

Supplementary Information: Spectroscopic Constants and Anharmonic Vibrational Frequencies of C(O)OC, c-C₂O₂, and their Silicon-containing Analogues

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C(O)OC dipole moment vector [a.u.]: 0.08929742, 0.03992090, 0.00000000. C(O)OC Cartesian coordinates [Bohr/a.u.]: O 0.000000000 0.059284581 -2.736156302; C 0.000000000 -0.347609661 -0.559243623; O 0.000000000 1.208339210 1.666460193; C 0.000000000 -1.340944172 1.984145457.

c-C₂O₂ dipole moment vector [a.u.]: 0.00000000, 0.00000000, 0.25822114. c-C₂O₂ Cartesian coordinates [Bohr/a.u.]: C -1.770561866 0.000000000 -0.231023337; C 1.770561866 0.000000000 -0.231023337; O 0.000000000 -1.874251686 0.173432835; O 0.000000000 1.874251686 0.173432835.

Si(O)OSi dipole moment vector [a.u.]: 2.05693724, -0.50201531, 0.00000000. Si(O)OSi Cartesian coordinates [Bohr/a.u.]: O 0.000000000 -0.038679051 -4.096222913; Si 0.000000000 -0.460667397 -1.265428612; O 0.000000000 1.829763565 0.985144156; Si 0.000000000 -0.559655459 3.037709450.

Table S1: C(O)OC Force Constants with motion coupling

F _{1,1,0,0}	15.023847793216
F _{2,1,0,0}	1.118790196621
F _{2,2,0,0}	2.796499259802
F _{3,1,0,0}	-0.096128921600
F _{3,2,0,0}	1.427517426504
F _{3,3,0,0}	5.871740163757
F _{4,1,0,0}	0.949357578032
F _{4,2,0,0}	1.120215060243
F _{4,3,0,0}	1.662271777467
F _{4,4,0,0}	1.656343785237
F _{5,1,0,0}	0.040760175155
F _{5,2,0,0}	2.531258112172
F _{5,3,0,0}	2.891526656896
F _{5,4,0,0}	2.124234146695
F _{5,5,0,0}	7.385054275053
F _{6,6,0,0}	0.267220080154
F _{1,1,1,0}	-106.029760641484
F _{2,1,1,0}	-3.040759320279
F _{2,2,1,0}	-2.128660304150
F _{2,2,2,0}	-10.882729611467
F _{3,1,1,0}	0.031884512560
F _{3,2,1,0}	-0.312812062132
F _{3,2,2,0}	-2.144327759126
F _{3,3,1,0}	0.472610710267
F _{3,3,2,0}	-3.589281654061
F _{3,3,3,0}	-34.382922408200
F _{4,1,1,0}	-2.784991403758
F _{4,2,1,0}	0.390207857911
F _{4,2,2,0}	-8.170465368670
F _{4,3,1,0}	-0.548170413529
F _{4,3,2,0}	-1.432345814775
F _{4,3,3,0}	-4.373503263910
F _{4,4,1,0}	-0.550252986838
F _{4,4,2,0}	-9.292976608105
F _{4,4,3,0}	0.074673012267
F _{4,4,4,0}	-11.938983888606

F _{5,1,1,0}	-0.405995660061
F _{5,2,1,0}	-1.222927625065
F _{5,2,2,0}	-2.869772028460
F _{5,3,1,0}	1.900335201178
F _{5,3,2,0}	-6.236264793530
F _{5,3,3,0}	-4.927692327901
F _{5,4,1,0}	-2.092722987053
F _{5,4,2,0}	-3.454855357075
F _{5,4,3,0}	-4.176315342550
F _{5,4,4,0}	-5.868797094476
F _{5,5,1,0}	-1.092262224457
F _{5,5,2,0}	-13.413277348064
F _{5,5,3,0}	-15.017969701043
F _{5,5,4,0}	-14.669145523104
F _{5,5,5,0}	-56.717523023035
F _{6,6,1,0}	-0.399076558296
F _{6,6,2,0}	-0.095405296434
F _{6,6,3,0}	-0.054881998380
F _{6,6,4,0}	-0.036655563606
F _{6,6,5,0}	-0.107957579665
F _{1,1,1,1}	613.522956496453
F _{2,1,1,1}	5.561914075058
F _{2,2,1,1}	4.771374752451
F _{2,2,2,1}	6.539270557335
F _{2,2,2,2}	34.182255274310
F _{3,1,1,1}	0.002955033735
F _{3,2,1,1}	1.511356544451
F _{3,2,2,1}	0.300599325294
F _{3,2,2,2}	3.410306535058
F _{3,3,1,1}	-2.184111870151
F _{3,3,2,1}	-0.599518547595
F _{3,3,2,2}	4.797882704805
F _{3,3,3,1}	2.367717959661
F _{3,3,3,2}	4.995458956744
F _{3,3,3,3}	195.717236042012
F _{4,1,1,1}	6.363841289446
F _{4,2,1,1}	1.956807810218
F _{4,2,2,1}	-1.005186164552
F _{4,2,2,2}	27.414577328014
F _{4,3,1,1}	2.102787490366
F _{4,3,2,1}	0.027466826447
F _{4,3,2,2}	4.802448694572
F _{4,3,3,1}	-0.536845288526
F _{4,3,3,2}	2.268647512143
F _{4,3,3,3}	10.586538505701
F _{4,4,1,1}	1.409145130466
F _{4,4,2,1}	-1.509524694200
F _{4,4,2,2}	30.051858624160
F _{4,4,3,1}	0.180591416890
F _{4,4,3,2}	7.172461539818
F _{4,4,3,3}	-4.621059560348
F _{4,4,4,1}	1.826298876741
F _{4,4,4,2}	31.486339984158
F _{4,4,4,3}	9.486273186144
F _{4,4,4,4}	35.092661282999
F _{5,1,1,1}	2.436673542813
F _{5,2,1,1}	-0.187560043434
F _{5,2,2,1}	1.894897940675
F _{5,2,2,2}	-7.985955076347
F _{5,3,1,1}	-3.271570578095
F _{5,3,2,1}	1.096057152232
F _{5,3,2,2}	13.937938000022
F _{5,3,3,1}	-2.462590476065
F _{5,3,3,2}	8.141363373667
F _{5,3,3,3}	-10.594231926130

F _{5,4,1,1}	3.569021759848
F _{5,4,2,1}	2.701340545304
F _{5,4,2,2}	-9.991678016418
F _{5,4,3,1}	-1.457485702714
F _{5,4,3,2}	15.992668443638
F _{5,4,3,3}	4.137993602957
F _{5,4,4,1}	6.332025629494
F _{5,4,4,2}	-10.967602978270
F _{5,4,4,3}	17.599729340752
F _{5,4,4,4}	-9.575234092274
F _{5,5,1,1}	-0.919062029966
F _{5,5,2,1}	3.153215271708
F _{5,5,2,2}	3.614022850359
F _{5,5,3,1}	-4.318542503375
F _{5,5,3,2}	39.701644808803
F _{5,5,3,3}	-15.048369649589
F _{5,5,4,1}	5.194985560466
F _{5,5,4,2}	5.695654812910
F _{5,5,4,3}	39.613138594868
F _{5,5,4,4}	7.118401095172
F _{5,5,5,1}	9.593971117882
F _{5,5,5,2}	78.666289061756
F _{5,5,5,3}	61.379164136641
F _{5,5,5,4}	88.113556058182
F _{5,5,5,5}	379.021117134932
F _{6,6,1,1}	-0.021150691023
F _{6,6,2,1}	0.424049817081
F _{6,6,2,2}	-0.443840908751
F _{6,6,3,1}	0.046155239127
F _{6,6,3,2}	-0.011317929404
F _{6,6,3,3}	-0.254001562584
F _{6,6,4,1}	0.244259013415
F _{6,6,4,2}	0.224541646957
F _{6,6,4,3}	-0.174018596477
F _{6,6,4,4}	-0.143347172980
F _{6,6,5,1}	0.773240151034
F _{6,6,5,2}	0.045177504543
F _{6,6,5,3}	-0.300228695434
F _{6,6,5,4}	-0.039160362177
F _{6,6,5,5}	0.131177887351
F _{6,6,6,6}	0.052307194813

Table S2: C(O)OC Force Constants

F _{1,1,0,0}	15.023846183669
F _{2,1,0,0}	1.462403198572
F _{2,2,0,0}	3.346629139121
F _{3,1,0,0}	-0.096129135831
F _{3,2,0,0}	2.184811491477
F _{3,3,0,0}	5.871737144875
F _{4,1,0,0}	0.119807637547
F _{4,2,0,0}	0.570080270357
F _{4,3,0,0}	-0.165996595882
F _{4,4,0,0}	1.106201868138
F _{5,1,0,0}	0.040760816240
F _{5,2,0,0}	3.291930955282
F _{5,3,0,0}	2.891529489643
F _{5,4,0,0}	0.287809578898
F _{5,5,0,0}	7.385053774333
F _{6,6,0,0}	0.267217148896
F _{1,1,1,0}	-106.029782952037
F _{2,1,1,0}	-4.120034932080

F _{2,2,1,0}	-0.949206748159
F _{2,2,2,0}	-26.596335774714
F _{3,1,1,0}	0.031990003766
F _{3,2,1,0}	-0.608727826777
F _{3,2,2,0}	-2.466826308173
F _{3,3,1,0}	0.472535932844
F _{3,3,2,0}	-5.631733619106
F _{3,3,3,0}	-34.382667989725
F _{4,1,1,0}	-0.180767225879
F _{4,2,1,0}	-0.789273017118
F _{4,2,2,0}	0.770536588411
F _{4,3,1,0}	0.166385703960
F _{4,3,2,0}	-1.109387097530
F _{4,3,3,0}	0.554308429050
F _{4,4,1,0}	-1.729494571065
F _{4,4,2,0}	-1.896547266760
F _{4,4,3,0}	0.397889712455
F _{4,4,4,0}	-0.817322973479
F _{5,1,1,0}	-0.405796203951
F _{5,2,1,0}	-2.344507321329
F _{5,2,2,0}	-7.823459453568
F _{5,3,1,0}	1.900448665987
F _{5,3,2,0}	-7.362774796784
F _{5,3,3,0}	-4.927439788697
F _{5,4,1,0}	0.614989923629
F _{5,4,2,0}	1.499604210996
F _{5,4,3,0}	-1.456549080433
F _{5,4,4,0}	-0.914056069226
F _{5,5,1,0}	-1.092462954470
F _{5,5,2,0}	-19.857858771652
F _{5,5,3,0}	-15.017814832873
F _{5,5,4,0}	0.888054020395
F _{5,5,5,0}	-56.717447396684
F _{6,6,1,0}	-0.399257019920
F _{6,6,2,0}	-0.094415409977
F _{6,6,3,0}	-0.054445669789
F _{6,6,4,0}	-0.041460859393
F _{6,6,5,0}	-0.107956935989
F _{1,1,1,1}	613.507539873684
F _{2,1,1,1}	8.385031475487
F _{2,2,1,1}	5.081319986367
F _{2,2,2,1}	0.259931091448
F _{2,2,2,2}	121.419796645773
F _{3,1,1,1}	0.000204326340
F _{3,2,1,1}	2.519265703407
F _{3,2,2,1}	0.179217069714
F _{3,2,2,2}	17.224908003272
F _{3,3,1,1}	-2.147015749649
F _{3,3,2,1}	-0.880221388353
F _{3,3,2,2}	2.299792148062
F _{3,3,3,1}	2.404091840619
F _{3,3,3,2}	11.029878183020
F _{3,3,3,3}	195.743896331034
F _{4,1,1,1}	-0.597729253968
F _{4,2,1,1}	1.689252858985
F _{4,2,2,1}	1.817542747435
F _{4,2,2,2}	-2.316422701579
F _{4,3,1,1}	-0.422250980819
F _{4,3,2,1}	0.099839732279
F _{4,3,2,2}	-2.977553910370
F _{4,3,3,1}	-0.095349720954
F _{4,3,3,2}	4.683249928072
F _{4,3,3,3}	-3.962230636405
F _{4,4,1,1}	1.178303928683
F _{4,4,2,1}	3.830702590650

F _{4,4,2,2}	2.262109689917
F _{4,4,3,1}	0.258533383505
F _{4,4,3,2}	0.352922741329
F _{4,4,3,3}	-2.107565890317
F _{4,4,4,1}	1.104872761414
F _{4,4,4,2}	1.833892427494
F _{4,4,4,3}	0.338062081774
F _{4,4,4,4}	3.606489679342
F _{5,1,1,1}	2.437037482165
F _{5,2,1,1}	2.382465297311
F _{5,2,2,1}	6.766637670852
F _{5,2,2,2}	-28.363273934773
F _{5,3,1,1}	-3.334498916731
F _{5,3,2,1}	-0.227582272348
F _{5,3,2,2}	31.705355708811
F _{5,3,3,1}	-2.485403624803
F _{5,3,3,2}	8.703032477840
F _{5,3,3,3}	-10.669924070152
F _{5,4,1,1}	-2.635931704665
F _{5,4,2,1}	-2.253587674494
F _{5,4,2,2}	0.874461073297
F _{5,4,3,1}	1.825889957403
F _{5,4,3,2}	-1.808886685769
F _{5,4,3,3}	2.844192586912
F _{5,4,4,1}	1.428675599104
F _{5,4,4,2}	1.203636276260
F _{5,4,4,3}	-0.265319284055
F _{5,4,4,4}	-0.485063001588
F _{5,5,1,1}	-0.967975893798
F _{5,5,2,1}	5.813287477986
F _{5,5,2,2}	11.000993048872
F _{5,5,3,1}	-4.304092341692
F _{5,5,3,2}	56.046926270403
F _{5,5,3,3}	-15.048713016114
F _{5,5,4,1}	-1.492234011241
F _{5,5,4,2}	-1.772503773778
F _{5,5,4,3}	0.058297367442
F _{5,5,4,4}	-0.354927959975
F _{5,5,5,1}	9.555286284065
F _{5,5,5,2}	117.942518574570
F _{5,5,5,3}	61.284061341174
F _{5,5,5,4}	-6.662577745709
F _{5,5,5,5}	379.013771138610
F _{6,6,1,1}	-0.085428774122
F _{6,6,2,1}	0.382932773053
F _{6,6,2,2}	-0.015781629336
F _{6,6,3,1}	0.102976321184
F _{6,6,3,2}	-0.084322237703
F _{6,6,3,3}	-0.309390460471
F _{6,6,4,1}	0.038025639424
F _{6,6,4,2}	-0.148894630905
F _{6,6,4,3}	0.043642806670
F _{6,6,4,4}	-0.465715171818
F _{6,6,5,1}	0.770482930980
F _{6,6,5,2}	-0.064153775112
F _{6,6,5,3}	-0.260019927203
F _{6,6,5,4}	0.076886972207
F _{6,6,5,5}	0.147995761765
F _{6,6,6,6}	0.085369898213

Table S3: c-C₂O₂ Force Constants

F _{1,1,0,0}	6.144290687282
F _{2,1,0,0}	0.506301066671
F _{2,2,0,0}	4.018328021919
F _{3,1,0,0}	-0.880295789094
F _{3,2,0,0}	0.476738180662
F _{3,3,0,0}	0.668832744253
F _{4,4,0,0}	0.575469297143
F _{5,5,0,0}	4.566411262153
F _{6,6,0,0}	4.744159089462
F _{1,1,1,0}	-20.023836667994
F _{2,1,1,0}	-2.844149149854
F _{2,2,1,0}	-5.728169023618
F _{2,2,2,0}	-5.545395393502
F _{3,1,1,0}	2.279670225683
F _{3,2,1,0}	-1.147157989024
F _{3,2,2,0}	0.115805543964
F _{3,3,1,0}	0.939623456961
F _{3,3,2,0}	1.052360822168
F _{3,3,3,0}	-3.187075234020
F _{4,4,1,0}	-15.657562263342
F _{4,4,2,0}	-0.193966360119
F _{4,4,3,0}	1.979613942702
F _{5,5,1,0}	-15.016605304680
F _{5,5,2,0}	-2.753789129591
F _{5,5,3,0}	2.211362572890
F _{6,5,4,0}	-12.897828871186
F _{6,6,1,0}	-13.871425814986
F _{6,6,2,0}	3.094628496373
F _{6,6,3,0}	3.075822443602
F _{1,1,1,1}	55.728802323570
F _{2,1,1,1}	9.427934700668
F _{2,2,1,1}	6.506666983001
F _{2,2,2,1}	7.173222650401
F _{2,2,2,2}	7.013726576884
F _{3,1,1,1}	-5.345994823154
F _{3,2,1,1}	2.330884806010
F _{3,2,2,1}	1.379717591864
F _{3,2,2,2}	-7.154849449354
F _{3,3,1,1}	-3.026696370397
F _{3,3,2,1}	-1.896937368771
F _{3,3,2,2}	3.275734671131
F _{3,3,3,1}	3.704427611122
F _{3,3,3,2}	-5.899865619615
F _{3,3,3,3}	-3.158543255830
F _{4,4,1,1}	55.637043394567
F _{4,4,2,1}	-0.629048065487
F _{4,4,2,2}	-16.214687133303
F _{4,4,3,1}	-5.469765738116
F _{4,4,3,2}	3.335930005115
F _{4,4,3,3}	-9.012541185509
F _{4,4,4,4}	86.436379729573
F _{5,5,1,1}	44.401189833975
F _{5,5,2,1}	3.336202451819
F _{5,5,2,2}	-5.278731304746
F _{5,5,3,1}	-4.940048379166
F _{5,5,3,2}	0.289728204883
F _{5,5,3,3}	-6.674596811052
F _{5,5,4,4}	32.644834440927
F _{5,5,5,5}	24.954105676999
F _{6,5,4,1}	49.471241501957
F _{6,5,4,2}	3.153889196585
F _{6,5,4,3}	-6.831392012890
F _{6,6,1,1}	39.484935855710

F _{6,6,2,1}	2.082756026583
F _{6,6,2,2}	-2.512810057511
F _{6,6,3,1}	-7.209767367066
F _{6,6,3,2}	4.649541858384
F _{6,6,3,3}	-0.023393203145
F _{6,6,4,4}	52.294338925882
F _{6,6,5,5}	32.702117371759
F _{6,6,6,6}	-26.046037786948

Table S4: Si(O)OSi Force Constants

F _{1,1,0,0}	8.888514564084
F _{2,1,0,0}	0.021106719732
F _{2,2,0,0}	3.136944072899
F _{3,1,0,0}	-0.012850770740
F _{3,2,0,0}	1.402690323127
F _{3,3,0,0}	4.462801171588
F _{4,1,0,0}	0.145508301209
F _{4,2,0,0}	0.385166358749
F _{4,3,0,0}	-0.232450095371
F _{4,4,0,0}	0.656200219994
F _{5,1,0,0}	-0.071849575760
F _{5,2,0,0}	1.068542462600
F _{5,3,0,0}	1.756356561283
F _{5,4,0,0}	0.243211050779
F _{5,5,0,0}	3.081100969213
F _{6,6,0,0}	0.143227893510
F _{1,1,1,0}	-52.958798328488
F _{2,1,1,0}	-0.247619356347
F _{2,2,1,0}	-0.111948955891
F _{2,2,2,0}	-22.127064757959
F _{3,1,1,0}	-0.096495884735
F _{3,2,1,0}	0.056736702963
F _{3,2,2,0}	-0.709203140326
F _{3,3,1,0}	-0.065309157885
F _{3,3,2,0}	-2.665460753613
F _{3,3,3,0}	-24.096481051791
F _{4,1,1,0}	-0.198443178073
F _{4,2,1,0}	-0.345435711190
F _{4,2,2,0}	-0.178638182668
F _{4,3,1,0}	0.107272106342
F _{4,3,2,0}	-0.064042126389
F _{4,3,3,0}	0.148078284496
F _{4,4,1,0}	-0.552703963666
F _{4,4,2,0}	-0.642931949085
F _{4,4,3,0}	0.012755736649
F _{4,4,4,0}	-0.465935265909
F _{5,1,1,0}	-0.236023391821
F _{5,2,1,0}	-0.184175010226
F _{5,2,2,0}	-3.203893654837
F _{5,3,1,0}	-0.005403523281
F _{5,3,2,0}	-2.273749360995
F _{5,3,3,0}	-3.225756451132
F _{5,4,1,0}	-0.006522679160
F _{5,4,2,0}	0.308336948715
F _{5,4,3,0}	-0.184221595260
F _{5,4,4,0}	-0.273430060252
F _{5,5,1,0}	-0.147288283792
F _{5,5,2,0}	-6.507325029478
F _{5,5,3,0}	-6.204083354151
F _{5,5,4,0}	0.098669034551
F _{5,5,5,0}	-19.265993818618

F _{6,6,1,0}	-0.103772458379
F _{6,6,2,0}	-0.086549800465
F _{6,6,3,0}	0.023711382110
F _{6,6,4,0}	0.026507654303
F _{6,6,5,0}	-0.101249858502
F _{1,1,1,1}	264.601953836922
F _{2,1,1,1}	0.079362395183
F _{2,2,1,1}	1.103024856515
F _{2,2,2,1}	0.845021492167
F _{2,2,2,2}	100.638379135728
F _{3,1,1,1}	0.473976546064
F _{3,2,1,1}	-0.248137044302
F _{3,2,2,1}	0.053357958664
F _{3,2,2,2}	2.452282552170
F _{3,3,1,1}	-0.040561261106
F _{3,3,2,1}	0.101127124530
F _{3,3,2,2}	2.934531630770
F _{3,3,3,1}	0.102596240001
F _{3,3,3,2}	2.273719749051
F _{3,3,3,3}	118.340743232783
F _{4,1,1,1}	0.082112999623
F _{4,2,1,1}	0.087874742588
F _{4,2,2,1}	-0.164577574213
F _{4,2,2,2}	-1.032062336582
F _{4,3,1,1}	0.427026121723
F _{4,3,2,1}	-0.047957953128
F _{4,3,2,2}	1.224193822113
F _{4,3,3,1}	0.246472099542
F _{4,3,3,2}	0.313034900015
F _{4,3,3,3}	0.592127294660
F _{4,4,1,1}	-0.198602058884
F _{4,4,2,1}	1.025665984387
F _{4,4,2,2}	0.485930828684
F _{4,4,3,1}	0.241056009558
F _{4,4,3,2}	-0.044679071412
F _{4,4,3,3}	-0.325226157074
F _{4,4,4,1}	0.925869604913
F _{4,4,4,2}	0.756977705769
F _{4,4,4,3}	0.088739428000
F _{4,4,4,4}	1.755642429848
F _{5,1,1,1}	-0.073754015832
F _{5,2,1,1}	-0.041416507778
F _{5,2,2,1}	0.180417812532
F _{5,2,2,2}	-3.225520809532
F _{5,3,1,1}	-0.648970172350
F _{5,3,2,1}	0.424209867294
F _{5,3,2,2}	7.672460819687
F _{5,3,3,1}	1.106248460593
F _{5,3,3,2}	5.707013941756
F _{5,3,3,3}	-1.142313592839
F _{5,4,1,1}	-0.874559145028
F _{5,4,2,1}	-0.517073903227
F _{5,4,2,2}	-1.174772682606
F _{5,4,3,1}	0.727216918991
F _{5,4,3,2}	0.342245380799
F _{5,4,3,3}	-1.620830065777
F _{5,4,4,1}	0.621049644828
F _{5,4,4,2}	-0.108073215219
F _{5,4,4,3}	-0.503126334840
F _{5,4,4,4}	-0.281848571252
F _{5,5,1,1}	-0.292849361611
F _{5,5,2,1}	0.268027250608
F _{5,5,2,2}	4.320894753533
F _{5,5,3,1}	0.635699879398
F _{5,5,3,2}	15.337453981708

F _{5,5,3,3}	3.221179169317
F _{5,5,4,1}	-0.173361803029
F _{5,5,4,2}	-0.537225653417
F _{5,5,4,3}	-0.520635891935
F _{5,5,4,4}	-0.340403004419
F _{5,5,5,1}	1.970657382656
F _{5,5,5,2}	29.279126747182
F _{5,5,5,3}	27.327572854401
F _{5,5,5,4}	-2.692939254157
F _{5,5,5,5}	101.348402507844
F _{6,6,1,1}	-0.350253563832
F _{6,6,2,1}	-0.310737974495
F _{6,6,2,2}	0.343270084455
F _{6,6,3,1}	0.616817861349
F _{6,6,3,2}	-0.150953541866
F _{6,6,3,3}	0.194021213085
F _{6,6,4,1}	0.287620644211
F _{6,6,4,2}	-0.022844990567
F _{6,6,4,3}	0.152225112967
F _{6,6,4,4}	0.200051278870
F _{6,6,5,1}	-1.220337284670
F _{6,6,5,2}	-1.166868535941
F _{6,6,5,3}	-0.570039395345
F _{6,6,5,4}	0.912009436852
F _{6,6,5,5}	-0.361593245021
F _{6,6,6,6}	-0.075363012381

Table S5: c-Si₂O₂ Force Constants

F _{1,1,0,0}	4.350447425724
F _{2,1,0,0}	-0.198394300695
F _{2,2,0,0}	2.094913742715
F _{3,3,0,0}	1.980375422923
F _{4,4,0,0}	0.229997430540
F _{5,5,0,0}	3.867805374562
F _{6,6,0,0}	3.942531087669
F _{1,1,1,0}	-11.516337862792
F _{2,1,1,0}	0.022022813881
F _{2,2,1,0}	-2.118226963454
F _{2,2,2,0}	-0.353687366606
F _{3,3,1,0}	-11.262445549545
F _{3,3,2,0}	0.535829518041
F _{4,4,1,0}	1.380036809300
F _{4,4,2,0}	-0.056911778451
F _{5,5,1,0}	-9.387241116609
F _{5,5,2,0}	-0.471549024622
F _{6,5,3,0}	-10.033974099665
F _{6,6,1,0}	-9.555603417617
F _{6,6,2,0}	1.476471147455
F _{1,1,1,1}	27.416231792620
F _{2,1,1,1}	0.595765779548
F _{2,2,1,1}	2.730152728978
F _{2,2,2,1}	-0.162636628443
F _{2,2,2,2}	6.097071492116
F _{3,3,1,1}	31.544731709657
F _{3,3,2,1}	-1.267316337003
F _{3,3,2,2}	-4.853526668049
F _{3,3,3,3}	45.602872874892
F _{4,4,1,1}	-2.607541355869
F _{4,4,2,1}	1.002402650758
F _{4,4,2,2}	0.257414252749
F _{4,4,3,3}	-4.727328226602

F _{4,4,4,4}	3.445543503331
F _{5,5,1,1}	22.172039623577
F _{5,5,2,1}	-0.310337240139
F _{5,5,2,2}	-3.208508023587
F _{5,5,3,3}	26.024552991015
F _{5,5,4,4}	-3.708162334288
F _{5,5,5,5}	7.688744310625
F _{6,5,3,1}	27.912398969239
F _{6,5,3,2}	-0.749887948318
F _{6,5,4,3}	0.325242098515
F _{6,6,1,1}	22.627498598712
F _{6,6,2,1}	-0.133764787208
F _{6,6,2,2}	-2.043271386450
F _{6,6,3,3}	28.279171170424
F _{6,6,4,4}	-3.892859893945
F _{6,6,5,5}	19.898142848520
F _{6,6,6,6}	9.724222396484

Table S6: C(O)OC Frequencies and ZPVE with motion coupling

	Description	Frequencies [cm ⁻¹]
ω_1	O ₁ –C ₁ stretch	2030.4
ω_2	O ₂ –C ₂ stretch	1236.1
ω_3	C ₁ –O ₂ –C ₂ bend	947.4
ω_4	(C ₁ –O ₂ stretch) + (O ₁ –C ₁ –O ₂ bend)	518.1
ω_5	out-of-plane bend	508.2
ω_6	(C ₁ –O ₂ stretch) - (O ₁ –C ₁ –O ₂ bend)	478.3
ν_1	O ₁ –C ₁ stretch	2006.9
ν_2	O ₂ –C ₂ stretch	1248.9
ν_3	C ₁ –O ₂ –C ₂ bend	919.6
ν_4	(C ₁ –O ₂ stretch) + (O ₁ –C ₁ –O ₂ bend)	454.2
ν_5	out-of-plane bend	492.4
ν_6	(C ₁ –O ₂ stretch) - (O ₁ –C ₁ –O ₂ bend)	310.6
ZPVE [cm ⁻¹]		2808.9

Table S7: C(O)OC Rotational Constants [MHz] with motion coupling

A_e	38841.1
B_e	8384.9
C_e	6896.1
A_0	38826.2
B_0	8274.5
C_0	6807.3
κ	-0.90835
A_1	38818.2
B_1	8232.2
C_1	6778.5
A_2	38374.6
B_2	8298.3
C_2	6811.8
A_3	38967.6
B_3	8252.8
C_3	6792.9
A_4	40153.9
B_4	8217.8
C_4	6755.1
A_5	42481.4
B_5	8278.3
C_5	6818.7
A_6	34131.2
B_6	8147.1
C_6	6709.0

Table S8: C(O)OC Quartic and Sextic Distortion Constants with motion coupling

Constant	Units	
Δ_J	kHz	3.456
Δ_K	kHz	151.182
Δ_{JK}	kHz	51.193
δ_J	Hz	682.262
δ_K	kHz	36.183
Φ_J	mHz	-11.976
Φ_K	Hz	-2.507
Φ_{JK}	mHz	-344.913
Φ_{KJ}	Hz	2.500
ϕ_j	mHz	-3.170
ϕ_{jk}	mHz	-257.387
ϕ_k	Hz	3.710

Table S9: C(O)OC Geometry [\AA or Deg] with motion coupling

Coordinate	r_e	r_0
$r(\text{O}_1-\text{C}_2)$	1.1717212	1.1703507
$r(\text{C}_2-\text{O}_3)$	1.4387036	1.4719814
$r(\text{O}_3-\text{C}_4)$	1.3594921	1.3566819
$\angle(\text{C}_2-\text{O}_1-\text{O}_3)$	134.4045544	133.3263362
$\angle(\text{O}_3-\text{C}_2-\text{C}_4)$	62.0919164	61.6193430

Table S10: C(O)OC Fermi Resonances with motion coupling

$2\nu_3 = \nu_3 + \nu_2 = \nu_1$
$\nu_6 + \nu_3 = \nu_2$
$2\nu_4 = 2\nu_5 = 2\nu_6 = \nu_6 + \nu_4 = \nu_3$

Table S11: C(O)OC Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{C}_2)$	1.1717212	1.1703483
$r(\text{C}_2-\text{O}_3)$	1.4387035	1.4720071
$r(\text{O}_3-\text{C}_4)$	1.3594921	1.3566750
$\angle(\text{C}_2-\text{O}_1-\text{O}_3)$	134.4045563	133.3254266
$\angle(\text{O}_3-\text{C}_2-\text{C}_4)$	62.0919179	61.6188493

Table S12: C(O)OC Fermi Resonances

$2\nu_3 = \nu_3 + \nu_2 = \nu_1$
$\nu_6 + \nu_3 = \nu_2$
$2\nu_4 = 2\nu_5 = 2\nu_6 = \nu_6 + \nu_4 = \nu_3$

Table S13: $^{12}\text{C}(^{16}\text{O})^{16}\text{O}^{13}\text{C}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	O_1-C_1 stretch	2027.5
ω_2	O_2-C_2 stretch	1210.9
ω_3	$\text{C}_1-\text{O}_2-\text{C}_2$ bend	933.2
ω_4	$(\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	514.8
ω_5	out-of-plane bend	506.2
ω_6	$(\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	474.4
ν_1	O_1-C_1 stretch	2004.0
ν_2	O_2-C_2 stretch	1225.7
ν_3	$\text{C}_1-\text{O}_2-\text{C}_2$ bend	906.4
ν_4	$(\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	445.9
ν_5	out-of-plane bend	490.9
ν_6	$(\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	313.7
ZPVE [cm^{-1}]		2782.8

Table S14: $^{12}\text{C}(^{16}\text{O})^{16}\text{O}^{13}\text{C}$ Rotational Constants [MHz]

A_e	37443.5
B_e	8235.0
C_e	6750.4
A_0	37442.9
B_0	8128.7
C_0	6665.5
κ	-0.90492
A_1	37439.2
B_1	8086.0
C_1	6636.8
A_2	37008.8
B_2	8150.8
C_2	6668.6
A_3	37596.4
B_3	8105.5
C_3	6651.3
A_4	38546.0
B_4	8070.3
C_4	6614.0
A_5	40767.8
B_5	8132.8
C_5	6676.7
A_6	33298.6
B_6	8013.9
C_6	6575.6

Table S15: $^{12}\text{C}(^{16}\text{O})^{16}\text{O}^{13}\text{C}$ Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	3.220
Δ_K	kHz	142.886
Δ_{JK}	kHz	49.644
δ_J	Hz	645.073
δ_K	kHz	34.593
Φ_J	mHz	-10.040
Φ_K	Hz	-2.308
Φ_{JK}	mHz	-328.667
Φ_{KJ}	Hz	2.355
ϕ_j	mHz	-2.688
ϕ_{jk}	mHz	-235.391
ϕ_k	Hz	3.452

Table S16: $^{12}\text{C}(^{16}\text{O})^{16}\text{O}^{13}\text{C}$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{C}_2)$	1.1717212	1.1703046
$r(\text{C}_2-\text{O}_3)$	1.4387035	1.4720723
$r(\text{O}_3-\text{C}_4)$	1.3594921	1.3565218
$\angle(\text{C}_2-\text{O}_1-\text{O}_3)$	134.4045563	133.3281560
$\angle(\text{O}_3-\text{C}_2-\text{C}_4)$	62.0919179	61.6165354

Table S17: $^{12}\text{C}(^{16}\text{O})^{16}\text{O}^{13}\text{C}$ Fermi Resonances

$2\nu_3 = \nu_3 + \nu_2 = \nu_1$
$2\nu_5 = \nu_6 + \nu_3 = \nu_2$
$2\nu_4 = 2\nu_5 = 2\nu_6 = \nu_6 + \nu_4 = \nu_3$

Table S18: $^{12}\text{C}(^{16}\text{O})^{18}\text{O}^{12}\text{C}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	O_1-C_1 stretch	2030.4
ω_2	O_2-C_2 stretch	1209.8
ω_3	$\text{C}_1-\text{O}_2-\text{C}_2$ bend	939.4
ω_4	$(\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	508.0
ω_5	out-of-plane bend	501.9
ω_6	$(\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	475.6
ν_1	O_1-C_1 stretch	2006.1
ν_2	O_2-C_2 stretch	1208.6
ν_3	$\text{C}_1-\text{O}_2-\text{C}_2$ bend	910.8
ν_4	$(\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	493.0
ν_5	out-of-plane bend	468.7
ν_6	$(\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	285.7
ZPVE [cm^{-1}]		2783.6

Table S19: $^{12}\text{C}(^{16}\text{O})^{18}\text{O}^{12}\text{C}$ Rotational Constants [MHz]

A_e	36682.3
B_e	8176.8
C_e	6686.3
A_0	36681.0
B_0	8067.0
C_0	6599.6
κ	-0.90244
A_1	36665.2
B_1	8027.7
C_1	6573.0
A_2	36277.6
B_2	8088.7
C_2	6603.6
A_3	36792.9
B_3	8049.0
C_3	6586.6
A_4	39952.8
B_4	8084.7
C_4	6610.3
A_5	36895.2
B_5	8026.0
C_5	6573.3
A_6	33499.7
B_6	7906.2
C_6	6477.7

Table S20: $^{12}\text{C}(^{16}\text{O})^{18}\text{O}^{12}\text{C}$ Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	3.468
Δ_K	kHz	131.734
Δ_{JK}	kHz	46.461
δ_J	Hz	705.886
δ_K	kHz	33.896
Φ_J	mHz	-13.394
Φ_K	Hz	-2.343
Φ_{JK}	mHz	-295.573
Φ_{KJ}	Hz	2.281
ϕ_j	mHz	-3.732
ϕ_{jk}	mHz	-246.490
ϕ_k	Hz	3.228

Table S21: $^{12}\text{C}(^{16}\text{O})^{18}\text{O}^{12}\text{C}$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{C}_2)$	1.1717212	1.1704133
$r(\text{C}_2-\text{O}_3)$	1.4387035	1.4712782
$r(\text{O}_3-\text{C}_4)$	1.3594921	1.3567044
$\angle(\text{C}_2-\text{O}_1-\text{O}_3)$	134.4045563	133.3380614
$\angle(\text{O}_3-\text{C}_2-\text{C}_4)$	62.0919179	61.6352607

Table S22: $^{12}\text{C}(^{16}\text{O})^{18}\text{O}^{12}\text{C}$ Fermi Resonances

$2\nu_3 = \nu_3 + \nu_2 = \nu_1$
$2\nu_4 = \nu_2$
$2\nu_4 = 2\nu_5 = 2\nu_6 = \nu_6 + \nu_5 = \nu_3$

Table S23: $^{12}\text{C}(^{18}\text{O})^{16}\text{O}^{12}\text{C}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	O_1-C_1 stretch	1996.5
ω_2	O_2-C_2 stretch	1231.7
ω_3	$\text{C}_1-\text{O}_2-\text{C}_2$ bend	931.3
ω_4	$(\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	512.2
ω_5	out-of-plane bend	503.7
ω_6	$(\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	475.0
ν_1	O_1-C_1 stretch	1973.6
ν_2	O_2-C_2 stretch	1242.0
ν_3	$\text{C}_1-\text{O}_2-\text{C}_2$ bend	904.0
ν_4	$(\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	439.5
ν_5	out-of-plane bend	488.7
ν_6	$(\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	318.2
ZPVE [cm^{-1}]		2775.4

Table S24: $^{12}\text{C}(^{18}\text{O})^{16}\text{O}^{12}\text{C}$ Rotational Constants [MHz]

A_e	38835.7
B_e	7856.1
C_e	6534.3
A_0	38815.3
B_0	7755.2
C_0	6451.5
κ	-0.91943
A_1	38810.6
B_1	7714.0
C_1	6423.0
A_2	38357.0
B_2	7778.4
C_2	6457.0
A_3	38966.3
B_3	7733.7
C_3	6436.8
A_4	39839.2
B_4	7694.4
C_4	6396.8
A_5	43117.7
B_5	7759.7
C_5	6462.4
A_6	33760.5
B_6	7649.1
C_6	6367.2

Table S25: $^{12}\text{C}(^{18}\text{O})^{16}\text{O}^{12}\text{C}$ Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	3.000
Δ_K	kHz	156.337
Δ_{JK}	kHz	46.223
δ_J	Hz	562.919
δ_K	kHz	32.658
Φ_J	mHz	-9.191
Φ_K	Hz	-2.177
Φ_{JK}	mHz	-274.488
Φ_{KJ}	Hz	2.115
ϕ_j	mHz	-2.295
ϕ_{jk}	mHz	-204.119
ϕ_k	Hz	3.464

Table S26: $^{12}\text{C}(^{18}\text{O})^{16}\text{O}^{12}\text{C}$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{C}_2)$	1.1717212	1.1703408
$r(\text{C}_2-\text{O}_3)$	1.4387035	1.4719488
$r(\text{O}_3-\text{C}_4)$	1.3594921	1.3566623
$\angle(\text{C}_2-\text{O}_1-\text{O}_3)$	134.4045563	133.3236999
$\angle(\text{O}_3-\text{C}_2-\text{C}_4)$	62.0919179	61.6165057

Table S27: $^{12}\text{C}(^{18}\text{O})^{16}\text{O}^{12}\text{C}$ Fermi Resonances

$2\nu_3 = \nu_3 + \nu_2 = \nu_1$ $\nu_6 + \nu_3 = \nu_2$ $2\nu_5 = 2\nu_6 = \nu_6 + \nu_4 = \nu_3$
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Table S28: $^{12}\text{C}(^{18}\text{O})^{18}\text{O}^{12}\text{C}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	O_1-C_1 stretch	1996.5
ω_2	O_2-C_2 stretch	1204.7
ω_3	$\text{C}_1-\text{O}_2-\text{C}_2$ bend	924.0
ω_4	$(\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	503.6
ω_5	out-of-plane bend	495.0
ω_6	$(\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	473.1
ν_1	O_1-C_1 stretch	1972.7
ν_2	O_2-C_2 stretch	1212.7
ν_3	$\text{C}_1-\text{O}_2-\text{C}_2$ bend	895.4
ν_4	$(\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	488.7
ν_5	out-of-plane bend	455.9
ν_6	$(\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	291.4
ZPVE [cm^{-1}]		2749.6

Table S29: $^{12}\text{C}(^{18}\text{O})^{18}\text{O}^{12}\text{C}$ Rotational Constants [MHz]

A_e	36673.3
B_e	7652.8
C_e	6331.6
A_0	36666.0
B_0	7552.7
C_0	6250.9
κ	-0.91440
A_1	36653.4
B_1	7514.4
C_1	6224.4
A_2	36254.4
B_2	7574.2
C_2	6255.9
A_3	36789.0
B_3	7534.3
C_3	6237.4
A_4	40350.9
B_4	7562.1
C_4	6261.1
A_5	36879.5
B_5	7516.0
C_5	6222.2
A_6	33053.8
B_6	7414.9
C_6	6143.0

Table S30: $^{12}\text{C}(^{18}\text{O})^{18}\text{O}^{12}\text{C}$ Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	3.002
Δ_K	kHz	136.321
Δ_{JK}	kHz	41.991
δ_J	Hz	580.245
δ_K	kHz	30.579
Φ_J	mHz	-10.228
Φ_K	Hz	-2.035
Φ_{JK}	mHz	-235.034
Φ_{KJ}	Hz	1.925
ϕ_j	mHz	-2.694
ϕ_{jk}	mHz	-195.277
ϕ_k	Hz	3.014

Table S31: $^{12}\text{C}(^{18}\text{O})^{18}\text{O}^{12}\text{C}$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{C}_2)$	1.1717212	1.1704062
$r(\text{C}_2-\text{O}_3)$	1.4387035	1.4712159
$r(\text{O}_3-\text{C}_4)$	1.3594921	1.3566927
$\angle(\text{C}_2-\text{O}_1-\text{O}_3)$	134.4045563	133.3363692
$\angle(\text{O}_3-\text{C}_2-\text{C}_4)$	62.0919179	61.6330167

Table S32: $^{12}\text{C}(^{18}\text{O})^{18}\text{O}^{12}\text{C}$ Fermi Resonances

$2\nu_3 = \nu_3 + \nu_2 = \nu_1$
$2\nu_4 = \nu_6 + \nu_3 = \nu_2$
$2\nu_4 = 2\nu_5 = 2\nu_6 = \nu_6 + \nu_5 = \nu_3$

Table S33: $^{13}\text{C}(^{16}\text{O})^{16}\text{O}^{12}\text{C}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	O_1-C_1 stretch	1978.2
ω_2	O_2-C_2 stretch	1234.9
ω_3	$\text{C}_1-\text{O}_2-\text{C}_2$ bend	940.4
ω_4	$(\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	517.0
ω_5	out-of-plane bend	493.5
ω_6	$(\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	466.4
ν_1	O_1-C_1 stretch	1957.0
ν_2	O_2-C_2 stretch	1246.1
ν_3	$\text{C}_1-\text{O}_2-\text{C}_2$ bend	912.0
ν_4	$(\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	451.8
ν_5	out-of-plane bend	479.3
ν_6	$(\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	308.5
ZPVE [cm^{-1}]		2767.4

Table S34: $^{13}\text{C}(^{16}\text{O})^{16}\text{O}^{12}\text{C}$ Rotational Constants [MHz]

A_e	38741.3
B_e	8372.9
C_e	6884.7
A_0	38706.2
B_0	8264.5
C_0	6796.8
κ	-0.90801
A_1	38698.2
B_1	8224.9
C_1	6769.9
A_2	38262.6
B_2	8288.8
C_2	6801.9
A_3	38832.3
B_3	8244.4
C_3	6783.3
A_4	39366.0
B_4	8204.4
C_4	6739.9
A_5	43600.0
B_5	8267.8
C_5	6807.8
A_6	33408.4
B_6	8140.5
C_6	6702.2

Table S35: $^{13}\text{C}(^{16}\text{O})^{16}\text{O}^{12}\text{C}$ Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	3.479
Δ_K	kHz	147.731
Δ_{JK}	kHz	51.114
δ_J	Hz	685.213
δ_K	kHz	36.072
Φ_J	mHz	-12.356
Φ_K	Hz	-2.386
Φ_{JK}	mHz	-364.548
Φ_{KJ}	Hz	2.451
ϕ_j	mHz	-3.226
ϕ_{jk}	mHz	-265.785
ϕ_k	Hz	3.612

Table S36: $^{13}\text{C}(^{16}\text{O})^{16}\text{O}^{12}\text{C}$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{C}_2)$	1.1717212	1.1704055
$r(\text{C}_2-\text{O}_3)$	1.4387035	1.4711731
$r(\text{O}_3-\text{C}_4)$	1.3594921	1.3569285
$\angle(\text{C}_2-\text{O}_1-\text{O}_3)$	134.4045563	133.3576373
$\angle(\text{O}_3-\text{C}_2-\text{C}_4)$	62.0919179	61.6300776

Table S37: $^{13}\text{C}(^{16}\text{O})^{16}\text{O}^{12}\text{C}$ Fermi Resonances

$2\nu_3 = \nu_3 + \nu_2 = \nu_1$
$\nu_6 + \nu_3 = \nu_2$
$2\nu_4 = 2\nu_5 = 2\nu_6 = \nu_6 + \nu_4 = \nu_3$

Table S38: $^{13}\text{C}(^{16}\text{O})^{16}\text{O}^{13}\text{C}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	O_1-C_1 stretch	1975.2
ω_2	O_2-C_2 stretch	1209.5
ω_3	$\text{C}_1-\text{O}_2-\text{C}_2$ bend	925.9
ω_4	$(\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	513.8
ω_5	out-of-plane bend	491.4
ω_6	$(\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	462.7
ν_1	O_1-C_1 stretch	1953.8
ν_2	O_2-C_2 stretch	1223.4
ν_3	$\text{C}_1-\text{O}_2-\text{C}_2$ bend	899.0
ν_4	$(\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	445.1
ν_5	out-of-plane bend	477.2
ν_6	$(\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{O}_1-\text{C}_1-\text{O}_2 \text{ bend})$	310.2
ZPVE [cm^{-1}]		2741.7

Table S39: $^{13}\text{C}(^{16}\text{O})^{16}\text{O}^{13}\text{C}$ Rotational Constants [MHz]

A_e	37358.0
B_e	8222.1
C_e	6739.0
A_0	37338.8
B_0	8117.8
C_0	6654.9
κ	-0.90464
A_1	37334.7
B_1	8077.8
C_1	6628.0
A_2	36911.2
B_2	8140.4
C_2	6658.5
A_3	37477.2
B_3	8096.1
C_3	6641.4
A_4	37891.7
B_4	8057.8
C_4	6599.4
A_5	41707.7
B_5	8121.3
C_5	6665.7
A_6	32671.8
B_6	8004.9
C_6	6568.0

Table S40: $^{13}\text{C}(^{16}\text{O})^{16}\text{O}^{13}\text{C}$ Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	3.241
Δ_K	kHz	139.535
Δ_{JK}	kHz	49.548
δ_J	Hz	647.794
δ_K	kHz	34.492
Φ_J	mHz	-10.369
Φ_K	Hz	-2.224
Φ_{JK}	mHz	-345.694
Φ_{KJ}	Hz	2.313
ϕ_j	mHz	-2.739
ϕ_{jk}	mHz	-242.919
ϕ_k	Hz	3.365

Table S41: $^{13}\text{C}(^{16}\text{O})^{16}\text{O}^{13}\text{C}$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{C}_2)$	1.1717212	1.1703610
$r(\text{C}_2-\text{O}_3)$	1.4387035	1.4712391
$r(\text{O}_3-\text{C}_4)$	1.3594921	1.3567757
$\angle(\text{C}_2-\text{O}_1-\text{O}_3)$	134.4045563	133.3604061
$\angle(\text{O}_3-\text{C}_2-\text{C}_4)$	62.0919179	61.6277284

Table S42: $^{13}\text{C}(^{16}\text{O})^{16}\text{O}^{13}\text{C}$ Fermi Resonances

$$\begin{array}{l}
2\nu_3 = \nu_3 + \nu_2 = \nu_1 \\
2\nu_4 = \nu_6 + \nu_3 = \nu_2 \\
2\nu_4 = 2\nu_5 = 2\nu_6 = \nu_6 + \nu_4 = \nu_3
\end{array}$$

Table S43: $\text{c-C}_2\text{O}_2$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{C}_2)$	1.3813041	1.3891670
$r(\text{O}_1-\text{C}_3)$	1.3813041	1.3891670
$r(\text{O}_1-\text{O}_4)$	1.9840284	1.9955788
$\angle(\text{O}_1-\text{O}_4-\text{C}_2)$	44.0962196	44.0885741
$\angle(\text{O}_1-\text{O}_4-\text{C}_3)$	44.0962197	44.0885743

Table S44: $\text{c-C}_2\text{O}_2$ Fermi Resonances

$$2\nu_5 = \nu_4$$

Table S45: $\text{c-}^{12}\text{C}^{12}\text{C}^{16}\text{O}^{18}\text{O}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	$(\text{O}_1-\text{O}_2 \text{ stretch}) + (\text{C}_1-\text{C}_2 \text{ stretch})$	1228.6
ω_2	$(\text{O}_1-\text{C}_1 \text{ stretch}) + (\text{O}_1-\text{C}_2 \text{ stretch}) - (\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{C}_2-\text{O}_2 \text{ stretch})$	1079.8
ω_3	$(\text{O}_1-\text{C}_1 \text{ stretch}) - (\text{O}_1-\text{C}_2 \text{ stretch}) + (\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{C}_2-\text{O}_2 \text{ stretch})$	1042.7
ω_4	$(\text{O}_1-\text{O}_2 \text{ stretch}) - (\text{C}_1-\text{C}_2 \text{ stretch})$	993.7
ω_5	out-of-plane bend	439.4
ω_6	$(\text{O}_1-\text{C}_1 \text{ stretch}) - (\text{O}_1-\text{C}_2 \text{ stretch}) - (\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{C}_2-\text{O}_2 \text{ stretch})$	370.0
ν_1	$(\text{O}_1-\text{O}_2 \text{ stretch}) + (\text{C}_1-\text{C}_2 \text{ stretch})$	1236.6
ν_2	$(\text{O}_1-\text{C}_1 \text{ stretch}) + (\text{O}_1-\text{C}_2 \text{ stretch}) - (\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{C}_2-\text{O}_2 \text{ stretch})$	1016.9
ν_3	$(\text{O}_1-\text{C}_1 \text{ stretch}) - (\text{O}_1-\text{C}_2 \text{ stretch}) + (\text{C}_1-\text{O}_2 \text{ stretch}) - (\text{C}_2-\text{O}_2 \text{ stretch})$	998.3
ν_4	$(\text{O}_1-\text{O}_2 \text{ stretch}) - (\text{C}_1-\text{C}_2 \text{ stretch})$	974.9
ν_5	out-of-plane bend	366.0
ν_6	$(\text{O}_1-\text{C}_1 \text{ stretch}) - (\text{O}_1-\text{C}_2 \text{ stretch}) - (\text{C}_1-\text{O}_2 \text{ stretch}) + (\text{C}_2-\text{O}_2 \text{ stretch})$	311.0
ZPVE [cm^{-1}]		2538.3

Table S46: c-¹²C¹²C¹⁶O¹⁸O Rotational Constants [MHz]

A_e	23278.3
B_e	14846.6
C_e	9282.8
A_0	23049.6
B_0	14768.8
C_0	9158.0
κ	-0.19220
A_1	22996.9
B_1	14735.6
C_1	9133.4
A_2	22943.0
B_2	14755.1
C_2	9121.4
A_3	23098.8
B_3	14716.4
C_3	9136.0
A_4	23077.4
B_4	14735.5
C_4	9145.2
A_5	22827.0
B_5	14807.0
C_5	9135.3
A_6	22897.7
B_6	14707.5
C_6	9026.9

Table S47: c-¹²C¹²C¹⁶O¹⁸O Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	8.995
Δ_K	kHz	-139.741
Δ_{JK}	kHz	176.181
δ_J	kHz	2.972
δ_K	kHz	100.084
Φ_J	mHz	12.872
Φ_K	Hz	6.801
Φ_{JK}	Hz	-1.047
Φ_{KJ}	Hz	-5.605
ϕ_j	mHz	6.163
ϕ_{jk}	mHz	-507.164
ϕ_k	Hz	1.397

Table S48: c-¹²C¹²C¹⁶O¹⁸O Geometry [Å or Deg]

Coordinate	r_e	r_0
r(O ₁ –C ₂)	1.3813041	1.3891216
r(O ₁ –C ₃)	1.3813041	1.3891216
r(O ₁ –O ₄)	1.9840284	1.9954322
\angle (O ₁ –O ₄ –C ₂)	44.0962196	44.0860097
\angle (O ₁ –O ₄ –C ₃)	44.0962197	44.0860099

Table S49: c-¹²C¹²C¹⁶O¹⁸O Fermi Resonances

$\nu_6 + \nu_3 = \nu_1$
$2\nu_5 = \nu_4$

Table S50: c-¹²C¹²C¹⁸O¹⁸O Frequencies and ZPVE

	Description	Frequencies [cm ⁻¹]
ω_1	(O ₁ -O ₂ stretch) + (C ₁ -C ₂ stretch)	1219.9
ω_2	(O ₁ -C ₁ stretch) + (O ₁ -C ₂ stretch) - (C ₁ -O ₂ stretch) - (C ₂ -O ₂ stretch)	1063.7
ω_3	(O ₁ -C ₁ stretch) - (O ₁ -C ₂ stretch) + (C ₁ -O ₂ stretch) - (C ₂ -O ₂ stretch)	1030.2
ω_4	(O ₁ -O ₂ stretch) - (C ₁ -C ₂ stretch)	972.7
ω_5	out-of-plane bend	434.5
ω_6	(O ₁ -C ₁ stretch) - (O ₁ -C ₂ stretch) - (C ₁ -O ₂ stretch) + (C ₂ -O ₂ stretch)	365.9
ν_1	(O ₁ -O ₂ stretch) + (C ₁ -C ₂ stretch)	1228.4
ν_2	(O ₁ -C ₁ stretch) + (O ₁ -C ₂ stretch) - (C ₁ -O ₂ stretch) - (C ₂ -O ₂ stretch)	1000.8
ν_3	(O ₁ -C ₁ stretch) - (O ₁ -C ₂ stretch) + (C ₁ -O ₂ stretch) - (C ₂ -O ₂ stretch)	987.0
ν_4	(O ₁ -O ₂ stretch) - (C ₁ -C ₂ stretch)	957.6
ν_5	out-of-plane bend	362.8
ν_6	(O ₁ -C ₁ stretch) - (O ₁ -C ₂ stretch) - (C ₁ -O ₂ stretch) + (C ₂ -O ₂ stretch)	308.3
ZPVE [cm ⁻¹]		2505.8

Table S51: c-¹²C¹²C¹⁸O¹⁸O Rotational Constants [MHz]

A_e	23260.6
B_e	14000.9
C_e	8947.6
A_0	23037.5
B_0	13926.5
C_0	8829.6
κ	-0.28253
A_1	22990.0
B_1	13896.4
C_1	8807.1
A_2	22924.9
B_2	13913.9
C_2	8793.8
A_3	23086.7
B_3	13877.9
C_3	8802.1
A_4	23070.9
B_4	13893.4
C_4	8824.1
A_5	22817.9
B_5	13961.3
C_5	8809.2
A_6	22888.7
B_6	13867.4
C_6	8705.6

Table S52: c-¹²C¹²C¹⁸O¹⁸O Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	8.011
Δ_K	kHz	-127.614
Δ_{JK}	kHz	164.701
δ_J	kHz	2.594
δ_K	kHz	93.688
Φ_J	mHz	10.458
Φ_K	Hz	6.301
Φ_{JK}	mHz	-955.975
Φ_{KJ}	Hz	-5.195
ϕ_j	mHz	4.988
ϕ_{jk}	mHz	-463.898
ϕ_k	Hz	1.607

Table S53: c-¹²C¹²C¹⁸O¹⁸O Geometry [Å or Deg]

Coordinate	r _e	r ₀
r(O ₁ –C ₂)	1.3813041	1.3889568
r(O ₁ –C ₃)	1.3813041	1.3889568
r(O ₁ –O ₄)	1.9840284	1.9952869
∠(O ₁ –O ₄ –C ₂)	44.0962196	44.0882770
∠(O ₁ –O ₄ –C ₃)	44.0962197	44.0882772

Table S54: c-¹²C¹²C¹⁸O¹⁸O Fermi Resonances

$$2\nu_5 = \nu_4$$

Table S55: c-¹³C¹²C¹⁶O¹⁶O Frequencies and ZPVE

	Description	Frequencies [cm ⁻¹]
ω_1	(O ₁ –O ₂ stretch) + (C ₁ –C ₂ stretch)	1221.4
ω_2	(O ₁ –C ₁ stretch) + (O ₁ –C ₂ stretch) - (C ₁ –O ₂ stretch) - (C ₂ –O ₂ stretch)	1078.9
ω_3	(O ₁ –C ₁ stretch) - (O ₁ –C ₂ stretch) + (C ₁ –O ₂ stretch) - (C ₂ –O ₂ stretch)	1044.1
ω_4	(O ₁ –O ₂ stretch) - (C ₁ –C ₂ stretch)	1012.0
ω_5	out-of-plane bend	439.0
ω_6	(O ₁ –C ₁ stretch) - (O ₁ –C ₂ stretch) - (C ₁ –O ₂ stretch) + (C ₂ –O ₂ stretch)	369.9
ν_1	(O ₁ –O ₂ stretch) + (C ₁ –C ₂ stretch)	1231.9
ν_2	(O ₁ –C ₁ stretch) + (O ₁ –C ₂ stretch) - (C ₁ –O ₂ stretch) - (C ₂ –O ₂ stretch)	1014.4
ν_3	(O ₁ –C ₁ stretch) - (O ₁ –C ₂ stretch) + (C ₁ –O ₂ stretch) - (C ₂ –O ₂ stretch)	1002.1
ν_4	(O ₁ –O ₂ stretch) - (C ₁ –C ₂ stretch)	989.4
ν_5	out-of-plane bend	365.7
ν_6	(O ₁ –C ₁ stretch) - (O ₁ –C ₂ stretch) - (C ₁ –O ₂ stretch) + (C ₂ –O ₂ stretch)	310.8
ZPVE [cm ⁻¹]		2543.8

Table S56: c-¹³C¹²C¹⁶O¹⁶O Rotational Constants [MHz]

A_e	22387.0
B_e	15727.4
C_e	9463.5
A_0	22163.0
B_0	15648.2
C_0	9334.5
κ	-0.01568
A_1	22108.3
B_1	15608.6
C_1	9307.6
A_2	22052.8
B_2	15687.1
C_2	9294.6
A_3	22214.5
B_3	15587.8
C_3	9306.6
A_4	22191.7
B_4	15570.2
C_4	9331.2
A_5	21948.7
B_5	15690.2
C_5	9309.2
A_6	22014.4
B_6	15587.2
C_6	9199.5

Table S57: c-¹³C¹²C¹⁶O¹⁶O Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	10.048
Δ_K	kHz	-148.516
Δ_{JK}	kHz	180.953
δ_J	kHz	3.424
δ_K	kHz	102.581
Φ_J	mHz	16.045
Φ_K	Hz	6.833
Φ_{JK}	Hz	-1.086
Φ_{KJ}	Hz	-5.618
ϕ_j	mHz	7.725
ϕ_{jk}	mHz	-524.101
ϕ_k	mHz	851.357

Table S58: c-¹³C¹²C¹⁶O¹⁶O Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{C}_2)$	1.3813041	1.3890322
$r(\text{O}_1-\text{C}_3)$	1.3813041	1.3891362
$r(\text{O}_1-\text{O}_4)$	1.9840284	1.9954515
$\angle(\text{O}_1-\text{O}_4-\text{C}_2)$	44.0962196	44.0865974
$\angle(\text{O}_1-\text{O}_4-\text{C}_3)$	44.0962197	44.0910515

Table S59: c-¹³C¹²C¹⁶O¹⁶O Fermi Resonances

$$2\nu_5 = \nu_4$$

Table S60: c-¹³C¹³C¹⁶O¹⁶O Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	(O ₁ -O ₂ stretch) + (C ₁ -C ₂ stretch)	1204.2
ω_2	(O ₁ -C ₁ stretch) + (O ₁ -C ₂ stretch) - (C ₁ -O ₂ stretch) - (C ₂ -O ₂ stretch)	1066.9
ω_3	(O ₁ -C ₁ stretch) - (O ₁ -C ₂ stretch) + (C ₁ -O ₂ stretch) - (C ₂ -O ₂ stretch)	1030.9
ω_4	(O ₁ -O ₂ stretch) - (C ₁ -C ₂ stretch)	1008.0
ω_5	out-of-plane bend	433.6
ω_6	(O ₁ -C ₁ stretch) - (O ₁ -C ₂ stretch) - (C ₁ -O ₂ stretch) + (C ₂ -O ₂ stretch)	365.6
ν_1	(O ₁ -O ₂ stretch) + (C ₁ -C ₂ stretch)	1215.8
ν_2	(O ₁ -C ₁ stretch) + (O ₁ -C ₂ stretch) - (C ₁ -O ₂ stretch) - (C ₂ -O ₂ stretch)	1003.9
ν_3	(O ₁ -C ₁ stretch) - (O ₁ -C ₂ stretch) + (C ₁ -O ₂ stretch) - (C ₂ -O ₂ stretch)	987.3
ν_4	(O ₁ -O ₂ stretch) - (C ₁ -C ₂ stretch)	986.8
ν_5	out-of-plane bend	362.1
ν_6	(O ₁ -C ₁ stretch) - (O ₁ -C ₂ stretch) - (C ₁ -O ₂ stretch) + (C ₂ -O ₂ stretch)	307.8
ZPVE [cm^{-1}]		2516.6

Table S61: c-¹³C¹³C¹⁶O¹⁶O Rotational Constants [MHz]

A_e	21519.4
B_e	15719.9
C_e	9307.4
A_0	21304.6
B_0	15643.2
C_0	9181.3
κ	0.06602
A_1	21249.6
B_1	15601.9
C_1	9153.6
A_2	21199.4
B_2	15636.3
C_2	9143.0
A_3	21364.5
B_3	15587.4
C_3	9153.0
A_4	21321.6
B_4	15610.1
C_4	9180.5
A_5	21100.9
B_5	15685.2
C_5	9145.2
A_6	21162.4
B_6	15584.3
C_6	9060.3

Table S62: c-¹³C¹³C¹⁶O¹⁶O Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	10.031
Δ_K	kHz	-144.671
Δ_{JK}	kHz	174.031
δ_J	kHz	3.458
δ_K	kHz	98.625
Φ_J	mHz	16.361
Φ_K	Hz	6.365
Φ_{JK}	Hz	-1.030
Φ_{KJ}	Hz	-5.223
ϕ_j	mHz	7.896
ϕ_{jk}	mHz	-496.365
ϕ_k	mHz	593.908

Table S63: c-¹³C¹³C¹⁶O¹⁶O Geometry [Å or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{C}_2)$	1.3813041	1.3890025
$r(\text{O}_1-\text{C}_3)$	1.3813041	1.3890025
$r(\text{O}_1-\text{O}_4)$	1.9840284	1.9953246
$\angle(\text{O}_1-\text{O}_4-\text{C}_2)$	44.0962196	44.0891104
$\angle(\text{O}_1-\text{O}_4-\text{C}_3)$	44.0962197	44.0891105

Table S64: c-¹³C¹³C¹⁶O¹⁶O Fermi Resonances

$$2\nu_5 = \nu_4$$

Table S65: Si(O)OSi Geometry [Å or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{Si}_2)$	1.5142983	1.5140618
$r(\text{Si}_2-\text{O}_3)$	1.7009711	1.7112598
$r(\text{O}_3-\text{Si}_4)$	1.6660867	1.6670303
$\angle(\text{Si}_2-\text{O}_1-\text{O}_3)$	125.7978085	125.4552259
$\angle(\text{O}_3-\text{Si}_2-\text{Si}_4)$	85.1391323	85.1899607

Table S66: Si(O)OSi Fermi Resonances

$2\nu_3=\nu_5+\nu_2=\nu_1$ $\nu_4+\nu_3=\nu_5+\nu_3=\nu_2$ $2\nu_5=\nu_3$ $2\nu_6=\nu_4$

Table S67: $^{28}\text{Si}(^{16}\text{O})^{16}\text{O}^{29}\text{Si}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	$\text{O}_1\text{--Si}_1$ stretch	1246.9
ω_2	$\text{O}_2\text{--Si}_2$ stretch	855.4
ω_3	$\text{Si}_1\text{--O}_2$ stretch	603.5
ω_4	$\text{Si}_1\text{--O}_2\text{--Si}_2$ bend	440.7
ω_5	$\text{O}_1\text{--Si}_1\text{--O}_2$ bend	206.9
ω_6	out-of-plane bend	166.7
ν_1	$\text{O}_1\text{--Si}_1$ stretch	1234.3
ν_2	$\text{O}_2\text{--Si}_2$ stretch	853.2
ν_3	$\text{Si}_1\text{--O}_2$ stretch	579.9
ν_4	$\text{Si}_1\text{--O}_2\text{--Si}_2$ bend	432.6
ν_5	$\text{O}_1\text{--Si}_1\text{--O}_2$ bend	203.9
ν_6	out-of-plane bend	166.0
ZPVE [cm^{-1}]		1750.9

Table S68: $^{28}\text{Si}(^{16}\text{O})^{16}\text{O}^{29}\text{Si}$ Rotational Constants [MHz]

A_e	26301.4
B_e	3028.8
C_e	2716.1
A_0	26272.2
B_0	3016.0
C_0	2703.2
κ	-0.97346
A_1	26310.1
B_1	3005.0
C_1	2694.9
A_2	26114.2
B_2	3015.3
C_2	2702.0
A_3	26085.5
B_3	3007.4
C_3	2690.0
A_4	26479.8
B_4	3007.3
C_4	2696.9
A_5	26326.1
B_5	3018.4
C_5	2701.4
A_6	26259.0
B_6	3017.0
C_6	2708.6

Table S69: $^{28}\text{Si}(^{16}\text{O})^{16}\text{O}^{29}\text{Si}$ Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	Hz	464.156
Δ_K	kHz	205.703
Δ_{JK}	kHz	-1.478
δ_J	Hz	67.442
δ_K	kHz	3.781
Φ_J	uHz	-83.199
Φ_K	Hz	3.651
Φ_{JK}	mHz	14.113
Φ_{KJ}	mHz	-497.433
ϕ_j	uHz	-11.585
ϕ_{jk}	mHz	2.328
ϕ_k	mHz	555.751

Table S70: $^{28}\text{Si}(^{16}\text{O})^{16}\text{O}^{29}\text{Si}$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{Si}_2)$	1.5142983	1.5140371
$r(\text{Si}_2-\text{O}_3)$	1.7009711	1.7112661
$r(\text{O}_3-\text{Si}_4)$	1.6660867	1.6670067
$\angle(\text{Si}_2-\text{O}_1-\text{O}_3)$	125.7978085	125.4553449
$\angle(\text{O}_3-\text{Si}_2-\text{Si}_4)$	85.1391323	85.1896935

Table S71: $^{28}\text{Si}(^{16}\text{O})^{16}\text{O}^{29}\text{Si}$ Fermi Resonances

$2\nu_3=\nu_5+\nu_2=\nu_1$
$\nu_4+\nu_3=\nu_5+\nu_3=\nu_2$
$2\nu_5=\nu_3$
$2\nu_6=\nu_4$

Table S72: $^{28}\text{Si}(^{16}\text{O})^{16}\text{O}^{30}\text{Si}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	O_1-Si_1 stretch	1246.8
ω_2	O_2-Si_2 stretch	851.6
ω_3	Si_1-O_2 stretch	602.5
ω_4	$\text{Si}_1-\text{O}_2-\text{Si}_2$ bend	437.7
ω_5	$\text{O}_1-\text{Si}_1-\text{O}_2$ bend	206.3
ω_6	out-of-plane bend	166.4
ν_1	O_1-Si_1 stretch	1234.1
ν_2	O_2-Si_2 stretch	849.8
ν_3	Si_1-O_2 stretch	578.9
ν_4	$\text{Si}_1-\text{O}_2-\text{Si}_2$ bend	429.8
ν_5	$\text{O}_1-\text{Si}_1-\text{O}_2$ bend	203.3
ν_6	out-of-plane bend	165.7
ZPVE [cm^{-1}]		1746.5

Table S73: $^{28}\text{Si}(^{16}\text{O})^{16}\text{O}^{30}\text{Si}$ Rotational Constants [MHz]

A_e	26192.0
B_e	2984.1
C_e	2678.9
A_0	26164.1
B_0	2971.5
C_0	2666.3
κ	-0.97402
A_1	26203.0
B_1	2960.7
C_1	2658.1
A_2	26009.5
B_2	2970.7
C_2	2665.0
A_3	25975.0
B_3	2963.2
C_3	2653.5
A_4	26372.1
B_4	2963.0
C_4	2660.1
A_5	26219.2
B_5	2973.8
C_5	2664.5
A_6	26150.4
B_6	2972.5
C_6	2671.6

Table S74: $^{28}\text{Si}(^{16}\text{O})^{16}\text{O}^{30}\text{Si}$ Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	Hz	453.245
Δ_K	kHz	206.769
Δ_{JK}	kHz	-1.672
δ_J	Hz	65.542
δ_K	kHz	3.673
Φ_J	uHz	-80.282
Φ_K	Hz	3.597
Φ_{JK}	mHz	13.659
Φ_{KJ}	mHz	-485.144
ϕ_j	uHz	-10.947
ϕ_{jk}	mHz	2.173
ϕ_k	mHz	549.076

Table S75: $^{28}\text{Si}(^{16}\text{O})^{16}\text{O}^{30}\text{Si}$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{Si}_2)$	1.5142983	1.5140137
$r(\text{Si}_2-\text{O}_3)$	1.7009711	1.7112720
$r(\text{O}_3-\text{Si}_4)$	1.6660867	1.6669844
$\angle(\text{Si}_2-\text{O}_1-\text{O}_3)$	125.7978085	125.4554615
$\angle(\text{O}_3-\text{Si}_2-\text{Si}_4)$	85.1391323	85.1894376

Table S76: $^{28}\text{Si}(^{16}\text{O})^{16}\text{O}^{30}\text{Si}$ Fermi Resonances

$2\nu_3=\nu_5+\nu_2=\nu_1$
$\nu_4+\nu_3=\nu_5+\nu_3=\nu_2$
$2\nu_5=\nu_3$
$2\nu_6=\nu_4$

Table S77: $^{28}\text{Si}(^{16}\text{O})^{18}\text{O}^{28}\text{Si}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	$\text{O}_1\text{--Si}_1$ stretch	1246.7
ω_2	$\text{O}_2\text{--Si}_2$ stretch	828.8
ω_3	$\text{Si}_1\text{--O}_2$ stretch	580.3
ω_4	$\text{Si}_1\text{--O}_2\text{--Si}_2$ bend	441.0
ω_5	$\text{O}_1\text{--Si}_1\text{--O}_2$ bend	206.4
ω_6	out-of-plane bend	166.9
ν_1	$\text{O}_1\text{--Si}_1$ stretch	1232.9
ν_2	$\text{O}_2\text{--Si}_2$ stretch	826.7
ν_3	$\text{Si}_1\text{--O}_2$ stretch	558.1
ν_4	$\text{Si}_1\text{--O}_2\text{--Si}_2$ bend	432.8
ν_5	$\text{O}_1\text{--Si}_1\text{--O}_2$ bend	203.5
ν_6	out-of-plane bend	166.2
ZPVE [cm^{-1}]		1726.3

Table S78: $^{28}\text{Si}(^{16}\text{O})^{18}\text{O}^{28}\text{Si}$ Rotational Constants [MHz]

A_e	24115.3
B_e	3065.7
C_e	2720.0
A_0	24096.9
B_0	3053.1
C_0	2707.4
κ	-0.96768
A_1	24133.3
B_1	3041.9
C_1	2699.2
A_2	23942.8
B_2	3052.7
C_2	2706.2
A_3	23947.7
B_3	3044.1
C_3	2694.3
A_4	24284.9
B_4	3044.4
C_4	2701.3
A_5	24149.7
B_5	3055.8
C_5	2705.7
A_6	24086.2
B_6	3053.9
C_6	2712.8

Table S79: $^{28}\text{Si}(^{16}\text{O})^{18}\text{O}^{28}\text{Si}$ Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	Hz	464.875
Δ_K	kHz	173.095
Δ_{JK}	kHz	-0.486
δ_J	Hz	72.651
δ_K	kHz	3.792
Φ_J	uHz	-82.136
Φ_K	Hz	3.040
Φ_{JK}	mHz	13.863
Φ_{KJ}	mHz	-434.923
ϕ_j	uHz	-14.181
ϕ_{jk}	mHz	2.511
ϕ_k	mHz	490.249

Table S80: $^{28}\text{Si}(^{16}\text{O})^{18}\text{O}^{28}\text{Si}$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{Si}_2)$	1.5142983	1.5140582
$r(\text{Si}_2-\text{O}_3)$	1.7009711	1.7109596
$r(\text{O}_3-\text{Si}_4)$	1.6660867	1.6669218
$\angle(\text{Si}_2-\text{O}_1-\text{O}_3)$	125.7978085	125.4581576
$\angle(\text{O}_3-\text{Si}_2-\text{Si}_4)$	85.1391323	85.1973788

Table S81: $^{28}\text{Si}(^{16}\text{O})^{18}\text{O}^{28}\text{Si}$ Fermi Resonances

$2\nu_3=\nu_3+\nu_2=\nu_1$
$\nu_4+\nu_3=\nu_5+\nu_3=\nu_2$
$2\nu_5=\nu_3$
$2\nu_6=\nu_4$

Table S82: $^{28}\text{Si}(^{18}\text{O})^{16}\text{O}^{28}\text{Si}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	O_1-Si_1 stretch	1207.2
ω_2	O_2-Si_2 stretch	858.3
ω_3	Si_1-O_2 stretch	603.7
ω_4	$\text{Si}_1-\text{O}_2-\text{Si}_2$ bend	437.2
ω_5	$\text{O}_1-\text{Si}_1-\text{O}_2$ bend	203.2
ω_6	out-of-plane bend	163.6
ν_1	O_1-Si_1 stretch	1198.6
ν_2	O_2-Si_2 stretch	855.2
ν_3	Si_1-O_2 stretch	580.2
ν_4	$\text{Si}_1-\text{O}_2-\text{Si}_2$ bend	429.1
ν_5	$\text{O}_1-\text{Si}_1-\text{O}_2$ bend	200.3
ν_6	out-of-plane bend	163.0
ZPVE [cm^{-1}]		1727.8

Table S83: $^{28}\text{Si}(^{18}\text{O})^{16}\text{O}^{28}\text{Si}$ Rotational Constants [MHz]

A_e	26417.7
B_e	2913.1
C_e	2623.8
A_0	26386.3
B_0	2901.0
C_0	2611.6
κ	-0.97566
A_1	26424.1
B_1	2890.2
C_1	2603.4
A_2	26224.6
B_2	2900.5
C_2	2610.5
A_3	26207.0
B_3	2892.6
C_3	2599.0
A_4	26587.2
B_4	2893.0
C_4	2605.6
A_5	26438.8
B_5	2903.7
C_5	2610.2
A_6	26373.4
B_6	2902.2
C_6	2617.0

Table S84: $^{28}\text{Si}(^{18}\text{O})^{16}\text{O}^{28}\text{Si}$ Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	Hz	418.418
Δ_K	kHz	204.919
Δ_{JK}	kHz	-1.018
δ_J	Hz	58.072
δ_K	kHz	3.619
Φ_J	uHz	-67.171
Φ_K	Hz	3.608
Φ_{JK}	mHz	13.259
Φ_{KJ}	mHz	-494.018
ϕ_j	uHz	-9.349
ϕ_{jk}	mHz	2.502
ϕ_k	mHz	542.068

Table S85: $^{28}\text{Si}(^{18}\text{O})^{16}\text{O}^{28}\text{Si}$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{Si}_2)$	1.5142983	1.5141699
$r(\text{Si}_2-\text{O}_3)$	1.7009711	1.7111853
$r(\text{O}_3-\text{Si}_4)$	1.6660867	1.6670135
$\angle(\text{Si}_2-\text{O}_1-\text{O}_3)$	125.7978085	125.4561284
$\angle(\text{O}_3-\text{Si}_2-\text{Si}_4)$	85.1391323	85.1861714

Table S86: $^{28}\text{Si}(^{18}\text{O})^{16}\text{O}^{28}\text{Si}$ Fermi Resonances

$2\nu_3=\nu_5+\nu_2=\nu_1$
$\nu_4+\nu_3=\nu_5+\nu_3=\nu_2$
$2\nu_5=\nu_3$
$2\nu_6=\nu_4$

Table S87: $^{28}\text{Si}(^{18}\text{O})^{18}\text{O}^{28}\text{Si}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	O_1-Si_1 stretch	1206.8
ω_2	O_2-Si_2 stretch	827.6
ω_3	Si_1-O_2 stretch	579.4
ω_4	$\text{Si}_1-\text{O}_2-\text{Si}_2$ bend	434.3
ω_5	$\text{O}_1-\text{Si}_1-\text{O}_2$ bend	202.2
ω_6	out-of-plane bend	163.5
ν_1	O_1-Si_1 stretch	1195.2
ν_2	O_2-Si_2 stretch	824.9
ν_3	Si_1-O_2 stretch	557.4
ν_4	$\text{Si}_1-\text{O}_2-\text{Si}_2$ bend	426.2
ν_5	$\text{O}_1-\text{Si}_1-\text{O}_2$ bend	199.3
ν_6	out-of-plane bend	162.8
ZPVE [cm^{-1}]		1698.4

Table S88: $^{28}\text{Si}(^{18}\text{O})^{18}\text{O}^{28}\text{Si}$ Rotational Constants [MHz]

A_e	24113.8
B_e	2902.0
C_e	2590.5
A_0	24095.1
B_0	2890.4
C_0	2578.7
κ	-0.97103
A_1	24132.7
B_1	2879.7
C_1	2570.8
A_2	23940.3
B_2	2890.1
C_2	2577.5
A_3	23950.8
B_3	2882.0
C_3	2566.5
A_4	24277.3
B_4	2882.6
C_4	2573.1
A_5	24147.8
B_5	2893.2
C_5	2577.3
A_6	24084.1
B_6	2891.5
C_6	2584.0

Table S89: $^{28}\text{Si}(^{18}\text{O})^{18}\text{O}^{28}\text{Si}$ Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	Hz	408.796
Δ_K	kHz	173.490
Δ_{JK}	kHz	-0.279
δ_J	Hz	60.709
δ_K	kHz	3.528
Φ_J	uHz	-63.524
Φ_K	Hz	2.966
Φ_{JK}	mHz	12.610
Φ_{KJ}	mHz	-420.109
ϕ_j	uHz	-10.809
ϕ_{jk}	mHz	2.507
ϕ_k	mHz	473.723

Table S90: $^{28}\text{Si}(^{18}\text{O})^{18}\text{O}^{28}\text{Si}$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{Si}_2)$	1.5142983	1.5141664
$r(\text{Si}_2-\text{O}_3)$	1.7009711	1.7108837
$r(\text{O}_3-\text{Si}_4)$	1.6660867	1.6669062
$\angle(\text{Si}_2-\text{O}_1-\text{O}_3)$	125.7978085	125.4590691
$\angle(\text{O}_3-\text{Si}_2-\text{Si}_4)$	85.1391323	85.1935991

Table S91: $^{28}\text{Si}(^{18}\text{O})^{18}\text{O}^{28}\text{Si}$ Fermi Resonances

$2\nu_3=\nu_5+\nu_2=\nu_1$
$\nu_4+\nu_3=\nu_5+\nu_3=\nu_2$
$2\nu_5=\nu_3$
$2\nu_6=\nu_4$

Table S92: $^{29}\text{Si}(^{16}\text{O})^{16}\text{O}^{28}\text{Si}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	$\text{O}_1\text{--Si}_1$ stretch	1237.9
ω_2	$\text{O}_2\text{--Si}_2$ stretch	858.5
ω_3	$\text{Si}_1\text{--O}_2$ stretch	603.0
ω_4	$\text{Si}_1\text{--O}_2\text{--Si}_2$ bend	441.8
ω_5	$\text{O}_1\text{--Si}_1\text{--O}_2$ bend	206.0
ω_6	out-of-plane bend	165.5
ν_1	$\text{O}_1\text{--Si}_1$ stretch	1225.8
ν_2	$\text{O}_2\text{--Si}_2$ stretch	855.8
ν_3	$\text{Si}_1\text{--O}_2$ stretch	579.5
ν_4	$\text{Si}_1\text{--O}_2\text{--Si}_2$ bend	433.7
ν_5	$\text{O}_1\text{--Si}_1\text{--O}_2$ bend	203.1
ν_6	out-of-plane bend	164.9
ZPVE [cm^{-1}]		1747.4

Table S93: $^{29}\text{Si}(^{16}\text{O})^{16}\text{O}^{28}\text{Si}$ Rotational Constants [MHz]

A_e	26336.2
B_e	3067.8
C_e	2747.6
A_0	26301.5
B_0	3054.7
C_0	2734.6
κ	-0.97284
A_1	26335.3
B_1	3043.7
C_1	2726.3
A_2	26143.4
B_2	3054.2
C_2	2733.5
A_3	26117.3
B_3	3045.7
C_3	2721.0
A_4	26504.4
B_4	3045.9
C_4	2728.1
A_5	26350.1
B_5	3057.3
C_5	2732.7
A_6	26289.3
B_6	3055.5
C_6	2740.0

Table S94: $^{29}\text{Si}(^{16}\text{O})^{16}\text{O}^{28}\text{Si}$ Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	Hz	475.674
Δ_K	kHz	199.357
Δ_{JK}	kHz	-1.281
δ_J	Hz	69.319
δ_K	kHz	3.860
Φ_J	uHz	-87.760
Φ_K	Hz	3.636
Φ_{JK}	mHz	14.166
Φ_{KJ}	mHz	-499.502
ϕ_j	uHz	-11.995
ϕ_{jk}	mHz	2.397
ϕ_k	mHz	540.053

Table S95: $^{29}\text{Si}(^{16}\text{O})^{16}\text{O}^{28}\text{Si}$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{Si}_2)$	1.5142983	1.5140580
$r(\text{Si}_2-\text{O}_3)$	1.7009711	1.7111886
$r(\text{O}_3-\text{Si}_4)$	1.6660867	1.6670751
$\angle(\text{Si}_2-\text{O}_1-\text{O}_3)$	125.7978085	125.4598827
$\angle(\text{O}_3-\text{Si}_2-\text{Si}_4)$	85.1391323	85.1882112

Table S96: $^{29}\text{Si}(^{16}\text{O})^{16}\text{O}^{28}\text{Si}$ Fermi Resonances

$2\nu_3=\nu_5+\nu_2=\nu_1$
$\nu_4+\nu_3=\nu_5+\nu_3=\nu_2$
$2\nu_5=\nu_3$
$2\nu_6=\nu_4$

Table S97: $^{30}\text{Si}(^{16}\text{O})^{16}\text{O}^{28}\text{Si}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	O_1-Si_1 stretch	1229.3
ω_2	O_2-Si_2 stretch	857.6
ω_3	Si_1-O_2 stretch	601.5
ω_4	$\text{Si}_1-\text{O}_2-\text{Si}_2$ bend	440.0
ω_5	$\text{O}_1-\text{Si}_1-\text{O}_2$ bend	204.7
ω_6	out-of-plane bend	164.1
ν_1	O_1-Si_1 stretch	1217.6
ν_2	O_2-Si_2 stretch	854.7
ν_3	Si_1-O_2 stretch	578.2
ν_4	$\text{Si}_1-\text{O}_2-\text{Si}_2$ bend	431.9
ν_5	$\text{O}_1-\text{Si}_1-\text{O}_2$ bend	201.8
ν_6	out-of-plane bend	163.6
ZPVE [cm^{-1}]		1739.8

Table S98: $^{30}\text{Si}(^{16}\text{O})^{16}\text{O}^{28}\text{Si}$ Rotational Constants [MHz]

A_e	26256.7
B_e	3059.7
C_e	2740.4
A_0	26218.5
B_0	3046.7
C_0	2727.3
κ	-0.97281
A_1	26249.4
B_1	3036.0
C_1	2719.2
A_2	26063.7
B_2	3046.4
C_2	2726.4
A_3	26034.0
B_3	3037.6
C_3	2713.7
A_4	26417.5
B_4	3037.9
C_4	2720.8
A_5	26263.3
B_5	3049.2
C_5	2725.4
A_6	26206.7
B_6	3047.4
C_6	2732.7

Table S99: $^{30}\text{Si}(^{16}\text{O})^{16}\text{O}^{28}\text{Si}$ Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	Hz	475.572
Δ_K	kHz	194.545
Δ_{JK}	kHz	-1.292
δ_J	Hz	69.171
δ_K	kHz	3.823
Φ_J	uHz	-89.214
Φ_K	Hz	3.574
Φ_{JK}	mHz	13.751
Φ_{KJ}	mHz	-488.989
ϕ_j	uHz	-11.752
ϕ_{jk}	mHz	2.300
ϕ_k	mHz	518.869

Table S100: $^{30}\text{Si}(^{16}\text{O})^{16}\text{O}^{28}\text{Si}$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{Si}_2)$	1.5142983	1.5140543
$r(\text{Si}_2-\text{O}_3)$	1.7009711	1.7111213
$r(\text{O}_3-\text{Si}_4)$	1.6660867	1.6671173
$\angle(\text{Si}_2-\text{O}_1-\text{O}_3)$	125.7978085	125.4642794
$\angle(\text{O}_3-\text{Si}_2-\text{Si}_4)$	85.1391323	85.1865688

Table S101: $^{30}\text{Si}(^{16}\text{O})^{16}\text{O}^{28}\text{Si}$ Fermi Resonances

$$\begin{array}{c}
2\nu_3=\nu_5+\nu_2=\nu_1 \\
\nu_4+\nu_3=\nu_5+\nu_3=\nu_2 \\
2\nu_5=\nu_3 \\
2\nu_6=\nu_4
\end{array}$$

Table S102: $\text{c-Si}_2\text{O}_2$ Geometry [\AA or Deg]

Coordinate	r_e	r_0
$r(\text{O}_1-\text{Si}_2)$	1.6867196	1.6915087
$r(\text{O}_1-\text{Si}_3)$	1.6867196	1.6915087
$r(\text{O}_1-\text{O}_4)$	2.3335636	2.3411308
$\angle(\text{O}_1-\text{O}_4-\text{Si}_2)$	46.2315078	46.2093635
$\angle(\text{O}_1-\text{O}_4-\text{Si}_3)$	46.2315078	46.2093635

Table S103: $\text{c-Si}_2\text{O}_2$ Fermi Resonances

$$2\nu_6=\nu_5$$

Table S104: $\text{c-}^{28}\text{Si}^{28}\text{Si}^{16}\text{O}^{18}\text{O}$ Frequencies and ZPVE

	Description	Frequencies [cm^{-1}]
ω_1	$(\text{O}_1-\text{O}_2 \text{ stretch}) + (\text{Si}_1-\text{Si}_2 \text{ stretch})$	846.4
ω_2	$(\text{O}_1-\text{Si}_1 \text{ stretch}) - (\text{O}_1-\text{Si}_2 \text{ stretch}) + (\text{Si}_1-\text{O}_2 \text{ stretch}) - (\text{Si}_2-\text{O}_2 \text{ stretch})$	813.9
ω_3	$(\text{O}_1-\text{Si}_1 \text{ stretch}) + (\text{O}_1-\text{Si}_2 \text{ stretch}) - (\text{Si}_1-\text{O}_2 \text{ stretch}) - (\text{Si}_2-\text{O}_2 \text{ stretch})$	768.3
ω_4	$(\text{O}_1-\text{Si}_1 \text{ stretch}) - (\text{O}_1-\text{Si}_2 \text{ stretch}) - (\text{Si}_1-\text{O}_2 \text{ stretch}) + (\text{Si}_2-\text{O}_2 \text{ stretch})$	566.6
ω_5	$(\text{O}_1-\text{O}_2 \text{ stretch}) - (\text{Si}_1-\text{Si}_2 \text{ stretch})$	556.9
ω_6	out-of-plane bend	233.1
ν_1	$(\text{O}_1-\text{O}_2 \text{ stretch}) + (\text{Si}_1-\text{Si}_2 \text{ stretch})$	832.8
ν_2	$(\text{O}_1-\text{Si}_1 \text{ stretch}) - (\text{O}_1-\text{Si}_2 \text{ stretch}) + (\text{Si}_1-\text{O}_2 \text{ stretch}) - (\text{Si}_2-\text{O}_2 \text{ stretch})$	800.6
ν_3	$(\text{O}_1-\text{Si}_1 \text{ stretch}) + (\text{O}_1-\text{Si}_2 \text{ stretch}) - (\text{Si}_1-\text{O}_2 \text{ stretch}) - (\text{Si}_2-\text{O}_2 \text{ stretch})$	757.4
ν_4	$(\text{O}_1-\text{Si}_1 \text{ stretch}) - (\text{O}_1-\text{Si}_2 \text{ stretch}) - (\text{Si}_1-\text{O}_2 \text{ stretch}) + (\text{Si}_2-\text{O}_2 \text{ stretch})$	553.4
ν_5	$(\text{O}_1-\text{O}_2 \text{ stretch}) - (\text{Si}_1-\text{Si}_2 \text{ stretch})$	553.8
ν_6	out-of-plane bend	236.5
ZPVE [cm^{-1}]		1887.6

Table S105: c-²⁸Si²⁸Si¹⁶O¹⁸O Rotational Constants [MHz]

A_e	10934.6
B_e	6087.9
C_e	3910.5
A_0	10882.5
B_0	6066.3
C_0	3891.4
κ	-0.37782
A_1	10859.2
B_1	6056.6
C_1	3888.5
A_2	10844.7
B_2	6064.4
C_2	3877.8
A_3	10897.0
B_3	6047.0
C_3	3881.1
A_4	10855.1
B_4	6051.5
C_4	3875.3
A_5	10886.0
B_5	6071.0
C_5	3889.1
A_6	10848.9
B_6	6064.3
C_6	3898.4

Table S106: c-²⁸Si²⁸Si¹⁶O¹⁸O Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	1.602
Δ_K	kHz	7.412
Δ_{JK}	kHz	1.979
δ_J	Hz	578.205
δ_K	kHz	3.697
Φ_J	mHz	1.316
Φ_K	mHz	50.480
Φ_{JK}	mHz	-8.078
Φ_{KJ}	mHz	-24.066
ϕ_j	uHz	651.299
ϕ_{jk}	mHz	-1.699
ϕ_k	mHz	29.735

Table S107: c-²⁸Si²⁸Si¹⁶O¹⁸O Geometry [Å or Deg]

Coordinate	r_e	r_0
r(O ₁ –Si ₂)	1.6867196	1.6914498
r(O ₁ –Si ₃)	1.6867196	1.6914498
r(O ₁ –O ₄)	2.3335636	2.3409727
\angle (O ₁ –O ₄ –Si ₂)	46.2315078	46.2093800
\angle (O ₁ –O ₄ –Si ₃)	46.2315078	46.2093800

Table S108: c-²⁸Si²⁸Si¹⁶O¹⁸O Fermi Resonances

$$2\nu_6=\nu_5$$

Table S109: c-²⁸Si²⁸Si¹⁸O¹⁸O Frequencies and ZPVE

	Description	Frequencies [cm ⁻¹]
ω_1	(O ₁ –O ₂ stretch) + (Si ₁ –Si ₂ stretch)	824.7
ω_2	(O ₁ –Si ₁ stretch) - (O ₁ –Si ₂ stretch) + (Si ₁ –O ₂ stretch) - (Si ₂ –O ₂ stretch)	798.2
ω_3	(O ₁ –Si ₁ stretch) + (O ₁ –Si ₂ stretch) - (Si ₁ –O ₂ stretch) - (Si ₂ –O ₂ stretch)	757.4
ω_4	(O ₁ –Si ₁ stretch) - (O ₁ –Si ₂ stretch) - (Si ₁ –O ₂ stretch) + (Si ₂ –O ₂ stretch)	556.5
ω_5	(O ₁ –O ₂ stretch) - (Si ₁ –Si ₂ stretch)	552.5
ω_6	out-of-plane bend	228.8
ν_1	(O ₁ –O ₂ stretch) + (Si ₁ –Si ₂ stretch)	811.7
ν_2	(O ₁ –Si ₁ stretch) - (O ₁ –Si ₂ stretch) + (Si ₁ –O ₂ stretch) - (Si ₂ –O ₂ stretch)	785.6
ν_3	(O ₁ –Si ₁ stretch) + (O ₁ –Si ₂ stretch) - (Si ₁ –O ₂ stretch) - (Si ₂ –O ₂ stretch)	746.8
ν_4	(O ₁ –Si ₁ stretch) - (O ₁ –Si ₂ stretch) - (Si ₁ –O ₂ stretch) + (Si ₂ –O ₂ stretch)	543.8
ν_5	(O ₁ –O ₂ stretch) - (Si ₁ –Si ₂ stretch)	549.5
ν_6	out-of-plane bend	232.0
ZPVE [cm ⁻¹]		1854.3

Table S110: c-²⁸Si²⁸Si¹⁸O¹⁸O Rotational Constants [MHz]

A_e	10312.3
B_e	6087.9
C_e	3828.0
A_0	10264.2
B_0	6066.7
C_0	3809.4
κ	-0.30060
A_1	10240.4
B_1	6057.4
C_1	3802.9
A_2	10228.9
B_2	6065.3
C_2	3799.9
A_3	10279.1
B_3	6047.2
C_3	3799.4
A_4	10239.2
B_4	6052.2
C_4	3794.1
A_5	10267.4
B_5	6071.5
C_5	3807.1
A_6	10234.0
B_6	6064.2
C_6	3816.1

Table S111: c-²⁸Si²⁸Si¹⁸O¹⁸O Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	1.589
Δ_K	kHz	6.382
Δ_{JK}	kHz	1.788
δ_J	Hz	585.110
δ_K	kHz	3.420
Φ_J	mHz	1.314
Φ_K	mHz	43.270
Φ_{JK}	mHz	-8.166
Φ_{KJ}	mHz	-19.999
ϕ_j	uHz	652.029
ϕ_{jk}	mHz	-1.904
ϕ_k	mHz	24.583

Table S112: c-²⁸Si²⁸Si¹⁸O¹⁸O Geometry [Å or Deg]

Coordinate	r _e	r ₀
r(O ₁ –Si ₂)	1.6867196	1.6913413
r(O ₁ –Si ₃)	1.6867196	1.6913413
r(O ₁ –O ₄)	2.3335636	2.3408221
∠(O ₁ –O ₄ –Si ₂)	46.2315078	46.2111774
∠(O ₁ –O ₄ –Si ₃)	46.2315078	46.2111774

Table S113: c-²⁸Si²⁸Si¹⁸O¹⁸O Fermi Resonances

$$2\nu_6=\nu_5$$

Table S114: c-²⁸Si²⁹Si¹⁶O¹⁶O Frequencies and ZPVE

	Description	Frequencies [cm ⁻¹]
ω_1	(O ₁ –O ₂ stretch) + (Si ₁ –Si ₂ stretch)	859.8
ω_2	(O ₁ –Si ₁ stretch) - (O ₁ –Si ₂ stretch) + (Si ₁ –O ₂ stretch) - (Si ₂ –O ₂ stretch)	825.4
ω_3	(O ₁ –Si ₁ stretch) + (O ₁ –Si ₂ stretch) - (Si ₁ –O ₂ stretch) - (Si ₂ –O ₂ stretch)	783.3
ω_4	(O ₁ –Si ₁ stretch) - (O ₁ –Si ₂ stretch) - (Si ₁ –O ₂ stretch) + (Si ₂ –O ₂ stretch)	576.3
ω_5	(O ₁ –O ₂ stretch) - (Si ₁ –Si ₂ stretch)	557.4
ω_6	out-of-plane bend	236.6
ν_1	(O ₁ –O ₂ stretch) + (Si ₁ –Si ₂ stretch)	845.9
ν_2	(O ₁ –Si ₁ stretch) - (O ₁ –Si ₂ stretch) + (Si ₁ –O ₂ stretch) - (Si ₂ –O ₂ stretch)	811.8
ν_3	(O ₁ –Si ₁ stretch) + (O ₁ –Si ₂ stretch) - (Si ₁ –O ₂ stretch) - (Si ₂ –O ₂ stretch)	772.1
ν_4	(O ₁ –Si ₁ stretch) - (O ₁ –Si ₂ stretch) - (Si ₁ –O ₂ stretch) + (Si ₂ –O ₂ stretch)	562.6
ν_5	(O ₁ –O ₂ stretch) - (Si ₁ –Si ₂ stretch)	554.4
ν_6	out-of-plane bend	240.1
ZPVE [cm ⁻¹]		1914.3

Table S115: c-²⁸Si²⁹Si¹⁶O¹⁶O Rotational Constants [MHz]

A_e	11604.4
B_e	5982.1
C_e	3947.4
A_0	11547.9
B_0	5960.7
C_0	3927.8
κ	-0.46643
A_1	11520.4
B_1	5951.9
C_1	3921.6
A_2	11506.9
B_2	5958.4
C_2	3917.8
A_3	11567.1
B_3	5940.9
C_3	3916.8
A_4	11518.3
B_4	5945.7
C_4	3910.9
A_5	11551.2
B_5	5965.1
C_5	3925.5
A_6	11510.1
B_6	5959.4
C_6	3935.0

Table S116: c-²⁸Si²⁹Si¹⁶O¹⁶O Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	1.566
Δ_K	kHz	8.675
Δ_{JK}	kHz	2.117
δ_J	Hz	549.056
δ_K	kHz	3.925
Φ_J	mHz	1.251
Φ_K	mHz	57.776
Φ_{JK}	mHz	-7.622
Φ_{KJ}	mHz	-28.007
ϕ_j	uHz	616.809
ϕ_{jk}	mHz	-1.368
ϕ_k	mHz	35.950

Table S117: c-²⁸Si²⁹Si¹⁶O¹⁶O Geometry [Å or Deg]

Coordinate	r _e	r ₀
r(O ₁ –Si ₂)	1.6867196	1.6914975
r(O ₁ –Si ₃)	1.6867196	1.6914876
r(O ₁ –O ₄)	2.3335636	2.3411121
∠(O ₁ –O ₄ –Si ₂)	46.2315078	46.2094396
∠(O ₁ –O ₄ –Si ₃)	46.2315078	46.2091193

Table S118: c-²⁸Si²⁹Si¹⁶O¹⁶O Fermi Resonances

$$2\nu_6=\nu_5$$

Table S119: c-²⁸Si³⁰Si¹⁶O¹⁶O Frequencies and ZPVE

	Description	Frequencies [cm ⁻¹]
ω_1	(O ₁ –O ₂ stretch) + (Si ₁ –Si ₂ stretch)	858.5
ω_2	(O ₁ –Si ₁ stretch) - (O ₁ –Si ₂ stretch) + (Si ₁ –O ₂ stretch) - (Si ₂ –O ₂ stretch)	822.7
ω_3	(O ₁ –Si ₁ stretch) + (O ₁ –Si ₂ stretch) - (Si ₁ –O ₂ stretch) - (Si ₂ –O ₂ stretch)	781.0
ω_4	(O ₁ –Si ₁ stretch) - (O ₁ –Si ₂ stretch) - (Si ₁ –O ₂ stretch) + (Si ₂ –O ₂ stretch)	574.6
ω_5	(O ₁ –O ₂ stretch) - (Si ₁ –Si ₂ stretch)	553.7
ω_6	out-of-plane bend	235.9
ν_1	(O ₁ –O ₂ stretch) + (Si ₁ –Si ₂ stretch)	844.7
ν_2	(O ₁ –Si ₁ stretch) - (O ₁ –Si ₂ stretch) + (Si ₁ –O ₂ stretch) - (Si ₂ –O ₂ stretch)	809.2
ν_3	(O ₁ –Si ₁ stretch) + (O ₁ –Si ₂ stretch) - (Si ₁ –O ₂ stretch) - (Si ₂ –O ₂ stretch)	769.9
ν_4	(O ₁ –Si ₁ stretch) - (O ₁ –Si ₂ stretch) - (Si ₁ –O ₂ stretch) + (Si ₂ –O ₂ stretch)	561.0
ν_5	(O ₁ –O ₂ stretch) - (Si ₁ –Si ₂ stretch)	550.7
ν_6	out-of-plane bend	239.3
ZPVE [cm ⁻¹]		1908.2

Table S120: c-²⁸Si³⁰Si¹⁶O¹⁶O Rotational Constants [MHz]

A_e	11604.4
B_e	5882.5
C_e	3903.6
A_0	11548.0
B_0	5861.5
C_0	3884.5
κ	-0.48403
A_1	11520.4
B_1	5853.1
C_1	3878.7
A_2	11507.2
B_2	5859.1
C_2	3874.7
A_3	11567.4
B_3	5842.2
C_3	3873.4
A_4	11518.5
B_4	5846.8
C_4	3867.8
A_5	11551.2
B_5	5865.8
C_5	3882.3
A_6	11510.0
B_6	5860.4
C_6	3891.6

Table S121: c-²⁸Si³⁰Si¹⁶O¹⁶O Quartic and Sextic Distortion Constants

Constant	Units	
Δ_J	kHz	1.519
Δ_K	kHz	8.751
Δ_{JK}	kHz	2.088
δ_J	Hz	528.926
δ_K	kHz	3.872
Φ_J	mHz	1.190
Φ_K	mHz	57.262
Φ_{JK}	mHz	-7.246
Φ_{KJ}	mHz	-27.808
ϕ_j	uHz	586.369
ϕ_{jk}	mHz	-1.249
ϕ_k	mHz	36.010

Table S122: c-²⁸Si³⁰Si¹⁶O¹⁶O Geometry [Å or Deg]

Coordinate	r_e	r_0
r(O ₁ –Si ₂)	1.6867196	1.6914868
r(O ₁ –Si ₃)	1.6867196	1.6914677
r(O ₁ –O ₄)	2.3335636	2.3410944
\angle (O ₁ –O ₄ –Si ₂)	46.2315078	46.2095086
\angle (O ₁ –O ₄ –Si ₃)	46.2315078	46.2088869

Table S123: c-²⁸Si³⁰Si¹⁶O¹⁶O Fermi Resonances

$$2\nu_6=\nu_5$$