

Supporting Information for

**On the Formation of 1H-Phenalene (C₁₃H₁₀) in the Taurus Molecular Cloud
via Methylidyne Addition-Cyclization-Aromatization (MACA)**

Alexander M. Mebel,^{1*} Ralf I. Kaiser,^{2*}

¹ *Department of Chemistry and Biochemistry, Florida International University, Miami, FL 33199*

mebela@fiu.edu

² *Department of Chemistry, University of Hawai`i at Mānoa, Honolulu, HI 96822*

ralfk@hawaii.edu

Table S1. Optimized Cartesian coordinates (Å) and vibrational frequencies for all the reactants, intermediates, and transition states involved in the CH + 1-vinylnaphthalene and 1-propynyl + naphthalene reactions calculated at the B3LYP/6-311G(d,p) level that are not covered in previous studies.

CH + 1-vinylnaphthalene

CH

C	0.000000	0.000000	0.161152
H	0.000000	0.000000	-0.966913

Frequencies:
2803.5542

1-Vinylnaphthalene

C	0.0119035652	-0.4303226854	0.3592533463
C	0.0014260039	-1.8653364434	0.3510385849
C	1.234017192	-2.57000817	0.3316549903
C	2.4330495393	-1.9034603194	0.3525033107
C	2.4489039305	-0.4928528947	0.4136415783
C	1.2740548485	0.2208011902	0.4167088303
C	-1.2443489936	0.2705532582	0.3624829703
C	-2.4159439384	-0.4639368929	0.4472046942
C	-2.4185710375	-1.8721291495	0.4495336229
C	-1.2338494667	-2.5607012945	0.3833604099
C	-1.381485132	1.7384312083	0.2680260197
C	-0.6727121443	2.5855494538	-0.4826427783
H	1.2084272264	-3.65461952	0.312130845
H	3.3664808943	-2.4548253713	0.3408876337
H	3.3965287854	0.031263089	0.4690843806
H	1.3067980026	1.2983985854	0.491799371
H	-3.3629637154	0.0646650071	0.4795905206
H	-3.3617704674	-2.4047789461	0.4940706243
H	-1.2236621329	-3.6454311839	0.3706318247
H	-2.2167898336	2.1451202768	0.8350030134
H	0.1375641094	2.2616527439	-1.1243550275
H	-0.9132262357	3.6423260582	-0.4973607652

Frequencies:

100.9129	122.5122	171.0253
213.1188	232.1434	353.4085
417.3442	443.9885	478.5346
488.4911	512.8239	564.7145

586.7194	631.8575	695.4445
719.8137	750.6625	793.7143
806.4728	822.6090	871.1344
883.2408	921.8342	949.2776
972.3138	985.6143	1000.7191
1010.3603	1032.0580	1049.3999
1095.9746	1108.5484	1168.7435
1186.1794	1195.9127	1237.3162
1246.7666	1288.3416	1331.9411
1370.0838	1385.9038	1423.6974
1454.9660	1473.2173	1493.4065
1546.9013	1613.1281	1630.4507
1658.9140	1686.9332	3120.9576
3143.1353	3156.6926	3158.0914
3165.0145	3168.7468	3183.4556
3184.4781	3212.6964	3225.8213

il

C	-0.0076784381	-0.3090762299	0.3014322825
C	0.0102902987	-1.7413885993	0.2931577152
C	1.2584773718	-2.4164738733	0.299623519
C	2.4416140773	-1.7192526354	0.3074675241
C	2.4275844066	-0.3069598003	0.3038431482
C	1.2353547674	0.3778660764	0.2991194685
C	-1.2684907268	0.372368384	0.3051726806
C	-2.4326330397	-0.3658726318	0.2871488846
C	-2.4115698965	-1.7784777201	0.2653121606
C	-1.2178834579	-2.452950491	0.2732977609
C	-1.3171198156	1.8703674123	0.3385821794
C	-1.3334531055	2.6648429329	-0.9921193827
C	-2.4989916782	2.6221546022	-0.1067548081
H	1.2611479966	-3.5016704046	0.2967034517
H	3.3877696968	-2.2487154	0.3120366912
H	3.3646995694	0.2386468508	0.3008295938
H	1.2400409497	1.4606076668	0.2824681837
H	-3.3828155131	0.1560713265	0.2959323703
H	-3.3483105068	-2.3245617608	0.2512531889
H	-1.1943560876	-3.5376512772	0.2644778495
H	-0.7388502526	2.3169990071	1.1476710199
H	-1.3417083961	2.059826261	-1.8954883672
H	-0.7526289394	3.5812185453	-1.077479848
H	-3.0806482804	3.4015187587	0.3647537333

Frequencies:

55.1889	96.6569	168.2013
174.9986	192.4717	301.6457
332.8467	423.6756	450.6731
480.0348	493.5029	535.2580
555.2696	598.3136	617.4495
660.3744	697.3320	745.8923
788.8980	794.8236	806.6405
813.1573	835.6228	865.3022
880.8908	924.0034	952.5531
965.0376	985.0301	995.9515
1022.9515	1041.7264	1047.8584
1058.8205	1077.2540	1099.8848
1122.7129	1168.3260	1180.7278
1187.5262	1228.3858	1234.1824
1260.7669	1285.1264	1357.5462
1380.6220	1394.7330	1426.5546
1463.0574	1471.0427	1493.6010
1546.3287	1617.4873	1637.0948
1662.7497	3074.8320	3076.6648
3149.2533	3155.9429	3158.3396
3166.7060	3170.5573	3181.5297
3183.4241	3193.6117	3205.0163

TS i1→i2

C	0.0596511791	-0.2755463218	0.6967417444
C	0.0245821754	-1.7058604847	0.6290660897
C	1.2414877681	-2.4332914276	0.6883692502
C	2.450110608	-1.7898835937	0.795614187
C	2.4909038343	-0.3807452939	0.8372457072
C	1.3271871655	0.3527781864	0.786003118
C	-1.1871060209	0.456773897	0.6603723723
C	-2.3768471293	-0.2563060134	0.5106125417
C	-2.3931306497	-1.658205447	0.4259348875
C	-1.2211128577	-2.3738586965	0.4917624583
C	-1.2313515935	1.895622044	0.7806498782
C	-1.9772483129	2.7954504843	-0.7884998021
C	-2.4163499322	2.7256794794	0.5368418115
H	1.198813778	-3.5166145028	0.6427490416
H	3.3717073959	-2.3592816876	0.838741519
H	3.4460754117	0.1281621203	0.903156984
H	1.3893203227	1.4333481552	0.7957863767
H	-3.3086602781	0.2973165648	0.4931086017
H	-3.3415970271	-2.1740521333	0.324199893
H	-1.2300985342	-3.4572095308	0.437671791

H	-0.3594737771	2.4094534549	1.169043833
H	-1.9312785352	1.9125556732	-1.4144423477
H	-1.744930969	3.7387014577	-1.2870191712
H	-2.6276530219	3.6164916159	1.1167872353

Frequencies:

777.0036i	76.5431	83.6946
173.0170	184.1928	202.3437
281.9170	339.5649	424.7076
446.3728	486.9017	491.9841
537.2732	563.8406	597.4070
654.8585	694.9377	741.3358
755.7118	773.3047	788.6746
802.8574	805.6194	816.2524
871.4870	877.8591	915.3537
937.6551	959.1178	983.4397
992.6682	1005.8447	1015.9333
1052.8741	1094.4197	1124.1323
1167.3255	1186.0356	1195.8952
1216.5973	1230.4168	1267.9651
1286.1097	1296.9708	1353.8482
1377.9887	1401.3394	1430.3200
1470.1978	1485.9881	1504.8333
1543.6045	1596.3759	1618.3111
1656.6060	3064.6381	3154.8163
3157.0309	3159.4885	3167.1774
3168.8651	3172.2298	3182.7240
3183.7226	3189.0396	3195.9864

1-propynyl + naphthalene

1-Propynyl

H	0.0167055274	1.0259043397	-1.4148818212
C	0.0002597056	-0.0306093734	-1.1238450291
C	0.0021694446	-0.1421862538	0.3258618251
H	0.8839501273	-0.5066354633	-1.5584394559
H	-0.8997971116	-0.4784495517	-1.5546481021
C	0.0067123067	0.131976018	1.5442789515

Frequencies:

92.7334	354.8879	862.0707
889.8638	981.0865	1392.2242
1453.6248	1455.5838	1545.6683
3015.0591	3071.5197	3083.7105

Naphthalene

C	0.000000	0.000000	0.715661
C	0.000000	0.000000	-0.715661
C	0.000000	1.243465	1.400275
C	0.000000	-1.243465	1.400275
C	0.000000	1.243465	-1.400275
C	0.000000	-1.243465	-1.400275
C	0.000000	2.429373	0.707395
C	0.000000	-2.429373	0.707395
C	0.000000	2.429373	-0.707395
C	0.000000	-2.429373	-0.707395
H	0.000000	1.241873	2.485452
H	0.000000	-1.241873	2.485452
H	0.000000	1.241873	-2.485452
H	0.000000	-1.241873	-2.485452
H	0.000000	3.372182	1.242827
H	0.000000	-3.372182	1.242827
H	0.000000	3.372182	-1.242827
H	0.000000	-3.372182	-1.242827

Frequencies:

174. 186. 366.
396. 480. 488.
519. 520. 635.
636. 729. 773.
787. 799. 809.
850. 897. 951.
957. 974. 993.
1000. 1036. 1046.
1151. 1169. 1172.
1185. 1232. 1270.
1287. 1391. 1399.
1418. 1491. 1492.
1549. 1614. 1641.
1671. 3156. 3158.
3160. 3164. 3174.
3175. 3187. 3188.

i0

C -0.0710275273 -0.807226587 -1.121738707

C	-1.3416931953	-0.2390905626	-1.100924749
C	1.1260459558	-0.024522677	-0.5693696469
C	-2.4413508861	-0.9109424494	-1.6301279069
C	-2.2757060123	-2.1806607393	-2.1899863971
C	-1.0198717967	-2.7624282365	-2.2163631588
C	0.1072636744	-2.0945166467	-1.6887372415
C	2.4255320619	-0.7970346708	-0.6128502785
C	1.4058603025	-2.7008929215	-1.7115949819
C	2.5195296379	-2.0434316849	-1.1660913361
C	0.8788899486	0.4954873077	0.7857916212
C	0.4754113447	1.4342250755	3.2435834056
C	0.7007426045	0.9267493632	1.8951676209
H	-1.4738115155	0.7405751795	-0.6541381902
H	1.2549975708	0.8579652752	-1.2218804324
H	-3.4216791025	-0.4491026151	-1.6038209908
H	-3.1280192192	-2.7100960315	-2.6010301737
H	-0.8855212573	-3.749702935	-2.6462482165
H	3.292513635	-0.3086295337	-0.1846481995
H	1.5135023906	-3.6884433429	-2.1447255973
H	3.4833776589	-2.5422908381	-1.179594867
H	-0.5278811815	1.1779518773	3.5964988118
H	0.5747921699	2.5231042108	3.280463654
H	1.1946367385	1.0087751824	3.9496359577

Frequencies:

30.7866	34.1811	65.7386
133.6251	170.1376	220.3335
262.3837	317.5670	364.5239
408.6304	430.6733	452.4817
480.9620	515.8673	543.0401
560.2310	635.8517	670.6501
708.4100	754.2964	782.0214
792.9876	799.0925	823.3197
882.6410	920.8235	957.3530
964.6205	985.7491	991.6058
1054.2571	1056.6161	1060.1673
1092.3992	1130.4385	1163.7845
1175.3073	1180.2155	1199.9308
1233.4027	1253.3591	1280.6773
1300.4292	1333.5518	1386.2995
1416.8605	1433.3284	1466.5258
1480.6941	1481.5194	1512.7832
1553.5844	1597.6225	1627.8725
2353.2902	2906.6500	3021.5231
3077.9278	3078.6968	3155.8420
3157.5577	3165.0905	3174.9682

3180.1197 3188.0990 3189.2621

TS i0→i1

C	0.1370221207	-0.8838343128	-1.0409383712
C	-1.0778853446	-0.2159798026	-0.7992267621
C	1.4279496243	-0.322756907	-0.6404803294
C	-2.2807397931	-0.7566310088	-1.2106119558
C	-2.3061155534	-1.9938541474	-1.8801755078
C	-1.1316447274	-2.6720993156	-2.1195123639
C	0.1180468104	-2.1465633046	-1.706654995
C	2.5933705015	-1.1244162312	-0.7912421526
C	1.3317341566	-2.8612100044	-1.9127545418
C	2.5296914841	-2.3562900457	-1.4390184388
C	1.4940655139	0.9438414077	0.0510722213
C	1.6420443698	3.2617594476	1.3556821738
C	1.5353898895	1.9192241343	0.8007510511
H	-1.0576762095	0.7366284971	-0.2830993389
H	-3.2067313811	-0.2279891225	-1.015046981
H	-3.2520731591	-2.4140698776	-2.2032169732
H	-1.1473835699	-3.6307153766	-2.6275802757
H	3.5370112601	-0.7443724957	-0.4203356401
H	1.2974960703	-3.8191569838	-2.4186884001
H	3.4415027266	-2.9312753929	-1.5594044448
H	1.6290849007	0.9424964224	-1.3398925206
H	0.7375741666	3.5278803763	1.9112060589
H	1.7935564476	4.0216882284	0.5777051583
H	2.4810936951	3.3276658155	2.0550373294

Frequencies:

1616.8522 <i>i</i>	63.4788	66.0317
70.7668	136.9484	170.6892
218.4943	264.1213	337.2634
371.5382	406.0500	468.8801
478.7300	487.1128	538.5729
561.0725	579.0691	660.2068
677.8849	694.7197	734.0658
783.1845	792.6437	804.3565
827.7125	842.7023	882.8059
944.0708	959.8919	965.7600
990.3513	991.8739	1043.3733
1052.9385	1067.2571	1093.3981
1116.1256	1162.0272	1179.1426
1204.1751	1234.8675	1265.7239
1299.3038	1325.6597	1366.4224

1407.1560	1414.8231	1465.5132
1472.5661	1474.7069	1475.2803
1539.0131	1569.2477	1596.1019
1643.5869	2160.1346	2989.2228
3051.2299	3075.2241	3158.6755
3162.9874	3169.8480	3179.9784
3181.4189	3191.0435	3193.0280

TS i0→p4

C	-0.0628429768	-1.0182633579	-0.9077259921
C	-1.2931621969	-0.327666769	-0.8832797198
C	1.0389736168	-0.6716793626	-0.0242914822
C	-2.3063679428	-0.6596746744	-1.755622358
C	-2.1285459989	-1.6971038449	-2.694691029
C	-0.9408843856	-2.387645298	-2.7395505837
C	0.119011396	-2.0743921575	-1.8504677595
C	2.1786050573	-1.4967056212	-0.0137844243
C	1.3394454671	-2.8015322977	-1.8626113683
C	2.3342940482	-2.5259968815	-0.9496235333
C	0.8292645697	0.2425552609	1.0615439998
C	0.4605260411	1.9008274072	3.1111029212
C	0.6580403226	0.9908278136	1.9909630185
H	-1.4261460589	0.4738226872	-0.1669489058
H	1.7345617875	0.6277185296	-1.1260917184
H	-3.2462310987	-0.1202449426	-1.7225113835
H	-2.9311834347	-1.9482614746	-3.3788875396
H	-0.7980310766	-3.1892765311	-3.456569233
H	2.9595197946	-1.2903220868	0.7071683279
H	1.4640372008	-3.5996023187	-2.5865120782
H	3.2454457771	-3.1133951811	-0.9449296313
H	-0.5993607531	1.9835997516	3.3690041357
H	0.8260112059	2.9044242104	2.8729555338
H	0.9944426385	1.5522531392	3.9999578029

Frequencies:

941.7729i	22.2981	71.0455
74.3209	161.5182	173.5609
250.7906	265.4267	347.5413
376.1949	401.7748	423.2863
443.2938	486.4246	495.0697
500.4960	539.0497	576.2168
588.8469	653.9959	687.1219
742.5791	786.5212	802.6276
814.4855	833.9776	882.6067

908.6754	955.5175	967.2310
980.8226	998.2882	1044.1647
1050.6640	1054.5602	1078.7138
1116.7833	1165.7183	1179.6810
1195.5139	1236.5234	1262.7731
1303.5858	1335.4013	1378.9808
1414.2614	1421.2431	1465.5526
1478.1372	1479.1635	1481.8976
1539.1667	1589.3242	1607.2685
1653.3893	2340.4410	3020.9941
3076.5934	3080.6442	3159.9709
3164.2856	3170.9727	3180.0723
3183.9659	3194.5105	3196.8413