

The Mechanism and Kinetics of the Atmospheric Oxidation of $\text{CF}_3(\text{CF}_2)_2\text{CH}=\text{CH}_2$ (HFC-1447fz) by hydroxyl radical: Ab Initio investigation

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(2) **Table S2.** The excitation energy T_V (in eV), wavelength λ (in nm) and oscillator strength f (in atomic units) of the calculated excited states of the intermediates involved in the reaction of HFC-1447fz + OH, calculated using TD-DFT calculations at the M06-2X/6-311++G(d, p) level.

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(6) **Global warming potential calculation.**

(7) **Photochemical ozone creation potential (POCP) calculation.**

Table S1: Cartesian Coordinates (in Å) of all species at M06-2X/6-311++G(d,p) level of theory.

Species		X	Y	Z
HFC-1447fz	C	-1.56910600	-0.08677600	-0.09282800
	C	-0.16838300	0.54059000	0.09125800
	C	1.01743100	-0.45160000	0.11462600
	C	2.29549500	0.20626500	0.53124500
	H	2.34240100	0.49229700	1.57545000
	C	3.28118300	0.42636400	-0.32430900
	H	4.19833000	0.90271000	-0.00182200
	H	3.19963200	0.13411600	-1.36439800
	F	1.11217800	-0.99745600	-1.11636200
	F	0.69372900	-1.44475900	0.98154400
	F	-0.18475800	1.21818500	1.25523600
	F	0.02655700	1.41143900	-0.91102000
	F	-1.59218700	-0.88034900	-1.15656600
	F	-1.91691000	-0.78653600	0.97853900
F	-2.45861900	0.88634300	-0.26794700	
OH	O	0.00000000	0.00000000	0.10800100
	H	0.00000000	0.00000000	-0.86401200
TS1	C	1.79674200	-0.06540600	0.00132200
	C	0.35319900	0.49679100	-0.06016800
	C	-0.74738900	-0.59820400	0.01801000
	C	-2.05916100	-0.24982800	-0.63063400
	H	-1.98711400	0.13886600	-1.63768400
	C	-3.21868100	-0.70478200	-0.11967000
	H	-4.14458100	-0.56730900	-0.66133800
	H	-3.25733600	-1.17744000	0.85461900
	F	-0.91288100	-0.92292100	1.31790000
	F	-0.24978000	-1.70000200	-0.60885100
	F	0.23848100	1.16722800	-1.21793300
	F	0.22591800	1.34733000	0.96540200
	F	1.92006800	-0.90780500	1.02228300
	F	2.11894500	-0.69038700	-1.12292200
	F	2.64563100	0.94234300	0.17653100
	O	-2.33817900	1.70574500	0.05084500
H	-2.53122900	1.56642600	0.99279300	
TS1a	C	1.83817200	-0.21806400	0.08717800
	C	0.51932800	0.54321100	-0.17965100
	C	-0.77865500	-0.28529600	-0.02331900
	C	-1.98244300	0.47434600	-0.50632100
	H	-2.17571100	0.40072800	-1.56851100

	C	-2.56816400	1.40669300	0.27139600
	H	-3.37130900	2.01825700	-0.11628200
	H	-2.28239100	1.53046800	1.30965700
	F	-0.89989700	-0.59519200	1.29047600
	F	-0.60990900	-1.42890900	-0.71245600
	F	0.57505100	1.01794900	-1.43732900
	F	0.47093300	1.58257900	0.67048000
	F	1.80198000	-0.81507200	1.27228800
	F	2.05824900	-1.12683900	-0.85168900
	F	2.84473000	0.65087300	0.07856500
	O	-3.39517000	-0.99939400	-0.14251300
	H	-3.34889600	-1.04815800	0.82652900
TS2	C	1.82960400	0.16699300	0.13556100
	C	0.35034500	0.37821000	-0.26011200
	C	-0.59399000	-0.82544500	-0.03345000
	C	-1.94923500	-0.62158200	-0.63127900
	H	-1.97591100	-0.55544700	-1.71190700
	C	-3.06012100	-0.50382300	0.12723700
	H	-4.03481000	-0.49387700	-0.33855200
	H	-3.01921100	-0.64102900	1.19972500
	F	-0.66397800	-1.03887000	1.29779500
	F	0.00346500	-1.90736700	-0.59511500
	F	0.32022300	0.71424300	-1.55966200
	F	-0.11551600	1.41877600	0.46215500
	F	1.92075100	-0.27137400	1.38456800
	F	2.41392400	-0.70257700	-0.67550200
	F	2.46865800	1.32900900	0.04306700
	O	-3.16125700	1.55445900	0.14770900
	H	-2.26737600	1.81200800	0.42556800
TS2a	C	-1.89884900	-0.23188700	-0.13826700
	C	-0.59995200	0.57184200	0.09709600
	C	0.69874700	-0.25880000	0.21902900
	C	1.87580200	0.57379300	0.61171000
	H	1.99184700	0.75274300	1.67303200
	C	2.75424000	1.02411400	-0.30696900
	H	2.56472100	0.90519300	-1.36615200
	H	3.56524900	1.67567500	-0.01562400
	F	0.90699800	-0.86211100	-0.97806100
	F	0.47819300	-1.23263600	1.13382700
	F	-0.76102100	1.27818000	1.22995600
	F	-0.45661000	1.42657800	-0.92896800
	F	-1.77751000	-1.01250500	-1.20497500
	F	-2.18711500	-0.98045400	0.91731500
	F	-2.90084200	0.61711500	-0.34243400

	O	3.97584100	-0.64804200	-0.14335300
	H	3.37268500	-1.33114500	-0.47996800
TS3	C	1.81426300	0.16007200	-0.06240700
	C	0.39286300	0.00663000	0.52491600
	C	-0.71320000	-0.38915700	-0.47929700
	C	-2.07155100	-0.37360400	0.13810300
	H	-2.53222600	0.76286000	0.28100800
	C	-2.77400200	-1.42277900	0.50730100
	H	-2.36838800	-2.42581900	0.40144000
	H	-3.76835900	-1.31357200	0.92379600
	F	-0.41194900	-1.61091700	-0.96715800
	F	-0.66792200	0.49288400	-1.51148400
	F	0.05911900	1.18056900	1.08405500
	F	0.44641900	-0.93339200	1.48175900
	F	2.18913800	-0.95184200	-0.68255700
	F	1.86301200	1.17204600	-0.91854500
	F	2.66461300	0.40240800	0.92951900
	O	-2.98755900	1.90307400	0.08348600
	H	-2.60264700	2.09916300	-0.78613100
TS4	C	1.77275200	-0.35699700	-0.09061100
	C	0.44078900	0.09718700	0.54848300
	C	-0.60980300	0.68028800	-0.42452100
	C	-1.77597800	1.28049000	0.30139600
	H	-1.62155600	2.30380800	0.63339800
	C	-2.88976100	0.62774900	0.55851700
	H	-3.75041700	1.02438800	1.08496900
	H	-3.07598400	-0.55102000	0.23015700
	F	-0.99430900	-0.32342500	-1.25040800
	F	0.00043400	1.61849200	-1.18229400
	F	0.73378800	1.03291700	1.46878800
	F	-0.10255300	-0.96389500	1.16342100
	F	1.54676800	-1.21846700	-1.07563900
	F	2.44424800	0.68175300	-0.56778100
	F	2.51561000	-0.95279500	0.83561500
	O	-3.24681400	-1.72590500	-0.13542800
	H	-2.50140600	-1.81346800	-0.74999900
TS5	C	2.02215700	-0.14009200	-0.06759500
	C	0.52159600	-0.49526300	0.03786900
	C	-0.45325700	0.69991200	0.14349500
	C	-1.86189800	0.24718300	0.40225700
	H	-2.04567200	-0.16899400	1.38719200
	C	-2.80132600	0.35807200	-0.51263700
	H	-3.93105300	-0.00320800	-0.19818600
	H	-2.69786400	0.74879400	-1.51843200

	F	-0.36152000	1.40683700	-1.00155700
	F	-0.02363200	1.49069600	1.15481800
	F	0.36580600	-1.26746000	1.12901300
	F	0.19503200	-1.21333800	-1.04851700
	F	2.23980700	0.66696000	-1.09818800
	F	2.44774400	0.44666200	1.04219700
	F	2.71664300	-1.25915400	-0.24839000
	O	-4.92830600	-0.68518400	0.14401900
	H	-4.68151300	-1.55481900	-0.20745300
TS6	C	2.04340200	-0.37313900	0.07671700
	C	0.80570800	0.45106600	-0.34747600
	C	-0.55046800	-0.04746800	0.21496000
	C	-1.73851500	0.65041500	-0.40128000
	H	-1.87266100	0.51740800	-1.46842300
	F	-0.54510900	0.21006600	1.55244700
	F	-0.61617600	-1.37078300	0.03199900
	F	0.74570400	0.43148400	-1.68934000
	F	0.99068100	1.71841800	0.05863600
	F	2.08132300	-0.50239600	1.39755200
	F	2.01780000	-1.57502000	-0.47870900
	F	3.14078900	0.25880900	-0.32374700
	O	-1.93913200	1.91689700	0.00674300
	H	-1.66318000	2.02785000	0.92615100
	C	-3.37545200	-0.47142100	0.22270800
	H	-4.02086400	0.40888300	0.06569100
	H	-2.97904400	-0.59199300	1.24849000
	O	-3.42429600	-1.43615500	-0.54489600
TS6a	C	1.97366800	0.06372300	0.01148300
	C	0.47387700	0.44698200	-0.05990500
	C	-0.48207500	-0.76479400	0.00920500
	C	-1.87173600	-0.53331900	-0.53018000
	H	-1.93583800	-0.18525200	-1.55410500
	F	-0.58086800	-1.17362400	1.30102600
	F	0.09464100	-1.79036200	-0.67274600
	F	0.27298200	1.08982800	-1.21945400
	F	0.22084400	1.26703100	0.96578200
	F	2.18359900	-0.76785100	1.02776500
	F	2.37218000	-0.51285700	-1.11296300
	F	2.69239300	1.16250400	0.20106100
	O	-2.73087100	-1.53210300	-0.25174800
	H	-2.53165200	-1.92184000	0.60981500
	C	-2.66573700	1.16215200	0.38551200
	H	-3.67892300	0.78510800	0.17225000
	H	-2.25501300	0.88720800	1.37553200

	O	-2.20269000	2.12139100	-0.23755400
TS7	C	-2.04837000	-0.05278300	0.05583000
	C	-0.56981900	-0.46467200	-0.14321300
	C	0.44412800	0.68550200	0.07102000
	F	0.68993800	0.80740200	1.37940400
	F	-0.12653000	1.83224500	-0.36958600
	F	-0.43651600	-0.92620500	-1.40365300
	F	-0.30678500	-1.45923000	0.71047900
	F	-2.18068800	0.61751400	1.19485600
	F	-2.46812000	0.70186200	-0.94948800
	F	-2.80150700	-1.14417100	0.10892400
	O	2.76804000	1.14192600	-0.24526900
	H	3.36825800	0.11043300	0.30705100
	C	1.77018900	0.54219000	-0.70137900
	H	1.65041900	0.35044100	-1.77251100
	O	2.20222100	-1.20744800	-0.20335700
	O	3.28929300	-1.00786000	0.41531400
TS8	C	1.96028400	0.14582200	0.01329400
	C	0.43454400	0.37287200	-0.10998600
	C	-0.43484200	-0.89271000	0.06386000
	C	-2.70904700	0.96770300	0.38218200
	H	-3.70086200	0.62611100	0.12050700
	H	-2.32529600	0.75702800	1.37621700
	F	-0.53575700	-1.15383000	1.37659100
	F	0.25000100	-1.91306400	-0.51329900
	F	0.19707800	0.92044500	-1.31536700
	F	0.09496800	1.28494500	0.83279200
	F	2.23125800	-0.54661600	1.11143500
	F	2.42804200	-0.49779300	-1.04409800
	F	2.56578300	1.32764600	0.08944300
	O	-2.37590400	2.12419300	-0.20497100
	H	-1.55590100	2.46935500	0.16542800
	C	-1.83941100	-0.86175100	-0.59013600
H	-1.89763700	-0.33604500	-1.55460800	
O	-2.63307400	-1.71215100	-0.23256700	
TS8a	C	-2.09157700	-0.15774900	0.02347700
	C	-0.57953700	-0.44571800	-0.13425700
	C	0.34101000	0.77856200	0.06415200
	C	2.50343700	-1.19849000	0.28188800
	H	2.22639800	-0.89269500	1.28771200
	H	1.99873300	-2.04355600	-0.17022300
	F	0.45359500	1.01311200	1.38096300
	F	-0.28382300	1.84302400	-0.50052200
	F	-0.38582100	-0.94749600	-1.37047200

	F	-0.25284000	-1.39593300	0.76072300
	F	-2.31203600	0.52739500	1.13862800
	F	-2.55160800	0.52778100	-1.01206300
	F	-2.74774800	-1.31158600	0.09134600
	O	3.77266700	-1.07357100	-0.09916400
	H	4.13261200	-0.23716300	0.23113800
	C	1.74057300	0.67104700	-0.57833300
	H	1.76111800	0.22341100	-1.58264400
	O	2.61736300	1.41824900	-0.16395700
TS9	O	1.19915800	0.51350300	0.00000000
	H	0.00000000	1.01093600	0.00000000
	C	0.88702900	-0.70615800	0.00000000
	H	0.93506800	-1.28698900	0.92843700
	H	0.93506800	-1.28698900	-0.92843700
	O	-1.10111100	0.73858600	0.00000000
	O	-0.99708500	-0.52709000	0.00000000
P1	C	1.79816200	-0.16880700	-0.00894000
	C	0.42607600	0.54372600	-0.09071300
	C	-0.78610900	-0.40186400	0.09451900
	C	-2.09895900	0.14671600	-0.46870000
	H	-1.93615300	0.31298000	-1.54081100
	C	-3.20389300	-0.82363400	-0.23636700
	H	-4.21826900	-0.46596200	-0.34344700
	H	-3.01064600	-1.88368800	-0.15501700
	F	-0.91551300	-0.64219600	1.41986600
	F	-0.49433200	-1.57985400	-0.50840000
	F	0.35231800	1.12907900	-1.29966600
	F	0.40819200	1.49134600	0.85465100
	F	1.85465200	-0.93772500	1.07348500
	F	2.00892000	-0.91601900	-1.08431100
	F	2.76075500	0.74364500	0.06420300
	O	-2.35307500	1.41927800	0.07730900
	H	-2.59691200	1.31115200	1.00354800
P1a	C	1.80752900	-0.15132800	0.00440400
	C	0.42678900	0.53924700	-0.09631300
	C	-0.78159400	-0.41019400	0.06991200
	C	-2.09897100	0.14840300	-0.47564400
	H	-1.98409600	0.24920200	-1.55567600
	C	-2.44305500	1.45380300	0.15445300
	H	-2.99764600	2.19037800	-0.40751400
	H	-2.31823800	1.58918300	1.22115100
	F	-0.92129800	-0.67911000	1.39263800
	F	-0.47930000	-1.57081600	-0.54779300
	F	0.35669000	1.12738500	-1.30676900

	F	0.38095000	1.49459600	0.84523200
	F	1.86156800	-0.91435100	1.09007500
	F	2.04208600	-0.89657100	-1.06591800
	F	2.75420400	0.77779500	0.08665800
	O	-3.10319700	-0.83202600	-0.28755000
	H	-3.29272600	-0.90250600	0.65446000
P2	C	-1.79589400	-0.25701300	0.17390000
	C	-0.32915400	-0.32525600	-0.30458900
	C	0.54671200	0.93059200	-0.06458700
	C	1.96540900	0.71143400	-0.43798500
	H	2.22663000	0.90685200	-1.47035200
	C	2.92260300	-0.00208300	0.45949300
	H	3.86055800	0.55517500	0.50735200
	H	2.51986600	-0.07100600	1.47432300
	F	0.42582900	1.24986000	1.24993900
	F	0.01035100	1.93981600	-0.78801000
	F	-0.33391800	-0.59247500	-1.61884800
	F	0.24930600	-1.36737900	0.33869400
	F	-1.85582100	-0.16389200	1.49507400
	F	-2.41463200	0.78470000	-0.36497700
	F	-2.42233000	-1.36831500	-0.20134700
	O	3.26508600	-1.27959100	-0.05582000
	H	2.48512300	-1.84116800	-0.01688100
P2a	C	-1.92403200	-0.12395400	0.12607000
	C	-0.45341700	-0.41045300	-0.24813900
	C	0.56046000	0.74029700	-0.02839700
	C	1.92979100	0.39636300	-0.47500800
	H	2.25375700	0.76789700	-1.43768900
	C	2.77656900	-0.56803600	0.27160800
	H	2.57284000	-0.48722600	1.34701000
	H	2.52478000	-1.59626500	-0.03365800
	F	0.53542000	1.03087700	1.30026300
	F	0.09715300	1.82066600	-0.69701000
	F	-0.42680200	-0.75939900	-1.54574200
	F	-0.04569000	-1.46554500	0.48599700
	F	-2.02774500	0.22328100	1.40211700
	F	-2.42070400	0.84533600	-0.63035700
	F	-2.64154600	-1.22646800	-0.07248900
	O	4.12438700	-0.26954300	-0.03451800
	H	4.68652800	-0.95210800	0.33867200
P3	C	-1.55298400	-0.07210900	-0.08874300
	C	-0.14645500	0.53939900	0.10728900
	C	1.02491700	-0.47041900	0.11233200
	C	2.29939300	0.17399500	0.49270800

	C	3.38027800	0.49303500	-0.16465900
	H	4.21853300	0.98269500	0.32003300
	H	3.46828800	0.26851200	-1.22757800
	F	1.11168100	-1.00998300	-1.12880200
	F	0.71051400	-1.46823900	0.96873900
	F	-0.15294300	1.19502500	1.28001900
	F	0.06043400	1.42191200	-0.88209300
	F	-1.58613300	-0.83556100	-1.17385300
	F	-1.90131000	-0.79840000	0.96416100
	F	-2.43310000	0.91362200	-0.23328400
P4	C	-1.52729100	-0.10703400	-0.10093300
	C	-0.13951500	0.54325600	0.10138800
	C	1.06510800	-0.42504700	0.11517700
	C	2.33867400	0.26988400	0.51934200
	H	2.39162000	0.56596900	1.56348900
	C	3.29999500	0.50056600	-0.33349500
	H	3.48578500	0.32229600	-1.38147000
	F	1.16823800	-0.97013200	-1.11389900
	F	0.77793300	-1.42067400	0.98759900
	F	-0.17189300	1.19929600	1.27662500
	F	0.04354900	1.43353800	-0.88557200
	F	-1.53734200	-0.85871800	-1.19482600
	F	-1.85404100	-0.85580600	0.94343800
	F	-2.43747100	0.85271800	-0.23457500
P5	C	-1.53764900	-0.08936000	-0.08697100
	C	-0.13618400	0.53830600	0.09047100
	C	1.05346400	-0.44916700	0.08433600
	C	2.34050300	0.22518800	0.46679800
	H	2.41617700	0.51818300	1.51332500
	C	3.28483200	0.44415200	-0.40781800
	H	4.26977500	0.88357600	-0.41601100
	F	1.12483300	-1.00147200	-1.14075000
	F	0.76530200	-1.43486000	0.96999900
	F	-0.13859800	1.19383800	1.26764400
	F	0.04283900	1.42738800	-0.89743300
	F	-1.58369500	-0.83527400	-1.18331500
	F	-1.85536300	-0.83744300	0.96106600
	F	-2.43484700	0.88599400	-0.19701300
PC1	C	1.75776600	0.14979900	-0.08277600
	C	0.36270200	-0.08466400	0.54155700
	C	-0.75886300	-0.48660700	-0.44433800
	C	-2.07999900	-0.53393700	0.20710300
	H	-1.80261600	2.49390400	0.60761800
	C	-2.90591700	-1.50591800	0.48467800

	H	-2.65904900	-2.53652900	0.23073600
	H	-3.85799800	-1.31614600	0.96911300
	F	-0.42646500	-1.68757600	-0.97746600
	F	-0.74924600	0.41759600	-1.45969200
	F	0.00868900	1.06602900	1.15135600
	F	0.48093100	-1.04373800	1.46862500
	F	2.14763400	-0.90652100	-0.78239900
	F	1.74199500	1.21514300	-0.87438100
	F	2.63298900	0.36293500	0.89423800
	O	-2.54068600	2.37476600	0.00474300
	H	-2.13771400	2.31380100	-0.86528500
PC2	C	1.66665100	-0.39992200	-0.21366400
	C	0.35555500	0.02054100	0.49044500
	C	-0.64442600	0.82276700	-0.37399700
	C	-1.76573700	1.39780400	0.44135100
	H	-1.49334100	2.24669800	1.06698300
	C	-2.96741300	0.88603300	0.39850400
	H	-3.92491700	1.06316200	0.86007300
	H	-2.77647300	-1.63083800	-0.92956800
	F	-1.10296600	-0.01394600	-1.33338900
	F	0.05347300	1.80799600	-0.98607500
	F	0.68975800	0.75578800	1.56373700
	F	-0.25729900	-1.10243800	0.91397000
	F	1.40327800	-1.00980300	-1.36329700
	F	2.43277600	0.65577500	-0.44554400
	F	2.32949900	-1.24066500	0.57359500
	O	-3.06339400	-2.03804000	-0.10782300
	H	-2.25673600	-2.12260000	0.40674900
PC3	C	1.95632800	-0.27852800	0.05604300
	C	0.45952200	-0.35525600	-0.32195800
	C	-0.45166000	0.72407100	0.30550700
	C	-1.90891900	0.43548500	0.06935400
	H	-2.33688300	-0.39352400	0.62811000
	C	-2.62015200	1.13721500	-0.77192700
	H	-4.69384400	-0.87910100	-0.61462700
	H	-2.46529000	1.97432900	-1.43591700
	F	-0.08771600	1.91655500	-0.21345200
	F	-0.18908700	0.75649900	1.63447200
	F	0.01568000	-1.56726300	0.05708000
	F	0.36973400	-0.26093000	-1.65814300
	F	2.44207900	0.93247300	-0.18774400
	F	2.13433500	-0.56780400	1.33792200
	F	2.63185600	-1.16223500	-0.67355000
	O	-4.45965000	-1.20673700	0.25735100

	H	-5.28942100	-1.45138800	0.67225400
PC4	C	2.11093600	-0.49547000	0.12851200
	C	0.96733400	0.41323000	-0.37376800
	C	-0.46650300	0.05438000	0.09073600
	C	-1.52274700	0.96604700	-0.41814500
	H	-1.87487500	0.87612300	-1.43485600
	F	-0.45728300	0.10630900	1.45667200
	F	-0.72138800	-1.21092400	-0.29268800
	F	0.98908800	0.39149700	-1.71563100
	F	1.23182900	1.66604400	0.04488200
	F	2.17722000	-0.47175300	1.45427400
	F	1.92829000	-1.74523500	-0.27455600
	F	3.26320800	-0.05244900	-0.36267700
	O	-1.68555600	2.16489300	0.16072400
	H	-1.29292600	2.17247500	1.04274900
	C	-3.90318800	-0.70008800	0.43691800
	H	-4.19970400	0.28598200	0.84008200
H	-3.18005500	-1.28122700	1.03820200	
O	-4.34770900	-1.11906300	-0.59374700	
PC5	C	1.99645300	-0.30355700	-0.24715600
	C	0.69007500	-0.07656700	0.54548900
	C	-0.40424900	0.73037300	-0.17505100
	F	-0.73443800	0.13644800	-1.32925000
	F	0.09029900	1.95565000	-0.45465500
	F	0.99962000	0.59416500	1.67357000
	F	0.19972500	-1.27624400	0.88285600
	F	1.75406100	-1.00831500	-1.34356100
	F	2.54532600	0.85516600	-0.58576300
	F	2.84996000	-0.97465300	0.51636200
	O	-2.67328600	1.33426400	0.14810100
	H	-3.44307400	-0.24824100	-0.60563600
	C	-1.67617300	0.94616500	0.68612400
	H	-1.57917300	0.81472800	1.77341700
	O	-2.41766500	-1.46833000	0.31274000
	O	-3.40347000	-1.22655000	-0.49337200
PC6	C	2.05137200	-0.42183100	-0.06951200
	C	0.50932900	-0.35726700	0.00923400
	C	-0.09518100	1.05150700	0.17061600
	C	-2.95485800	-1.57626400	-0.04641900
	H	-2.59032500	-1.61240900	-1.06606500
	H	-2.87231400	-2.43690000	0.60081800
	F	0.30002400	1.81739200	-0.85070200
	F	0.36075600	1.58615500	1.32532200
	F	0.12128700	-1.10309900	1.05826300

	F	0.02102200	-0.89907600	-1.11864900
	F	2.49453800	0.25471500	-1.11952300
	F	2.59558800	0.07748800	1.03217900
	F	2.41965200	-1.69213100	-0.19170200
	O	-4.00996500	-0.77700500	0.24003400
	H	-4.03653200	-0.03799300	-0.37911500
	C	-1.63680400	1.01319900	0.24885300
	H	-2.04236900	0.67350600	1.21396100
	O	-2.30471300	1.37509900	-0.67289900
PC7	O	1.45637600	-0.01270300	0.00000000
	H	0.00000000	1.12926900	0.00000000
	C	0.99162100	-1.12540000	0.00000000
	H	0.77926200	-1.66168700	0.93848400
	H	0.77926200	-1.66168700	-0.93848400
	O	-0.98530900	1.17889500	0.00000000
	O	-1.40959800	-0.04787900	0.00000000
IM1	C	-1.79667200	0.21898000	-0.11769700
	C	-0.28073000	0.37139600	0.13945100
	C	0.55677300	-0.92863700	0.12664700
	C	1.98483700	-0.67735900	0.49623200
	H	2.15104100	-0.39552300	1.52940800
	C	2.96703800	-0.77639100	-0.39015500
	H	2.77095300	-1.04868700	-1.42077200
	H	3.99195300	-0.58379500	-0.10093000
	F	0.44319600	-1.46932500	-1.10560200
	F	-0.01888700	-1.78295400	1.00754000
	F	-0.13048800	0.96966100	1.33214500
	F	0.20594800	1.19698100	-0.81461100
	F	-2.01967000	-0.37276400	-1.28357100
	F	-2.36630700	-0.48894100	0.84686900
	F	-2.35049200	1.42782600	-0.14062600
	O	3.05265400	1.92628200	0.03923300
	H	2.20762900	2.04546000	-0.42774200
IM1a	C	1.86487400	-0.34142400	0.10254000
	C	0.65861200	0.56954600	-0.21989000
	C	-0.73949800	-0.03381100	0.03511300
	C	-1.84754200	0.85258800	-0.43776300
	H	-1.83562300	1.08151500	-1.49701900
	C	-2.79794900	1.27933400	0.38283100
	H	-3.61648900	1.88239900	0.01160100
	H	-2.79132300	1.02734100	1.43625500
	F	-0.83855800	-0.31378700	1.34897600
	F	-0.79255200	-1.22644200	-0.63309600
	F	0.74676000	0.90508700	-1.52069600

	F	0.77893100	1.68128600	0.52173900
	F	1.82438700	-0.74465200	1.36580100
	F	1.87979200	-1.40297100	-0.69269300
	F	2.98536700	0.34743000	-0.08947600
	O	-3.85053500	-1.19002400	-0.17081800
	H	-3.04040600	-1.64201800	-0.46627900
IM2	C	-1.79683100	0.21882100	-0.11766200
	C	-0.28089000	0.37129600	0.13934900
	C	0.55701100	-0.92848700	0.12660000
	C	1.98499900	-0.67654200	0.49618300
	H	2.15099400	-0.39368300	1.52910900
	C	2.96740300	-0.77636000	-0.38992100
	H	3.99221900	-0.58321200	-0.10066900
	H	2.77157000	-1.04984600	-1.42030200
	F	0.44356400	-1.46936400	-1.10554900
	F	-0.01829700	-1.78293700	1.00761000
	F	-0.13069300	0.96961300	1.33202700
	F	0.20553800	1.19690700	-0.81478800
	F	-2.01989900	-0.37314900	-1.28342400
	F	-2.36637600	-0.48898400	0.84705600
	F	-2.35067900	1.42762000	-0.14072400
	O	3.05234800	1.92635600	0.03916700
	H	2.20786900	2.04616900	-0.42863400
IM3	C	2.21632700	-0.57877900	0.00550500
	C	1.10864300	0.46432500	-0.27876900
	C	-0.27961400	0.08896400	0.29535400
	C	-1.44173200	0.84675900	-0.34355300
	H	-1.41558200	0.67242000	-1.42105300
	F	-0.25796200	0.36304300	1.62631300
	F	-0.45821300	-1.23921300	0.15543000
	F	1.00871000	0.59600700	-1.61275800
	F	1.50442500	1.63269300	0.24503800
	F	2.21591100	-0.90616100	1.29331600
	F	2.03386400	-1.67055900	-0.72237700
	F	3.39625000	-0.05504800	-0.30384500
	O	-1.27668400	2.22422500	-0.14305600
	H	-1.14458200	2.40391400	0.79478000
	C	-2.78072400	0.35327200	0.19948100
	H	-3.53614500	1.11653500	0.00695700
	H	-2.75306700	0.10651800	1.26306600
	O	-3.13454500	-0.83314500	-0.53430300
	O	-4.22313300	-1.37026700	-0.07788100
IM3a	C	-2.11556700	-0.30493400	0.03932600
	C	-0.57850300	-0.39759900	-0.12202300

	C	0.16504700	0.94513400	0.03067300
	C	1.62895700	0.96083200	-0.42585700
	H	1.64601700	0.79110200	-1.50456000
	F	0.12304600	1.29913200	1.34285900
	F	-0.52398800	1.87573700	-0.65912500
	F	-0.32889800	-0.89290900	-1.34465200
	F	-0.12437700	-1.25523300	0.80663900
	F	-2.42360900	0.34298100	1.15719600
	F	-2.65982700	0.32240000	-0.99308900
	F	-2.61755700	-1.53218700	0.10247200
	O	2.13952900	2.24762100	-0.20262300
	H	2.00510300	2.49326800	0.71963000
	C	2.50066400	-0.08739700	0.26172500
	H	3.54331100	0.21683400	0.15735100
	H	2.25286100	-0.23994600	1.31412500
	O	2.32321900	-1.33430600	-0.43384500
	O	2.78050200	-2.33791000	0.24892700
IM4	C	2.00173400	-0.35558500	0.01016300
	C	0.75128700	0.51796000	-0.25177000
	C	-0.57391100	-0.10899500	0.24613100
	C	-1.83078800	0.49048000	-0.37887900
	H	-1.75417100	0.40159100	-1.46345500
	F	-0.62593100	0.07062300	1.59316200
	F	-0.52993800	-1.43694300	0.01547300
	F	0.67079300	0.72321000	-1.57774200
	F	0.94379400	1.69514200	0.35991700
	F	2.01989500	-0.76035500	1.27576700
	F	2.01352800	-1.41434600	-0.78680100
	F	3.09358000	0.36324400	-0.22463100
	O	-1.90918800	1.85702400	-0.06999600
	H	-1.84749900	1.97749700	0.88427300
	C	-3.07435600	-0.27926000	0.08957800
	H	-3.94946100	0.32535000	-0.21022800
	H	-3.12536900	-0.35661600	1.18693000
	O	-3.24566100	-1.49459700	-0.50314900
IM4a	C	1.97468500	-0.01788800	0.03837300
	C	0.50714500	0.45214300	-0.11046500
	C	-0.54155200	-0.67300100	0.00589500
	C	-1.96272000	-0.31182100	-0.43376100
	H	-1.94112400	-0.10251300	-1.50459300
	F	-0.58494900	-1.06897300	1.30751400
	F	-0.09510000	-1.72146600	-0.71572200
	F	0.39141700	1.03575200	-1.31370400
	F	0.27484300	1.36479200	0.84860400

	F	2.11120300	-0.77693600	1.11967900
	F	2.36024300	-0.70499800	-1.02703400
	F	2.75849200	1.04726300	0.16172500
	O	-2.77719900	-1.43973500	-0.24414300
	H	-2.70562700	-1.73727600	0.66967900
	C	-2.53905600	0.90508400	0.30467300
	H	-3.62759500	0.90165800	0.11912800
	H	-2.42878100	0.81634300	1.39762600
	O	-2.08195500	2.11670600	-0.12331800
IM5	C	-1.59670500	-0.20090300	-0.00764800
	C	-0.27183900	0.59637000	-0.04380600
	C	1.00954900	-0.25110200	0.08680200
	C	2.20846900	0.57781800	0.34011100
	H	2.22282900	1.30496000	1.13624600
	F	1.18738400	-0.95540500	-1.06327800
	F	0.78275500	-1.18438300	1.06382400
	F	-0.30329500	1.48444300	0.96793500
	F	-0.22544300	1.26780500	-1.20336700
	F	-1.54245100	-1.22354200	-0.85363100
	F	-1.84151300	-0.65669400	1.21190000
	F	-2.59447600	0.59988800	-0.36735300
	O	3.40266000	0.11378200	-0.05427800
	H	3.29240600	-0.53731400	-0.75903200
IM6	C	-2.03386000	-0.04890100	-0.04540000
	C	-0.55517900	-0.50189600	0.01971900
	C	0.45845400	0.66614300	0.04282700
	F	0.52063600	1.16404200	1.29593000
	F	0.00734700	1.64200200	-0.76830900
	F	-0.30846000	-1.25504600	-1.06922300
	F	-0.40311900	-1.25095800	1.11440900
	F	-2.26449800	0.87556300	0.88067100
	F	-2.32319400	0.44712600	-1.23946900
	F	-2.81874600	-1.09357000	0.18205200
	O	2.75331100	1.31455900	-0.21920600
	H	2.69987800	1.62123400	0.69529000
	C	1.87569400	0.28872800	-0.41581500
	H	1.88482100	0.01201000	-1.46928500
	O	2.22046300	-0.87131200	0.36552400
	O	3.18309500	-1.54576200	-0.19613700
IM7	C	2.21827200	-0.19254800	-0.04424600
	C	0.80096600	0.42534800	-0.13128900
	C	-0.35012600	-0.55854000	0.17195100
	C	-2.21610200	1.21855800	0.43752200
	H	-3.30357300	1.21154200	0.34406300

	H	-1.95867800	1.19741100	1.50048800
	F	-0.33900400	-0.80726700	1.49776800
	F	-0.06979600	-1.71239300	-0.47080900
	F	0.64965100	0.92631400	-1.36551400
	F	0.74739200	1.44077800	0.75814200
	F	2.36130100	-0.87182600	1.08575400
	F	2.43713700	-0.99776100	-1.07196300
	F	3.11401900	0.78793100	-0.07369400
	O	-1.73905500	2.36627100	-0.21873800
	H	-0.95734600	2.70008000	0.22589400
	C	-1.72837100	-0.06065700	-0.25288700
	H	-1.75974500	0.06093300	-1.33700400
	O	-2.59634800	-1.15422400	0.11297800
	O	-3.72394600	-1.09391200	-0.52635300
IM7a	C	2.28660800	-0.09013700	-0.08781500
	C	0.87147400	0.53117600	-0.15951300
	C	-0.26642500	-0.40603000	0.31514100
	C	-2.14835300	1.31674500	0.32094400
	H	-2.31380700	1.22376600	1.39968800
	H	-1.39417200	2.09043500	0.14593200
	F	-0.25962600	-0.41247700	1.66405200
	F	0.02471600	-1.65351300	-0.10527700
	F	0.64345900	0.89047900	-1.43642600
	F	0.87394300	1.64032600	0.59947000
	F	2.49038700	-0.62553000	1.10913700
	F	2.43917400	-1.02029300	-1.01799700
	F	3.18645500	0.86550200	-0.29081900
	O	-3.33788900	1.58611100	-0.38252000
	H	-3.84785000	2.24839900	0.08813800
	C	-1.64859500	-0.01383000	-0.20517300
	H	-1.65549900	-0.04054800	-1.29580600
	O	-2.55342700	-1.02765000	0.26663000
	O	-2.85162200	-1.89721700	-0.65144900
IM8	C	1.97088700	0.04686900	0.02115200
	C	0.47605800	0.43286600	-0.10458700
	C	-0.50793200	-0.75035100	0.04738300
	C	-2.61747000	0.70732100	0.36345700
	H	-3.69135100	0.53608900	0.28042000
	H	-2.34780400	0.64336700	1.42184700
	F	-0.51434600	-1.11176000	1.34432300
	F	-0.00813200	-1.77772600	-0.66984500
	F	0.30533900	1.01750500	-1.29866700
	F	0.21171900	1.34290800	0.85884200
	F	2.16667800	-0.70494500	1.09582900

	F	2.37455100	-0.61008600	-1.05482100
	F	2.69052500	1.15753000	0.13600700
	O	-2.35176000	1.96716500	-0.19878600
	H	-1.57395900	2.35269000	0.20963000
	C	-1.94207200	-0.43506400	-0.42756600
	H	-1.86867000	-0.17044600	-1.49119400
	O	-2.62724500	-1.61621000	-0.24180800
IM8a	C	-2.08878500	-0.08441000	-0.03953700
	C	-0.60056100	-0.51085000	-0.04653400
	C	0.39942700	0.66530600	0.09198600
	C	2.44160700	-0.84390600	0.31657500
	H	2.49848700	-0.59936600	1.38236300
	H	1.83800300	-1.74644300	0.17542000
	F	0.43526000	1.02058300	1.38867100
	F	-0.09457200	1.70702200	-0.61005300
	F	-0.36933700	-1.16652600	-1.19859100
	F	-0.41480700	-1.36469200	0.97345900
	F	-2.32439300	0.74025800	0.97300000
	F	-2.41156200	0.51171300	-1.17741100
	F	-2.84597800	-1.16643500	0.10178500
	O	3.72036800	-0.98923300	-0.26310500
	H	4.22894600	-1.62579100	0.24351800
	C	1.81264300	0.33448100	-0.42268300
	H	1.72163100	0.11339500	-1.49358300
	O	2.54906500	1.48388000	-0.20743200
IM9	C	0.68166800	0.02837700	-0.06582500
	H	1.11374700	0.99155600	0.17563400
	H	1.23210500	-0.88473700	0.09971900
	O	-0.66683000	-0.12530300	0.02372700
	H	-1.10122400	0.72533900	-0.07022000
IM10	O	1.67124800	-0.16879600	-0.04600300
	H	1.77971000	-0.68043100	0.76107500
	C	0.48033200	0.50478500	-0.01206500
	H	0.42489800	1.15782700	-0.88143600
	H	0.28713300	1.04958500	0.91549300
	O	-0.59499800	-0.47520100	-0.13151300
	O	-1.74796600	0.07453600	0.08717300
HO ₂	O	0.70984800	0.02831100	-0.00000700
	O	-0.58857600	-0.12464100	-0.00001400
	H	-0.97017400	0.77064400	0.00016600
HCHO	O	0.00000000	0.00000000	0.67103700
	C	0.00000000	0.00000000	-0.52559400
	H	0.00000000	0.93967600	-1.10736700
	H	0.00000000	-0.93967600	-1.10736700

O ₂	O	0.00000000	0.00000000	0.59437700
	O	0.00000000	0.00000000	-0.59437700
NO ₂	O	0.00000000	1.09098300	-0.13784700
	N	0.00000000	0.00000000	0.31507800
	O	0.00000000	-1.09098300	-0.13784700
NO	N	0.00000000	0.00000000	-0.60707600
	O	0.00000000	0.00000000	0.53119100
C ₃ F ₇ CHO	C	-1.56351500	-0.08365000	-0.10710200
	C	-0.16116400	0.51645000	0.13685500
	C	1.01995200	-0.47057400	0.07169800
	F	1.07372100	-1.01788700	-1.14500700
	F	0.82233400	-1.44409700	0.98821900
	F	-0.15824600	1.07679900	1.36242400
	F	0.04462900	1.47699000	-0.77534800
	F	-1.62195100	-0.64835300	-1.30511400
	F	-1.84944000	-0.99033500	0.81718900
	F	-2.46415600	0.88971400	-0.04503200
	O	3.11877200	0.54189400	-0.45057900
	C	2.35497500	0.23437600	0.40610600
	H	2.52632200	0.39975500	1.48331300

Table S2. The excitation energy T_V (in eV), wavelength λ (in nm) and oscillator strength f (in atomic units) of the calculated excited states of the intermediates involved in the reaction of HFC-1447fz + OH, calculated using TD-DFT calculations at the M06-2X/6-311++G(d, p) level.

Species	Parameters	Excited state				
		1	2	3	4	5
IM1	T_V	0.3895	3.7886	4.5250	5.0276	6.8651
	λ	3182.96	327.25	274.00	246.61	180.60
	f	0.0000	0.0032	0.0050	0.0807	0.0039
IM1a	T_V	0.3939	3.7918	4.5057	5.1063	6.9831
	λ	3147.47	326.98	275.17	242.80	177.55
	f	0.0000	0.0051	0.0032	0.0923	0.0020
IM2	T_V	0.1664	5.4972	5.6328	7.1365	7.1882
	λ	7450.88	225.54	220.11	173.73	172.48
	f	0.0000	0.0748	0.0035	0.0001	0.0012
IM2a	T_V	0.2216	5.5097	5.6566	7.0721	7.1511
	λ	5596.13	225.03	219.18	175.32	173.38
	f	0.0000	0.0704	0.0018	0.0004	0.0015
IM3	T_V	0.3791	3.8032	5.6171	6.2494	7.1109
	λ	3270.15	326.00	220.73	198.39	174.36
	f	0.0000	0.0009	0.0081	0.0086	0.0014
IM3a	T_V	0.3910	3.7841	5.6870	6.1002	7.1805
	λ	3171.34	327.64	218.01	203.25	172.67
	f	0.0000	0.0012	0.0011	0.0099	0.0017
IM4	T_V	4.8199	5.7455	6.1112	6.3528	6.6484
	λ	257.23	215.79	202.88	195.17	186.49
	f	0.0009	0.0061	0.0155	0.0026	0.0522
IM5	T_V	0.4082	5.6078	5.8197	6.3980	7.0703
	λ	3037.60	221.09	213.04	193.79	175.36
	f	0.0000	0.0168	0.0502	0.0102	0.0002
IM6	T_V	0.1669	5.2880	5.6962	6.4532	6.9584
	λ	7426.57	234.46	217.66	192.13	178.18
	f	0.0000	0.0617	0.0031	0.0112	0.0006
IM6a	T_V	0.1734	5.7527	5.7741	6.2443	6.9435
	λ	7152.02	215.52	214.73	198.56	178.56
	f	0.0000	0.0581	0.0283	0.0007	0.0000
IM7	T_V	0.3074	3.3928	4.4584	5.4170	6.3662
	λ	4033.92	365.43	278.09	228.88	194.76
	f	0.0000	0.0007	0.0181	0.0115	0.0291
IM7a	T_V	0.2569	3.4391	4.6090	5.6754	6.1057
	λ	4826.32	360.51	269.01	218.46	203.06
	f	0.0000	0.0003	0.0028	0.0161	0.0290
IM8	T_V	3.6433	4.5956	5.1087	6.0243	6.2169
	λ	340.31	269.79	242.69	205.81	199.43

	f	0.0037	0.0120	0.0011	0.0247	0.0097
	T_v	0.1333	5.4251	5.9434	6.4948	7.0053
IM9	λ	9300.55	228.54	208.61	190.90	176.99
	f	0.0000	0.0563	0.0024	0.0096	0.0002

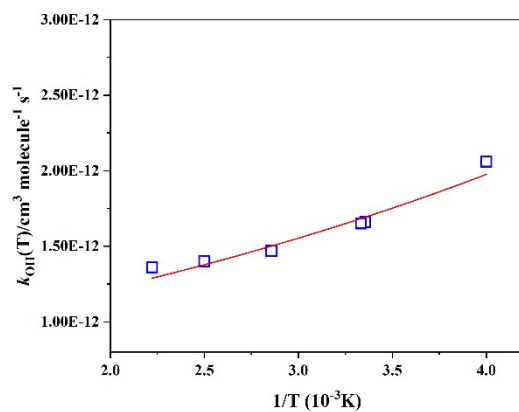


Figure S1. Arrhenius plot for the reaction between HFC-1447fz and OH radical.

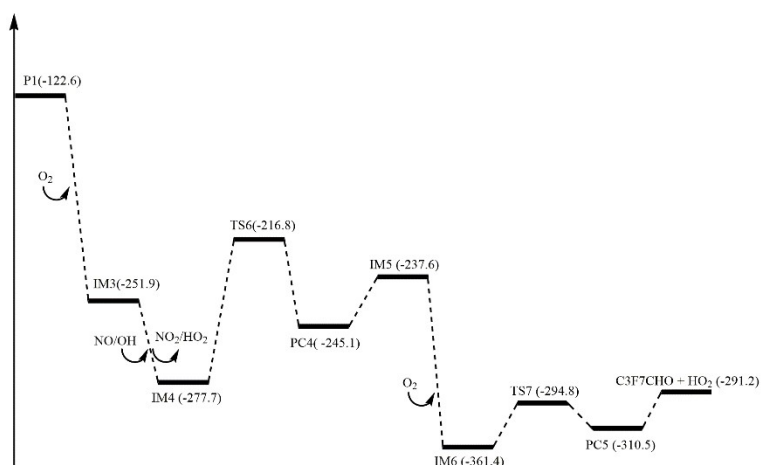


Figure S2. Potential energy profile of the degradation of P1 calculated at the CCSD(T)/cc-pVTZ//M06-2X/6-311++G (d, p) level of theory.

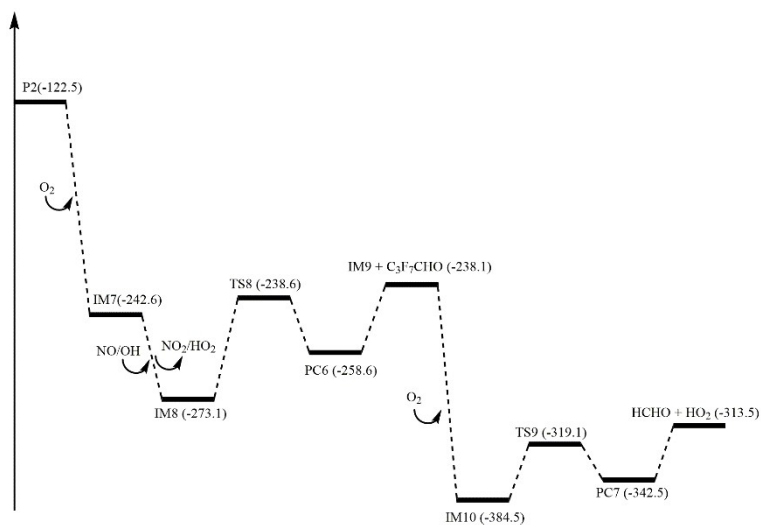


Figure S3. Potential energy profile of the degradation of P2 calculated at the

CCSD(T)/cc-pVTZ//M06-2X/6-311++G (d, p) level of theory.

Global warming potential calculation.

GWP^{1,2} of HFC-1447fz relative to CO₂ is calculated using equation (1):

$$\text{GWP} = \frac{a_0 \int_0^{\text{TH}} e^{-\frac{t}{\tau}} dt}{\text{AGWP}_{\text{CO}_2}} \quad (1)$$

where a_0 is the total instantaneous infrared radiative forcing ($\text{W m}^{-2} \text{ppbv}^{-1}$), TH is the time horizon and $\text{AGWP}_{(\text{CO}_2)}$ is the absolute GWP of CO₂ for the same time horizon. a_0 can be obtained from the radiative forcing function per unit cross section per wave-number ($\text{W m}^{-2} (\text{cm}^{-1})^{-1} (\text{cm}^2 \text{ per molecule})^{-1}$), $F(\nu_k)$ evaluated at the scaled band centre frequency³ ν_k and the intensity A_k of the corresponding vibrational mode of HFC-1447fz calculated at the UM06-2X/6-311++G** level of theory as

$$a_0 = \sum_k A_k F(\nu_k) \quad (2)$$

Then the radiative efficiency can be calculated using the method proposed by Pinnock et al.². The very short-lived substance (VSLS) lifetime need to be adjusted and the correction factor $f(\tau)$ was calculated based on the atmospheric lifetime of the compound using following formula⁴:

$$f(\tau) = \frac{\alpha \tau^b}{1 + c \tau^d} \quad (3)$$

where a, b, c, and d are the constants and are equal to 2.962, 0.9312, 2.994 and 0.9302, respectively, and τ is the atmospheric lifetime in years.

Photochemical ozone creation potential (POCP) calculation.

The POCP was estimated using the following expression^{5,6}:

$$\varepsilon^{\text{POCP}} = \alpha_1 \times \gamma_s \times \gamma_R^\beta (1 - \alpha_2 \times n_c) \quad (4)$$

In which $\varepsilon^{\text{POCP}}$ is the estimated POCP, α_1 , α_2 and β are constants with the values 111, 0.04 and 0.5. γ_s is a structure-based index,

$$\gamma_s = \left(\frac{n_b}{M}\right) \times \left(\frac{28}{6}\right) \quad (5)$$

γ_R^β is the scaled OH reactivity relative to ethylene,

$$\gamma_R^\beta = \left(\frac{k_{\text{OH}}}{n_B}\right) \times \left(\frac{6}{8.64 \times 10^{-12}}\right) \quad (6)$$

where M is the molecular mass, n_B is the total number of C–C and C–H bonds, n_C is number of carbons.

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