The Regulation of Hydroboration of Olefins by Oriented External Electric Field

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Contents

1. Coordinates of structures in gas phase:

Hydroboration of C_2H_4 with BH_3

C_2H_4:

C,0,-0.0423144608,0.0069985627,-0.725843711

C,0,-0.0924835106,0.0004835503,0.6223372936

H,0,-0.0088431545,-0.9239043601,-1.3014542928

H,0,-0.1013880157,-0.93589998,1.1900733093

H,0,-0.126313266,0.9313465194,1.1981570637

H,0,-0.0337376825,0.9433836377,-1.2933131628

BH_3:

B,0,1.9954603302,0.0326793967,-0.0425141941

H,0,2.0956159553,1.0751434914,0.5545129546

H,0,1.7689013595,0.037859288,-1.2264617578

H,0,2.119981625,-1.0132433361,0.5440796472

Q:

C,0,-0.0661804712,0.1147204107,-0.6653517503

C,0,-0.0445269625,-0.0941259642,0.6890741569

H,0,-0.1964884141,-0.7184415439,-1.3588505933

H,0,-0.1570623997,-1.0980740541,1.1032114288

H,0,-0.0423675858,0.7402785658,1.3939349135

B,0,1.8575271115,0.0922786728,-0.0061069416

H,0,2.0861557411,1.2664986164,0.171057693

H,0,2.1074742048,-0.3708660786,-1.1011409815

H,0,2.1392065279,-0.6774918338,0.8906711192

H,0,-0.0820731419,1.1226680289,-1.0858797248

TS:

C,0,0.0710319656,0.0092750769,-0.7483037448

C,0,0.0304562107,0.002203966,0.6542946442

H,0,-0.0453407883,-0.9175176557,-1.3149859042

H,0,-0.1467590327,-0.9335869078,1.1852145448

H,0,-0.1723658291,0.927804579,1.1938675295

B,0,1.7436135463,0.0284336868,0.0909246378

H,0,2.1596456739,1.0984918652,0.4635537188

H,0,1.8164006993,0.0351304763,-1.1523967346

H,0,2.1890450851,-1.0331092428,0.4537978953

H,0,-0.0708483508,0.9377209259,-1.3063934369

P:

C,0,0.02032524,-0.01807811,-0.83698015

C,0,-0.00306375,-0.04011847,0.72448564

H,0,-0.97855929,-0.2527402,-1.24192728

H,0,-0.32981105,-1.04201522,1.05502062

H,0,-0.74615072,0.69877866,1.07332385

B,0,1.46621489,0.30652225,1.18962411

H,0,1.81209754,1.45685338,1.3359701

H,0,0.72907426,-0.76245876,-1.24177747

H,0,2.29548312,-0.56551854,1.31676335

H,0,0.31360967,0.9743514,-1.22345281

Hydroboration of C_3H_6 with BH_3

C_3H_6:

C,0,-0.0953659904,0.0174469189,-0.6812914531

C,0,0.1023030396,-0.0150175795,0.6529379815

H,0,-0.2679421667,-0.9277376878,-1.2142091705

H,0,0.0938214649,-0.9581902654,1.2079286719

C,0,-0.0978244721,1.2751802368,-1.5205474978

H,0,0.6846807128,1.2297656491,-2.2995571234

H,0,-1.0661512238,1.4007416893,-2.0379392829

H,0,0.0823560516,2.1680501549,-0.8983420197

H,0,0.2788615839,0.9026558837,1.226136894

Q(A-M):

C,0,-0.1160042904,0.0088749634,-0.6666557556

C,0,-0.0349411841,-0.0796655695,0.6999982375

H,0,-0.2901000055,-0.9096358264,-1.2368764768

H,0,-0.1786891907,-1.0332823816,1.2104016099

B,0,1.8524751379,-0.1382066991,-0.0268515297

H,0,2.1820669534,1.0149987092,0.1371157038

H,0,1.9834669127,-0.566584098,-1.1580055095

H,0,2.1431982196,-0.9567741599,0.8188782214

C,0,-0.1864030019,1.3081993575,-1.4342293875

H,0,0.5050020343,1.2993024022,-2.2917999317

H,0,-1.2128714541,1.4379278678,-1.8218212142

H,0,0.0597336755,2.1639278617,-0.786377421

H,0,0.0137863532,0.8203917728,1.3190969234

TSM:

C,0,0.0955230208,0.0505995351,-0.7264010165

C,0,0.1169118561,0.0470165582,0.6864218017

H,0,-0.165466689,-0.8920847194,-1.2150998144

H,0,-0.1013963865,-0.8637561656,1.2492693465

B,0,1.7620367815,-0.1055447766,-0.1413606908

H,0,2.1281929445,-1.2196138642,-0.4248778127

H,0,1.780496077,-0.0508288737,1.1114162031

H,0,2.3119068986,0.9046630616,-0.5055854729

C,0,-0.1705184176,1.3215999261,-1.5186703658

H,0,0.3829850947,1.3164336188,-2.4716932405

H,0,-1.2478806172,1.4182169435,-1.7458146303

H,0,0.1470254392,2.2101188157,-0.9475423288

H,0,0.0196799978,0.9861989405,1.2397590214

PM:

C,0,0.0529663124,0.0846076782,-0.7904092712

C,0,-0.0217633969,-0.0401668521,0.7638831451

H,0,-0.5731985122,-0.7272623098,-1.207761561

H,0,0.3123478524,-1.0309987991,1.1192877174

B,0,1.5790355837,-0.1612579885,-1.1210184275

H,0,2.0202411961,-1.284920196,-1.198937117

H,0,0.5995870574,0.7298265127,1.2585009961

H,0,2.3441359433,0.7733568768,-1.2111878673

C,0,-0.5034186014,1.4492081852,-1.2429943632

H,0,-0.4718018638,1.55738595,-2.3417292022

H,0,-1.5537138147,1.5812624875,-0.9229469572

H,0,0.0902735228,2.2747211206,-0.8093862727

H,0,-1.0630893292,0.1074694045,1.1025740107

TSAM:

C,0,-0.0369026483,0.0501723799,-0.7258367316

C,0,-0.0388471622,0.0440796914,0.6807384111

H,0,-0.2187546134,-0.8954226212,-1.2469699462

H,0,-0.2862745174,-0.8707266007,1.2203428052

B,0,1.6524016837,-0.0599760265,0.1067358762

H,0,2.1553226813,0.99368079,0.4218317952

H,0,1.6858340341,-0.1057005598,-1.1360606528

H,0,2.045844495,-1.1356881445,0.4902481962

C,0,-0.2430494948,1.3206022904,-1.5245690425

H,0,0.230279965,1.2601195807,-2.5170647601

H,0,-1.3277295114,1.4793197811,-1.6594278655

H,0,0.1719251919,2.1851984181,-0.9820137272

H,0,-0.1782311635,0.987425681,1.2134405521

PAM:

C,0,0.0447695142,-0.0010465388,-0.7900287979

C,0,0.0160082302,-0.0109542736,0.7705005424

H,0,0.0038422647,-1.0389426298,-1.1714489636

H,0,-0.948515836,-0.4442294294,1.0939339281

B,0,1.25605984,-0.8635619934,1.2520402388

H,0,2.3371056838,-0.3451314301,1.415900375

H,0,1.0015397969,0.4277325691,-1.1437655512

H,0,1.1685824946,-2.0634272607,1.3822722069

C,0,-1.1225096662,0.8042692768,-1.3866374138

H,0,-1.0873602738,0.8011945891,-2.4902052343

H,0,-2.0919331882,0.3775685912,-1.0736231926

H,0,-1.0874360269,1.854219283,-1.045745749

H,0,0.0586205867,1.0365665768,1.1219451411

Coordinates of structures in OEEF ($\times 10^{-4}$ a.u.):

Hydroboration of C_2H_4 with BH_3

1) **$F_Z = 20$**

C_2H_4:

C	-0.024323172262	0.005460590025	-0.725828887127
C	-0.066356066948	-0.000492112431	0.622578795261
H	0.008316038898	-0.925151474761	-1.301612930722
H	-0.073136510891	-0.936835651629	1.190867429787
H	-0.097960051927	0.930829476648	1.198200950671
H	-0.016630236870	0.941123172146	-1.294249357871

BH_3:

B	1.995447162808	0.032849066251	-0.043424536902
H	2.095618649667	1.075146883503	0.555237017575
H	1.769060703012	0.037434072308	-1.226397687110
H	2.119832484512	-1.012991022068	0.544201206420

Q:

C	-0.062256393974	-0.037817606229	-0.669974392942
C	-0.049635399740	0.102161671328	0.693574577918
H	-0.034312561070	-1.022533679544	-1.142059422405
H	-0.016305467347	-0.766916559548	1.354198464639
H	-0.204444838038	1.078469480032	1.157119480161
B	1.857655025394	0.034163121351	-0.000374120824
H	2.118671546415	0.823965867003	0.885044709746
H	2.073774368427	0.496244068089	-1.103020092295
H	2.138363922342	-1.129326815491	0.173899861074
H	-0.226636202372	0.822895452321	-1.321328065289

TS:

C	0.063124736738	0.009230462289	-0.747367851473
C	0.026473165188	0.002120005055	0.653206712937

H	-0.048590951120	-0.917563386063	-1.314818582161
H	-0.144161779806	-0.934017053604	1.185866729839
H	-0.169722647563	0.928105659827	1.194768490189
B	1.746991141094	0.028521383361	0.083418743829
H	2.157167273485	1.097184473286	0.468366504132
H	1.829888033871	0.035432246496	-1.156133866864
H	2.186571469428	-1.031943714121	0.458406922393
H	-0.073987441316	0.937837923462	-1.306108802829

P:

C	0.015612304988	0.004920892921	-0.836765295206
C	-0.002428057606	0.027550224719	0.725775688411
H	0.208562027837	-1.010795131842	-1.225096366365
H	-0.814623278925	-0.634676366057	1.074928208573
H	-0.227575346701	1.057098460992	1.056894811391
B	1.426018025280	-0.463090574806	1.184950168531
H	2.339358018099	0.321566490248	1.308372127770
H	0.792505788948	0.676576844050	-1.242597981087
H	1.655264162352	-1.641522287857	1.339820722087
H	-0.956437244715	0.336935756565	-1.238127813849

2) **F_Z = -20**

C_2H_4:

C	-0.024450355838	0.005458292410	-0.726335193447
C	-0.066610347896	-0.000494652396	0.622057411723
H	0.008414764734	-0.926021127392	-1.301367449783
H	-0.073044423133	-0.935948854819	1.191136197317
H	-0.097856530511	0.929944379222	1.198445819023
H	-0.016543107357	0.941995962967	-1.293980784833

BH_3:

B	1.994127182532	0.032832399661	-0.041425318895

H	2.096057988925	1.075154336707	0.554568295825
H	1.769500232083	0.037442338271	-1.227061867463
H	2.120273596557	-1.012990076761	0.543534893412

Q:

C	-0.064297819897	-0.071244939838	-0.663586078862
C	-0.046047756219	0.148590042838	0.689452214814
H	-0.054817048224	-1.082727403072	-1.075376067170
H	-0.016210749325	-0.679825971918	1.400865846432
H	-0.188765386603	1.151176735808	1.097574200947
B	1.856055914664	0.017556653568	-0.015287088709
H	2.101316344152	0.743319986842	0.927959153097
H	2.104771755513	0.552388686502	-1.077573191615
H	2.125242077775	-1.154752067119	0.109196202500
H	-0.222374331952	0.752823278307	-1.362144186394

TS:

C	0.078048429372	0.009453700466	-0.749234096701
C	0.034135853671	0.001982060641	0.655272967942
H	-0.042968838611	-0.917001147007	-1.315821372818
H	-0.149198309408	-0.933625716088	1.184444227251
H	-0.175313800342	0.927077887206	1.193099276114
B	1.740494913103	0.028510435107	0.098110107048
H	2.161592007245	1.100006646551	0.458843907020
H	1.803513317031	0.034169580705	-1.148857718023
H	2.191157545897	-1.033992983537	0.449998563462
H	-0.067708117959	0.938327535948	-1.306250861316

P:

C	0.015495686130	0.005061531245	-0.835745605548
C	-0.003312985532	0.027370745040	0.724982989956
H	0.208997515923	-1.011430159712	-1.223580949538
H	-0.815111350916	-0.634228342935	1.075204213348

H	-0.228492854598	1.056043872226	1.057580410400
B	1.425937984408	-0.463077803768	1.189132512908
H	2.338827575918	0.322516393828	1.303540716952
H	0.794592175972	0.676087048138	-1.240544128358
H	1.655080476753	-1.641587752240	1.337728591040
H	-0.955757824073	0.337808778223	-1.240144481102

3) **$F_X = 20$**

C_2H_4:

C	-0.019996000891	0.005497307839	-0.725748049926
C	-0.063573341649	-0.000430088927	0.622610232926
H	0.006293822138	-0.925689387584	-1.301358633052
H	-0.074664257955	-0.936644432884	1.190502428525
H	-0.099550527385	0.930617164662	1.197904093533
H	-0.018599694263	0.941583436894	-1.293954072001

BH_3:

B	1.992079589168	0.033006056851	-0.042383470123
H	2.096788333771	1.074734009819	0.555122919200
H	1.770166754745	0.037172623611	-1.226859114853
H	2.120924322319	-1.012473690124	0.543734666026

Q:

C	-0.059107540759	-0.048013649834	-0.668684316374
C	-0.045242164493	0.112919275963	0.692994194851
H	-0.038630671857	-1.040477895793	-1.124283478947
H	-0.012945130543	-0.746096255463	1.366787918499
H	-0.203429632267	1.095265778032	1.142262631247
B	1.848803773701	0.032906273396	-0.007562082271
H	2.108894835263	0.784641157290	0.911656573702
H	2.087015102611	0.541200501287	-1.085845792098
H	2.138459335638	-1.133921824636	0.131041792213

H	-0.228942907391	0.802879641598	-1.331285441078

TS:

C	0.073428532986	0.009342339318	-0.749196458972
C	0.034971201661	0.002271296219	0.654787190876
H	-0.045955708754	-0.917364277793	-1.315447774917
H	-0.150743487306	-0.933448333699	1.182971184377
H	-0.176447250983	0.927550055960	1.191630604350
B	1.741463992506	0.028355146539	0.096216158746
H	2.166144724468	1.097958602350	0.462433015370
H	1.807084638414	0.035315061295	-1.149126630726
H	2.195432001370	-1.032694247859	0.452146158803
H	-0.071626644388	0.937621357666	-1.306808448333

P:

C	0.016397897211	0.003429084243	-0.835341246710
C	-0.003248092532	0.028833198905	0.726678777985
H	0.205952969596	-1.014060670647	-1.221511462759
H	-0.815737071712	-0.632269192152	1.075645181116
H	-0.229110546413	1.058177132482	1.056468015048
B	1.424020429986	-0.461995978060	1.186295274623
H	2.337441754096	0.323459227803	1.313676891878
H	0.796017332058	0.672503575486	-1.242140610893
H	1.658817509833	-1.641345917142	1.326154024089
H	-0.954295182202	0.337833538863	-1.237769844350

4) **F_X = -20**

C_2H_4:

C	-0.026142539172	0.005412570011	-0.726094030814
C	-0.069244127777	-0.000512210628	0.622237418346
H	0.009325480098	-0.925708212944	-1.301242677455
H	-0.071786536993	-0.936465444190	1.190743191036

H	-0.096681963101	0.930520002662	1.198142227094
H	-0.015559313055	0.941686295089	-1.293830128207

BH_3:

B	1.997921497444	0.033051925201	-0.042734000202
H	2.094792507055	1.075124349565	0.555008386882
H	1.768307523588	0.037158123718	-1.226279001625
H	2.118937471900	-1.012896398323	0.543620614447

Q:

C	-0.069721650038	-0.058078023665	-0.665468693883
C	-0.053572285292	0.136397894403	0.690472953894
H	-0.046059417295	-1.060965148968	-1.097761195320
H	-0.017599545758	-0.704667645546	1.386538541561
H	-0.195043334446	1.131856706471	1.116338710277
B	1.869067215906	0.018312862892	-0.006590000728
H	2.116352177602	0.790167616259	0.897474330371
H	2.091693315329	0.497362968061	-1.100015660117
H	2.123441043054	-1.151187940235	0.160702929746
H	-0.223684519053	0.778106710094	-1.350610915482

TS:

C	0.067982460860	0.009344562707	-0.747399141873
C	0.025381363641	0.002017476394	0.653789987717
H	-0.045024811923	-0.917411025128	-1.314786663500
H	-0.143131689881	-0.933966259479	1.187281789026
H	-0.168651767108	0.927841658644	1.196266639747
B	1.746036321429	0.028527648056	0.085546571507
H	2.153053321507	1.098984488284	0.465009291372
H	1.825908431164	0.035049400785	-1.155766057446
H	2.182537255278	-1.033577112653	0.455509800716
H	-0.070337885152	0.938098162028	-1.305847220325

P:

C	0.014573284004	0.005723789095	-0.836898363957
C	-0.002382527767	0.027182767160	0.724294907799
H	0.211797414023	-1.009306856447	-1.225608482117
H	-0.814406642077	-0.634688147379	1.075336709491
H	-0.226185680370	1.056392107345	1.057382356058
B	1.427675654407	-0.463969485102	1.187989024101
H	2.339799959305	0.320771401303	1.304320114711
H	0.790643875738	0.679064996695	-1.241906494920
H	1.652791332250	-1.642147648737	1.343867060518
H	-0.958049668573	0.335542077032	-1.240621833031

Hydroboration of C_3H_6 with BH_3

1) **$F_Z = 10$**

C_3H_6:

C	-0.095007036566	0.017770854932	-0.681413048242
C	0.102783421104	-0.015215802727	0.652947372218
H	-0.267885658197	-0.927114659716	-1.214376275456
H	0.094106932134	-0.958659936304	1.207776031998
C	-0.097920059801	1.275379075247	-1.520338438576
H	0.684271148359	1.229987606684	-2.299329126516
H	-1.066140265793	1.399826613168	-2.038185982862
H	0.081127405470	2.168350316916	-0.898105969371
H	0.279402872019	0.902571630924	1.226143796073

BH_3:

B	1.995116747061	0.032844951747	-0.042926811865
H	2.095726459779	1.075141101480	0.555058670523
H	1.769175218804	0.037436073135	-1.226539475053
H	2.119940574354	-1.012983126435	0.544023616202

Q(A-M):

C	-0.113543332363	0.009258751274	-0.667385564059

C	-0.034340323724	-0.074977738796	0.699807317621
H	-0.284402657739	-0.911256669945	-1.235268887899
H	-0.177294944966	-1.027309144222	1.212692957268
B	1.854099836802	-0.139936458260	-0.021830013412
H	2.188506280081	1.009032723104	0.160705090797
H	1.983651909688	-0.548715876699	-1.159454914186
H	2.142044666490	-0.973821597575	0.809588525364
C	-0.188352225620	1.306290313549	-1.437965763871
H	0.492680384666	1.293597390821	-2.303473562133
H	-1.218824062945	1.435996804788	-1.814674227577
H	0.065707504460	2.163798225994	-0.795416024637
H	0.010787124536	0.827517476475	1.315548536336

TSM:

C	0.098449512369	0.050590146796	-0.727810899768
C	0.119042987265	0.047372469288	0.685820922356
H	-0.164022008970	-0.892100762301	-1.215722123112
H	-0.101746022653	-0.862999150770	1.248516041397
B	1.762113133692	-0.106035995013	-0.142495355685
H	2.129741247274	-1.221127713103	-0.419226046347
H	1.775086860992	-0.048712667009	1.111691500179
H	2.315002518252	0.903744529355	-0.502611826821
C	-0.170888455877	1.321514900977	-1.519309716442
H	0.377161413516	1.315440699195	-2.475351289363
H	-1.249282929978	1.417884376751	-1.741217837682
H	0.149678905994	2.210391155575	-0.950457799926
H	0.019158838683	0.987057011457	1.237995433069

PM:

C	0.052946083126	0.084872903333	-0.790530718282
C	-0.021753282671	-0.040408468078	0.763495741452
H	-0.572894489956	-0.726992881873	-1.208164076827

H	0.311728559636	-1.031785189772	1.118373900927
B	1.579295689914	-0.161180766976	-1.121738640961
H	2.020748246166	-1.285031161844	-1.193862461376
H	0.600551810584	0.729027570005	1.258192358846
H	2.343926020271	0.773490099497	-1.213924201349
C	-0.503710575032	1.449367840351	-1.242838538789
H	-0.472574344650	1.557359893692	-2.341340162592
H	-1.554020878211	1.581291518421	-0.922631957776
H	0.090309502849	2.274998089590	-0.809726535672
H	-1.062950391060	0.108222623633	1.102570122792

TSAM:

C	-0.039872991447	0.051071691392	-0.725797466958
C	-0.039909044468	0.044481276495	0.679905119171
H	-0.218737416392	-0.894832024954	-1.247354296826
H	-0.285259609737	-0.870686240013	1.219912004619
B	1.654281826758	-0.060939989664	0.104612106157
H	2.155815084816	0.991605444302	0.426703817908
H	1.693141387422	-0.105213498092	-1.136645227732
H	2.044463027459	-1.136601630041	0.492678823988
C	-0.244563714426	1.321097399971	-1.525036345649
H	0.227001905795	1.259089976642	-2.517994103269
H	-1.329242624761	1.480293124559	-1.659123870907
H	0.171653324622	2.185868254696	-0.983738069130
H	-0.176952215682	0.987850874757	1.213272418634

PAM:

C	0.044849917905	-0.001323640676	-0.790433644445
C	0.016862004033	-0.009937578774	0.770561927796
H	0.003634602903	-1.039412489225	-1.170847617917
H	-0.947988872771	-0.442766312705	1.093951876219
B	1.256126531813	-0.863324733587	1.250887203294

H	2.336544722332	-0.345399658632	1.421655361406
H	1.001323571086	0.427103907895	-1.145034562614
H	1.168152611873	-2.063638184993	1.378498213838
C	-1.122879469152	0.803814366908	-1.386304281632
H	-1.087887361736	0.800461595277	-2.489584398524
H	-2.092126175050	0.376733209345	-1.073154901929
H	-1.087716567121	1.853911130148	-1.045786682721
H	0.059877903959	1.038035719022	1.120729037214

2) $F_Z = -10$

C_3H_6:

C	-0.094280422375	0.016710207943	-0.681861269906
C	0.103155212512	-0.015076818986	0.652366000266
H	-0.267477752547	-0.928478164459	-1.214437894823
H	0.093861069523	-0.957545653449	1.208474491494
C	-0.097944212073	1.275022760421	-1.520551311256
H	0.684436807286	1.231397861582	-2.299981304231
H	-1.067063208883	1.400913485628	-2.036981959909
H	0.081357852729	2.167217883967	-0.897413366845
H	0.278693412185	0.902734136792	1.225504974782

BH_3:

B	1.994456730883	0.032836618278	-0.041927188493
H	2.095946130742	1.075144854802	0.554724268116
H	1.769395006257	0.037440205333	-1.226871495344
H	2.120161132163	-1.012982679545	0.543690416972

Q(A-M):

C	-0.119326546407	0.010265945809	-0.665034480059
C	-0.037471957913	-0.081632685488	0.700763546448
H	-0.294946309117	-0.906860791403	-1.237038809097
H	-0.179212308773	-1.036554140908	1.209285403853

B	1.856046550246	-0.140183341737	-0.033576585213
H	2.181222809969	1.016408750419	0.112175421624
H	1.986475155204	-0.589743578908	-1.156374222352
H	2.142979102780	-0.940605853364	0.829746976048
C	-0.186856839502	1.311024676025	-1.430799343636
H	0.517445656128	1.308089437877	-2.278136561898
H	-1.208338192835	1.436312091357	-1.832906390984
H	0.045438720842	2.166782937535	-0.777927972495
H	0.017264319327	0.816170755154	1.322696489672

TSM:

C	0.093236350947	0.050739414108	-0.724744655354
C	0.114691173098	0.048066149078	0.687416108231
H	-0.166954697785	-0.892391475271	-1.213023197319
H	-0.101939040028	-0.862517428544	1.251082030371
B	1.761679511949	-0.105119198732	-0.139221379356
H	2.126541642617	-1.218481402590	-0.427708382519
H	1.785438262124	-0.051489682227	1.112122439165
H	2.309484360603	0.904828283682	-0.507962728643
C	-0.169787801790	1.320732024976	-1.519497741316
H	0.389862646063	1.315534257529	-2.469228906680
H	-1.245982983543	1.415755528047	-1.753199534685
H	0.142920963144	2.210181506931	-0.947316117759
H	0.020305612490	0.987181022297	1.241103065034

PM:

C	0.052805027064	0.084250039643	-0.790515772907
C	-0.021328784264	-0.039813799941	0.764207046268
H	-0.573669865419	-0.727900603252	-1.207035225529
H	0.311482089481	-1.030826170581	1.119822891048
B	1.578710931821	-0.161324716461	-1.119835175511
H	2.020432797349	-1.284760123438	-1.199503160094

H	0.600854377499	0.729443810325	1.258556064416
H	2.343311892213	0.773684450042	-1.212422415927
C	-0.503484737234	1.448839990688	-1.243361146939
H	-0.469986862976	1.557806711566	-2.342222561796
H	-1.554204490661	1.580427472135	-0.924709770139
H	0.088990167886	2.274255237578	-0.808077415926
H	-1.062310592943	0.109149771298	1.102971472637

TSAM:

C	-0.033867853348	0.049452669909	-0.725898314634
C	-0.037756062632	0.043914376107	0.681526223237
H	-0.218490745973	-0.895912180038	-1.246612612657
H	-0.287420714259	-0.870458883332	1.220771872289
B	1.650611574736	-0.059341841820	0.109038416354
H	2.155134771496	0.995005868813	0.418145292439
H	1.678927158297	-0.105511054456	-1.135257477636
H	2.046781845012	-1.135493695431	0.487424195931
C	-0.241626337849	1.320157985218	-1.524293938671
H	0.233128046756	1.261042885064	-2.516440358093
H	-1.326319657146	1.478199910391	-1.659666351783
H	0.172095032394	2.184731955942	-0.980820183090
H	-0.179378118330	0.987296664808	1.213478146569

PAM:

C	0.044667614693	-0.000965299530	-0.789276358874
C	0.015678747233	-0.010703400205	0.770726163173
H	0.003911230486	-1.039054177378	-1.170612518865
H	-0.948609726973	-0.443869240165	1.094761530798
B	1.256076942775	-0.863548675749	1.252869856941
H	2.337384475876	-0.345052587682	1.413388419296
H	1.001628738074	0.427837337149	-1.142899601450
H	1.168172344022	-2.063335796836	1.381968400855

C	-1.122316712304	0.804044591514	-1.387052342449
H	-1.086814859401	0.800545703822	-2.490907909938
H	-2.091882726070	0.377715231388	-1.074043540579
H	-1.087590847260	1.854070238090	-1.046442847633
H	0.058468198858	1.036573405569	1.122658278718

3) **F_Z = -57**

C_3H_6:

C	-0.092338471113	0.014327214015	-0.682878064140
C	0.103790163628	-0.014795783225	0.651304198719
H	-0.266232373933	-0.931540085858	-1.214781153821
H	0.093128915634	-0.955096707334	1.210413620991
C	-0.097924933774	1.274219603383	-1.521156694703
H	0.684534359037	1.234573063394	-2.302252181321
H	-1.069351058240	1.403540572527	-2.034129975321
H	0.082334108876	2.164712732670	-0.896107952085
H	0.276798047977	0.902955089574	1.224706561001

BH_3:

B	2.011953141265	-0.160104314475	-0.000268610804
H	2.152233690960	0.920189540500	0.512169180445
H	1.852953251981	-0.239231076716	-1.196552722608
H	2.032867915868	-1.161596148326	0.666683141926

Q(A-M):

C	-0.122819468354	0.011691034246	-0.661648822545
C	-0.040568169521	-0.093017504974	0.702627729212
H	-0.305792478624	-0.899975666292	-1.240335934772
H	-0.181303550056	-1.052288225977	1.203468820351
B	1.854067956218	-0.139929150111	-0.053574500229
H	2.169683728909	1.025111230813	0.029843973794
H	1.993674663698	-0.657760661866	-1.147711237416

H	2.137946742152	-0.882237462043	0.859833696638
C	-0.184380700008	1.319006999750	-1.419045708415
H	0.549647311523	1.332421860549	-2.241950593083
H	-1.194178239370	1.438934214751	-1.852267721193
H	0.018380079090	2.171127238039	-0.752033743036
H	0.026361124642	0.796390092990	1.335668040976

TSM:

C	0.079789000000	0.051665000000	-0.716818000000
C	0.103481000000	0.049564000000	0.691603000000
H	-0.173965000000	-0.892520000000	-1.206832000000
H	-0.102613000000	-0.861952000000	1.257266000000
B	1.762381000000	-0.102913000000	-0.131208000000
H	2.118548000000	-1.211589000000	-0.451939000000
H	1.814071000000	-0.060629000000	1.113181000000
H	2.296216000000	0.908210000000	-0.520817000000
C	-0.167758000000	1.319332000000	-1.519479000000
H	0.420026000000	1.316765000000	-2.453329000000
H	-1.238107000000	1.409590000000	-1.782360000000
H	0.123713000000	2.210370000000	-0.939175000000
H	0.023714000000	0.987127000000	1.249730000000

PM:

C	0.052935111412	0.083503950157	-0.790330211246
C	-0.020828535657	-0.039015990140	0.766276301451
H	-0.574767904624	-0.729255030351	-1.205020422744
H	0.311990760400	-1.028898769958	1.123254895369
B	1.577549012438	-0.161518259141	-1.116016544700
H	2.019534597136	-1.284303680047	-1.210869620740
H	0.599341605118	0.730656831117	1.260884289066
H	2.342984814695	0.773214924990	-1.212507397057
C	-0.502778433119	1.448299327652	-1.244210221493

H	-0.464303773816	1.559567026992	-2.344191853479
H	-1.554354115213	1.579111759341	-0.928755259174
H	0.086234192946	2.273350068690	-0.804281096753
H	-1.061935382235	0.108519910995	1.103641971518

TSAM:

C	-0.021398000000	0.046071000000	-0.726192000000
C	-0.033194000000	0.042694000000	0.685050000000
H	-0.218981000000	-0.897982000000	-1.245155000000
H	-0.291653000000	-0.870024000000	1.222833000000
B	1.643816000000	-0.056154000000	0.118886000000
H	2.154045000000	1.002061000000	0.399713000000
H	1.648554000000	-0.106538000000	-1.132464000000
H	2.051898000000	-1.133586000000	0.475898000000
C	-0.235717000000	1.318365000000	-1.522748000000
H	0.247609000000	1.266277000000	-2.512669000000
H	-1.320400000000	1.473318000000	-1.662556000000
H	0.171119000000	2.182637000000	-0.973696000000
H	-0.183879000000	0.985946000000	1.214494000000

PAM:

C	0.044245348974	-0.000298697018	-0.786128824812
C	0.014576204724	-0.009554117413	0.771672926077
H	0.004354609369	-1.039261448935	-1.167306110792
H	-0.948619080082	-0.442308073279	1.098452094744
B	1.256285012365	-0.864067410471	1.256921530997
H	2.338206670518	-0.345309929651	1.405719388542
H	1.001918310561	0.428948749050	-1.139429871975
H	1.166911696503	-2.063938579671	1.376626283433
C	-1.121812029727	0.803334842525	-1.388758213429
H	-1.084534587609	0.799128829078	-2.494184386545
H	-2.091839890882	0.377760638411	-1.076419650770

H	-1.089366514409	1.853380913472	-1.048306597166
H	0.058447669777	1.036441613929	1.126278961685

4) **F_Z = -58**

C_3H_6:

C	-0.092293117088	0.014278064230	-0.682899194018
C	0.103799878317	-0.014790457020	0.651286231336
H	-0.266200474952	-0.931603237048	-1.214791657904
H	0.093110751593	-0.955047151313	1.210459437893
C	-0.097923364375	1.274203007664	-1.521171156793
H	0.684531231874	1.234638245842	-2.302312569076
H	-1.069401972727	1.403598044940	-2.034067916424
H	0.082362600785	2.164661709768	-0.896085195416
H	0.276753224578	0.902957472445	1.224700380055

BH_3:

B	2.011944345096	-0.160103382323	-0.000193085500
H	2.152232231782	0.920216865688	0.512131144929
H	1.852968893313	-0.239227438573	-1.196560824533
H	2.032862529791	-1.161628045041	0.666653760434

Q(A-M):

C	-0.123509207971	0.011698035607	-0.661507168461
C	-0.041606674461	-0.093333079684	0.702657129158
H	-0.306131980196	-0.899874632095	-1.240487895360
H	-0.181534908914	-1.052885226236	1.203241031009
B	1.855332805089	-0.140009563700	-0.054015368356
H	2.169568115409	1.025359973168	0.030283088789
H	1.994294374287	-0.657024605682	-1.148667192449
H	2.138539960478	-0.882340352432	0.859498143208
C	-0.184414102885	1.319132666664	-1.418803035772
H	0.550549784846	1.332559669548	-2.240896989320

H	-1.193740588983	1.439288824000	-1.853072671440
H	0.017789560100	2.171145455352	-0.751484026715
H	0.025583862142	0.795757833572	1.336127952736

TSM:

C	0.079789000000	0.051665000000	-0.716818000000
C	0.103481000000	0.049564000000	0.691603000000
H	-0.173965000000	-0.892520000000	-1.206832000000
H	-0.102613000000	-0.861952000000	1.257266000000
B	1.762381000000	-0.102913000000	-0.131208000000
H	2.118548000000	-1.211589000000	-0.451939000000
H	1.814071000000	-0.060629000000	1.113181000000
H	2.296216000000	0.908210000000	-0.520817000000
C	-0.167758000000	1.319332000000	-1.519479000000
H	0.420026000000	1.316765000000	-2.453329000000
H	-1.238107000000	1.409590000000	-1.782360000000
H	0.123713000000	2.210370000000	-0.939175000000
H	0.023714000000	0.987127000000	1.249730000000

PM:

C	0.052933709616	0.083482996448	-0.790328555764
C	-0.020813760573	-0.038994500705	0.766322372083
H	-0.574799462729	-0.729289494052	-1.204973289979
H	0.312010950204	-1.028850766746	1.123335548207
B	1.577523289837	-0.161525844294	-1.115928031667
H	2.019509174585	-1.284295044392	-1.211151235699
H	0.599313592632	0.730693926512	1.260928467351
H	2.342977631167	0.773208224378	-1.212454491562
C	-0.502764104951	1.448284240423	-1.244234177676
H	-0.464191122928	1.559594193791	-2.344244017059
H	-1.554356061491	1.579087257315	-0.928842106513
H	0.086182175655	2.273327800500	-0.804216461264

H	-1.061924061551	0.108509081121	1.103660809559

TSAM:

C	-0.021398000000	0.046071000000	-0.726192000000
C	-0.033194000000	0.042694000000	0.685050000000
H	-0.218981000000	-0.897982000000	-1.245155000000
H	-0.291653000000	-0.870024000000	1.222833000000
B	1.643816000000	-0.056154000000	0.118886000000
H	2.154045000000	1.002061000000	0.399713000000
H	1.648554000000	-0.106538000000	-1.132464000000
H	2.051898000000	-1.133586000000	0.475898000000
C	-0.235717000000	1.318365000000	-1.522748000000
H	0.247609000000	1.266277000000	-2.512669000000
H	-1.320400000000	1.473318000000	-1.662556000000
H	0.171119000000	2.182637000000	-0.973696000000
H	-0.183879000000	0.985946000000	1.214494000000

PAM:

C	0.044233032724	-0.000239829222	-0.786065934229
C	0.014478740259	-0.009637143687	0.771686529132
H	0.004423000337	-1.039185771907	-1.167355814267
H	-0.948678123471	-0.442420749868	1.098513228955
B	1.256266608533	-0.864095328415	1.257027329587
H	2.338337252626	-0.345377819096	1.404781570838
H	1.001927894660	0.429084738007	-1.139258436390
H	1.166854732700	-2.063880246083	1.377346694684
C	-1.121781563034	0.803360652630	-1.388821701045
H	-1.084400409187	0.799188815286	-2.494285113356
H	-2.091826919050	0.377765738476	-1.076572377029
H	-1.089419525031	1.853392377034	-1.048322511948
H	0.058358698013	1.036301896873	1.126464065058

5) $F_X = 10$

C_3H_6:

C	-0.092401628415	0.017206598686	-0.681838746427
C	0.102991599324	-0.015048296251	0.652871035349
H	-0.266918388539	-0.927659119343	-1.214581017477
H	0.090288743721	-0.957898494989	1.208532844503
C	-0.096795129153	1.275031233683	-1.520643478277
H	0.682816108439	1.229462713167	-2.302614860796
H	-1.066732453503	1.400955386413	-2.034477905348
H	0.085340052302	2.167679605762	-0.898565048130
H	0.276151095796	0.903165372870	1.226434176603

BH_3:

B	2.010954643816	-0.160110012728	-0.004789725657
H	2.153232079949	0.918423752574	0.514456592338
H	1.851637257882	-0.239789222699	-1.196735228017
H	2.034184018138	-1.159265518393	0.669099313527

Q(A-M):

C	-0.11298754	0.00876135	-0.66739123
C	-0.03232802	-0.07815052	0.69980311
H	-0.28798598	-0.91041321	-1.23620341
H	-0.17932239	-1.03080535	1.21098061
B	1.84830830	-0.13807833	-0.02404266
H	2.18429590	1.01308091	0.14486630
H	1.98387663	-0.56036893	-1.15732985
H	2.14320771	-0.96170135	0.81585507
C	-0.18642697	1.30720840	-1.43589647
H	0.49820600	1.29598462	-2.29887246
H	-1.21563573	1.43750255	-1.81559101
H	0.06514742	2.16340335	-0.79077280
H	0.01236567	0.82304950	1.31746782

TSM:

C	0.098634136975	0.050480389205	-0.727444242953
C	0.117506338189	0.047708400141	0.686038985548
H	-0.165252831429	-0.892181335288	-1.214657557893
H	-0.103308016739	-0.862464645532	1.248882094825
B	1.762136655515	-0.105710183445	-0.142173171094
H	2.131761671452	-1.220019746655	-0.421566876193
H	1.775643275565	-0.050003097983	1.111441304835
H	2.316220701886	0.903777437320	-0.503247664787
C	-0.170763336178	1.321238455056	-1.519241332284
H	0.378166045302	1.315176962907	-2.474966114952
H	-1.248925269212	1.417493415623	-1.741496234656
H	0.149095486085	2.210209199150	-0.950117361278
H	0.018582142589	0.987312749497	1.238369170880

PM:

C	0.052580161129	0.084589334003	-0.791519714902
C	-0.020669208803	-0.039841723237	0.763281984499
H	-0.574109102832	-0.727239467488	-1.207684449978
H	0.313452357624	-1.030623183130	1.119013390443
B	1.577961949469	-0.161645186512	-1.119978004224
H	2.020092448870	-1.285209021831	-1.200407239719
H	0.600461121206	0.730888907731	1.257253614661
H	2.345215390256	0.772475913008	-1.204748454201
C	-0.504001764016	1.449248813211	-1.243660380299
H	-0.474652552236	1.556807705544	-2.342481545330
H	-1.553490431048	1.581479847775	-0.922026058242
H	0.090573394174	2.274821225664	-0.811163000394
H	-1.061809764280	0.107480835332	1.101993857535

TSAM:

C	-0.035326222110	0.050548710618	-0.726658152687

C	-0.036302128158	0.044170161982	0.680720905990
H	-0.218768797011	-0.894896298294	-1.247529123235
H	-0.288922360871	-0.870178600446	1.218731664660
B	1.651664898740	-0.060366581867	0.109895903309
H	2.159206041785	0.992507633378	0.421729381522
H	1.681777708807	-0.105809754277	-1.133809420637
H	2.048871067740	-1.136298504705	0.490013776606
C	-0.242871264609	1.320928653736	-1.524926807694
H	0.229216893188	1.261007857114	-2.518083894862
H	-1.327798237579	1.477900979984	-1.658587165302
H	0.171014210010	2.185980102506	-0.982273376285
H	-0.179943809964	0.987589640265	1.212172308576

PAM:

C	0.04321562	-0.00376858	-0.78969255
C	0.01479588	-0.01183540	0.77119543
H	-0.00197206	-1.04207697	-1.16941774
H	-0.94849637	-0.44723070	1.09478831
B	1.25634957	-0.86123679	1.25168566
H	2.33521353	-0.33896767	1.42287265
H	1.00165120	0.42104111	-1.14458754
H	1.17555572	-2.06259038	1.37301971
C	-1.12125179	0.80545155	-1.38652272
H	-1.08728007	0.79988950	-2.49006638
H	-2.09202198	0.38363044	-1.07193505
H	-1.08147935	1.85584935	-1.04770347
H	0.05449609	1.03610155	1.12149969

6) **F_X = -10**

C_3H_6:

C	-0.097095121407	0.017505478493	-0.681244626717

C	0.101563760512	-0.015047336669	0.652882569013
H	-0.267353134448	-0.927868586883	-1.214492315380
H	0.096657402213	-0.958485533990	1.207622606758
C	-0.098744693294	1.275323316255	-1.520357827909
H	0.684990804396	1.229878144420	-2.297812222850
H	-1.066232571108	1.401102969817	-2.039536112900
H	0.081019649804	2.168031427374	-0.897792855715
H	0.279932902657	0.902455121181	1.225849785733

BH_3:

B	2.014052911813	-0.160241022488	-0.004190318057
H	2.151902891226	0.919298677852	0.513669676674
H	1.851371507142	-0.239669563449	-1.196015530551
H	2.032680689822	-1.160130091832	0.668566170330

Q(A-M):

C	-0.120079970203	0.009291033273	-0.665657933627
C	-0.037942057301	-0.080883673530	0.700293214682
H	-0.293300553376	-0.908684847720	-1.237110950801
H	-0.178357554203	-1.035485342258	1.209903404419
B	1.858068718976	-0.138467432804	-0.029877733808
H	2.180529652806	1.017254148821	0.126676352042
H	1.983811302601	-0.576311236399	-1.157530478649
H	2.143550758330	-0.949161326319	0.824699168115
C	-0.186763490763	1.309113549349	-1.432910997243
H	0.509963158354	1.300908382140	-2.286181153439
H	-1.210873047276	1.439461294739	-1.826911995002
H	0.056160763113	2.164525624283	-0.783418610448
H	0.015953319010	0.817913826429	1.320900713854

TSM:

C	0.09296727	0.05076435	-0.72517901
C	0.11626133	0.04780637	0.68717489

H	-0.16580898	-0.89243340	-1.21408713
H	-0.10047326	-0.86283868	1.25083154
B	1.76168138	-0.10543660	-0.13959237
H	2.12475467	-1.21954296	-0.42560569
H	1.78469550	-0.05050410	1.11232188
H	2.30835081	0.90489677	-0.50708208
C	-0.16999728	1.32092396	-1.51962818
H	0.38897196	1.31593652	-2.46941462
H	-1.24641775	1.41612495	-1.75300681
H	0.14341845	2.21017520	-0.94748827
H	0.02109191	0.98714763	1.24057585

PM:

C	0.05344605	0.08474672	-0.78927561
C	-0.02281760	-0.04014046	0.76456987
H	-0.57192879	-0.72742504	-1.20776239
H	0.31164512	-1.03081378	1.11989651
B	1.58019671	-0.16100583	-1.12183877
H	2.02024542	-1.28500112	-1.19564894
H	0.59843305	0.72948737	1.25967746
H	2.34348278	0.77364923	-1.21906239
C	-0.50301093	1.44906406	-1.24254545
H	-0.46978985	1.55741817	-2.34125594
H	-1.55393171	1.58105159	-0.92349863
H	0.09004331	2.27471325	-0.80850933
H	-1.06441255	0.10748685	1.10312862

TSAM:

C	-0.038553835843	0.049837948032	-0.724896088584
C	-0.041578835697	0.044005072837	0.680774568348
H	-0.218850638379	-0.895855695348	-1.246389210123
H	-0.284119029127	-0.871218817417	1.221862795714

B	1.653178009606	-0.059698374221	0.103557307511
H	2.151672950616	0.994823389137	0.421454079315
H	1.689557030935	-0.105977888185	-1.138287019027
H	2.043041804690	-1.135130502481	0.490463694817
C	-0.242999786682	1.320359405089	-1.524112730527
H	0.231937668726	1.259530494559	-2.515791140360
H	-1.327428543115	1.480603653346	-1.660520197206
H	0.172688953454	2.184513440716	-0.981384644328
H	-0.176726748733	0.987292874590	1.214663585504

PAM:

C	0.04625908	0.00155619	-0.79066804
C	0.01711849	-0.01066765	0.76941047
H	0.00951660	-1.03577408	-1.17414958
H	-0.94863299	-0.44173560	1.09281424
B	1.25586837	-0.86578797	1.25296235
H	2.33952248	-0.35097446	1.40536635
H	1.00143576	0.43427806	-1.14304934
H	1.16117958	-2.06339023	1.39728100
C	-1.12371769	0.80319224	-1.38694010
H	-1.08743137	0.80265030	-2.49053050
H	-2.09185842	0.37180252	-1.07550349
H	-1.09313064	1.85265036	-1.04392550
H	0.06264273	1.03645732	1.12206814

2. The number of imaginary frequencies of structures:

Table S1. The number of imaginary frequencies of stationary points in hydroboration reaction of C_2H_4 with and without OEEF.

	OEEF	Q	TS[a]	P
	0	0	1 (−480.42 i)	0
F_Z[b]	20	0	1 (−439.44 i)	0
	40	0	1 (−388.18 i)	0
	60	0	1 (−322.81 i)	0
	80	0	1 (−216.06 i)	0
	−10	0	1 (−499.94 i)	0
	−15	0	1 (−509.08 i)	0
	−20	0	1 (−517.93 i)	0
F_X[c]	20	0	1 (−505.11 i)	0
	−20	0	1 (−453.91 i)	0

[a] The values of imaginary frequencies of TSs are listed in brackets, and the unit is given in cm^{-1}; [b] represents the external electric field is oriented to parallel the direction of C=C bond, and [c] is perpendicular to C=C bond.

Table S2. The number of imaginary frequencies of stationary points in hydroboration reaction of C_3H_6 with and without OEEF.

	OEEF	Q(A-M)	TSM[a]	PM	TSAM[a]	PAM
	0	0	1 (−617.32 i)	0	1 (−471.51 i)	0
F_Z[b]	10	0	1 (−630.05 i)	0	1 (−454.73 i)	0
	30	0	1 (−653.44 i)	0	1 (−416.63 i)	0
	50	0	1 (−675.89 i)	0	1 (−372.30 i)	0
	70	0	1 (−696.82 i)	0	1 (−318.21 i)	0
	−10	0	1 (−605.38 i)	0	1 (−487.73 i)	0
	−30	0	1 (−577.33 i)	0	1 (−517.68 i)	0
	−50	0	1 (−549.96 i)	0	1 (−545.35 i)	0
	−55	0	1 (−542.14 i)	0	1 (−551.92 i)	0
	−56	0	1 (−542.28 i)	0	1 (−555.97 i)	0
	−57	0	1 (−538.00 i)	0	1 (−555.90 i)	0
	−58	0	1 (−538.15 i)	0	1 (−555.83 i)	0
	−59	0	1 (−538.29 i)	0	1 (−555.75 i)	0
	−60	0	1 (−533.75 i)	0	1 (−558.36 i)	0
	−70	0	1 (−519.51 i)	0	1 (−570.06 i)	0
F_X[c]	10	0	1 (−626.41 i)	0	1 (−482.71 i)	0
	−10	0	1(−609.13 i)	0	1 (−460.18 i)	0

[a] The values of imaginary frequencies of TSMs and TSAMs are respectively listed in brackets, and the unit is given in cm^{-1}; [b] represents the external electric field is oriented to parallel the direction of C=C bond, and [c] is perpendicular to C=C bond.

3. Computed total electronic energies (with ZPE) of optimized structures:

Table S3. The total electronic energies (with ZPE) of stationary points in hydroboration reaction of C_2H_4 with and without OEEF.

OEEF / Total energy (with ZPE)	**0**	**20**[a]	**40**[a]	**60**[a]	**80**[a]
BH_3	−26.4848024	−26.484844	−26.484961	−26.4851683	−26.485456
C_2H_4	−78.3072254	−78.307297	−78.307515	−78.3078795	−78.30839
Q	−104.7998707	−104.799978	−104.800325	−104.8010709	−104.801911
TS	−104.7981522	−104.798913	−104.799833	−104.8009093	−104.802143
P	−104.8376414	−104.837933	−104.838409	−104.8390698	−104.839916
	−10[a]	**−15**[a]	**−20**[a]	**20**[b]	**−20**[b]
BH_3	−26.484813	−26.484826	−26.484844	−26.484829	−26.484829
C_2H_4	−78.307242	−78.307265	−78.307297	−78.307274	−78.307274
Q	−104.799916	−104.799946	−104.800004	−104.8021	−104.797894
TS	−104.797831	−104.797685	−104.797549	−104.800203	−104.796306
P	−104.837563	−104.837542	−104.837532	−104.838176	−104.837294

[a] The energies of stationary points are calculated when the OEEF parallel to the direction of C=C bond; [b] The energies of stationary points are calculated when the OEEF are perpendicular to the direction of C=C bond.

Table S4. The total electronic energies (with ZPE) of stationary points in hydroboration reaction of C_3H_6 with and without OEEF.

OEEF / Total energy (with ZPE)	**0**	**10**[a]	**30**[a]	**50**[a]	**70**[a]
BH_3	−26.484802	−26.48481	−26.484889	−26.48505	−26.4853
C_3H_6	−117.481994	−117.4821	−117.4826	−117.4833	−117.4841
Q(A-M)	−143.977575	−143.9778	−143.97844	−143.9793	−143.9805
TSM	−143.971721	−143.9715	−143.97111	−143.971	−143.9711
PM	−144.009519	−144.0095	−144.00958	−144.0099	−144.0104
TSAM	−143.975918	−143.9764	−143.97751	−143.9788	−143.9804
PAM	−144.009529	−144.0097	−144.01018	−144.0109	−144.0119
	−10[a]	**−30**[a]	**−50**[a]	**−60**[a]	**−70**[a]
BH_3	−26.484813	−26.48489	−26.485056	−26.48517	−26.48531
C_3H_6	−117.481894	−117.4819	−117.48202	−117.4822	−117.4824
Q(A-M)	−143.977469	−143.9774	−143.97769	−143.9779	−143.9782
TSM	−143.972037	−143.9728	−143.97386	−143.9745	−143.9751
PM	−144.009614	−144.01	−144.01057	−144.0109	−144.0114
TSAM	−143.9755	−143.9748	−143.9744	−143.9743	−143.9742
PAM	−144.009429	−144.0094	−144.00963	−144.0098	−144.0101
	−55[a]	**−56**[a]	**−57**[a]	**−58**[a]	**−59**[a]
BH_3	−26.485111	−26.48512	−26.485134	−26.48515	−26.48516
C_3H_6	−117.482088	−117.4821	−117.48212	−117.4821	−117.4822
Q(A-M)	−143.977783	−143.9778	−143.97783	−143.9779	−143.9779
TSM	−143.974154	−143.9742	−143.97427	−143.9743	−143.9744
PM	−144.010752	−144.0108	−144.01083	−144.0109	−144.0109
TSAM	−143.974323	−143.9743	−143.9743	−143.9743	−143.9743
PAM	−144.009724	−144.0097	−144.00977	−144.0098	−144.0098
	10[b]	**−10**[b]			
BH_3	−26.484804	−26.484804			
C_3H_6	−117.482025	−117.481999			
Q(A-M)	−143.978745	−143.976486			
TSM	−143.972723	−143.970783			
PM	−144.009771	−144.009328			
TSAM	−143.977003	−143.974894			
PAM	−144.009739	−144.009383			

[a] The energies of stationary points are calculated when the OEEF parallel to the direction of C=C bond; [b] The energies of stationary points are calculated when the OEEF are perpendicular to the direction of C=C bond.

4. Computed relative energies (with ZPE) of optimized structures:

Table S5. The relative energies of stationary points along potential surface in hydroboration of C_2H_4 and the dipole moment of C_2H_4 with and without OEEF when the electric field is along $-F_Z$.

F_Z[a]	Q[b]	TS[b]	P[b]	μ[c]
−10	−20.64	−15.16	−119.48	0.09
−15	−20.62	−14.69	−119.33	0.13
−20	−20.64	−14.20	−119.17	0.18

[a] F_Z is given in the unit of ($\times 10^{-4}$) a.u.; [b] The relative energies of Q, TS, and P is given in kJ/mol; [c] The dipole moment is given in Debye (D).

Table S6. The relative energies of stationary points along potential surface in hydroboration of C_2H_4 and the dipole moment of C_2H_4 with and without OEEF when the electric field is along F_X and $-F_X$.

F_X[a]	Q[b]	TS[b]	P[b]	μ[c]
0	−20.59	−16.08	−119.76	0.000
20	−26.25	−21.27	−120.96	0.002
−20	−15.20	−11.03	−118.65	−0.002

[a] F_X is given in the unit of ($\times 10^{-4}$) a.u.; [b] The relative energies of Q, TS, and P is given in kJ/mol; [c] The dipole moment is given in Debye (D), and the number of digits is given in three due to they are too close to zero.

Table S7. The relative energies of stationary points along potential surface in hydroboration of C_3H_6 and the dipole moment of C_3H_6 with and without OEEF when the electric field is along F_X and $-F_X$.

F_X[a]	Q(A-M) [b]	TSM[b]	PM[b]	TSAM[b]	PAM[b]	μ[c]
0	−28.3	−12.93	−112.17	−23.95	−112.2	−0.32
10	−31.2855	−15.4747	−112.744	−26.7118	−112.66	−0.32
−10	−25.4227	−10.4495	−111.649	−21.2429	−111.794	−0.31

[a] F_X is given in the unit of ($\times 10^{-4}$) a.u.; [b] The relative energies of Q, TS, and P is given in kJ/mol; [c] The dipole moment is given in Debye (D).

5. Variations of charge quantity of carbon atoms with the change of electric field in hydroboration reactions of C_3H_6 with BH_3:

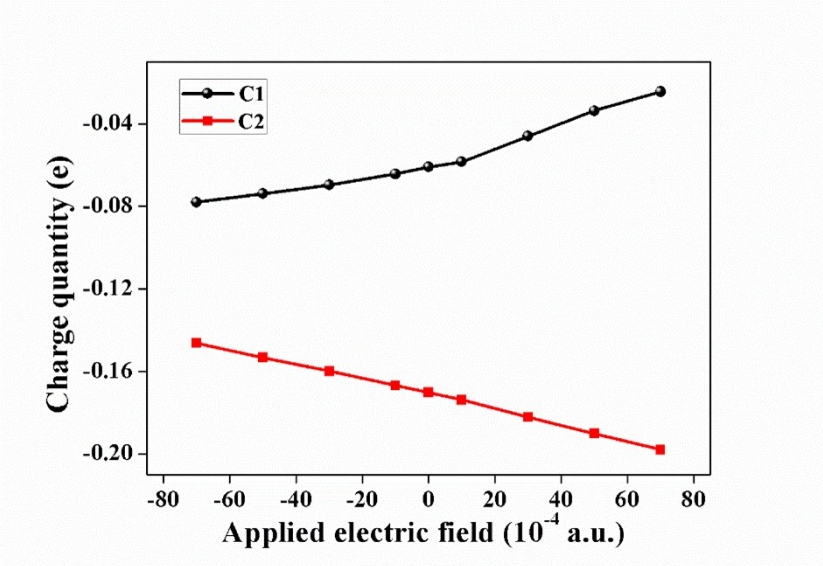

Fig. S1 The variations of charge quantity of carbon atoms with the change of electric field in the hydroboration reactions of C_3H_6 with BH_3.

6. Frontier molecular orbitals of stationary points along potential energy surface in hydroboration reactions of C_3H_6 with BH_3:

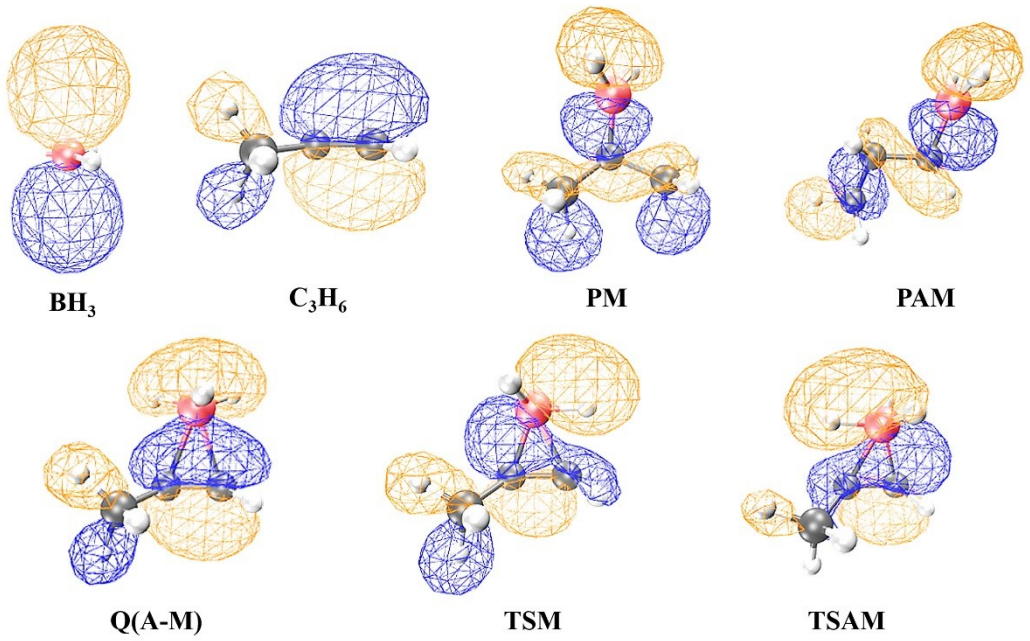

Fig. S2 The frontier molecular orbitals of the stationary points along potential energy surface in the hydroboration reactions of C_3H_6 with BH_3. Noted: The Isovalves are set for 0.03; Orange color represents the positive, and blue color represents the negative; Except the BH_3 molecule, all of the frontier molecular orbitals are given in their HOMO.

7. Frontier molecular orbitals of precursor complex Q(A-M) along potential energy surface in hydroboration reactions of C_3H_6 with BH_3 in presence of field:

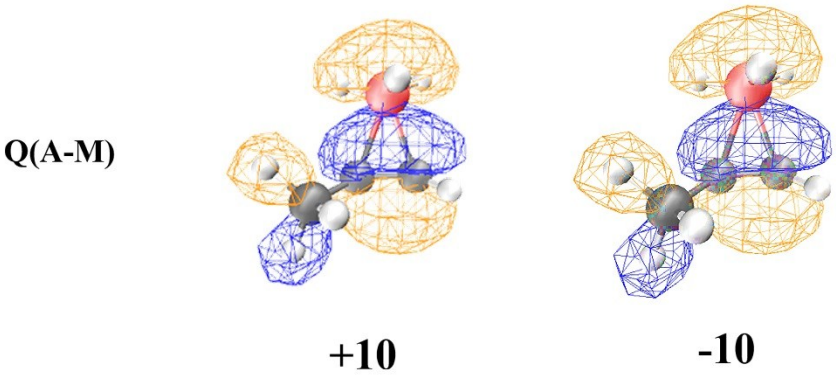

Fig. S3 Frontier molecular orbitals of precursor complex Q(A-M) along potential energy surface in hydroboration reactions of C_3H_6 with BH_3 as $F_X = \pm 10$ ($\times 10^{-4}$) a.u.