Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2023

Electronic Supplementary Information for: Bridging the gap: viable reaction pathways from tetrahedrane to benzene and benzyne

Cartesian Coordinates for each structure at the CCSD(T)-F12b/cc-pVTZ-F12 level of theory, and transition states at the B3LYP/aug-CC-pVTZ level of theory.

Tetrahedrane (C_4H_4)

C	0.7394447926	0.0000000000	0.5228484649
C	-0.7394447926	0.0000000000	0.5228484649
C	0.0000000000	-0.7394447926	-0.5228484649
C	0.0000000000	0.7394447926	-0.5228484649
H	1.6118611566	0.0000000000	1.1398238501
H	-1.6118611566	0.0000000000	1.1398238501
H	0.0000000000	-1.6118611566	-1.1398238501
H	0.0000000000	1.6118611566	-1.1398238501

Benzvalyne (C_6H_4)

C	-0.624235799	0.000000000	1.255064411
C	0.624235799	0.000000000	1.255064411
C	-1.069102992	0.000000000	-0.140443387
C	1.069102992	0.000000000	-0.140443387
C	0.000000000	0.758178537	-0.929585749
C	0.000000000	-0.758178537	-0.929585749
H	-2.099093572	0.000000000	-0.462623651
H	2.099093572	0.000000000	-0.462623651
H	0.000000000	1.465344051	-1.742327724
H	0.000000000	-1.465344051	-1.742327724

Benzyne (C_6H_4)

C	0.000000000	-0.711729735	-1.120345871
C	0.000000000	0.711729735	-1.120345871
C	0.000000000	1.475234669	0.079087260
C	0.000000000	-1.475234669	0.079087260
C	0.000000000	0.640023260	1.209501735
C	0.000000000	-0.640023260	1.209501735
H	0.000000000	-2.571130469	0.078749014
H	0.000000000	2.571130469	0.078749014
H	0.000000000	1.240194489	-2.083598667
H	0.000000000	-1.240194489	-2.083598667

Benzvalene (C_6H_6)

C	-0.726407878	0.000000000	1.012120875
C	0.726407878	0.000000000	1.012120875
C	0.000000000	1.073793413	0.210180028
C	0.000000000	-1.073793413	0.210180028
H	0.000000000	-2.099784319	0.549500747
H	0.000000000	2.099784319	0.549500747
C	0.000000000	-0.671124591	-1.243148218
C	0.000000000	0.671124591	-1.243148218
H	0.000000000	1.346767996	-2.083675061
H	0.000000000	-1.346767996	-2.083675061
H	1.478709265	0.000000000	1.783454017
H	-1.478709265	0.000000000	1.783454017

Benzene (C_6H_6)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	1.39354993	-0.00000000
C	0.00000000	2.09032489	-1.20684964
C	0.00000000	1.39354993	-2.41369928
C	0.00000000	-0.00000000	-2.41369928
C	0.00000000	-0.69677496	-1.20684964
H	0.00000000	-1.77945859	-1.20684964
H	0.00000000	-0.54134181	-3.35133080
H	0.00000000	1.93489174	-3.35133080
H	0.00000000	3.17300851	-1.20684964
H	0.00000000	1.93489174	0.93763152
H	0.00000000	-0.54134181	0.93763152

Diatomic Carbon (C_2)

C	0.0000000000	0.0000000000	-0.6223020365
C	0.0000000000	0.0000000000	0.6223020365

Ethynyl Radical (C_2H)

C	0.0000000000	0.0000000000	-0.6722923016
C	0.0000000000	0.0000000000	0.5378422902
H	0.0000000000	0.0000000000	1.6021579524

Acetylene (HCCH)

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.20548154
H	0.00000000	0.00000000	2.26860752
H	0.00000000	-0.00000000	-1.06312599

Vinylidene ($H_2C=C:$)

C	0.0000000000	0.0000000000	-0.7431849209
C	0.0000000000	0.0000000000	0.5583543031
H	0.0000000000	0.9406248706	1.1012563002
H	0.0000000000	-0.9406248706	1.1012563002

Diatomic Hydrogen (H2)

H	0.0000000000	0.0000000000	-0.3708352481
H	0.0000000000	0.0000000000	0.3708352481

C_2H Addition to C_4H_4

I1

C	-0.722789032	0.000000000	1.160725439
C	0.722789032	0.000000000	1.160725439
C	0.000000000	0.979627472	0.239614112
C	0.000000000	-0.979627472	0.239614112
H	0.000000000	-2.057532772	0.261456726
H	0.000000000	2.057532772	0.261456726
C	0.000000000	0.000000000	-0.923666596
C	0.000000000	0.000000000	-2.231962026
H	1.545873127	0.000000000	1.853400654
H	-1.545873127	0.000000000	1.853400654

TS1

C	-0.923245	-0.245197	-0.727239
C	-0.476022	1.016375	-0.000338
C	0.212622	-0.941271	0.000184
C	-0.923385	-0.244471	0.727158
H	-1.628921	-0.480685	-1.505610
H	-0.984574	1.964497	-0.000647
H	0.366941	-2.007805	0.001559
H	-1.628690	-0.479328	1.506047
C	0.975755	0.769875	0.000416
C	1.780148	-0.188092	-0.000405

C_2H Addition to C_4H_4

I1

C	-0.007934417	-0.541555995	-1.367429612
C	0.995835288	-0.094423929	-0.307746591
C	-0.004335865	0.874721549	-0.888366596
C	-0.997829973	-0.083880329	-0.302333364
H	-2.081032601	-0.091488116	-0.342606343
C	0.017879528	-0.398453286	0.817906994
C	0.037424469	0.209351245	2.190334801
H	-0.431071560	-0.331616009	3.004247227
H	0.001163611	1.731836638	-1.534755810
H	2.075477593	-0.117968862	-0.367858081
H	-0.025670375	-0.724267689	-2.433091655

I2

C	-0.728304040	-0.138905636	-0.972347839
C	0.728304040	-0.138905636	-0.972347839
C	0.000000000	-1.064854840	-0.002369896
C	0.000000000	1.058922165	-0.370820884
H	0.000000000	2.017183498	-0.865242506
C	0.000000000	0.863067048	1.114782824
C	0.000000000	-0.443623112	1.385643079
H	0.000000000	-0.972299038	2.323084313
H	1.480932435	-0.265186667	-1.733585205
H	-1.480932435	-0.265186667	-1.733585205
H	0.000000000	-2.132621996	-0.169323170

I3

C	-0.138714159	-0.729845636	-0.971733306
C	-0.138714159	0.729845636	-0.971733306
C	1.058900288	0.000000000	-0.370741992
C	-1.065060124	0.000000000	-0.002636775
H	-2.132402953	0.000000000	-0.169432828
C	-0.443490675	0.000000000	1.385352525
C	0.862901125	0.000000000	1.114457752
H	-0.972788932	0.000000000	2.322913189
H	-0.265872546	1.478197395	-1.736109864
H	-0.265872546	-1.478197395	-1.736109864
H	2.017339964	0.000000000	-0.864937885

TS

C	0.00000000	0.00000000	0.00000000
C	0.77756800	-1.08495779	-0.74066600
C	-0.03363600	-0.00004926	-1.44297900
C	0.77750267	1.08495507	-0.74073855
H	0.43870600	2.10924435	-0.73062805
C	2.22524514	0.66193673	-0.83802027
C	2.22528500	-0.66185879	-0.83797600
H	-0.81380300	-0.00009750	-2.18349300
H	0.43883300	-2.10926679	-0.73048700
H	-0.75733899	0.00000280	0.76550701
H	2.70673999	0.00008727	0.17306499

C_6H_4 Isomer 1

C	0.00000000	0.00000000	0.00000000
C	0.72299249	-1.09533484	-0.73907077
C	-0.00022490	0.00012116	-1.47774182
C	0.93525309	0.99276590	-0.73893187
H	0.68918106	2.05151151	-0.73880761
C	2.34770738	0.39192258	-0.73919609
C	2.07395224	-0.92434256	-0.73926235
H	3.27992902	0.93336444	-0.73929357
H	-0.79865791	0.08403125	-2.19767542
H	-0.79821385	0.08379201	0.72019034

C_6H_4 Isomer 2

C	0.9501417263	-0.3099239985	0.7327315399
C	0.5303586467	0.9391636041	-0.0000674061
C	0.9503443623	-0.3101434404	-0.7323748481
C	-0.2097702820	-0.9531642943	0.0001144602
C	-1.5517569634	-0.2831847385	-0.0001753599
C	-0.9982784744	0.9112542221	-0.0002872151
H	-2.5385940325	-0.7011523065	-0.0002452893
H	1.6586423928	-0.5825817707	-1.4962222529
H	1.0818256503	1.8675638328	-0.0001260609
H	1.6582289734	-0.5821321101	1.4968564321

C_6H_4 Isomer 3

C	0.5876550957	0.9878689759	0.1760421993
C	0.9346202409	-0.4310719498	0.7220650858
C	-0.2978065316	-1.0972525893	0.1509578494
C	0.9403303815	-0.3257369578	-0.6385047890
H	1.0602794560	-0.4587250676	-1.6979511550
H	-0.3408031368	-2.1704291798	0.0417674911
C	-1.3163790204	-0.1349061769	-0.0469205455
C	-0.8127295490	1.2123774095	-0.0643226419
H	-2.3603541611	-0.3945941524	-0.1740091168
H	1.3703052241	1.7311506884	0.2059866223

HCCH and $H_2C{=}C$: Addition to C_4H4

I1

C	0.00000000	0.00000000	0.00000000
C	-0.13149581	1.29264067	0.74444418
C	0.00000383	-0.00004048	1.48881739
C	1.17266593	-0.57350855	0.74439008
H	1.23494175	-1.65689554	0.74436047
C	2.46601750	0.09181872	0.74440484
C	3.54233680	0.64169176	0.74441702
H	4.48872027	1.12565575	0.74442774
H	-0.66766199	-0.48725508	2.17757849
H	0.70302237	1.98740926	0.74446092
H	-1.11482598	1.74829944	0.74445910
H	-0.66766937	-0.48717715	-0.68878415

TS1

C	0.00000000	0.00000000	0.00000000
C	-0.49647201	1.21691205	-0.72830262
C	-0.00001329	0.00005170	-1.45670067
C	-1.01428500	-0.83449700	-0.72837070
H	-1.03201999	-1.91937004	-0.72840904
C	-2.27334302	-0.03149391	-0.72833071
C	-3.48871299	0.27657496	-0.72830869
H	-4.55054100	0.14766100	-0.72830358
H	0.71572600	-0.23464400	-2.22216500
H	0.07579699	2.14231503	-0.72827499
H	0.71575326	-0.23475004	0.76543461
H	-2.52553399	1.21788594	-0.72828407

I2

C	0.0000000000	-0.7191854474	-1.2914237997
C	0.0000000000	0.7191854474	-1.2914237997
C	0.9894981441	0.0000000000	-0.3687838730
C	-0.9894981441	0.0000000000	-0.3687838730
H	-2.0672763956	0.0000000000	-0.4328088955
H	2.0672763956	0.0000000000	-0.4328088955
C	0.0000000000	0.0000000000	0.7676693596
C	0.0000000000	0.0000000000	2.0967923893
H	-0.9289112643	0.0000000000	2.6509483020
H	0.9289112643	0.0000000000	2.6509483020
H	0.0000000000	1.5341569879	-1.9901626083
H	0.0000000000	-1.5341569879	-1.9901626083

TS2

C	0.975732	-0.092322	-0.724622
C	0.099671	-1.082777	0.003913
C	1.002641	-0.077602	0.711942
C	0.289780	1.073238	-0.006920
H	0.755531	2.047419	-0.034186
C	-1.198508	0.897059	0.107182
C	-1.291437	-0.502142	0.041545
H	-2.192260	-1.071393	0.235449
H	-1.661640	0.178176	-0.959343
H	1.775602	-0.143502	1.457522
H	0.332544	-2.137935	-0.001453
H	1.722951	-0.165477	-1.496235

I3

C	0.00000000	0.00000000	0.00000000
C	-0.00000000	-1.49323943	-0.27972840
C	-0.00000000	-1.55082113	-1.77772512
C	0.74325777	-0.34265506	-2.29630859
C	-0.00000000	0.59588895	-1.37558213
C	-0.74325777	-0.34265506	-2.29630859
H	-1.33593504	-0.17751476	-3.17786451
H	0.00000000	1.66440675	-1.57766795
H	1.33593504	-0.17751476	-3.17786451
H	-0.00000000	-2.47374099	-2.35286677
H	0.87695010	0.22794172	0.60128391
H	-0.87695010	0.22794172	0.60128391

TS3

C	-0.969668	-0.220599	0.753582
C	0.093690	-1.048572	0.018447
C	-1.014240	-0.292371	-0.688424
C	-0.520436	1.019407	-0.032989
H	-1.154564	1.893316	-0.053041
C	0.997082	1.115278	0.047527
C	1.236494	-0.116965	-0.177972
H	-1.759579	-0.550513	-1.422842
H	0.129434	-2.126276	0.033891
H	-1.690843	-0.406504	1.533265
H	2.680715	-0.743491	-0.187877
H	2.857304	-0.803599	0.575567

TS6

C	0.00000000	0.00000000	0.00000000
C	-1.31158800	0.39844000	-0.38197800
C	-2.11280800	-0.72690139	-0.59117404
C	-1.31160293	-1.85216120	-0.38148259
C	-0.00000964	-1.45357047	0.00031996
C	0.76642100	-0.72707925	-1.31245302
H	-0.01027400	-0.72724372	-2.08298891
H	0.71213700	-2.07635900	0.51667000
H	-1.61181149	-2.87511700	-0.55794125
H	-3.11378300	-0.72698282	-0.99125605
H	-1.61178300	1.42132200	-0.55888700
H	0.71215490	0.62300635	0.51607581

I5

C	-0.529355638	-0.323550517	-0.828861689
C	-0.176627298	-1.199671351	0.317839779
C	0.217522701	-0.434200995	1.383939161
C	0.113598708	0.950006792	1.003688640
C	-0.341909548	1.057909170	-0.286505561
H	-0.542280001	1.965754408	-0.831892770
H	0.355043047	1.785935633	1.646257386
H	0.620966246	-0.795055056	2.313153323
H	-0.137351118	-2.277479454	0.253038469
C	0.683412652	-0.046077672	-1.669795325
H	1.537640840	-0.141951956	-0.974800321
H	-1.436507248	-0.526760701	-1.393021150

TS7

C	-0.513844	0.925750	-0.364902
C	0.966613	0.992467	-0.107993
C	1.383383	-0.251294	0.170527
C	0.316980	-1.259433	0.009521
C	-0.937718	-0.768475	-0.255044
H	-1.684999	-1.298265	-0.831881
H	0.564053	-2.309658	-0.091784
H	2.400365	-0.523186	0.416436
H	1.569180	1.886755	-0.136702
C	-1.390395	0.474393	0.617911
H	-0.948010	0.473231	1.613242
H	-0.850705	1.090674	-1.389425

TS8

C	0.823166	-0.596200	-0.517917
C	-0.454811	-1.184451	-0.003889
C	-1.446365	-0.248264	0.130507
C	-0.900780	1.031095	-0.056170
C	0.506194	0.980795	-0.076737
H	1.076725	1.816361	-0.463664
H	-1.457823	1.950620	-0.157164
H	-2.453378	-0.445464	0.467382
H	-0.491234	-2.214537	0.317781
C	1.405657	-0.048942	0.624192
H	2.471344	0.135802	0.722274
H	1.255992	-0.846976	-1.486529