Electronic Supplementary Material (ESI) for RSC Advances.

Distortion–Interaction Analysis along the Reaction Pathway to Reveal the Reactivity of the Alder-Ene Reaction of Enes

Supporting Information

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1. Complete reference for Gaussian 09

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, **2013**.

2. B3LYP absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{(elec\text{-}B3LYP)}$[1]	$H_{(corr\text{-}B3LYP)}$[2]	$G_{(corr\text{-}B3LYP)}$[3]	IF[4]
2-ts	-196.504203338	0.136697	0.101489	-1251.85
3	-196.593182611	0.143823	0.106776	-
5-ts	-447.900975727	0.128393	0.090424	-363.65
6	-447.997480505	0.133106	0.092381	-
8-ts	-212.552372284	0.125348	0.090268	-1291.85
9	-212.638952966	0.132668	0.095971	-
11-ts	-499.165914608	0.119372	0.082454	-1139.94
12	-499.241751964	0.125629	0.085877	-
14-ts	-232.432594442	0.112354	0.077392	-1039.34
15	-232.506492415	0.120021	0.083939	-
17-ts	-555.413110167	0.110511	0.074025	-1203.63
18	-555.483614854	0.116948	0.078581	-

[1]The electronic energy calculated by B3LYP in gas phase. [2]The thermal correction to enthalpy calculated by B3LYP in gas phase. [3]The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. [4]The B3LYP calculated imaginary frequencies for the transition states.

3. M11 absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{(elec\text{-}M11)}$[1]	$H_{(corr\text{-}M11)}$[2]	$G_{(corr\text{-}M11)}$[3]	IF[4]
2-ts	-196.345221298	0.136597	0.101678	-1209.70
3	-196.437949724	0.143419	0.106688	-
5-ts	-447.734474951	0.127903	0.090028	-446.33
6	-447.837228022	0.132551	0.091822	-
8-ts	-212.397611674	0.125566	0.090749	-1400.31
9	-212.49086203	0.132268	0.095529	-
11-ts	-499.005642423	0.119636	0.083083	-1006.30

12	-499.085097188	0.125376	0.085498	-
14-ts	-232.279526128	0.112376	0.077638	-1323.69
15	-232.361052258	0.119882	0.084079	-
17-ts	-555.258929811	0.110595	0.074450	-1156.97
18	-555.334739374	0.116907	0.079042	-

[1]The electronic energy calculated by M11 in gas phase. [2]The thermal correction to enthalpy calculated by M11 in gas phase. [3]The thermal correction to Gibbs free energy calculated by M11 in gas phase. [4]The M11 calculated imaginary frequencies for the transition states.

4. G3B3 absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{(elec\text{-}G3B3)}$[1]	$H_{(elec\text{-}G3B3)}$[2]	$G_{(elec\text{-}G3B3)}$[3]	IF[4]
2-ts	-196.232006	-196.231062	-196.266420	-1194.43
3	-196.320609	-196.319665	-196.356934	-
5-ts	-447.502946	-447.502002	-447.540369	-363.92
6	-447.598378	-447.597434	-447.638477	-
8-ts	-212.279105	-212.278160	-212.313430	-1311.02
9	-212.364205	-212.363261	-212.400058	-
11-ts	-498.776229	-498.775285	-498.812445	-1112.30
12	-498.852250	-498.851306	-498.891303	-
14-ts	-232.155523	-232.154579	-232.189723	-1145.15
15	-232.230057	-232.229113	-232.265412	-
17-ts	-555.030902	-555.029958	-555.066678	-1205.44
18	-555.102398	-555.101453	-555.140092	-

[1]The electronic energy calculated by G3B3 in gas phase. [2]The thermal correction to enthalpy calculated by G3B3 in gas phase. [3]The thermal correction to Gibbs free energy calculated by G3B3 in gas phase. [4]The G3B3 calculated imaginary frequencies for the transition states.

5. CBS-QB3 absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{(elec\text{-}CBS\text{-}QB3)}$[1]	$H_{(elec\text{-}CBS\text{-}QB3)}$[2]	$G_{(elec\text{-}CBS\text{-}QB3)}$[3]	IF[4]
2-ts	-196.003289	-196.002345	-196.037593	-1251.13
3	-196.089993	-196.089048	-196.126148	-
5-ts	-447.026787	-447.025843	-447.063887	-372.99
6	-447.121200	-447.120256	-447.160969	-
8-ts	-212.050711	-212.049767	-212.084872	-1301.49
9	-212.134292	-212.133348	-212.170000	-
11-ts	-498.295395	-498.294450	-498.331411	-1129.39
12	-498.369109	-498.368165	-498.407508	-
14-ts	-231.928464	-231.927519	-231.962500	-1076.22
15	-232.002288	-232.001344	-232.037464	-
17-ts	-554.545307	-554.544363	-554.580898	-1198.56
18	-554.615307	-554.614363	-554.652760	-

[1]The electronic energy calculated by CBS-QB3 in gas phase. [2]The thermal correction to enthalpy calculated by CBS-QB3 in gas phase. [3]The thermal correction to Gibbs free energy calculated by CBS-QB3 in gas phase. [4]The CBS-QB3 calculated imaginary frequencies for the transition states.

6. Geometries for all the optimized compounds and transition states.

6.1 B3LYP geometries for all the optimized compounds and transition states.

1

C	-1.23400100	0.16278200	-0.00001200
H	-1.80743100	-0.15322900	-0.87854500
H	-1.80735700	-0.15298800	0.87865900
H	-1.18222700	1.25419600	-0.00016300
C	0.13370900	-0.45386900	0.00003300
H	0.16548500	-1.54232200	0.00004800
C	1.28163000	0.22031400	-0.00000100
H	2.23963300	-0.28736600	-0.00001500
H	1.30387100	1.30634600	-0.00010900

2-ts

C	-0.55247200	1.25804100	0.26633500
H	-0.42017100	1.22519800	1.34288100
C	-1.30515300	0.26807300	-0.34304100
H	-1.59922200	0.41135700	-1.38079900
C	-1.25565300	-1.05076400	0.15940700
H	0.06508700	-1.23038700	0.02063600
H	-1.77825200	-1.83506500	-0.38292200
H	-1.28868200	-1.18224000	1.24059700
C	1.43246500	0.54370300	-0.10801400
H	1.54308900	1.01462200	-1.07730300
H	1.81421500	1.13155100	0.71776200
C	1.46045400	-0.85923100	-0.02287200

H	1.67481800	-1.42971600	-0.92298100
H	1.82120900	-1.31763300	0.89405300
H	-0.50993600	2.25337300	-0.16281900

3

C	-1.52360000	0.52298300	0.00001300
H	-2.13493600	1.42446200	0.00003500
C	0.86186700	-0.46766000	0.00004800
H	0.63320700	-1.08354800	-0.87679900
H	0.63324500	-1.08329200	0.87708400
C	2.35187700	-0.11312700	-0.00004300
H	2.62006700	0.47558100	0.88297100
H	2.97409100	-1.01215100	0.00008400
H	2.62002600	0.47530500	-0.88325400
C	-2.14082000	-0.65741400	0.00008100
H	-3.22307900	-0.72292800	0.00014000
H	-1.60023000	-1.59752000	0.00009900
C	-0.03815100	0.77050800	-0.00009200
H	0.20525100	1.39604200	-0.87074700
H	0.20531800	1.39630400	0.87035300

4

Si	-1.15326400	0.10186100	0.00000500
H	-1.43197800	1.55341900	-0.00015900
H	-2.33866800	-0.77756000	0.00001100
C	0.44166700	-0.53290500	-0.00006200
H	0.53311900	-1.61780000	-0.00007300
C	1.74124000	0.22590600	0.00004700
H	2.34639100	-0.02548200	0.87942600
H	2.34657700	-0.02550500	-0.87919700
H	1.59282300	1.30886800	0.00001700

5-ts

C	1.41820800	0.33594600	-0.40656300
H	1.77081600	0.36856400	-1.43503200
Si	0.61637900	-1.12543200	0.16464600
H	0.46915700	-1.30881400	1.62805400
C	-1.55359200	-0.54701600	-0.24842000
H	-1.86698200	-1.30412900	0.46898500
H	-1.62521000	-0.86670900	-1.28342300
C	-1.86936500	0.77504300	0.04923600
H	-2.14388200	1.07239100	1.05455300
H	-0.20464100	1.61258200	0.08953100
H	-2.06190300	1.49384900	-0.73757600
C	0.96084200	1.59243900	0.18276700
H	1.10177100	1.67411300	1.26476700
H	1.33463900	2.49680300	-0.30232700
H	0.86037000	-2.42107700	-0.51469600

6

C	-1.72410300	-0.30253800	-0.40216100
H	-1.85035200	-0.94660100	-1.27324800
Si	-0.07397500	0.55662600	-0.16507000
H	-0.17077900	1.42145500	1.04462700
C	1.34503900	-0.68253600	0.02743000
H	1.34673200	-1.34041100	-0.84989500
H	1.12043700	-1.32687700	0.88507900
C	2.72985300	-0.03347900	0.19979400
H	2.76648500	0.60304600	1.08888800
H	3.51415600	-0.78876500	0.30617500
H	2.99019200	0.59038200	-0.66035000
C	-2.76246200	-0.17904500	0.43025400
H	-2.71601300	0.44717400	1.31737100
H	-3.70486200	-0.69426700	0.26252100
H	0.20969100	1.42768900	-1.34208700

7

C	-0.18899200	0.40501100	-0.00013400
H	-0.26986000	1.50180600	0.00019300
H	-2.07138600	0.19185000	0.00028600
C	1.20575500	-0.14099400	0.00001000
H	1.75385200	0.21571000	-0.87880800
H	1.75293400	0.21405100	0.88008400
H	1.18751500	-1.23122800	-0.00093000
N	-1.20766200	-0.35375600	-0.00001200

8-ts

C	1.30169500	0.29660900	0.27947400
H	1.78627200	0.48846000	1.24286300
C	1.26641400	-1.02255900	-0.20205600
H	1.12161700	-1.16842300	-1.26860300
H	1.87710500	-1.77436300	0.28731800
N	0.50664400	1.19446000	-0.27752200
H	0.50671000	2.06620700	0.25000100
C	-1.44838000	0.53889800	-0.05201900
H	-1.72029400	0.94020700	-1.01731300
H	-1.62376000	1.20141700	0.78653500
C	-1.43929200	-0.85137100	0.15228900
H	-1.65303900	-1.22145300	1.15236000
H	-1.81780100	-1.48193300	-0.64822200
H	-0.10594000	-1.18080700	0.09158500

9

C	1.41702300	0.54474900	0.00127600
H	1.93522300	1.49906800	0.03566600
C	-0.83220300	-0.47702500	0.05775900
H	-0.64213700	-1.00950700	1.00302000
H	-0.59455800	-1.17829900	-0.74953000
C	-2.29805700	-0.06649700	-0.03015100
H	-2.51264900	0.41933300	-0.98546100
H	-2.94548500	-0.94151500	0.06159900
H	-2.56479500	0.62634700	0.77481700
C	2.12616300	-0.59537800	-0.00944300
H	3.20643900	-0.55228800	-0.00269700
H	1.66742500	-1.57510200	-0.04147300
N	0.04285000	0.67659900	-0.07240700
H	-0.32696400	1.54067500	0.29425500

10

C	-0.37435300	0.53009000	0.00009400
H	-0.45447800	1.61478500	-0.00009800
P	1.12847100	-0.22201900	0.00000200
H	1.92277000	0.96630100	-0.00019800
C	-1.67703400	-0.20995000	-0.00003500
H	-2.27434700	0.06062500	0.87860700
H	-2.27468400	0.06135800	-0.87821300
H	-1.53799900	-1.29362200	-0.00049000

11-ts

C	-1.14036100	0.69291700	0.41445500
H	-1.45601900	0.86164400	1.44003000
P	-1.03381700	-0.90396600	-0.23477000
H	-1.47060100	-1.61483600	0.92583500
C	1.38647000	-0.97580200	0.08490100
H	1.50132000	-1.61601800	-0.78020100

H	1.30473500	-1.49660800	1.03136200
C	1.94785200	0.30873200	0.05601600
H	2.30440500	0.74368900	0.98586100
H	2.48750000	0.62193000	-0.83306100
H	0.81709900	1.24977200	-0.04683200
C	-0.39234400	1.70700500	-0.23191800
H	-0.42261700	2.71415400	0.17999600
H	-0.36826900	1.69865600	-1.32216300

12

C	-1.56572900	0.33572000	0.37369300
H	-1.50374400	1.07956700	1.16707900
C	1.23089000	0.65677300	-0.10217700
H	1.10436800	1.37519300	0.71308400
H	1.04753500	1.19504200	-1.03687400
C	2.65073400	0.07927500	-0.09484300
H	2.79913700	-0.62909700	-0.91459900
H	3.39407100	0.87421500	-0.20315300
H	2.86338200	-0.44588600	0.84094700
C	-2.70372800	0.19937400	-0.30695200
H	-3.57536300	0.80951200	-0.08926300
H	-2.80570100	-0.52999400	-1.10510700
P	-0.07998400	-0.68620300	0.00389400
H	0.20307300	-1.06236000	1.35116000

13

C	0.23341300	0.39665300	0.00008100
H	0.30842700	1.50631100	-0.00016700
O	1.23428400	-0.27638500	-0.00002300
C	-1.16831600	-0.14827600	-0.00003000
H	-1.70486500	0.22690400	-0.87853500
H	-1.16400300	-1.23814300	-0.00067900
H	-1.70441300	0.22573900	0.87925700

14-ts

C	-1.25113700	-0.34771000	0.29551100
H	-1.69051700	-0.55504800	1.28652300
C	-1.34861500	0.95220400	-0.20429100
H	-1.15497800	1.12670300	-1.25779200
H	0.13912400	1.12007300	0.11092600
O	-0.48407600	-1.21096900	-0.21940000
C	1.48834700	-0.52203000	-0.03698200
H	1.61705600	-1.18154900	0.80953600
H	1.68328200	-0.95862200	-1.00552600
C	1.41721600	0.86917100	0.12965400
H	1.75518300	1.48579400	-0.70071300
H	1.67314000	1.26731300	1.10986600
H	-1.98454600	1.67328900	0.29902400

15

C	1.35892700	-0.55635700	0.00005900
H	1.84224700	-1.52724600	0.00004400
C	-0.79397200	0.46787200	-0.00003000
H	-0.55514400	1.06679600	-0.88741900
H	-0.55512300	1.06685600	0.88731300
C	-2.24920800	0.04209100	-0.00000600
H	-2.47854900	-0.55365100	0.88624800
H	-2.89567400	0.92369900	-0.00034900
H	-2.47836600	-0.55419500	-0.88594300
C	2.06109400	0.57980600	0.00000100
H	3.14105900	0.52268700	-0.00005800
H	1.61337000	1.56394400	-0.00005300
O	0.01314200	-0.71367000	0.00000800

16

S	-1.14469700	-0.12577600	0.00000400
C	0.34828400	0.51290600	-0.00002500
H	0.45524000	1.60109900	0.00007800
C	1.63760500	-0.23973400	-0.00000700
H	2.23260600	0.04521800	-0.87674200
H	2.23233200	0.04483700	0.87704000
H	1.47963600	-1.31777300	-0.00024700

17-ts

C	-1.18059000	0.59253100	0.40184200
H	-1.55510900	0.76025000	1.41123200
C	-0.53536900	1.65022600	-0.25627700
H	0.73688000	1.21271100	-0.03128700
H	-0.45571800	1.60224900	-1.33958700
S	-0.98526800	-0.98289300	-0.13477500
C	1.47964500	-0.89167400	0.07516400
H	1.55803900	-1.50221100	-0.81361900
H	1.41684200	-1.42710400	1.01261200
C	1.90653200	0.43918000	0.05102900
H	2.26237100	0.88053500	0.97901700
H	2.39860200	0.80378100	-0.84698100
H	-0.61893000	2.65450100	0.15446600

18

C	1.68287300	-0.31164700	-0.00009300
H	2.37985700	-1.14467300	-0.00017400
C	-0.96176700	0.64311700	0.00045500
H	-0.69253700	1.22254100	-0.88568100
H	-0.69328500	1.22164300	0.88740400
C	-2.45153300	0.30750800	-0.00033400
H	-2.73142100	-0.26925100	0.88439400
H	-3.03841400	1.22991200	-0.00011600
H	-2.73068700	-0.26836300	-0.88587400
C	2.13484800	0.94502200	-0.00014600
H	3.20200700	1.13229700	-0.00025800
H	1.48578500	1.81121300	-0.00009600
S	0.02451100	-0.90245700	0.00006900

6.2 M11 geometries for all the optimized compounds and transition states.

1

C	-1.23057200	0.16245900	-0.00000400
H	-1.80248200	-0.15245300	-0.88247300
H	-1.80243200	-0.15225300	0.88256800
H	-1.16813100	1.25627000	-0.00012800
C	0.13636700	-0.45853500	0.00003500
H	0.17456300	-1.55069300	0.00009700
C	1.27420800	0.22343600	-0.00002200
H	2.23954400	-0.27921400	-0.00001200
H	1.27891900	1.31418000	-0.00011100

2-ts

C	-0.50900600	1.24389400	0.27776900
H	-0.38559800	1.17315200	1.35878200

C	-1.28500900	0.29075800	-0.35016900
H	-1.58254600	0.45283200	-1.38780100
C	-1.27138300	-1.02442400	0.15761000
H	0.01873800	-1.23880100	0.01590200
H	-1.81595500	-1.80247800	-0.37834000
H	-1.30308800	-1.13886300	1.24443000
C	1.41024400	0.52397900	-0.11656800
H	1.51905100	0.98285400	-1.09725100
H	1.81811300	1.11808200	0.69836900
C	1.44728000	-0.86967100	-0.02078600
H	1.62950900	-1.45685300	-0.92032800
H	1.78959200	-1.32993700	0.90556700
H	-0.44056800	2.25279500	-0.12646800

3

C	-1.51930000	0.52581100	0.00000000
H	-2.15100100	1.41822500	-0.00005800
C	0.84332300	-0.46724000	-0.00004000
H	0.60414400	-1.07941300	-0.88132100
H	0.60406200	-1.07931900	0.88128400
C	2.33151800	-0.11663500	0.00000100
H	2.59466800	0.47604700	0.88592100
H	2.95789300	-1.01634300	0.00010100
H	2.59474900	0.47590600	-0.88598900
C	-2.10466100	-0.66526500	0.00018400
H	-3.18940000	-0.75721000	0.00026400
H	-1.53068000	-1.59150700	0.00026600
C	-0.03557900	0.78121300	-0.00014200
H	0.21181700	1.40303400	-0.87556600
H	0.21194100	1.40327200	0.87507600

4

Si	-1.14385700	0.10240500	-0.00004600
H	-1.40309200	1.56489000	-0.00007800
H	-2.34946700	-0.76066200	-0.00007400
C	0.43522400	-0.54077000	0.00002700
H	0.52997500	-1.62889200	0.00004700
C	1.73111700	0.22791900	0.00006200
H	2.33452500	-0.02199600	0.88337500
H	2.33458000	-0.02200700	-0.88321100
H	1.56942800	1.31210700	0.00005000

5-ts

C	1.32548200	0.50236200	-0.43731800
H	1.66598000	0.60255500	-1.46790700
Si	0.79292900	-1.04214400	0.16063500
H	0.62645500	-1.21345200	1.62963500
C	-1.51195300	-0.71734500	-0.23252700
H	-1.67678400	-1.48598900	0.52475100
H	-1.52296800	-1.07014700	-1.26219200
C	-1.91924200	0.56884000	0.04103700
H	-2.23375000	0.85220500	1.04404600
H	-0.44767700	1.53276500	0.09288200
H	-2.20354800	1.24107700	-0.76612900
C	0.72608600	1.66420700	0.19955300
H	0.84213200	1.71173300	1.28953900
H	0.97333600	2.63157500	-0.24803200
H	1.15358600	-2.32069700	-0.50995700

6

C	-1.72125700	-0.32484300	-0.39309900
H	-1.87537900	-1.01844100	-1.22491500
Si	-0.06881600	0.52502400	-0.19613000
H	-0.16714100	1.43656200	0.98710900
C	1.33882300	-0.69562500	0.04902600
H	1.36387400	-1.38255300	-0.80863100
H	1.11690200	-1.31415700	0.92941200
C	2.69972400	0.00119600	0.21118300
H	2.70225300	0.67111500	1.08040100
H	3.50977200	-0.72446000	0.35075400
H	2.94440900	0.60609500	-0.67112100
C	-2.73650300	-0.13021900	0.44680400
H	-2.65390500	0.55096500	1.29619200
H	-3.69515100	-0.63735500	0.32539600
H	0.23306400	1.35883200	-1.40227000

7

C	-0.19087900	0.40494100	-0.00017800
H	-0.28349700	1.50412900	0.00027300
H	-2.06928800	0.18471600	0.00033600
C	1.20520800	-0.13969200	0.00001600
H	1.75181100	0.21629400	-0.88271500
H	1.75078500	0.21451300	0.88412300
H	1.17717600	-1.23250400	-0.00099300
N	-1.20185200	-0.35409200	-0.00000800

8-ts

C	1.28327000	0.31420600	0.28045700
H	1.77542300	0.52747900	1.23911700
C	1.27347900	-1.00014600	-0.20775300
H	1.12117300	-1.12607800	-1.27959100
H	1.90825100	-1.74497300	0.26821000
N	0.45844100	1.18048400	-0.26807600
H	0.44048600	2.06233800	0.24023600
C	-1.41153300	0.52045300	-0.06595800
H	-1.71258200	0.89591300	-1.03912400
H	-1.62330300	1.19198900	0.76432900
C	-1.42691500	-0.85892700	0.16541400
H	-1.60424600	-1.21882800	1.17857500
H	-1.78231700	-1.51505300	-0.62781000
H	-0.04177800	-1.18969700	0.09962600

9

C	1.41047000	0.55045800	0.00462800
H	1.94789600	1.49857100	0.04458900
C	-0.81174500	-0.47847300	0.02230800
H	-0.58165900	-1.04684400	0.94117000
H	-0.59006300	-1.14333800	-0.82590000
C	-2.27839400	-0.06961300	-0.00256800
H	-2.51223200	0.47330000	-0.92584300
H	-2.92743200	-0.94976200	0.05219500
H	-2.51947900	0.57744500	0.85103700
C	2.08873000	-0.60413200	0.00354800
H	3.17324000	-0.58918400	0.02912600
H	1.59426400	-1.57113600	-0.03616900
N	0.04432500	0.68520000	-0.07424700
H	-0.34916900	1.56510100	0.22203200

10

C	-0.36510000	0.52998500	0.00003300
H	-0.43876600	1.61945400	-0.00004900
P	1.11990500	-0.22334900	0.00000000
H	1.91488000	0.96629800	-0.00005700
C	-1.67096100	-0.20839200	-0.00001800
H	-2.26526400	0.06440000	0.88269200

H	-2.26571000	0.06513100	-0.88219000
H	-1.52735000	-1.29460500	-0.00047700

11-ts

C	-1.13726200	0.65393600	0.43114400
H	-1.43418800	0.80650800	1.46864100
P	-0.99153500	-0.91160000	-0.24180600
H	-1.39523300	-1.65503700	0.91242900
C	1.37236200	-0.94033500	0.09209200
H	1.50879700	-1.59481800	-0.76530700
H	1.29547800	-1.44870200	1.05110200
C	1.92936800	0.33526500	0.04961500
H	2.25654300	0.80408000	0.97724400
H	2.45217000	0.65820100	-0.84964300
H	0.76739300	1.28664600	-0.05816800
C	-0.43881400	1.69174400	-0.23274800
H	-0.49277500	2.70189300	0.17695300
H	-0.43909400	1.67156700	-1.32677900

12

C	-1.54877900	0.33889300	0.37309600
H	-1.47561500	1.09885600	1.15570500
C	1.21126800	0.66044700	-0.12005600
H	1.06964000	1.39166300	0.68536900
H	1.03627300	1.18313900	-1.06853900
C	2.62759500	0.07989100	-0.08315800
H	2.78101800	-0.64248800	-0.89399100
H	3.38040000	0.86980600	-0.18866000
H	2.81687300	-0.43820300	0.86546800
C	-2.68598700	0.19310800	-0.29724400
H	-3.55782200	0.81251600	-0.08501100
H	-2.78688600	-0.55532900	-1.08440100
P	-0.07413500	-0.68774700	0.00152400
H	0.22356000	-1.03778400	1.35537600

13

C	0.23541300	0.39958300	-0.00002100
H	0.32180200	1.51120100	0.00003100
O	1.22678400	-0.27930600	0.00000100
C	-1.16599200	-0.14724200	-0.00001800
H	-1.70212300	0.22496000	-0.88241400
H	-1.14894400	-1.23972500	-0.00056400
H	-1.70153600	0.22396600	0.88316900

14-ts

C	-1.23240900	-0.35988200	0.29487400
H	-1.67824600	-0.59160500	1.28028600
C	-1.34027500	0.93405200	-0.20509900
H	-1.13774600	1.09196800	-1.26360900
H	0.07576300	1.11978900	0.12041600
O	-0.43595900	-1.19405600	-0.21977900
C	1.43801100	-0.51120900	-0.04012100
H	1.60185100	-1.17058600	0.80737300
H	1.67062300	-0.93650900	-1.01134300
C	1.40225200	0.87300200	0.13564300
H	1.71545600	1.50248800	-0.69718900
H	1.63082300	1.27093300	1.12470700
H	-1.99632700	1.65019500	0.28580400

15

C	1.35412500	-0.55861600	0.00013500
H	1.85790400	-1.52432400	0.00018300
C	-0.77717500	0.46121100	0.00003200
H	-0.52739100	1.05745500	-0.89166700
H	-0.52754500	1.05747100	0.89176400
C	-2.23450300	0.04775600	-0.00008900
H	-2.46060800	-0.55091900	0.88866100
H	-2.88070300	0.93287700	-0.00029500
H	-2.46039900	-0.55117700	-0.88872000
C	2.02789200	0.59004800	-0.00011000
H	3.11263000	0.55621700	-0.00024600
H	1.54977600	1.56460800	-0.00031800
O	0.01428700	-0.72307500	0.00010300

16

S	-1.13663800	-0.12696200	-0.00009200
C	0.34155100	0.51484600	0.00017800
H	0.44105200	1.60744500	0.00003900
C	1.63089200	-0.23931400	0.00004500
H	2.22334300	0.04516600	-0.88088100
H	2.22323000	0.04475200	0.88118200
H	1.46393000	-1.31915800	-0.00020400

17-ts

C	-1.18391200	0.53561000	0.41792000
H	-1.54571100	0.67299900	1.44023700
C	-0.60586000	1.62479200	-0.25095200
H	0.64995300	1.26485800	-0.03890800
H	-0.55015800	1.56652800	-1.33942400
S	-0.90942600	-1.00226400	-0.14735900
C	1.44965200	-0.83423100	0.09711500
H	1.57925100	-1.47558900	-0.77038500
H	1.42324000	-1.34187200	1.05759300
C	1.87324500	0.48839500	0.03392300
H	2.20284200	0.97967600	0.94932200
H	2.32744100	0.85390800	-0.88641100
H	-0.73479700	2.62831700	0.15769200

18

C	1.66980500	-0.30941200	-0.00009400
H	2.39167200	-1.12616500	-0.00018200
C	-0.92912000	0.63919300	0.00000600
H	-0.65057400	1.21433900	-0.89093200
H	-0.65058800	1.21429100	0.89097900
C	-2.42069900	0.31660600	-0.00004200
H	-2.69804100	-0.26279700	0.88780500
H	-3.00651900	1.24266400	-0.00002000
H	-2.69804000	-0.26274800	-0.88792400
C	2.08409400	0.95469600	0.00001600
H	3.14992700	1.17104400	-0.00000100
H	1.40399500	1.80273800	0.00017900
S	0.02085500	-0.91249100	0.00004900

6.3 G3B3 geometries for all the optimized compounds and transition states.

1

C	-1.23509400	0.16290100	0.00000300
H	-1.81225000	-0.15077400	-0.88040700
H	-1.81216300	-0.15054400	0.88055400
H	-1.18169000	1.25681600	-0.00014000
C	0.13380300	-0.45543800	0.00001500

H	0.16398600	-1.54622800	0.00009000
C	1.28315500	0.22040200	-0.00002400
H	2.24518500	-0.28511200	0.00002200
H	1.30574400	1.30865200	-0.00007700

2-ts

C	-0.52567900	1.25410900	0.26907100
H	-0.40311500	1.21590200	1.34963200
C	-1.30873800	0.28413400	-0.34106300
H	-1.59607900	0.43341000	-1.38241200
C	-1.26510800	-1.04292100	0.15660900
H	0.02854000	-1.24380000	0.02117300
H	-1.80817600	-1.81808000	-0.38504200
H	-1.32024500	-1.17230800	1.24066300
C	1.42385300	0.53522800	-0.11127300
H	1.54046100	0.99940300	-1.08647300
H	1.82582200	1.12590500	0.70699500
C	1.46195300	-0.86829900	-0.02202200
H	1.66897000	-1.44430900	-0.92303500
H	1.82073500	-1.32734500	0.89807400
H	-0.47460300	2.25771300	-0.14751100

3

C	-1.52465400	0.52433600	0.00000300
H	-2.13971000	1.42604500	-0.00002000
C	0.85929500	-0.46600200	0.00004300
H	0.62680700	-1.08234400	-0.87854400
H	0.62685000	-1.08211900	0.87879900
C	2.35106100	-0.11630000	-0.00004300
H	2.62145200	0.47326600	0.88471100
H	2.97178900	-1.01939500	0.00006800
H	2.62140800	0.47301900	-0.88497500
C	-2.13705300	-0.66077900	0.00009900
H	-3.22121300	-0.73517300	0.00015300
H	-1.59064200	-1.60012200	0.00012600
C	-0.03785200	0.77584600	-0.00009200
H	0.20920500	1.40198900	-0.87261600
H	0.20927800	1.40223200	0.87223600

4

Si	-1.15479000	0.10175400	0.00000800
H	-1.43606100	1.55616300	-0.00016300
H	-2.34168400	-0.78185000	0.00000700
C	0.44268400	-0.53292800	-0.00006500
H	0.53887400	-1.61978800	-0.00007400
C	1.74268600	0.22636900	0.00004500
H	2.34968700	-0.02558900	0.88128000
H	2.34987200	-0.02561100	-0.88105500
H	1.59415400	1.31147800	0.00001600

5-ts

C	1.42097400	0.36592400	-0.40479100
H	1.78497300	0.41832500	-1.43081200
Si	0.65198000	-1.11534600	0.15683500
H	0.50816200	-1.31470700	1.62100300
C	-1.57034300	-0.58128600	-0.22823400
H	-1.86133900	-1.32438400	0.51526700
H	-1.64788000	-0.93240500	-1.25526000
C	-1.89138200	0.74686500	0.03503300
H	-2.16952600	1.07058900	1.03385100
H	-0.23961600	1.60695800	0.07856700
H	-2.09130700	1.44411500	-0.77275500
C	0.92542800	1.60887100	0.18829700
H	1.05096400	1.68292400	1.27561400
H	1.29115100	2.52823300	-0.28124700
H	0.93862900	-2.40704300	-0.52175000

6

C	-1.72962200	-0.30952100	-0.40127900
H	-1.86941900	-0.96854300	-1.26174300
Si	-0.07545800	0.54350200	-0.17731500
H	-0.17271000	1.42321800	1.02428100
C	1.35308700	-0.68713600	0.03178000
H	1.37009800	-1.35457300	-0.84119500
H	1.13381200	-1.32923700	0.89560400
C	2.72819000	-0.01820800	0.20654400
H	2.74987700	0.62868500	1.09151300
H	3.52435100	-0.76320100	0.32527100
H	2.98558000	0.60263700	-0.65962300
C	-2.76194400	-0.16277200	0.43936100
H	-2.70253900	0.47769600	1.31798500
H	-3.71457900	-0.67053500	0.29093200
H	0.21367000	1.41065100	-1.35905000

7

C	-0.19036800	0.40904600	-0.00015100
H	-0.26139100	1.50886900	0.00022600
H	-2.07026600	0.19886200	0.00030400
C	1.20572000	-0.14159300	0.00001600
H	1.75868000	0.21005200	-0.88103700
H	1.75783500	0.20854600	0.88221600
H	1.17862700	-1.23408900	-0.00084400
N	-1.20794200	-0.35670800	-0.00000800

8-ts

C	1.30161000	0.30770500	0.27627700
H	1.79390000	0.50636500	1.23735500
C	1.26704700	-1.01817100	-0.20095400
H	1.13823900	-1.15967900	-1.27331900
H	1.89936400	-1.76100200	0.28099400
N	0.48324300	1.19156600	-0.27591300
H	0.47436000	2.06081900	0.26314900
C	-1.43135700	0.53403500	-0.05736500
H	-1.72100800	0.92714600	-1.02436200
H	-1.62389500	1.20149600	0.77749300
C	-1.43591500	-0.85770700	0.15741900
H	-1.65038500	-1.21996500	1.16281100
H	-1.82308100	-1.49280000	-0.63858000
H	-0.07850900	-1.19851800	0.09358500

9

C	1.41700100	0.54441900	0.00190200
H	1.93967000	1.49905900	0.03778100
C	-0.82553600	-0.47173200	0.05980900
H	-0.62926500	-1.00223300	1.00847600
H	-0.58269700	-1.17635900	-0.74566300
C	-2.29604100	-0.07289200	-0.02956000
H	-2.50986800	0.41719600	-0.98536000
H	-2.93972100	-0.95408100	0.05876900
H	-2.57015400	0.61847700	0.77779600
C	2.11899000	-0.60021500	-0.00660100
H	3.20237200	-0.56760100	-0.00342800
H	1.65396200	-1.57957200	-0.04055000
N	0.03817300	0.68930800	-0.08932300
H	-0.31799700	1.52247900	0.36414400

10

C	-0.37562400	0.53222300	-0.00006200
H	-0.46484400	1.61877400	0.00003100
P	1.13033200	-0.22214800	-0.00000500
H	1.92736700	0.96734300	0.00017300
C	-1.67825300	-0.21111700	0.00001400
H	-2.27845000	0.05786800	0.88052900
H	-2.27883900	0.05835100	-0.88007800
H	-1.53695000	-1.29675100	-0.00029300

11-ts

C	-1.15696600	0.68131100	0.41378800
H	-1.47928400	0.85420600	1.43933700
P	-1.01998700	-0.91568800	-0.23390300
H	-1.45381700	-1.63645200	0.92478600
C	1.39813500	-0.96204400	0.08134000
H	1.52502600	-1.59936900	-0.78760900
H	1.32605700	-1.49201500	1.02669500
C	1.94766400	0.32979800	0.06042300
H	2.30131200	0.76197400	0.99560900
H	2.48855700	0.65336100	-0.82732800
H	0.79694400	1.26792800	-0.04345500
C	-0.41346200	1.70365600	-0.23312700
H	-0.46333900	2.71586900	0.17228100
H	-0.39388100	1.69349300	-1.32631300

12

C	-1.56391100	0.33971100	0.37563700
H	-1.49964400	1.09604800	1.16056700
C	1.23285500	0.65772500	-0.11494800
H	1.10354200	1.39480900	0.68719600
H	1.06210800	1.18380000	-1.06220500
C	2.65155700	0.07579300	-0.08487900
H	2.80330400	-0.65111400	-0.89093000
H	3.40072100	0.86749900	-0.20259700
H	2.85407300	-0.43341300	0.86476600
C	-2.70721600	0.19531300	-0.30027300
H	-3.58254900	0.80658000	-0.08773900
H	-2.81293500	-0.54400100	-1.09164400
P	-0.08175100	-0.68455300	0.00151100
H	0.21792700	-1.06316000	1.34670200

13

C	0.23411600	0.39956400	0.00001300
H	0.30185200	1.51172900	-0.00003300
O	1.23790400	-0.27701000	-0.00000500
C	-1.17107800	-0.14849900	-0.00001700
H	-1.71397300	0.21984300	-0.88050100
H	-1.15583600	-1.24071900	-0.00059000
H	-1.71350500	0.21883400	0.88118900

14-ts

C	-1.24953200	-0.35427100	0.29306700
H	-1.69442100	-0.56710500	1.28364500
C	-1.33871000	0.95364500	-0.20123400
H	-1.16442500	1.11958500	-1.26256400
H	0.11560500	1.13933900	0.10914400
O	-0.46721100	-1.20924800	-0.22036000
C	1.46725800	-0.52269700	-0.03576700
H	1.60874700	-1.18067500	0.81301700
H	1.67849900	-0.95963200	-1.00353400
C	1.41203200	0.87221600	0.13002300
H	1.75976200	1.48656800	-0.70120300
H	1.67321200	1.26925000	1.11199500
H	-1.98557400	1.67329200	0.29584800

15

C	1.35630400	-0.55665600	0.00004800
H	1.83872100	-1.53081400	0.00013900
C	-0.78915300	0.46704000	-0.00004600
H	-0.54812500	1.06931200	-0.88777900
H	-0.54809800	1.06944300	0.88759000
C	-2.24801000	0.04562700	0.00000000
H	-2.47726100	-0.55262600	0.88754300
H	-2.89592700	0.92890100	-0.00019200
H	-2.47719200	-0.55296300	-0.88733400
C	2.06108100	0.57959300	-0.00002000
H	3.14360000	0.52521700	0.00002100
H	1.61308400	1.56628100	-0.00011000
O	0.00873400	-0.71704800	0.00002900

16

S	-1.14739500	-0.12583500	0.00000500
C	0.34891300	0.51399700	-0.00002700
H	0.46153400	1.60396300	0.00007800
C	1.64089500	-0.24002900	-0.00000700
H	2.23859100	0.04304400	-0.87865300
H	2.23831600	0.04266300	0.87895100
H	1.48103100	-1.32011100	-0.00024800

17-ts

C	-1.19590700	0.58018000	0.40015100
H	-1.57770400	0.74741000	1.40969500
C	-0.55269200	1.64694700	-0.25519700
H	0.71761000	1.23180300	-0.02965400
H	-0.48139100	1.60245000	-1.34207700
S	-0.96880400	-0.99312100	-0.13497700
C	1.48415200	-0.87865800	0.07467700
H	1.57512500	-1.49051800	-0.81530600
H	1.43485000	-1.41895500	1.01326000
C	1.90281000	0.45793100	0.05271000
H	2.26068100	0.89863000	0.98315100
H	2.39556200	0.82699900	-0.84619900
H	-0.65405400	2.65372700	0.15271800

18

C	1.68478900	-0.31195700	-0.00005200
H	2.38773500	-1.14301000	-0.00009500
C	-0.95862600	0.64294600	0.00025700
H	-0.68819000	1.22589900	-0.88659100
H	-0.68861300	1.22538700	0.88756900
C	-2.45053500	0.31096300	-0.00018700
H	-2.73073600	-0.26727300	0.88640000
H	-3.03699900	1.23639200	-0.00008000
H	-2.73031700	-0.26679600	-0.88721900
C	2.13130300	0.94853000	-0.00008200
H	3.19951100	1.14420400	-0.00014200
H	1.47752100	1.81433600	-0.00005900
S	0.02303100	-0.90700200	0.00003800

6.4 CBS-QB3 geometries for all the optimized compounds and transition states.

1

C	-1.23346700	0.16234400	0.00000300
H	-1.80749700	-0.15332100	-0.87832500
H	-1.80720900	-0.15298000	0.87861900
H	-1.18188100	1.25364200	-0.00020300
C	0.13462700	-0.45370200	-0.00003500
H	0.16672100	-1.54206300	0.00010100
C	1.28040800	0.22044700	-0.00003000
H	2.23888300	-0.28624400	0.00008200
H	1.30157300	1.30642800	0.00009300

2-ts

C	0.55455100	1.25717900	-0.26553900
H	0.42198000	1.22484600	-1.34208200
C	1.30577300	0.26681600	0.34283200
H	1.59920800	0.40906500	1.38096300
C	1.25510900	-1.05138100	-0.15970500
H	-0.06546300	-1.22923300	-0.02075800
H	1.77793800	-1.83630100	0.38150600
H	1.28863300	-1.18200800	-1.24101400
C	-1.43259700	0.54428500	0.10737200
H	-1.54298200	1.01616900	1.07611100
H	-1.81282900	1.13221700	-0.71893700
C	-1.46269600	-0.85761800	0.02335700
H	-1.67717800	-1.42696500	0.92404800
H	-1.82432000	-1.31629300	-0.89276400
H	0.51416900	2.25281500	0.16301500

3

C	1.52385800	0.52222200	-0.00001900
H	2.13626800	1.42288800	-0.00013400
C	-0.86077500	-0.46678600	-0.00023500
H	-0.63091800	-1.08248400	0.87631200
H	-0.63123500	-1.08195300	-0.87723600
C	-2.35099100	-0.11360100	0.00013000
H	-2.61961400	0.47499800	-0.88267700
H	-2.97256900	-1.01292500	0.00002000
H	-2.61928200	0.47455200	0.88333500
C	2.13798700	-0.65783500	0.00009300
H	3.22005300	-0.72583700	0.00004200
H	1.59520500	-1.59659600	0.00026600
C	0.03870900	0.77153800	0.00000500
H	-0.20531900	1.39691600	0.87065200
H	-0.20531600	1.39722100	-0.87042500

4

Si	-1.15074400	0.10220200	0.00003600
H	-1.42626500	1.55024000	-0.00037400
H	-2.33363500	-0.77382100	0.00014500
C	0.43880300	-0.53304600	-0.00009900
H	0.52841000	-1.61814100	-0.00017000
C	1.73851800	0.22534000	0.00003400
H	2.34416100	-0.02554800	0.87924900
H	2.34439000	-0.02540400	-0.87906900
H	1.58943700	1.30808000	0.00010100

5-ts

C	1.41202600	0.35179900	-0.40599200
H	1.76126700	0.38814100	-1.43560800
Si	0.63439900	-1.11607200	0.16397300
H	0.48683500	-1.30116700	1.62295700
C	-1.54904700	-0.56547600	-0.24650600
H	-1.84416200	-1.32582000	0.47502900
H	-1.61577400	-0.89010700	-1.28015400
C	-1.87710300	0.75293800	0.04855400
H	-2.15489000	1.04904500	1.05320100
H	-0.23078200	1.60274000	0.08961400
H	-2.08417400	1.46552900	-0.74017500
C	0.93641100	1.60138500	0.18243600
H	1.07511500	1.68578000	1.26451200
H	1.29512300	2.51185700	-0.30263100
H	0.89613100	-2.40486300	-0.51332300

6

C	-1.85808100	-0.31528600	-0.00003200
H	-2.59769100	-1.11679200	-0.00011900
C	1.10490100	0.67684400	-0.00017800
H	0.87633300	1.29529800	0.87556300
H	0.87653900	1.29487300	-0.87627300
C	2.59820100	0.30130000	0.00009500
H	2.86237000	-0.29010200	-0.88121500
H	3.23360100	1.19171500	-0.00005500
H	2.86215600	-0.28965800	0.88176600
C	-2.30980300	0.94114300	0.00001700
H	-3.37126300	1.17537200	-0.00002100
H	-1.64016300	1.79667700	0.00009800
Si	-0.05326300	-0.81176400	0.00003800
H	0.21626200	-1.65817800	1.19287900
H	0.21623500	-1.65852200	-1.19256500

7

C	-0.19102400	0.40709400	-0.00012200
H	-0.26589500	1.50495000	0.00030000
H	-2.06762100	0.19299900	0.00011700
C	1.20468900	-0.14092000	-0.00008800
H	1.75559000	0.21170600	-0.87863400
H	1.75428700	0.20918000	0.88067100
H	1.17737700	-1.23076400	-0.00128000
N	-1.20510400	-0.35501700	0.00001300

8-ts

C	1.29931100	0.29981200	0.27893100
H	1.78774400	0.49261000	1.24069600
C	1.26669000	-1.02013200	-0.20184000
H	1.12290200	-1.16299300	-1.26897100
H	1.88495500	-1.76885800	0.28264300
N	0.49933100	1.19245800	-0.27745800
H	0.49429900	2.05987700	0.25773700
C	-1.44071600	0.53696100	-0.05415500
H	-1.71881200	0.93487300	-1.01905200
H	-1.62107200	1.20081400	0.78238900
C	-1.43806000	-0.85235300	0.15412200
H	-1.65121700	-1.21930100	1.15534700
H	-1.81901100	-1.48419700	-0.64394800
H	-0.09844900	-1.18575700	0.09301900

9

C	1.41576100	0.54289000	-0.00042500
H	1.93513700	1.49703700	0.03188900
C	-0.83037200	-0.47501800	0.06989600

H	-0.64892700	-0.99600900	1.02385200
H	-0.58435300	-1.18739800	-0.72477000
C	-2.29610500	-0.06841200	-0.03913600
H	-2.49323400	0.41807000	-0.99760500
H	-2.94580800	-0.94248500	0.04405700
H	-2.57387800	0.62644800	0.76038500
C	2.12380400	-0.59542200	-0.01275900
H	3.20424200	-0.55400200	-0.01501400
H	1.66452700	-1.57494400	-0.04140100
N	0.04042900	0.68007000	-0.07487500
H	-0.31923500	1.52856300	0.33727900

10

C	-0.37148600	0.53044800	0.00005100
H	-0.44973800	1.61491500	-0.00016300
P	1.12571600	-0.22195400	-0.00000900
H	1.92244800	0.95919200	0.00000000
C	-1.67484100	-0.20937600	-0.00001200
H	-2.27207200	0.06001400	0.87886800
H	-2.27319500	0.06160200	-0.87774200
H	-1.53523000	-1.29285400	-0.00107100

11-ts

C	-1.14589400	0.68106100	0.41604300
H	-1.46051300	0.84328000	1.44282500
P	-1.02259100	-0.90780300	-0.23610300
H	-1.44840600	-1.62733700	0.91737100
C	1.38860400	-0.96540800	0.08777900
H	1.50848100	-1.60918800	-0.77410300
H	1.31047700	-1.48280800	1.03634400
C	1.94421200	0.32075200	0.05326200
H	2.30088100	0.76021300	0.98078300
H	2.47973100	0.63432700	-0.83798900
H	0.80465100	1.25665000	-0.04909600
C	-0.40734500	1.70287100	-0.22994200
H	-0.44593600	2.70937100	0.18284500
H	-0.38795500	1.69687900	-1.32028600

12

C	-1.72799900	-0.29680300	0.14227100
H	-2.42108700	-1.09432000	0.40624200
C	1.00045900	0.65149800	-0.00647200
H	0.67096600	1.21997000	0.86720900
H	0.81012100	1.27076600	-0.88847500
C	2.49695300	0.32725500	0.08315600
H	2.83868900	-0.23383000	-0.79072200
H	3.08903500	1.24454100	0.14307000
H	2.72323100	-0.27015900	0.97071400
C	-2.20196300	0.93944200	-0.01452700
H	-3.25465500	1.16063400	0.12928900
H	-1.57096600	1.77688300	-0.29187400
P	-0.03295000	-0.89115300	-0.19141400
H	0.20421700	-1.43554100	1.09918600

13

C	0.23550400	0.39707200	-0.00011700
H	0.30483500	1.50860300	0.00008700
O	1.23324800	-0.27647400	0.00002700
C	-1.16883600	-0.14788800	-0.00002300
H	-1.70812000	0.22358900	-0.87820800
H	-1.15591800	-1.23755500	-0.00097400
H	-1.70679700	0.22204800	0.87971900

14-ts

C	-1.24818200	-0.34964300	0.29487300
H	-1.69372300	-0.55513400	1.28469900
C	-1.34581800	0.95035700	-0.20643600
H	-1.15095000	1.11926800	-1.26066300
H	0.13057000	1.12509800	0.11144300
O	-0.47624700	-1.20936400	-0.21519800
C	1.47898500	-0.52052400	-0.04228900
H	1.61545400	-1.18585100	0.79810800
H	1.67764400	-0.94816400	-1.01385300
C	1.41405200	0.86934900	0.13450600
H	1.75614700	1.49126300	-0.68997800
H	1.66789600	1.25980800	1.11818000
H	-1.98728400	1.67138700	0.28972000

15

C	1.35609200	-0.55540100	0.00012600
H	1.83691200	-1.52787500	-0.00017000
C	-0.79267800	0.47050900	0.00011200
H	-0.55490500	1.07114000	-0.88667400
H	-0.55512700	1.07074800	0.88721900
C	-2.24721000	0.04162000	-0.00005800
H	-2.47146500	-0.55637400	0.88578900
H	-2.89974700	0.91850900	-0.00094700
H	-2.47085400	-0.55750700	-0.88532500
C	2.06222400	0.57654000	-0.00000500
H	3.14198900	0.51696900	-0.00036200
H	1.61761200	1.56200800	-0.00020200
O	0.01062800	-0.71215300	-0.00004700

16

S	-1.14215700	-0.12612900	0.00000000
C	0.34614800	0.51343700	0.00000300
H	0.45054300	1.60159300	-0.00000900
C	1.63517000	-0.23936500	-0.00000400
H	2.23052300	0.04466000	-0.87667000
H	2.23028200	0.04421100	0.87697400
H	1.47525900	-1.31684200	-0.00029000

17-ts

C	-1.18575700	0.57920100	0.40315700
H	-1.56129900	0.73895600	1.41347500
C	-0.55114300	1.64492800	-0.25327300
H	0.72189200	1.22102800	-0.03345200
H	-0.47736900	1.59999200	-1.33701500
S	-0.97044700	-0.98715400	-0.13725000
C	1.47927400	-0.87998300	0.08008900
H	1.56370400	-1.49586400	-0.80446800
H	1.42432700	-1.41000200	1.02108200
C	1.90039100	0.45202000	0.04698400
H	2.25797700	0.90042900	0.97075100
H	2.38540900	0.81519700	-0.85521300
H	-0.64407300	2.64774200	0.15910600

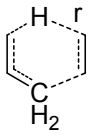
18

C	1.68030400	-0.31155100	0.00068100
H	2.37568700	-1.14610600	0.00240200
C	-0.95828500	0.64111400	-0.00021200
H	-0.68850500	1.21958400	-0.88685900
H	-0.68751300	1.21961600	0.88611600
C	-2.44902700	0.30835900	0.00053600

H	-2.72852200	-0.26812800	0.88548700	H	3.19914100	1.13212700	0.00092000
H	-3.03538300	1.23092400	0.00064300	H	1.48287700	1.80910600	-0.00180200
H	-2.72936400	-0.26841100	-0.88396900	S	0.02375400	-0.90103700	-0.00050100
C	2.13226100	0.94339200	-0.00016000				

7. The date of distortion, interaction, and total energies along the reaction pathways of the Ene-reaction between the C-H bond in hetero enes and ethylene.

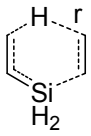
7.1 The data of distortion, interaction and total energies along the reaction pathways of the Ene-reaction between propylene and ethylene.



Step	r	$\Delta E^{\neq}$	$\Delta E^{\neq}_{dist}$	$\Delta E^{\neq}_{int}$
1	2.98	0.4	0.0	0.4
2	2.91	1.2	0.1	1.1
3	2.76	1.8	0.1	1.7
4	2.72	2.1	0.2	1.9
5	2.67	2.4	0.2	2.1
6	2.62	2.7	0.3	2.4
7	2.58	3.1	0.4	2.7
8	2.53	3.5	0.5	3.0
9	2.48	4.1	0.6	3.4
10	2.44	4.7	0.7	3.9
11	2.39	5.3	0.9	4.5
12	2.34	6.1	1.0	5.1
13	2.30	7.0	1.2	5.8
14	2.25	8.0	1.3	6.6
15	2.21	8.5	1.6	7.0
16	2.16	9.8	1.8	8.0
17	2.11	11.2	2.2	9.1

18	2.01	14.7	2.7	12.0
19	1.96	16.8	3.6	13.2
20	1.91	19.6	5.5	14.2
21	1.86	22.1	7.3	14.8
22	1.80	24.7	9.9	14.8
23	1.73	27.0	13.9	13.1
24	1.66	29.8	20.1	9.6
25	1.55	32.0	30.4	1.6
26	1.45	32.9	42.0	-9.1
27	1.37	32.4	51.9	-19.5
28	1.24	29.3	69.0	-39.7
29	1.16	25.4	85.7	-60.3

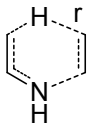
7.2 The data of distortion, interaction and total energies along the reaction pathways of the Ene-reaction between ethylidenesilane and ethylene.



Step	r	$\Delta E^{\neq}$	$\Delta E^{\neq}_{dist}$	$\Delta E^{\neq}_{int}$
1	3.17	1.8	0.3	1.5
2	2.84	2.7	1.1	1.5
3	2.62	4.3	2.2	2.1
4	2.54	5.0	2.6	2.4
5	2.41	6.6	3.2	3.5
6	2.35	7.6	4.1	3.5
7	2.29	8.6	5.1	3.5
8	2.22	9.1	6.3	2.8
9	2.15	10.2	8.6	1.6
10	2.08	11.1	10.8	0.2

11	2.00	11.7	14.0	-2.3
12	1.92	11.8	18.5	-6.7
13	1.85	11.5	22.4	-10.9
14	1.78	10.8	27.5	-16.7
15	1.62	8.4	42.6	-34.1
16	1.40	1.4	66.6	-65.2
17	1.19	-12.4	92.4	-104.8

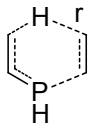
7.3 The data of distortion, interaction and total energies along the reaction pathways of the Ene-reaction between ethanimine and ethylene.



Step	r	$\Delta E^{\neq}$	$\Delta E^{\neq}_{dist}$	$\Delta E^{\neq}_{int}$
1	3.05	0.0	0.0	0.0
2	2.97	0.3	0.0	0.3
3	2.89	0.6	0.0	0.6
4	2.80	1.6	0.1	1.6
5	2.70	1.6	0.2	1.5
6	2.50	3.5	0.5	3.0
7	2.40	4.8	0.7	4.2
8	2.16	10.3	0.7	9.5
9	2.11	11.8	1.0	10.8
10	2.06	13.5	1.3	12.2
11	2.01	15.4	2.0	13.4
12	1.96	17.5	2.7	14.8
13	1.90	20.0	3.8	16.2
14	1.84	23.3	5.3	17.9
15	1.78	26.3	8.3	17.9

16	1.71	29.0	12.2	16.8
17	1.61	32.5	19.2	13.3
18	1.38	37.1	43.4	-6.3
19	1.28	36.2	55.9	-19.7
20	1.18	33.8	72.1	-38.2

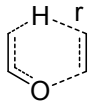
7.4 The data of distortion, interaction and total energies along the reaction pathways of the Ene-reaction between ethylidenephosphine and ethylene.



Step	r	$\Delta E^{\neq}$	$\Delta E^{\neq}_{dist}$	$\Delta E^{\neq}_{int}$
1	3.09	-0.1	0.0	-0.1
2	2.96	0.3	0.1	0.2
3	2.88	0.5	0.1	0.4
4	2.80	0.9	0.2	0.6
5	2.71	1.4	0.4	1.0
6	2.61	2.1	0.6	1.5
7	2.52	3.0	0.9	2.1
8	2.42	4.0	1.2	2.9
9	2.38	4.7	1.3	3.4
10	2.19	8.0	2.2	5.7
11	2.14	9.0	2.6	6.4
12	2.09	10.8	3.0	7.8
13	1.99	13.4	4.4	9.1
14	1.93	14.9	5.3	9.6
15	1.88	16.5	6.6	9.9
16	1.82	18.2	8.4	9.7
17	1.75	19.3	11.1	8.2

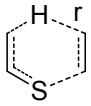
18	1.67	21.0	15.5	5.6
19	1.58	22.4	23.2	-0.8
20	1.45	22.9	35.9	-13.0
21	1.15	15.1	76.8	-61.7

7.5 The data of distortion, interaction and total energies along the reaction pathways of the Ene-reaction between acetaldehyde and ethylene.



Step	r	$\Delta E^{\neq}$	$\Delta E^{\neq}_{dist}$	$\Delta E^{\neq}_{int}$
1	2.99	-0.1	0.0	-0.2
2	2.89	0.2	0.1	0.1
3	2.79	0.6	0.1	0.5
4	2.68	1.2	0.2	1.0
5	2.57	2.0	0.3	1.7
6	2.46	3.2	0.5	2.7
7	2.09	11.0	0.7	10.4
8	1.97	15.2	2.4	12.9
9	1.90	17.9	3.6	14.3
10	1.76	25.4	9.7	15.7
11	1.66	29.2	16.3	12.9
12	1.53	34.7	28.1	6.7
13	1.39	39.1	43.4	-4.3
14	1.31	40.0	52.7	-12.8
15	1.22	39.8	65.7	-25.9
16	1.17	38.5	78.6	-40.1

7.6 The data of distortion, interaction and total energies along the reaction pathways of the Ene-reaction between ethanethial and ethylene.



Step	r	$\Delta E^{\neq}$	$\Delta E^{\neq}_{dist}$	$\Delta E^{\neq}_{int}$
1	3.01	-0.2	0.0	-0.3
2	2.93	-0.1	0.2	-0.2
3	2.84	0.1	0.2	-0.1
4	2.75	0.4	0.3	0.1
5	2.66	0.9	0.5	0.4
6	2.57	1.4	0.7	0.8
7	2.47	2.1	0.8	1.3
8	2.38	3.1	1.0	2.0
9	2.33	3.6	1.1	2.5
10	2.29	4.2	1.3	2.9
11	2.24	4.9	1.4	3.5
12	2.19	5.7	1.5	4.2
13	2.15	6.6	1.7	4.9
14	2.10	7.5	1.9	5.6
15	2.00	9.9	2.5	7.3
16	1.95	11.2	3.0	8.2
17	1.77	16.8	6.4	10.4
18	1.70	18.2	9.2	8.9
19	1.63	20.3	14.3	6.0
20	1.51	22.3	23.7	-1.4
21	1.41	23.4	34.5	-11.1
22	1.38	23.4	37.5	-14.0
23	1.19	20.6	61.9	-41.3