

Laboratory IR spectroscopy of protonated hexa-peri-hexabenzocoronene and dicoronylene

Supplementary Information

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This Supplementary Information file lists computational results for the title species having the ionizing proton attached to different sites in the molecule. The isomers are labeled A and B for HBC+H⁺ and A through E for DC+H⁺, see Figures 4 and 5 of the main text for a definition of these sites. Unscaled harmonic frequencies follow the optimized geometries. All calculations were performed at the B3LYP/6-311++G(d,p) level of theory using Gaussian16 Revision A.03.

OPTIMIZED GEOMETRIES PROTONATED HEXA-PERI-HEXABENZOCORONENE

Supplementary Table 1: Atom positions for HBC+H⁺ isomer A.

Atom	X (Å)	Y (Å)	Z (Å)
C	-1.453357	0.112477	-0.008071
C	-0.648427	1.28301	0.010673
C	0.775387	1.166953	-0.00878
C	1.384884	-0.1117	-0.00158
C	0.58279	-1.280968	0.000662
C	-0.840073	-1.171989	0.000212
C	1.590996	2.341225	-0.015096
C	3.017991	2.225823	-0.057736
C	3.621249	0.938482	-0.061009
C	2.823181	-0.222439	-0.027515
C	3.445352	-1.51181	-0.001336
C	2.637053	-2.685269	0.065663
C	1.20609	-2.568802	0.043155
C	-1.652667	-2.361027	-0.023387
C	0.412652	-3.749304	0.063577
C	-1.042314	-3.647981	-0.004703
C	-2.892556	0.225927	-0.014508
C	-3.702366	-0.941903	-0.058462
C	-3.071758	-2.258036	-0.065933
C	-1.262371	2.586033	0.03357
C	-2.680143	2.706714	0.05943
C	-3.508908	1.507191	0.005382
C	-0.456902	3.761207	0.057976
C	0.997559	3.635077	0.001795
C	1.83048	4.754816	-0.037404
C	3.221308	4.642378	-0.08248
C	3.809863	3.399397	-0.088641
C	5.116761	0.835628	-0.100868
C	5.67367	-0.53285	-0.105635
C	4.886073	-1.616961	-0.056716
C	3.223618	-3.972103	0.158513

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Supplementary Table 1 – *Continued from previous page*

Atom	X (Å)	Y (Å)	Z (Å)
C	2.441253	-5.101715	0.21393
C	1.052871	-4.98767	0.16067
C	-1.850591	-4.788022	-0.061161
C	-3.833425	-3.432425	-0.11496
C	-3.23144	-4.679804	-0.117703
C	-5.095711	-0.802642	-0.085717
C	-4.906927	1.590027	-0.028274
C	-5.69048	0.448649	-0.073883
C	-3.249286	3.985057	0.133509
C	-2.459065	5.121206	0.173977
C	-1.077056	5.011813	0.132187
H	1.404649	5.747922	-0.038349
H	3.8319	5.536498	-0.112173
H	4.888034	3.333467	-0.120493
H	5.499642	1.369739	-0.982035
H	6.752058	-0.636418	-0.151553
H	5.348314	-2.591336	-0.069993
H	4.295232	-4.089318	0.201108
H	2.899247	-6.079507	0.29727
H	0.469784	-5.896308	0.205103
H	-1.414843	-5.776561	-0.069948
H	-3.841574	-5.573917	-0.16366
H	-4.911536	-3.385202	-0.15557
H	-5.734948	-1.672597	-0.117424
H	-6.770166	0.534455	-0.100346
H	-5.400975	2.55044	-0.024494
H	-4.321839	4.10628	0.168055
H	-2.921408	6.098927	0.238313
H	-0.491019	5.918847	0.166375
H	5.547914	1.382587	0.749881

Supplementary Table 2: Atom positions for HBC+H⁺ isomer B.

Atom	X (Å)	Y (Å)	Z (Å)
C	0.003689	-1.42779	-0.031079
C	1.243812	-0.71468	0.003124
C	1.245096	0.695241	0.018853
C	-0.003649	1.411003	-0.030796
C	-1.248685	0.688776	0.018823
C	-1.240103	-0.721116	0.003047
C	2.488858	1.416215	0.099373
C	2.496158	2.836156	0.06015
C	1.244308	3.54039	-0.231862
C	-0.007278	2.810618	-0.142975
C	-1.262605	3.533917	-0.231746
C	-2.510788	2.823204	0.060193
C	-2.496157	1.403315	0.099292
C	-2.485253	-1.450705	0.060224
C	-3.717622	0.697303	0.272362
C	-3.716276	-0.757869	0.216421
C	0.007391	-2.858834	-0.141968
C	-1.223924	-3.576766	-0.216855
C	-2.48592	-2.86745	-0.035645
C	2.492719	-1.437811	0.060246
C	2.500716	-2.854531	-0.035612
C	1.242419	-3.570371	-0.21684
C	3.720136	-0.738633	0.216484

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Supplementary Table 2 – Continued from previous page

Atom	X (Å)	Y (Å)	Z (Å)
C	3.713961	0.716518	0.272408
C	4.888942	1.457364	0.47932
C	4.87142	2.840291	0.50667
C	3.682024	3.528868	0.290425
C	1.229575	4.839588	-0.64181
C	-0.014453	5.575959	-0.917195
C	-1.254627	4.833184	-0.641636
C	-3.700187	3.509789	0.290531
C	-4.886023	2.815077	0.506758
C	-4.896409	1.43208	0.479354
C	-4.907515	-1.493494	0.299128
C	-3.700645	-3.556037	0.064815
C	-4.898351	-2.876276	0.230982
C	-1.190681	-4.953185	-0.460807
C	1.216349	-4.946913	-0.460917
C	0.014585	-5.625673	-0.595185
C	3.718959	-3.536859	0.064953
C	4.913145	-2.85091	0.231052
C	4.915161	-1.468093	0.299138
H	5.830775	0.95298	0.638925
H	5.786009	3.388729	0.697421
H	3.689011	4.610239	0.330197
H	2.1582	5.370924	-0.806996
H	-0.015415	5.932316	-1.962665
H	-2.186009	5.359713	-0.806735
H	-3.71278	4.591117	0.330353
H	-5.803407	3.358798	0.697586
H	-5.835611	0.922834	0.638994
H	-5.856528	-0.990277	0.414466
H	-5.827383	-3.428353	0.306514
H	-3.723082	-4.635527	0.027016
H	-2.107898	-5.513972	-0.565611
H	0.017351	-6.689481	-0.801507
H	2.136481	-5.502886	-0.565871
H	3.746941	-4.616228	0.027259
H	5.845019	-3.398169	0.30662
H	5.861567	-0.959984	0.414454
H	-0.016875	6.522047	-0.347579

OPTIMIZED GEOMETRIES
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Supplementary Table 3: Atom positions for DC+H⁺ isomer A.

Atom	X (Å)	Y (Å)	Z (Å)
C	-7.778299	1.262141	-0.002327
C	-7.106435	0.039348	0.000477
C	-5.692239	0.025019	0.003933
C	-4.971112	1.253023	-0.004826
C	-5.676556	2.487393	-0.003796
C	-7.080305	2.462476	-0.004453
C	-7.868963	-1.254817	0.00381
C	-7.045051	-2.486602	0.004518
C	-5.684037	-2.476826	0.003837
C	-4.968379	-1.207258	-0.001269

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Supplementary Table 3 – Continued from previous page

Atom	X (Å)	Y (Å)	Z (Å)
C	-4.932479	3.711553	-0.006262
C	-3.549784	1.24818	0.003082
C	-2.835075	2.479622	-0.00371
C	-3.570853	3.708028	-0.005796
C	-3.564206	-1.20307	0.00606
C	-2.833476	0.026672	-0.003981
C	-4.918823	-3.704133	0.003488
C	-3.567479	-3.68415	0.002425
C	-2.839723	-2.439341	0.000647
C	-1.453191	-2.415546	-0.000348
C	-0.708255	-1.221834	-0.00081
C	-1.409434	0.025643	0.003033
C	-0.700192	1.273275	-0.001086
C	-1.4342	2.456323	-0.003306
C	0.74707	-1.228602	0.000286
C	1.457213	0.016611	-0.001738
C	0.764564	1.266166	0.001902
C	1.474561	-2.420102	-0.000871
C	2.876108	-2.455023	-0.001603
C	3.592609	-1.226865	-0.004566
C	2.879012	0.005666	0.004138
C	1.505248	2.444865	0.00414
C	2.910051	2.462136	0.004257
C	3.610036	1.227199	-0.001651
C	5.014295	-1.240138	0.001695
C	5.737144	-0.014677	-0.003682
C	5.032291	1.220267	0.00487
C	5.749987	2.446659	0.0032
C	5.020358	3.67198	0.005727
C	3.65413	3.681383	0.006049
C	3.603495	-3.68522	-0.003315
C	4.968824	-3.693856	-0.003981
C	5.714571	-2.477396	-0.003371
C	7.133547	-2.46019	-0.00392
C	7.828695	-1.276387	-0.002918
C	7.155066	-0.024835	-0.000873
C	7.848047	1.2167	0.000487
C	7.169606	2.409294	0.002709
H	-5.459025	-4.644026	0.005028
H	-3.003251	-4.609812	0.001648
H	-7.571383	-3.436083	0.006975
H	-8.54802	-1.286921	0.870214
H	-8.862951	1.275635	-0.003312
H	-7.62524	3.40009	-0.00605
H	-5.477097	4.6492	-0.007767
H	-3.02127	4.642562	-0.008102
H	-0.926969	3.411321	-0.007485
H	-0.943831	-3.368716	-0.00342
H	0.962931	-3.373068	0.000744
H	3.050766	-4.618259	-0.003463
H	5.508404	-4.634364	-0.005669
H	7.667898	-3.403629	-0.005717
H	8.913209	-1.285326	-0.002993
H	8.932506	1.209461	0.000448
H	7.716789	3.345396	0.003511
H	5.571702	4.605686	0.006675
H	3.114593	4.622124	0.008246
H	1.004258	3.403883	0.007946
H	-8.551908	-1.28967	-0.859322

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Supplementary Table 3 – *Continued from previous page*

Atom	X (Å)	Y (Å)	Z (Å)
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Supplementary Table 4: Atom positions in Å for DC+H⁺ isomer B, calculated with B3LYP/6-311++G(d,p).

Atom	X (Å)	Y (Å)	Z (Å)
C	-7.830095	1.321507	-0.000698
C	-7.153306	0.04798	0.000453
C	-5.699157	0.01998	-0.003236
C	-4.9849	1.236809	0.004191
C	-5.693358	2.481042	-0.001501
C	-7.127002	2.481413	-0.001139
C	-7.84421	-1.130161	0.000247
C	-7.183902	-2.44968	0.000586
C	-5.6881	-2.448523	-0.00076
C	-4.987859	-1.217815	0.003896
C	-4.956749	3.681875	-0.001961
C	-3.557586	1.229324	-0.004083
C	-2.844096	2.454007	0.000514
C	-3.578386	3.667959	-0.001357
C	-3.56384	-1.212394	-0.004085
C	-2.837592	0.008622	0.005766
C	-4.970575	-3.649457	-0.002024
C	-3.587394	-3.647165	-0.001788
C	-2.854309	-2.43871	0.000069
C	-1.440458	-2.418187	0.000317
C	-0.703251	-1.245616	0.001917
C	-1.409158	0.007071	-0.000891
C	-0.70001	1.255416	0.002089
C	-1.434545	2.432079	0.00079
C	0.768882	-1.247391	0.001394
C	1.469349	0.001287	0.000808
C	0.772139	1.252175	0.001544
C	1.495421	-2.427761	0.001131
C	2.904302	-2.457874	0.00073
C	3.613033	-1.229892	-0.002533
C	2.892053	-0.000815	0.003993
C	1.502191	2.430078	0.00134
C	2.91136	2.456065	0.000927
C	3.616624	1.226079	-0.002432
C	5.036919	-1.234792	0.00299
C	5.752918	-0.005025	-0.003488
C	5.040508	1.226821	0.003081
C	5.750831	2.456406	-0.000329
C	5.014743	3.675807	0.000111
C	3.647048	3.677424	0.000456
C	3.636507	-3.681423	0.000187
C	5.00418	-3.683773	-0.000151
C	5.743707	-2.466512	-0.000513
C	7.164779	-2.440874	-0.001038
C	7.853188	-1.255208	-0.001481
C	7.171398	-0.007085	-0.001007
C	7.856798	1.238917	-0.001382
C	7.171753	2.426643	-0.000844
H	-5.505706	-4.592828	-0.003839
H	-3.049141	-4.588684	-0.001926
H	-7.56045	-3.025655	-0.860289
H	-8.929686	-1.115099	0.001617
H	-8.913813	1.328704	-0.000271

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Supplementary Table 4 – *Continued from previous page*

Atom	X (Å)	Y (Å)	Z (Å)
H	-7.641991	3.435185	-0.002441
H	-5.48858	4.626224	-0.003848
H	-3.033477	4.605943	-0.001135
H	-0.929823	3.388443	0.002273
H	-0.938582	-3.376121	0.001556
H	0.989781	-3.384764	0.002276
H	3.089495	-4.618079	0.000631
H	5.547085	-4.622615	-0.000887
H	7.703459	-3.3821	-0.001698
H	8.937755	-1.257055	-0.001575
H	8.941364	1.237659	-0.001473
H	7.713184	3.366291	-0.001431
H	5.56032	4.613101	-0.000565
H	3.102752	4.615646	0.000966
H	0.999337	3.388509	0.002544
H	-7.558041	-3.022624	0.864673

Supplementary Table 5: Atom positions for DC+H⁺ isomer C.

Atom	X (Å)	Y (Å)	Z (Å)
C	-7.808658	-1.318908	0.100702
C	-7.136268	-0.0634	0.011704
C	-5.717053	-0.042794	0.003989
C	-4.989143	-1.258043	0.08996
C	-5.683806	-2.498225	0.172448
C	-7.106859	-2.490851	0.179355
C	-7.829993	1.160782	-0.07428
C	-7.151297	2.364266	-0.161906
C	-5.752942	2.402661	-0.165006
C	-5.019901	1.196148	-0.074277
C	-4.933574	-3.704308	0.2492
C	-3.572237	-1.235732	0.071246
C	-2.851047	-2.452075	0.14514
C	-3.565796	-3.683484	0.235219
C	-3.589293	1.205561	-0.077338
C	-2.858394	-0.000329	0.007364
C	-5.025041	3.705178	-0.261039
C	-3.5523	3.633251	-0.245723
C	-2.858297	2.454792	-0.152793
C	-1.430384	2.429701	-0.127471
C	-0.705474	1.268216	-0.030617
C	-1.421634	0.009112	-0.004914
C	-0.713827	-1.224746	0.022676
C	-1.448759	-2.408463	0.113312
C	0.765343	1.259025	0.036674
C	1.460157	0.008855	-0.000851
C	0.75654	-1.23607	-0.040718
C	1.495185	2.433688	0.129806
C	2.903854	2.455847	0.155561
C	3.607596	1.226285	0.079426
C	2.882023	0.00385	-0.004324
C	1.476661	-2.416398	-0.127677
C	2.88696	-2.44886	-0.153834
C	3.599159	-1.225844	-0.073833
C	5.031481	1.223743	0.080391
C	5.740837	-0.007483	0.003194
C	5.022498	-1.232739	-0.085742

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Supplementary Table 5 – *Continued from previous page*

Atom	X (Å)	Y (Å)	Z (Å)
C	5.726455	-2.463337	-0.169164
C	4.984009	-3.67532	-0.25193
C	3.615667	-3.670251	-0.244349
C	3.642552	3.672144	0.249443
C	5.010027	3.666584	0.256363
C	5.744123	2.44834	0.171648
C	7.164621	2.41545	0.172671
C	7.84708	1.228721	0.089294
C	7.159263	-0.012441	0.000841
C	7.838622	-1.259335	-0.086702
C	7.148027	-2.440491	-0.169836
H	-5.351429	4.376824	0.549599
H	-3.007195	4.569811	-0.308227
H	-7.710496	3.291139	-0.229243
H	-8.91442	1.154075	-0.071749
H	-8.892777	-1.330834	0.105613
H	-7.632492	-3.436583	0.246143
H	-5.464532	-4.646966	0.316263
H	-3.00499	-4.609705	0.291494
H	-0.928599	-3.355489	0.170659
H	-0.930602	3.386853	-0.185193
H	0.991145	3.390067	0.189321
H	3.100738	4.609654	0.312835
H	5.55761	4.600062	0.326573
H	7.7084	3.351235	0.240823
H	8.931625	1.22525	0.090173
H	8.923159	-1.263296	-0.087696
H	7.684785	-3.38044	-0.236189
H	5.524078	-4.613326	-0.319482
H	3.067	-4.603874	-0.306247
H	0.968462	-3.370431	-0.1846
H	-5.34004	4.242343	-1.170694

Supplementary Table 6: Atom positions for DC+H⁺ isomer D.

Atom	X (Å)	Y (Å)	Z (Å)
C	-7.792306	-1.274639	-0.004407
C	-7.122908	-0.041387	-0.001687
C	-5.694246	-0.029391	0.003462
C	-4.974928	-1.25961	-0.00515
C	-5.682193	-2.494588	-0.004488
C	-7.089923	-2.468597	-0.005874
C	-7.838661	1.20771	0.000259
C	-7.183013	2.390967	0.002703
C	-5.737578	2.447211	0.004105
C	-4.987126	1.195994	-0.000749
C	-4.941403	-3.715908	-0.006795
C	-3.557963	-1.253763	0.00318
C	-2.843261	-2.485281	-0.003494
C	-3.577182	-3.711889	-0.00598
C	-3.568239	1.199937	0.00683
C	-2.841566	-0.028432	-0.003161
C	-5.07138	3.633863	0.00615
C	-3.592677	3.731322	0.006965
C	-2.847719	2.424526	0.00355
C	-1.46893	2.406844	0.00169
C	-0.71819	1.21375	0.000245

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Supplementary Table 6 – *Continued from previous page*

Atom	X (Å)	Y (Å)	Z (Å)
C	-1.416988	-0.028199	0.003784
C	-0.706916	-1.279367	-0.000412
C	-1.440526	-2.460907	-0.00291
C	0.739035	1.224291	0.000767
C	1.449353	-0.020171	-0.001329
C	0.756874	-1.270785	0.002785
C	1.465066	2.415021	-0.00116
C	2.867898	2.450906	-0.00243
C	3.584637	1.223714	-0.004993
C	2.8712	-0.009065	0.00433
C	1.498304	-2.449469	0.005355
C	2.902724	-2.466086	0.005332
C	3.602395	-1.230575	-0.001235
C	5.006599	1.237137	0.000752
C	5.729526	0.011801	-0.004129
C	5.024729	-1.223396	0.005009
C	5.742579	-2.449719	0.003751
C	5.013284	-3.675308	0.006944
C	3.647184	-3.68521	0.007531
C	3.594909	3.680747	-0.004899
C	4.960631	3.68994	-0.005921
C	5.706774	2.474209	-0.004919
C	7.126113	2.457141	-0.005828
C	7.82136	1.273743	-0.004459
C	7.147518	0.02211	-0.001719
C	7.840371	-1.219402	0.000054
C	7.162082	-2.412135	0.002934
H	-5.631599	4.563473	0.008779
H	-3.282921	4.33326	0.874955
H	-7.729888	3.32689	0.004201
H	-8.922307	1.179678	-0.001132
H	-8.876147	-1.286823	-0.006112
H	-7.631333	-3.408458	-0.007589
H	-5.485222	-4.653967	-0.008608
H	-3.027923	-4.646562	-0.008256
H	-0.933422	-3.416007	-0.007157
H	-0.956189	3.359253	-0.000452
H	0.95348	3.368207	0.000111
H	3.042278	4.613913	-0.005347
H	5.499671	4.630792	-0.00816
H	7.660222	3.400746	-0.008164
H	8.905865	1.282578	-0.00481
H	8.924842	-1.212145	-0.000233
H	7.709424	-3.348153	0.004036
H	5.565	-4.608804	0.008197
H	3.107872	-4.626082	0.010244
H	0.997868	-3.408797	0.009611
H	-3.281501	4.33939	-0.856129

Supplementary Table 7: Atom positions for DC+H⁺ isomer E.

Atom	X (Å)	Y (Å)	Z (Å)
C	7.814488	1.290775	-0.000948
C	7.146085	0.041608	-0.000146
C	5.724515	0.022715	0.003047
C	4.996371	1.239913	-0.003348
C	5.691681	2.474344	-0.001751

Continued on next page

Supplementary Table 7 – Continued from previous page

Atom	X (Å)	Y (Å)	Z (Å)
C	7.109358	2.469621	-0.001943
C	7.852453	-1.199453	0.00026
C	7.184401	-2.388465	0.000322
C	5.754384	-2.434398	0.000603
C	5.024459	-1.214891	-0.001913
C	4.94138	3.686668	-0.003345
C	3.564765	1.219223	0.002744
C	2.846979	2.455725	-0.002076
C	3.574071	3.679819	-0.003444
C	3.598809	-1.235592	0.003815
C	2.856596	-0.000227	-0.002049
C	5.043189	-3.648455	0.000482
C	3.659227	-3.660239	0.000802
C	2.929452	-2.466631	0.001333
C	1.431149	-2.510693	0.0027
C	0.698181	-1.199025	0.000817
C	1.410293	0.007573	0.002627
C	0.703828	1.272919	-0.000342
C	1.442234	2.443697	-0.001908
C	-0.735817	-1.207223	0.001842
C	-1.452931	0.035552	-0.001149
C	-0.757982	1.276962	0.002052
C	-1.461805	-2.408596	0.00075
C	-2.859266	-2.446111	0.000221
C	-3.580455	-1.21615	-0.004055
C	-2.872178	0.019161	0.005247
C	-1.500603	2.459244	0.002829
C	-2.903773	2.474559	0.002812
C	-3.604029	1.238891	-0.002577
C	-5.000528	-1.232278	0.002796
C	-5.725889	-0.007878	-0.004135
C	-5.02493	1.228675	0.004308
C	-5.745319	2.454021	0.001111
C	-5.017329	3.68101	0.002712
C	-3.651356	3.693206	0.003187
C	-3.586069	-3.678947	-0.001282
C	-4.950139	-3.688792	-0.002132
C	-5.698447	-2.471952	-0.002306
C	-7.115857	-2.457827	-0.003078
C	-7.813472	-1.273884	-0.002831
C	-7.143503	-0.02123	-0.001302
C	-7.839933	1.218776	-0.001014
C	-7.164672	2.41342	0.00045
H	5.591972	-4.583711	0.000581
H	3.131805	-4.608408	0.000219
H	7.732777	-3.323891	0.000621
H	8.936464	-1.181116	-0.000214
H	8.898533	1.305324	-0.001539
H	7.635491	3.417753	-0.0025
H	5.478189	4.629206	-0.004071
H	3.023192	4.613393	-0.005099
H	0.944934	3.403976	-0.004786
H	1.103519	-3.090293	0.874742
H	-0.941265	-3.357428	0.002674
H	-3.0319	-4.611016	-0.000861
H	-5.489015	-4.629581	-0.003587
H	-7.649145	-3.401725	-0.004584
H	-8.897953	-1.285838	-0.003063
H	-8.92431	1.208764	-0.001235
H	-7.714438	3.347888	0.000345

Continued on next page

Supplementary Table 7 – Continued from previous page

Atom	X (Å)	Y (Å)	Z (Å)
H	-5.570242	4.613677	0.002642
H	-3.114012	4.635114	0.004598
H	-0.998748	3.417948	0.00584
H	1.101761	-3.094878	-0.865506

VIBRATIONAL SPECTRA
PROTONATED HEXA-PERI-HEXABENZOCORONENE

Supplementary Table 8: Theoretical vibrational spectrum for HBC+H⁺ isomer A.

Frequency cm ⁻¹	IR Intensity km mol ⁻¹
10.3526	0.0043
11.7785	0.0337
22.9926	0.0022
81.3727	6.9162
87.3919	0.0326
107.8821	0.0219
113.5689	0.0057
116.9192	0.0177
126.0703	0.0879
152.9349	0.5058
196.9307	0.0942
208.2626	0.2378
264.9350	1.1096
269.7741	0.7249
273.9824	2.7803
277.5015	1.8934
279.2292	4.1459
285.1339	1.6619
292.6002	0.0732
336.4116	2.1191
339.6025	2.4752
345.6337	0.8681
350.2838	0.2918
353.4593	0.1524
359.3291	0.3418
381.4301	0.0119
394.6913	0.3097
399.2278	0.4612
439.1787	1.6948
452.5187	0.1209
468.7078	0.0587
474.7314	0.2956
503.6900	1.7134
507.2852	5.0372
512.4765	0.0952
513.4038	0.9194
529.0004	0.2115
540.4965	0.7865
549.3311	0.2397
551.4546	1.9806
553.1668	3.8518
554.3218	1.7403

Continued on next page

Supplementary Table 8 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
597.5407	2.2698
600.0137	0.6339
602.8563	2.7069
617.6330	4.0438
623.3983	1.0633
626.5886	1.4428
627.4323	0.6123
634.6797	1.3856
662.2561	0.297
666.6658	1.0552
676.1467	0.3296
681.6850	3.7853
686.6936	1.5278
688.3802	3.6377
693.6153	3.0122
713.3874	0.0945
726.0424	8.9857
736.8604	4.2372
753.9598	0.2709
763.6140	2.4066
772.8449	74.8722
789.5574	117.3716
792.6168	29.8222
793.5877	1.3655
795.2013	1.7802
800.3690	0.1796
809.3545	0.4011
825.5532	0.3482
831.4775	0.1959
839.1951	1.0149
846.3986	3.5432
886.5871	2.1385
892.5859	1.6269
901.3054	8.8746
906.7334	0.2528
912.4488	0.0501
920.2835	0.0511
932.4439	0.1845
935.8481	0.0497
942.6876	6.4909
984.9617	23.0009
989.8257	0.0238
994.0775	0.0226
997.5296	0.071
1000.4263	0.0571
1002.8899	0.0308
1006.3319	0.0035
1014.8556	0.1591
1018.4721	9.3275
1032.8635	24.6519
1077.9916	1.6096
1085.6068	0.0628
1100.8958	0.1077
1107.3385	26.9846
1118.3991	2.2931
1122.9206	0.357
1124.2857	0.9161
1145.5035	1.3711
1154.1787	2.35

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Supplementary Table 8 – *Continued from previous page*

Frequency cm^{-1}	IR Intensity km mol^{-1}
1164.0533	0.9712
1182.3060	12.2441
1193.1483	0.2971
1195.7886	2.1626
1212.9972	0.6287
1217.4137	38.1337
1236.2774	6.6384
1237.4144	3.6561
1246.4974	5.1545
1250.6410	35.6281
1258.9823	17.6475
1263.6189	138.3463
1271.6343	51.1864
1285.1613	11.4185
1300.5856	137.905
1312.2711	2.4074
1317.2624	154.022
1333.5060	92.276
1340.2135	16.9859
1346.1187	65.7963
1360.1569	112.2256
1361.7038	54.7928
1368.9843	8.158
1372.9682	0.8595
1383.9574	28.4593
1385.2336	12.1073
1392.8291	51.4782
1397.1907	88.7854
1403.6028	67.4117
1407.7169	3.4416
1413.3691	40.7024
1423.5842	18.9375
1427.2208	4.7773
1441.1288	8.3483
1453.8448	11.0346
1461.5582	2.0535
1479.6092	7.8118
1488.1645	12.3385
1493.6502	2.7525
1497.7992	65.5675
1519.9967	48.9752
1524.6670	57.4708
1536.6148	9.3619
1545.1940	59.4957
1563.9064	1.7688
1569.5420	84.9693
1584.1712	84.9104
1603.3488	79.9042
1614.5401	111.0884
1617.9687	30.5193
1624.3582	6.947
1631.4008	40.5618
1632.0219	3.819
1633.8157	42.3902
1634.8777	101.6189
1643.5723	7.9082
1679.0959	119.8427
2997.1300	2.8214
3011.0952	0.1604

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Supplementary Table 8 – *Continued from previous page*

Frequency cm^{-1}	IR Intensity km mol^{-1}
3182.2279	0.5882
3184.1025	0.2268
3184.9400	4.7921
3185.8994	10.4028
3189.3317	4.9386
3191.8636	5.2169
3207.4511	1.1335
3208.2880	0.2833
3211.1509	0.0519
3213.6569	0.0241
3217.7762	1.2109
3224.1492	0.5904
3227.2595	5.5215
3228.0956	4.1093
3231.4824	5.5929
3232.5745	12.6173
3249.0720	4.4123

Supplementary Table 9: Theoretical vibrational spectrum for $\text{HBC}+\text{H}^+$ isomer B.

Frequency cm^{-1}	IR Intensity km mol^{-1}
19.8021	0.0248
28.3006	0.1823
43.7701	0.7421
80.9286	6.3556
107.5268	0.0113
118.0242	0.0124
121.1824	0.8704
122.1307	0.2745
130.4845	0.2436
187.0672	0.2634
204.7532	0.2229
210.3629	0.0411
243.6825	6.9597
267.3585	1.2884
270.0301	0.1141
276.1180	1.6872
279.9862	4.5394
291.7150	0.1894
293.7393	0.9985
307.4972	0.6439
335.2961	0.4589
340.4322	1.1269
348.2049	0.0659
351.5302	0.0968
358.0552	0.2127
384.7285	0.0062
394.4065	1.1047
407.2382	0.8325
440.6654	1.9615
450.5079	3.7053
466.5702	0.2426
466.5789	0.0873
506.8706	0.4706

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Supplementary Table 9 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
506.9902	0.7173
512.5016	1.0026
516.4479	1.5926
532.9887	0.6318
542.0470	0.2339
548.0275	0.9138
550.9157	0.0047
556.7291	1.523
561.2750	0.0983
596.8358	5.6439
603.0355	3.9406
618.4676	0.2328
620.5793	3.3034
622.0792	0.0242
623.3019	0.0356
628.0242	0.0892
649.2904	1.6397
662.7118	0.0303
671.6302	0.0296
675.0996	2.8983
687.7050	2.6411
689.8947	0.8634
692.0663	1.4994
707.3216	4.1978
718.1320	0.4763
719.4015	1.8091
736.0391	0.1508
762.9384	33.561
788.6828	39.2141
789.9816	2.8502
795.9403	138.2807
796.2421	1.5343
797.9472	0.1842
803.6376	3.0158
818.3297	23.8213
823.5928	11.1092
829.6960	0.2111
833.5892	0.0203
844.5171	7.9204
848.5409	0.0865
865.7057	0.7078
890.1677	2.5601
892.2680	5.9419
914.3394	0.0011
916.7837	0.2629
920.1570	0.1913
925.2921	0.3801
927.5258	0.0126
947.0013	4.2268
961.6897	11.1635
979.0191	26.6434
994.4901	0.1086
995.5253	0.009
1001.5984	0.1877
1002.7202	0.0036
1005.9550	0.2436
1014.1614	10.9871
1016.8119	1.5812
1043.8358	24.9422

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Supplementary Table 9 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
1064.7593	4.2784
1065.2797	2.4043
1102.1491	2.858
1114.5954	0.0236
1116.6232	1.2007
1120.6844	1.8366
1123.9268	0.0174
1131.0847	0.3015
1140.4976	13.6307
1159.6665	2.5796
1165.6399	2.7201
1169.2326	0.2891
1192.5255	0.0828
1193.6035	0.3481
1214.1722	0.1347
1231.9040	35.6234
1234.0683	13.1304
1246.3745	40.4822
1248.7153	29.1961
1259.6979	0.5157
1268.1484	78.2643
1277.1809	119.4662
1281.9948	5.8847
1297.3095	15.8933
1307.9918	1.2717
1326.5399	71.1532
1329.4908	78.1511
1337.1484	22.2761
1346.3096	151.2024
1354.4800	238.1362
1361.9703	110.6372
1362.5660	0.3263
1369.0777	9.9244
1369.3978	5.3092
1377.1681	1.985
1386.6180	12.2319
1391.5479	10.0059
1397.5998	9.9643
1406.8748	1.23
1410.1830	1.122
1417.9481	144.4158
1420.5477	101.8536
1435.5822	24.5691
1455.7515	10.1716
1471.1132	2.7345
1472.5725	14.1836
1483.1966	359.0143
1492.5088	5.3712
1508.8198	6.6266
1514.6808	23.7509
1530.1415	20.015
1539.7326	6.2095
1548.3792	40.2569
1561.4377	145.0513
1580.4154	63.3161
1592.8500	0.0003
1612.0360	341.7512
1612.9886	31.5402
1623.9855	0.6671

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Supplementary Table 9 – *Continued from previous page*

Frequency cm ⁻¹	IR Intensity km mol ⁻¹
1624.0174	6.5889
1629.9510	43.2391
1632.2674	2.2501
1633.5712	73.7648
1634.4523	25.8352
1638.7742	36.6729
1653.6408	68.9934
2957.4213	1.9771
2961.4754	7.6922
3183.3491	1.4504
3183.3996	0.0737
3183.9564	2.343
3186.0475	9.4593
3186.5153	5.8814
3194.6529	0.7739
3195.1525	2.8897
3204.3424	1.7631
3204.6636	3.3126
3208.0665	0.0225
3209.5971	0.2425
3211.6949	0.0131
3212.6553	0.2288
3227.4042	0.7932
3228.4574	5.8606
3229.2727	18.0046
3229.5815	5.394

**VIBRATIONAL SPECTRA
PROTONATED DICORONYLENE**

Supplementary Table 10: Theoretical vibrational spectrum for DC+H⁺ isomer A.

Frequency cm ⁻¹	IR Intensity km mol ⁻¹
12.3173	0.0262
22.0242	0.8342
52.0335	0.0331
82.5219	0.0013
91.3251	0.8167
95.5302	0.1865
101.5621	0.7846
112.1345	0.1227
137.6200	11.3563
150.9307	0.1313
173.4591	0.0021
182.5375	8.9085
193.1064	0.4845
218.7106	0.726
224.0312	0.3206
247.1206	0.9237
267.0355	0.6037
280.0650	0.0497
292.0761	0.0001

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Supplementary Table 10 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
299.7113	0.1393
306.6082	0.1743
314.0262	0.3171
331.2258	0.2151
361.7190	0.5228
368.4256	7.2008
369.8677	1.4523
375.1415	1.1398
382.8974	3.828
391.8308	0.045
401.0885	7.9201
417.3236	2.3259
421.5429	4.8452
448.8453	0.6116
451.7033	0.047
458.2535	0.1981
476.3774	0.0682
476.8918	8.9048
485.7201	7.0731
504.4794	1.9289
516.3092	4.4569
516.6402	5.5596
528.7504	0.8111
531.5142	1.0945
533.4611	6.5843
537.4890	3.3447
538.1437	2.6422
542.0693	4.1204
557.1382	6.75
563.0958	2.0983
566.1097	20.6491
568.6690	11.4512
596.7731	7.6107
617.3373	1.1546
623.0519	0.3285
632.0246	1.2083
633.1896	4.096
638.3221	5.3941
649.5022	0.3532
656.9344	0.0011
662.8393	0.0758
670.2764	0.0824
674.0447	0.4899
684.0511	1.3736
687.5603	0.3109
688.9091	0.6911
690.0071	2.1382
697.4693	12.6716
699.8122	0.2743
719.1272	0.6069
725.8979	0.2345
728.5252	1.362
731.7180	0.0503
737.9748	18.3876
749.4834	0.0498
785.5124	11.5836
791.2340	0.1972
794.0891	0.0131
799.1468	8.2915

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Supplementary Table 10 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
806.5463	5.7462
808.1858	3.5259
811.5285	0.9008
815.9500	6.0919
823.1784	0.5583
825.7636	0.3334
830.2845	1.2793
847.4048	0.0045
865.0303	34.5507
872.3153	81.651
886.7760	0.5849
893.7204	1.9597
908.2645	0.2873
908.6146	11.9204
912.5590	99.1689
921.6316	5.0962
948.9870	1.763
950.6746	1.3137
979.1053	0.0023
984.4610	0.4484
984.7940	0.0032
990.7104	0.0017
994.3447	0.0068
996.3013	0.0084
997.4484	0.0821
1004.1674	10.9279
1013.1983	61.0877
1017.8286	2.9525
1034.3728	85.3927
1060.7233	3.9755
1078.2665	4.8845
1082.7642	21.9945
1118.5269	47.7051
1168.1735	2.0253
1170.6654	38.0587
1173.0613	9.1553
1173.7516	16.9226
1175.5543	4.3715
1183.2054	23.2864
1195.9420	151.0889
1198.2827	0.7758
1205.2845	86.9062
1207.2690	11.9676
1210.7526	0.5472
1224.9386	13.4542
1228.6791	71.9853
1241.1545	207.9778
1248.9590	15.2766
1253.1490	96.2715
1256.9863	20.9385
1259.0971	1.5361
1265.1821	13.8653
1269.5992	226.7155
1292.1220	45.0694
1327.3412	322.8944
1330.8010	226.4244
1333.5135	555.2456
1338.6682	44.8979
1343.5515	151.4614

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Supplementary Table 10 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
1356.8650	3.0477
1370.0209	208.3542
1378.5111	113.5046
1384.5820	102.2039
1387.2841	65.8138
1393.5588	33.1125
1400.3993	186.279
1406.5594	12.3381
1408.1371	10.612
1418.7920	4.0903
1421.0101	67.1789
1426.5780	7.692
1429.1393	9.3903
1435.1288	17.8203
1441.7480	2.406
1450.3507	24.8481
1460.6238	18.9836
1466.9955	15.5676
1469.2836	73.1788
1471.7618	41.7966
1479.6674	17.3894
1484.7622	17.0562
1498.4947	2.3622
1500.2405	43.9687
1508.7138	0.0678
1520.5575	160.935
1524.6522	4.5835
1546.0741	3.3825
1551.7341	23.106
1557.6610	469.2991
1571.2540	13.3558
1580.9246	60.5889
1586.3213	129.2169
1601.1834	1861.6943
1621.7089	18.6498
1633.0162	34.7371
1635.7845	67.5024
1639.5692	96.6374
1645.4708	221.3645
1646.2817	29.492
1650.5937	5.3077
1650.8971	4.5432
1661.3909	297.8893
2980.6953	5.4545
2987.6653	0.0167
3168.0001	0.8021
3168.0664	6.0307
3168.3922	0.4233
3168.5248	1.146
3169.4459	0.1226
3170.7916	0.0779
3171.8705	0.0378
3174.2552	0.0771
3184.0001	8.5739
3184.0632	2.2393
3184.6055	0.0969
3185.8436	26.712
3186.6597	51.9585
3187.8437	13.3445

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Supplementary Table 10 – *Continued from previous page*

Frequency cm^{-1}	IR Intensity km mol^{-1}
3190.2621	8.8366
3192.1537	0.1953
3196.1380	0.3256
3210.8287	6.2522
3217.2039	5.2771

Supplementary Table 11: Theoretical vibrational spectrum for DC+H⁺ isomer B.

Frequency cm^{-1}	IR Intensity km mol^{-1}
4.6982	0.0346
22.7748	1.06
54.0893	0.0011
77.9027	0.7845
94.4433	2.6361
94.8330	0.9056
96.8726	0.0758
111.1219	0.0042
140.2654	7.6759
155.2489	1.9201
172.4314	0.0054
181.5579	2.7244
191.3138	0.866
207.7143	1.2503
222.3744	0.2299
243.4229	0.6507
273.1785	0.1636
275.6729	0.0343
291.3526	0.0002
296.0344	0.0193
314.0418	1.3926
315.3998	1.7031
330.0918	0.4167
356.9882	0.1729
367.7087	3.8565
369.5711	9.5534
375.0187	0.022
386.5038	0.3869
395.2804	0.0023
404.8769	3.6657
414.0071	8.7087
424.5358	0.4053
445.9021	0.234
447.9320	0.0255
452.2680	0.1559
475.3913	0.5365
477.4461	0.2383
477.8930	0.2183
485.8459	3.1036
503.4222	0.1533
504.5577	1.3908
515.2855	4.2344
523.1624	0.3485
532.3856	0.06
534.0065	4.0749

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Supplementary Table 11 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
535.4521	3.2503
537.1756	0.8456
541.3922	7.2862
554.4424	4.5512
561.2441	0.3495
571.3874	28.2811
587.4576	9.5743
603.2811	0.4546
621.2254	0.0677
628.8343	0.1758
631.8407	4.4499
639.3274	1.138
640.3623	0.4398
641.7541	0.0349
650.9809	1.0073
658.2635	0.0154
675.3411	1.9193
676.0547	2.8863
684.1793	0.2765
685.3876	0.2314
689.4592	0.0298
696.0075	0.5856
697.0593	0.7211
716.3603	0.2402
719.9987	0.5813
728.4527	0.0286
729.4850	0.4524
740.8797	4.4133
749.4977	0.5149
783.4203	2.7628
784.7896	0.0895
791.7160	0.0055
793.4678	1.0845
805.7880	14.9249
808.6981	0.799
814.4934	4.6313
819.9203	2.5223
823.0918	0.9375
826.9545	0.7151
841.7772	8.249
843.4748	0.7898
861.0189	24.3652
868.6113	79.6971
886.9066	0.3314
890.7876	0.797
901.9345	0.5994
909.9149	118.4359
911.5872	3.6691
916.7327	3.4124
945.6874	2.8202
951.0707	0.0732
975.5250	0.0005
980.3779	0.1377
986.7291	0.0004
989.9581	0.1967
990.5076	0.3263
992.3278	0.0089
999.6072	0.0353
1006.4549	28.5238

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Supplementary Table 11 – *Continued from previous page*

Frequency cm^{-1}	IR Intensity km mol^{-1}
1014.9949	32.2863
1018.9886	0.0184
1035.1993	11.5201
1058.7158	3.843
1076.8078	9.6869
1082.2756	5.1806
1125.4227	21.6326
1163.8839	5.6421
1168.9552	15.3392
1172.5428	3.7818
1173.5032	7.8009
1177.9710	4.4915
1182.5873	2.3902
1182.7990	0.9391
1205.5894	21.1597
1211.0254	2.9045
1214.3806	4.6794
1218.0565	8.3098
1222.8802	1.5638
1228.1593	1.6605
1242.1773	41.0453
1246.8734	17.6355
1249.3733	22.6896
1256.2130	9.2471
1258.2059	45.7178
1259.3609	9.2486
1263.5985	33.4391
1278.1061	12.6847
1316.6935	26.7178
1324.3371	37.833
1331.8999	8.7038
1338.0778	24.4459
1350.3311	163.3465
1368.3763	96.3853
1369.5210	20.2193
1369.9687	297.2906
1374.6708	31.0858
1379.0634	250.3214
1385.8638	23.26
1392.9330	41.6207
1399.3766	15.2407
1406.5391	26.3785
1417.9252	0.0576
1422.9353	6.5078
1425.2537	1.7749
1426.4795	36.7511
1437.2812	11.5207
1438.3895	2.7789
1440.4899	2.3033
1454.7544	46.6607
1465.1234	2.3439
1465.8283	2.2457
1468.6647	18.7463
1480.4684	0.3024
1483.0101	0.9299
1487.9097	14.0745
1505.2238	0.0067
1518.6033	6.2786
1524.7114	43.2159

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Supplementary Table 11 – *Continued from previous page*

Frequency cm^{-1}	IR Intensity km mol^{-1}
1531.3742	11.9655
1535.5185	8.1586
1540.4548	45.3461
1561.2349	71.1906
1567.5216	33.8445
1579.8346	8.3033
1584.2092	32.3756
1610.3666	323.2561
1610.4627	193.6705
1624.5393	116.8866
1632.0075	33.2052
1635.8229	22.2482
1641.3513	0.9745
1648.0261	15.4568
1649.3480	31.2998
1651.8842	7.2276
1654.5584	69.045
2979.8293	14.8258
2987.1446	1.1967
3164.4011	1.1447
3164.6176	1.0611
3166.4097	0.5033
3167.8779	0.039
3170.0352	2.1811
3172.1253	1.0701
3173.5093	1.4213
3178.6302	3.2711
3181.0800	7.825
3181.4519	0.3306
3183.0537	26.6974
3184.2554	53.4021
3185.1927	7.2781
3187.4321	3.4001
3187.7207	5.7773
3189.6639	3.9635
3194.1110	7.8037
3209.0485	3.7382
3209.4846	5.2235

Supplementary Table 12: Theoretical vibrational spectrum for DC+H⁺ isomer C.

Frequency cm^{-1}	IR Intensity km mol^{-1}
9.5769	0.1374
22.6002	0.3452
51.9764	0.4595
84.3324	0.9098
92.4448	2.8305
94.8558	0.7891
100.8488	0.05
112.9863	0.0507
133.3817	3.6312
148.6035	5.7097
172.0108	0.0769
179.7637	0.9108

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Supplementary Table 12 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
192.9965	0.8644
216.9232	0.2531
230.4709	0.6887
257.6480	1.7139
260.8653	0.3276
280.3384	0.1029
290.7453	0.0087
293.7561	0.0962
301.3357	0.0378
313.0291	0.9977
330.7664	0.6523
361.1824	0.6863
367.5616	15.1827
370.2568	1.4052
375.4131	0.4061
384.9614	1.534
404.6391	2.2683
410.1511	2.0241
419.1599	4.6191
423.8385	1.8875
446.7425	1.574
454.5329	0.2277
462.3851	0.1472
475.3472	0.041
477.2773	0.1393
484.7065	2.9039
495.9289	0.0658
504.0086	0.9717
507.7894	0.2366
518.7136	1.8781
521.7274	2.257
531.1613	1.566
532.9063	4.6158
535.0399	0.1543
539.0977	8.8374
539.7833	1.4153
554.3272	3.5377
560.5569	1.8107
576.2582	29.4707
593.9551	1.531
597.2662	2.5367
615.6509	5.18
630.5150	1.6433
635.1921	1.6348
639.1797	1.3147
649.9095	0.0325
652.5008	0.6072
659.1134	0.2917
667.9248	0.9937
671.5661	2.3262
681.5717	2.0841
685.2780	0.3642
687.8284	1.2258
689.8314	0.2869
696.2417	2.5587
713.5760	0.5585
715.2389	0.458
727.2494	2.4441
730.5813	0.3409

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Supplementary Table 12 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
740.7339	0.4006
743.6770	2.5431
748.8402	0.298
783.9603	0.1315
789.5025	1.1308
791.8155	0.1048
794.0507	1.1536
806.1172	13.9227
806.9915	5.3764
811.5792	7.4973
814.8383	4.8801
826.2575	0.336
828.2986	2.584
841.4239	0.1264
843.4684	0.0211
864.6628	0.5539
869.6018	76.0349
877.1239	51.4495
893.3273	8.3148
898.9911	51.6781
909.5487	1.5023
920.0244	16.3329
927.0211	39.1597
939.7172	3.1005
949.4018	1.3075
976.1618	0.0013
980.9808	0.1433
985.7634	0.2738
987.2472	0.005
992.7689	0.0527
992.8426	0.0723
1000.7080	0.0141
1008.3464	12.0089
1016.0456	21.5804
1018.7953	3.3034
1023.9207	23.3762
1059.7944	3.1199
1071.8044	6.6574
1101.8082	13.0137
1127.1021	12.4477
1166.4161	0.4345
1171.6496	13.6953
1173.3507	12.8591
1175.0103	3.4618
1177.3374	2.3111
1181.8903	0.9152
1183.1864	0.8948
1196.0915	20.1894
1207.0902	27.2035
1212.5617	0.0262
1217.5000	27.978
1222.0884	6.0561
1237.8905	38.1662
1241.7064	2.4822
1244.4398	33.8931
1248.7504	2.5597
1253.9005	18.3138
1256.2330	2.4746
1259.9095	40.1011

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Supplementary Table 12 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
1267.6073	38.3362
1278.5339	20.8455
1311.6539	64.657
1331.3571	42.1895
1334.2163	27.0814
1335.4741	107.3324
1343.3232	83.4439
1359.8592	66.8503
1368.0827	53.5646
1373.3885	97.2127
1377.1025	27.3095
1380.8391	40.7996
1382.9655	34.635
1393.3420	75.7986
1398.6682	243.092
1407.2051	6.5871
1418.2737	13.5509
1424.0505	18.3235
1425.1646	13.2183
1426.9941	30.4284
1433.5027	11.1957
1438.4250	2.085
1451.5228	3.47
1455.2683	1.7205
1465.9717	28.0476
1466.0468	0.605
1471.1093	17.9073
1482.4569	3.0509
1482.9039	7.4464
1487.7824	7.389
1504.0599	2.2062
1514.7651	6.3714
1525.5968	56.0732
1525.9803	43.9305
1537.0636	8.2852
1544.2648	69.7386
1560.0319	22.3706
1565.9943	7.6031
1580.1750	108.2085
1584.4617	6.3613
1606.3071	219.9322
1613.6108	95.346
1621.5481	48.7431
1634.8939	28.5898
1638.8737	113.947
1641.4526	6.5963
1646.4173	23.5514
1648.8765	17.6347
1651.6502	1.5721
1652.8825	14.1763
2977.0075	8.943
2983.7098	0.961
3164.6923	0.9172
3165.0594	1.1258
3166.9066	0.5106
3168.3900	0.011
3170.4141	1.5239
3172.0891	1.8002
3174.1826	0.0769

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Supplementary Table 12 – *Continued from previous page*

Frequency cm^{-1}	IR Intensity km mol^{-1}
3175.5789	0.6154
3181.2868	6.7762
3181.7088	1.7751
3183.3561	17.9411
3184.3574	34.9337
3184.7835	25.5276
3185.6119	5.3582
3186.0204	4.7178
3189.4547	3.2616
3190.9658	15.3312
3206.6653	2.7188
3207.4652	4.3481

Supplementary Table 13: Theoretical vibrational spectrum for DC+H⁺ isomer D.

Frequency cm^{-1}	IR Intensity km mol^{-1}
12.4778	0.0913
21.7523	0.2575
50.6565	0.5481
81.9211	1.0953
92.4435	2.4236
95.2394	0.1266
100.4476	0.3351
113.0069	0.0031
138.5012	7.4297
152.7515	1.8053
177.2326	0.0355
181.7940	13.3058
192.3716	1.2602
203.3329	0.3727
223.2521	0.0125
243.2980	0.5021
267.3622	0.9826
283.9480	0.0478
291.7680	0.0027
295.1731	0.0595
300.8347	0.1747
316.1489	1.0391
330.7824	0.0349
361.0339	0.1057
368.2059	1.8315
369.9323	2.1647
374.1003	0.7172
385.0244	6.5528
400.6589	0.042
403.6927	12.8997
417.7835	9.6221
422.0117	17.39
447.5029	0.2848
455.6840	0.1725
465.7392	0.0516
477.8675	0.6442
478.0076	0.0358
484.5150	4.5382

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Supplementary Table 13 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
499.0360	0.2467
504.3995	0.1675
517.4360	8.8333
529.8681	0.6705
531.7310	6.4011
532.2133	1.2033
536.4245	1.5935
537.6183	1.8607
538.3749	5.8773
555.8984	0.556
562.9508	1.4674
564.5340	13.5874
584.0137	10.8081
593.3424	11.381
609.6155	0.2312
616.5071	0.3757
631.2349	2.0146
637.6137	1.2084
640.1955	0.2317
648.8669	0.3512
658.1876	0.1408
663.3984	0.0173
663.9376	0.1266
681.8872	1.9484
683.8909	3.0151
690.0040	2.788
692.9519	0.3174
695.8820	0.3612
696.0838	0.2341
715.2432	0.1185
719.5321	0.488
719.7343	0.5559
727.7957	0.2652
732.1021	0.0482
740.6756	8.0871
748.8414	0.2938
787.6048	0.3373
789.0555	12.3063
791.3462	0.1538
793.8185	0.009
805.6054	3.0927
807.3434	14.1505
812.5481	5.7683
815.7078	6.3179
824.0336	0.4542
827.0132	6.9023
831.4425	0.6092
846.8044	0.0035
871.3259	28.4602
874.2996	70.8467
884.7534	8.4022
894.7157	2.3243
904.6981	36.629
912.2598	84.1979
916.2578	0.3326
919.0558	45.9282
948.4020	0.0073
949.8649	1.1008
978.7424	0.0089

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Supplementary Table 13 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
983.3555	0.0659
984.2400	0.1209
990.2226	0.0017
994.8150	0.1198
995.7331	0.0064
1000.3128	0.1006
1000.6786	11.2246
1012.8967	35.2739
1018.1364	0.0919
1023.9633	29.2457
1060.7485	18.768
1076.7819	1.8439
1092.2229	4.3584
1123.0563	34.8424
1165.8348	18.7088
1169.1717	6.3426
1173.3504	8.0054
1174.8277	0.9291
1175.6154	5.359
1181.1895	167.7073
1185.5029	9.2889
1200.7292	0.4129
1204.5735	150.4583
1207.6654	7.2846
1223.8266	40.9876
1232.9363	173.6931
1234.9245	151.0829
1241.6051	103.8915
1248.0114	0.2923
1253.2312	1.5139
1256.1952	68.2397
1257.9268	40.3012
1264.5839	0.5384
1267.8778	180.7529
1285.3422	33.9134
1322.1061	714.9802
1331.8676	161.956
1335.6711	248.6514
1337.3212	4.7328
1341.8876	72.7512
1363.7858	60.6762
1370.9441	425.3972
1373.2381	65.0295
1377.4158	88.5966
1383.2536	60.4409
1395.7293	11.863
1400.4866	54.269
1406.2744	13.7611
1416.3885	7.5496
1420.0531	0.4457
1423.8937	15.2844
1425.9437	33.251
1426.8332	1.4881
1434.7642	10.4737
1442.4340	21.8861
1444.2835	3.1596
1458.1477	12.1305
1464.1917	7.7653
1469.7247	27.8745

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Supplementary Table 13 – *Continued from previous page*

Frequency cm^{-1}	IR Intensity km mol^{-1}
1474.9046	15.3423
1481.8171	55.2306
1485.6603	5.176
1491.7130	81.0245
1500.6109	67.7972
1507.8449	6.3162
1520.1136	207.3299
1524.2196	15.0651
1543.8839	30.166
1553.0361	148.3065
1558.2705	30.3052
1567.0358	189.1478
1578.8006	2.4852
1581.2406	37.9682
1604.9764	1379.945
1619.8824	138.9971
1632.2071	20.6542
1634.2352	41.4445
1636.2081	243.9395
1644.7255	156.6858
1645.0096	32.6162
1649.1776	2.6937
1650.7840	2.3186
1663.1557	74.6965
2985.3500	3.5534
2994.4153	0.0078
3167.5213	0.7827
3168.0096	0.5095
3169.1647	0.1952
3170.5782	0.0987
3170.8191	0.115
3171.9352	1.2625
3173.7780	1.2921
3175.7828	0.8212
3183.7593	3.2229
3184.2770	0.0468
3185.5597	26.3651
3186.4535	51.7615
3187.7430	3.5962
3188.8077	14.5391
3189.9286	0.1818
3191.6233	21.7556
3191.8955	0.2127
3209.1552	5.6458
3210.5941	5.8846

Supplementary Table 14: Theoretical vibrational spectrum for DC+H⁺ isomer E.

Frequency cm^{-1}	IR Intensity km mol^{-1}
15.0388	0
20.9827	0.0482
52.7280	0.434
73.5461	0.6602
93.7146	0.102

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Supplementary Table 14 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
93.9315	1.3356
99.3769	1.1305
113.2152	0.4233
133.6588	7.2777
141.5583	4.2812
171.0090	0.0292
180.0381	10.6042
189.9335	0.2401
224.2976	0.0287
228.8172	0.0011
250.3565	0.3388
266.3686	0.0006
280.1774	0.0009
292.0366	0.0027
303.7216	0.2034
313.5332	0.1778
318.3288	0.9814
325.4227	0.135
368.8540	4.0895
369.5207	0.6172
373.5391	0.4218
382.8185	0.2708
384.6184	17.3456
405.2835	1.9813
417.1137	6.5713
423.5748	1.324
425.2935	9.7207
449.7263	2.8195
456.3141	0.078
461.3085	0.0708
477.8732	15.0652
478.9886	0.4753
483.1366	2.1769
489.8451	0.1111
498.2223	1.0584
502.9926	2.398
518.5645	0.1551
518.7980	18.7882
529.5170	4.9641
535.4729	0.0603
538.8742	6.2765
539.2626	4.397
545.7438	6.8275
553.5502	0.3911
560.8564	0.2763
576.1928	31.236
587.0922	0.7166
600.8853	2.8364
613.9805	0.2546
629.0050	0.0693
632.4370	14.7271
640.0590	0.1055
641.7947	0.1442
650.3354	1.0549
658.0954	0.0689
660.8794	0.0329
674.3222	3.3963
678.7793	0.4497
684.1673	0.0689

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Supplementary Table 14 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
690.2393	2.0721
698.4994	5.4503
707.1591	0.7116
712.4128	0.031
718.7860	0.1772
724.9874	1.5394
726.4403	0.1954
732.5774	0.0461
743.1026	24.327
744.3594	4.9649
786.2590	0.2906
794.3788	0.148
795.9567	0.0063
796.7444	1.305
805.5411	17.9076
816.3464	7.2139
819.7349	4.1848
821.5326	0.1686
822.1644	1.9875
826.0213	0.2581
847.6700	0.2943
850.0004	0.4106
870.5642	55.0318
874.8360	47.2945
894.9899	34.4416
899.9814	44.8681
912.9748	2.1159
914.9224	50.1852
921.6304	18.5032
923.2513	3.0485
950.9904	0.1869
979.4567	0.114
981.2970	0.0249
984.3094	0.1641
987.1188	0.1835
992.8871	0.0036
995.0744	0.0204
998.4697	0.0082
999.5962	0.0641
1009.4532	5.721
1015.5163	0.5024
1016.8824	1.1252
1043.8486	63.5035
1055.3319	4.8399
1066.4814	18.5772
1119.9271	0.4689
1155.5351	100.7079
1165.5994	10.7835
1173.7572	6.9443
1174.0516	3.7785
1176.1388	90.2778
1177.5800	100.2034
1179.8657	6.3659
1187.1813	3.9364
1200.9588	134.6692
1208.3024	83.2829
1221.4952	102.1183
1226.5404	40.7947
1233.5751	406.1411

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Supplementary Table 14 – Continued from previous page

Frequency cm^{-1}	IR Intensity km mol^{-1}
1234.9920	0.3595
1240.8683	190.161
1246.5792	152.3324
1249.8344	0.2464
1250.6556	12.64
1252.6318	23.3554
1257.8285	5.7736
1261.5945	88.871
1279.0152	110.5346
1301.0702	473.515
1325.8937	583.0683
1335.4806	37.5132
1337.3365	9.7831
1351.2543	135.6526
1356.4388	3.7488
1371.0209	409.5198
1378.2714	496.0991
1379.2976	25.7742
1384.1491	4.9008
1392.0512	70.665
1405.7811	14.5831
1411.2416	80.3445
1418.9880	44.9957
1422.5313	4.2562
1425.3327	3.7675
1427.9650	16.4292
1433.9460	27.6674
1437.7994	79.0571
1445.9609	50.9824
1450.6761	51.2969
1454.4793	12.6548
1464.3202	20.713
1467.8512	41.5399
1469.4696	1.4915
1477.8774	27.61
1485.1948	68.3713
1489.9063	284.7843
1499.3540	4.0392
1502.5443	36.5461
1512.9898	236.6528
1523.8568	172.1247
1536.5858	78.3797
1542.3676	134.2248
1558.6576	96.8838
1561.7172	695.4676
1577.3573	84.7388
1579.7928	4.899
1599.6655	282.522
1616.4698	163.4086
1630.8749	20.5626
1633.3203	136.8023
1636.5664	47.8717
1641.2941	27.172
1645.2625	172.0991
1648.2085	56.9567
1650.4093	13.1179
1653.0137	27.7139
3011.1048	4.5117
3032.1680	0.0255

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Supplementary Table 14 – *Continued from previous page*

Frequency cm⁻¹	IR Intensity km mol⁻¹
3164.7512	2.3614
3169.9311	0.6064
3170.3794	0.1132
3170.4299	0.2374
3171.3115	0.1059
3171.5217	0.4878
3172.6094	0.0514
3173.0093	0.6459
3183.4983	5.3209
3185.7008	1.1813
3186.2580	0.2467
3186.4751	0.4593
3187.3768	6.2751
3187.5028	32.9905
3188.1829	45.9579
3188.6875	29.7341
3192.1679	0.1661
3198.7847	1.7959
3209.8564	5.1626