

## Supplementary Information

### Atomic coordinates of the optimized geometries

#### 1. Pyrolysis mechanism of thiophene

Thiophene

S	0.00009100	-1.20006100	0.00000000
C	-0.00017200	0.01025800	1.24350400
H	0.00081000	-0.28275900	2.28433500
C	-0.00017200	0.01025800	-1.24350400
H	0.00081000	-0.28275900	-2.28433500
C	-0.00017200	1.27469100	-0.71527900
H	0.00052700	2.17356000	-1.32134500
C	-0.00017200	1.27469100	0.71527900
H	0.00052700	2.17356000	1.32134500

a-1-1m

S	0.00097500	-0.82103500	-0.43430500
C	-0.00087400	1.35192200	1.39347900
H	-0.00076400	1.51352800	2.46741900
C	0.00024700	0.52114300	-1.43216200
H	-0.00013900	0.36090500	-2.51071200
C	0.00028500	1.85713400	-0.98964900
H	0.00026000	2.63787200	-1.74784400
C	0.00038200	2.24760300	0.37885700
H	0.00143200	3.32276600	0.58607300

b-1-1t

S	-1.21743300	-0.14605900	-0.05378400
C	0.36151500	-1.48555300	-0.05092100
C	-0.15658500	1.23772300	0.01897200
H	-0.55545900	2.24271400	0.05820900
C	1.15297100	0.85975600	-0.00467800
H	1.96363700	1.58301100	0.02857400
C	1.37994700	-0.55706600	-0.01190300
H	2.39171600	-0.96117800	-0.00497400
H	-0.74805200	-0.85676300	1.06992000

b-1-1m

S	-1.15029800	-0.09605100	-0.09832100
C	0.16381700	-1.47086000	0.02225700
C	-0.02155000	1.28373700	0.04088800

H	-0.34571500	2.31363700	-0.00790400
C	1.22491700	0.75877700	0.00365700
H	2.11141300	1.38867900	-0.01228500
C	1.29722500	-0.70108400	-0.00021400
H	2.26422900	-1.19885600	0.02470800
H	-1.61161000	-0.19006100	1.16908900

c-1-1t

S	-1.21477000	-0.05526500	-0.00167100
C	0.04461500	1.24442200	-0.02356400
H	-0.29205200	2.25721100	-0.22339900
C	0.06990400	-1.21882300	0.00185000
H	-0.17842100	-2.27437100	0.03566500
C	1.32416900	-0.66725100	0.00066300
H	2.21672600	-1.28364100	0.03267100
C	1.37996600	0.77766800	-0.11167800
H	0.77815000	1.36894300	0.97816300

c-1-1m

S	-1.25341300	0.00092300	0.00012700
C	0.27108000	1.32994200	-0.00014100
H	0.10321000	1.93747100	-0.89542200
C	-0.05324400	-1.18496400	0.00000000
H	-0.35705500	-2.22976900	-0.00077400
C	1.29522500	-0.77309900	0.00005900
H	2.08819400	-1.51580100	-0.00042900
C	1.50658500	0.60349800	0.00044200
H	0.10237300	1.94107700	0.89242900

**2. Possible H2S formation pathways based on Mode A**

a-1-2t

S	1.26709300	-0.20831800	1.29832500
C	0.30759500	1.19600700	1.40604000
H	0.02286300	1.54222500	2.40016300
C	-0.63197300	0.93311200	-1.88079500
H	-0.63576300	0.61765900	-2.91542100
C	0.12485000	1.66457500	-1.09407100
H	1.01699100	2.15418300	-1.51372800
C	-0.14255600	1.94129600	0.33917600
H	-0.72781300	2.83544800	0.56056000

a-1-2m

S	-2.94246900	1.27436200	-0.79342900
C	0.93795200	1.27491900	1.60833600

H	1.18100000	1.27524500	2.66307800
C	-1.35310400	1.27473100	-1.34838400
H	-1.19106900	1.27356900	-2.42703900
C	-0.19486300	1.27462800	-0.55821100
H	0.76615600	1.27416500	-1.06866700
C	-0.17966700	1.27494700	0.87017800
H	-1.15650400	1.27547000	1.36880300

a-1-2m-1

C	0.91463400	1.27503900	1.64391200
H	1.13567000	1.27538500	2.70249200
C	-1.21185800	1.27437500	-1.36709000
H	-1.43438700	1.27405000	-2.42528300
C	-0.13855900	1.27442400	-0.59622800
H	0.85390200	1.27404700	-1.06208600
C	-0.15863500	1.27498300	0.87302800
H	-1.15086600	1.27537000	1.33934800

a-2-1t

S	-3.11578200	1.43164300	-1.13129600
C	0.99014200	1.23712200	1.61470500
H	1.28027700	1.17564700	2.65504100
C	-1.39722900	1.42611000	-1.19401600
H	-2.27783800	0.92833800	-2.23986200
C	-0.24162900	1.35710000	-0.53187100
H	0.68910900	1.35675100	-1.09709000
C	-0.14111500	1.28720900	0.92653200
H	-1.08849100	1.27156100	1.47963500

a-2-1m

S	-1.69601500	0.12174600	-0.74635800
C	2.17461000	-0.11376900	1.93297500
H	2.44284700	-0.21168000	2.97508600
C	-0.00532300	0.07213700	-1.05016500
H	-2.05515700	-0.92107600	-1.52894200
C	1.08110900	0.07481000	-0.27971100
H	2.04956800	0.23433900	-0.75079300
C	1.09135100	-0.14452000	1.18131400
H	0.11497200	-0.34672300	1.63759700

a-2-1m-1

C	2.18638000	-0.11291700	1.93863000
H	2.45270400	-0.22970200	2.97993600
C	0.09829000	0.07372800	-1.14965100

C	1.03576200	0.05787900	-0.23735900
H	1.96993600	0.25261100	-0.79444900
C	1.08410800	-0.14431800	1.21161700
H	0.12195300	-0.33268700	1.69757900

a-3-1t

S	-2.90398300	1.50716100	-0.83226000
C	0.83759100	1.61130800	1.63016600
H	1.04196400	1.52300800	2.68950000
C	-1.27303000	1.49269900	-1.46615000
H	-1.10017500	1.79368400	-2.50012100
C	-0.14329700	1.55689200	-0.58150400
H	-0.77286000	0.42184400	-1.38689500
C	-0.08052800	1.13961900	0.78616800
H	-0.83224300	0.42561000	1.15828200

a-3-1m

S	-1.65032500	0.01130900	-0.47596100
C	2.02961900	0.09182000	1.89548400
H	2.21523100	-0.10505600	2.94645500
C	-0.01099800	-0.00025100	-1.24598200
H	0.03903700	0.60161000	-2.15734900
C	1.11077700	0.25563600	-0.32625400
H	0.25447600	-1.03652100	-1.54653600
C	1.07863200	-0.23754800	1.01625800
H	0.24821000	-0.88500200	1.34960700

a-3-2t

S	-1.99634500	0.61983400	-0.96864400
C	1.88598900	0.32824800	1.99954300
H	2.37209800	0.13496100	2.94615900
C	-0.23418300	0.09071500	-1.12482800
H	0.18389800	0.23063900	-2.12379800
C	0.65945300	-0.00684300	-0.08273300
H	-0.91667600	-0.85329500	-1.12280600
C	1.16030400	-0.42260100	1.11398400
H	0.99257800	-1.48264400	1.37491500

a-3-2m

S	1.88474100	-0.42292000	0.07672700
C	-2.62111800	-0.70643600	-0.41675700
H	-3.52689600	-0.99779200	0.15576100
C	0.56971100	0.72186600	-0.33260000
H	0.81204200	1.55636700	-0.98813900
C	-0.66641700	0.53204100	0.02705900

H	2.79573000	0.52276200	0.39005200
C	-1.93438900	0.27269700	0.37831700
H	-2.32345100	0.76437800	1.27858400

a-3-2m-1

C	1.70700300	-0.45264900	0.00000100
H	2.78744500	-0.39515900	-0.00000700
C	-1.86916700	-0.15844100	0.00000500
H	-2.91061100	-0.38641500	-0.00001700
C	-0.68021400	0.07856300	-0.00000300
C	0.70618500	0.41490900	0.00000100
H	0.94032200	1.48728200	0.00000000

a-4-1t

S	1.89624300	-0.29682500	0.20060700
C	-2.51596000	-0.83906800	-0.25009700
H	-3.51264300	-1.01449200	0.20222000
C	0.51271500	0.75188800	-0.43479400
H	1.02272700	-0.60583900	-0.91378000
C	-0.68456600	0.55738800	-0.03464100
H	2.85891100	0.21881400	-0.59857700
C	-2.01142100	0.37003800	0.25437400
H	-2.51349900	1.10923200	0.89136700

a-4-1m

S	1.95740000	0.10708100	-0.14333300
C	-2.68244200	0.78804000	0.19196200
H	-3.70285900	0.77737400	-0.24314400
C	0.50725900	-0.49688300	0.45266400
H	1.76824200	1.34050000	-0.74780900
C	-0.69878200	-0.45250000	0.09494300
H	2.52132400	0.68463800	0.95267900
C	-2.03515300	-0.38800100	-0.21723600
H	-2.45040500	-1.21973800	-0.80239400

a-4-1m-1

C	-2.78376800	0.67173300	0.04503800
H	-3.81658400	0.93984600	-0.14502500
C	0.59231500	-0.53195500	0.45883000
C	-0.65334300	-0.45687700	0.14994600
C	-1.98545700	-0.38635200	-0.23635200
H	-2.41554500	-1.22810200	-0.79564100

a-5-1t

S	-2.69146000	1.16002400	-0.37504200
C	0.77903700	1.07333700	1.69312800
H	0.72027000	1.30187900	2.75294200
C	-1.30368200	1.22598300	-1.36050200
H	-1.40497500	1.21896600	-2.43881700
C	-0.04062600	1.29962000	-0.70497900
H	0.85916400	1.42602800	-1.30636100
C	0.00456300	1.34873700	0.67559000
H	-1.73191600	1.46636300	0.72375300

a-5-1m

S	-1.60220800	-0.58179000	-0.00000100
C	2.42266700	-0.78336400	0.00002900
H	3.16310000	-1.55051600	0.00001700
C	-0.72299500	0.93726400	0.00030400
H	-1.38749700	1.79606900	-0.00076900
C	0.61541800	1.13228600	-0.00006200
H	0.98099300	2.15645200	-0.00024900
C	1.58461800	0.09642900	-0.00000700
H	-0.51952100	-1.38905400	-0.00057000

a-5-1m-1

C	-1.86912700	-0.15849700	-0.00014900
H	-2.91060200	-0.38640300	-0.00036300
C	1.70693300	-0.45268100	-0.00001800
H	2.78739200	-0.39541900	-0.00090300
C	0.70622900	0.41500100	0.00041900
H	0.94020700	1.48735400	-0.00121600
C	-0.68020200	0.07858900	0.00016200

a-6-1t

S	1.60893600	-0.59359200	-0.00374700
C	-2.45877600	-0.74309900	0.01844800
C	0.67879400	0.96322400	-0.00879200
H	1.35627800	1.79947400	-0.17956800
C	-0.70239600	1.18725300	-0.12751700
H	0.11649700	1.34874800	1.02219300
C	-1.59777700	0.12494800	-0.01670100
H	0.52096700	-1.39352000	-0.02336500
H	-3.25580100	-1.45119100	0.04805700

a-6-1m

S	1.60521600	-0.61289100	-0.05767400
C	-2.48465900	-0.77651200	0.01180300

C	0.70090100	1.01848500	0.07082400
H	1.22096100	1.70166700	-0.60908700
C	-0.74396600	1.13292800	-0.08402200
H	0.87858200	1.45207200	1.07121200
C	-1.63873400	0.14332000	-0.03015000
H	0.71350900	-1.32943700	0.65626000
H	-3.49775500	-1.12737600	-0.00633500

a-6-2t

S	2.06130300	-0.50233200	-0.02730300
C	-2.85227800	-0.78157900	-0.00147900
C	0.35180000	1.18779300	0.03036900
H	0.89037500	1.98660300	-0.46191700
C	-0.94903400	0.94324500	-0.04719200
H	0.81453700	0.84295000	0.99379700
C	-1.91129900	0.01246600	-0.00825200
H	1.13486100	-1.48036800	0.05939300
H	-3.65576300	-1.48342200	0.00489600

Diacetylene

C	1.89886900	0.00078200	-0.00011000
C	-1.89885500	0.00056700	0.00019300
H	-2.96509300	-0.00160900	-0.00061000
C	-0.68451500	-0.00029200	-0.00003300
C	0.68449300	-0.00041200	-0.00004400
H	2.96514400	-0.00226900	0.00056900

a-7-1t

S	1.94141600	-0.49182600	-0.07407900
C	-2.29344400	-1.23051100	-0.01058800
C	0.12908900	1.57527500	-0.00956400
H	1.53962600	0.86908600	-0.07380300
C	-1.10555700	1.10871100	0.01143800
H	-1.75471900	2.00187900	0.04643100
C	-1.72430100	-0.16175500	0.00250600
H	1.88638700	-0.56696300	1.27177600
H	-2.76867200	-2.18510000	-0.02190300

a-7-1m

S	1.46154700	-0.50863400	-0.10360200
C	-2.29031600	-0.86127000	0.00533400
C	0.72230000	1.17258900	0.02176200
H	2.33754500	-0.41191500	0.91481200
C	-0.63331400	1.19348600	0.01054500

H	-1.07287300	2.19188800	0.01963200
C	-1.54428100	0.09913600	0.00745700
H	0.79245600	-1.58148300	0.46185900
H	-2.96821400	-1.68398900	-0.00926400

a-7-1m-1

C	1.80875600	-0.10634800	0.00049500
C	-1.91202000	-0.39398200	0.00014500
C	-0.78325600	0.26808600	0.00003600
H	-1.20101000	1.30218900	0.00070200
C	0.60945700	0.05939200	-0.00080900
H	2.86338700	-0.26507800	0.00009300

**3. Possible H2S formation pathways based on Mode B**

b-1-1m-1

C	1.74818500	-0.59509900	-0.00002900
C	-1.53472300	-0.51968100	0.00009800
H	-2.61213600	-0.61052300	-0.00027900
C	-0.65340100	0.46459200	-0.00003800
H	-1.01374400	1.49826300	-0.00006700
C	0.80160400	0.30186000	-0.00000900
H	1.45588900	1.20222300	0.00021300

b-2-1t

S	1.49990100	0.31686200	-0.10950000
C	-1.17511000	0.68658200	0.85480900
C	0.14865600	-0.79717600	0.26021000
H	0.44557400	-1.66428300	0.84952000
C	-1.11422500	-0.79211500	-0.31682100
H	-1.75243400	-1.67136700	-0.20652500
C	-1.64654300	0.55075500	-0.39307900
H	-2.37519600	1.04619200	-1.01673000
H	2.40696500	-0.66860200	-0.30497100

b-2-1m

S	-1.54796800	-0.24516800	-0.13725900
C	1.06444100	-0.51750800	0.86156000
C	-0.01111300	0.54736100	0.45641000
H	-0.23732300	1.33027500	1.18263800
C	1.13676900	0.74407700	-0.44703100
H	1.73458900	1.66031300	-0.47024500
C	1.64268200	-0.57587100	-0.38623000
H	2.41910500	-1.14878900	-0.87100800
H	-2.14555300	0.89254400	-0.55348900

## b-2-1m-1

C	-0.00002200	-0.96513000	0.26908200
C	-1.04764700	-0.08203100	-0.18033900
H	-2.12710200	-0.08050800	-0.15610900
C	0.00001300	0.86928300	0.02490400
H	0.00006600	1.72071200	0.71227000
C	1.04765000	-0.08206200	-0.18030300
H	2.12706800	-0.08056300	-0.15622300

## b-3-1t

S	1.47865100	-0.58861700	0.00695100
C	-2.25799500	-1.11991400	-0.03795800
C	0.63417800	0.95899700	-0.00991700
H	1.25405700	1.84831400	-0.03809600
C	-0.70834800	1.09230200	-0.00470000
H	-1.13504800	2.08949800	-0.02311800
C	-1.61625000	-0.01847800	-0.00302100
H	2.71989300	-0.06722600	0.02302600
H	-2.80682500	0.06984300	0.26055600

## b-3-1m

S	1.48518200	0.64476500	0.00003200
C	-2.43265300	0.79507700	-0.00051000
C	0.70629800	-0.93918800	-0.00033700
H	1.36743800	-1.79930300	-0.00078100
C	-0.63099000	-1.12493200	0.00017900
H	-1.00241700	-2.14710300	0.00055000
C	-1.59461200	-0.08361600	0.00038200
H	2.74785100	0.17549900	0.00062900
H	-3.16404900	1.57063300	0.00080900

## b-3-2t

S	1.57861200	-0.59513100	-0.08434700
C	-2.46454700	-0.79387300	-0.00493400
C	0.70319100	0.96665400	0.01000000
H	1.32237500	1.85902600	0.01119700
C	-0.63647700	1.10084000	0.00885200
H	-1.03946800	2.11370100	0.02725600
C	-1.59418500	0.05079300	-0.00045400
H	1.61873200	-0.83830200	1.24413200
H	-3.20731700	-1.55881200	-0.01382100

## b-3-2m

S	2.25902400	-0.19898800	-0.00067300
C	0.60180300	0.15685200	0.00060400
C	-2.94640600	-0.49869300	0.00073000
H	-2.67507100	-1.54953300	0.00260200
C	-2.01731400	0.47418900	-0.00069300
H	-4.00262600	-0.25187000	-0.00016900
C	-0.61239500	0.26668100	-0.00036700
H	-2.33575400	1.51633100	-0.00265800
H	2.71493300	1.07470800	0.00935300

b-3-2m-1

C	-2.04401300	-0.26774800	-0.00001100
C	1.56048700	-0.37125100	-0.00000300
H	1.37978500	-1.44146300	-0.00004800
C	0.51342800	0.51616500	-0.00002900
H	2.58940300	-0.02388900	0.00009500
C	-0.81278900	0.10281800	0.00003700
H	0.72813400	1.58544700	-0.00001400

b-6-1t

S	-1.33460100	0.53408400	-0.03462000
C	-0.76741200	-1.09737300	0.05577600
C	1.74444600	1.10046900	0.15900700
H	2.15016400	1.89919800	-0.44921200
C	1.42656700	-0.13865500	-0.06774500
H	2.61599100	-0.04422900	0.09213900
C	0.62220000	-1.27146700	-0.03086700
H	1.06330700	-2.26103000	-0.04437400
H	-2.63065200	0.30286500	0.25833600

b-6-1m

S	1.52559400	-0.55456000	-0.08448600
C	0.86910700	0.96929000	0.27764700
C	-2.36517200	-0.72654100	0.09290900
H	-2.72278400	-1.34480800	-0.72766000
C	-1.45284300	0.18737700	-0.09659000
H	-2.79661600	-0.90216200	1.07723400
C	-0.51490100	1.13031200	-0.13927400
H	-0.83342700	2.15706700	-0.32672000
H	2.72617800	-0.39976800	0.52076900

b-6-2t

S	2.03765200	-0.34611100	-0.00880400
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C	0.74348600	0.74755800	0.11192800
C	-3.02463200	-0.33824500	0.09077700
H	-3.34637200	-1.34086300	-0.17821100
C	-1.75010900	-0.00943900	-0.03130000
H	-3.77205700	0.34787200	0.47704800
C	-0.50376400	0.39334400	-0.20215300
H	-1.31091200	1.30040900	-0.37213400
H	3.03701400	0.47104700	0.39864200

b-6-2m

S	2.25902400	-0.19898800	-0.00067300
C	0.60180300	0.15685200	0.00060400
C	-2.94640600	-0.49869300	0.00073000
H	-2.67507100	-1.54953300	0.00260200
C	-2.01731400	0.47418900	-0.00069300
H	-4.00262600	-0.25187000	-0.00016900
C	-0.61239500	0.26668100	-0.00036700
H	-2.33575400	1.51633100	-0.00265800
H	2.71493300	1.07470800	0.00935300

b-6-2m-1

C	-2.04401300	-0.26774800	-0.00001100
C	1.56048700	-0.37125100	-0.00000300
H	1.37978500	-1.44146300	-0.00004800
C	0.51342800	0.51616500	-0.00002900
H	2.58940300	-0.02388900	0.00009500
C	-0.81278900	0.10281800	0.00003700
H	0.72813400	1.58544700	-0.00001400

b-7-1t

S	2.04593300	-0.34935700	-0.01179300
C	0.71301200	0.75774900	0.17118100
C	-3.09038700	-0.27452700	0.03535000
H	-3.45865100	-1.29219100	-0.09002100
C	-1.80632200	0.00521900	-0.00573900
H	-3.84077500	0.49757400	0.20548500
C	-0.55113600	0.30995100	-0.05636200
H	-0.05800300	1.03728100	-0.95275600
H	3.03150200	0.55669000	0.15940100

b-7-1m

S	2.02000300	-0.40999800	0.00009100
C	0.67312100	0.75010200	0.00011000
C	-3.09163400	-0.31512900	-0.00007400

H	-3.38368700	-1.36206000	-0.00032600
C	-1.81896800	0.04141300	0.00000700
H	-3.88628600	0.42644400	0.00007900
C	-0.59731500	0.38740900	0.00003200
H	0.95804100	1.79914900	0.00019700
H	3.00065900	0.51367500	-0.00184800

b-7-2t

S	2.49698300	0.36624500	0.07888000
C	0.18280200	-1.22156900	-0.01381200
C	-3.26326100	0.55696400	0.00821100
H	-3.37503400	1.63761400	0.06461500
C	-2.07837600	0.00575700	-0.00020400
H	-4.16547500	-0.04856900	-0.03967100
C	-0.90523400	-0.54109400	-0.00626300
H	1.56526300	-0.79595800	0.04096800
H	2.40792600	0.54664900	-1.25558600

b-7-2m

C	2.13301100	0.00098000	0.00017200
C	-1.75661400	0.00029000	0.00012600
H	-2.31463700	0.93320700	0.00005900
C	-0.45029100	0.00045800	-0.00013100
H	-2.31242900	-0.93402500	0.00006200
C	0.84507100	-0.00159200	-0.00018800

**4. Possible H<sub>2</sub>S formation pathways based on Mode C**

c-1-1t

S	-1.21477000	-0.05526500	-0.00167100
C	0.04461500	1.24442200	-0.02356400
H	-0.29205200	2.25721100	-0.22339900
C	0.06990400	-1.21882300	0.00185000
H	-0.17842100	-2.27437100	0.03566500
C	1.32416900	-0.66725100	0.00066300
H	2.21672600	-1.28364100	0.03267100
C	1.37996600	0.77766800	-0.11167800
H	0.77815000	1.36894300	0.97816300

c-1-1m

S	-1.25341300	0.00092300	0.00012700
C	0.27108000	1.32994200	-0.00014100
H	0.10321000	1.93747100	-0.89542200
C	-0.05324400	-1.18496400	0.00000000
H	-0.35705500	-2.22976900	-0.00077400

C	1.29522500	-0.77309900	0.00005900
H	2.08819400	-1.51580100	-0.00042900
C	1.50658500	0.60349800	0.00044200
H	0.10237300	1.94107700	0.89242900

c-1-2t

S	-1.00437500	0.54360000	-0.11049600
C	-0.48620200	-1.24812300	0.31864000
H	-0.36636800	-1.35899700	1.40786900
C	0.73443700	1.03368800	0.12482400
H	0.98577700	2.07136300	0.31753400
C	1.58699200	-0.06701900	-0.07776000
H	1.51377700	0.35939700	1.08933800
C	0.69725800	-1.02900200	-0.52671700
H	-1.25810000	-1.90662100	-0.08072700

c-1-2m

S	0.88324500	-0.75904500	0.00019300
C	-1.05871300	-0.92063300	-0.00029900
H	-1.34684300	-1.47705800	-0.89355100
C	0.85549900	1.15834900	-0.00038100
H	1.35089700	1.53492000	-0.89773400
C	-0.59957100	1.27146200	0.00044200
C	-1.55393400	0.49576800	0.00015900
H	-1.34725500	-1.47803700	0.89218700
H	1.35159200	1.53522700	0.89647800

c-2-1t

S	1.27519000	0.06851900	0.00000600
C	-0.41715400	1.34177900	0.00001100
H	-0.26409500	1.94212600	0.90119300
C	0.14070100	-1.16892900	-0.00001000
H	0.49754600	-2.19716400	-0.00001800
C	-1.24307200	-0.85508200	-0.00001300
H	-1.97773900	-1.65513700	-0.00002400
C	-1.54625400	0.49418600	-0.00000200
H	-0.26408800	1.94214400	-0.90115900

c-2-1m

S	1.65034000	-0.63174100	-0.00009300
C	-2.43732500	-0.70815100	0.00017100
H	-2.84060300	-1.10343200	-0.93009800
C	0.89736600	0.82443600	0.00048600
H	1.50934400	1.73055300	0.00099500
C	-0.53526000	1.10245800	-0.00035800

H	-0.82817600	2.15252900	-0.00113200
C	-1.49222100	0.18630900	-0.00012300
H	-2.84136500	-1.10210200	0.93067200

c-2-2t

S	1.36526800	-0.46631700	-0.01200100
C	-1.41816400	-1.19677600	0.06516000
H	-1.78714000	-2.11983100	-0.35108600
C	0.54609800	1.01940400	-0.03374400
H	1.15684500	1.90155400	0.15041000
C	-0.84220400	1.22744800	-0.04309800
H	-1.24118900	2.21146600	0.17003800
C	-1.58558800	0.06168300	-0.02004500
H	-0.17365500	-1.20267100	0.41301700

**5. Effect of hydrogen radical on thiophene pyrolysis**

d-1-1t

S	1.20209700	-0.05557200	-0.05053800
C	-0.00273800	1.20486400	-0.10993600
H	0.29190700	2.21625900	-0.35093300
C	-0.01974000	-1.27815300	0.07585900
H	0.26249300	-2.31597700	0.18930700
C	-1.28455300	-0.74402600	0.02481300
H	-2.18537700	-1.34403500	0.08495300
C	-1.27907300	0.67185100	-0.11281700
H	-2.17272400	1.28148400	-0.17821100
H	0.08677400	1.92422000	1.79597800

d-1-1m

S	1.24569800	-0.03059900	-0.00001700
C	-0.03840800	1.31079600	0.00002800
H	0.11131900	1.94315400	-0.88467700
C	0.01800000	-1.28288300	0.00001200
H	0.31254600	-2.32362800	0.00006000
C	-1.28320500	-0.77151100	0.00000300
H	-2.15305200	-1.42117200	0.00000200
C	-1.36635300	0.60679000	-0.00001800
H	-2.29347300	1.16904800	-0.00009200
H	0.11129400	1.94303700	0.88482900

e-1-1t

C	-0.14085000	1.25740100	0.00477800
C	1.15877200	0.85522400	-0.08990100
C	1.29950200	-0.58074900	-0.10202000

C	0.07035400	-1.21922200	-0.10817700
S	-1.23716200	-0.09571600	0.03795600
H	-0.52746000	2.26572800	0.06297500
H	1.99771500	1.54070800	-0.11539300
H	2.22597900	-1.09109400	-0.33636500
H	-0.12563100	-2.28186000	-0.14171800
H	1.89732800	-0.77795600	1.69512000

e-1-1m

C	0.08437300	1.26201200	-0.00000300
C	-1.19156600	0.85047700	0.00000200
C	-1.38527700	-0.64617500	-0.00001800
C	-0.00742200	-1.24298600	0.00011600
S	1.26929100	-0.05779500	-0.00001100
H	0.44293100	2.28406200	0.00000800
H	-2.03178400	1.53763000	0.00001000
H	-1.97567400	-0.96975000	0.87685500
H	0.23071900	-2.29745700	-0.00026800
H	-1.97550300	-0.96973800	-0.87701600

**6. Possible H2S formation pathways based on Mode D**

d-1-2m

S	-1.61337000	-0.52404100	-0.00016800
C	1.72927100	-1.12887200	0.00028400
H	0.80621900	-1.69525100	0.00127300
C	-0.75772400	0.92345600	0.00025500
H	-1.35069300	1.84014100	0.00070200
C	0.63068500	1.13987800	0.00006500
H	0.91424900	2.19214900	0.00016700
C	1.74150200	0.23269600	-0.00030000
H	2.71481100	0.72158600	-0.00107200
H	2.66693300	-1.67692400	-0.00021000

d-1-3t

S	1.48167200	-0.46732900	-0.09867500
C	-1.46060300	-1.26116300	0.04252500
H	1.72812400	-0.63598100	1.21977800
C	0.56303100	1.06330400	0.03187100
H	1.15778900	1.97163100	0.05633400
C	-0.78043700	1.13814600	0.01075600
H	-1.21193500	2.13827600	0.02566600
C	-1.74428300	0.03234700	-0.02472300
H	-2.79510800	0.33599400	-0.10531200
H	-2.05187300	-2.16846200	0.01975000

d-1-3m

S	-1.40844500	-0.50733900	0.00010900
C	1.43049700	-1.24880900	-0.00042500
H	-2.64970800	0.02822300	-0.00048700
C	-0.55580200	1.03792900	0.00000700
H	-1.18082600	1.92402700	-0.00019700
C	0.78923700	1.15114000	-0.00009000
H	1.20677700	2.15412100	-0.00042100
C	1.73794200	0.04129400	0.00014100
H	2.79935500	0.31925800	0.00118400
H	1.94828600	-2.19752700	0.00038200

d-1-3m-1

C	1.41036500	-1.24306100	0.00003300
C	-0.50316000	1.11704100	-0.00024800
H	-1.32645500	1.81856600	-0.00041800
C	0.81975500	1.18039400	0.00005500
H	1.28933700	2.17203200	0.00017900
C	1.74601600	0.03802100	0.00024800
H	2.81332000	0.29230500	0.00060900
H	1.92628900	-2.19386500	0.00012200

d-2-1t

S	-1.30186600	-0.31895700	-0.08645300
C	0.93435800	-1.44483900	-0.02846500
H	-2.43626800	0.36339500	0.43037600
C	-0.28392900	1.14752700	0.00813100
H	-0.82183400	2.08398700	0.06289700
C	1.05751900	0.98507100	-0.00584500
H	1.67155600	1.88402500	0.02417200
C	1.69257500	-0.32047900	0.00721800
H	2.78724500	-0.34935100	0.04334600
H	-0.77397200	-1.08242500	0.93622200

d-2-1m

S	-1.24249900	-0.27306100	-0.10483200
C	0.71583500	-1.42050500	0.05132400
H	-2.40399000	0.56035000	0.06601300
C	-0.18664600	1.16812200	0.03631300
H	-0.68249000	2.12587100	0.11332000
C	1.14259300	0.92368700	0.02341100
H	1.82955700	1.76775900	0.05006700
C	1.64160600	-0.44176500	-0.03319100

H	2.71557200	-0.61563900	-0.12505000
H	-1.45899700	-0.84659300	1.10582300

d-2-1m-1

C	1.74810800	-0.59514300	0.00000100
C	-1.53465000	-0.51974700	-0.00000100
H	-2.61209100	-0.61042100	0.00000000
C	-0.65341600	0.46462500	0.00000100
H	-1.01377400	1.49827600	0.00000400
C	0.80162000	0.30191200	-0.00000100
H	1.45589000	1.20226200	-0.00000600

d-3-1t

S	-1.76069100	-0.41500200	-0.04052500
C	1.79375400	-1.13633600	0.05285900
H	0.86318900	-1.67536800	0.20125800
C	-0.57635000	0.82848400	-0.02125300
H	-1.89875500	0.91840100	0.58097300
C	0.72020700	1.14484100	0.00770200
H	0.97378100	2.20361800	0.04473500
C	1.84766700	0.20430100	-0.04057400
H	2.82145400	0.67652400	-0.16495900
H	2.69972300	-1.73088100	-0.00601800

d-3-1m

S	-1.67467800	-0.39634300	-0.04560900
C	1.75938900	-1.14478000	-0.01760600
H	0.83898700	-1.67980000	-0.22834300
C	-0.60504700	0.93841200	0.00033800
H	-2.57841000	0.06389700	0.84958600
C	0.70864000	1.15389400	-0.06733800
H	1.01195400	2.19458500	-0.19648700
C	1.81773200	0.19440600	0.07151100
H	2.78507700	0.65683200	0.26373600
H	2.65296200	-1.74562000	0.11981300

d-3-2t

S	-1.42705100	-0.38289600	-0.08306400
C	1.48328200	-1.23515700	-0.07780700
H	-0.73354900	-1.44697700	0.50355200
C	-0.61181100	1.21573800	-0.01353100
H	-2.31013100	-0.23008500	0.92846800
C	0.74164400	1.18597900	-0.03012400
H	1.20987800	2.17049400	-0.04917000

C	1.69580100	0.06613700	0.06847100
H	2.72165900	0.36681400	0.32518300
H	2.09145600	-2.13008900	-0.06106800

d-3-2m

S	-1.44021600	-0.37677200	-0.08011100
C	1.49404900	-1.23757600	-0.09267700
H	-0.85722700	-1.46189600	0.57371400
C	-0.59330400	1.21414400	-0.02757100
H	-2.36536000	-0.15745300	0.87883000
C	0.75872100	1.17790200	-0.02669700
H	1.22689800	2.16245400	-0.05674600
C	1.71067000	0.05847400	0.08149600
H	2.73415900	0.35172800	0.35543900
H	2.08416800	-2.14415000	-0.07676600

**7. Possible H2S formation pathways based on Mode E**

e-1-2m

C	-1.20576800	1.77942100	-0.21945500
C	-1.63322700	0.53773600	-0.27397700
C	-0.89726500	-0.77047000	-0.04172000
C	0.55656900	-0.81887200	0.31121100
S	1.63337700	0.38324000	0.52216000
H	-0.30703900	2.34221800	-0.02283000
H	-2.68654000	0.37475700	-0.52434500
H	-1.42489200	-1.33723900	0.74526100
H	0.90801400	-1.84898800	0.43821200
H	-1.01962500	-1.40780300	-0.93484600

e-1-3t

C	-1.59203100	-1.32944500	0.13278800
C	-1.79546500	-0.04425900	-0.02118900
C	-0.76867000	1.08993600	-0.18347700
C	0.63122900	0.83769300	0.30481500
S	1.60243900	-0.40604300	-0.09912000
H	-0.79589600	-2.05443400	0.20986100
H	-2.82554900	0.31828900	-0.06994000
H	-0.71854900	1.33059100	-1.25693300
H	1.01687400	1.59534300	0.99371700
H	-1.16629000	1.98334400	0.31159100

e-1-3m

C	2.19551700	1.03501000	-0.08919600
C	1.96614500	-0.25827000	-0.12757800
C	0.60528000	-0.94781200	-0.01441600

C	-0.48477500	-0.06918100	0.52234900
S	-1.93374500	0.19805200	-0.16685100
H	1.65313600	1.96484800	0.01789600
H	2.80638000	-0.94182100	-0.27000600
H	0.31420600	-1.36787700	-0.98370000
H	-0.24686600	0.41228400	1.47648700
H	0.72006800	-1.79475100	0.68198700

e-1-4t

C	2.48787200	0.85157300	-0.11982800
C	2.02678100	-0.37854200	-0.10802200
C	0.58244200	-0.80324400	0.13817700
C	-0.38992300	0.31145300	0.34316400
S	-2.02313200	0.06912900	-0.14110400
H	2.11554900	1.85749800	0.01578100
H	2.71223000	-1.20987400	-0.29060900
H	0.24783300	-1.51544700	-0.63751700
H	-1.50065200	1.23640900	0.55677500
H	0.55212100	-1.36209400	1.09228500

e-1-4m

C	2.47467700	0.84755400	-0.11982300
C	1.99724600	-0.37657000	-0.11453600
C	0.54713200	-0.78276900	0.14427800
C	-0.37272800	0.37365200	0.41127300
S	-1.92914300	0.04179800	-0.14871700
H	2.11563800	1.85631400	0.02898900
H	2.66861100	-1.21565400	-0.31330600
H	0.23073100	-1.51184300	-0.62329900
H	-2.56104500	1.16966600	0.25867000
H	0.53439800	-1.33845200	1.10125900

e-1-4m-1

C	2.57476600	0.70527000	-0.45772400
C	2.02236900	-0.22497200	0.27920700
C	0.51906600	-0.61275600	0.18796400
C	-0.23396800	-0.82508100	1.38236800
H	2.28407200	1.41381000	-1.22219700
H	2.58913700	-0.78000600	1.02410800
H	0.00415300	-0.10667700	-0.64150000
H	0.43610900	-1.71735500	-0.03739200

e-2-1t

C	-1.18092500	-1.53425100	-0.08130500
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C	-1.63215900	-0.30948500	0.01126900
C	-1.01851000	1.06862900	-0.00728600
C	0.48357500	1.07378300	0.06895000
S	1.48923200	-0.34229900	-0.03705500
H	0.76780000	-1.16624000	0.76481300
H	-2.72547800	-0.39419600	0.12324400
H	-1.34674900	1.58496400	-0.92549000
H	1.00450200	2.00250500	-0.14129000
H	-1.43968200	1.65769600	0.82183800

e-2-1m

C	-0.86311500	-1.35901700	0.03170700
C	-1.62968300	-0.24655200	0.08349400
C	-1.11899600	1.18787900	0.04272200
C	0.36975600	1.12110100	-0.04415200
S	0.87857800	-0.56683300	-0.20515800
H	1.46047600	-0.79764600	1.00537200
H	-2.70471500	-0.39438600	0.18796800
H	-1.53365100	1.74986700	-0.81181300
H	1.05216600	1.94802900	-0.20151200
H	-1.43037600	1.75323300	0.93889800

e-2-1m-1

C	-1.18040900	-1.49711900	0.07125500
C	-1.59010900	-0.26130900	0.08987700
C	-0.98944500	1.11877300	0.02427400
C	0.48398800	1.17653400	-0.09725000
H	-2.68737000	-0.37949800	0.18089300
H	-1.43455700	1.67980300	-0.81985700
H	0.83370000	2.22139300	-0.13644300
H	-1.29441100	1.70157700	0.91456300

e-3-1t

C	0.38465000	1.45078900	-0.12290700
C	1.42616000	0.63883400	-0.03505000
C	1.20487500	-0.87572700	0.22831100
C	-0.07635600	-1.18059200	-0.48141500
S	-1.26124500	0.12974900	-0.01070300
H	-1.37359600	0.50624200	1.31456700
H	2.44874500	0.99561200	-0.14584600
H	2.00341000	-1.51231900	-0.16932400
H	-1.70857900	-1.22813200	0.32077500
H	1.17396800	-1.03720700	1.31744800

e-3-1m

C	-1.55642800	-1.44311000	-0.24862400
C	-1.67172800	-0.19076300	0.07785900
C	-0.88242800	1.11379900	0.13927300
C	0.52376300	1.12033900	-0.41292200
S	1.39128600	-0.37819600	0.01881500
H	1.66093000	-0.71344700	1.35499500
H	-2.72501300	-0.18679800	0.42963200
H	-1.44196600	1.87964700	-0.41140400
H	2.65656800	0.02825400	-0.20143800
H	-0.89016900	1.44189100	1.19365000

e-3-1m-1

C	-1.51366400	-1.45497500	-0.22196000
C	-1.69798500	-0.20530500	0.09082300
C	-0.86462700	1.05925900	0.20216700
C	0.39934600	1.17898000	-0.48861000
H	-2.76726400	-0.17069600	0.37204200
H	-1.32598000	1.87358500	-0.41925900
H	-0.87379400	1.45415600	1.23226100

e-4-1t

C	0.03543900	1.26795900	-0.00973300
C	-1.24459800	0.81240300	-0.00938700
C	-1.37180300	-0.62340700	-0.01887900
C	-0.01118800	-1.27286600	0.02094000
S	1.26562100	-0.01859700	-0.00819500
H	0.36139500	2.29954100	0.01956400
H	-2.10284500	1.47594200	-0.00252300
H	-0.90176700	-1.17326700	1.02743100
H	0.17811900	-2.25612800	-0.39501900
H	-2.23194400	-1.15306700	-0.41597500