

Principal axis coordinates (Å) for inertial fit ( $r_0$ ) and MP2/6-311++G(2d,2p) ab initio ( $r_e$ ) structures of BZ<sup>-</sup>HCC<sup>+</sup>H.

$r_0$  fit of  $R_{cm}$

	<b>a</b>	<b>b</b>	<b>c</b>
C	-3.717425	0.000020	0.000000
H	-4.778425	0.000037	0.000000
H	-1.453425	-0.000015	0.000000
C	-2.514425	0.000001	0.000000
C	1.038623	-1.209755	0.698400
C	1.038623	-1.209755	-0.698400
C	1.038642	-0.000004	1.396850
C	1.038642	-0.000004	-1.396850
C	1.038661	1.209747	0.698400
C	1.038661	1.209747	-0.698400
H	1.038608	-2.146361	1.239150
H	1.038608	-2.146361	-1.239150
H	1.038642	-0.000004	2.478350
H	1.038642	-0.000004	-2.478350
H	1.038676	2.146354	1.239150
H	1.038676	2.146354	-1.239150

$r_0$  fit of  $R_{cm}$ ,  $\theta$ , and  $\phi$

	<b>a</b>	<b>b</b>	<b>c</b>
C	-3.715182	0.057451	0.000020
H	-4.771144	0.160726	0.000035
H	-1.461933	-0.162921	-0.000013
C	-2.517894	-0.059646	0.000002
C	1.028900	-0.697980	-1.209745
C	1.048754	0.698679	-1.209764
C	1.018991	-1.396343	0.000015
C	1.058701	1.397075	-0.000022
C	1.028938	-0.697948	1.209757
C	1.048792	0.698711	1.209738
H	1.021199	-1.238688	-2.146344
H	1.056426	1.239362	-2.146378
H	1.003618	-2.477734	0.000030
H	1.074074	2.478465	-0.000037
H	1.021266	-1.238631	2.146370
H	1.056493	1.239419	2.146337

$r_0$  fit of  $R_{cm}$  and  $\theta$

	<b>a</b>	<b>b</b>	<b>c</b>
C	-3.713887	-0.051881	0.000013
H	-4.766908	-0.181757	0.000013
H	-1.466913	0.225254	0.000015
C	-2.519934	0.095378	0.000014
C	1.034078	-0.705473	-1.209848
C	1.043824	0.691293	-1.209663
C	1.029224	-1.404065	-0.000189
C	1.048716	1.389566	0.000180
C	1.034116	-0.705792	1.209654
C	1.043862	0.690974	1.209838
H	1.030290	-1.246086	-2.146525
H	1.047582	1.232154	-2.146198
H	1.021678	-2.485539	-0.000332
H	1.056263	2.471040	0.000323
H	1.030358	-1.246653	2.146189
H	1.047650	1.231587	2.146516

$r_0$  fit of  $R_{cm}$  and  $\phi$

	<b>a</b>	<b>b</b>	<b>c</b>
C	-3.717451	0.000008	0.022276
H	-4.778432	0.000021	0.028634
H	-1.453492	-0.000020	0.008710
C	-2.514473	-0.000007	0.015067
C	1.022089	-1.209367	-0.705093
C	1.055182	-1.210135	0.691315
C	1.005560	0.000768	-1.402682
C	1.071748	-0.000769	1.390234
C	1.022127	1.210135	-0.703762
C	1.055220	1.209366	0.692645
H	1.009262	-2.145676	-1.246206
H	1.067978	-2.147039	1.231398
H	0.979937	0.001363	-2.483878
H	1.097371	-0.001364	2.471430
H	1.009330	2.147039	-1.243846
H	1.068046	2.145675	1.233758

Ab Initio

	<b>a</b>	<b>b</b>	<b>c</b>
C	-3.635215	0.000001	0.000001
H	-4.695929	0.000001	0.000001
H	-1.359490	0.000003	0.000000
C	-2.422479	0.000002	0.000000
C	1.009897	-0.901978	-1.066377
C	1.009902	0.901976	1.066377
C	1.009900	-0.472522	1.314323
C	1.009899	0.472521	-1.314324
C	1.009902	1.374498	-0.247946
C	1.009898	-1.374499	0.247946
H	1.005853	-1.599949	-1.891566
H	1.005862	1.599948	1.891566
H	1.005858	-0.838170	2.331378
H	1.005857	0.838169	-2.331379
H	1.005854	-2.438118	0.439812
H	1.005862	2.438117	-0.439813

Electric fields and observed transition frequencies for BZ...HCCH Stark effects. -- denotes transitions that were not fitted.

$J'$	$K'$	$J''$	$K''$	$2M'$	$2M''$	Field / (V cm <sup>-1</sup> )	Obs. Freq. / MHz	Obs. - Calc. / MHz	Calc. Freq. / MHz
3	0	2	0	2	2	0	6893.2463	-0.00272--	6893.2490
3	0	2	0	2	2	167.1	6893.2438	-0.0010	6893.2448
3	0	2	0	2	2	199.5	6893.2390	-0.0040	6893.2430
3	0	2	0	2	2	231.9	6893.2359	-0.0050	6893.2409
3	0	2	0	2	2	264.3	6893.2331	-0.0054	6893.2385
3	0	2	0	2	2	296.7	6893.2327	-0.0030	6893.2357
3	0	2	0	2	2	329.2	6893.2289	-0.0038	6893.2327
3	0	2	0	4	4	0	6893.2463	-0.00272--	6893.2490
3	0	2	0	4	4	167.1	6893.2849	0.0078	6893.2771
3	0	2	0	4	4	199.5	6893.2933	0.0042	6893.2891
3	0	2	0	4	4	231.9	6893.3109	0.0077	6893.3032
3	1	2	1	0	0	0	6893.1333	0.00414--	6893.1292
3	1	2	1	0	0	134.6	6893.1296	0.00318--	6893.1264
3	1	2	1	0	0	167.1	6893.1220	-0.0029	6893.1249
3	1	2	1	0	0	199.5	6893.1183	-0.0049	6893.1231
3	1	2	1	0	0	231.9	6893.1156	-0.0054	6893.1210
3	1	2	1	0	0	264.3	6893.1138	-0.0048	6893.1186
3	1	2	1	0	0	296.7	6893.1121	-0.0038	6893.1159
3	1	2	1	0	0	329.2	6893.1089	-0.0039	6893.1128
4	0	3	0	6	6	0	9190.8690	0.00544--	9190.8636
4	0	3	0	6	6	231.9	9190.8873	-0.0027	9190.8900
4	0	3	0	6	6	264.3	9190.8898	-0.0081	9190.8979
4	0	3	0	6	6	296.7	9190.8966	-0.0103	9190.9068
4	0	3	0	6	6	329.2	9190.9077	-0.0091	9190.9168

Standard deviation = 0.0058 MHz  
 $\mu_a = 0.438 \pm 0.011$  D