

Theoretical study on the mechanisms and kinetics of nitrous acid with simplest aromatic Criegee intermediate

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Table S1 Cartesian coordinates for all optimized structures at the M06-2X/6-311++G (d,p) level of theory

species		Cartesian coordinates		
PhCH=CH ₂	C	-0.29115600	2.00230100	0.00000000
	H	0.58820600	2.64215800	0.00000000
	C	-1.49234100	2.57746300	0.00000000
	H	-1.58847500	3.65581600	0.00000000
	H	-2.41345200	2.00637600	0.00000000
	C	0.00000000	0.55651600	0.00000000
	C	1.33381000	0.13885100	0.00000000
	C	-1.00101100	-0.42201800	0.00000000
	C	1.66376200	-1.21195800	0.00000000
	H	2.12093600	0.88575600	0.00000000
	C	-0.67485600	-1.77035500	0.00000000
	H	-2.04454300	-0.12956300	0.00000000
	C	0.65947800	-2.17216200	0.00000000
	H	2.70485600	-1.51314000	0.00000000
	H	-1.46422900	-2.51300000	0.00000000
	H	0.91058200	-3.22623300	0.00000000
O ₃	O	0.00000000	1.05807800	-0.21002600
	O	0.00000000	0.00000000	0.42005300
	O	0.00000000	-1.05807800	-0.21002600
TS1	C	0.75013100	-1.07143600	0.53070800
	C	1.64229800	-0.57113900	1.43493400
	H	2.55023500	-1.11061800	1.67221400
	H	1.37382500	0.24907900	2.08840200
	O	2.67747500	0.92857700	0.18707900
	O	2.81981200	0.22549200	-0.85150800
	O	1.72804300	-0.12589900	-1.37244500
	H	0.94288000	-2.03881600	0.07667300
	C	-0.56444800	-0.47339700	0.27473200
	C	-1.62420700	-1.27584600	-0.15571100
	C	-0.77294900	0.90079900	0.43590700
	C	-2.87897700	-0.72478100	-0.38428300
	H	-1.46158700	-2.33836600	-0.30304700
	C	-2.02520200	1.45098200	0.20176000
	H	0.06142700	1.53612800	0.71154600
	C	-3.08275100	0.63927100	-0.20183300
	H	-3.69635300	-1.35809200	-0.70789200
	H	-2.17664200	2.51708900	0.32284800

	H	-4.05979900	1.07151800	-0.38303900
C1	C	-0.93772300	-0.77932600	-0.05922700
	O	-1.59887300	-0.13091800	-1.14946500
	O	-2.89291600	0.15313800	-0.65085300
	O	-2.60206500	0.70393400	0.61266500
	C	-1.76599500	-0.29462700	1.16755200
	H	-2.36525000	-1.10634000	1.58568400
	H	-1.15425800	0.18174600	1.93149400
	H	-1.02257800	-1.86392500	-0.16713600
	C	0.50224800	-0.34629500	-0.05219400
	C	1.52333900	-1.28880600	-0.00464800
	C	0.81551400	1.01430300	-0.06524400
	C	2.85384200	-0.87973900	0.04070500
	H	1.28058700	-2.34639100	-0.00795100
	C	2.14151300	1.42135900	-0.02575300
	H	0.01290900	1.74229400	-0.12259300
	C	3.16304900	0.47455400	0.02996100
	H	3.64544900	-1.61855100	0.07721100
	H	2.38163500	2.47789800	-0.04173700
	H	4.19762300	0.79549700	0.05933500
TS2A	C	0.89235500	-0.37992000	0.79716500
	O	1.60493200	0.60494500	1.17147800
	O	2.94912000	0.80116500	-0.27014500
	O	2.89415000	-0.45604400	-0.60495600
	C	1.65433600	-0.79485600	-0.89344400
	H	1.09339500	-0.06773800	-1.47249000
	H	1.55092300	-1.85059300	-1.11908600
	H	1.07706800	-1.34774400	1.28872400
	C	-0.53965800	-0.14988600	0.38961700
	C	-1.43220000	-1.21713300	0.35988200
	C	-0.96634500	1.12705000	0.03092200
	C	-2.75423300	-1.01030800	-0.02358700
	H	-1.09757200	-2.20830400	0.65198600
	C	-2.28555100	1.33101400	-0.35313500
	H	-0.25695900	1.94641200	0.07379900
	C	-3.18091700	0.26352900	-0.38256600
	H	-3.44923300	-1.84140100	-0.03777400
	H	-2.62002500	2.32504700	-0.62557300
	H	-4.20993800	0.42685600	-0.67972100

CH ₂ OO	C	1.05982600	-0.18797900	0.00000000
	H	1.01164500	-1.27314700	0.00000000
	O	0.00000000	0.45689000	0.00000000
	H	1.96879400	0.40072300	0.00000000
	O	-1.16742400	-0.20685300	0.00000000
PhCHO	C	-0.29968100	2.02235400	0.00000000
	H	0.59084800	2.68231300	0.00000000
	C	0.00000000	0.56889600	0.00000000
	C	1.32651900	0.14345600	0.00000000
	C	-1.03847700	-0.36408800	0.00000000
	C	1.62100400	-1.21565200	0.00000000
	H	2.12587500	0.87816700	0.00000000
	C	-0.74406600	-1.71913800	0.00000000
	H	-2.06117600	-0.00483100	0.00000000
	C	0.58496600	-2.14364600	0.00000000
	H	2.65112000	-1.55074900	0.00000000
	H	-1.54510500	-2.44856100	0.00000000
	H	0.81109000	-3.20364900	0.00000000
	O	-1.40928100	2.48677700	0.00000000
TS2B	C	1.80782200	0.62265200	1.16924000
	O	3.01981900	0.37189400	0.89005200
	O	2.87249500	-0.49664600	-0.87867400
	O	1.60208300	-0.77055400	-0.76910400
	C	0.90945400	0.32216800	-0.45740200
	H	1.24746600	1.21515600	-0.97878300
	H	1.25912500	-0.06902600	1.82341600
	H	1.50385700	1.67715500	1.24505100
	C	-0.53449600	0.12555300	-0.24797500
	C	-1.40349200	1.19280900	-0.47289700
	C	-1.03273400	-1.09459300	0.21720900
	C	-2.76579000	1.04155700	-0.24184700
	H	-1.01298600	2.13880400	-0.83345700
	C	-2.39491500	-1.24409300	0.43386300
	H	-0.35059100	-1.91729300	0.39832800
	C	-3.26201300	-0.17689600	0.20866900
	H	-3.43878900	1.87167900	-0.41825700
	H	-2.78214300	-2.19239500	0.78650800
	H	-4.32413100	-0.29657600	0.38583800
HCHO	C	0.00000000	0.00000000	-0.52559400
	H	0.00000000	0.93967600	-1.10736700

	O	0.00000000	0.00000000	0.67103700
	H	0.00000000	-0.93967600	-1.10736700
trans-PhCHOO	C	-1.43896900	0.53226200	0.00023900
	O	-2.28621000	-0.38397500	-0.00035300
	C	-0.02315200	0.22697300	0.00017900
	C	0.88268600	1.29231200	0.00001600
	C	0.44500000	-1.09426300	0.00020000
	C	2.24829700	1.04159200	-0.00013000
	H	0.51289400	2.31193800	0.00000700
	C	1.80836900	-1.33526200	0.00005400
	H	-0.26520300	-1.91215600	0.00030400
	C	2.71009400	-0.27035300	-0.00012000
	H	2.94945800	1.86675900	-0.00023800
	H	2.17491200	-2.35435000	0.00004100
	H	3.77560200	-0.46675100	-0.00029200
	H	-1.82267800	1.55186000	0.00071300
	O	-3.60365700	-0.03563300	-0.00004200
cis-PhCHOO	O	-2.64016100	0.97581600	0.00019000
	O	-2.56334900	-0.37736600	0.00005300
	C	-1.44675400	-0.95042900	-0.00024000
	H	-1.55114900	-2.03268700	0.00016400
	C	-0.12315700	-0.37595700	-0.00012900
	C	0.93090100	-1.30925700	0.00001800
	C	0.16753800	1.00047700	-0.00013800
	C	2.24652200	-0.88513600	0.00010500
	H	0.70554000	-2.37056400	0.00004600
	C	1.49494600	1.41108000	-0.00005000
	H	-0.64838800	1.70559100	-0.00024000
	C	2.52842900	0.48099500	0.00007100
	H	3.05169300	-1.60911400	0.00019800
	H	1.72131200	2.47032300	-0.00007600
	H	3.55852100	0.81820800	0.00014300
trans-HONO	N	-0.16162800	0.48087000	0.00001100
	O	1.01721300	-0.25463200	0.00001100
	O	-1.08972100	-0.21824500	-0.00002600
	H	1.71145900	0.41693200	0.00004500
cis-HONO	N	-0.15994300	-0.51612800	-0.00009100
	O	1.06914800	0.06839400	0.00004400

	O	-1.04522500	0.25390400	0.00001300
	H	0.92821300	1.03451500	0.00017300
trans-TSot	O	1.61088600	-1.46444200	0.00000000
	O	-0.01784500	-0.89059700	0.00000000
	C	0.00000000	0.32668700	0.00000000
	H	0.97671300	0.82894500	0.00000000
	N	3.32031300	-2.27958500	0.00000000
	O	2.96874100	-3.58387400	0.00000000
	O	4.46985700	-2.08837900	0.00000000
	H	1.99824700	-3.48809000	0.00000000
	C	-1.21756200	1.14260300	0.00000000
	C	-1.09073000	2.53218700	0.00000000
	C	-2.48202300	0.54535700	0.00000000
	C	-2.22841000	3.32988100	0.00000000
	H	-0.10313300	2.98150700	0.00000000
	C	-3.61336700	1.34454300	0.00000000
	H	-2.55490200	-0.53575700	0.00000000
	C	-3.48533600	2.73423900	0.00000000
	H	-2.13637900	4.40881400	0.00000000
	H	-4.59740100	0.89217600	0.00000000
	H	-4.37389000	3.35485100	0.00000000
cis-TSot	O	-2.15589900	-0.14984400	-0.09568800
	O	-0.53586300	-0.68139300	0.02899500
	C	0.21626500	0.26574700	-0.10229500
	H	-0.22297400	1.25783000	-0.27090200
	N	-3.96345600	0.25517600	-0.00493600
	O	-4.73163800	-0.62961000	-0.68468300
	O	-4.51687400	0.82416000	0.85842600
	H	-5.61441200	-0.59813000	-0.27093600
	C	1.67602300	0.13296100	-0.04372800
	C	2.46290000	1.27194500	-0.21592200
	C	2.27059900	-1.11284900	0.17955800
	C	3.84770000	1.16903000	-0.16698600
	H	1.98810000	2.23246100	-0.38750500
	C	3.65136200	-1.21060100	0.22835800
	H	1.63716500	-1.98233000	0.31030400
	C	4.43775700	-0.07093500	0.05496800
	H	4.46366000	2.04966700	-0.30043700
	H	4.12143200	-2.17118400	0.40033400
	H	5.51777200	-0.15283800	0.09357500

HNO ₃	O	1.03999400	-0.74083600	-0.00009100
	N	0.14180800	0.03384600	0.00001900
	O	-1.11020600	-0.54973800	0.00007000
	O	0.16144400	1.23567700	-0.00000900
	H	-1.72250800	0.20225800	0.00011100
trans-TSoz	O	2.59438600	-1.02434300	0.88196500
	O	1.25534800	-1.13595700	0.85303400
	C	0.71517000	0.05362600	0.58888600
	O	2.52654500	-0.36322100	-0.91642200
	H	1.08362700	0.86636700	1.21259200
	O	2.25662700	1.76097400	-0.48739000
	N	1.67504300	0.49333300	-0.80120000
	H	1.75066100	2.37969300	-1.02773200
	C	-0.72999900	0.00697000	0.28744700
	C	-1.55947800	1.02736400	0.74537000
	C	-1.25313600	-1.04149600	-0.47015200
	C	-2.91860900	0.99867400	0.45190000
	H	-1.14407000	1.83628200	1.33698100
	C	-2.61066400	-1.06915400	-0.75532800
	H	-0.59289500	-1.82459900	-0.82452700
	C	-3.44243100	-0.04972000	-0.29590600
	H	-3.56650800	1.78920300	0.81006400
	H	-3.02276800	-1.88324000	-1.33899600
	H	-4.50171300	-0.07425000	-0.52277500
cis-TSoz	O	2.58366600	-0.94948900	0.88060300
	O	1.24147500	-0.98508900	0.99031700
	C	0.71677800	0.19097800	0.55761900
	O	2.37123900	-0.51310300	-0.94998600
	H	1.03181200	1.06074200	1.13216600
	O	2.32063800	1.65725000	-0.61736700
	H	3.22946400	1.39109200	-0.40240500
	N	1.62738900	0.44951500	-0.79550100
	C	-0.73589100	0.08198500	0.27490600
	C	-1.58508600	1.13038700	0.61613100
	C	-1.23701800	-1.05584200	-0.35664200
	C	-2.94299000	1.04141700	0.33078800
	H	-1.18509000	2.01338400	1.10255600
	C	-2.59384700	-1.14251100	-0.63560300
	H	-0.56197900	-1.86243200	-0.61801700
	C	-3.44586300	-0.09482600	-0.29302600
	H	-3.60536200	1.85585100	0.59709600

	H	-2.98892900	-2.02574300	-1.12239400
	H	-4.50428100	-0.16557600	-0.51405200
trans-ozonide	O	2.55504100	-0.80239300	0.82914000
	O	1.23076400	-0.64847400	1.25623500
	C	0.74122600	0.41143500	0.44618200
	O	2.33011000	-0.80657100	-0.59895200
	H	0.96477600	1.38546900	0.88360700
	O	2.41468900	1.43791100	-0.78181000
	N	1.57406800	0.31198800	-0.81030800
	H	2.60111400	1.60424300	-1.71185400
	C	-0.71822300	0.19168600	0.19872800
	C	-1.63802700	1.17847700	0.53123900
	C	-1.14788500	-1.00851200	-0.36629800
	C	-2.99473500	0.97106400	0.29612400
	H	-1.29611200	2.10802900	0.97368800
	C	-2.49972700	-1.21374300	-0.59921800
	H	-0.41805200	-1.77111100	-0.61475100
	C	-3.42368100	-0.22384100	-0.26778100
	H	-3.71196100	1.73984200	0.55652000
	H	-2.83747700	-2.14544500	-1.03673600
	H	-4.47928800	-0.38811300	-0.44907400
cis-ozonide	O	-2.76288000	1.05661400	0.03948400
	O	-1.40353900	1.21776100	0.25757500
	C	-0.79756500	0.24555500	-0.59070800
	O	-2.84973700	-0.46547400	-0.36985400
	H	-1.03088100	0.47295300	-1.63407100
	O	-1.37363300	-1.34713500	1.06360400
	H	-1.41267200	-0.55934400	1.63079500
	N	-1.62158500	-0.92666200	-0.24153200
	C	0.66462700	0.12860500	-0.29773800
	C	1.30015900	-1.10744500	-0.38936700
	C	1.39241000	1.27391500	0.01583500
	C	2.66880600	-1.19340900	-0.16834800
	H	0.72161400	-1.99524000	-0.61540000
	C	2.76181600	1.17975600	0.23873900
	H	0.88912000	2.23089400	0.08951900
	C	3.40043700	-0.05168000	0.14527100
	H	3.16310000	-2.15495600	-0.23518100
	H	3.32766100	2.06960100	0.48656400
	H	4.46731400	-0.12316900	0.31992600

trans-TS1ca	C	0.57954400	0.04749100	-0.54993100
	O	1.13784400	-1.10128700	-0.79070800
	O	2.48903400	-0.96475600	-0.81450400
	O	1.47301700	0.19590100	1.09660900
	H	1.06723700	0.92156200	-0.97387300
	O	3.13393100	1.21366700	0.25387100
	N	2.66668200	0.04263000	0.83941200
	H	4.04557400	1.00307200	0.01398100
	C	-0.85251000	0.04585000	-0.26845400
	C	-1.59400600	1.19713300	-0.53289000
	C	-1.46793800	-1.08481600	0.27441900
	C	-2.95793600	1.21409400	-0.27146800
	H	-1.10257300	2.07255200	-0.94294400
	C	-2.83045000	-1.06228400	0.53053200
	H	-0.87182400	-1.96192500	0.49500100
	C	-3.57429800	0.08431700	0.25700600
	H	-3.53759200	2.10496600	-0.47921300
	H	-3.31443600	-1.93495700	0.95136700
	H	-4.63819400	0.09742000	0.46236900
cis-TS1ca	C	0.54015100	0.08498600	-0.62848400
	O	1.11905800	-1.04542800	-0.87644400
	O	2.46512800	-0.87657000	-0.89748000
	O	1.49061700	0.25811100	1.03539000
	H	0.99365300	0.96632700	-1.07390900
	O	3.41420100	1.02301500	0.42280900
	H	2.79093800	1.75668100	0.29065500
	N	2.67917500	-0.05627300	0.81921500
	C	-0.87725800	0.06270700	-0.29538700
	C	-1.65945200	1.18434400	-0.57286500
	C	-1.44082500	-1.06436000	0.30865900
	C	-3.01298900	1.17406900	-0.26374700
	H	-1.20922900	2.05701600	-1.03351500
	C	-2.79365800	-1.06939100	0.61110100
	H	-0.81110400	-1.91480300	0.53987300
	C	-3.57805200	0.04684400	0.32474900
	H	-3.62485400	2.04066500	-0.48145900
	H	-3.23894800	-1.93904800	1.07820200
	H	-4.63421800	0.03885500	0.56728900
trans-RCca	C	-0.66841700	-0.19573400	0.83624900
	O	-1.34911000	-1.25889900	0.21788800

	O	-1.69918700	-0.59901900	-1.02817900
	O	-1.45778000	0.95045800	0.49175700
	H	-0.76036000	-0.36106800	1.91209100
	O	-3.52549500	0.30786300	-0.09961700
	N	-2.27576300	0.57303300	-0.60208700
	C	0.76245100	-0.05151300	0.38113700
	C	1.53876900	-1.19697000	0.22193800
	C	1.31984600	1.20645700	0.17755400
	C	2.87409700	-1.08208600	-0.14387300
	H	1.09157100	-2.17392700	0.36817200
	C	2.65883000	1.31695700	-0.18393200
	H	0.70393400	2.09015400	0.28967700
	C	3.43635900	0.17560200	-0.34343600
	H	3.47465400	-1.97394900	-0.27653800
	H	3.09252000	2.29661900	-0.34559900
	H	4.47778600	0.26393900	-0.62907200
	H	-3.42880100	-0.39249300	0.56726100
cis-RCca	C	-0.65857400	-0.11033700	0.79955900
	O	-1.33203400	-1.23897400	0.31288900
	O	-1.80378900	-0.72762600	-0.95712900
	O	-1.41328800	1.00400900	0.27742500
	H	-0.77751200	-0.13098000	1.88475400
	O	-3.49197400	0.24894700	0.12602800
	H	-4.18566400	0.63697100	-0.41773600
	N	-2.33632000	0.48251700	-0.62185300
	C	0.78259800	-0.01804000	0.36052800
	C	1.52966800	-1.18400000	0.21590200
	C	1.38004800	1.22347500	0.16097000
	C	2.87383000	-1.10651900	-0.13083100
	H	1.05353100	-2.14685400	0.36078400
	C	2.72557000	1.29673000	-0.18204900
	H	0.78877600	2.12596000	0.25868000
	C	3.47404900	0.13316800	-0.32697500
	H	3.45105000	-2.01554400	-0.25059300
	H	3.18800500	2.26365600	-0.34130400
	H	4.52160200	0.19146100	-0.59794900
trans-TS2ca	C	-0.60300400	1.17904100	0.66605900
	O	-0.95943400	2.14546100	0.00078300
	O	-3.42336200	-0.93340900	-0.37725100
	O	-1.62740800	0.13237400	1.05665200
	H	-0.81010400	1.17042900	1.85429400

	O	-1.50432400	-0.85223200	-1.29082300
	N	-2.29922000	-0.71682400	-0.23081000
	H	-0.60447600	-0.60712700	-0.98564900
	C	0.71844900	0.47678800	0.36829500
	C	1.11362300	-0.68229700	1.04093300
	C	1.53916500	1.02563300	-0.61646200
	C	2.32206200	-1.29092400	0.72279900
	H	0.47139000	-1.09920000	1.80907600
	C	2.74710800	0.41202300	-0.93323100
	H	1.20761800	1.92996600	-1.11385700
	C	3.13802300	-0.74417000	-0.26487000
	H	2.62884200	-2.18909600	1.24527900
	H	3.38490800	0.83840000	-1.69829800
	H	4.08002100	-1.21972500	-0.51120600
cis-TS2ca	C	0.60512000	0.59056900	-0.93108700
	O	1.12809800	1.67435500	-0.69811900
	O	3.52950200	-0.29579700	0.40839500
	O	1.55341900	-0.64149900	-0.92150400
	H	0.80151100	0.10131300	-2.01951900
	O	1.62420300	-0.21926400	1.42001000
	H	2.13102400	0.47445100	1.88657800
	N	2.41102000	-0.64835900	0.41770200
	C	-0.76684900	0.21881000	-0.44299800
	C	-1.27989700	-1.06663200	-0.60729800
	C	-1.53490300	1.20992100	0.16285900
	C	-2.55720700	-1.36324600	-0.14877300
	H	-0.67259500	-1.82940700	-1.08081900
	C	-2.81248900	0.90998200	0.61962200
	H	-1.11347000	2.20251100	0.26922400
	C	-3.32338900	-0.37584800	0.46508000
	H	-2.95650400	-2.36314500	-0.26976900
	H	-3.41097800	1.67798900	1.09498700
	H	-4.32021500	-0.60890000	0.82071800
PhCOOH	C	-0.05571100	1.73662900	0.00000000
	O	-1.08578700	2.34346500	0.00000000
	O	1.11455100	2.40548700	0.00000000
	H	1.86394700	1.80491800	0.00000000
	C	0.00000000	0.23307400	0.00000000
	C	1.18304000	-0.50760900	0.00000000
	C	-1.22500200	-0.43509400	0.00000000
	C	1.14073300	-1.89707800	0.00000000

	H	2.16014000	-0.03457100	0.00000000
	C	-1.26716500	-1.82211000	0.00000000
	H	-2.13241100	0.15583500	0.00000000
	C	-0.08394400	-2.55509300	0.00000000
	H	2.06385200	-2.46343100	0.00000000
	H	-2.22245700	-2.33261800	0.00000000
	H	-0.11489400	-3.63805400	0.00000000
trans-RCha	O	-1.99814000	2.01069800	-0.35161400
	O	-0.73071900	1.61261300	0.06913700
	C	-0.15237400	0.76312400	-0.63917800
	H	-0.67333500	0.41486000	-1.53088700
	N	-3.38654600	-0.80040100	0.66325100
	O	-2.83504300	-0.38314700	-0.50046900
	H	-2.69532200	0.62096700	-0.40597500
	O	-3.56339500	-1.96212300	0.67524800
	C	1.15407600	0.27046000	-0.27429500
	C	1.74225700	-0.69228700	-1.10156000
	C	1.82254700	0.73556500	0.86752400
	C	2.99923200	-1.19022300	-0.79018600
	H	1.20998100	-1.04722700	-1.97733000
	C	3.07617700	0.23478500	1.16807000
	H	1.35065700	1.47923900	1.49828200
	C	3.66250700	-0.72544700	0.34088400
	H	3.45891800	-1.93766300	-1.42417600
	H	3.60232500	0.58616100	2.04679300
	H	4.64444800	-1.11371500	0.58456200
trans-TSha	O	-2.74428900	-1.51177100	-0.06166000
	O	-1.37247800	-1.49993800	-0.41969200
	C	-0.66962700	-0.97993900	0.50414800
	H	-1.08135100	-0.95444800	1.50788100
	N	-2.09293000	1.60797000	-0.43122700
	O	-2.23388000	0.74606300	0.55291400
	H	-2.79550000	-0.43341100	0.17223200
	O	-1.20746500	2.39018000	-0.25879000
	C	0.67456100	-0.57067900	0.22905500
	C	1.47083200	-0.17783300	1.31259500
	C	1.16768900	-0.52064000	-1.08391600
	C	2.77099600	0.24137600	1.08679900
	H	1.05905900	-0.19213000	2.31536600
	C	2.46701300	-0.10032900	-1.29794700
	H	0.52293200	-0.79402400	-1.91028600

	C	3.26432100	0.27591900	-0.21522200
	H	3.39500500	0.55047000	1.91539900
	H	2.86151100	-0.04886400	-2.30465800
	H	4.27903000	0.61309900	-0.39259200
Ph-HMPH	O	-2.64713100	-1.81283500	0.24105300
	O	-1.38352900	-1.40476100	-0.27972400
	C	-0.86973800	-0.45613100	0.60415800
	H	-1.01046700	-0.80108900	1.63170700
	N	-1.54942400	1.34475800	-0.70770000
	O	-1.62572800	0.74630600	0.56567000
	O	-2.19657100	2.30761700	-0.73603400
	C	0.59296500	-0.24597700	0.27394600
	C	1.21901500	0.92201600	0.70804100
	C	1.33227500	-1.22168000	-0.38888300
	C	2.57492900	1.11339600	0.47481000
	H	0.64360200	1.68146400	1.22490700
	C	2.68951700	-1.02385400	-0.62371400
	H	0.84699400	-2.12761500	-0.72761300
	C	3.31319800	0.14097500	-0.19283500
	H	3.05443700	2.02405900	0.81322800
	H	3.25785600	-1.78358800	-1.14687200
	H	4.37000000	0.29272500	-0.37728700
	H	-2.60574900	-2.76234700	0.07496000

Table S2 Frequencies for all optimized structures at the M06-2X/6-311++G(d,p) level of theory

species	frequencies
PhCH=CH ₂	21.54, 213.28, 246.44, 407.17, 447.70, 449.65, 554.30, 631.20, 662.45, 713.09, 791.72, 813.58, 860.05, 943.24, 960.29, 994.36, 1016.97, 1017.16, 1041.48, 1047.83, 1068.01, 1118.91, 1176.69, 1204.80, 1236.33, 1317.63, 1342.25, 1360.05, 1455.39, 1490.36, 1541.35, 1654.06, 1678.81, 1718.66, 3163.36, 3165.56, 3175.07, 3176.08, 3197.77, 3204.72, 3213.80, 3253.05
O ₃	798.04, 1365.82, 1367.56
TS1	-287.50, 45.24, 73.31, 98.65, 189.33, 231.31, 238.93, 348.26, 409.52, 449.05, 471.06, 522.14, 572.79, 629.65, 701.43, 724.57, 790.10, 800.93, 807.00, 869.62, 948.83, 958.30, 1004.52, 1006.20, 1017.91, 1022.56, 1046.14, 1065.34, 1116.86, 1180.41, 1198.48, 1205.42, 1241.45, 1270.37, 1302.56, 1336.46, 1355.23, 1451.86, 1491.51, 1538.57, 1608.83, 1661.17, 1678.58, 3169.78, 3180.25, 3186.78, 3187.59, 3197.53, 3206.84, 3213.15, 3265.12
C1	45.06, 78.85, 124.84, 217.13, 313.05, 338.98, 413.14, 426.23, 540.02, 739.43, 772.56, 794.42, 806.38, 874.63, 879.80, 950.78, 984.69, 999.49, 1005.57, 1020.13, 1025.25, 1044.79, 1062.63, 1073.64, 1077.33, 1118.39, 1179.32, 1204.04, 1234.98, 1251.07, 1312.69, 1323.30, 1351.80, 1358.38, 1404.86, 1499.50, 1510.20, 1544.44, 1667.02, 1685.84, 3078.05, 3102.37, 3163.49, 3179.91,

	3183.53, 3194.27, 3201.44, 3213.56
TS2A	-545.58, 55.58, 73.78, 108.50, 231.82, 257.88, 350.22, 413.21, 431.03, 507.74, 528.29, 605.20, 626.46, 628.30, 652.89, 716.92, 782.06, 833.67, 874.79, 909.02, 948.66, 1006.82, 1009.24, 1019.00, 1023.46, 1059.95, 1108.32, 1109.97, 1163.57, 1179.85, 1193.22, 1222.52, 1271.52, 1310.31, 1325.67, 1350.60, 1374.45, 1464.58, 1498.31, 1515.38, 1538.13, 1670.27, 1680.90, 3015.78, 3125.66, 3169.20, 3182.91, 3190.29, 3200.68, 3208.18, 3256.47
CH ₂ OO	545.08, 705.03, 911.84, 1019.29, 1263.91, 1438.99, 1625.16, 3138.44, 3297.03
PhCHO	117.76, 225.79, 238.48, 412.06, 444.48, 460.52, 627.35, 662.94, 704.85, 766.71, 845.12, 873.49, 953.79, 1013.29, 1020.61, 1030.13, 1048.25, 1056.88, 1110.54, 1182.13, 1193.02, 1238.63, 1336.39, 1351.66, 1423.80, 1498.47, 1537.48, 1665.55, 1678.74, 1845.32, 2962.86, 3165.00, 3183.59, 3200.16, 3209.43, 3215.08
TS2B	-556.76, 50.39, 97.21, 129.26, 200.05, 253.27, 341.53, 410.33, 426.04, 447.97, 542.63, 546.41, 596.56, 630.32, 677.64, 711.44, 786.86, 871.55, 878.17, 920.10, 956.61, 1011.64, 1019.20, 1030.10, 1031.59, 1062.75, 1113.65, 1156.61, 1182.54, 1189.61, 1207.45, 1219.20, 1242.87, 1299.08, 1338.27, 1357.03, 1414.19, 1438.91, 1504.66, 1546.90, 1553.66, 1662.53, 1685.27, 2985.43, 3068.92, 3165.48, 3188.64, 3194.40, 3201.33, 3209.62, 3223.16

HCHO	1224.08, 1276.63, 1545.51, 1880.36, 2957.59, 3028.40
trans-PhCHOO	91.38, 152.53, 174.10, 292.39, 379.99, 405.59, 443.19, 495.61, 626.83, 651.71, 688.07, 771.77, 869.78, 884.31, 948.27, 958.69, 1001.00, 1006.97, 1018.15, 1022.13, 1059.60, 1119.89, 1186.36, 1204.35, 1248.29, 1346.25, 1359.04, 1400.77, 1492.88, 1541.78, 1617.76, 1662.89, 1680.50, 3172.95, 3187.53, 3194.93, 3200.54, 3209.30, 3217.54
cis-PhCHOO	80.56, 160.10, 230.72, 322.04, 403.64, 409.68, 483.50, 552.47, 626.61, 689.47, 736.48, 770.55, 868.87, 873.17, 916.53, 932.59, 971.14, 1013.56, 1014.87, 1035.83, 1061.37, 1116.50, 1185.87, 1203.82, 1235.04, 1346.98, 1354.94, 1428.54, 1486.43, 1528.25, 1619.98, 1647.41, 1673.83, 3182.93, 3187.19, 3196.96, 3205.09, 3216.19, 3248.86
trans-HONO	607.95, 706.16, 908.70, 1340.55, 1858.89, 3831.94
cis-HONO	689.81, 707.05, 979.83, 1367.69, 1786.31, 3664.61
trans-TSot	-597.81, 30.55, 42.65, 60.27, 104.30, 144.60, 151.78, 168.53, 264.82, 308.17, 408.79, 456.13, 457.62, 502.91, 503.45, 627.46, 674.97, 695.99, 729.95, 733.57, 771.96, 867.08, 871.43, 960.46, 1011.87, 1020.14, 1027.16, 1035.06, 1053.68, 1058.29, 1115.42, 1186.27, 1196.50, 1245.00, 1341.88, 1355.91, 1398.84, 1411.73, 1497.64, 1539.74, 1663.11, 1676.52, 1765.90, 1847.24, 3106.94, 3170.54, 3185.70, 3208.49, 3212.22, 3225.16, 3689.31

cis-TSot	-659.52, 37.35, 45.90, 58.27, 102.09, 128.43, 142.11, 175.89, 265.79, 344.81, 410.96, 415.65, 454.50, 482.71, 523.50, 627.37, 674.65, 682.54, 693.51, 723.14, 768.15, 866.85, 874.75, 959.20, 1002.32, 1009.09, 1020.22, 1028.67, 1057.20, 1058.65, 1116.79, 1182.57, 1199.94, 1245.64, 1342.09, 1356.22, 1391.69, 1400.07, 1496.15, 1540.64, 1659.53, 1680.10, 1766.10, 1783.13, 3104.63, 3181.52, 3190.20, 3197.94, 3203.72, 3218.56, 3676.78
HNO ₃	464.39, 624.79, 710.55, 815.32, 981.84, 1362.41, 1429.16, 1831.92, 3797.70
trans-TSoz	-365.63, 34.01, 89.88, 104.57, 195.70, 230.37, 290.49, 334.05, 357.59, 403.44, 410.10, 431.05, 554.02, 623.41, 645.01, 657.74, 681.68, 685.60, 711.38, 788.74, 871.18, 893.14, 914.41, 955.80, 1006.82, 1021.53, 1026.34, 1062.65, 1086.39, 1115.10, 1144.37, 1185.15, 1205.16, 1232.18, 1291.28, 1315.82, 1340.21, 1356.67, 1432.44, 1477.46, 1506.78, 1550.50, 1671.60, 1688.26, 3162.90, 3175.99, 3187.12, 3197.76, 3203.63, 3213.36, 3864.64
cis-TSoz	-248.49, 41.04, 98.36, 103.90, 190.79, 247.07, 262.83, 342.98, 359.18, 405.37, 413.37, 459.75, 580.61, 627.04, 653.77, 676.38, 704.74, 711.44, 722.91, 797.56, 874.09, 897.24, 957.13, 969.23, 1009.64, 1022.33, 1028.12, 1062.89, 1088.97, 1111.25, 1147.48, 1183.16, 1203.99, 1237.62, 1267.76, 1338.10, 1354.85, 1382.63, 1416.05, 1478.81, 1504.42, 1549.50, 1672.24, 1690.94, 3173.81, 3182.14, 3188.55, 3196.47, 3205.84, 3212.60, 3757.87

trans-ozonide	19.19, 75.38, 107.45, 197.66, 284.26, 328.54, 345.08, 380.67, 410.99, 433.47, 530.29, 627.08, 635.19, 669.82, 693.57, 713.49, 751.29, 782.33, 842.19, 865.09, 881.66, 942.70, 967.45, 992.07, 1001.45, 1013.74, 1021.56, 1023.09, 1061.11, 1064.10, 1086.24, 1123.95, 1182.49, 1205.96, 1243.39, 1327.39, 1335.73, 1356.00, 1398.55, 1423.30, 1502.88, 1547.76, 1671.21, 1690.22, 3141.54, 3178.97, 3182.07, 3192.86, 3199.78, 3213.07, 3888.60
cis-ozonide	35.30, 105.67, 143.59, 215.46, 242.76, 303.49, 334.32, 383.01, 408.57, 411.02, 458.21, 501.76, 601.72, 630.67, 675.59, 713.96, 754.51, 786.79, 847.57, 860.21, 880.27, 938.27, 967.86, 1012.96, 1022.46, 1028.50, 1030.48, 1040.44, 1066.86, 1116.66, 1132.61, 1134.25, 1181.22, 1211.30, 1258.99, 1322.36, 1350.73, 1358.39, 1412.93, 1434.41, 1495.86, 1550.55, 1665.23, 1691.63, 3135.51, 3188.84, 3196.42, 3203.31, 3217.26, 3222.47, 3748.77
trans-TS1ca	-362.87, 42.84, 85.24, 112.55, 183.05, 241.39, 316.70, 351.76, 404.26, 410.38, 421.75, 472.12, 536.84, 576.36, 625.31, 631.15, 671.75, 705.65, 735.70, 787.44, 871.62, 899.57, 932.49, 960.25, 1010.03, 1020.92, 1029.36, 1061.53, 1077.06, 1106.29, 1119.39, 1186.67, 1203.61, 1246.84, 1294.09, 1340.28, 1346.78, 1357.11, 1471.74, 1503.37, 1517.81, 1554.13, 1667.34, 1686.48, 3184.04, 3192.97, 3194.57, 3204.33, 3215.11, 3222.29, 3853.72
cis-TS1ca	-367.55, 47.07, 80.51, 92.45, 164.29, 233.01, 329.03, 352.16, 392.75, 410.05, 421.19, 457.16, 536.13, 566.38,

	629.38, 650.63, 670.07, 705.88, 714.04, 790.04, 877.55, 898.16, 964.19, 975.29, 1014.53, 1020.08, 1033.76, 1058.96, 1064.70, 1082.43, 1118.06, 1186.29, 1201.65, 1242.64, 1275.47, 1342.55, 1348.20, 1354.57, 1463.97, 1472.99, 1519.82, 1552.99, 1665.44, 1681.41, 3183.29, 3186.04, 3197.06, 3207.56, 3217.78, 3222.57, 3731.17
trans-RCca	18.43, 71.31, 133.66, 183.05, 255.33, 326.49, 407.58, 419.54, 446.32, 472.88, 582.84, 604.09, 630.47, 669.47, 710.92, 733.43, 753.02, 808.64, 869.22, 873.36, 904.55, 918.81, 964.31, 971.00, 1006.25, 1017.57, 1020.77, 1022.93, 1037.03, 1061.30, 1087.12, 1114.59, 1180.38, 1202.34, 1254.03, 1280.07, 1341.51, 1350.19, 1378.53, 1447.78, 1493.15, 1543.52, 1666.64, 1688.26, 3132.21, 3177.48, 3191.42, 3196.10, 3212.32, 3216.81, 3754.17
cis-RCca	32.46, 62.05, 142.22, 162.64, 253.53, 298.19, 335.70, 408.40, 452.83, 459.28, 569.55, 623.04, 630.79, 659.37, 713.77, 753.54, 764.10, 813.55, 873.47, 887.75, 910.53, 947.91, 963.17, 990.00, 1005.95, 1010.67, 1016.08, 1020.27, 1022.99, 1065.08, 1105.13, 1120.76, 1182.39, 1212.88, 1256.33, 1281.03, 1339.80, 1358.25, 1386.70, 1419.83, 1492.89, 1546.11, 1665.97, 1687.71, 3130.14, 3181.60, 3192.69, 3199.44, 3214.73, 3217.54, 3882.80
trans-TS2ca	-1098.54, 43.64, 48.47, 60.33, 95.46, 167.97, 208.54, 226.35, 292.25, 409.53, 417.47, 450.11, 526.42, 564.77, 624.38, 646.83, 656.46, 703.78, 744.57, 756.74, 808.24, 883.01, 888.15, 916.16, 976.17, 1020.59, 1021.92, 1033.69,

	1056.79, 1086.96, 1103.77, 1115.46, 1175.48, 1184.71, 1216.36, 1329.72, 1344.64, 1432.18, 1487.73, 1526.69, 1643.88, 1671.37, 1675.06, 1888.59, 2239.19, 3182.60, 3188.94, 3197.03, 3205.29, 3209.84, 3557.37
cis-TS2ca	-1206.49, 41.92, 43.69, 68.66, 112.38, 186.49, 195.77, 281.08, 361.72, 410.69, 435.13, 442.38, 498.16, 545.54, 586.60, 627.17, 666.06, 699.15, 722.23, 748.41, 815.19, 841.59, 878.56, 917.15, 969.81, 1014.94, 1019.69, 1022.43, 1025.54, 1060.35, 1081.52, 1112.47, 1176.76, 1197.56, 1234.27, 1337.64, 1349.89, 1407.14, 1492.02, 1534.19, 1648.56, 1673.65, 1680.62, 1735.56, 2207.79, 3184.57, 3192.20, 3199.87, 3216.29, 3224.27, 3667.90
PhCOOH	-159.20, 156.24, 214.45, 242.84, 391.70, 413.53, 443.39, 494.73, 628.55, 660.07, 682.77, 711.29, 797.30, 805.75, 856.09, 941.98, 1011.84, 1019.52, 1037.31, 1064.28, 1110.75, 1133.12, 1184.69, 1203.25, 1222.27, 1336.08, 1353.63, 1362.32, 1494.29, 1543.51, 1666.83, 1683.34, 1885.50, 3149.89, 3188.16, 3202.00, 3216.79, 3234.83, 3924.47
trans-RCha	23.30, 41.83, 66.67, 113.87, 123.43, 146.85, 155.16, 221.91, 267.02, 327.98, 384.18, 405.85, 445.33, 495.82, 622.87, 650.18, 692.52, 778.34, 782.07, 874.23, 883.20, 941.17, 965.03, 1013.29, 1016.63, 1019.52, 1033.34, 1038.72, 1056.23, 1118.31, 1173.18, 1178.87, 1200.55, 1258.60, 1347.17, 1357.76, 1417.41, 1465.10, 1491.01, 1538.13, 1628.24, 1663.05, 1678.95, 1795.04, 2795.90,

	3186.08, 3191.17, 3197.86, 3200.73, 3209.95, 3214.32
trans-TSha	-218.25, 26.95, 45.76, 83.25, 108.39, 126.77, 163.16, 284.43, 332.74, 355.51, 403.04, 418.60, 474.62, 542.52, 624.10, 655.52, 683.49, 780.40, 859.17, 869.82, 886.60, 960.84, 986.82, 994.04, 996.70, 1017.92, 1020.47, 1034.77, 1058.12, 1124.66, 1188.87, 1204.53, 1264.17, 1312.52, 1338.23, 1356.85, 1367.96, 1430.94, 1495.26, 1538.98, 1595.40, 1658.10, 1674.10, 1683.56, 1946.31, 3188.95, 3192.86, 3209.04, 3220.64, 3223.50, 3228.89
Ph-HMPH	31.58, 76.76, 91.82, 145.94, 201.35, 207.23, 232.85, 238.44, 333.35, 355.19, 411.48, 429.53, 478.10, 575.34, 629.52, 655.74, 691.77, 713.88, 763.94, 868.53, 912.61, 961.85, 1011.39, 1020.37, 1025.93, 1032.30, 1063.56, 1093.69, 1106.84, 1156.38, 1179.42, 1203.13, 1239.00, 1327.42, 1349.04, 1363.82, 1405.56, 1432.66, 1494.50, 1542.13, 1666.57, 1687.43, 1860.36, 3115.15, 3186.08, 3195.98, 3203.07, 3210.49, 3217.62, 3854.22

Table S3 Electronic energy (E) at M06-2X/6-311++G(d,p) and CCSD(T)/6-311++G(3df,3pd) level, T1 diagnostic value for various species at CCSD(T)/6-311++G(3df,3pd) level

species	E/ M06-2X	E/ CCSD(T)	T1 diagnostic/ CCSD(T)
PhCH=CH ₂	-309.581961	-309.245663	0.018
O ₃	-225.375293	-225.130468	0.02
TS1	-534.961925	-534.380796	0.016
C1	-535.073743	-534.492492	0.019
TS2A	-535.034184	-534.452976	0.017
CH ₂ OO	-189.551583	-189.316282	0.02
PhCHO	-345.515956	-345.140622	0.02
TS2B	-535.035508	-534.454299	0.017
HCHO	-114.487213	-114.336076	0.016
trans-PhCHOO	-420.583605	-420.126725	0.018
cis-PhCHOO	-420.581731	-420.125853	0.02
trans-HONO	-205.685454	-205.436452	0.02
cis-HONO	-205.684771	-205.435691	0.02
trans-TSot	-626.254045	-625.573746	0.016
cis-TSot	-626.242105	-625.561818	0.019
HNO ₃	-280.862511	-280.523901	0.018
trans-TSoz	-626.236076	-625.555796	0.016
cis-TSoz	-626.239440	-625.559156	0.019
trans-ozonide	-626.252631	-625.572333	0.018
cis-ozonide	-626.250311	-625.570015	0.02
trans-TS1ca	-626.263040	-625.582730	0.017
cis-TS1ca	-626.254998	-625.574697	0.019
trans-RCca	-626.295164	-625.614819	0.018
cis-RCca	-626.295164	-625.614819	0.02

trans-TS2ca	-626.259936	-625.579630	0.017
cis-TS2ca	-626.253819	-625.573520	0.019
PhCOOH	-420.761837	-420.304763	0.02
trans-RCha	-626.291115	-625.610775	0.019
trans-TSha	-626.280263	-625.599935	0.016
Ph-HMPH	-626.336365	-625.655976	0.018

Table S4 The activation energy and reaction energy of each reaction calculated at CCSD(T)/6-311++G(3df,3pd) level (kcal/mol)

Reaction	Activation Energy	Reaction Energy
(1) $\text{PhCH=CH}_2 + \text{O}_3 \rightarrow \text{TS1} \rightarrow \text{C1}$	1.46	-63.43
(2) $\text{C1} \rightarrow \text{TS2A} \rightarrow \text{CH}_2\text{OO} + \text{PhCHO}$	22.62	-0.50
(3) $\text{C1} \rightarrow \text{TS2B} \rightarrow \text{PhCHOO} + \text{HCHO}$	18.79	-2.17
(4) $\text{trans-PhCHOO} + \text{trans-HONO}$ $\rightarrow \text{trans-TSot} \rightarrow \text{PhCHO} + \text{HNO}_3$	8.25	-69.83
(5) $\text{trans-PhCHOO} + \text{cis-HONO}$ $\rightarrow \text{cis-TSot} \rightarrow \text{PhCHO} + \text{HNO}_3$	16.98	-69.83
(6) $\text{trans-PhCHOO} + \text{trans-HONO}$ $\rightarrow \text{trans-TSoz} \rightarrow \text{trans-Ozonide}$	19.52	9.13
(7) $\text{trans-PhCHOO} + \text{trans-HONO}$ $\rightarrow \text{cis-TSoz} \rightarrow \text{cis-Ozonide}$	15.31	10.16
(8) $\text{trans-PhCHOO} + \text{trans-HONO}$ $\rightarrow \text{trans-TS1ca} \rightarrow \text{trans-RCca}$	2.60	-17.56
(9) $\text{trans-RCca} \rightarrow \text{trans-TS2ca} \rightarrow$ $\text{PhCOOH} + \text{trans-HONO}$	22.11	-95.46
(10) $\text{trans-PhCHOO} + \text{cis-HONO}$ $\rightarrow \text{cis-TS1ca} \rightarrow \text{cis-RCca}$	7.22	-17.99
(11) $\text{cis-RCca} \rightarrow \text{cis-TS2ca} \rightarrow$ $\text{PhCOOH} + \text{cis-HONO}$	25.95	-95.03
(12) $\text{trans-RCha} \rightarrow \text{trans-TSha} \rightarrow \text{Ph-HMPH}$	9.35	-25.85

Table S5 K_{eq} , rate constant (k_2 and k_{ha}) corrected by tunneling effect for hydrogen atom transfer reaction pathway in 238-338 K ($\text{cm}^3/(\text{molecule}\cdot\text{s})$)

T	K_{eq}	k_2	$k_{ha} = K_{eq} \times k_2$
238	3.03×10^{12}	2.26×10^{-24}	6.85×10^{-12}
248	7.82×10^{11}	6.64×10^{-24}	5.19×10^{-12}
258	2.63×10^{11}	1.15×10^{-23}	3.02×10^{-12}
268	7.03×10^{10}	2.36×10^{-23}	1.66×10^{-12}
278	2.05×10^{10}	4.62×10^{-23}	9.47×10^{-13}
288	8.24×10^9	8.68×10^{-23}	7.15×10^{-13}
298	3.57×10^9	1.59×10^{-22}	5.68×10^{-13}
308	1.29×10^9	2.73×10^{-22}	3.52×10^{-13}
318	4.90×10^8	4.61×10^{-22}	2.26×10^{-13}
328	1.35×10^8	7.54×10^{-22}	1.02×10^{-13}
338	7.44×10^7	1.20×10^{-21}	8.93×10^{-14}

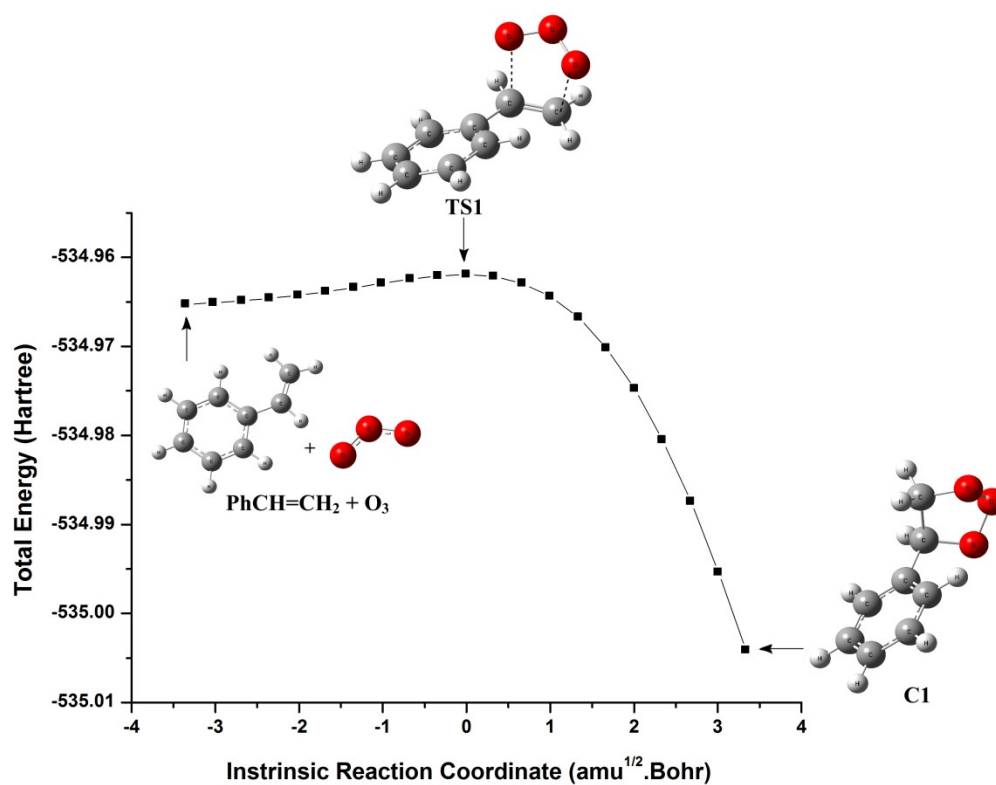


Fig. S1(a) Intrinsic reaction coordinate (IRC) profile for the reaction of PhCH=CH₂ + O₃ → TS1 → C1 at M06-2X/6-311++G(d,p) level

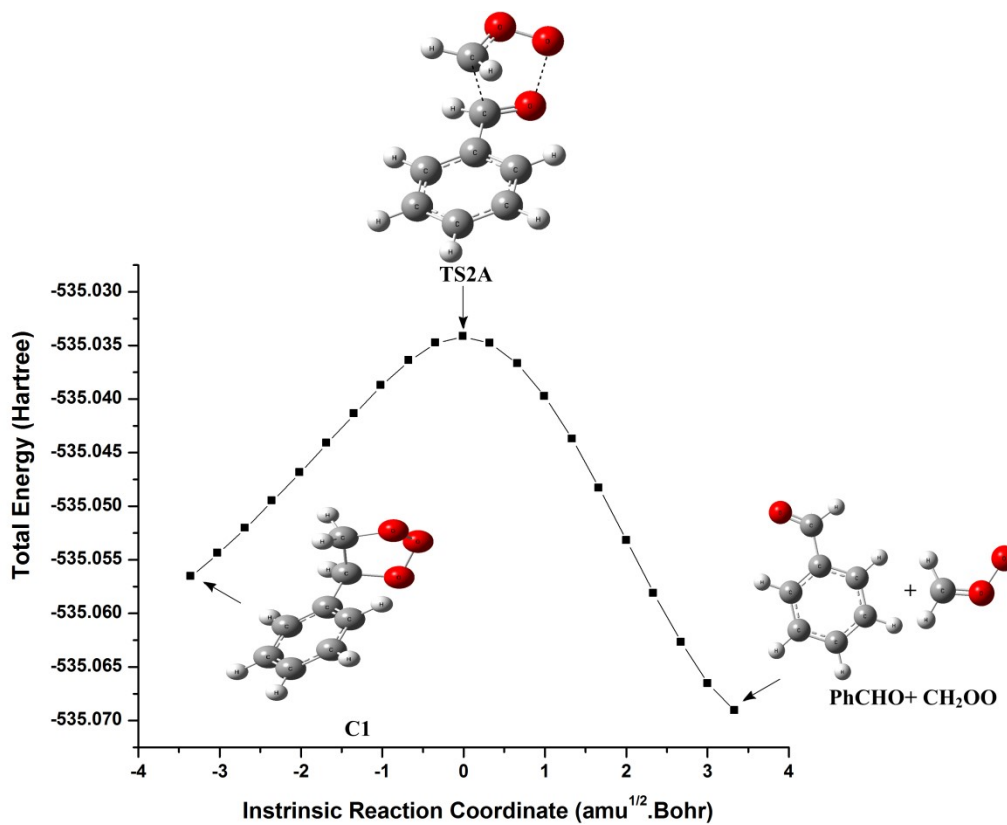


Fig. S1(b) Intrinsic reaction coordinate (IRC) profile for the reaction of

C1→TS2A→PhCHO + CH₂OO at M06-2X/6-311++G(d,p) level

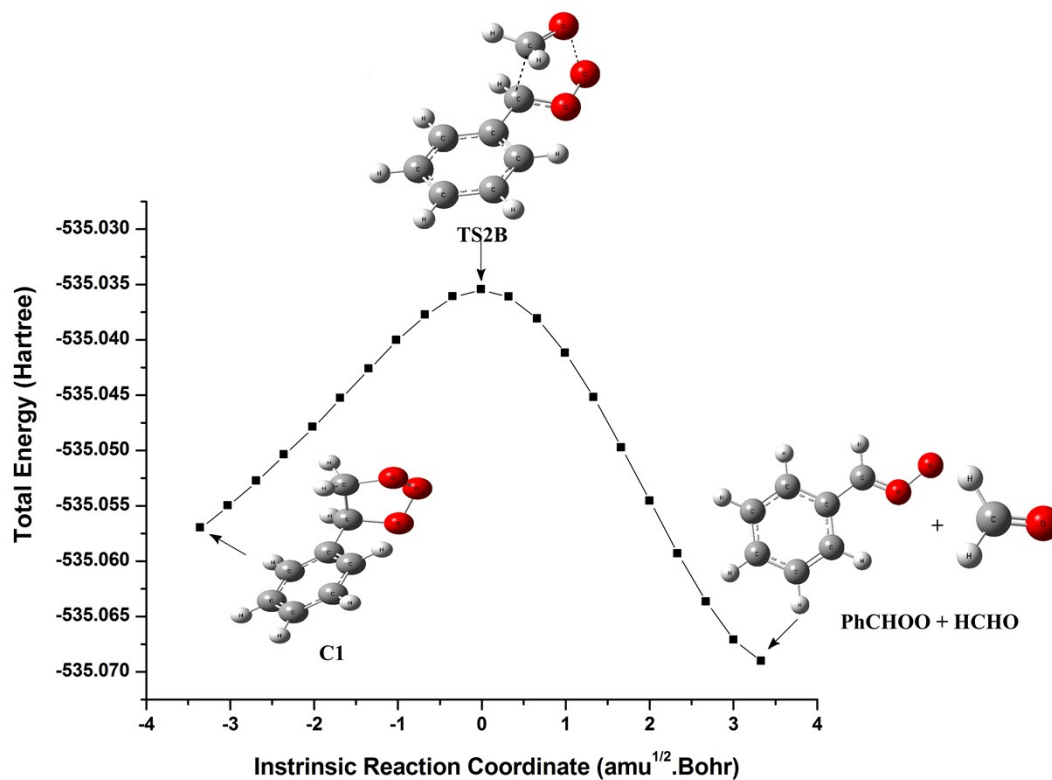


Fig. S1(c) Intrinsic reaction coordinate (IRC) profile for the reaction of C1→TS2B→PhCHOO + HCHO at M06-2X/6-311++G(d,p) level

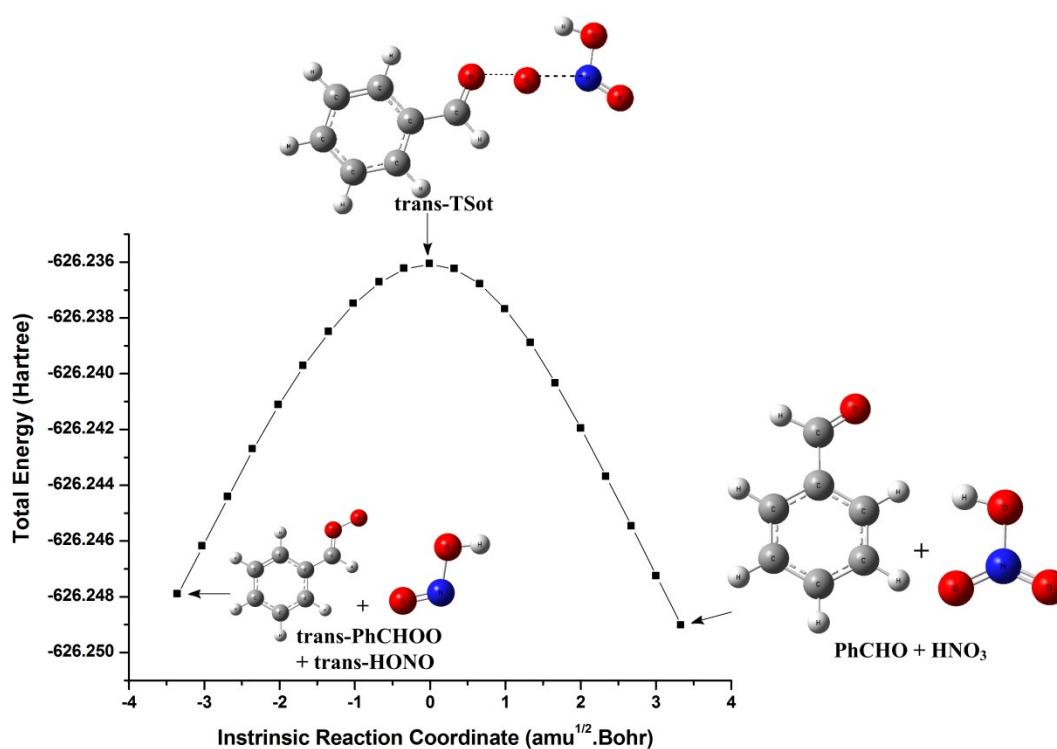


Fig. S1(d) Intrinsic reaction coordinate (IRC) profile for the reaction of trans-PhCHO

+ trans-HONO $\rightarrow$ trans-TSot $\rightarrow$ PhCHO + HNO₃ at M06-2X/6-311++G(d,p) level

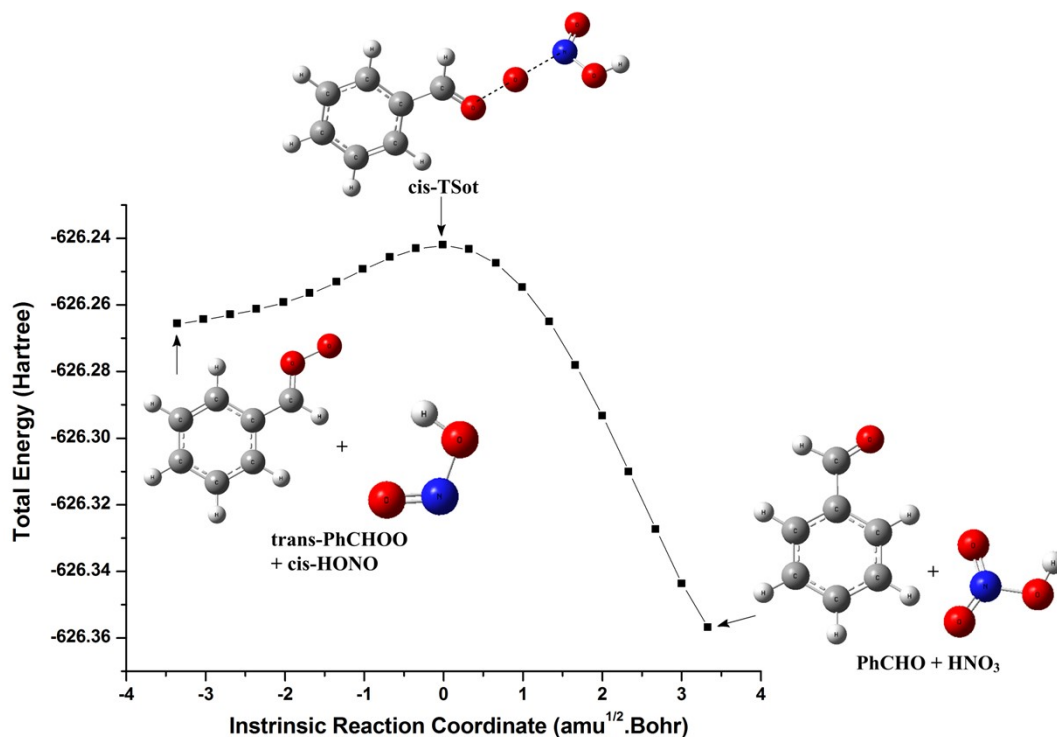


Fig. S1(e) Intrinsic reaction coordinate (IRC) profile for the reaction of trans-PhCHO

+ cis-HONO $\rightarrow$ cis-TSot $\rightarrow$ PhCHO + HNO₃ at M06-2X/6-311++G(d,p) level

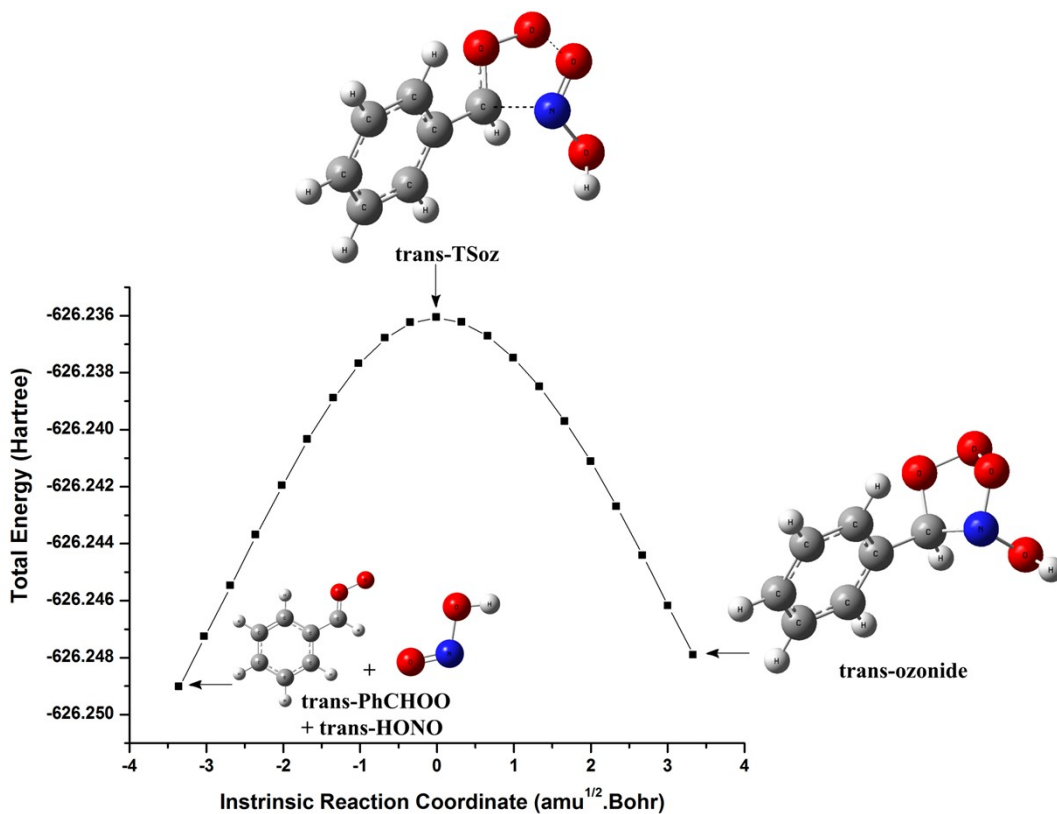


Fig. S1(f) Intrinsic reaction coordinate (IRC) profile for the reaction of trans-PhCHO + trans-HONO $\rightarrow$ trans-TSoz $\rightarrow$ trans-ozonide at M06-2X/6-311++G(d,p) level

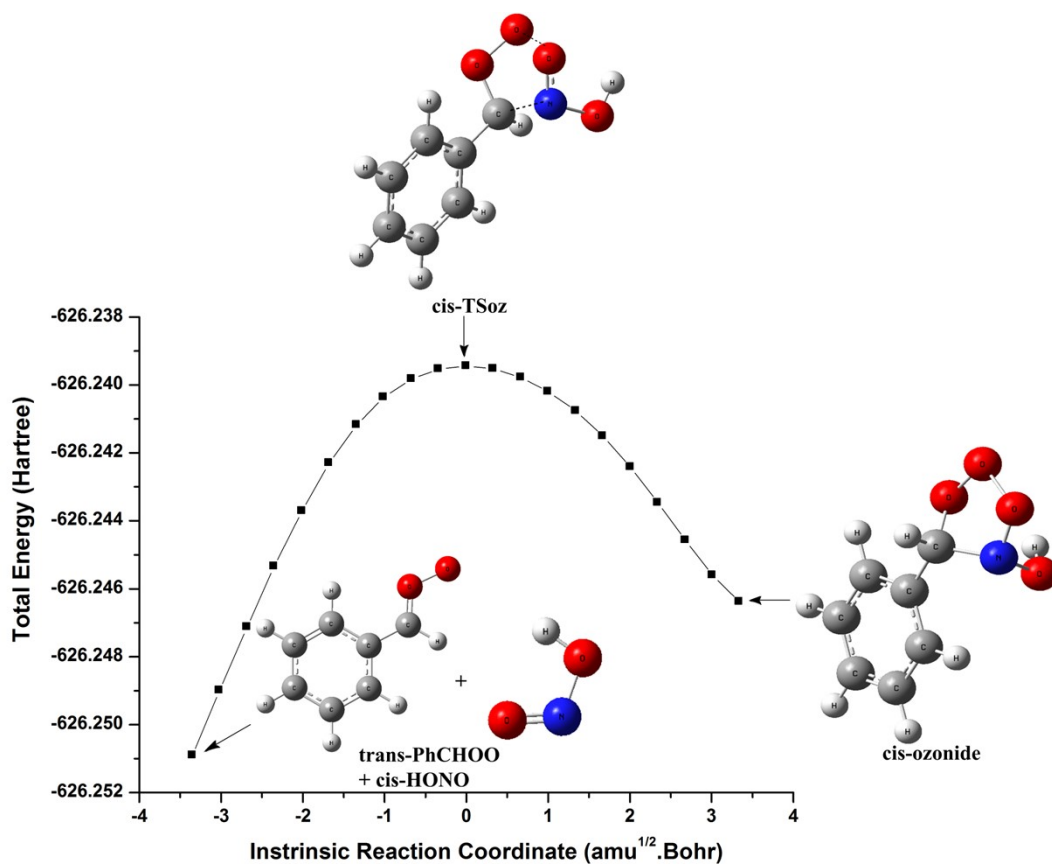


Fig. S1(g) Intrinsic reaction coordinate (IRC) profile for the reaction of trans-PhCHO + cis-HONO $\rightarrow$ cis-TSoz $\rightarrow$ cis-ozonide at M06-2X/6-311++G(d,p) level

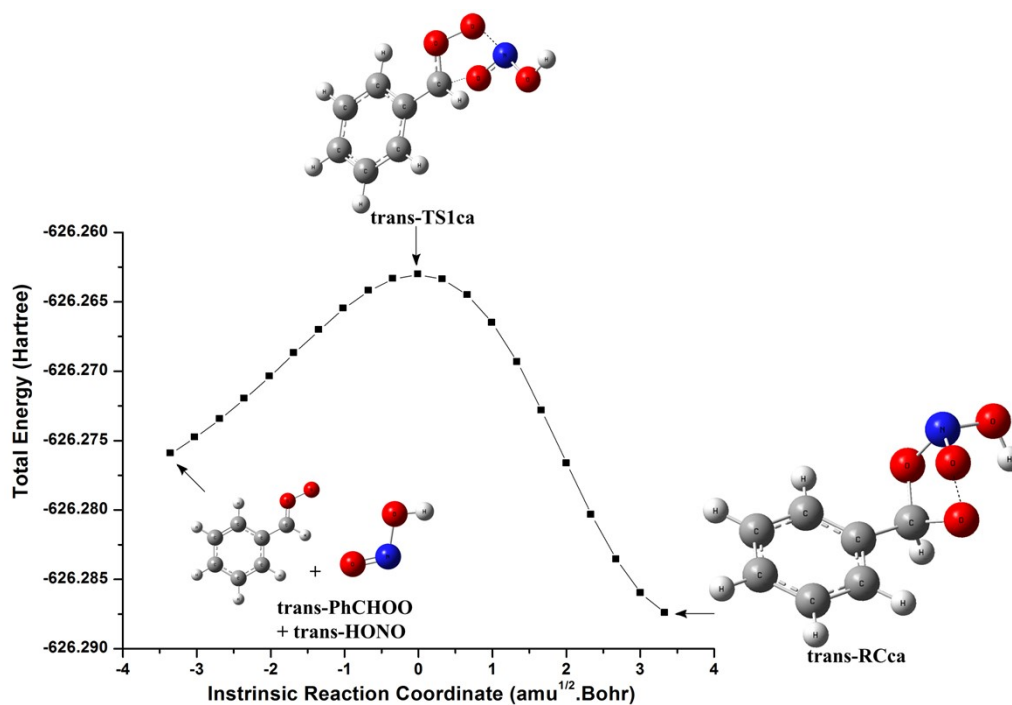


Fig. S1(h) Intrinsic reaction coordinate (IRC) profile for the reaction of trans-PhCHO + trans-HONO $\rightarrow$ trans-TS1ca $\rightarrow$ trans-RCca at M06-2X/6-311++G(d,p) level

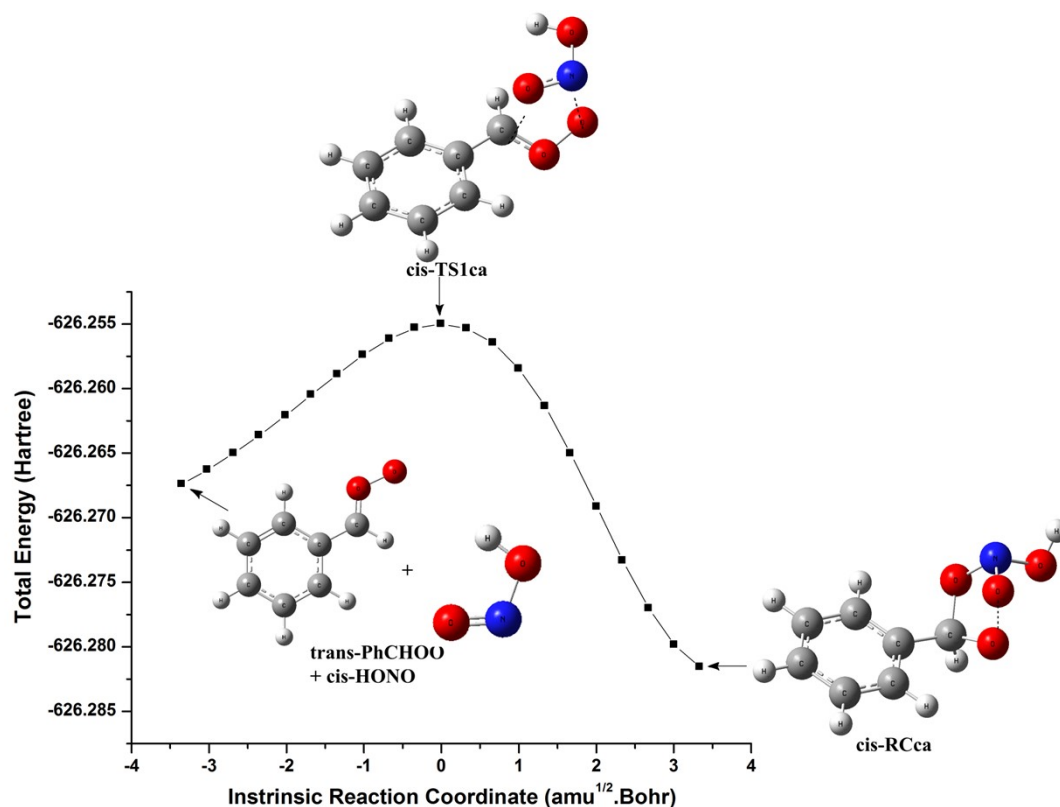


Fig. S1(i) Intrinsic reaction coordinate (IRC) profile for the reaction of trans-PhCHO + cis-HONO $\rightarrow$ cis-TS1ca $\rightarrow$ cis-RCca at M06-2X/6-311++G(d,p) level

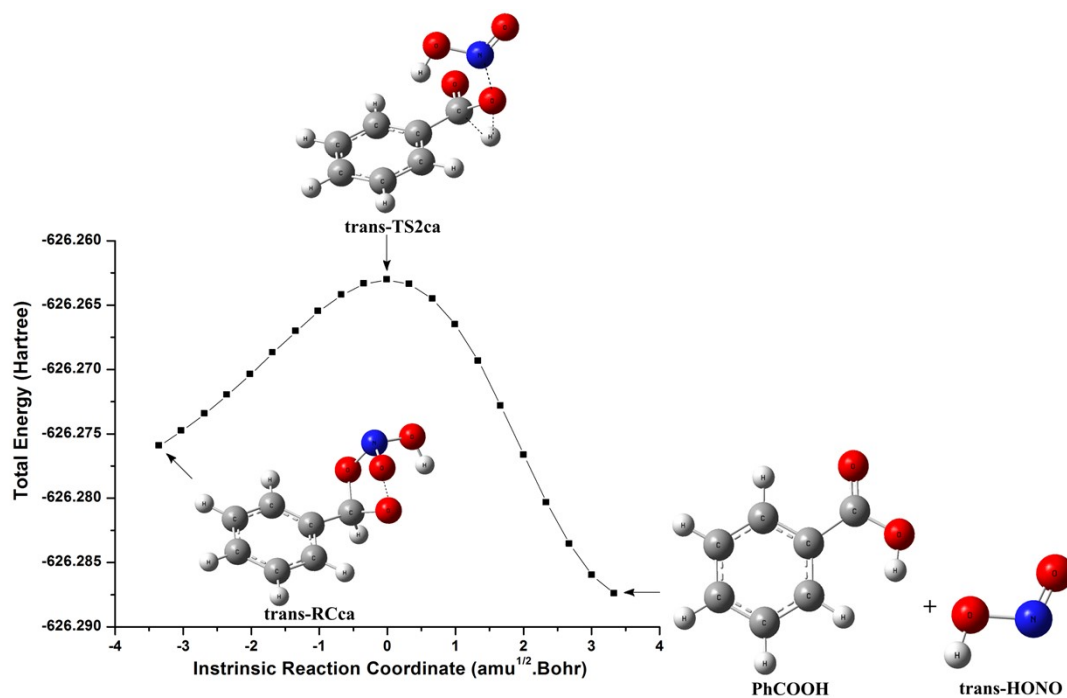


Fig. S1(j) Intrinsic reaction coordinate (IRC) profile for the reaction of trans-RCca $\rightarrow$ trans-TS2ca $\rightarrow$ PhCOOH+ trans-HONO at M06-2X/6-311++G(d,p) level

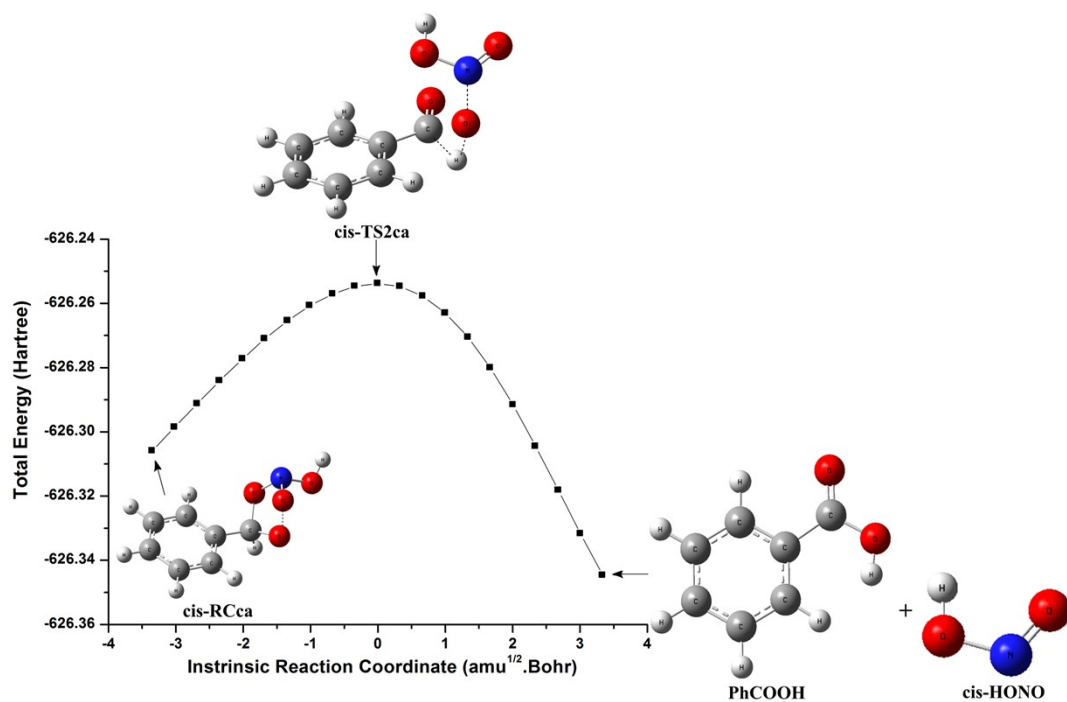


Fig. S1(k) Intrinsic reaction coordinate (IRC) profile for the reaction of cis-RCca $\rightarrow$ cis-TS2ca $\rightarrow$ PhCOOH+ cis-HONO at M06-2X/6-311++G(d,p) level

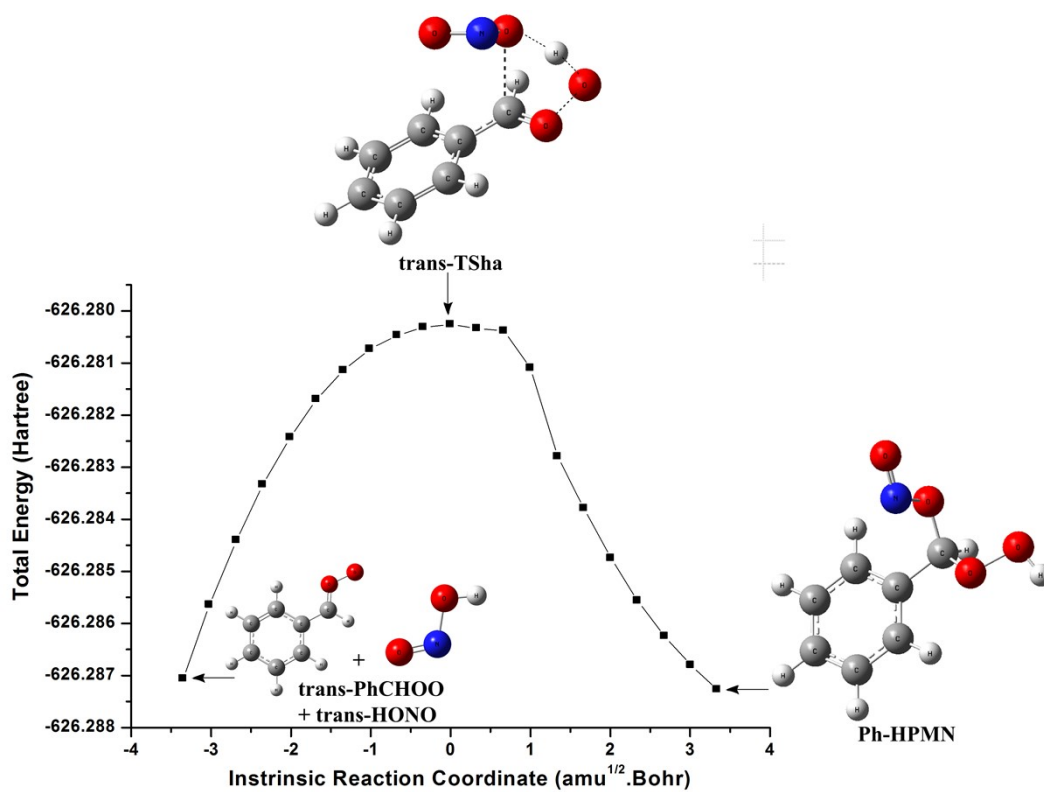


Fig. S1(l) Intrinsic reaction coordinate (IRC) profile for the reaction of trans-PhCHO + trans-HONO $\rightarrow$ TSha $\rightarrow$ Ph-HPMN at M06-2X/6-311++G(d,p) level