Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY INFORMATION FOR:

Interstellar hide and go seek: C_3H_4O. There and back (again).

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C_3H_4O potential energy surface

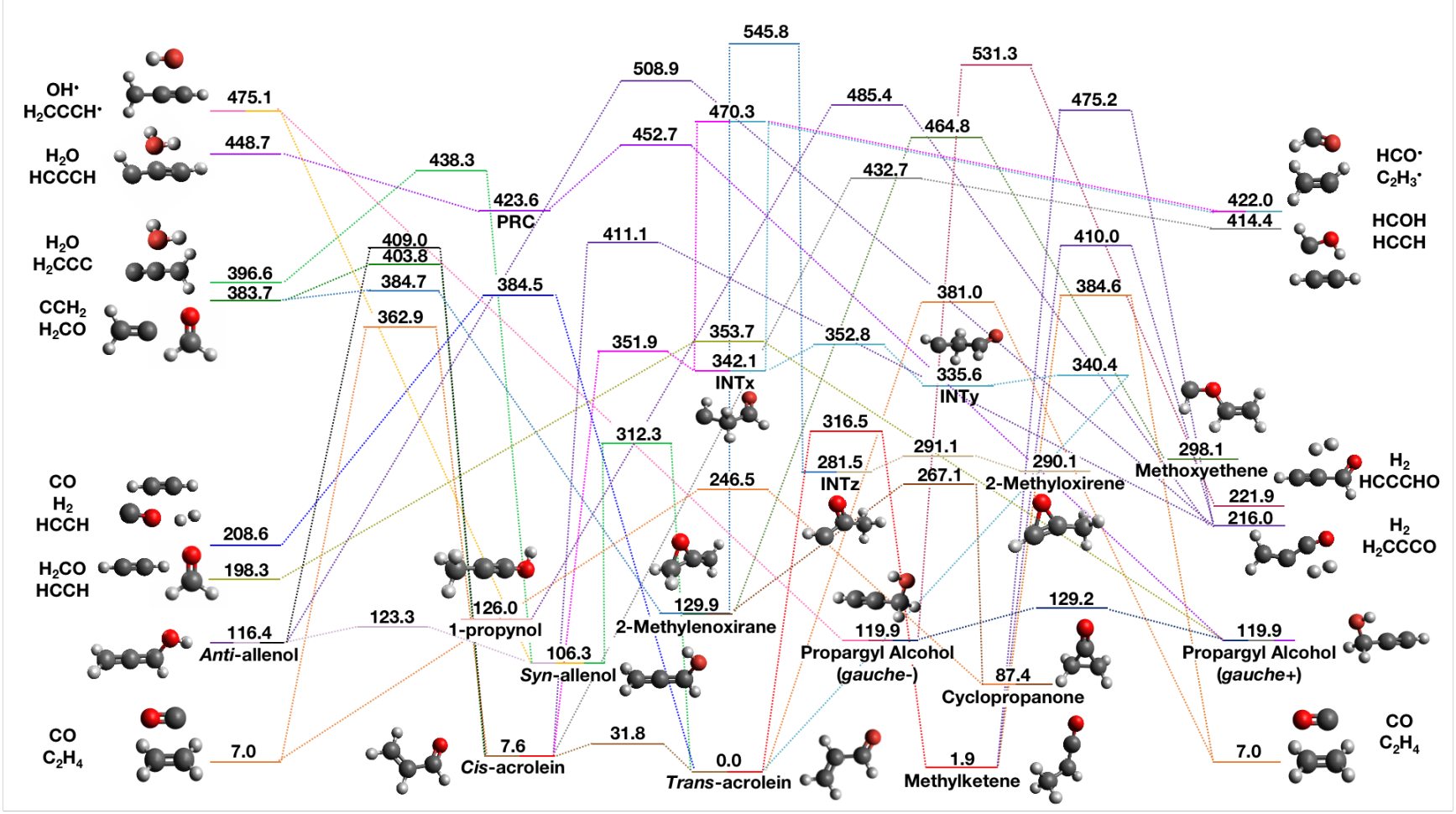

Figure 1: CCSD(T)/cc-pVTZ potential energy profile (in kJ/mol) of C_3H_4O. All energies are relative to the *trans*-acrolein isomer.

Fragments

Carbon Monoxide (CO)

CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −113.155578732807797 a.u.

O	0.0000000000	0.0000000000	-0.4868216639
C	0.0000000000	0.0000000000	0.6488892450

Ethene (C_2H_4)

CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −78.438803500228616 a.u.

C	0.6685648118	0.0000000000	0.0000000000
C	-0.6685648118	0.0000000000	0.0000000000
H	1.2337640611	-0.9240306111	0.0000000000
H	1.2337640611	0.9240306111	0.0000000000
H	-1.2337640611	-0.9240306111	0.0000000000
H	-1.2337640611	0.9240306111	0.0000000000

Molecular hydrogen (H_2)

CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −1.172336686229020 a.u.

H	0.0000000000	0.0000000000	-0.3713000000
H	0.0000000000	0.0000000000	0.3713000000

Propadienone (CH_2CCO)

CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −190.340377579525438 a.u.

O	1.7708565846	-0.0791178091	0.0000000000
C	0.6015800581	-0.0129906188	0.0000000000
C	-1.8928353114	-0.1699364786	0.0000000000
C	-0.6622392069	0.3528456792	0.0000000000
H	-2.7668613342	0.4732643385	0.0000000000
H	-2.0779938646	-1.2407987423	0.0000000000

Acetylene (HCCH)

CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −77.187648309540037 a.u.

C	0.0000000000	0.0000000000	-0.6048497702
C	0.0000000000	0.0000000000	0.6048497702
H	0.0000000000	0.0000000000	-1.6685443176
H	0.0000000000	0.0000000000	1.6685443176

Propynal (HC_2CHO)
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −190.338154327067429 a.u.

O	1.5786412993	-0.3712735255	0.0000000000
C	-1.9030676943	-0.1710326005	0.0000000000
C	0.6931208376	0.4577253132	0.0000000000
C	-0.7239658386	0.1145281810	0.0000000000
H	0.9098495181	1.5366116768	0.0000000000
H	-2.9372654414	-0.4214997808	0.0000000000

Vinylidene ($C{=}CH_2$)
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −77.117041851652488 a.u.

C	0.0000000000	0.0000000000	-0.7463316738
C	0.0000000000	0.0000000000	0.5606675129
H	0.0000000000	-0.9399037378	1.1053356744
H	0.0000000000	0.9399037378	1.1053356744

Formaldehyde (H_2CO)
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −114.333871977680431 a.u.

O	0.0000000000	0.0000000000	0.6040626032
C	0.0000000000	0.0000000000	-0.6055037698
H	0.0000000000	-0.9365775042	-1.1886411118
H	0.0000000000	0.9365775042	-1.1886411118

***Trans*-hydroxymethylene (HCOH)**
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −114.251574775138863 a.u.

O	-0.5637907858	0.0832384806	0.0000000000
C	0.7390893381	-0.1222244238	0.0000000000
H	-0.9893897270	-0.7843360672	0.0000000000
H	1.1369484957	0.9185862345	0.0000000000

Water (H_2O)
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −76.332216515443406 a.u.

O	0.0000000000	0.0000000000	-0.0664141525
H	0.0000000000	0.7538793394	0.5270204125
H	0.0000000000	-0.7538793394	0.5270204125

Propadienylidene (H_2CCC)
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −115.113788571712320 a.u.

C	0.0000000000	0.0000000000	-1.4083360318
C	0.0000000000	0.0000000000	1.2212534325
C	0.0000000000	0.0000000000	-0.1127996341
H	-0.9278792114	0.0000000000	1.7853231740
H	0.9278792114	0.0000000000	1.7853231740

Propargylene (HCCCH)
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −115.093939594437458 a.u.

C	0.0266427833	0.0574015549	0.0000000000
C	-1.3297032984	-0.1094660714	0.0000000000
C	1.2638369925	-0.0313184241	0.0000000000
H	2.3159214121	0.1333990809	0.0000000000
H	-1.8488936550	0.8594272608	0.0000000000

Vinyl radical ($C_2H_3^\bullet$)
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −77.752223046059115 a.u.

C	0.6903333065	-0.0848126188	0.0000000529
C	-0.6198649736	0.0230277618	-0.0000003069
H	-1.2675159703	-0.8473167590	0.0000014817
H	-1.1082645699	0.9979240913	0.0000012065
H	1.5367261696	0.5850543447	0.0000003281

Formyl radical ($HCO^\bullet$)
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −113.684112129896135 a.u.

O	0.5524508878	-0.0293175626	0.0000000000
C	-0.6226425773	0.1018564814	0.0000000000
H	-1.3540979621	-0.7474966522	0.0000000000

Propargyl radical ($H_2CCCH^\bullet$)
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −115.778386380690918 a.u.

C	0.0000000000	0.0000000000	-0.0883836604
C	0.0000000000	0.0000000000	1.2934490475
C	0.0000000000	0.0000000000	-1.3146516929
H	0.0000000000	0.0000000000	-2.3775795629
H	0.9315189295	0.0000000000	1.8412024870
H	-0.9315189295	0.0000000000	1.8412024870

OH radical ($OH^{\bullet}$)
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −75.637723243447155 a.u.

O	0.0000000000	0.0000000000	0.0575849730
H	0.0000000000	0.0000000000	-0.9139153033

$H_2CCCHO^{\bullet}$
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −190.912054341751940 a.u.

O	-1.6254631881	0.3805010061	0.0000000000
C	0.6447285042	-0.1347717773	0.0000000000
C	1.9107417646	0.1711198406	0.0000000000
C	-0.7225348957	-0.4651272541	0.0000000000
H	-0.9476595553	-1.5412067451	0.0000000000
H	2.4602462463	0.3038900261	0.9283677743
H	2.4602462463	0.3038900261	-0.9283677743

***Syn*-HCCCHOH$^{\bullet}$**
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −190.907221094641756 a.u.

O	1.6168631211	-0.3421089586	0.0000000000
C	-1.9190488049	-0.2142761027	0.0000000000
C	0.5782209784	0.5436518290	0.0000000000
C	-0.7465927275	0.1415673921	0.0000000000
H	1.2447623329	-1.2309579135	0.0000000000
H	0.8851239334	1.5759957147	0.0000000000
H	-2.9361183386	-0.5229593740	0.0000000000

***Anti*-HCCCHOH$^{\bullet}$**
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −190.903851252468968 a.u.

O	1.5541195855	-0.4168153556	0.0000000000
C	-1.9227672223	-0.2130474378	0.0000000000
C	0.5750095763	0.5378165386	0.0000000000
C	-0.7511894574	0.1391439773	0.0000000000
H	2.4039896776	0.0320224204	0.0000000000
H	0.8632695586	1.5783856379	0.0000000000
H	-2.9404613227	-0.5189794372	0.0000000000

$HCCCH_2O^{\bullet}$
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −190.872893415023299 a.u.

O	-1.5844900732	0.4655799229	-0.0000053500
C	-0.6586634981	-0.5513541414	-0.0000024130
C	1.9151549229	0.2165039442	0.0000002646
C	0.7548289692	-0.1296609834	-0.0000009419
H	-0.8667800199	-1.1924718153	0.8706711026
H	-0.8667218633	-1.1926606681	-0.8705507359
H	2.9320618246	0.5268962728	0.0000013124

$H_2CCCOH^\bullet$
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −190.893298706993789 a.u.

C	0.6847518306	-0.0064076538	0.0000000000
C	2.0697602000	0.0145633971	0.0000000000
C	-0.5374145491	-0.0249130352	0.0000000000
H	2.6034287721	0.9537529255	0.0000000000
H	2.6316190125	-0.9080382396	0.0000000000
O	-1.8563121274	-0.0448830733	0.0000000000
H	-2.1726271189	0.8661384031	0.0000000000

Pathway stationary points

***Trans*-acrolein: 0.0 kJ/mol**
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.597058266929565 a.u.

O	-1.7168987936	0.1028058836	0.0000000000
C	-0.5954923766	-0.3641440633	0.0000000000
C	1.8415089918	-0.1535964694	0.0000000000
C	0.6411788626	0.4449121751	0.0000000000
H	-0.4303938851	-1.4597209578	0.0000000000
H	1.9168895183	-1.2361070939	0.0000000000
H	2.7657242275	0.4091316914	0.0000000000
H	0.5256966386	1.5222471551	0.0000000000

TS: 316.5 kJ/mol
Mechanism: *Trans*-acrolein → Methylketene
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.476506943916974 a.u.
Imaginary frequency: 1943.3721i cm^{-1}

O	1.6740684835	-0.1362235856	0.0782364009
C	-1.6075132735	-0.4027899942	0.0589421010
C	-0.6689416866	0.6943183551	-0.0299004831
C	0.4958115122	-0.0401479000	-0.1259511916
H	-2.3981095341	-0.3930607318	0.8136809989
H	-1.8455875143	-1.0147628289	-0.8038275068
H	-0.8381568278	1.7610510572	0.0092689205
H	-0.2850113473	-1.1844043494	-0.1069051340

Methylketene: 1.9 kJ/mol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.596319319108289 a.u.

O	1.7505728608	-0.2437804384	0.0000000000
C	0.6449556006	0.1421121166	0.0000000000
C	-1.7870706284	-0.3702346871	0.0000000000
C	-0.6024597253	0.5697575979	0.0000000000
H	-0.7339492066	1.6427136573	0.0000000000
H	-2.4088078788	-0.2156482963	0.8840110630
H	-2.4088078788	-0.2156482963	-0.8840110630
H	-1.4589440303	-1.4102343388	0.0000000000

***Cis*-acrolein: 7.6 kJ/mol**
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.594181705482015 a.u.

O	-1.3638095552	0.5184032531	0.0001605524
C	-0.7341134103	-0.5213687413	-0.0002290597
C	1.5013347264	0.5180405286	-0.0001097090
C	0.7527536101	-0.5945634800	0.0001754011
H	-1.2597437482	-1.4931130106	-0.0008630299
H	2.5825996517	0.4763760807	0.0002410826
H	1.0215110559	1.4894965709	-0.0007157334
H	1.2021992838	-1.5812015541	0.0007347679

TS: 31.8 kJ/mol
Mechanism: *Cis*-acrolein → *Trans*-acrolein
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.584965461192525 a.u.
Imaginary frequency: $204.3481i$ cm^{-1}

O	1.6740684835	-0.1362235856	0.0782364009
C	-1.6075132735	-0.4027899942	0.0589421010
C	-0.6689416866	0.6943183551	-0.0299004831
C	0.4958115122	-0.0401479000	-0.1259511916
H	-2.3981095341	-0.3930607318	0.8136809989
H	-1.8455875143	-1.0147628289	-0.8038275068
H	-0.8381568278	1.7610510572	0.0092689205
H	-0.2850113473	-1.1844043494	-0.1069051340

TS: 362.9 kJ/mol
Mechanism: CO + C_2H_4 → *Cis*-acrolein
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.458843972428127 a.u.
Imaginary frequency: 1616.7312i cm^{-1}

O	-1.5737914586	0.3727789289	0.0149742927
C	1.6072786734	0.5408754741	0.0124740836
C	0.7526309204	-0.5936267833	0.1015044251
C	-0.6753659884	-0.3912968412	-0.0490494498
H	1.1756518212	1.5175687943	0.1915040499
H	2.4662050362	0.4981496766	-0.6465191183
H	1.0097643899	-1.5783582107	0.4711737921
H	0.2680191959	-1.0664271446	-1.0269108229

TS: 381.0 kJ/mol
Mechanism: CO + C_2H_4 → *Trans*-acrolein
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.451934524771445 a.u.
Imaginary frequency: 1764.1130i cm^{-1}

O	-1.7016034438	0.0417097296	0.3341521225
C	1.7710390449	-0.3751481825	0.1896202001
C	0.9427411756	0.6187871136	-0.1481670209
C	-0.8931762489	-0.2772566939	-0.4497936765
H	1.4898252853	-1.4118855517	-0.0170361048
H	2.7313983727	-0.2423576184	0.6811938174
H	1.1357303085	1.6730538814	0.0325469409
H	-0.0288920777	-0.2804934489	-1.1379010042

TS: 384.6 kJ/mol
Mechanism: CO + C_2H_4 → Methylketene
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.450578342550045 a.u.
Imaginary frequency: 1350.0972i cm^{-1}

O	-1.7353079440	0.2658379749	0.0893843451
C	1.8266769737	0.4098823981	0.0703803889
C	0.6412672617	-0.5118592726	0.0967502437
C	-0.6908822961	-0.2053301443	-0.2189026676
H	2.7818896347	-0.0357035096	-0.1773597188
H	1.6579918723	1.4398375460	-0.2132919918
H	0.7309833375	-1.4917046688	0.5491614161
H	1.2105594006	-0.4724188720	-0.9606633348

TS: 246.5 kJ/mol
Mechanism: CO + C_2H_4 → Cyclopropanone
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.503158862394201 a.u.
Imaginary frequency: 697.8370i cm^{-1}

O	-1.5573709404	0.2239290842	0.0000001799
C	-0.5110759263	-0.3136565849	-0.0000006615
C	0.9059562817	-0.7017176607	0.0000004233
C	1.2860963784	0.7203293484	0.0000002646
H	1.1336421751	-1.2858768809	0.8913744374
H	1.1336456041	-1.2858693402	-0.8913777236
H	1.2171094402	1.2654388332	-0.9301069576
H	1.2171077891	1.2654393412	0.9301070688

TS: 410.0 kJ/mol
Mechanism: H_2 + H_2CCCO → Methylketene
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.440898765052907 a.u.
Imaginary frequency: 976.1950i cm^{-1}

O	-1.6963068399	-0.2618031043	-0.0132939697
C	-0.6226483295	0.1585112825	0.0287024205
C	0.6415460693	0.6232259794	0.0613961869
C	1.5962960653	-0.4045184512	-0.2513193515
H	1.9529190911	-1.2508208938	0.8788061550
H	0.7774730246	1.6797941867	0.2657396485
H	2.5908880545	0.0209144131	-0.4301482357
H	2.3685044906	-0.7863621864	1.4162151106

TS: 411.1 kJ/mol
Mechanism: H_2 + H_2CCCO → *Cis*-acrolein
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.440466128624536 a.u.
Imaginary frequency: 1978.5584i cm^{-1}

O	-1.7202270751	-0.2509646493	0.0753022400
C	-0.6407085987	0.1204787103	-0.1800049383
C	0.7027548639	0.3104459342	0.2490652258
C	1.8612115096	-0.2800541048	-0.0609108097
H	-0.4965519793	1.5680205267	-0.8176383663
H	2.7799417597	0.1163833600	0.3502600398
H	1.9299427600	-1.1270670737	-0.7326563790
H	0.1880186663	1.6292645964	-0.0921008766

TS: 475.2 kJ/mol
Mechanism: H_2 + H_2CCCO → Methylketene
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.416049271948253 a.u.
Imaginary frequency: 1623.9461i cm^{-1}

O	-1.8126807276	-0.1677027844	0.0126473627
C	1.8150773343	-0.1929311563	0.1204067528
C	0.5577683148	0.5269915617	-0.0497613890
C	-0.6519832650	0.0627191512	0.0038896486
H	2.2619854920	-0.9536869794	-0.9654119862
H	1.4232328318	-0.4928227932	-1.0224863137
H	2.7151727028	0.4159872462	0.0854468907
H	1.8781539289	-1.0322987998	0.8142529231

TS: 485.4 kJ/mol
Mechanism: H_2 + H_2CCCO → 1-Propynol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.412163207422822 a.u.
Imaginary frequency: 1886.5454i cm^{-1}

O	-1.4472572937	0.3485792670	0.0112589762
C	-0.5590581896	-0.5172781270	-0.0575210801
C	0.6728856288	-0.7304786294	0.0581588551
C	1.4820010186	0.4287263418	-0.0258244266
H	-0.5094500874	1.3512082521	0.1586940921
H	2.1477230903	0.6746105402	0.7996666549
H	1.8579723628	0.7612533874	-0.9927763291
H	0.4715220595	1.4327767234	0.1556206676

TS: 384.5 kJ/mol
Mechanism: HCCH + CO + H_2 → *Trans*-acrolein
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.450612453152559 a.u.
Imaginary frequency: 1046.8228i cm^{-1}

O	-1.8528174091	0.0867011784	0.0000000000
C	1.8805434129	-0.2251387516	0.0000000000
C	0.9649747800	0.6262240278	0.0000000000
C	-0.7810905491	-0.3279044178	-0.0000000053
H	1.0608051866	-1.6051812053	0.0000000000
H	2.8952195573	-0.5593084058	-0.0000000106
H	0.6428727378	1.6467066912	0.0000000106
H	0.2258730433	-1.7295796215	0.0000000265

TS: 531.3 kJ/mol
Mechanism: H_2 + Propynal → (*Gauche*-propargyl alcohol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.394709110942983 a.u.
Imaginary frequency: 2289.1868i cm^{-1}

O	-1.5703348729	-0.4612799979	0.0070104926
C	1.9468505023	-0.2044745335	0.0257327942
C	0.7804048306	0.1197429899	-0.0169977447
C	-0.6406938029	0.4726437406	-0.1220199073
H	2.9690679675	-0.4966167030	0.0651274951
H	-0.7294504750	1.3238367547	1.0505385183
H	-0.8036425541	1.3038595674	-0.8229304086
H	-1.3579516001	0.5709645983	0.9448662191

***Gauche*-propargyl alcohol: 119.9 kJ/mol**
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.551400496057255 a.u.

O	-1.5211594418	0.4542134072	-0.0582551231
C	-0.5889423052	-0.6139061414	0.0223238344
C	1.9293070699	0.2545938315	-0.0122292492
C	0.6701359232	-0.1796721811	0.0050479276
H	-1.2789068969	1.0760867514	0.6448604810
H	-0.7521247200	-1.1745048083	0.9548516086
H	-0.7352570470	-1.2944128010	-0.8297384274
H	2.9695055971	0.6017304503	-0.0257218350

TS: 403.8 kJ/mol
Mechanism: CCH_2 + H_2CO → *Cis*-acrolein
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.443273074713943 a.u.
Imaginary frequency: 938.9174i cm^{-1}

O	-1.3962347747	0.5542793751	-0.0000001852
C	-1.0765581848	-0.5865531123	-0.0000003281
C	1.4793207729	0.5960373603	0.0000003704
C	1.3251139557	-0.7181646589	0.0000009737
H	2.4823894408	1.0077020962	-0.0000069111
H	-1.7757613275	-1.4460183363	0.0000070539
H	0.2428918810	-1.2110171865	-0.0000136581
H	0.6362090574	1.2906537110	0.0000043922

TS: 432.7 kJ/mol
Mechanism: HCOH + HCCH → *Cis*-acrolein
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.432262340323888 a.u.
Imaginary frequency: 610.8577i cm^{-1}

O	-1.2052248706	0.5990242378	0.0000000000
C	1.2102691574	-0.6593102638	0.0000000000
C	1.4123204243	0.5629675341	0.0000000000
C	-1.1037742575	-0.6637445575	0.0000000000
H	1.3173531110	-1.7184090655	0.0000000000
H	2.0464421527	1.4233029001	0.0000000000
H	-0.1897083028	0.9147797567	0.0000000000
H	-2.1305674179	-1.0763937641	0.0000000000

TS: 438.3 kJ/mol
Mechanism: H_2O + H_2CCC → *Syn*-allenol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.430117881843188 a.u.
Imaginary frequency: 1391.5918i cm^{-1}

O	-1.8554863674	0.4316811617	0.0644970545
C	1.9652202025	0.3403383792	0.0088388529
C	0.7447384322	-0.1797382700	-0.0065959722
C	-0.3669612389	-0.8255108198	-0.0176779915
H	2.4704461960	0.6095285120	-0.9114078498
H	2.4812767874	0.5185990223	0.9450065781
H	-1.5895588240	-0.7651716962	-0.0094262238
H	-1.8119175800	0.7029287516	-0.8640043477

***Syn*-allenol: 106.3 kJ/mol**
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.556554800095739 a.u.

O	-1.6802514911	0.3266811346	0.0000000000
C	-0.5943899310	-0.5188014378	0.0000000000
C	1.9353894226	0.2064314045	0.0000000000
C	0.6702473732	-0.1562573631	0.0000000000
H	-1.3451603171	1.2295198479	0.0000000000
H	2.4780504731	0.3620005515	-0.9267508626
H	2.4780504731	0.3620005515	0.9267508626
H	-0.8917020246	-1.5583215280	0.0000000000

TS: 312.3 kJ/mol
Mechanism: *Syn*-allenol → *Trans*-acrolein
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.478119410534902 a.u.
Imaginary frequency: 1475.1098i cm^{-1}

O	-1.6151543284	0.1641434694	0.0010000550
C	1.8392342863	-0.0511614544	0.0009196095
C	0.5674077176	0.4211150637	-0.0015890875
C	-0.5284998704	-0.5048388104	-0.0009025965
H	2.6921492167	0.6196316752	0.0011981208
H	2.0757912278	-1.1163367296	0.0031508166
H	-0.9051986480	1.0912444886	0.0003272697
H	-0.5917872203	-1.5935604306	-0.0018293816

TS: 123.3 kJ/mol
Mechanism: *Syn*-allenol → *Anti*-allenol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.550087096572327 a.u.
Imaginary frequency: 304.4499i cm^{-1}

O	-1.6477247277	0.3663035245	-0.0687996783
C	0.6711423760	-0.1570608447	0.0053368002
C	1.9298478415	0.2191814382	-0.0027189974
C	-0.5890537024	-0.5337486843	0.0134021388
H	-0.8589184780	-1.5822700212	0.0859201868
H	2.4518917811	0.4472069734	0.9194723206
H	2.4805175609	0.3118029776	-0.9317757551
H	-1.8786870909	0.6253522242	0.8275373358

***Anti*-allenol: 123.3 kJ/mol**
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.552735925123017 a.u.

O	-1.6212160485	0.4051795787	0.0000000000
C	0.6741904423	-0.1539189765	0.0000000000
C	1.9388284821	0.2043602154	0.0000000000
C	-0.5906765249	-0.5122630243	0.0000000000
H	-0.8664198248	-1.5607898806	0.0000000000
H	2.4808789043	0.3579261989	0.9271014161
H	2.4808789043	0.3579261989	-0.9271014161
H	-2.4451472372	-0.0867236314	0.0000000000

TS: 409.0 kJ/mol
Mechanism: *Anti*-allenol → *Cis*-acrolein
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.441267443520701 a.u.
Imaginary frequency: 533.9838i cm^{-1}

O	-1.6251999594	-0.3718100107	0.0127245009
C	1.9199077654	-0.3646383783	-0.1110127507
C	0.6941635549	0.2324938709	0.0698344844
C	-0.5984021159	0.5465241872	-0.0235787518
H	-1.2489147656	-1.2497389221	-0.1054377837
H	2.4451099884	-0.4043147920	0.8598982603
H	1.5387411813	1.0540218222	-0.1161282119
H	-0.9420615638	1.5669787302	-0.0692285923

TS: 470.3 kJ/mol
Mechanism: HCO + $CHCH_2$ → INTx
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.417940232507192 a.u.
Imaginary frequency: 1369.2804i cm^{-1}

O	-1.4557826567	0.4830549855	-0.0139101966
C	1.6201341986	0.6073969702	0.0969044777
C	0.9938965233	-0.5546679393	-0.0821472377
C	-0.7934627925	-0.5083560028	0.0498196144
H	1.2536911988	-1.5704253304	0.1899201642
H	-1.0609764601	-1.4671384194	0.5147979421
H	0.1056480523	-0.7021005839	-0.9523410965
H	1.1287739984	1.4983034880	-0.3005176483

INTx: 342.1 kJ/mol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.466753279607815 a.u.

O	-1.3706875048	0.5087419635	-0.0603205654
C	1.6270239805	0.5901671812	0.1111377265
C	0.7769914204	-0.5908742467	-0.1076241853
C	-0.7319946428	-0.5018132500	0.1201314113
H	1.1999978641	-1.5380933572	0.2317174620
H	-1.2194537747	-1.4305215340	0.4694050489
H	0.9277469488	-0.5734460745	-1.2146527506
H	0.9370495938	1.4513801559	-0.0013578635

TS: 351.9 kJ/mol
Mechanism: INTx → *Cis*-acrolein
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.463013688426372 a.u.
Imaginary frequency: 815.8445i cm^{-1}

O	-1.3899077516	-0.5015476930	0.0671644623
C	1.6469643900	-0.5304225936	-0.1078106886
C	0.7644411670	0.5596854498	0.0806627209
C	-0.7423169647	0.5041946694	-0.1120688932
H	0.9916796357	-1.4100982662	-0.2305482237
H	1.2314739513	0.0106452365	1.0786827309
H	1.1785535858	1.5632456017	0.1917876095
H	-1.2164144346	1.4443459192	-0.4482395941

TS: 352.8 kJ/mol
Mechanism: INTx → INTy
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.462667760458203 a.u.
Imaginary frequency: 252.2270i cm^{-1}

O	-1.4154593344	0.3920084258	-0.1465843840
C	1.5337613747	0.6152787849	0.2063652997
C	0.8020003795	-0.5903325015	-0.2728133354
C	-0.6255055321	-0.4012688689	0.3016781975
H	1.2131573222	-1.5284445668	0.1001104611
H	-0.8705338393	-1.0458611365	1.1612560357
H	0.6704055549	-0.6127341990	-1.3608148036
H	1.0876099193	1.4463902685	-0.3749963298

INTy: 335.6 kJ/mol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.469249095512339 a.u.

O	1.6825055321	-0.0931066785	-0.1669067536
C	0.6113391132	0.3563963633	0.1685183206
C	-0.6697378602	-0.4522215788	0.1517110850
C	-1.8744081266	0.3070620310	-0.1888895862
H	-1.0088802512	-0.5252707779	1.2214768829
H	0.4828730544	1.4048431604	0.4925738999
H	-0.5101775791	-1.4725268937	-0.2098954306
H	-2.6527987392	-0.4445354697	-0.4190646976

TS: 340.4 kJ/mol
Mechanism: INTy → *Trans*-acrolein
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.467415403983892 a.u.
Imaginary frequency: 589.4461i cm^{-1}

O	1.6950377141	-0.1198715059	-0.1061152099
C	0.6125336409	0.3786369105	0.1020388200
C	-0.6629439864	-0.4291998866	0.1002578740
C	-1.8745909044	0.2552757611	-0.1635048901
H	-1.2666713029	0.0202112741	1.0653715894
H	0.4652659038	1.4615902764	0.2569644662
H	-0.5096623139	-1.5118478908	0.0995452521
H	-2.6697507737	-0.5049860010	-0.1996433146

TS: 353.7 kJ/mol
Mechanism: H_2CO + HCCH → *Gauche*-propargyl alcohol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.462339062057993 a.u.
Imaginary frequency: 345.0615i cm^{-1}

C	-0.3704310541	-0.3036100649	-0.5085237944
C	0.9633506979	0.7640965191	-0.1070440853
C	1.3537694488	-0.3707393316	0.2841175510
O	-1.4330095720	0.0387871419	0.3101116794
H	-0.2944389998	-1.3954258638	-0.4934323048
H	-0.4579516794	0.0083698484	-1.5460988724
H	1.7293990503	-1.2959563740	0.6710318150
H	-1.4130000519	0.9988286775	0.3933242674

TS: 129.2 kJ/mol
Mechanism: *Gauche*-propargyl alcohol (+) → *Gauche*-propargyl alcohol (−)
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.547852228525102 a.u.
Imaginary frequency: 255.2360 cm^{-1}

C	0.7785710356	-0.1437445331	0.0017516349
C	1.9253857554	0.2452317282	0.0098945139
C	-0.6143205825	-0.6161850750	-0.0081384974
H	2.9346519673	0.5787580563	0.0172339642
H	-0.7649201729	-1.2468166942	-0.8890103804
H	-0.7799539240	-1.2394269509	0.8752905712
O	-1.5174648268	0.4855271481	-0.0422790449
H	-2.1874501621	0.3302369199	0.6257199600

PRC: 423.6 kJ/mol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.435701467252301 a.u.

O	-1.5985530909	0.4889882425	0.0568078339
C	-0.4459259941	-0.9138625867	-0.1001555152
C	0.7904290776	-0.2194127998	0.0237907931
C	1.8590697018	0.3773508775	-0.0075908889
H	-1.9197088847	0.4680478786	-0.8525635673
H	-0.7368517121	-1.3560748095	0.8557525058
H	-1.0116241463	1.2578517755	0.1097123187
H	2.8008187388	0.8702405322	-0.0148377332

TS: 452.7 kJ/mol
Mechanism: PRC → *Gauche*-propargyl alcohol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.424626304130896 a.u.
Imaginary frequency: 1181.6454 cm^{-1}

O	-1.7190086233	0.5288841642	0.0025667584
C	-0.3689980898	-0.8629610535	-0.0878161707
C	0.8496406991	-0.1635522620	0.0221016223
C	1.9415712236	0.3807172121	0.0078817194
H	-2.4007729361	0.0899848290	0.5294698523
H	-0.6301633608	-1.4033983795	0.8225280011
H	-1.4213167762	-0.2457326209	-0.7196736131
H	2.8932822923	0.8547542553	0.0155450103

TS: 384.7 kJ/mol
Mechanism: CCH_2 + H_2CO → 2-Methylenoxirane
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.450518773168881 a.u.
Imaginary frequency: 323.1556i cm^{-1}

O	-1.0692084314	0.7103707406	-0.0002485281
C	-1.2492085066	-0.5106564633	0.0003531517
C	0.8486978640	-0.6800653152	-0.0004616648
C	1.7080185908	0.3119929416	0.0002425854
H	-1.4234926896	-1.0676699173	0.9308742541
H	-1.4245870493	-1.0684286411	-0.9295011926
H	2.7372531157	-0.0478296857	0.0001884612
H	1.5116672138	1.3727027652	0.0007863997

2-Methylenoxirane: 129.9 kJ/mol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.547589016019771 a.u.

O	-0.7538214739	0.7782944823	-0.0000022490
C	-1.0206416283	-0.6838482816	-0.0000018997
C	0.2909993159	-0.0908945800	0.0000105359
C	1.6158353531	-0.0738965971	-0.0000039000
H	-1.4509943910	-1.0516345343	0.9236625366
H	-1.4509770181	-1.0516401754	-0.9236762105
H	2.1587442754	-1.0067035758	-0.0000036196
H	2.1551722814	0.8624847887	-0.0000034608

TS: 545.8 kJ/mol
Mechanism: 2-Methylenoxirane → INTz
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.389157356426836 a.u.
Imaginary frequency: 1909.8842i cm^{-1}

O	-0.8045115425	-0.8086298909	-0.0489266436
C	-0.8755405598	0.9025769716	-0.1174928648
C	0.1676406113	-0.0287312766	0.2456851802
C	1.5214159340	0.0311506326	-0.0481216698
H	0.4970137658	0.8469343808	-0.8642601096
H	-1.5483343128	1.2077141733	0.6827195571
H	2.0781939095	0.8552803209	0.3795916997
H	2.0549131215	-0.8520219914	-0.3749373371

INTz: 281.5 kJ/mol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.489833963797139 a.u.

O	-0.7006439547	0.9361988514	0.0042425569
C	-1.0149666627	-0.9240283356	0.0931259617
C	0.0601260927	-0.0883761196	-0.0313729347
C	1.5426962150	-0.1103659214	-0.0024888159
H	1.8964230696	0.4099905567	0.8890955092
H	-1.6066844391	-1.1908019594	-0.7774841638
H	1.9149281281	-1.1333978275	-0.0068035313
H	1.9155648289	0.4246885712	-0.8777890393

TS: 291.1 kJ/mol
Mechanism: INTz → 2-Methyloxirene
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.486198715320654 a.u.
Imaginary frequency: 192.2925i cm^{-1}

O	1.6223991000	1.5563241600	0.0043999800
C	-3.0418859700	-0.0341674200	0.0052190900
C	-0.2755824600	-0.2949163600	0.0010858300
C	1.8118568900	-1.5286976700	-0.0397358200
H	-3.9452213400	-1.8828752800	0.0102726400
H	-3.6377404000	1.0260075100	-1.6612275800
H	3.3804894600	-2.7473450400	0.2995657800
H	-3.6191200700	1.0245044700	1.6796142700

2-Methyloxirene: 291.0 kJ/mol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.486244400175110 a.u.

C	0.1608120817	-0.1671762160	-0.0000939819
C	-0.9558817579	-0.7910608411	-0.0003556336
C	1.6204836037	-0.0049541309	0.0000802815
O	-0.8826536281	0.8060843049	0.0000611411
H	-1.7796626603	-1.4684883347	0.0029282817
H	2.1137302202	-0.9758516003	-0.0001242244
H	1.9229508680	0.5596008979	0.8843829000
H	1.9232728935	0.5601486493	-0.8837597250

TS: 464.8 kJ/mol
Mechanism: 2-Methyleneoxirane → Methoxyethene
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.420042084187429 a.u.
Imaginary frequency: 565.5885i cm^{-1}

O	-0.6387932787	0.7221065743	0.0108019946
C	-1.4270300595	-0.5241957278	0.0153234597
C	0.3572151328	-0.1677286082	0.0900043663
C	1.6788953897	-0.0920140756	-0.0534406102
H	-0.1406095601	-1.1814073276	0.4409029801
H	-1.4064497425	-0.8342413448	-1.0552674102
H	2.2858530211	-0.9761545754	0.0624512975
H	2.1471024130	0.8656682344	-0.2373345356

Methoxyethene: 298.1 kJ/mol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.483517640924930 a.u.

O	-0.5837199396	0.4140180612	0.0000000000
C	-1.7983030400	-0.0790539215	0.0000000000
C	0.5480855988	-0.4204970376	0.0000000000
C	1.7633425005	0.1168032886	0.0000000000
H	0.3068992613	-1.4781288911	0.0000000000
H	-1.6806080084	-1.1992495598	0.0000000000
H	2.6315415939	-0.5257601134	0.0000000000
H	1.8965340540	1.1896823950	0.0000000000

TS: 267.1 kJ/mol
Mechanism: 2-Methyleneoxirane → Cyclopropanone
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.495325410782812 a.u.
Imaginary frequency: 688.0266i cm^{-1}

O	0.5663445687	-1.1002595152	-0.0392097640
C	-0.1118846178	-0.0011715667	0.0168984658
C	0.9243647389	1.0015682969	0.0242056098
C	-1.4666999537	0.2032522717	0.0218647625
H	1.0556115342	1.7207777898	-0.7783342024
H	1.7448253133	0.8358196001	0.7100616058
H	-2.1564925786	-0.6247704626	0.1147513773
H	-1.8425601336	1.1984475494	-0.1739505209

Cyclopropanone: 84.7 kJ/mol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.563771793756217 a.u.

O	-1.5031326802	-0.0000188123	-0.0000007461
C	-0.3017061698	-0.0000043340	0.0000009843
C	0.9434699902	0.7893417982	0.0000002752
C	0.9435347827	-0.7893215784	0.0000002699
H	1.2449427135	1.2830482645	-0.9157774939
H	1.2449358554	1.2830593031	0.9157743347
H	1.2450210635	-1.2830046338	0.9157813199
H	1.2450279375	-1.2829935846	-0.9157844843

1-Propynol: 126.0 kJ/mol
CCSD(T)/cc-pVTZ optimized geometry (Å)
E: −191.549059777398725 a.u.

O	1.9130740498	-0.0639703749	0.0000000000
C	-2.0872858943	0.0000713701	0.0000000000
C	0.5893549841	0.0108397356	0.0000000000
C	-0.6186187347	0.0059799463	0.0000000000
H	2.2650424855	0.8326905274	0.0000000000
H	-2.4620933819	-1.0248134183	0.0000000000
H	-2.4817143059	0.5031301552	0.8843334960
H	-2.4817143059	0.5031301552	-0.8843334960

Barrierless pathway energies

Table 1: UCCSD(T)/cc-pVTZ energies as a function of bond distance (r(HO$^{\bullet}$(O−C)H$_2$CCCH$^{\bullet}$) for the formation of *gauche*-propargyl alcohol.

Bond distance (Å)	E(Hartree)
2.56	-191.428
2.46	-191.432
2.36	-191.438
2.26	-191.447
2.16	-191.458
2.05	-191.472
1.96	-191.487
1.86	-191.503
1.76	-191.518
1.66	-191.532
1.56	-191.544
1.42	-191.551

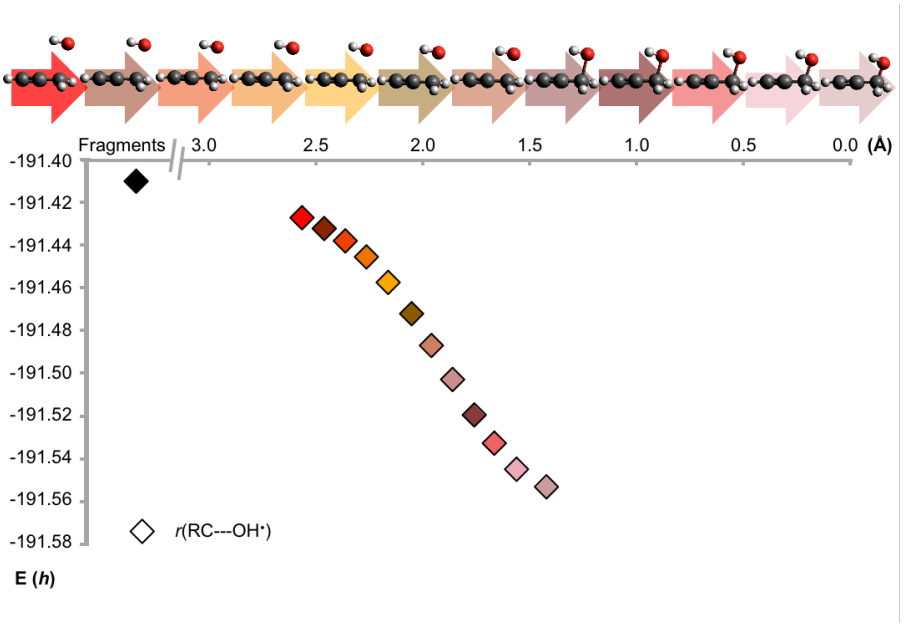

Figure 2: UCCSD(T)/cc-pVTZ one-dimensional potential energy curve as a function of C−OH$^{\bullet}$ bond formation (Å) for the reaction of OH$^{\bullet}$ + H$_2$CCCH$^{\bullet}$ → *gauche*-propargyl alcohol (E_{h}).

Table 2: UCCSD(T)/cc-pVTZ energies as a function of bond distance (r(HO$^{\bullet}$(O−C)H$_2$CCCH$^{\bullet}$) for the formation of *syn*-allenol.

Bond distance (Å)	E(Hartree)
2.50	-191.424
2.40	-191.427
2.30	-191.431
2.20	-191.439
2.10	-191.451
2.00	-191.465
1.90	-191.482
1.80	-191.501
1.70	-191.519
1.60	-191.535
1.50	-191.548
1.37	-191.557

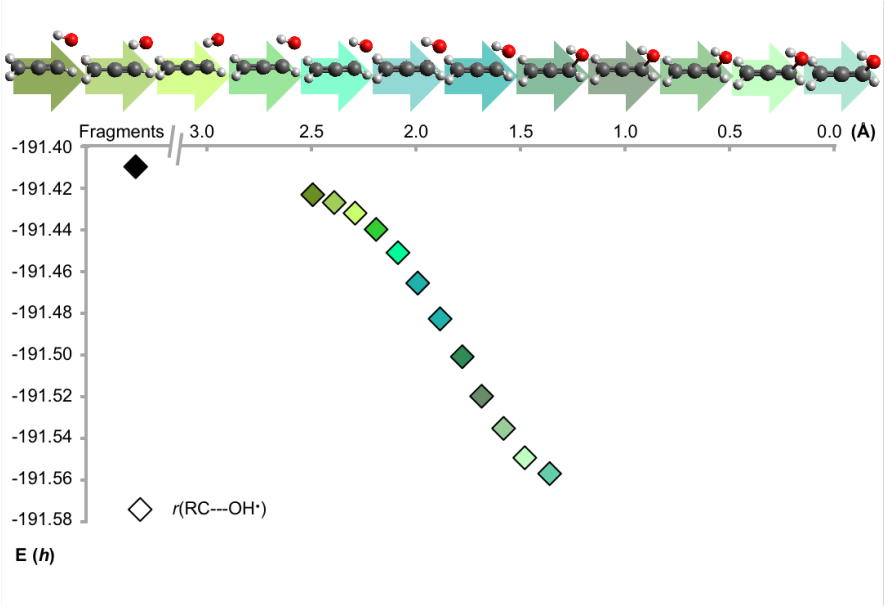

Figure 3: UCCSD(T)/cc-pVTZ one-dimensional potential energy curve as a function of C−OH$^{\bullet}$ bond formation (Å) for the reaction of OH$^{\bullet}$ + H$_2$CCCH$^{\bullet}$ → *syn*-allenol (E_{h}).

DFT, RASSCF and CCSD(T) discrepancies

Considerable attention has been paid to the direct formation of *trans*-acrolein from acetylene and formaldehyde. [Chin & Lee(2011), Martìnez-Nùñez(2015), Pham & Tue Trang(2020)] report a saddle point which corresponds to the transfer of a H atom from H_2CO to the HCCH moiety, Figure 4. After hydrogen migration, at B3LYP/6-311G(d,p) [Chin & Lee(2011), Martìnez-Nùñez(2015)] and M06-2X/aug-cc-pVTZ [Pham & Tue Trang(2020)] optimization levels, subsequent rearrangement directly produces *trans*-acrolein on the C_3H_4O surface. Unfortunately, large discrepancies arise when attempting to locate this DFT transition state with RASSCF and CCSD(T) methods. Initiating a RASSCF/cc-pVDZ TRIM [Helgaker(1991)] walk, from the M06-2X/aug-cc-pVTZ equilibrium geometry, results in the structure degenerating into the interaction between CO and ethene (C_2H_4), for the formation of *trans*-acrolein (orange path in Figure 1). Applying the ALTRUISM [Field-Theodore & Taylor(2020)] procedure to investigate the energy landscape, we search for a stationary point with a Hessian index of two. After 7 steps we locate a converged geometry, 2.31 kJ/mol below the DFT equilibrium structure, Figure 4. The two imaginary frequencies correspond to hydrogen transfer from H_2CO to the HCCH moiety (1427i cm^{-1}), and a combined H migration and in-plane bending (scissoring), in which H_2CO and HCCH move back and forth, but in opposite direction (449i cm^{-1}). Proceeding downhill with a target Hessian index of one, we arrive at the CO and C_2H_4 transition state after 20 steps, in accordance with the TRIM calculation. Similar issues occur using a higher-level treatment of electron correlation: investigating the CCSD(T) PES with a step-size of 0.005 a_0, we converge to the first-order stationary point corresponding to CO and C_2H_4 (1764i cm^{-1}; as per TRIM results), not the saddle point for H_2CO and HCCH, Figure 4. Conversely, using a step-size of 0.300 a_0 (which is the default in the CFOUR program), we locate a first order-stationary point with an imaginary frequency of 1412i cm^{-1}, Figure 4. The $\mathcal{T}_1$ diagnostic for this saddle point geometry is 0.038, which indicates this interaction possesses large nondynamical correlation effects, and single-reference treatments should be regarded with caution.

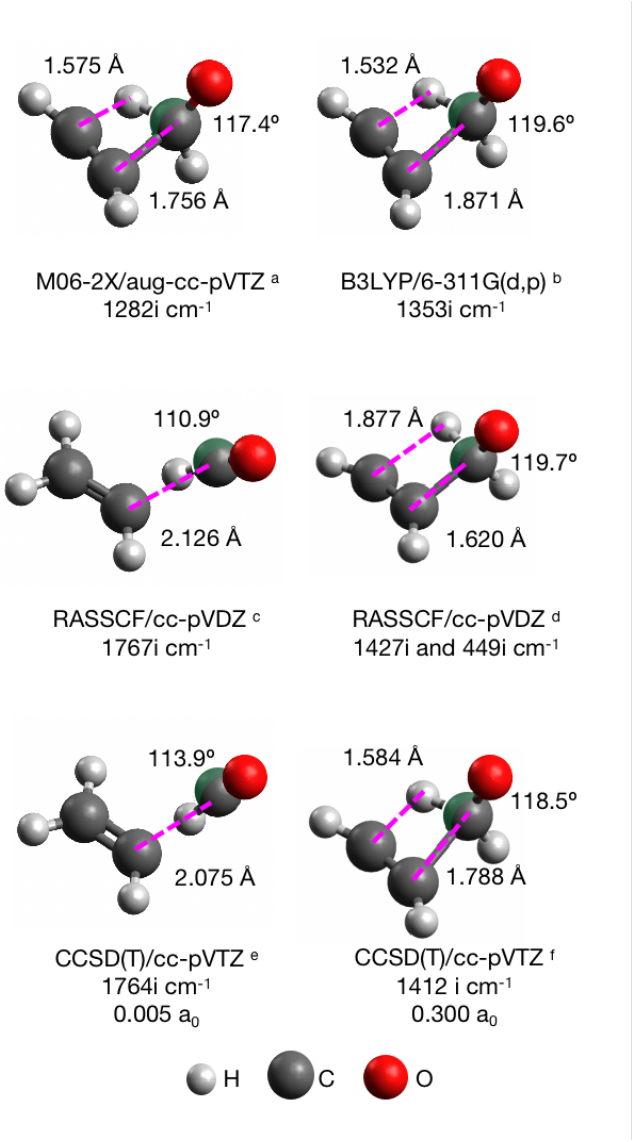

Figure 4: Comparison of DFT, RASSCF and CCSD(T) optimized stationary points.
[a] Ref. Pham & Tue Trang(2020)
[b] Ref. Chin & Lee(2011)
[c] Results from this work explored with TRIM [Helgaker(1991)]
[d] Results from this work explored with ALTRUISM [Field-Theodore & Taylor(2020)]
[e] Results from this work (step-size of 0.005 a_0)
[f] Results from this work (default step-size of 0.300 a_0)

H_2CO + HCCH: Ref. Pham & Tue Trang(2020)
M06-2X/aug-cc-pVTZ optimized geometry (Å)
Imaginary frequency: 1282i cm^{-1}

O	1.5048877584	-0.0325288811	-0.3789396566
C	0.5799125996	-0.1098916284	0.4147743967
C	-0.9141125367	0.7116909980	-0.0040832833
C	-1.2393516570	-0.4851765998	-0.1296606388
H	-1.7206939629	-1.3687952981	-0.5008909798
H	-1.0680330279	1.7565261723	-0.1733233425
H	0.5426973379	0.1566505202	1.4750136520
H	-0.0171775113	-1.1894102831	0.5710428521

H_2CO + HCCH: Ref. Chin & Lee(2011)
B3LYP/6-311G(d,p) optimized geometry (Å)
Imaginary frequency: 1353i cm^{-1}

O	-1.6426730000	-1.3561600000	-0.4497350000
C	-0.0366900000	0.0541750000	1.5174930000
C	-1.2614400000	0.0461500000	1.8019880000
C	-1.3181660000	-0.2689830000	-0.0409100000
H	-0.0873200000	0.0898860000	-0.0132630000
H	-1.7110330000	0.7301160000	-0.2314940000
H	-1.9993030000	-0.0130210000	2.5787010000
H	1.0172550000	-0.0986470000	1.6684710000

H_2CO + HCCH: Results from this work (default step-size of 0.300 a_0)
CCSD(T)/cc-PVTZ optimized geometry (Å)
Imaginary frequency: 1412i cm^{-1}

O	-1.5066955988	-0.0095503211	0.3004035365
C	1.3444070968	-0.5184115136	0.1328529118
C	0.9849413890	0.6904264840	0.0268104214
C	-0.5453656701	-0.1011291643	-0.4492104491
H	0.0834914908	-1.1849559373	-0.5572854776
H	-0.4419548469	0.1691228633	-1.5028491470
H	1.1940843242	1.7210154804	0.2348689771
H	1.8351538165	-1.3976370257	0.5052314334

H_2CO + $C{=}CH_2$: Ref. Pham & Tue Trang(2020)
M06-2X/aug-cc-pVTZ optimized geometry (Å)
Imaginary frequency: 577i cm^{-1}

O	-0.8899589225	-2.0697691166	-0.4189143724
C	-0.3194840591	-1.0526021964	-0.3728224056
C	1.5934151494	-0.6349441348	-1.3298419988
C	2.0879395766	-0.2796328513	-0.1615101633
H	-0.3644991667	-0.2608876275	0.3991247503
H	1.5645053516	-0.1222824711	0.7820246701
H	3.1612401815	-0.1226014137	-0.1272231667
H	0.3873860491	-0.7504579788	-1.4788822635

H_2CO + $C{=}CH_2$: Ref. Chin & Lee(2011)
B3LYP/6-311G(d,p) optimized geometry (Å)
Imaginary frequency: 644i

O	-3.8142310000	0.2983790000	0.3593270000
C	-2.6687170000	0.0635890000	0.4229950000
C	-0.0460210000	-0.2054250000	1.1498140000
C	-0.9299800000	0.3626080000	1.9401490000
H	0.9818130000	-0.2830740000	1.4947800000
H	-0.2345610000	-0.6221260000	0.1519900000
H	-2.0172410000	-0.4367680000	-0.3362390000
H	-2.0682350000	0.5025020000	1.6750870000

H_2CO + $C{=}CH_2$: Results from this work
CCSD(T)/cc-PVTZ optimized geometry (Å)
Imaginary frequencies: 615i and 22i cm^{-1}

O	-1.9822951542	0.0710531902	-0.0000237283
C	-0.8465202837	-0.2522731618	0.0000333223
C	1.2709973639	0.7666151594	0.0000088743
C	1.8824991091	-0.4145535568	-0.0000161717
H	-0.4204463318	-1.2788412524	0.0000819590
H	0.0419434884	0.7734713757	0.0000427046
H	2.9677048175	-0.4139496650	-0.0000438318
H	1.4024904171	-1.3965100051	-0.0000140761

Rotational spectra

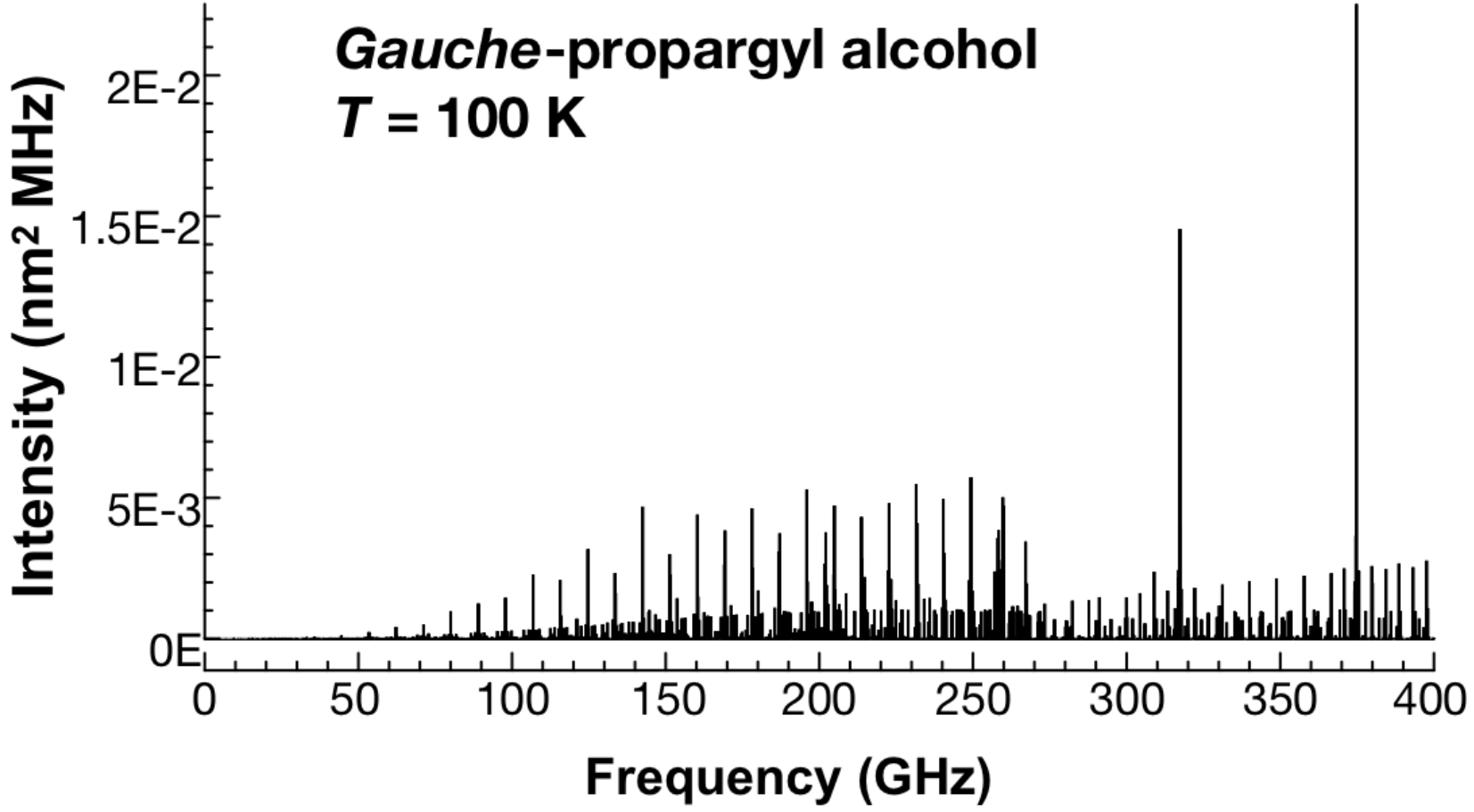

Figure 5: Simulated rotational spectra of *gauche*-propargyl alcohol: 0–400 GHz. Intensity in nm^2 MHz.

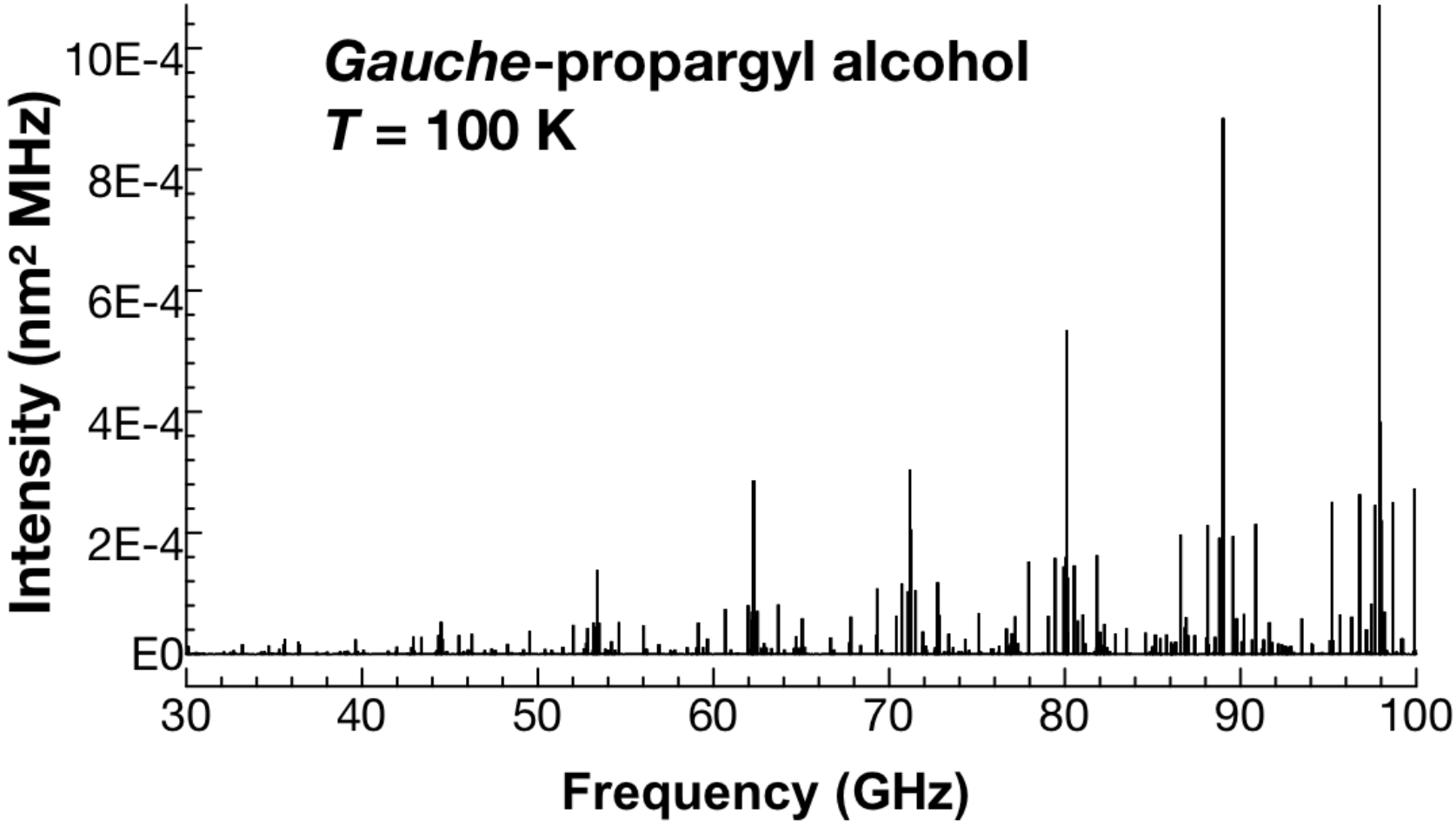

Figure 6: Simulated rotational spectra of *gauche*-propargyl alcohol: 30–100GHz. Intensity in nm^2 MHz.

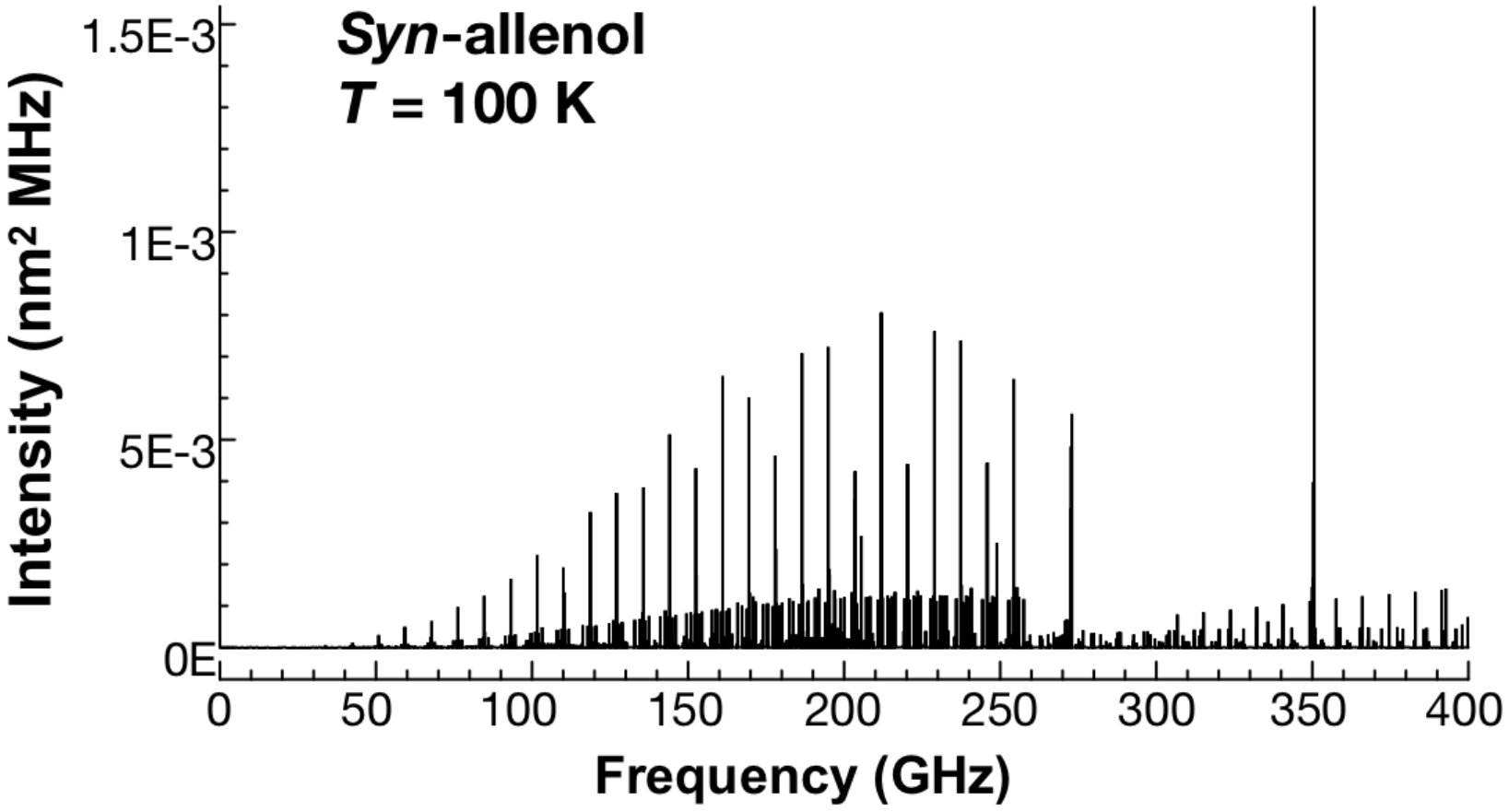

Figure 7: Simulated rotational spectra of *syn*-allenol: 0–400 GHz. Intensity in nm^2 MHz.

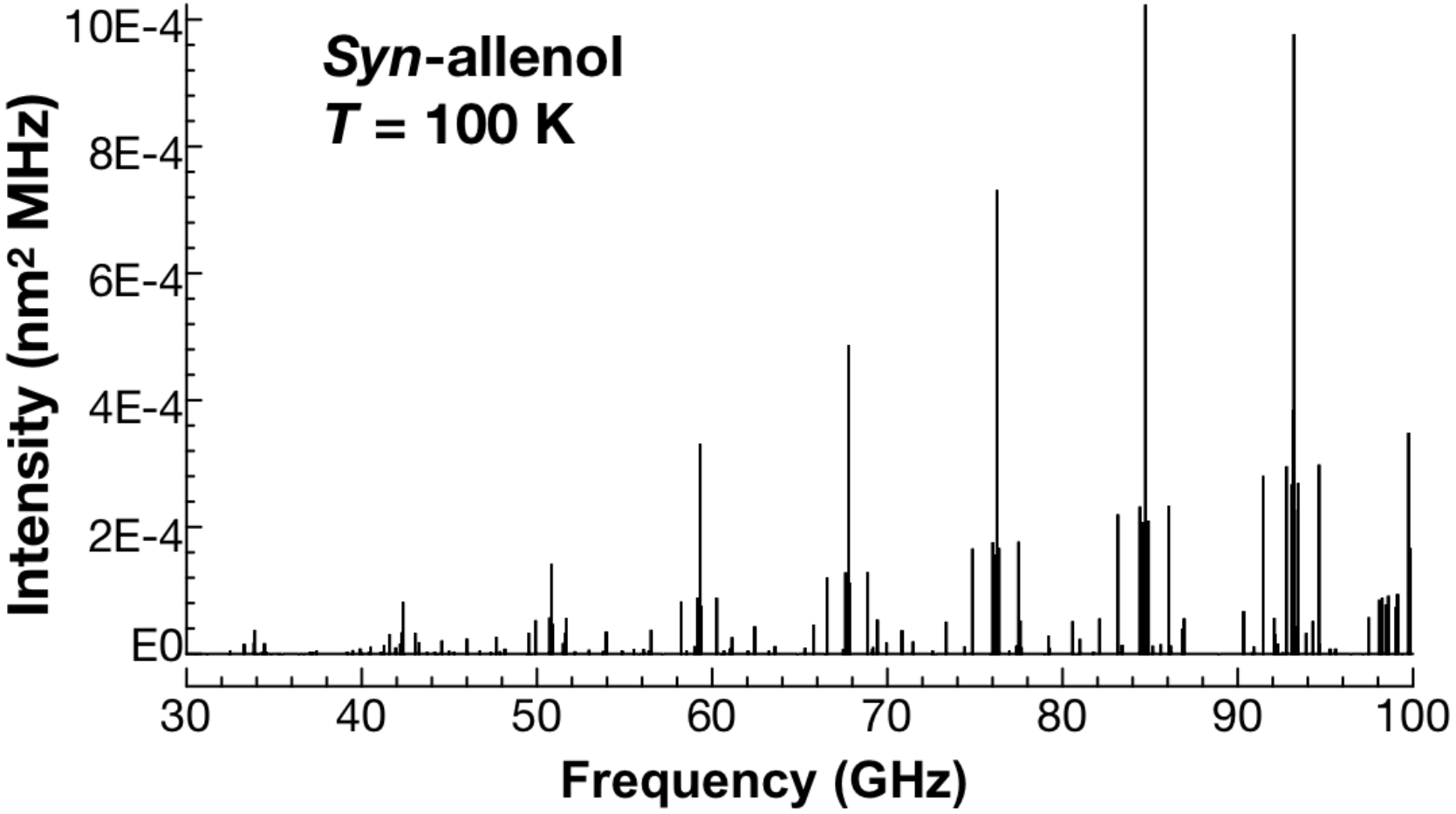

Figure 8: Simulated rotational spectra of *syn*-allenol: 30–100GHz. Intensity in nm^2 MHz.

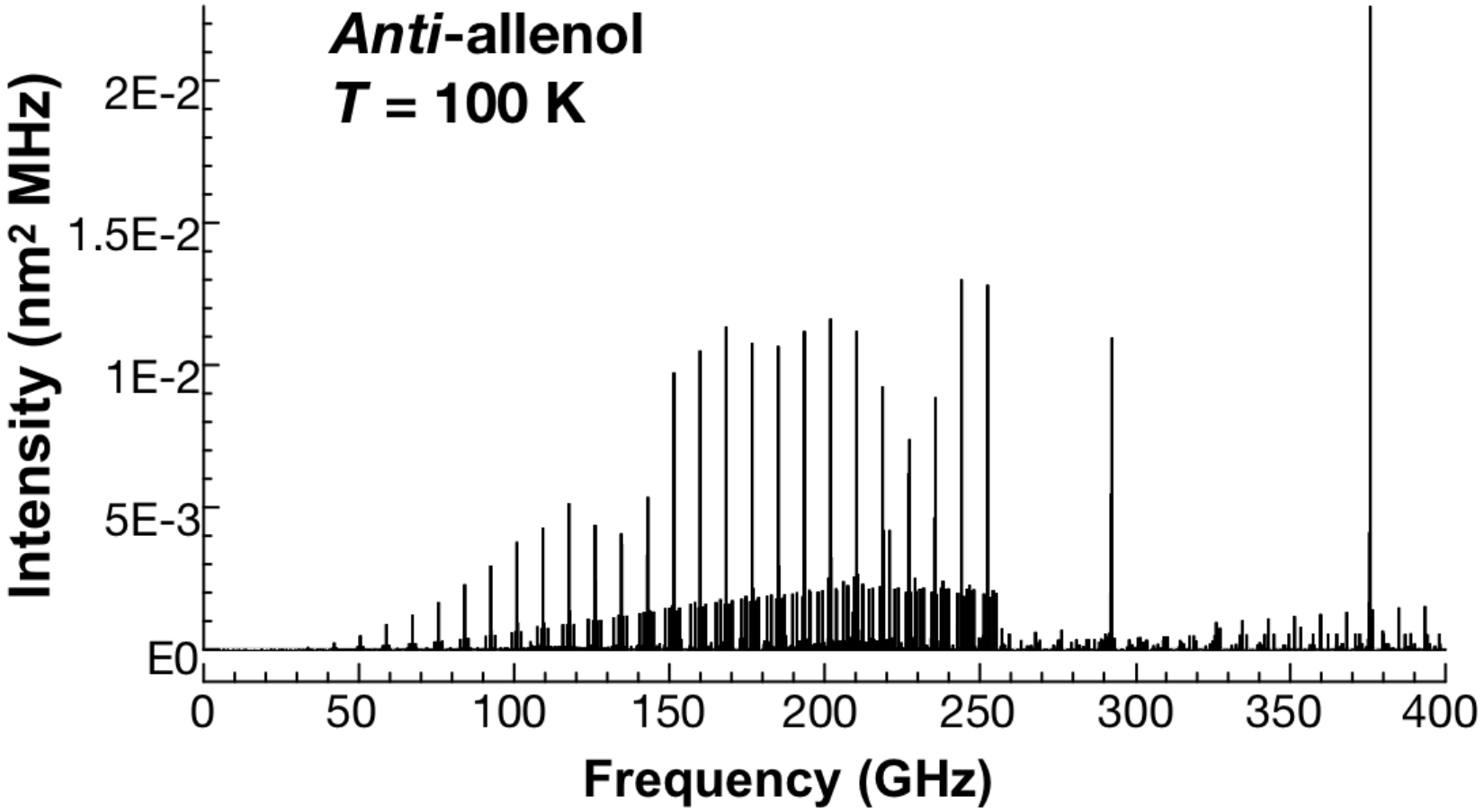

Figure 9: Simulated rotational spectra of *anti*-allenol: 0–400 GHz. Intensity in nm^2 MHz.

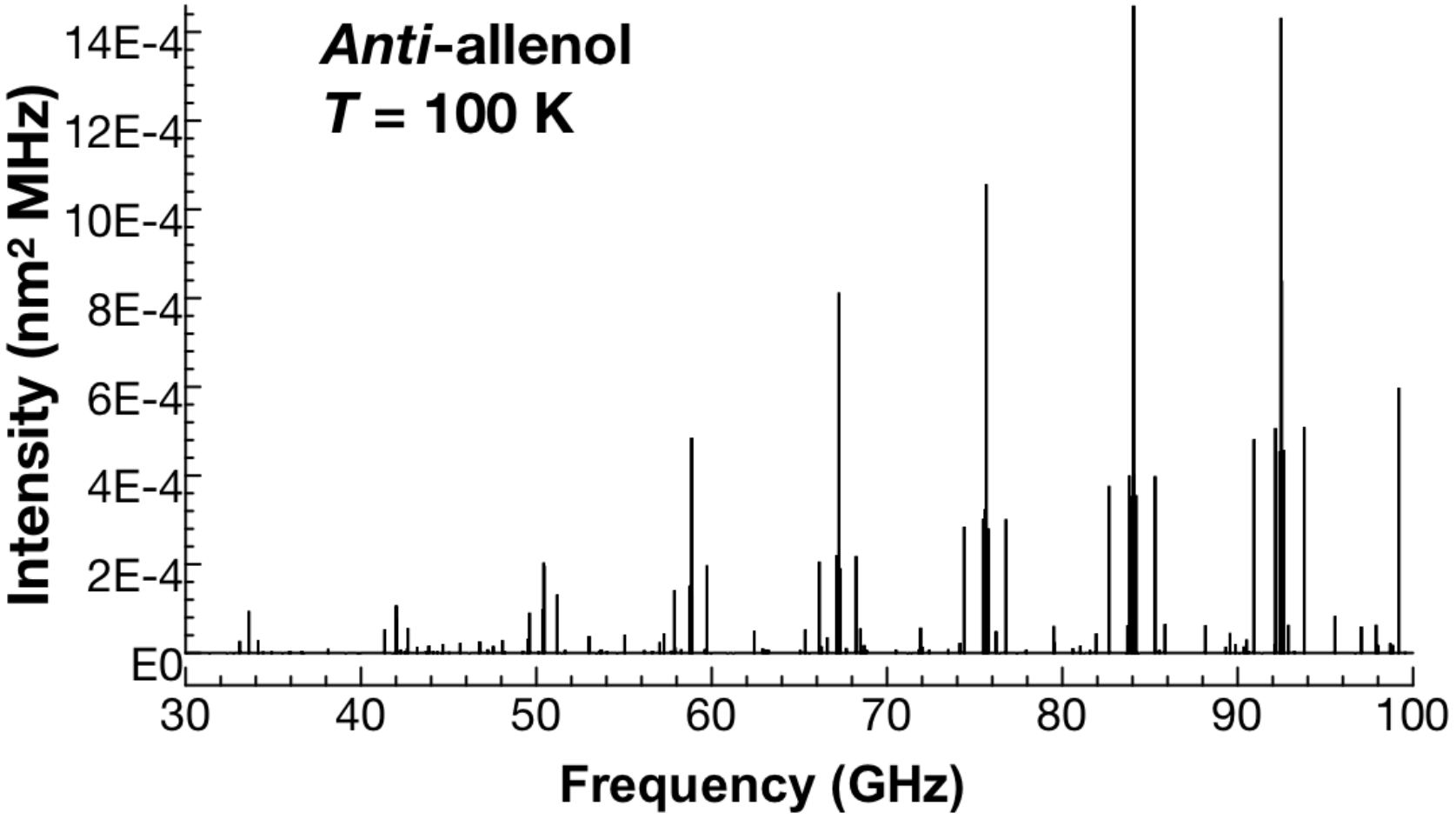

Figure 10: Simulated rotational spectra of *anti*-allenol: 30–100GHz. Intensity in nm^2 MHz.

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