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SUPPORTING INFORMATION

C-doped boron nitride fullerene as a novel catalyst for acetylene hydrochlorination: a DFT study

Fei Zhao, Yang Wang, Mingyuan Zhu, Lihua Kang*

College of Chemistry and Chemical Engineering/ Key Laboratory for Green Processing of Chemical Engineering of Xinjiang Bingtuan. Shihezi University, Shihezi, Xinjiang, 832000, PR China

*Corresponding author.E-mail: kanglihua@shzu.edu.cn

Tel: +86-0993-2057213; Fax: +86-0993-2057270

Cartesian coordinates, imaginary vibrational modes, energies [in B3LYP/6-31+G(d, p) level of theory] for the key structures involved in this study. Bond lengths are in Å and angles are in °.

Reactant

HCl Energy=-460.796499(a.u.)

Atom	Bond	Angle	X	Y	Z
Cl			0.000000	0.000000	0.071482
H	1.286683		0.000000	0.000000	-1.215201

C_2H_2 Energy=-77.310319(a.u.)

Atom	Bond	Angle	X	Y	Z
C			0.000000	0.000000	0.604031
C	1.208062		0.000000	0.000000	-0.604031
H	1.066461	180.000000	0.000000	0.000000	1.670492
H	3.340984	0.000000	0.000000	0.000000	-1.670492

Catalysts

$B_{12}N_{12}$ Energy=-956.036748(a.u.)

Atom	Bond	Angle	X	Y	Z
B			0.000000	0.961353	1.971396
B	1.9227060		0.000000	-0.961353	1.971396
B	2.4147026	66.5389968	-1.971396	0.000000	0.961353
B	2.4147026	60.0000000	-0.961353	1.971396	0.000000
B	2.4147026	66.5389968	1.971396	0.000000	0.961353
B	1.9227060	114.7265980	0.961353	1.971396	0.000000
B	2.4147026	98.6309250	0.000000	0.961353	-1.971396
B	1.9227060	114.7265980	1.971396	0.000000	-0.961353
B	1.9227060	114.7265980	0.000000	-0.961353	-1.971396
B	2.4147026	114.7265980	-0.961353	-1.971396	0.000000
B	1.9227060	66.5389968	0.961353	-1.971396	0.000000
N	1.4392013	35.0217960	-1.123613	0.000000	2.124351
N	1.4392013	125.6734204	0.000000	2.124351	1.123613
N	1.4392013	35.0217960	-2.124351	1.123613	0.000000

N	1.4392013	94.3195928	-2.124351	-1.123613	0.000000
N	1.4392013	143.9093196	0.000000	-2.124351	1.123613
N	1.4392013	143.9093196	2.124351	1.123613	0.000000
N	1.4392013	35.0217960	0.000000	2.124351	-1.123613
N	1.4392013	143.9093196	1.123613	0.000000	-2.124351
N	1.4866408	49.7096565	-1.123613	0.000000	-2.124351
N	1.4392013	143.9093196	0.000000	-2.124351	-1.123613
N	1.4392013	143.9093196	2.124351	-1.123613	0.000000
B	1.4392013	111.2278810	-1.971396	0.000000	-0.961353
N	1.4392013	35.0217960	1.123613	0.000000	2.124351

$B_{11}N_{12}C$ Energy=-969.134294(a.u.)

Atom	Bond	Angle	X	Y	Z
B			-2.307917	-0.302131	0.375770
B	2.1029741		-1.075375	-1.97104	0.719402

B	2.5756304	65.9053932	-1.084297	-1.155714	-1.723759
B	2.5756299	114.0950867	-1.354935	1.375312	-1.330653
B	2.5756295	65.9054148	-0.611523	0.019271	2.287004
B	2.1029740	65.9053755	-1.118550	1.962799	0.674710
B	2.5756300	65.9054196	1.066998	1.971304	-0.688073
B	2.1029744	114.0951006	1.075920	1.155978	1.755088
B	2.1029741	114.095072	2.299540	0.302395	-0.344441
B	2.5756295	114.0950976	1.110173	-1.962535	-0.643382
B	2.1029740	65.9053754	1.346558	-1.375048	1.361981
N	1.4870269	44.9999881	-1.809839	-1.430329	-0.455095
N	1.4870268	44.9999893	-2.080463	1.100702	-0.062013
N	1.4870272	125.2643652	-0.856847	0.247094	-2.161533
N	1.4870279	90.0002834	0.375696	-1.421815	-1.817901
N	1.4870274	106.7787997	0.384644	-2.237145	0.625258
N	1.4870272	90.0000091	-1.573454	-0.842842	1.550268
N	1.4870272	90.0003225	-0.384073	1.422079	1.849230
N	1.4870265	45.0000289	-0.393021	2.237409	-0.593929

N	1.4870269	90.0003446	1.801462	1.430593	0.486424
N	1.4870272	45.0000225	1.565077	0.843106	-1.518939
N	1.4870260	45.0000040	2.072086	-1.100438	0.093342
N	1.4870272	45.0000176	0.848470	-0.246830	2.192862
C	1.4870272	89.9999926	0.603146	-0.019007	-2.255675

$B_{12}N_{11}C$ Energy=-939.253191(a.u.)

Atom	Bond	Angle	X	Y	Z
B			-0.834981	0.989420	1.886393
B	2.0242148		-0.846855	-1.034549	1.857167
B	2.4689139	65.8069712	-2.190078	0.011701	0.068891
B	2.4095097	60.2833333	-0.868933	1.981953	-0.353507
B	2.5468318	66.6000235	1.491713	-0.033468	1.723460
B	1.9257429	114.4588039	0.884156	1.952262	0.442912
B	2.4174656	98.3918973	0.809473	0.982635	-1.777746
B	1.9356630	112.7560338	2.194637	-0.011539	-0.079928
B	1.9230474	114.7026666	0.798425	-0.940177	-1.805734
B	2.4093524	100.072444	-0.891650	-1.960359	-0.410737

		6			
B	1.9254963	114.4530787	0.861205	-1.973841	0.386040
N	1.4445523	33.5567144	-1.869584	-0.010735	1.477263
N	1.4472011	123.0069501	-0.462681	2.120147	1.063447
N	1.4417832	35.0449777	-1.935694	1.147659	-0.848192
N	1.4418025	35.0476338	-1.948736	-1.099915	-0.880843
N	1.4470813	140.7375087	-0.487515	-2.144847	1.001505
N	1.4437146	144.6064680	1.962821	1.099294	0.882502
N	1.4381922	34.8201135	0.470386	2.128218	-0.977086
N	1.4362070	146.6192263	1.893905	0.010469	-1.484124
N	1.4867781	49.7061167	-0.159429	0.035458	-2.389824
N	1.4380348	143.4151390	0.445909	-2.104168	-1.038400
N	1.4436326	144.6257164	1.949711	-1.146833	0.850031
B	1.4380956	111.3961125	-1.409870	0.032537	-1.679537

C	1.5458221	35.4196640	0.166689	-0.037683	2.519613

Single adsorption configurations

C_2H_2 adsorb on $B_{12}N_{12}$ Energy=-1033.348320(a.u.)

Atom	Bond	Angle	X	Y	Z
B			-0.901130	-1.053173	1.332844
B	1.9292860		-1.730535	0.057934	-0.008675
B	2.4105257	66.8175612	-0.355897	1.283256	1.566199
B	2.4135443	60.0683779	1.328457	-0.394038	1.984329
B	2.4106966	66.8096739	-0.426899	-1.770124	-0.919387
B	1.9225147	114.6315449	1.293803	-1.884437	0.770421
B	2.4140275	66.5396959	2.673325	-0.055947	0.008140
B	1.9233714	114.7141614	1.317386	-1.283744	-1.567663
B	1.9233494	114.7331948	1.864013	1.056793	-1.335771
B	2.4121078	98.6143530	-0.331100	1.883541	-0.769889
B	1.9200631	114.7516734	-0.367059	0.395455	-1.982716
N	1.4375695	35.0322789	-1.424569	0.332580	1.422111
N	1.4408701	125.7442868	0.357392	-1.51330	1.862478
N	1.4394730	35.0898825	0.992072	0.998378	2.126122
N	1.4397886	35.1266845	0.045971	2.297799	0.556459
N	1.4425160	142.5586753	-1.431258	0.945055	-1.106082

N	1.4393424	143.9418901	0.916312	-2.296181	-0.556106
N	1.4396032	35.0640694	2.395024	-0.943631	1.106786
N	1.4400398	143.9054373	2.388272	-0.331706	-1.42434
N	1.4866980	130.9908569	2.428315	1.410352	-0.006292
N	1.4391528	143.914505	0.605815	1.514769	-1.863366
N	1.4400472	143.8918584	-0.029934	-0.997246	-2.125778
B	1.4397920	111.1869865	1.388364	1.773307	0.920944
N	1.4383621	35.1338412	-1.467569	-1.409959	0.005909
C	3.2460675	107.4906591	-4.907170	-0.609810	-0.000805
C	1.2084775	81.4849223	-4.977899	0.596587	0.003835
H	1.0667433	98.2267338	-4.839378	-1.674389	-0.004938
H	1.0667656	179.7614056	-5.044754	1.661249	0.007576

HCl adsorb on $B_{12}N_{12}$ Energy=-1416.837874(a.u.)

Atom	Bond	Angle	X	Y	Z
B			0.167009	-2.057337	0.609281
B	1.9244553		1.072061	-1.859332	-1.077492
B	2.4134462	66.5540633	-1.115066	-0.839795	-1.035751
B	2.4145421	114.7439488	-1.142682	-0.144416	1.284156
B	2.4150648	66.5421334	2.364731	-1.073739	0.805162

B	1.9202169	66.6373131	0.553352	-0.259411	2.177172
B	2.4139061	109.5743667	0.186581	1.859785	1.076356
B	1.9241841	114.7016923	2.374340	0.836909	1.032794
B	1.9244245	114.8069350	1.091588	2.057124	-0.610484
B	2.4140129	114.7506101	0.709672	0.259326	-2.176319
B	1.9216627	66.5805076	2.405675	0.143931	-1.280191
N	1.4356500	35.0762084	-0.373686	-2.041304	-0.775323
N	1.4399060	125.5755821	-0.374862	-1.331585	1.728651
N	1.4502910	94.5636039	-1.790048	0.012513	-0.004112
N	1.4421240	94.0995019	-0.717057	0.241354	-1.966932
N	1.4389639	143.8980194	1.622329	-0.897845	-1.995841
N	1.4378423	143.9325343	1.976812	-0.242325	1.975033
N	1.4393517	34.8444516	-0.364260	0.897516	1.994150
N	1.4402641	143.8152089	1.629393	2.042148	0.774311

N	1.4865409	93.1520084	-0.352683	2.176057	-0.272336
N	1.4394861	143.8110957	1.632956	1.332398	-1.730222
N	1.4387846	143.8249012	3.031424	-0.012755	0.005884
B	1.4355217	111.4396778	-1.105661	1.077167	-0.807301
N	1.4400619	34.9811729	1.608325	-2.176691	0.271191
Cl	3.3107991	116.4454458	-5.100822	-0.000186	-0.001854
H	2.0045703	115.9896871	-3.794530	0.005732	0.013433

C_2H_2 adsorb on $B_{11}N_{12}C$

Configuration A Energy=-1046.485839(a.u.)

Atom	Bond	Angle	X	Y	Z
B			-1.065665	1.779615	-1.117058
B	1.9173884		-1.270876	0.099999	-2.018810
B	2.3879184	66.3537689	0.996501	0.634606	-1.494071
B	2.3825160	99.9128872	0.679570	1.788743	0.566003
B	2.4148378	66.6199288	-2.588075	0.272954	-0.001853

B	1.9147036	114.6376531	-1.084349	1.647023	1.297163
B	2.3504979	98.6952169	0.438479	-0.071688	1.982164
B	1.9261770	114.6819881	-1.844985	-0.637433	1.524309
B	1.9112102	114.8634201	0.231948	-1.745125	1.082343
B	2.3485399	114.9427203	0.263334	-1.619229	-1.262610
B	1.9154923	67.4513444	-1.508376	-1.814446	-0.561151
N	1.4380978	35.9186185	-0.198119	1.122338	-2.128993
N	1.4393678	125.2384804	-0.604154	2.388480	0.102807
N	1.4307631	35.1841040	1.638574	1.144130	-0.277720
N	1.4300946	93.8558769	1.404889	-0.758526	-1.297438
N	1.4392064	143.4452313	-1.057600	-1.317109	-1.886020
N	1.4404876	35.0186934	-2.259336	0.904827	-1.253920
N	1.4398734	142.767691	-2.238953	0.788183	1.347350
N	1.4333202	36.6501590	0.242778	1.345979	1.902614
N	1.4393818	144.0340652	-0.620895	-1.106276	2.118960

N	1.4714351	91.7914600	1.400368	-0.856065	1.191820
N	1.4330949	145.8165207	-0.216560	-2.403037	-0.109191
N	1.4400149	142.7441983	-2.480093	-1.179553	0.291093
C	1.4627882	121.3384465	2.056270	-0.290898	0.012783
C	1.5138081	112.0446351	3.553839	-0.510863	0.035531
C	1.3121279	124.7330826	4.450914	0.443178	-0.046578
H	1.0907435	113.8409155	3.844246	-1.556715	0.143136
H	1.0811510	138.1861947	4.475801	1.519531	-0.145231

Configuration B Energy=-1046.485568(a.u.)

Atom	Bond	Angle	X	Y	Z
B			-1.281016	0.039977	2.018886
B	1.9175083		-1.095610	1.743924	1.159219
B	2.3878341	66.3621408	0.980338	0.615878	1.512558

B	2.3810249	61.1312190	0.276206	-1.640157	1.223104
B	2.4150332	66.6165013	-2.597350	0.245583	0.004593
B	1.9154836	114.6583286	-1.491930	-1.840778	0.514215
B	2.3481687	98.7830569	0.249910	-1.709239	-1.123901
B	1.9260786	114.6677939	-1.840530	-0.617762	-1.541899
B	1.9108394	114.9163441	0.436136	-0.011781	-1.981376
B	2.3506458	114.8982256	0.652963	1.816649	-0.520087
B	1.9151483	67.4342271	-1.108590	1.669712	-1.257063
N	1.4387418	35.9060839	-0.222169	1.072517	2.157101
N	1.4393514	125.2734084	-1.049532	-1.370746	1.851529
N	1.429775	35.2156107	1.407708	-0.768156	1.282887
N	1.4289162	93.7687217	1.613605	1.160414	0.309566
N	1.4393500	143.4432144	-0.640110	2.388079	-0.044655
N	1.4404263	35.0311308	-2.278831	0.850712	1.272344
N	1.4400343	142.7774387	-2.471132	-1.198316	-0.323702

N	1.4331529	36.7602919	-0.192125	-2.402107	0.050180
N	1.4393286	144.0422779	-0.609836	-1.056318	-2.145826
N	1.4719431	49.5314985	1.407711	-0.804264	-1.210254
N	1.4329309	145.6488531	0.222384	1.400588	-1.868173
N	1.4403232	142.8185933	-2.252641	0.797788	-1.330730
C	1.4643609	121.1906784	2.053924	-0.257779	-0.015216
C	2.4995443	124.1556287	4.430242	0.512989	0.066950
C	1.3122948	29.6346579	3.547055	-0.451636	-0.040739
H	1.0810880	167.5787712	5.505988	0.620325	0.066093
H	1.0954470	121.1574606	3.858834	-1.493137	-0.175177

C_2H_2 adsorb on $B_{12}N_{11}C$

Configuration C Energy=-1016.607454(a.u.)

Atom	Bond	Angle	X	Y	Z

B			-1.516133	1.141638	-0.405083
B	1.9918404		-1.305442	-0.601812	-1.344987
B	2.4619665	66.4030790	0.432839	1.044130	-1.919907
B	2.4029267	99.7450085	0.632594	2.178218	0.189121
B	2.4974101	66.6229501	-1.345242	-0.815768	1.142923
B	1.9227470	114.3725394	-0.226622	1.281276	1.656840
B	2.4154275	98.3461132	2.068703	0.589842	1.306682
B	1.9328950	113.5295235	0.407893	-1.035685	1.926656
B	1.9240813	114.6955631	2.264563	-1.094825	0.398043
B	2.4051539	60.5235611	1.031822	-1.271973	-1.671610
B	1.9238763	114.3464553	0.172260	-2.159814	-0.197096
N	1.4423903	32.9273619	-0.973713	0.782993	-1.735764
N	1.4466027	122.1188421	-0.807715	2.015781	0.504135
N	1.4407570	35.2083095	1.239278	1.978881	-1.102382
N	1.4407137	35.1626898	1.465778	0.010569	-2.163976
N	1.4459062	141.5209626	-0.377821	-1.700314	-1.498145

N	1.4412569	144.1711378	-0.636606	-0.004937	2.161608
N	1.4388516	34.9085896	1.188297	1.713807	1.485237
N	1.4359022	146.1087668	1.816256	-0.795263	1.783387
N	1.4860991	49.6641885	2.798362	0.249597	0.057340
N	1.4386304	143.5235120	1.618217	-1.997935	-0.516444
N	1.4416182	144.3939555	-0.411049	-1.968588	1.107299
B	1.4378912	111.4362426	2.142906	0.797634	-1.099191
C	1.5853895	39.1462460	-2.220056	-0.261919	-0.057665
C	2.5207725	127.2705420	-4.647860	0.413266	0.007042
C	1.3165652	29.3346255	-3.715432	-0.515480	-0.029738
H	1.0826732	109.2577698	-4.717464	1.493286	0.036930
H	1.0923175	118.8045245	-4.018132	-1.564937	-0.042786

Reaction pathway 1

Co-ads Energy=-1507.286448(a.u.)

Atom	Bond	Angle	X	Y	Z
B			-1.317137	0.528705	2.105806
B	1.9181589		-0.571745	1.973092	1.087243
B	2.3887011	66.3364107	0.876135	0.082099	1.270770
B	2.3850378	99.8120897	-0.741601	-1.670418	1.266316
B	2.4151098	66.6287806	-2.716498	1.224750	0.264593
B	1.9131276	114.7596928	-2.515787	-1.121940	0.806432
B	2.3494101	98.8016664	-1.143812	-1.782507	-1.045694
B	1.9274531	114.6193868	-2.629139	0.083730	-1.286380
B	1.9107094	114.8315724	-0.402866	-0.342570	-2.059790
B	2.3485153	115.0099646	0.766984	1.258877	-0.801878
B	1.9116134	67.5754654	-0.981793	1.853623	-1.294140
N	1.4341928	35.8379383	0.085164	1.017537	2.016578
N	1.4387541	125.1762006	-1.720426	-0.850409	2.032213

N	1.432383	34.9232911	0.645154	-1.351785	1.101681
N	1.4419563	94.2546466	1.511594	0.280283	-0.048786
N	1.4391572	143.3240207	-0.077919	2.332058	-0.216004
N	1.4412366	34.9763269	-1.985317	1.667112	1.425133
N	1.4391622	142.6517271	-3.250590	-0.144588	0.047462
N	1.4332244	36.6164720	-1.650759	-2.190576	0.231262
N	1.4396375	144.0203598	-1.797700	-0.849493	-2.000775
N	1.4712271	49.5670965	0.257913	-1.450076	-1.351757
N	1.4328122	145.7407296	0.010445	1.029210	-2.041229
N	1.4381365	142.7169521	-2.378834	1.545911	-1.146403
C	1.4599537	122.3524993	1.236094	-1.226340	-0.291300
C	1.5128149	112.1048858	2.504497	-2.021329	-0.50983
C	1.3121401	124.6747259	3.025732	-2.850320	0.363554
H	1.0908337	113.955653	2.963971	-1.862637	-1.486364

		8			
H	1.0809644	138.5281536	2.818501	-3.211749	1.361005
Cl	3.3450834	106.5334234	4.676190	1.359904	0.047824
H	2.0434823	108.7330522	3.469567	0.860456	0.025786

Ts1 Energy=-1507.228954 (a.u.) , ν=-1058.17cm^{-1}

Atom	Bond	Angle	X	Y	Z
B			-1.418735	0.565193	2.092942
B	1.9186339		-0.722843	2.031768	1.070177
B	2.3872762	66.3298824	0.810696	0.217472	1.313317
B	2.3867503	61.0510621	-0.718275	-1.615155	1.295910
B	2.4157701	66.6318202	-2.810647	1.167970	0.212733
B	1.9136799	114.6913552	-2.506693	-1.159375	0.789949
B	2.3521163	98.8850619	-1.066133	-1.776030	-1.024772
B	1.9264694	114.6182607	-2.632983	0.014216	-1.319772
B	1.9134888	114.774134	-0.372912	-0.311679	-2.042888

		3			
B	2.3520286	115.0013691	0.694931	1.360236	-0.779381
B	1.9143314	67.4158774	-1.072746	1.861248	-1.316940
N	1.4334192	35.8817503	-0.041840	1.120777	2.028798
N	1.4398885	125.1186280	-1.751155	-0.834261	2.027335
N	1.4351903	35.3276769	0.660187	-1.238980	1.161351
N	1.4333536	93.7734029	1.443621	0.422387	0.004459
N	1.4393894	143.3188900	-0.218042	2.397650	-0.227185
N	1.4404981	34.9376696	-2.127202	1.659535	1.381622
N	1.4386030	142.7053114	-3.271547	-0.229864	0.002176
N	1.4317866	36.5088204	-1.576449	-2.191247	0.246914
N	1.4412515	143.9909945	-1.739692	-0.886784	-2.003465
N	1.4763362	91.8157823	0.328681	-1.384110	-1.308429
N	1.4311791	145.7443660	-0.025918	1.076762	-2.032863
N	1.4386690	142.7686186	-2.456465	1.486793	-1.194982

C	1.4575896	120.8747028	1.253937	-1.075490	-0.225275
C	1.5214458	110.5707259	2.577397	-1.797312	-0.430760
C	1.3705556	125.3539739	3.090360	-2.763430	0.395017
H	1.0912667	114.2297703	3.064329	-1.577610	-1.382333
H	1.0867981	122.6152961	2.640044	-3.016156	1.351299
Cl	2.4176414	107.4213115	5.287418	-2.030817	1.088706
H	1.3550142	118.3483867	3.606397	-1.503412	0.400411

De-ads	Energy=-1507.327953(a.u.)				
Atom	Bond	Angle	X	Y	Z
B			1.455745	1.491370	1.552003
B	1.9174703		2.106616	-0.29219	1.820281
B	2.3866875	66.3248085	-0.274781	-0.138209	1.766547
B	2.3809332	61.1469295	-0.541360	1.619077	0.182336
B	2.4149728	66.6235197	2.988066	0.761983	-0.166159

B	1.9156455	114.5439732	1.060131	2.095434	-0.754685
B	2.3502049	98.6174561	-0.242707	0.368150	-1.784756
B	1.9261637	114.6236175	2.147852	0.209670	-1.809052
B	1.9087463	114.9093345	0.404962	-1.40740	-1.517811
B	2.3505645	114.9800435	0.778677	-2.000897	0.725680
B	1.9157412	67.4279323	2.400343	-1.581037	-0.203826
N	1.4380196	35.9752077	0.912396	0.386950	2.385190
N	1.4388818	125.2868359	0.683923	2.320038	0.664320
N	1.4298043	35.1155352	-1.202242	0.553209	0.868995
N	1.4305621	93.8234230	-0.470022	-1.466661	1.174958
N	1.4396328	143.4218856	2.118983	-1.615737	1.254054
N	1.4404536	35.0391436	2.787458	0.901436	1.253424
N	1.4404963	142.7463479	2.316931	1.566795	-1.219469
N	1.4325859	36.6730754	-0.282458	1.703339	-1.267076
N	1.4395038	144.055516	0.935245	-0.317693	-2.377949

		4			
N	1.4724466	49.6209134	-0.900943	-0.809511	-1.193404
N	1.4331342	145.7854068	1.167480	-2.275857	-0.670331
N	1.4397334	142.8245299	3.078886	-0.523457	-0.906632
C	1.4630043	121.4756758	-1.413017	-0.790241	0.176921
C	1.5360719	112.9716279	-2.848598	-1.325293	0.288022
C	1.4881498	114.4596751	-3.843889	-0.596692	-0.544520
H	1.0937945	108.2019225	-3.137829	-1.311130	1.342788
H	1.0982579	106.2972745	-2.813079	-2.373225	-0.038700
H	1.0823582	123.3107430	-3.900008	-0.689798	-1.621405
Cl	1.7277955	120.7592326	-4.761955	0.709282	0.116437

Reaction pathway 2

Co-ads Energy=-1507.286356(a.u.)

Atom	Bond	Angle	X	Y	Z
B			-1.251171	-1.082950	-1.913855
B	1.9182023		-0.381663	-2.142764	-0.572121
B	2.3874422	66.3744166	0.873025	-0.223530	-1.243729
B	2.3821611	61.0746791	-0.907318	1.302777	-1.662605
B	2.4151107	66.6449007	-2.602732	-1.428898	0.057531
B	1.9141410	114.7540486	-2.626345	0.713634	-1.061113
B	2.3476953	98.8056419	-1.355096	1.948521	0.549675
B	1.9274145	114.5932427	-2.650605	0.068485	1.270164
B	1.9107457	114.9795757	-0.488257	0.896376	1.888529
B	2.3499954	114.8512715	0.853958	-0.845618	1.060040
B	1.9131768	67.5259634	-0.835805	-1.468225	1.706033
N	1.4348884	35.9075011	0.189804	-1.391906	-1.720186
N	1.4390371	125.2083337	-1.790324	0.223108	-2.186535

N	1.4313714	34.9989602	0.500911	1.176632	-1.439440
N	1.4399876	94.2053349	1.503667	-0.019360	0.075794
N	1.4385636	143.3095117	0.126266	-2.110454	0.773401
N	1.4406556	34.9932678	-1.814362	-2.074199	-0.961070
N	1.4395028	142.6340239	-3.272317	-0.108463	-0.071646
N	1.4326650	36.7246661	-1.880774	1.974198	-0.782816
N	1.4398010	144.0690408	-1.926730	1.229823	1.717742
N	1.4705801	49.5613302	0.067816	1.848248	0.915221
N	1.4326627	145.5143706	0.058829	-0.388028	2.210283
N	1.4393392	142.7361322	-2.255365	-1.348909	1.500338
C	1.4614492	121.6587287	1.089844	1.449108	-0.050170
C	2.5004767	123.6264299	3.497189	2.099856	0.133135
C	1.3113159	29.5699288	2.243208	2.417068	-0.082405
H	1.0805451	168.4302790	4.462943	2.582574	0.176498

H	1.0954825	121.1979390	1.947249	3.450907	-0.291372
Cl	3.4334768	102.3854700	4.666728	-1.350654	-0.031278
H	2.1673636	106.4928049	3.582076	-0.632419	0.032905

Ts1 Energy= -1507.207261 (a.u.) , ν=-2480.00cm^{-1}

Atom	Bond	Angle	X	Y	Z
B			-1.345065	-0.047543	2.022589
B	1.9179080		-1.208963	1.687863	1.217472
B	2.3861639	66.3509933	0.900058	0.629281	1.580876
B	2.3790639	61.2048907	0.293146	-1.640700	1.208332
B	2.4151887	66.6193395	-2.629879	0.168996	-0.011004
B	1.9157239	114.6476086	-1.452105	-1.888279	0.458131
B	2.3482872	98.8192666	0.313204	-1.638018	-1.139868
B	1.9262457	114.6489144	-1.809820	-0.616633	-1.566868
B	1.9112536	114.9856019	0.448195	0.090546	-1.944066

B	2.3497429	114.8731755	0.567727	1.880201	-0.426127
B	1.9152022	67.4238580	-1.173693	1.687132	-1.199548
N	1.4375555	35.9565113	-0.330159	1.020436	2.213434
N	1.4395939	125.2207282	-1.054004	-1.442391	1.817374
N	1.4304756	35.2596218	1.388719	-0.727632	1.319179
N	1.4310173	93.7807326	1.534452	1.232844	0.407049
N	1.4391915	143.4353703	-0.755258	2.384853	0.042896
N	1.4404428	35.0147174	-2.358511	0.746967	1.280191
N	1.4400193	142.7543278	-2.439628	-1.258501	-0.379624
N	1.4328493	36.7435849	-0.121831	-2.383587	0.003779
N	1.4393465	144.0997160	-0.55205	-0.989012	-2.159377
N	1.4716745	49.5134990	1.434960	-0.685867	-1.176405
N	1.4323218	145.6058456	0.177312	1.488869	-1.792868
N	1.4403769	142.8849409	-2.281359	0.774568	-1.321976
C	1.4656253	121.335279	2.041593	-0.151066	0.045905

		7			
C	2.5888842	121.4492262	4.544083	0.506004	0.136039
C	1.3284190	25.3546240	3.529287	-0.346209	0.043200
H	1.0828683	151.1940427	5.594326	0.242625	0.151034
H	1.0931537	115.8615235	3.799791	-1.398178	-0.079982
Cl	1.9882339	103.2073992	4.494371	2.404379	0.724915
H	2.4245504	80.8574063	3.603441	2.654783	-0.477464

Ims1 Energy=-1507.258448(a.u.)

Atom	Bond	Angle	X	Y	Z
B			1.870501	-0.257995	-1.954416
B	1.9168790		1.225437	1.509693	-1.588907
B	2.3877552	66.3522943	-0.492672	-0.148726	-1.630613
B	2.3808723	61.1020536	0.706316	-2.002370	-0.738994
B	2.4153810	66.6340818	2.957021	0.787080	-0.067260
B	1.9148175	114.6793205	2.416268	-1.565853	0.004002

B	2.3492801	98.7707086	0.583068	-1.445930	1.540107
B	1.9265790	114.6529393	2.320041	0.199511	1.653416
B	1.9112124	114.9543959	-0.060609	0.315978	1.906294
B	2.3489768	114.8228980	-0.603232	1.582791	0.004075
B	1.9153660	67.4606952	1.087030	2.076748	0.757499
N	1.4382097	35.9134883	0.608552	0.406549	-2.370493
N	1.4394318	125.2750927	1.970181	-1.587691	-1.412257
N	1.4300648	35.2271971	-0.593553	-1.486282	-1.037455
N	1.4299039	93.7440612	-1.318360	0.513101	-0.619608
N	1.4387878	143.4034028	0.546565	2.311287	-0.605703
N	1.4405795	34.9981187	2.591967	0.940368	-1.452362
N	1.4395542	142.8015555	3.153361	-0.505212	0.639652
N	1.4330676	36.7085964	1.257127	-2.290035	0.598399
N	1.4397251	144.0428131	1.189494	-0.357219	2.349637
N	1.4723399	91.8611701	-0.760212	-0.866113	1.375195

N	1.4322768	145.6006520	-0.181104	1.655990	1.415106
N	1.4404504	142.7849537	2.397866	1.566394	1.067572
C	1.4668859	121.8006737	-1.433549	-0.833711	0.072382
C	2.5883621	117.3561968	-4.020257	-0.926118	0.067783
C	1.3326607	25.5903525	-2.798868	-1.453185	0.147745
H	1.0835898	146.3339719	-4.900555	-1.550479	0.164817
H	1.0883780	115.6407757	-2.759707	-2.527067	0.320402
Cl	1.7454193	102.0456421	-4.444271	0.751578	-0.160333
H	3.5090357	95.5925728	-3.350113	3.216223	1.453170

Ts2 Energy=-1507.256224 (a.u.), ν=-475.15cm^{-1}

Atom	Bond	Angle	X	Y	Z
B			-1.610117	-0.110856	1.952331
B	1.9170465		-1.549099	1.538700	0.977493
B	2.3864789	66.3581934	0.595936	0.549471	1.325769

B	2.3816038	61.1774217	0.010710	-1.756135	1.208601
B	2.4147189	66.6290465	-3.004866	-0.110965	-0.018847
B	1.9153897	114.5987656	-1.767011	-2.096647	0.582121
B	2.3487377	98.8201875	-0.095092	-1.982610	-1.126797
B	1.9261134	114.7175524	-2.256855	-1.034340	-1.534687
B	1.9108261	114.9425248	-0.034877	-0.338897	-2.099339
B	2.3459965	114.8416802	0.133035	1.587039	-0.770326
B	1.9152040	67.5048779	-1.643356	1.302651	-1.427262
N	1.4376284	35.9349930	-0.606388	0.983571	1.983606
N	1.4395242	125.2481851	-1.305576	-1.515260	1.867867
N	1.4290573	35.1748235	1.091257	-0.821771	1.168767
N	1.4283958	93.9661201	1.155914	1.042077	0.064569
N	1.4392106	143.3671944	-1.171383	2.122177	-0.282750
N	1.4400946	35.0364826	-2.676769	0.593771	1.193412
N	1.4400784	142.8293295	-2.809528	-1.564847	-0.257029
N	1.4328792	36.7463108	-0.455289	-2.618171	0.105868
N	1.4398396	143.9775501	-1.024771	-1.446783	-2.155169
N	1.4726429	91.8172678	1.007138	-1.024622	-1.316600
N	1.4319069	145.7269459	-0.321979	1.063656	-2.071501
N	1.4405570	142.7048793	-2.739340	0.368153	-1.400115
C	1.4633837	121.8030568	1.667487	-0.374487	-0.184012
C	2.5800359	134.5005491	4.124613	-0.042407	0.529318

C	1.3433450	26.9944765	3.168655	-0.518832	-0.285384
H	1.0834961	148.0054415	5.168295	-0.287097	0.371779
H	1.0859936	115.8029033	3.499243	-1.229327	-1.037242
Cl	1.7367350	99.7757783	3.898175	1.029634	1.876798
H	2.1678834	102.2988503	3.291349	0.828956	-1.978940

De-ads Energy=-1507.327953(a.u.)

Atom	Bond	Angle	X	Y	Z
B			1.455745	1.491370	1.552003
B	1.9174703		2.106616	-0.29219	1.820281
B	2.3866875	66.3248085	-0.274781	-0.138209	1.766547
B	2.3809332	61.1469295	-0.541360	1.619077	0.182336
B	2.4149728	66.6235197	2.988066	0.761983	-0.166159
B	1.9156455	114.5439732	1.060131	2.095434	-0.754685
B	2.3502049	98.6174561	-0.242707	0.368150	-1.784756
B	1.9261637	114.6236175	2.147852	0.209670	-1.809052
B	1.9087463	114.9093345	0.404962	-1.40740	-1.517811
B	2.3505645	114.980043	0.778677	-2.000897	0.725680

		5			
B	1.9157412	67.4279323	2.400343	-1.581037	-0.203826
N	1.4380196	35.9752077	0.912396	0.386950	2.385190
N	1.4388818	125.2868359	0.683923	2.320038	0.664320
N	1.4298043	35.1155352	-1.202242	0.553209	0.868995
N	1.4305621	93.8234230	-0.470022	-1.466661	1.174958
N	1.4396328	143.4218856	2.118983	-1.615737	1.254054
N	1.4404536	35.0391436	2.787458	0.901436	1.253424
N	1.4404963	142.7463479	2.316931	1.566795	-1.219469
N	1.4325859	36.6730754	-0.282458	1.703339	-1.267076
N	1.4395038	144.0555164	0.935245	-0.317693	-2.377949
N	1.4724466	49.6209134	-0.900943	-0.809511	-1.193404
N	1.4331342	145.7854068	1.167480	-2.275857	-0.670331
N	1.4397334	142.8245299	3.078886	-0.523457	-0.906632
C	1.4630043	121.4756758	-1.413017	-0.790241	0.176921

C	1.5360719	112.9716279	-2.848598	-1.325293	0.288022
C	1.4881498	114.4596751	-3.843889	-0.596692	-0.544520
H	1.0937945	108.2019225	-3.137829	-1.311130	1.342788
H	1.0982579	106.2972745	-2.813079	-2.373225	-0.038700
H	1.0823582	123.3107430	-3.900008	-0.689798	-1.621405
Cl	1.7277955	120.7592326	-4.761955	0.709282	0.116437

Reaction pathway 3

Co-ads Energy=-1477.408310(a.u.)

Atom	Bond	Angle	X	Y	Z
B			0.066226	1.598603	-1.145595
B	1.9904681		-0.849468	2.018671	0.571091
B	2.4628094	66.3773507	-2.315753	0.948857	-1.093522
B	2.4037792	99.8128123	-0.724822	-0.49294	-2.174408
B	2.4959756	66.5827716	1.161901	0.567102	0.849005

B	1.9206129	114.3202452	0.943263	-0.671979	-1.239426
B	2.4169895	98.3730467	-0.724314	-2.290474	-0.558639
B	1.9406592	113.4529503	0.732515	-1.310482	1.086627
B	1.9253153	114.6382839	-1.605149	-1.876698	1.102613
B	2.4050597	60.5191908	-2.526804	0.352452	1.226838
B	1.9214377	114.3905429	-0.854107	0.171208	2.154824
N	1.4426918	32.8888848	-1.329999	1.967167	-0.823905
N	1.4465402	122.1224153	0.388377	0.473098	-1.995263
N	1.4391664	35.1847230	-2.124155	-0.200757	-2.007986
N	1.4398077	35.1438779	-3.151375	0.281561	-0.068512
N	1.4457896	141.4863742	-1.553082	1.383633	1.662861
N	1.4519738	144.9645026	1.587333	-0.632147	0.061272
N	1.4386678	34.9165176	-0.028702	-1.707375	-1.674831
N	1.4321161	145.9655087	-0.219968	-2.350735	0.838421

N	1.4852898	93.0025829	-2.167200	-2.118858	-0.250883
N	1.4383261	143.5653554	-1.968596	-0.798489	1.982473
N	1.4447646	143.8394857	0.544967	-0.147274	1.985987
B	1.4384097	111.5055257	-2.689445	-0.909610	-0.828812
C	1.5813532	39.1942481	0.737193	1.974311	0.265855
C	2.5211521	128.3289467	2.219749	3.895283	-0.418325
C	1.3160045	29.3879048	1.641996	3.168421	0.514274
H	1.0825158	109.4862294	2.291331	3.929450	-1.497931
H	1.0920588	118.8944476	1.805996	3.427488	1.562406
Cl	3.3214086	114.1075650	4.814515	-1.415408	0.001660
H	2.0160147	113.9042968	3.548879	-1.095407	0.016074

Ts1 Energy=-1477.342315 (a.u.), ν=-1780.75cm^{-1}

Ato	Bond	Angle	X	Y	Z

m					
B			-1.478432	1.121170	-0.271481
B	1.9951720		-1.325681	-0.666144	-1.144915
B	2.4635343	66.2834950	0.324240	0.975493	-1.952250
B	2.4051455	99.7930454	0.693964	2.215011	0.075464
B	2.4994070	66.6535395	-1.134259	-0.761056	1.345343
B	1.9233014	114.2794888	-0.012889	1.376076	1.655222
B	2.4162932	98.2980339	2.253592	0.700701	1.130404
B	1.9318562	113.5668836	0.685544	-0.916695	1.974757
B	1.9244783	114.6857239	2.395331	-1.023325	0.287041
B	2.4042433	60.4806179	0.984031	-1.316574	-1.649776
B	1.9238176	114.4978740	0.278044	-2.147397	-0.064724
N	1.4434845	32.8500895	-1.055051	0.702639	-1.625517
N	1.4451267	122.3706009	-0.709316	2.047352	0.527918
N	1.4408843	35.1362589	1.183118	1.960325	-1.255705
N	1.4404526	35.1499209	1.348527	-0.054095	-2.239855
N	1.4442668	141.384298	-0.396654	-1.756536	-1.328928

N	1.4413446	144.1949437	-0.352667	0.109709	2.253837
N	1.4390598	34.8702103	1.372150	1.819603	1.335371
N	1.4353806	146.1007981	2.069803	-0.663506	1.691844
N	1.4861183	49.6480039	2.871645	0.310347	-0.163505
N	1.4388349	143.5754285	1.685367	-1.978485	-0.521579
N	1.4418329	144.1935371	-0.187304	-1.899414	1.277229
B	1.4375602	111.4690945	2.104983	0.793436	-1.279495
C	1.5885972	39.2828030	-2.127635	-0.271970	0.206203
C	2.5265470	128.1392155	-4.567404	0.347420	0.423741
C	1.3125362	27.9446625	-3.593536	-0.531551	0.381999
H	1.0805483	107.9204119	-4.642944	1.424103	0.372437
H	1.1080687	114.9301163	-3.912887	-1.587680	0.484091
Cl	2.0396914	145.184652	-6.461110	-0.368415	0.672335

		3			
H	2.3644062	104.7523067	-5.695237	-1.718386	0.649251

Ims1	Energy=-1477.387214(a.u.)				
Atom	Bond	Angle	X	Y	Z
B			0.881479	-1.213326	0.139629
B	1.9933767		0.654492	-0.092036	-1.492773
B	2.4624176	66.3636324	-1.083466	-1.816568	-1.230110
B	2.4036036	99.8023316	-1.256064	-1.861849	1.166861
B	2.4979135	66.6431559	0.719976	1.237670	0.620794
B	1.9235584	114.2968157	-0.384374	-0.392683	2.051047
B	2.4156055	98.2797749	-2.685460	0.064880	1.449159
B	1.9322879	113.5255739	-1.025265	1.792170	1.237560
B	1.9244106	114.7583535	-2.899102	1.147773	-0.127247
B	2.4040224	60.5174196	-1.688945	0.356448	-2.061206
B	1.9233442	114.4264964	-0.817853	1.820507	-1.168467
N	1.4433636	32.8703793	0.324426	-1.499925	-1.200514

N	1.4460351	122.1982072	0.187204	-1.573683	1.355829
N	1.4404396	35.1763814	-1.876437	-2.273526	-0.066235
N	1.4403080	35.1636064	-2.122701	-1.008408	-1.907873
N	1.4445714	141.4555160	-0.278790	0.815104	-2.119565
N	1.4417271	144.1595673	0.026308	0.981603	1.905255
N	1.4386904	34.8989955	-1.798895	-0.853904	2.112234
N	1.4356465	146.1214702	-2.433744	1.514203	1.236100
N	1.4861581	93.0838253	-3.430363	-0.203230	0.191422
N	1.4390068	143.4693281	-2.265813	1.531280	-1.361187
N	1.4412653	144.2849244	-0.219649	2.245486	0.072013
B	1.4374253	111.4121912	-2.786041	-1.220647	-0.593373
C	1.5880452	39.3010024	1.589041	0.193443	-0.201522
C	2.5024367	127.7569859	3.988239	-0.421578	0.155952
C	1.3351456	29.7596982	3.065254	0.424703	-0.307212

H	1.0843589	94.6688894	3.765706	-1.350548	0.669107
H	1.0887959	118.6437612	3.394810	1.342046	-0.792342
Cl	1.7529938	152.5899723	5.709619	-0.130230	-0.002018
H	3.7428718	118.4865077	2.993035	4.206307	0.792511

Ts2 Energy=-1477.385072 (a.u.), ν=-459.88cm^{-1}

Atom	Bond	Angle	X	Y	Z
B			-0.995686	1.089149	-0.398692
B	1.9942369		-0.803259	-0.697626	-1.263208
B	2.4652077	66.1687217	0.818849	0.976673	-2.064917
B	2.4053872	99.8792684	1.148246	2.234265	-0.041097
B	2.5052574	66.5955575	-0.625026	-0.772622	1.236158
B	1.9234405	114.3053281	0.449203	1.388949	1.538904
B	2.4161487	98.3518136	2.733249	0.760948	1.033555
B	1.9328638	113.5110987	1.195088	-0.885247	1.876832
B	1.9245847	114.676316	2.918639	-0.964412	0.201215

		4			
B	2.4046987	60.4995061	1.526871	-1.298822	-1.743353
B	1.9228415	114.486253 2	0.828075	-2.134564	-0.158885
N	1.4422371	32.8376369	-0.555402	0.676206	-1.746795
N	1.4458270	122.434579 1	-0.254315	2.037058	0.402715
N	1.4403669	35.1516495	1.651889	1.983647	-1.367065
N	1.4405542	35.1568417	1.868139	-0.032090	-2.338435
N	1.4454340	140.964399 5	0.154857	-1.767011	-1.429668
N	1.4414296	144.280115 4	0.132712	0.119776	2.144505
N	1.4392274	34.8835863	1.825950	1.861454	1.226092
N	1.4353315	146.169091 3	2.575430	-0.603680	1.601964
N	1.4858859	93.0161946	3.368437	0.377120	-0.253717
N	1.438576	143.558369 2	2.235160	-1.939163	-0.606385
N	1.4425349	144.256915 6	0.348143	-1.890005	1.179309
B	1.4378445	111.456883	2.598577	0.836738	-1.377756

		8			
C	1.5871506	38.7863577	-1.616770	-0.317298	0.083695
C	2.5083973	125.6630404	-4.022724	0.321529	0.392471
C	1.3472865	29.9040185	-3.079213	-0.622792	0.210192
H	1.0842285	94.1804724	-3.822106	1.387035	0.393324
H	1.0882586	118.4659866	-3.369865	-1.668526	0.289367
Cl	1.7443786	152.6520928	-5.712349	-0.058761	0.600806
H	2.0898207	99.0052535	-3.384495	-1.002222	-1.822094

De-ads Energy=-1477.444564(a.u.)

Atom	Bond	Angle	X	Y	Z
B			1.245773	-0.708743	0.273461
B	1.9943454		0.895675	0.491951	-1.279980
B	2.467820	66.3297836	-0.356003	-1.633048	-1.368394
B	2.4016403	99.7945435	-0.743744	-1.976698	0.976694
B	2.4905883	66.5158091	0.399260	1.546406	0.921094
B	1.9198577	114.4390832	-0.377650	-0.445245	2.075093
B	2.4149881	98.3997993	-2.649647	-0.516550	1.236827
B	1.9338856	113.9027461	-1.482497	1.583599	1.365527

B	1.9245474	114.5576968	-2.980704	0.641646	-0.264128
B	2.4025239	60.6608366	-1.423497	0.393049	-2.094692
B	1.9211793	114.2504794	-1.055304	1.919518	-0.987779
N	1.4405271	32.7467296	0.908213	-0.979998	-1.143890
N	1.4492883	121.8137503	0.547010	-1.360051	1.363399
N	1.4408905	35.2751871	-1.113056	-2.398033	-0.350804
N	1.4401957	35.2684605	-1.500674	-1.045051	-2.103397
N	1.449608	141.2572499	-0.183765	1.194590	-1.945165
N	1.4424998	144.1832051	-0.326922	0.996253	2.092867
N	1.4384340	34.9499420	-1.623202	-1.249900	1.927986
N	1.4360397	145.9637478	-2.763726	0.964966	1.170705
N	1.4856274	49.6708712	-3.171539	-0.824676	-0.120704
N	1.4387987	143.6113113	-2.353454	1.302456	-1.377694
N	1.4415612	144.4108536	-0.712921	2.344914	0.346354
B	1.4384188	111.3502831	-2.208926	-1.556711	-0.899517
C	1.5827382	39.1600023	1.585259	0.860798	0.128372
C	1.5582385	117.7290322	3.013053	1.461615	0.297282
C	1.4888911	114.7055604	4.084859	0.735116	-0.437720
H	1.0979792	108.9036387	3.264322	1.486662	1.365830
H	1.0969966	109.6908747	3.022045	2.499075	-0.059085
H	1.0839475	123.9995112	4.393182	0.971546	-1.449639
Cl	1.7354321	118.9225730	4.527413	-0.859801	0.083922

Product Energy=-538.153156(a.u.)

Atom	Bond	Angle	X	Y	Z
C			-1.646061	-0.284826	0.000007
C	1.3292864		-0.575978	0.503796	0.000013
H	1.0855618	119.2375927	-2.634874	0.163162	0.000025
H	1.0846226	122.5432566	-1.573311	-1.367006	-0.000013
H	1.0838770	124.1780755	-0.617796	1.586866	0.000034
Cl	1.7514107	123.4508429	1.068131	-0.099814	-0.000010