVPP	21.354	18.457
cc-PVDZ	21.394	17.076
aug-cc-PVDZ	19.458	13.511

Table S-2 Comparison of the performances of various DFT methods with def2-SVP basis set

DFT Method	$\Delta G^{\ddagger}_1$ (kcal mol^{-1})	ΔG^{0}_1 (kcal mol^{-1})
B3LYP-D3	23.618	21.876
M06-2X	**21.084**	**17.835**
PBE1PBE	29.055	26.379
TPSSH	30.861	28.902
ωB97XD	24.052	22.147
MP2/def2-SVP	$\Delta G^{\ddagger}_1$ (kcal mol^{-1})	$\Delta G^{\ddagger}_1$ (kcal mol^{-1})
	20.640	**17.688**

According to the data shown in Table S-1 and Table S-2, the values of $\Delta G^{\ddagger}_1$ and ΔG^{0}_1 calculated at the M06-2X/def2SVP level of theory are the closest to those calculated at the MP2/Def2-SVP level. We therefore chose M06-2X as the functional and def2-SVP as the basis set for all calculations performed in this DFT mechanistic study.