

Electronic supplementary information (ESI)

DFT Studies on the Heterogeneous Oxidation of SO₂ by Oxygen Functional Groups on Graphene

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Table S1 Cartesian coordinates of the reactant, transition states, intermediate, and product for SO₂ oxidation.

Reactant complex				Transition state 1			Intermediate				
C	3.05906700	3.67360000	0.00420800	C	3.00019100	3.67702900	-0.05538500	C	3.04572000	3.66460200	-0.04862600
C	1.64299600	3.71389700	0.08323600	C	1.57676300	3.69771400	-0.00929300	C	1.61796800	3.69394400	-0.01504800
C	0.90424200	2.49732500	0.19420600	C	0.85391900	2.48059200	0.05676200	C	0.88640200	2.49011400	0.03179600
C	1.59948500	1.27972400	0.21430800	C	1.56175300	1.24792200	0.04255500	C	1.58447300	1.23213000	0.01056400
C	2.98946000	1.21899400	0.04593100	C	2.96619400	1.22160900	-0.04715800	C	2.99373800	1.20839700	-0.06312400
C	3.73450800	2.43247200	-0.04291700	C	3.69510100	2.44737500	-0.08624700	C	3.73148400	2.43101500	-0.07797000
C	-0.53061300	2.53892800	0.15915100	C	-0.57263500	2.50700900	0.05810600	C	-0.53130500	2.52667300	0.01853000
C	-0.65764900	0.07919600	0.42401800	C	-0.60583800	0.04075500	0.41216800	C	-0.58227800	0.05114100	0.41853800
C	-1.29467500	1.36394500	0.14634400	C	-1.31306500	1.31525100	0.09948300	C	-1.27788500	1.33041200	0.04954600
C	-1.36201500	-1.15570200	0.08236200	C	-1.34460700	-1.20583000	0.06201900	C	-1.32764000	-1.18660800	0.00530000
C	-0.66724500	-2.37278700	0.05949200	C	-0.63841000	-2.41570600	-0.00668600	C	-0.63188000	-2.40724500	-0.06036200
C	0.76611900	-2.41457000	0.09527500	C	0.78537900	-2.42755500	-0.01731900	C	0.78392900	-2.42567900	-0.04362800
C	1.52891400	-1.23968600	0.15921300	C	1.52665400	-1.21596400	-0.00353800	C	1.53410500	-1.19789800	-0.03074700
C	2.92017200	-1.25119900	-0.00426200	C	2.93233700	-1.22647800	-0.08779900	C	2.94386900	-1.23073400	-0.09985000
C	3.65789600	-0.03471000	-0.03336400	C	3.65514900	-0.01210700	-0.10095300	C	3.67428100	-0.02555700	-0.10354300
C	0.96856100	4.95495000	0.03610500	C	0.88498500	4.93448300	-0.04421100	C	0.93519900	4.93996100	-0.04488900
C	-0.44638800	4.99577800	0.00215200	C	-0.52479100	4.96095300	-0.07928900	C	-0.46870500	4.97841700	-0.08531400
C	-1.19238600	3.79563700	0.01861400	C	-1.25401500	3.75132600	-0.06021600	C	-1.20603400	3.77227500	-0.07937400
C	-2.60268400	3.83547200	-0.12766400	C	-2.66545100	3.77019700	-0.16928200	C	-2.61801500	3.80141000	-0.17779100
C	-3.34450100	2.63421200	-0.20615500	C	-3.38441500	2.55662700	-0.21842000	C	-3.34132800	2.59309900	-0.22785600
C	-2.67484100	1.38094800	-0.09087300	C	-2.69059700	1.31518600	-0.10793300	C	-2.65109000	1.34634400	-0.13834200
C	-2.74338100	-1.08844600	-0.13933100	C	-2.72737300	-1.16143900	-0.12368900	C	-2.70700100	-1.13645800	-0.17783900
C	-3.40813200	0.16710700	-0.19941300	C	-3.41076600	0.08563500	-0.18036400	C	-3.38161100	0.11680500	-0.21555200
C	5.14093500	2.38901800	-0.15740400	C	5.10555300	2.42759700	-0.14790800	C	5.14178600	2.40328100	-0.12463300
C	5.81007000	1.13730800	-0.22308800	C	5.79936800	1.18543100	-0.19202900	C	5.83069300	1.15500800	-0.16184800
C	-4.74465500	2.67071600	-0.38073000	C	-4.78787100	2.57124600	-0.35878800	C	-4.74543500	2.61653800	-0.34731900
C	-4.80978100	0.20954700	-0.39104600	C	-4.81386600	0.10651900	-0.34273000	C	-4.78501400	0.14826900	-0.35127300
C	-5.55004300	-0.99719200	-0.50628500	C	-5.54056800	-1.11315500	-0.42025800	C	-5.52046300	-1.06699100	-0.41930600
C	-5.48040100	1.45872900	-0.47175700	C	-5.50522100	1.34699800	-0.41604800	C	-5.46940100	1.39462500	-0.40107300
C	5.06712000	-0.07208800	-0.17149600	C	5.07531000	-0.03102000	-0.17060200	C	5.10135100	-0.05434700	-0.15576700
C	5.74055100	-1.31876300	-0.26852100	C	5.76474400	-1.26589300	-0.22709100	C	5.77989300	-1.29183500	-0.19491000
C	3.59523200	-2.50097800	-0.13612600	C	3.62641200	-2.47072000	-0.15745000	C	3.63010200	-2.48169700	-0.14550800
C	5.00184700	-2.53270300	-0.24817100	C	5.03638900	-2.48880100	-0.21675800	C	5.03976500	-2.51125500	-0.19013100
C	2.85085900	-3.70338200	-0.13055600	C	2.89721800	-3.68168300	-0.15237800	C	2.89332200	-3.68678100	-0.14376000
C	-3.48330900	-2.29831800	-0.28371900	C	-3.45554800	-2.38303800	-0.23793100	C	-3.44553100	-2.35244900	-0.27717600
C	-4.88411800	-2.25065000	-0.44954800	C	-4.85885500	-2.35706600	-0.36889900	C	-4.84877900	-2.31656300	-0.38482800
C	-2.81096600	-3.54069100	-0.24074600	C	-2.76974500	-3.61567600	-0.20467100	C	-2.77142000	-3.58900400	-0.24196100
C	1.43499700	-3.66677600	-0.05147900	C	1.47492200	-3.66431600	-0.10216800	C	1.46678700	-3.65884300	-0.11061600
C	0.69098200	-4.86528800	-0.13150000	C	0.74897400	-4.87934500	-0.14565300	C	0.73284200	-4.87323200	-0.15645100
C	-0.72423700	-4.82395100	-0.15792900	C	-0.66315300	-4.86553300	-0.16207900	C	-0.67432900	-4.85331100	-0.18836900

C	-1.40026500	-3.58481600	-0.10742300	C	-1.35688500	-3.63776000	-0.12200400	C	-1.35968400	-3.62067100	-0.16381700
C	-1.48078600	-6.03702100	-0.27562000	C	-1.40314900	-6.09396800	-0.23596800	C	-1.42414000	-6.08004300	-0.25246800
C	1.38079400	-6.11938100	-0.22732200	C	1.45991700	-6.12505600	-0.20271000	C	1.43874900	-6.12546800	-0.19632300
C	-1.13188300	6.25249000	-0.09056600	C	-1.23007300	6.21078900	-0.15480600	C	-1.16858300	6.23665600	-0.14518100
C	1.72899000	6.17017500	-0.02297800	C	1.63216500	6.16087200	-0.07988300	C	1.69451600	6.16301400	-0.06314300
C	7.15592200	-1.34727800	-0.39126800	C	7.18437000	-1.27787000	-0.29183700	C	7.19980100	-1.31559400	-0.24043300
C	7.22483100	1.09032700	-0.34710100	C	7.21811600	1.15953300	-0.25821200	C	7.24985200	1.12126800	-0.20830800
C	-6.95909500	-0.94565800	-0.68193900	C	-6.95409400	-1.08339700	-0.55833700	C	-6.93594100	-1.02798200	-0.53073200
C	-6.88962300	1.49209500	-0.64998700	C	-6.91736900	1.35852300	-0.55679600	C	-6.88165800	1.41669500	-0.51644000
C	3.52921800	-4.95602100	-0.24351300	C	3.59299600	-4.92433600	-0.21492000	C	3.57932600	-4.93162900	-0.19017300
C	5.67262200	-3.78886300	-0.34893700	C	5.72521400	-3.73642400	-0.27360400	C	5.72034400	-3.76181700	-0.23000600
C	-3.55584400	-4.75278300	-0.37165200	C	-3.49941900	-4.84053400	-0.29777200	C	-3.51030000	-4.80863400	-0.31907100
C	-5.62285700	-3.46695900	-0.56541600	C	-5.58553300	-3.58366700	-0.44929800	C	-5.58678900	-3.53632200	-0.45036100
C	-5.41185700	3.92966500	-0.46913800	C	-5.47786500	3.81723200	-0.43862100	C	-5.43022400	3.86407600	-0.40720800
C	-3.27627000	5.09118900	-0.23313900	C	-3.35981700	5.01641100	-0.26142500	C	-3.30588800	5.05250100	-0.24982300
C	3.80769600	4.88885000	-0.06960800	C	3.73065400	4.90076000	-0.09483200	C	3.78269500	4.88094400	-0.07025900
C	5.88198600	3.60799400	-0.21546500	C	5.82880300	3.65582200	-0.17569900	C	5.87311600	3.62460900	-0.13493700
C	-7.54040700	2.77376200	-0.72786700	C	-7.59261600	2.62622000	-0.63017600	C	-7.55317200	2.68606600	-0.57056800
C	-7.59788900	0.29340400	-0.74682400	C	-7.60873900	0.14653900	-0.62000800	C	-7.58078100	0.20674900	-0.57381300
C	7.80967600	-2.62655700	-0.48289300	C	7.85450500	-2.55167400	-0.34442300	C	7.86066000	-2.59513100	-0.27919500
C	7.86655400	-0.14651500	-0.42329700	C	7.88030700	-0.06863500	-0.30446800	C	7.90431000	-0.11122100	-0.24553600
C	5.20835700	4.82144000	-0.16737900	C	5.13333600	4.85890600	-0.14680300	C	5.18388800	4.83296300	-0.10702900
C	3.10590300	6.11870600	-0.05995800	C	3.00737200	6.12357400	-0.09310000	C	3.06580700	6.11368700	-0.06557900
C	1.00787400	7.42425400	-0.06295200	C	0.89618400	7.40723700	-0.11710400	C	0.96732500	7.41616700	-0.09210700
C	-0.33864800	7.46292400	-0.09537300	C	-0.45039500	7.43074300	-0.15433600	C	-0.37828600	7.45100100	-0.13241600
C	-2.50633000	6.27937800	-0.19159300	C	-2.60412400	6.21809400	-0.23502900	C	-2.53959100	6.25305800	-0.21837100
C	7.95001300	2.33310400	-0.39347700	C	7.92363100	2.41450300	-0.27740300	C	7.96300300	2.37246600	-0.21425200
C	-2.85518300	-5.98335000	-0.36531100	C	-2.77903200	-6.06223600	-0.29287500	C	-2.79721100	-6.03875800	-0.30865500
C	-0.75782800	-7.28991500	-0.31748400	C	-0.65849300	-7.33500200	-0.25967900	C	-0.68556200	-7.32579700	-0.26212700
C	0.58898800	-7.32903300	-0.29546400	C	0.68891100	-7.34976500	-0.24364400	C	0.66106900	-7.34722600	-0.23583900
C	2.75852400	-6.14428600	-0.26896100	C	2.83645200	-6.12581700	-0.22786800	C	2.81237100	-6.13227400	-0.20497300
C	4.93166000	-4.96372700	-0.34119300	C	4.99733100	-4.91959400	-0.26970600	C	4.98251800	-4.94046700	-0.22821300
C	7.10841500	-3.78349500	-0.46226900	C	7.16490100	-3.71546700	-0.33562200	C	7.16132600	-3.75281500	-0.27408300
C	-4.95182000	-4.68194100	-0.52175800	C	-4.89904600	-4.79088700	-0.40861200	C	-4.90893100	-4.75041800	-0.41546500
C	-7.05059700	-3.38102900	-0.73251700	C	-7.01827100	-3.51828600	-0.57763900	C	-7.02084100	-3.46105600	-0.55461300
C	-7.68249700	-2.18590700	-0.78879900	C	-7.66641900	-2.33202200	-0.63046400	C	-7.66080700	-2.26985600	-0.59382900
C	-6.84154800	3.92919700	-0.64236600	C	-6.91039000	3.79381100	-0.57419500	C	-6.86376500	3.85039600	-0.51969400
C	-4.67290900	5.10322600	-0.39254600	C	-4.75697700	5.00630000	-0.38771800	C	-4.70100800	5.05231600	-0.35803700
C	7.31509800	3.52627700	-0.33070100	C	7.26678200	3.59688300	-0.23858100	C	7.31190800	3.55792100	-0.17961400
H	-1.33395300	-8.20673300	-0.37940200	H	-1.21867900	-8.26282900	-0.29647200	H	-1.25039200	-8.25090000	-0.29467700
H	1.11375300	-8.27705500	-0.34084300	H	1.23024300	-8.28909700	-0.26827700	H	1.19819600	-8.28915100	-0.24846700
H	3.27219400	-7.09754600	-0.34631900	H	3.36696500	-7.07218700	-0.27148100	H	3.33949700	-7.08116600	-0.23529900
H	5.44674000	-5.91572800	-0.42398000	H	5.52478500	-5.86727300	-0.31478900	H	5.50291100	-5.89248000	-0.26110500
H	7.61975300	-4.73711300	-0.53527700	H	7.68889100	-4.66407600	-0.37651100	H	7.67790400	-4.70585000	-0.30376000

H	8.89044500	-2.64180400	-0.57247900	H	8.93793900	-2.55699900	-0.39207800	H	8.94450700	-2.60945400	-0.31231000
H	8.94784700	-0.17503900	-0.51679000	H	8.96463300	-0.08284400	-0.35367900	H	8.98911300	-0.13286600	-0.27911600
H	9.03006100	2.29110700	-0.48360200	H	9.00682400	2.39111600	-0.32552500	H	9.04657100	2.34338900	-0.24745300
H	7.87893200	4.45188000	-0.36926700	H	7.81689300	4.53129100	-0.25541400	H	7.86711000	4.48943000	-0.18512700
H	5.77560400	5.74564900	-0.21768500	H	5.68658800	5.79247900	-0.17200700	H	5.74294600	5.76329900	-0.11910900
H	3.67245800	7.04350700	-0.10726200	H	3.56429200	7.05525500	-0.11987000	H	3.63186200	7.04019700	-0.07857700
H	1.58592700	8.34173900	-0.07985800	H	1.46391800	8.33117300	-0.12436600	H	1.54256100	8.33548000	-0.08848100
H	-0.86175200	8.41196500	-0.13928200	H	-0.98401800	8.37406600	-0.19165000	H	-0.90441300	8.39877300	-0.16106100
H	-3.01676500	7.23466900	-0.26553300	H	-3.13041000	7.16550900	-0.29537400	H	-3.06181100	7.20341200	-0.26487500
H	-5.18447100	6.05774100	-0.46820000	H	-5.28729200	5.95094900	-0.45431100	H	-5.22843500	5.99940900	-0.40905200
H	-7.35014100	4.88494400	-0.70610900	H	-7.43559900	4.74076200	-0.63147700	H	-7.38497300	4.80022000	-0.56177500
H	-8.61665500	2.79211100	-0.86074300	H	-8.67222000	2.62527700	-0.73294800	H	-8.63439100	2.69047600	-0.65374600
H	-8.67477400	0.32540600	-0.88109500	H	-8.68960300	0.16258700	-0.72395100	H	-8.66355800	0.23091000	-0.65708400
H	-8.75837800	-2.14027600	-0.91818800	H	-8.74594700	-2.29974700	-0.72901700	H	-8.74164000	-2.22819500	-0.67184900
H	-7.61233200	-4.30502700	-0.81537900	H	-7.57041300	-4.44993100	-0.63280400	H	-7.58072100	-4.38849400	-0.59994700
H	-5.51653600	-5.60430600	-0.61576600	H	-5.45530500	-5.72061300	-0.47387700	H	-5.47365700	-5.67566800	-0.46827700
H	-3.41920700	-6.90644600	-0.45639300	H	-3.33221900	-6.99428000	-0.35177200	H	-3.35846500	-6.96647400	-0.35679700
C	0.87995500	0.03268100	0.46429100	C	0.85570800	0.02339900	0.12164800	C	0.87357000	0.02982400	0.04890200
O	0.07954800	0.03027500	1.64407500	O	-0.10762800	0.00784900	1.76724500	O	-0.43774200	0.04436000	1.85006200
S	-1.75750700	-1.00075100	3.41336000	S	-1.54285800	-0.48357600	3.14732100	S	-1.81061300	-0.60631600	3.00719500
O	-1.94190800	-2.33518400	2.89897100	O	-2.56388900	0.45727700	2.69460600	O	-2.96617600	0.19537400	2.57976300
O	-2.54442200	0.05503700	2.82558600	O	-1.77615500	-1.87045900	2.75796100	O	-1.89161200	-2.00926600	2.56625100

Transition state 2				Product complex			
C	3.00670300	3.67693200	-0.07277500	C	3.04942100	3.69381400	-0.10797300
C	1.58144100	3.69624100	-0.03783900	C	1.62967700	3.73649200	-0.12985200
C	0.85758500	2.48354600	0.00064100	C	0.88482500	2.52709300	-0.17250500
C	1.56191600	1.23497100	-0.02161200	C	1.56367000	1.27439300	-0.17904000
C	2.97121400	1.21878300	-0.09152700	C	2.97349800	1.23337100	-0.15700900
C	3.70034700	2.44654400	-0.10032000	C	3.72233400	2.44922000	-0.11469800
C	-0.55665400	2.50616500	-0.00795000	C	-0.52071500	2.56734200	-0.19147700
C	-0.58838200	0.03858600	0.27843100	C	-0.59521900	0.11245700	-0.23898300
C	-1.29471800	1.30057900	0.02153800	C	-1.26888000	1.35567400	-0.23649100
C	-1.32716500	-1.20144300	0.00244900	C	-1.33770600	-1.09521300	-0.29151000
C	-0.62074800	-2.42236400	-0.06173600	C	-0.65805600	-2.35152400	-0.27941900
C	0.79098400	-2.43379400	-0.05413100	C	0.74716600	-2.38862200	-0.26296200
C	1.52887800	-1.20427700	-0.05125900	C	1.49459900	-1.17550900	-0.22325700
C	2.93915400	-1.22479100	-0.11872000	C	2.90375500	-1.21480800	-0.19869000
C	3.65998400	-0.01250200	-0.12273900	C	3.64335500	-0.01067800	-0.15782400
C	0.88956600	4.93386400	-0.06124000	C	0.95643000	4.97785500	-0.11941600
C	-0.51712900	4.95800300	-0.09544300	C	-0.45471900	5.01801000	-0.13928200
C	-1.24436000	3.74609900	-0.09200700	C	-1.19643000	3.81659600	-0.17836400
C	-2.65847900	3.76262200	-0.18370400	C	-2.61611500	3.85385400	-0.19417000
C	-3.37580700	2.54819000	-0.23507400	C	-3.35820900	2.64929300	-0.23132200
C	-2.67883100	1.30468400	-0.15036900	C	-2.67919800	1.39342000	-0.24828900

C	-2.71866100	-1.16181000	-0.16799900	C	-2.75173500	-1.05458300	-0.28960300
C	-3.39943600	0.07826800	-0.23164500	C	-3.41994100	0.19004100	-0.28641000
C	5.11036900	2.42771500	-0.14761200	C	5.13155800	2.40719000	-0.09082700
C	5.80715900	1.18434800	-0.18086700	C	5.80798900	1.15342200	-0.09634600
C	-4.78081600	2.56282300	-0.35182800	C	-4.76780700	2.68683800	-0.24225400
C	-4.81013900	0.09901500	-0.35502600	C	-4.84415600	0.22962300	-0.29110700
C	-5.53487400	-1.11880700	-0.42050100	C	-5.58382100	-0.97522700	-0.32043400
C	-5.50124600	1.33738600	-0.40950900	C	-5.51478400	1.47404700	-0.27470800
C	5.08638600	-0.03095400	-0.17520900	C	5.06790300	-0.05123500	-0.13400400
C	5.77423000	-1.26424900	-0.20635000	C	5.73861300	-1.29611500	-0.13652200
C	3.63494300	-2.47094200	-0.15195000	C	3.58283900	-2.47154500	-0.19773700
C	5.04432700	-2.48901400	-0.19803900	C	4.99208900	-2.50957400	-0.17177800
C	2.90817900	-3.68345400	-0.14526600	C	2.84128700	-3.67619400	-0.23198800
C	-3.44516600	-2.38607700	-0.26162600	C	-3.49856500	-2.27133900	-0.32709700
C	-4.84908600	-2.36248700	-0.37278100	C	-4.90739400	-2.22874800	-0.33410600
C	-2.75809900	-3.61853900	-0.22013900	C	-2.82475100	-3.51526100	-0.33141100
C	1.48409600	-3.66631500	-0.11001400	C	1.42166600	-3.63832600	-0.25812900
C	0.75971800	-4.88306200	-0.14342000	C	0.67905000	-4.83947000	-0.28870600
C	-0.65002400	-4.86969200	-0.16827600	C	-0.73189700	-4.79994500	-0.31229200
C	-1.34341100	-3.64132000	-0.14722600	C	-1.40489700	-3.55898900	-0.31579400
C	-1.39206200	-6.10067100	-0.22252400	C	-1.49578700	-6.01854300	-0.33776000
C	1.47315800	-6.13082900	-0.17788300	C	1.37221900	-6.09991800	-0.28796300
C	-1.22738900	6.20962800	-0.14786500	C	-1.14818800	6.27803100	-0.12367600
C	1.63804100	6.16312800	-0.07745900	C	1.71999800	6.19646500	-0.08139000
C	7.19442300	-1.27725900	-0.25145500	C	7.15850300	-1.33039200	-0.10834300
C	7.22657100	1.16042400	-0.22658000	C	7.22760200	1.10661300	-0.06892800
C	-6.95099100	-1.09142900	-0.53128900	C	-7.00367300	-0.92883600	-0.32957700
C	-6.91497100	1.34984900	-0.52248200	C	-6.93486900	1.50820200	-0.28519300
C	3.60382600	-4.92422000	-0.18389100	C	3.51914100	-4.92875300	-0.23314000
C	5.73490200	-3.73523800	-0.23048600	C	5.66523500	-3.76659400	-0.17484800
C	-3.48709000	-4.84310700	-0.29071000	C	-3.57229300	-4.72697300	-0.35335600
C	-5.57535300	-3.58932900	-0.43444300	C	-5.65047300	-3.44549200	-0.35814900
C	-5.47268200	3.80689300	-0.40932300	C	-5.44107900	3.94356100	-0.22242600
C	-3.35465900	5.00746900	-0.24999600	C	-3.29427600	5.10616600	-0.17563300
C	3.73514900	4.89935300	-0.09170700	C	3.79723400	4.90579900	-0.07035100
C	5.83348900	3.65471800	-0.15692500	C	5.87468600	3.62392600	-0.05399700
C	-7.59101800	2.61796600	-0.57566200	C	-7.58879900	2.79121500	-0.26509600
C	-7.60781000	0.13716500	-0.57876200	C	-7.64789300	0.30882700	-0.31251300
C	7.86565400	-2.55145300	-0.28471500	C	7.81232700	-2.61362300	-0.11405100
C	7.88948000	-0.06765100	-0.26011800	C	7.87164300	-0.13113500	-0.07559900
C	5.13720700	4.85859400	-0.12879900	C	5.19996900	4.83891100	-0.04528800
C	3.01042500	6.12625700	-0.08345900	C	3.09292200	6.14187900	-0.05916600
C	0.89821000	7.40912100	-0.09970600	C	0.99379700	7.45064100	-0.06793000
C	-0.44788500	7.43100700	-0.13430500	C	-0.35250600	7.48897100	-0.08766000

C	-2.59888500	6.21374800	-0.21667600	C	-2.52206000	6.30096300	-0.14130000
C	7.93151700	2.41609400	-0.23430500	C	7.95297000	2.35044900	-0.03373500
C	-2.76555600	-6.06780400	-0.27521800	C	-2.86844800	-5.96347300	-0.35738500
C	-0.64593200	-7.34218400	-0.22876000	C	-0.76983900	-7.27284700	-0.33879400
C	0.70088700	-7.35643600	-0.20755700	C	0.57636900	-7.31100300	-0.31531200
C	2.84733500	-6.13018500	-0.19030400	C	2.74588800	-6.12312500	-0.26196300
C	5.00774800	-4.91977300	-0.22244500	C	4.92324700	-4.94165500	-0.20517300
C	7.17574500	-3.71471600	-0.27453800	C	7.10614400	-3.76686600	-0.14520300
C	-4.88691500	-4.79597000	-0.38945400	C	-4.97517500	-4.65989800	-0.36754800
C	-7.01025800	-3.52676100	-0.54390400	C	-7.08900600	-3.36451800	-0.36939300
C	-7.66169700	-2.34221600	-0.59035000	C	-7.72911600	-2.17282800	-0.35574000
C	-6.90702600	3.78481200	-0.52260300	C	-6.88221700	3.94423400	-0.23554000
C	-4.75128300	4.99759300	-0.35648500	C	-4.69867100	5.11824900	-0.19063000
C	7.27266000	3.59729200	-0.20124600	C	7.31310700	3.54233600	-0.02649800
H	-1.20585200	-8.27051200	-0.25499900	H	-1.34584100	-8.19162100	-0.35739100
H	1.24231700	-8.29596000	-0.21758800	H	1.10002400	-8.26071700	-0.31580500
H	3.38062100	-7.07554500	-0.21640900	H	3.26448300	-7.07681800	-0.26267800
H	5.53680300	-5.86717200	-0.25016300	H	5.44156600	-5.89542200	-0.20699100
H	7.69996200	-4.66369100	-0.29992300	H	7.61745700	-4.72322100	-0.14859300
H	8.94958900	-2.55705300	-0.31763900	H	8.89639200	-2.63450400	-0.09201400
H	8.97447500	-0.08151700	-0.29304200	H	8.95664400	-0.16198900	-0.05384600
H	9.01525300	2.39385900	-0.26719500	H	9.03651200	2.30984800	-0.01244800
H	7.82181500	4.53236900	-0.20784100	H	7.87706600	4.46828400	0.00037500
H	5.69117800	5.79198600	-0.14030800	H	5.77042300	5.76212100	-0.01780800
H	3.56890200	7.05718800	-0.09543200	H	3.66382900	7.06483800	-0.03158900
H	1.46424000	8.33412600	-0.09552000	H	1.56970000	8.36930400	-0.04121100
H	-0.98297600	8.37393900	-0.15770200	H	-0.87619300	8.43860400	-0.07605600
H	-3.12955400	7.15971900	-0.25856400	H	-3.04132000	7.25416400	-0.12717400
H	-5.28428000	5.94191200	-0.40386200	H	-5.21718700	6.07183800	-0.17484700
H	-7.43279900	4.73227300	-0.56345900	H	-7.39325700	4.90060300	-0.21950500
H	-8.67222600	2.61840500	-0.65946400	H	-8.67302300	2.81205900	-0.27357700
H	-8.69035900	0.15320000	-0.66257600	H	-8.73306900	0.33929300	-0.32004000
H	-8.74270900	-2.31262800	-0.67175200	H	-8.81281100	-2.13249600	-0.36355500
H	-7.56142400	-4.45958400	-0.58721100	H	-7.65296500	-4.29064900	-0.38754900
H	-5.44337000	-5.72657300	-0.43853400	H	-5.54567100	-5.58336800	-0.38294300
H	-3.32103300	-6.99933700	-0.31860100	H	-3.44003400	-6.88623500	-0.37332900
C	0.85822800	0.02339100	0.01008700	C	0.82386300	0.06983900	-0.22286300
O	-0.38806200	0.04224600	1.94063000	O	0.02018000	-1.18237400	2.66856300
S	-1.55735400	-0.43388500	2.97074100	S	-1.40833300	-1.11726700	2.61233200
O	-2.68115600	0.50000400	2.85350900	O	-2.06804400	0.15199200	2.65852700
O	-1.84775000	-1.83946000	2.64783200	O	-2.17772900	-2.32378100	2.61023900

Table S2 Cartesian coordinates of the reactant, transition state, and product for H₂SO₃ oxidation.

Reactant complex			Transition state			Product complex					
C	2.68793900	3.77705100	-0.19549400	C	2.78175700	3.75199000	-0.27611600	C	2.77507900	3.68560900	-0.34124700
C	1.26836100	3.76006800	-0.11642600	C	1.35812600	3.74727200	-0.23841400	C	1.35371300	3.68763600	-0.33405600
C	0.57125000	2.52415900	0.02242400	C	0.65286400	2.51820500	-0.21127300	C	0.64120500	2.45934400	-0.35051200
C	1.31804700	1.27836800	0.01314700	C	1.38067800	1.28220700	-0.25563300	C	1.35380000	1.22460300	-0.35856100
C	2.72266100	1.31146400	-0.15725100	C	2.79245600	1.29219500	-0.29776100	C	2.76788900	1.22286300	-0.36797900
C	3.41626300	2.56199500	-0.21299800	C	3.49817800	2.53287900	-0.30966400	C	3.48382700	2.46122800	-0.34520100
C	-0.81623000	2.53168100	0.06749200	C	-0.75608600	2.51601800	-0.17807400	C	-0.76378000	2.45770500	-0.33006800
C	-0.76985600	-0.01666200	0.35460300	C	-0.74159400	0.04500600	0.02143300	C	-0.77312200	-0.00107700	-0.34630700
C	-1.54686500	1.29000700	0.34635300	C	-1.46750500	1.28854900	-0.13866800	C	-1.47723000	1.22466900	-0.33443500
C	-1.49958300	-1.25482500	0.07378200	C	-1.46070000	-1.19707500	-0.21617100	C	-1.47808700	-1.22597800	-0.33306600
C	-0.75516700	-2.44816500	-0.09659600	C	-0.73818800	-2.40895100	-0.28896600	C	-0.76469200	-2.45889200	-0.32822900
C	0.65392500	-2.41619000	-0.17055100	C	0.67323300	-2.39767800	-0.30173000	C	0.64049500	-2.46105300	-0.35195600
C	1.35728600	-1.16287100	-0.13557900	C	1.39070300	-1.15791300	-0.29499500	C	1.35459300	-1.22861800	-0.36223300
C	2.75948100	-1.13641400	-0.28482100	C	2.80037700	-1.15240200	-0.32770500	C	2.76581400	-1.22855600	-0.37120400
C	3.44483000	0.10092600	-0.25905700	C	3.50045200	0.07277400	-0.33127200	C	3.47355700	-0.00471400	-0.35885400
C	0.54313300	4.96809100	-0.18992700	C	0.64379200	4.96898100	-0.22358400	C	0.64701900	4.91010800	-0.32063000
C	-0.86982300	4.95021400	-0.19707200	C	-0.76672200	4.96672000	-0.20707700	C	-0.76451100	4.90969900	-0.30635300
C	-1.55592000	3.72297400	-0.08892900	C	-1.47087400	3.74300200	-0.18965000	C	-1.47289600	3.68790200	-0.31213200
C	-2.98431100	3.68957900	-0.14597300	C	-2.89023700	3.73622200	-0.19069300	C	-2.89314600	3.68647600	-0.28686400
C	-3.68318900	2.44867900	-0.10781000	C	-3.59055500	2.50799500	-0.19908400	C	-3.60093300	2.46164800	-0.28328300
C	-2.98170500	1.22920000	0.06027300	C	-2.87155700	1.27501800	-0.18366100	C	-2.88674800	1.22461300	-0.29759200
C	-2.88107400	-1.24381200	0.02715000	C	-2.85546700	-1.19018900	-0.24973600	C	-2.88779000	-1.22439300	-0.29549400
C	-3.62607000	0.00296800	0.01861900	C	-3.56690300	0.04325000	-0.21711200	C	-3.59261700	0.00036400	-0.28945700
C	4.81884300	2.58246600	-0.33356200	C	4.90769000	2.53844400	-0.33887500	C	4.89373200	2.45698600	-0.34856100
C	5.55199700	1.35936400	-0.40223600	C	5.62603600	1.30698500	-0.36593800	C	5.60500000	1.22177700	-0.35104100
C	-5.08600500	2.42298400	-0.23420000	C	-4.99957300	2.49918400	-0.22280100	C	-5.01068700	2.46043100	-0.25252900
C	-5.04654000	-0.03082000	-0.13873900	C	-4.98733900	0.03663000	-0.25490400	C	-5.01768400	0.00099900	-0.25335000
C	-5.72990900	-1.27108700	-0.20129600	C	-5.69041100	-1.19421800	-0.30280700	C	-5.72412700	-1.22392200	-0.23952500
C	-5.77002400	1.17860700	-0.23143300	C	-5.70069400	1.26127700	-0.24658000	C	-5.72310500	1.22654000	-0.24177100
C	4.86964200	0.12505500	-0.38567900	C	4.92718000	0.07952700	-0.35583800	C	4.89954300	-0.00385600	-0.36022600
C	5.58922000	-1.08725400	-0.48326300	C	5.63628400	-1.14208300	-0.38391600	C	5.60393100	-1.22969700	-0.35552300
C	3.49014900	-2.36233700	-0.38609100	C	3.51731600	-2.38593100	-0.35646300	C	3.48061800	-2.46523200	-0.35413000
C	4.89629900	-2.33408500	-0.48815800	C	4.92740700	-2.37925100	-0.37814800	C	4.89067600	-2.46323200	-0.35578700
C	2.79964800	-3.59357200	-0.39927700	C	2.81047000	-3.60946600	-0.35355800	C	2.77182300	-3.68948700	-0.34735500
C	-3.58556600	-2.48442600	-0.11288400	C	-3.56871900	-2.42636100	-0.31502100	C	-3.60295400	-2.46075500	-0.27969900
C	-4.99608800	-2.49925300	-0.18658800	C	-4.97814800	-2.42732600	-0.33259800	C	-5.01272900	-2.45835900	-0.24814700
C	-2.86322100	-3.69561200	-0.18411700	C	-2.85858200	-3.64672700	-0.34466500	C	-2.89573000	-3.68598400	-0.28187200
C	1.37557500	-3.61855300	-0.30280200	C	1.38571200	-3.61610800	-0.33723800	C	1.35106800	-3.69032300	-0.33763900
C	0.68720800	-4.85877700	-0.35463700	C	0.68265100	-4.84618300	-0.35874000	C	0.64333300	-4.91230300	-0.32178700
C	-0.71528100	-4.88894000	-0.30477100	C	-0.72546200	-4.85902200	-0.36433000	C	-0.76817300	-4.91098900	-0.30404000
C	-1.44452700	-3.68077400	-0.19714700	C	-1.44075000	-3.64163900	-0.33572200	C	-1.47533600	-3.68840600	-0.30923500
C	-1.42826300	-6.14121400	-0.37489800	C	-1.44814600	-6.10381300	-0.39758200	C	-1.49744100	-6.15077100	-0.28411600
C	1.43920000	-6.08424500	-0.46629100	C	1.41914500	-6.08210500	-0.38645400	C	1.37175900	-6.15276700	-0.31523500

C	-1.61901500	6.17276900	-0.30551100	C	-1.49993000	6.20491300	-0.20400000	C	-1.49265200	6.15009300	-0.28821500
C	1.24989000	6.21868700	-0.28863500	C	1.36828800	6.21163500	-0.24045600	C	1.37682900	6.14979300	-0.31246800
C	7.00449900	-1.05769700	-0.59145000	C	7.05633600	-1.13053300	-0.41065200	C	7.02463700	-1.22377400	-0.35408200
C	6.96829000	1.37857500	-0.51861700	C	7.04641000	1.30770600	-0.39493800	C	7.02550700	1.21490000	-0.34991100
C	-7.13915800	-1.28962700	-0.31409100	C	-7.10888600	-1.19238600	-0.32736500	C	-7.14450700	-1.21706400	-0.20874900
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C	3.52784100	-4.81055900	-0.50884400	C	3.52786300	-4.83802600	-0.38142900	C	3.48485100	-4.92269800	-0.33813300
C	5.61996900	-3.55530400	-0.58870500	C	5.63925700	-3.61277600	-0.40207500	C	5.59875000	-3.70088800	-0.34889800
C	-3.55976600	-4.94053200	-0.28062600	C	-3.56826200	-4.88407700	-0.38596200	C	-3.60957800	-4.91840400	-0.26162500
C	-5.68252900	-3.73830400	-0.27973400	C	-5.68282700	-3.66478100	-0.37769800	C	-5.72182100	-3.69545000	-0.22926300
C	-5.80962400	3.65196400	-0.35319500	C	-5.71526500	3.73388400	-0.22325100	C	-5.71882000	3.69807900	-0.23562700
C	-3.70737300	4.89676900	-0.28277900	C	-3.60863400	4.96574100	-0.19688100	C	-3.60586100	4.91945200	-0.26814800
C	3.37779000	5.01737900	-0.28838300	C	3.48819300	4.98719000	-0.28956200	C	3.48932100	4.91819300	-0.32993000
C	5.50683400	3.83100600	-0.39362300	C	5.60907000	3.77914300	-0.34743400	C	5.60252100	3.69416900	-0.33910500
C	-7.90089200	2.40211300	-0.45477600	C	-7.82060000	2.50750700	-0.26748100	C	-7.83292200	2.48522800	-0.19560500
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C	7.71119500	-2.30839500	-0.68829000	C	7.74984000	-2.39265100	-0.43214300	C	7.71395800	-2.48827400	-0.35217800
C	7.66346400	0.17343300	-0.60356000	C	7.73062000	0.09186600	-0.41608400	C	7.70363000	-0.00482900	-0.35225300
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C	-0.87809900	7.41661800	-0.37815700	C	-0.74221600	7.44022100	-0.21220400	C	-0.73095700	7.38310500	-0.28605000
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C	7.63658300	2.65511700	-0.55288000	C	7.72903300	2.57635100	-0.40167400	C	7.71583200	2.47887000	-0.34426000
C	-2.79820600	-6.14676500	-0.35827300	C	-2.82177600	-6.09661500	-0.40906700	C	-2.87129700	-6.13469600	-0.26465500
C	-0.64573200	-7.35855900	-0.46761900	C	-0.67892800	-7.33187600	-0.41770800	C	-0.73697100	-7.38455800	-0.28328800
C	0.69946500	-7.33116500	-0.50967500	C	0.66780100	-7.32131100	-0.41090200	C	0.60992300	-7.38569300	-0.29786000
C	2.80709000	-6.04295600	-0.53298500	C	2.79203400	-6.05796000	-0.39277400	C	2.74581100	-6.13848000	-0.32457600
C	4.92597900	-4.76196300	-0.59725500	C	4.93113900	-4.80980000	-0.40205400	C	4.88920600	-4.89591200	-0.34132200
C	7.05580400	-3.49198200	-0.68612200	C	7.07950400	-3.56784600	-0.42755400	C	7.03946500	-3.66078600	-0.34920900
C	-4.95351400	-4.93228400	-0.31128900	C	-4.96986200	-4.86110300	-0.40179400	C	-5.01360700	-4.89128700	-0.23654700
C	-7.11699100	-3.72251500	-0.35885200	C	-7.12194000	-3.62744200	-0.39584900	C	-7.16211000	-3.65427400	-0.20047900
C	-7.80911500	-2.55783700	-0.37639700	C	-7.79752100	-2.45482400	-0.37267400	C	-7.83496500	-2.48082700	-0.19082000
C	-7.24946900	3.58447800	-0.45731700	C	-7.15553600	3.68485100	-0.24374000	C	-7.15912100	3.65809800	-0.20717000
C	-5.11855800	4.84864100	-0.37105700	C	-5.01343200	4.93302100	-0.20867400	C	-5.00984000	4.89347200	-0.24410500
C	6.94560000	3.81509000	-0.49651300	C	7.04996200	3.74597800	-0.37970000	C	7.04308900	3.65241700	-0.33883900
H	-1.17906100	-8.30211100	-0.50594500	H	-1.22217900	-8.27023500	-0.43752000	H	-1.28771300	-8.31880100	-0.26959700
H	1.26624700	-8.25308900	-0.58123700	H	1.22571800	-8.25118300	-0.42552600	H	1.15953000	-8.32065900	-0.29615200
H	3.36725100	-6.96921000	-0.61445200	H	3.34192700	-6.99392700	-0.41223600	H	3.29062600	-7.07738400	-0.31986000
H	5.48074500	-5.69156500	-0.67812600	H	5.47648700	-5.74821900	-0.42091100	H	5.43364200	-5.83505300	-0.33635600
H	7.60473900	-4.42430100	-0.76041700	H	7.62026200	-4.50774000	-0.44342900	H	7.57688800	-4.60273300	-0.34672900
H	8.79264500	-2.28015100	-0.76440500	H	8.83402100	-2.38002100	-0.45155700	H	8.79836200	-2.47916600	-0.35181300
H	8.74570000	0.19213200	-0.68781100	H	8.81598000	0.09642400	-0.43678900	H	8.78925400	-0.00516900	-0.35059000
H	8.71807300	2.66322500	-0.63296800	H	8.81324800	2.57274200	-0.42438100	H	8.80023100	2.46856000	-0.34349600

H	7.46507700	4.76631800	-0.53234200	H	7.58326200	4.69017700	-0.38468100	H	7.58172900	4.59361700	-0.33391400
H	5.30716200	5.96091400	-0.42867100	H	5.43022700	5.91274400	-0.33146200	H	5.43882800	5.82831300	-0.32408600
H	3.15286700	7.16717500	-0.39075200	H	3.28296400	7.14077600	-0.27839400	H	3.29629700	7.07285500	-0.31199900
H	1.00426300	8.37859800	-0.42357100	H	1.15290200	8.37890600	-0.23531800	H	1.16624400	8.31782000	-0.29396900
H	-1.44220500	8.34050100	-0.44425500	H	-1.29452300	8.37344100	-0.20539600	H	-1.28089600	8.31781400	-0.27335500
H	-3.55389200	7.05110500	-0.43144200	H	-3.42236000	7.12138000	-0.19739400	H	-3.41115900	7.07407200	-0.25599700
H	-5.66785200	5.77985100	-0.46774300	H	-5.56259300	5.86916200	-0.21109600	H	-5.55402700	5.83263800	-0.22898700
H	-7.79879000	4.51587600	-0.53954500	H	-7.69944700	4.62291600	-0.24045100	H	-7.69655000	4.59996100	-0.19390000
H	-8.98194900	2.37096400	-0.53628600	H	-8.90475700	2.48986100	-0.28374600	H	-8.91714700	2.47569700	-0.17362400
H	-8.92600100	-0.09963500	-0.46658900	H	-8.87760200	0.02168600	-0.32793500	H	-8.90837600	0.00269000	-0.17353800
H	-8.89123500	-2.56329900	-0.44739200	H	-8.88178100	-2.44573800	-0.38770100	H	-8.91918600	-2.47039200	-0.16879600
H	-7.63818000	-4.67180200	-0.41604900	H	-7.65840400	-4.56926000	-0.42916900	H	-7.70031100	-4.59568500	-0.18571700
H	-5.48801900	-5.87442900	-0.38265100	H	-5.51307500	-5.80024900	-0.43368800	H	-5.55843900	-5.83008800	-0.22047700
H	-3.33088900	-7.09085000	-0.41705200	H	-3.36150300	-7.03798300	-0.43558300	H	-3.41674300	-7.07320800	-0.24868400
C	0.66576000	0.04205200	0.05480400	C	0.69589200	0.05769200	-0.22922500	C	0.64708200	-0.00284600	-0.37861100
O	-1.16355200	0.63769800	1.56162900	O	-0.79634200	0.13203800	1.69260800	O	-0.12554400	1.24466400	2.56360200
S	1.22262000	-0.84429700	3.63414400	S	0.17721000	-0.63911500	3.14362600	S	0.48346200	0.01433200	2.96124000
O	0.90819200	0.73547100	3.38762600	O	1.45314000	0.35862300	2.89496700	O	2.04694100	0.08724600	2.65560400
O	0.33789100	-1.56424500	2.71587900	O	0.54276700	-1.95676700	2.63017500	O	-0.01966000	-1.25963700	2.53673100
O	2.72676400	-0.85509400	3.01113000	O	0.47740200	-0.79723400	4.77511000	O	0.55713200	0.00470300	4.55124100
H	2.72496100	-0.52908400	2.09595800	H	1.12099600	-1.51540500	4.87012900	H	0.63822300	-0.90853000	4.85808600
H	0.15911700	0.81801500	2.75987200	H	1.17902300	0.94987500	2.18109600	H	2.20757100	0.61228900	1.85237400

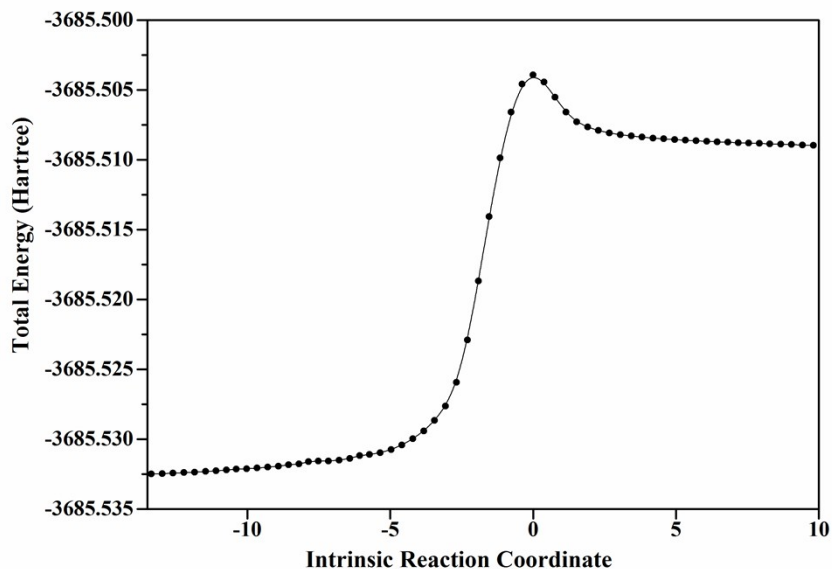


Fig. S1 IRC path of the first reaction step for SO₂ oxidation.

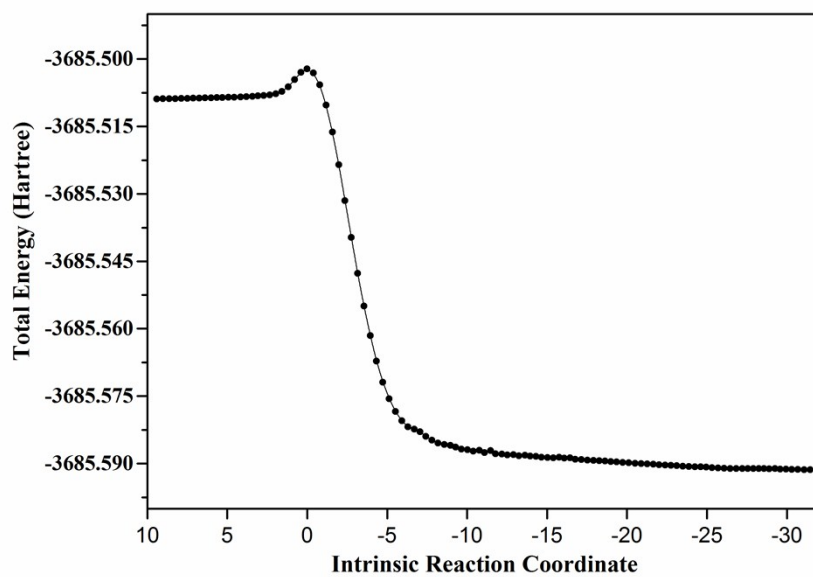


Fig. S2 IRC path of the second reaction step for SO₂ oxidation.

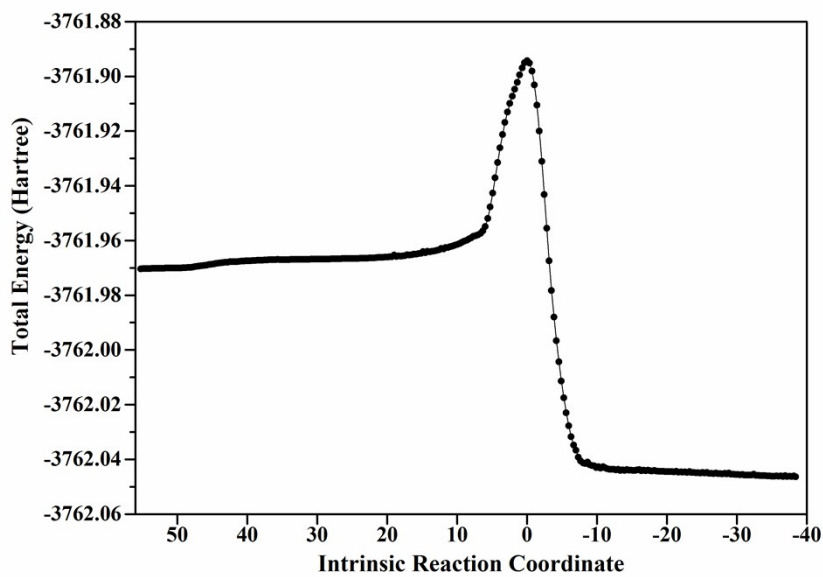


Fig. S3 IRC path for H₂SO₃ oxidation.