Supporting Information

A Theoretical Study of the Reactivity of Ethene and Benzophenone with a Hyper-Coordinated Alkene Containing a So-Called E=E (E = C, Si, Ge, Sn, and Pb) Unit

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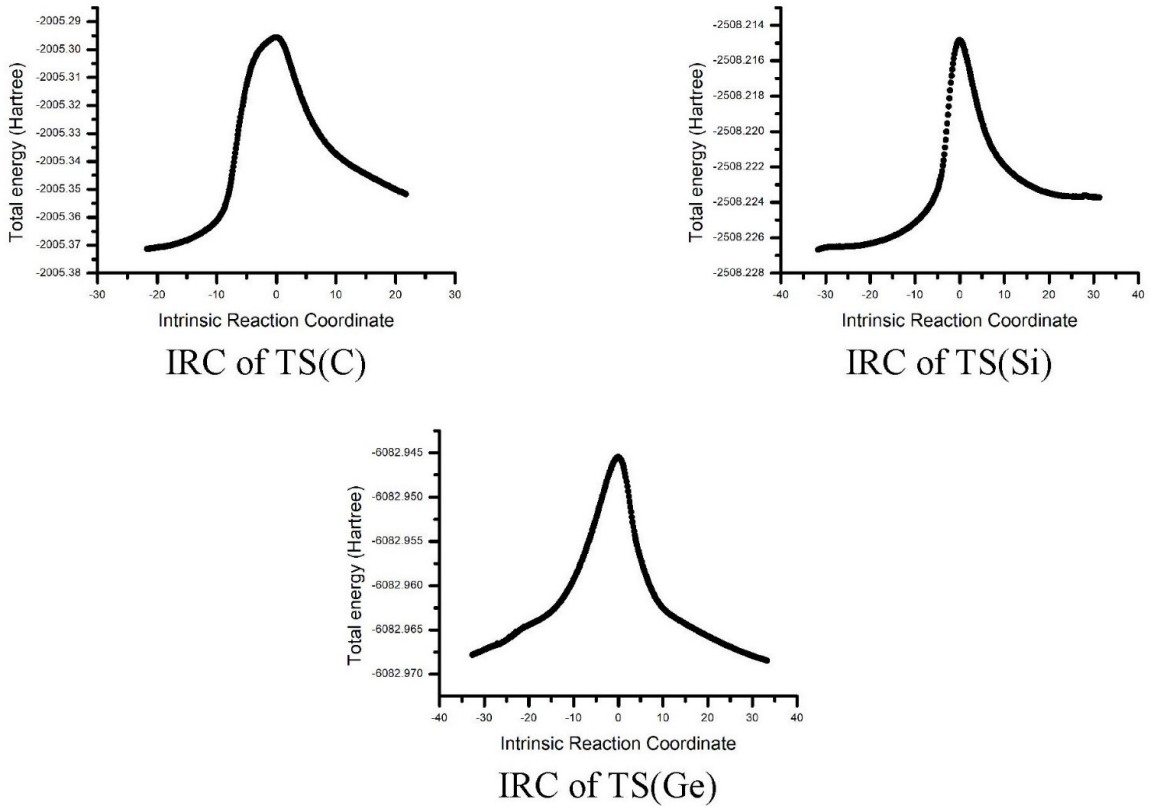
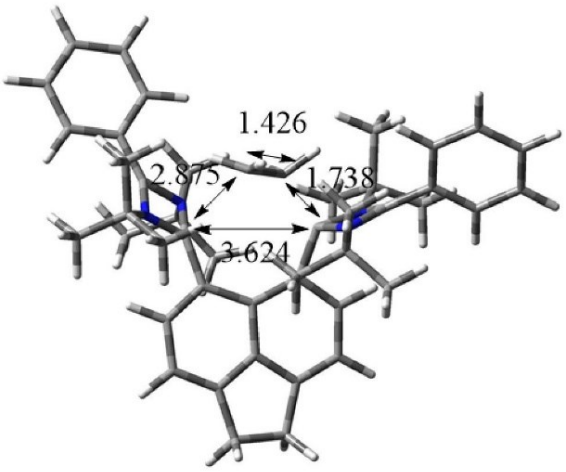
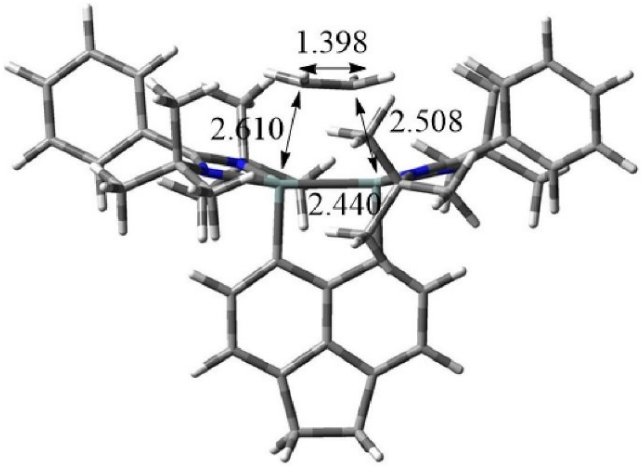


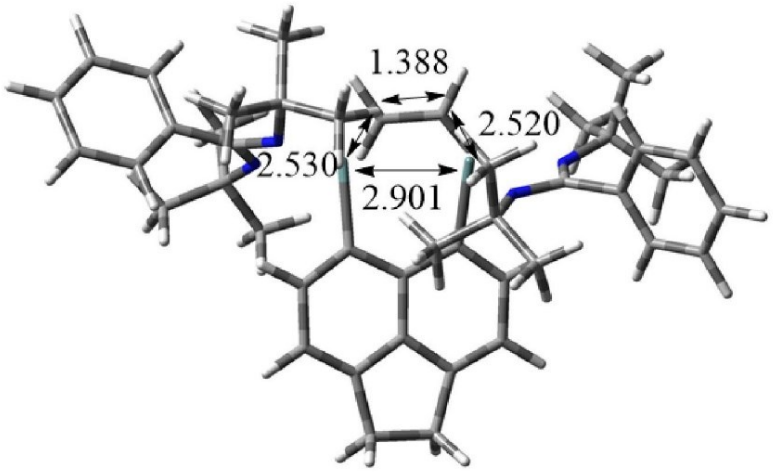
Figure S1. The curve of intrinsic reaction coordinate (IRC) of transition state for C_2H_2 + **Rea-E** (E = C, Si, and Ge) at B3PW91/def2-SVP level of theory.



TS-C_2H_4-C



TS-C_2H_4-Si



TS-C_2H_4-Ge

Figure S2. The optimized **TS-C_2H_2-E** (E = C, Si, and Ge) structures at the B3PW91/def2-SVP level of theory. The hydrogen is omitted for clarity.

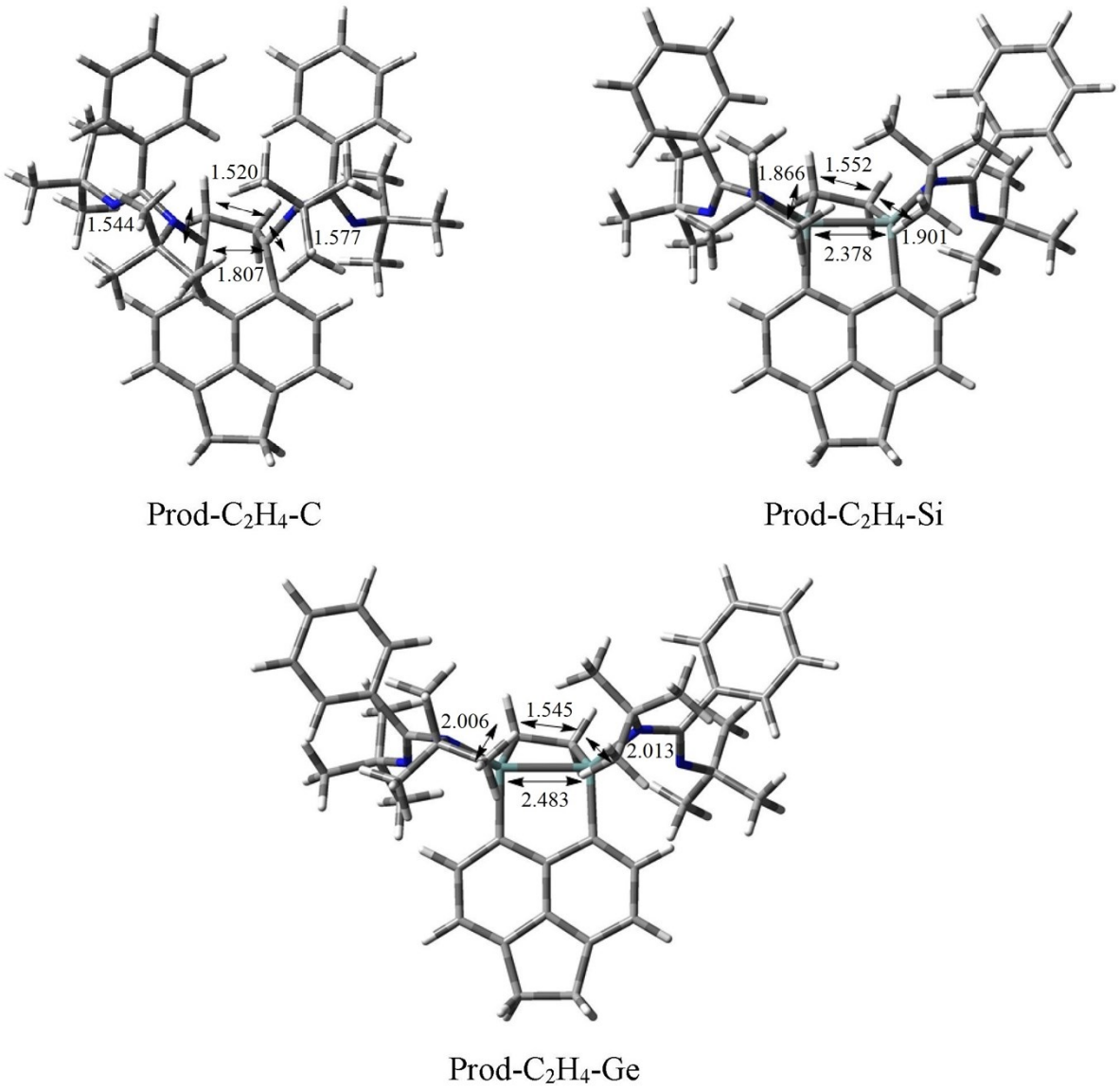


Figure S3. The optimized **Prod-C_2H_2-E** (E = C, Si, and Ge) structures at the B3PW91/def2-SVP level of theory. The hydrogen is omitted for clarity.

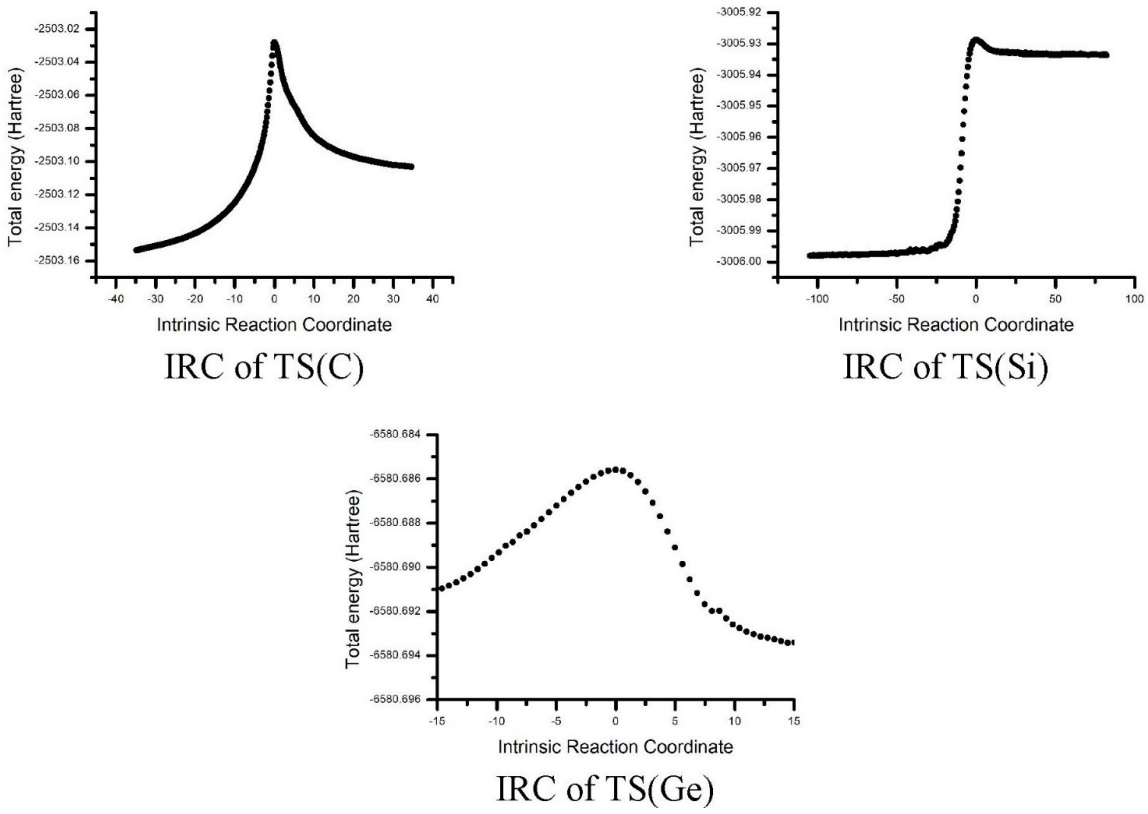


Figure S4. The curve of intrinsic reaction coordinate (IRC) of transition state for Ph_2CO + **Rea-E** (E = C, Si, Ge) at B3PW91/def2-SVP level of theory.

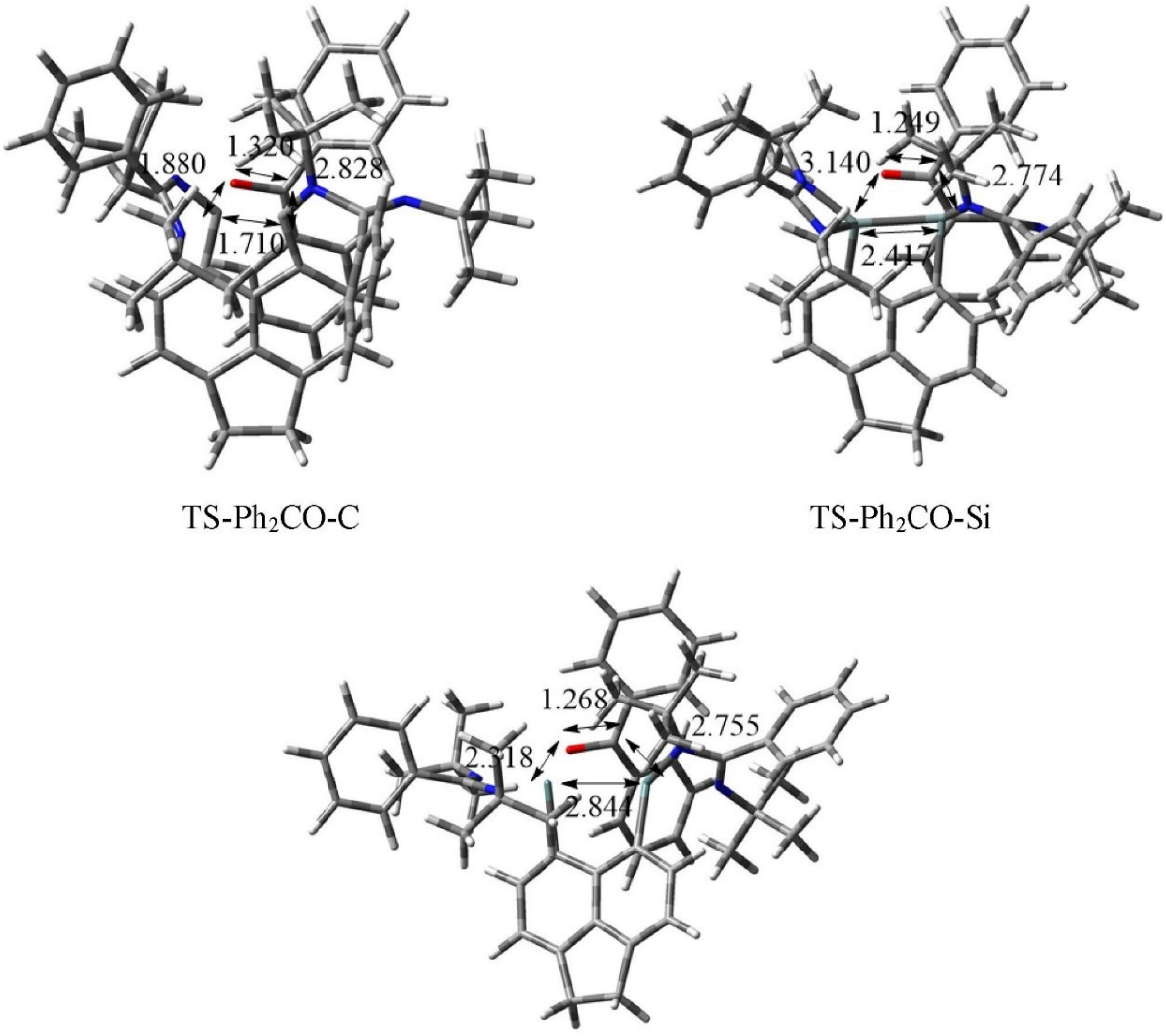
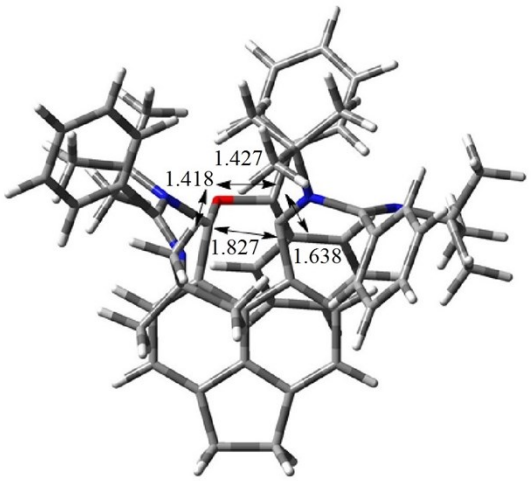
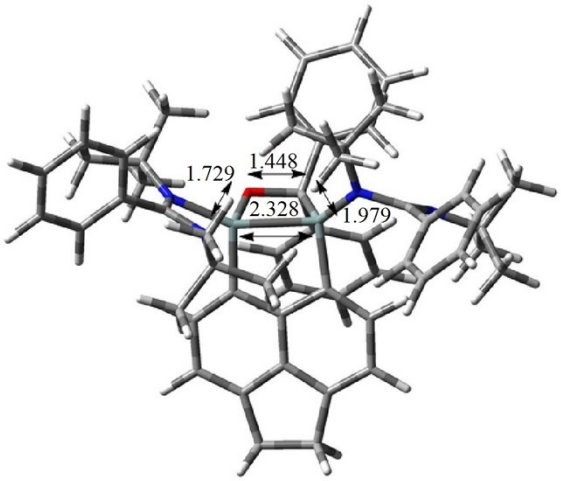


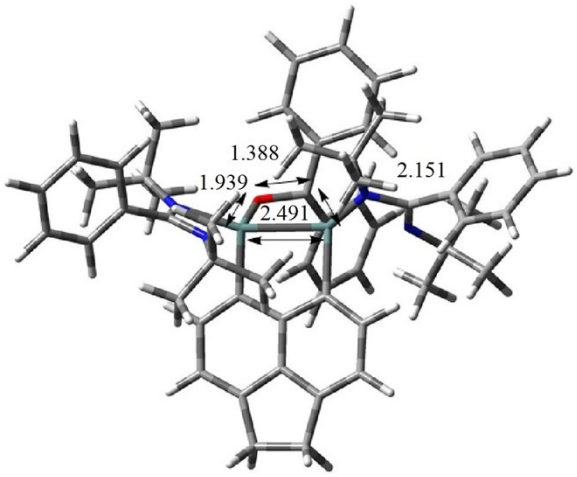
Figure S5. The optimized **TS-Ph_2CO-E** (E = C, Si, and Ge) structures at the B3PW91/def2-SVP level of theory. The hydrogen is omitted for clarity.



Prod-Ph_2CO-C



Prod-Ph_2CO-Si



Prod-Ph_2CO-Ge

Figure S6. The optimized **Prod-Ph_2CO-E** (E = C, Si, and Ge) structures at the B3PW91/def2-SVP level of theory. The hydrogen is omitted for clarity.

Table S1. Relative energies for the reaction of **Rea-E** + C_2H_4 and Ph_2CO

Table. Relative Energies (in kcal/mol) for Singlet and Triplet Group 14 Analogues (E = C, Si, Ge) for the Addition Reactions with C_2H_4: Reactant (Rea-E) → Transition State → Prod-E [a, b]

system	ΔE_{st} [c]	ΔG_{TS} [d]	ΔG_{Prod} [e]
E = C	29.7 [33.8]	54.8 [55.3]	-29.9 [-38.5]
E = Si	19.5 [30.7]	15.5 [16.6]	-13.3 [-16.3]
E = Ge	46.9 [42.6]	29.6 [30.0]	15.5 [3.8]

[a] All at the B3LYP-D3/def2-SVp level of theory. The values in bracket are obtained at M06-2X/def2-SVP level of theory.

[b] Energy differences have used the Gibbs free energy (ΔG).

[c] Energy relative to the corresponding singlet state. A positive value means the singlet is the ground state.

[d] The energy of the transition state is relative to the corresponding reactant.

[e] The energy of product is relative to the corresponding reactant.

Table. Relative Energies (in kcal/mol) for Singlet and Triplet Group 14 Analogues (E = C, Si, Ge) for the Addition Reactions with Ph_2CO: Reactant (Rea-E) → Transition State → Prod-E [a, b]

system	ΔE_{st} [c]	ΔG_{TS} [d]	ΔG_{Prod} [e]
E = C	29.7 [33.8]	44.2 [52.2]	0.1 [-6.0]
E = Si	19.5 [30.7]	13.2 [21.6]	-27.2 [-28.8]
E = Ge	46.9 [42.6]	10.7 [15.9]	7.7 [2.2]

[a] All at the B3LYP-D3/def2-SVp level of theory. The values in bracket are obtained at M06-2X/def2-SVP level of theory.

[b] Energy differences have used the Gibbs free energy (ΔG).

[c] Energy relative to the corresponding singlet state. A positive value means the singlet is the ground state.

[d] The energy of the transition state is relative to the corresponding reactant.

[e] The energy of product is relative to the corresponding reactant.

Table S2. EDA energy decomposition results describing the transition state between C_2H_4 and **Rea-Si**.

Table. BP86 ETS[(a)] energy decomposition results (in kcal mol^{-1}) describing the bond between C_2H_4 and Rea-Si for Rea. → Transition State → Prod. Singlet and triplet spin states were considered in ETS-NOCV analysis.

ETS results	Rea	TS	Prod	$\Delta E^{\#}$[ΔE(TS)-ΔE(Rea)]	ΔE_{rxn}[ΔE(Prod)-ΔE(Rea)]
Fragments in the singlet spin state					
ΔE_{total}[(b)]	0.0	15.0	-34.0	15.0	-34.0
ΔE_{orb}	0.0	-101.2	-474.0	-101.2	-474.0
ΔE_{Pauli}	0.0	232.5	606.2	232.5	606.2
ΔE_{elstat}	0.0	-114.8	-261.8	-114.8	-261.8
ΔE_{disper}	0.0	-17.9	-12.9	-17.9	-12.9
ΔE_{dist}	0.0	16.4	108.5	16.4	108.5
Fragments in the triplet spin state					
ΔE_{total}[(c)]	0.0	15.0	-34.0	15.0	-34.0
ΔE_{orb}	-77.9	-152.7	-294.0	-74.8	-216.1
ΔE_{Pauli}	0.0	88.0	387.7	88.0	387.7
ΔE_{elstat}	0.0	-59.6	-257.8	-59.6	-257.8
ΔE_{disper}	0.0	-16.5	-12.9	-16.5	-12.9
ΔE_{dist}	77.9	155.8	143.0	77.9	65.1

[(a)] $\Delta E_{total} = \Delta E_{orb} + \Delta E_{Pauli} + \Delta E_{elstat} + \Delta E_{disper} + \Delta E_{dist}$

[(b)] Fragments in singlet state were considered in ETS analysis.

[(c)] Fragments in triplet state were considered in ETS analysis. Distortion energy, ΔE_{dist}, calculated with respect to the singlet ground state of C_2H_4 and Rea-Si.

- It wad said that the smallest ΔE_{orb} value indicates which fragments are the best choice for describing the bonding situation, because the least alteration of the electronic charge distribution is required to yield the electronic structure of the molecule. See reference (76).
- Accordingly, a singlet reference state is more appropriate for a description of the TS and the triplet reference state can be a description of the product.

Table S3. EDA energy decomposition results describing the transition state between Ph_2CO and **Rea-Si**.

Table. BP86-D3 ETS[(a)] energy decomposition results (in kcal mol^{-1}) describing the bond between Ph_2CO and Rea-Si for Rea → Transition State → Prod. Singlet and triplet spin states were considered in ETS-NOCV analysis.

ETS results	Rea	TS	Prod	$\Delta E^{\#}$[ΔE(TS)-ΔE(Rea)]	ΔE_{rxn}[ΔE(Prod)-ΔE(Rea)]
Fragments in the singlet spin state					
ΔE_{total}[(b)]	0.0	14.8	-26.8	14.8	-26.8
ΔE_{orb}	0.0	-41.5	-406.4	-41.5	-406.4
ΔE_{Pauli}	0.0	123.4	614.4	123.4	614.4
ΔE_{elstat}	0.0	-55.7	-294.3	-55.7	-294.3
ΔE_{disper}	0.0	-30.0	-32.9	-30.0	-32.9
ΔE_{dist}	0.0	18.6	92.4	18.6	92.4
Fragments in the triplet spin state					
ΔE_{total}[(c)]	0.0	14.8	-26.8	14.8	-26.8
ΔE_{orb}	-75.0	-133.9	-429.5	-58.9	-354.5
ΔE_{Pauli}	0.0	70.1	600.4	70.1	600.4
ΔE_{elstat}	0.0	-45.7	-292.9	-45.7	-292.9
ΔE_{disper}	0.0	-30.0	-32.9	-30.0	-32.9
ΔE_{dist}	75.0	154.3	128.1	79.3	53.1

[(a)] $\Delta E_{total} = \Delta E_{orb} + \Delta E_{Pauli} + \Delta E_{elstat} + \Delta E_{disper} + \Delta E_{dist}$

[(b)] Fragments in singlet state were considered in ETS analysis.

[(c)] Fragments in triplet state were considered in ETS analysis. Distortion energy, ΔE_{dist}, calculated with respect to the singlet ground state of Ph_2CO and Rea-Si.

- It wad said that the smallest ΔE_{orb} value indicates which fragments are the best choice for describing the bonding situation, because the least alteration of the electronic charge distribution is required to yield the electronic structure of the molecule. See reference (76).
- Accordingly, a singlet reference state is more appropriate for a description of the TS and the singlet reference state can be a description of the product.

Table S4
B3LYP-D3/def2-SVP
C_2H_4
G = -78.503293 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	-0.666610	-0.000000
1	-0.931140	-1.242636	-0.000000
1	0.931140	-1.242636	-0.000000
6	0.000000	0.666610	-0.000000
1	0.931140	1.242636	-0.000000
1	-0.931140	1.242636	-0.000000

Table S5
B3LYP-D3/def2-SVP
Ph_2CO
G = -576.083392 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.000009	2.311371	0.000027
6	-0.000029	1.091668	0.000028
6	1.303084	0.341876	0.024646
6	1.450816	-0.916462	0.633242
1	0.588044	-1.406450	1.088286
6	-1.303139	0.341955	-0.024595
6	-1.450762	-0.916443	-0.633216
1	-0.587905	-1.406287	-1.088271
6	2.704757	-1.531448	0.687139
1	2.812073	-2.504146	1.173763
6	-3.818825	-0.902164	-0.124002
1	-4.797219	-1.388461	-0.158956
6	-3.681853	0.355520	0.476861
1	-4.553326	0.852189	0.910931
6	-2.704625	-1.531436	-0.687174
1	-2.811940	-2.504163	-1.173742
6	-2.435456	0.978662	0.513771
1	-2.312176	1.969500	0.955640
6	3.818854	-0.902114	0.123985
1	4.797301	-1.388305	0.158914
6	3.681768	0.355621	-0.476888
1	4.553210	0.852266	-0.911050
6	2.435392	0.978669	-0.513803
1	2.311979	1.969473	-0.955700

Table S6
B3LYP-D3/def2-SVP
Rea-C (Singlet)
E = -1926.83192151 Hartree
G = -1926.026270 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.631559	0.562513	0.197757
7	-1.672509	-0.557950	1.060600
7	-2.952723	0.238524	-0.214644
6	-3.580629	-0.563091	-2.472343
1	-2.533433	-0.664077	-2.785640
1	-4.189071	-0.337829	-3.362524
1	-3.913737	-1.527127	-2.062981
6	0.000059	2.581941	-0.000029
6	-5.200126	0.759427	-1.057433
1	-5.659603	-0.182064	-0.732690
1	-5.763486	1.123020	-1.930940
1	-5.298913	1.497290	-0.246712
6	-3.197352	1.878067	-2.042226
1	-3.366189	2.734290	-1.376893
1	-3.727844	2.064251	-2.988457
1	-2.122917	1.825073	-2.258014
6	0.163798	-1.970571	1.895959
1	-0.277312	-2.888847	1.483876
1	0.753627	-2.250845	2.782234
1	0.836413	-1.535270	1.148146
6	-1.052110	4.815172	0.503500
6	-0.284630	0.288144	2.901423
1	0.416186	0.749358	2.195368
1	0.272464	-0.000952	3.805802
1	-1.043500	1.033999	3.177599
6	-1.230002	1.967349	0.450385
6	-1.907859	-1.581644	3.279987
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1	-1.360938	-1.849817	4.197234
1	-2.373513	-2.494270	2.883970
6	-2.877515	-3.363344	0.274411
1	-1.802660	-3.295499	0.109209
6	0.000084	4.008372	-0.000015
6	-2.946818	-0.880766	0.613686
6	-3.610185	-2.178799	0.514240
6	-3.720397	0.566577	-1.434146
6	-0.929049	-0.955114	2.274145
6	-2.233328	2.790403	0.977513
1	-3.142933	2.299362	1.332622
6	-4.899478	-4.699712	0.371819
1	-5.397048	-5.671039	0.315769
6	-2.167681	4.202389	1.027534
1	-2.997467	4.775967	1.449769
6	-3.512418	-4.604527	0.214167
1	-2.920186	-5.503873	0.024009
6	-0.690696	6.279103	0.362302
1	-0.629378	6.762636	1.352036
1	-1.457114	6.832941	-0.204603
6	-5.005325	-2.298173	0.695813

1	-5.584374	-1.406950	0.942533
6	-5.641415	-3.537082	0.610233
1	-6.723548	-3.598911	0.753913
6	1.631648	0.562486	-0.197821
7	1.672405	-0.558098	-1.060479
7	2.952793	0.238438	0.214544
6	3.580803	-0.563198	2.472220
1	2.533600	-0.664274	2.785471
1	4.189190	-0.337884	3.362424
1	3.914008	-1.527207	2.062878
6	5.200206	0.759407	1.057266
1	5.659674	-0.182038	0.732380
1	5.763612	1.122906	1.930783
1	5.298932	1.497370	0.246628
6	3.197435	1.877944	2.042179
1	3.366242	2.734198	1.376882
1	3.727940	2.064106	2.988407
1	2.123004	1.824907	2.257980
6	-0.164045	-1.970512	-1.895871
1	0.276912	-2.888741	-1.483518
1	-0.753744	-2.250912	-2.782190
1	-0.836759	-1.535001	-1.148267
6	1.052306	4.815152	-0.503508
6	0.284790	0.288067	-2.901501
1	-0.416088	0.749392	-2.195586
1	-0.272186	-0.001021	-3.805955
1	1.043785	1.033824	-3.177600
6	1.230107	1.967307	-0.450443
6	1.907770	-1.581986	-3.279767
1	2.707916	-0.873673	-3.540372
1	1.360870	-1.850249	-4.197000
1	2.373330	-2.494592	-2.883589
6	2.877293	-3.363551	-0.274566
1	1.802416	-3.295682	-0.109530
6	2.946743	-0.880957	-0.613650
6	3.610039	-2.179013	-0.514192
6	3.720503	0.566490	1.434037
6	0.928966	-0.955228	-2.274060
6	2.233455	2.790348	-0.977567
1	3.143038	2.299293	-1.332709
6	4.899227	-4.699983	-0.371748
1	5.396754	-5.671332	-0.315679
6	2.167855	4.202338	-1.027551
1	2.997660	4.775891	-1.449782
6	3.512146	-4.604760	-0.214309
1	2.919854	-5.504099	-0.024303
6	0.690934	6.279091	-0.362283
1	0.629628	6.762643	-1.352008
1	1.457367	6.832899	0.204632
6	5.005205	-2.298427	-0.695575
1	5.584322	-1.407211	-0.942161
6	5.641239	-3.537362	-0.609978
1	6.723392	-3.599217	-0.753502

Table S7
B3LYP-D3/def2-SVP
Rea-C (Triplet)
E = -1926.78459137 Hartree
G = -1925.983833 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.424669	-1.262277	0.350060
7	-0.096975	-1.402594	0.843642
7	-1.494106	-2.648639	-0.005141
6	-1.120436	-3.957087	-2.106723
1	-0.418720	-3.194331	-2.470905
1	-1.641369	-4.387830	-2.975036
1	-0.539870	-4.758148	-1.635982
6	-2.401755	1.141194	0.058069
6	-3.093615	-4.423202	-0.596947
1	-2.535860	-5.152647	0.007274
1	-3.587600	-4.967612	-1.417153
1	-3.875102	-3.980525	0.038378
6	-3.002344	-2.347001	-1.998005
1	-3.827055	-1.899873	-1.432827
1	-3.431361	-2.898665	-2.847862
1	-2.382703	-1.536322	-2.399165
6	1.733365	-0.432269	2.200244
1	2.468822	-1.169811	1.855649
1	2.044130	-0.104166	3.204472
1	1.758999	0.426587	1.522583
6	-4.926535	1.163066	0.331602
6	-0.654067	0.008617	2.826416
1	-0.754254	0.864544	2.153911
1	-0.264492	0.366667	3.791400
1	-1.651777	-0.418641	2.995779
6	-2.456963	-0.298911	0.379815
6	0.297437	-2.259759	3.178645
1	-0.681688	-2.762491	3.142592
1	0.472552	-1.929658	4.214351
1	1.072147	-2.993787	2.924509
6	2.201603	-3.491729	0.434943
1	2.511286	-2.454735	0.314050
6	-3.683049	1.779982	0.013857
6	-0.152439	-2.764394	0.428755
6	0.803708	-3.796643	0.468688
6	-2.165691	-3.331717	-1.160978
6	0.321806	-1.026360	2.254120
6	-3.737542	-0.874351	0.703520
1	-3.742732	-1.921888	1.007642
6	2.771937	-5.848263	0.597407
1	3.526661	-6.636027	0.646708
6	-4.940977	-0.175067	0.699018
1	-5.866907	-0.680900	0.986560
6	3.153503	-4.498405	0.495059
1	4.213689	-4.234671	0.449065
6	-6.055538	2.158802	0.201491
1	-6.570636	2.306561	1.167205
1	-6.827832	1.807737	-0.504672
6	0.435802	-5.175311	0.572280

1	-0.618659	-5.441826	0.645091
6	1.403428	-6.167970	0.635833
1	1.091934	-7.211881	0.730397
6	0.145602	1.686911	-0.148838
7	1.082859	1.124026	-1.044902
7	1.127396	2.617146	0.253422
6	2.442568	3.236875	2.268868
1	2.272439	2.261120	2.741899
1	2.538958	3.992565	3.063963
1	3.394889	3.193597	1.726089
6	1.505323	4.995333	0.721087
1	2.413339	5.004643	0.104122
1	1.623095	5.751581	1.512791
1	0.656474	5.290975	0.087599
6	-0.014709	3.661423	2.195928
1	-0.887892	3.985235	1.617516
1	0.141130	4.380386	3.014345
1	-0.238598	2.685491	2.640956
6	1.439471	-1.008601	-2.269852
1	2.516122	-1.059610	-2.062257
1	1.260706	-1.529488	-3.223430
1	0.913145	-1.543365	-1.472673
6	-3.896246	3.128429	-0.362301
6	-0.513664	0.466823	-2.808848
1	-1.157203	-0.024851	-2.070713
1	-0.611090	-0.073598	-3.762629
1	-0.881985	1.492096	-2.947645
6	-1.289665	1.993219	-0.287253
6	1.799208	1.206387	-3.399658
1	1.472822	2.253437	-3.480372
1	1.687882	0.724230	-4.383991
1	2.865563	1.199089	-3.135372
6	4.086892	0.611486	-0.508259
1	3.438300	-0.256363	-0.397575
6	2.047814	2.044056	-0.624858
6	3.495235	1.893745	-0.587856
6	1.264341	3.607060	1.346789
6	0.952784	0.448126	-2.361872
6	-1.547990	3.315173	-0.718445
1	-0.688732	3.907343	-1.036820
6	6.315562	1.564526	-0.593856
1	7.401064	1.439375	-0.596958
6	-2.820711	3.901645	-0.753421
1	-2.945193	4.934929	-1.089247
6	5.472410	0.450093	-0.524009
1	5.897844	-0.555257	-0.457709
6	-5.369446	3.468859	-0.290336
1	-5.749364	3.785338	-1.276737
1	-5.552234	4.313825	0.394745
6	4.364078	3.006013	-0.673900
1	3.940270	4.006074	-0.776642
6	5.748864	2.843507	-0.661279
1	6.394286	3.723772	-0.726436

Table S8
B3LYP-D3/def2-SVP
Rea-Si (Singlet)
E = -2429.68331488 Hartree
G = -2428.896504 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-1.288416	0.080605	-0.402569
7	-2.367645	-0.704330	0.959330
7	-3.133923	-0.158964	-0.982089
6	-3.582280	-1.633238	-2.928973
1	-2.522778	-1.933907	-2.927687
1	-3.948979	-1.651785	-3.968086
1	-4.155976	-2.375059	-2.354277
6	0.000003	2.627233	-0.000006
6	-5.214330	0.194927	-2.308679
1	-5.843891	-0.545105	-1.797980
1	-5.586378	0.295378	-3.340677
1	-5.334328	1.166230	-1.803942
6	-2.951090	0.784695	-3.191276
1	-3.027585	1.799361	-2.773447
1	-3.347251	0.793553	-4.218350
1	-1.883819	0.517620	-3.237082
6	-1.223433	-2.263603	2.459537
1	-1.685189	-3.141337	1.979726
1	-1.004033	-2.518480	3.509073
1	-0.275607	-2.036932	1.946935
6	-1.174273	4.828558	0.003565
6	-1.521468	0.170410	3.066839
1	-0.569660	0.427705	2.582399
1	-1.325702	-0.049010	4.128675
1	-2.184175	1.046580	3.001771
6	-1.276677	1.965231	-0.045404
6	-3.479219	-1.366580	3.126032
1	-4.210699	-0.552472	3.013858
1	-3.254246	-1.474379	4.198179
1	-3.947426	-2.299869	2.789618
6	-4.461617	-3.098906	0.266931
1	-3.484735	-3.518831	0.015884
6	0.000003	4.040566	-0.000012
6	-3.419343	-0.832586	0.138213
6	-4.606124	-1.706546	0.366496
6	-3.732001	-0.222327	-2.326288
6	-2.169726	-1.050374	2.381644
6	-2.422487	2.762454	-0.033109
1	-3.399583	2.271404	-0.077902
6	-6.799815	-3.394145	0.824652
1	-7.654341	-4.051072	1.005341
6	-2.396015	4.186683	0.002784
1	-3.336045	4.746774	0.008949
6	-5.555144	-3.938708	0.490810
1	-5.434746	-5.021838	0.408342
6	-0.783562	6.294846	0.006407
1	-1.182304	6.811981	0.895430
1	-1.198244	6.822729	-0.868803
6	-5.856613	-1.166387	0.695840

1	-5.967544	-0.083119	0.778811
6	-6.947814	-2.007100	0.928011
1	-7.917414	-1.577773	1.192226
14	1.288416	0.080607	0.402583
7	2.367638	-0.704350	-0.959305
7	3.133926	-0.158968	0.982109
6	3.582187	-1.633297	2.928981
1	2.522674	-1.933925	2.927668
1	3.948864	-1.651875	3.968101
1	4.155867	-2.375130	2.354285
6	5.214322	0.194815	2.308750
1	5.843869	-0.545236	1.798060
1	5.586348	0.295242	3.340758
1	5.334371	1.166119	1.804026
6	2.951089	0.784657	3.191309
1	3.027635	1.799327	2.773498
1	3.347229	0.793482	4.218391
1	1.883806	0.517626	3.237089
6	1.223457	-2.263675	-2.459475
1	1.685243	-3.141388	-1.979653
1	1.004054	-2.518575	-3.509004
1	0.275630	-2.037021	-1.946868
6	1.174281	4.828556	-0.003597
6	1.521420	0.170339	-3.066817
1	0.569611	0.427620	-2.582372
1	1.325647	-0.049105	-4.128647
1	2.184105	1.046527	-3.001772
6	1.276681	1.965230	0.045398
6	3.479218	-1.366606	-3.125993
1	4.210666	-0.552463	-3.013858
1	3.254244	-1.474461	-4.198134
1	3.947464	-2.299861	-2.789538
6	4.461637	-3.098879	-0.267044
1	3.484751	-3.518825	-0.016050
6	3.419353	-0.832569	-0.138205
6	4.606142	-1.706512	-0.366512
6	3.731977	-0.222383	2.326320
6	2.169717	-1.050418	-2.381610
6	2.422492	2.762451	0.033096
1	3.399587	2.271400	0.077894
6	6.799849	-3.394072	-0.824732
1	7.654382	-4.050984	-1.005447
6	2.396022	4.186680	-0.002809
1	3.336052	4.746769	-0.008978
6	5.555173	-3.938662	-0.490956
1	5.434776	-5.021798	-0.408562
6	0.783572	6.294844	-0.006451
1	1.182314	6.811972	-0.895479
1	1.198254	6.822735	0.868755
6	5.856634	-1.166326	-0.695798
1	5.967564	-0.083053	-0.778698
6	6.947844	-2.007020	-0.928000
1	7.917448	-1.577672	-1.192167

Table S9
B3LYP-D3/def2-SVP
Rea-Si(Triplet)
E = -2429.65217020 Hartree
G = -2428.862471 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	1.212818	0.543134	-0.167103
7	1.969049	-0.553811	-1.379131
7	2.377208	-0.423771	0.802698
6	3.572996	-1.088638	2.903261
1	2.607510	-1.429254	3.307736
1	4.174679	-0.690381	3.735814
1	4.103848	-1.956029	2.492903
6	0.218690	3.130165	0.091688
6	4.706283	0.367192	1.188969
1	5.150668	-0.502013	0.683746
1	5.417383	0.722622	1.951902
1	4.572994	1.167808	0.444824
6	2.794941	1.252354	2.549927
1	2.695867	2.105108	1.865154
1	3.472754	1.552982	3.363459
1	1.808006	1.053707	2.992426
6	0.272259	-2.261334	-2.024655
1	0.787703	-3.028701	-1.427580
1	-0.228811	-2.758366	-2.871220
1	-0.503518	-1.799212	-1.394758
6	1.438346	5.251132	-0.313097
6	0.549880	-0.080000	-3.277483
1	-0.169953	0.433019	-2.623292
1	-0.004474	-0.486717	-4.137391
1	1.269147	0.668758	-3.642202
6	1.374204	2.404427	-0.357306
6	2.255367	-1.867468	-3.510142
1	3.058953	-1.169394	-3.789518
1	1.710998	-2.149854	-4.425453
1	2.708431	-2.775907	-3.095825
6	3.359946	-3.393645	0.626722
1	2.595819	-3.268144	1.394544
6	0.299341	4.531077	0.113061
6	2.693779	-1.199948	-0.341062
6	3.492329	-2.390544	-0.379926
6	3.356654	0.005642	1.839763
6	1.281156	-1.203193	-2.522426
6	2.484614	3.125600	-0.792268
1	3.364686	2.580907	-1.148633
6	5.101317	-4.747751	-0.394833
1	5.717061	-5.650090	-0.401488
6	2.533970	4.549185	-0.781647
1	3.433236	5.062097	-1.133707
6	4.144462	-4.541226	0.612274
1	3.999429	-5.298330	1.388774
6	1.159350	6.734861	-0.158574
1	1.239830	7.255795	-1.127365
1	1.896263	7.211335	0.509292
6	4.476622	-2.617075	-1.387374

1	4.651541	-1.845088	-2.137132
6	5.255852	-3.768603	-1.389761
1	6.013624	-3.899514	-2.168076
14	-1.030683	0.685682	0.272110
7	-1.822575	-0.703106	1.253999
7	-2.651693	0.122855	-0.556804
6	-3.410428	-0.581782	-2.815533
1	-2.364840	-0.793677	-3.083122
1	-3.935947	-0.239200	-3.720712
1	-3.883773	-1.516382	-2.486451
6	-4.934026	0.750371	-1.296131
1	-5.423398	-0.172033	-0.955963
1	-5.512087	1.144105	-2.146726
1	-4.973964	1.491038	-0.482040
6	-2.905106	1.815400	-2.293528
1	-2.950598	2.627217	-1.555679
1	-3.488517	2.112536	-3.178105
1	-1.856626	1.697847	-2.600906
6	-0.491440	-2.746294	1.640665
1	-1.100352	-3.331619	0.935917
1	-0.098592	-3.435057	2.405171
1	0.363653	-2.319052	1.098631
6	-0.756364	5.379397	0.536319
6	-0.437562	-0.809965	3.239978
1	0.413445	-0.387867	2.692345
1	-0.038776	-1.455426	4.037661
1	-1.004734	0.012442	3.701953
6	-1.037302	2.518371	0.484977
6	-2.474352	-2.248043	3.121667
1	-3.161546	-1.467946	3.483505
1	-2.048491	-2.762455	3.996942
1	-3.053003	-2.986734	2.553331
6	-3.583248	-3.095862	-0.454451
1	-2.662661	-3.178922	-1.035718
6	-2.807925	-0.856918	0.341347
6	-3.816701	-1.942404	0.313833
6	-3.475533	0.504125	-1.724472
6	-1.329582	-1.632836	2.297949
6	-2.070234	3.373744	0.897797
1	-3.032212	2.941035	1.191267
6	-5.695640	-4.028072	0.283299
1	-6.426682	-4.840009	0.272670
6	-1.941619	4.791724	0.936938
1	-2.790741	5.396145	1.269796
6	-4.519815	-4.131944	-0.467562
1	-4.327214	-5.026526	-1.064765
6	-0.294817	6.820158	0.424493
1	-0.304484	7.322423	1.406944
1	-0.959262	7.410557	-0.228911
6	-4.999493	-1.842603	1.066240
1	-5.181115	-0.948694	1.666540
6	-5.932107	-2.879914	1.048989
1	-6.849348	-2.792662	1.636512

Table S10
B3LYP-D3/def2-SVP
Rea-Ge (Singlet)
E = -6004.43256621 Hartree
G = -6003.654441 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	-1.434041	-0.293719	-0.556239
7	-2.801677	-0.743402	0.915275
7	-3.418378	-0.326796	-1.135438
6	-4.205326	-1.865744	-2.920623
1	-3.235069	-2.385254	-2.880826
1	-4.582195	-1.911499	-3.955325
1	-4.915327	-2.406338	-2.278051
6	-0.000010	2.336045	-0.000045
6	-5.407395	0.317300	-2.502783
1	-6.170948	-0.215998	-1.922085
1	-5.765404	0.385360	-3.542474
1	-5.315279	1.339777	-2.104432
6	-3.085465	0.327310	-3.423721
1	-2.940283	1.371415	-3.107649
1	-3.486731	0.322011	-4.448792
1	-2.099274	-0.163574	-3.442486
6	-2.136346	-2.454359	2.537370
1	-2.831466	-3.199586	2.119689
1	-1.988146	-2.681448	3.605619
1	-1.167869	-2.553871	2.023356
6	-1.163434	4.556257	-0.122832
6	-1.704890	-0.005755	2.940679
1	-0.722221	-0.087253	2.453788
1	-1.565726	-0.181464	4.019034
1	-2.072844	1.019945	2.789735
6	-1.278734	1.698747	-0.198692
6	-4.028392	-0.889925	3.114850
1	-4.497207	0.084528	2.911512
1	-3.829421	-0.953933	4.195882
1	-4.747988	-1.678715	2.862535
6	-5.354952	-2.744601	0.380126
1	-4.512186	-3.404692	0.162360
6	-0.000013	3.759902	-0.000096
6	-3.814103	-0.793792	0.053719
6	-5.167478	-1.354945	0.351804
6	-4.044273	-0.402213	-2.463646
6	-2.696471	-1.030128	2.353785
6	-2.410467	2.507635	-0.305220
1	-3.380161	2.025557	-0.456770
6	-7.682620	-2.431159	0.972795
1	-8.662066	-2.850017	1.217020
6	-2.382405	3.928518	-0.257642
1	-3.313458	4.496158	-0.348901
6	-6.608844	-3.280231	0.685788
1	-6.747077	-4.364213	0.703259
6	-0.778501	6.022142	-0.073384
1	-1.266859	6.532142	0.774131
1	-1.105191	6.554007	-0.982664
6	-6.248445	-0.508497	0.634321

1	-6.099983	0.573344	0.617192
6	-7.499672	-1.044393	0.946784
1	-8.335250	-0.377232	1.172655
32	1.434052	-0.293684	0.556347
7	2.801632	-0.743470	-0.915202
7	3.418429	-0.326701	1.135451
6	4.205768	-1.865433	2.920656
1	3.235590	-2.385102	2.880986
1	4.582746	-1.911064	3.955323
1	4.915793	-2.405953	2.278048
6	5.407439	0.317785	2.502589
1	6.171002	-0.215377	1.921779
1	5.765576	0.385889	3.542233
1	5.315100	1.340254	2.104268
6	3.085584	0.327462	3.423738
1	2.940192	1.371523	3.107618
1	3.486948	0.322296	4.448770
1	2.099480	-0.163593	3.442624
6	2.136106	-2.454516	-2.537128
1	2.831173	-3.199771	-2.119407
1	1.987852	-2.681682	-3.605353
1	1.167637	-2.553897	-2.023075
6	1.163406	4.556271	0.122578
6	1.704875	-0.005903	-2.940653
1	0.722213	-0.087240	-2.453722
1	1.565659	-0.181707	-4.018985
1	2.072946	1.019773	-2.789826
6	1.278715	1.698762	0.198645
6	4.028287	-0.890310	-3.114785
1	4.497198	0.084118	-2.911546
1	3.829288	-0.954398	-4.195807
1	4.747814	-1.679144	-2.862414
6	5.354909	-2.744651	-0.379947
1	4.512148	-3.404708	-0.162062
6	3.814096	-0.793792	-0.053685
6	5.167451	-1.354990	-0.351775
6	4.044430	-0.401955	2.463616
6	2.696366	-1.030321	-2.353682
6	2.410445	2.507664	0.305109
1	3.380141	2.025600	0.456682
6	7.682554	-2.431302	-0.972757
1	8.661984	-2.850198	-1.216980
6	2.382378	3.928543	0.257428
1	3.313431	4.496192	0.348641
6	6.608781	-3.280329	-0.685606
1	6.747001	-4.364315	-0.702962
6	0.778468	6.022150	0.073023
1	1.266824	6.532089	-0.774529
1	1.105157	6.554083	0.982264
6	6.248416	-0.508585	-0.634427
1	6.099966	0.573259	-0.617412
6	7.499623	-1.044531	-0.946888
1	8.335199	-0.377404	-1.172869

Table S11
B3LYP-D3/def2-SVP
Rea-Ge (Triplet)
E = -6004.35784949 Hartree
G = -6003.581508 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	-1.216853	0.127357	-0.462399
7	-2.455762	-0.656484	0.943478
7	-3.078571	-0.473241	-1.141597
6	-3.415548	-2.227749	-2.856658
1	-2.352393	-2.504542	-2.774401
1	-3.742319	-2.414605	-3.892373
1	-3.998471	-2.883574	-2.193356
6	-0.000014	2.688304	0.000017
6	-5.098684	-0.357747	-2.603977
1	-5.747575	-1.028918	-2.027073
1	-5.413580	-0.411130	-3.658147
1	-5.256637	0.672710	-2.249765
6	-2.801437	0.136599	-3.453209
1	-2.893014	1.198789	-3.180213
1	-3.163575	0.003077	-4.484185
1	-1.732841	-0.127616	-3.426852
6	-1.525600	-2.023382	2.745778
1	-2.028177	-2.936005	2.388067
1	-1.376895	-2.113935	3.833862
1	-0.537270	-1.959148	2.264059
6	-1.160395	4.890059	-0.199257
6	-1.654478	0.490714	2.924450
1	-0.647957	0.592722	2.490341
1	-1.542931	0.446778	4.019152
1	-2.224559	1.392951	2.658689
6	-1.253059	2.047121	-0.302309
6	-3.733302	-0.866922	3.113756
1	-4.385590	-0.031699	2.818829
1	-3.575132	-0.806600	4.201639
1	-4.259402	-1.807007	2.905359
6	-4.599308	-3.100810	0.485009
1	-3.644980	-3.612813	0.341389
6	-0.000022	4.108907	0.000034
6	-3.416191	-0.938064	0.064267
6	-4.658436	-1.703143	0.368296
6	-3.611806	-0.745395	-2.484460
6	-2.367306	-0.776359	2.410560
6	-2.412275	2.841229	-0.480096
1	-3.363003	2.344319	-0.696466
6	-6.968365	-3.169466	0.988581
1	-7.868327	-3.739651	1.231568
6	-2.376982	4.248774	-0.420874
1	-3.297997	4.820930	-0.571003
6	-5.751444	-3.830164	0.789034
1	-5.697619	-4.918287	0.875629
6	-0.779002	6.356400	-0.098442
1	-1.288498	6.842856	0.752580
1	-1.077901	6.923221	-0.996980
6	-5.882163	-1.045161	0.563077

1	-5.926521	0.042219	0.473097
6	-7.029556	-1.775221	0.876264
1	-7.977257	-1.254306	1.033543
32	1.216848	0.127363	0.462378
7	2.455784	-0.656433	-0.943503
7	3.078556	-0.473251	1.141589
6	3.415500	-2.227770	2.856643
1	2.352340	-2.504547	2.774383
1	3.742266	-2.414636	3.892358
1	3.998414	-2.883599	2.193338
6	5.098662	-0.357789	2.603980
1	5.747546	-1.028961	2.027068
1	5.413556	-0.411190	3.658150
1	5.256629	0.672670	2.249782
6	2.801416	0.136584	3.453203
1	2.893012	1.198774	3.180214
1	3.163544	0.003049	4.484180
1	1.732816	-0.127614	3.426835
6	1.525590	-2.023167	-2.745916
1	2.028079	-2.935851	-2.388237
1	1.376921	-2.113647	-3.834010
1	0.537247	-1.958879	-2.264231
6	1.160343	4.890067	0.199343
6	1.654698	0.490927	-2.924467
1	0.648151	0.592989	-2.490433
1	1.543234	0.447062	-4.019181
1	2.224829	1.393104	-2.658611
6	1.253038	2.047129	0.302331
6	3.733409	-0.866875	-3.113724
1	4.385800	-0.031794	-2.818617
1	3.575313	-0.806350	-4.201607
1	4.259360	-1.807069	-2.905452
6	4.599298	-3.100820	-0.485012
1	3.644972	-3.612826	-0.341388
6	3.416178	-0.938075	-0.064274
6	4.658424	-1.703153	-0.368301
6	3.611779	-0.745416	2.484454
6	2.367386	-0.776231	-2.410594
6	2.412245	2.841246	0.480138
1	3.362979	2.344341	0.696501
6	6.968354	-3.169471	-0.988589
1	7.868318	-3.739654	-1.231578
6	2.376937	4.248792	0.420947
1	3.297945	4.820954	0.571090
6	5.751436	-3.830172	-0.789038
1	5.697613	-4.918295	-0.875631
6	0.778933	6.356406	0.098561
1	1.288423	6.842888	-0.752451
1	1.077825	6.923211	0.997111
6	5.882148	-1.045168	-0.563087
1	5.926503	0.042212	-0.473111
6	7.029542	-1.775226	-0.876275
1	7.977242	-1.254309	-1.033559

Table S12
B3LYP-D3/def2-SVP
TS-C (with C_2H_4)
1st frequency = -264.4 cm^{-1}
G = -2004.442300 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.460952	-0.139306	0.169178
6	-2.069357	0.600563	-0.183537
6	-0.042382	2.163749	0.271167
6	-0.418854	-1.445175	-1.347880
1	-1.482881	-1.630290	-1.261039
1	0.033960	-1.636324	-2.325387
6	1.106823	1.308017	0.583805
6	2.213747	1.924680	1.199895
1	3.072455	1.298229	1.424228
6	0.205878	3.573937	0.441164
7	2.455058	-0.230987	-0.929649
7	-3.147480	0.157704	-0.959056
6	3.297024	-0.920874	-0.126945
6	5.763076	-1.218031	0.161861
1	5.776134	-0.337231	0.806326
6	5.736337	-3.427029	-1.552601
1	5.721399	-4.294765	-2.216792
6	4.547751	-2.753062	-1.271173
1	3.603697	-3.097413	-1.697142
6	4.543907	-1.639014	-0.407245
6	2.565573	-1.482845	2.285553
6	-2.664795	0.040969	2.285285
6	-3.453168	0.211240	-2.418187
6	2.642004	0.425161	-2.241902
6	-1.591107	1.004576	2.806710
1	-0.582984	0.678495	2.539587
1	-1.658511	1.053935	3.904057
1	-1.729950	2.019572	2.414712
7	2.562169	-0.736753	1.007426
6	-2.240667	2.953223	-0.564530
1	-3.263945	2.704329	-0.841928
7	-2.422654	-0.309825	0.842011
6	-1.878143	4.305617	-0.531389
1	-2.582145	5.074677	-0.860739
6	1.435580	1.328778	-2.529061
1	0.498492	0.789378	-2.335696
1	1.460981	1.636444	-3.585156
1	1.449546	2.233873	-1.910004
6	-1.406729	1.879723	-0.173336
6	-0.657024	4.621174	0.021660
6	-4.302103	-1.941861	0.103354
6	-0.021966	5.969104	0.280413
6	0.389299	-1.464431	-0.172954
1	1.200612	-2.222831	-0.182876
1	-0.214933	-1.574637	0.735936
6	-5.655489	-1.935056	-0.322935
1	-6.086306	-1.010173	-0.710546
6	-3.793115	-3.152513	0.642730
1	-2.739668	-3.197027	0.923007

6	-3.467939	-0.777385	0.018589
6	-4.600840	-4.280964	0.762903
1	-4.178211	-5.201410	1.175926
6	-6.447297	-3.076910	-0.223305
1	-7.487184	-3.039932	-0.560129
6	-5.932799	-4.258075	0.328056
1	-6.560065	-5.148497	0.414253
6	6.940418	-3.005576	-0.975056
1	7.869722	-3.537043	-1.193925
6	6.948435	-1.900006	-0.117156
1	7.886479	-1.558971	0.328096
6	-2.296849	0.881132	-3.174119
1	-2.146134	1.924981	-2.873925
1	-2.520946	0.864071	-4.251583
1	-1.368665	0.325846	-2.987625
6	1.408261	-0.969271	3.146860
1	1.496101	0.110633	3.328815
1	1.413768	-1.490168	4.115753
1	0.442510	-1.162092	2.666943
6	3.891614	-1.186343	3.014676
1	4.747887	-1.634842	2.494792
1	3.857500	-1.611853	4.029316
1	4.057532	-0.101892	3.102996
6	2.751764	-0.645013	-3.345348
1	3.639050	-1.276471	-3.204438
1	2.841444	-0.156268	-4.327806
1	1.858079	-1.284581	-3.354617
6	3.930423	1.268562	-2.193370
1	3.868033	2.011023	-1.383143
1	4.063045	1.802291	-3.147508
1	4.819160	0.640958	-2.027208
6	-3.642854	-1.206749	-2.992460
1	-2.745768	-1.819793	-2.839485
1	-3.827241	-1.126713	-4.074861
1	-4.497459	-1.727941	-2.545762
6	-4.751878	1.017502	-2.611512
1	-5.590129	0.560367	-2.066463
1	-5.017258	1.050960	-3.679689
1	-4.637651	2.052893	-2.258729
6	2.434676	-3.006358	2.080743
1	1.453865	-3.279084	1.670824
1	2.555944	-3.517108	3.049013
1	3.211531	-3.380973	1.397926
6	-4.038312	0.726699	2.420841
1	-4.183549	1.081521	3.454097
1	-4.857754	0.039034	2.168692
1	-4.095795	1.596396	1.748074
6	-2.637464	-1.249474	3.118654
1	-1.681363	-1.779214	2.992382
1	-3.447827	-1.931967	2.834312
1	-2.759884	-1.005012	4.185345
6	2.348557	3.295182	1.486783
1	3.250817	3.663179	1.982641
6	1.356677	4.136585	1.053100
6	1.237099	5.641159	1.130074
1	2.144901	6.149284	0.766963
1	1.102031	5.956886	2.179681
1	-0.709411	6.664530	0.788969
1	0.258825	6.451684	-0.672930

Table S13
B3LYP-D3/def2-SVP
TS-Si (with C_2H_4)
1st frequency = -167.9 cm^{-1}
G = -2507.375045 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	1.185779	-0.054070	0.471346
14	-1.114117	-0.163912	-0.336036
6	-0.026858	2.477912	-0.108439
6	-0.467975	-2.666216	0.029604
1	-1.483822	-2.855462	0.385847
1	-0.246611	-3.055702	-0.966862
6	1.198667	1.874073	0.362206
6	2.249330	2.725575	0.701470
1	3.184218	2.280675	1.053689
6	-0.062792	3.890291	-0.195874
7	2.424480	-0.549632	-0.874753
7	-2.824463	-0.608854	-1.135581
6	3.425384	-0.717144	0.006035
6	5.918601	-0.624945	-0.372123
1	5.885668	0.455762	-0.219954
6	5.982012	-3.388079	-0.798199
1	6.003742	-4.468289	-0.962135
6	4.771605	-2.754358	-0.508171
1	3.845816	-3.330922	-0.448155
6	4.733792	-1.368603	-0.288398
6	3.553583	-0.518673	2.548231
6	-2.609238	-0.213231	2.434563
6	-3.241609	-1.054040	-2.475065
6	2.408228	-0.561822	-2.353987
6	-1.324367	0.456915	2.943986
1	-0.457013	-0.194127	2.773886
1	-1.407403	0.656323	4.023355
1	-1.139355	1.409571	2.426598
7	2.995668	-0.313554	1.199735
6	-2.306668	2.508658	-0.946178
1	-3.213655	1.975520	-1.248269
7	-2.444133	-0.456186	0.986151
6	-2.314894	3.931081	-1.028298
1	-3.208403	4.450219	-1.388622
6	1.610829	0.670622	-2.825726
1	0.586661	0.661718	-2.430616
1	1.551076	0.683980	-3.925300
1	2.089385	1.599637	-2.483234
6	-1.215994	1.760562	-0.503497
6	-1.183481	4.624083	-0.648827
6	-4.717654	-1.362680	0.341832
6	-0.851784	6.104666	-0.612929
6	0.572850	-2.441757	0.934818
1	1.594713	-2.739188	0.677927
1	0.367104	-2.421068	2.010406
6	-5.863730	-0.557203	0.266767
1	-5.758270	0.501437	0.020877

6	-4.853512	-2.723708	0.654525
1	-3.962291	-3.352076	0.712017
6	-3.364665	-0.793827	0.068188
6	-6.118580	-3.270840	0.885995
1	-6.214111	-4.332912	1.124672
6	-7.126659	-1.103231	0.506465
1	-8.012780	-0.466240	0.450175
6	-7.256669	-2.461587	0.814766
1	-8.245340	-2.889128	0.999418
6	7.161700	-2.640665	-0.883065
1	8.107969	-3.135448	-1.115775
6	7.127022	-1.258370	-0.672270
1	8.044961	-0.669847	-0.744793
6	-2.195921	-0.492039	-3.455564
1	-2.146444	0.605123	-3.386588
1	-2.452532	-0.769025	-4.489388
1	-1.196258	-0.892735	-3.232934
6	2.512029	0.043944	3.532058
1	2.289288	1.097617	3.305463
1	2.886352	-0.021868	4.565045
1	1.573058	-0.524505	3.471941
6	4.871391	0.259433	2.731968
1	5.679374	-0.161175	2.119574
1	5.191801	0.212248	3.784877
1	4.739970	1.318557	2.462387
6	1.708051	-1.847403	-2.826979
1	2.268179	-2.736972	-2.499059
1	1.630629	-1.869147	-3.925793
1	0.697859	-1.901983	-2.399701
6	3.809097	-0.473419	-2.986019
1	4.368341	0.390101	-2.596547
1	3.694409	-0.340897	-4.072722
1	4.409684	-1.376806	-2.824614
6	-3.251584	-2.591965	-2.565099
1	-2.272619	-2.997766	-2.271611
1	-3.472358	-2.915799	-3.594984
1	-4.017425	-3.022781	-1.904109
6	-4.623816	-0.492059	-2.857957
1	-5.428383	-0.933144	-2.255666
1	-4.836139	-0.715948	-3.915328
1	-4.648154	0.601057	-2.728350
6	3.781264	-2.011354	2.856294
1	2.851652	-2.581597	2.714623
1	4.108314	-2.136860	3.900932
1	4.556069	-2.443811	2.207767
6	-3.787789	0.743818	2.701190
1	-3.808314	1.025523	3.765776
1	-4.755522	0.283912	2.462310
1	-3.673543	1.660144	2.101526
6	-2.807881	-1.542047	3.189391
1	-1.983987	-2.235989	2.962317
1	-3.755788	-2.025247	2.915933
1	-2.822542	-1.363816	4.276550
6	2.184175	4.146578	0.609488
1	3.051374	4.749694	0.895766
6	1.019334	4.730328	0.156536
6	0.613170	6.176325	-0.061335
1	1.291332	6.682073	-0.769050
1	0.664811	6.751025	0.878877
1	-1.557068	6.658845	0.028995

1	-0.929771	6.555267	-1.616826

Table S14
B3LYP-D3/def2-SVP
TS-Ge (with C_2H_4)
1st frequency = -184.3 cm^{-1}
G = -6082.110512 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	1.382546	-0.441533	0.995004
32	-1.481600	-0.238767	0.579182
6	0.182387	2.064877	-0.222772
6	-0.991062	-0.025295	3.051789
1	-1.401653	0.985698	3.025337
1	-1.708735	-0.811470	3.298022
6	1.292497	1.548197	0.537223
6	2.392050	2.381154	0.730577
1	3.251109	1.989114	1.280869
6	0.344378	3.351415	-0.802215
7	2.664297	-0.758710	-0.711428
7	-2.837166	-1.252594	-0.598196
6	3.750752	-0.797653	0.038230
6	5.967164	-0.033372	-0.861936
1	5.631892	0.994432	-0.707805
6	6.801399	-2.670758	-1.255785
1	7.124073	-3.703777	-1.408277
6	5.542071	-2.410168	-0.705830
1	4.881242	-3.236185	-0.434446
6	5.117413	-1.090675	-0.503782
6	4.375811	-0.700178	2.489486
6	-4.309463	1.291391	1.553919
6	-2.738440	-2.616063	-1.164108
6	2.485051	-0.950772	-2.160941
6	-3.427370	2.547322	1.708199
1	-2.461345	2.315537	2.174302
1	-3.940151	3.287566	2.341668
1	-3.216747	3.004072	0.732051
7	3.482960	-0.526188	1.324277
6	-1.962582	1.989002	-1.377122
1	-2.900793	1.468641	-1.595042
7	-3.523898	0.269566	0.832682
6	-1.746013	3.254837	-1.989613
1	-2.492339	3.665112	-2.676494
6	1.203341	-0.195345	-2.552371
1	0.353445	-0.495241	-1.930237
1	0.942812	-0.397735	-3.602963
1	1.335726	0.888022	-2.425532
6	-1.061489	1.400990	-0.496401
6	-0.596090	3.949883	-1.673135
6	-5.319602	-1.068048	-0.280567
6	-0.073564	5.306175	-2.109017
6	0.365110	-0.205227	3.288447
1	0.721226	-1.146376	3.712805
1	0.998708	0.670076	3.442968

6	-5.944259	-0.657579	-1.467335
1	-5.376827	-0.074138	-2.195379
6	-6.043725	-1.821028	0.653812
1	-5.559364	-2.142560	1.578171
6	-3.902184	-0.677645	-0.008924
6	-7.376989	-2.159763	0.404434
1	-7.933067	-2.750981	1.136249
6	-7.278208	-0.986230	-1.710847
1	-7.759596	-0.655554	-2.634501
6	-7.997701	-1.739245	-0.775681
1	-9.041804	-1.998649	-0.967782
6	7.642245	-1.612951	-1.613282
1	8.624780	-1.815958	-2.046754
6	7.221318	-0.292504	-1.414711
1	7.874191	0.538123	-1.694537
6	-1.312795	-2.752113	-1.717849
1	-1.140752	-2.030963	-2.529408
1	-1.145740	-3.765428	-2.113939
1	-0.568918	-2.567352	-0.928670
6	3.667161	-0.106130	3.718121
1	3.388600	0.943957	3.542136
1	4.334826	-0.143499	4.592189
1	2.762593	-0.670487	3.967701
6	5.722371	0.044584	2.342379
1	6.394022	-0.431176	1.619303
1	6.242131	0.057932	3.313298
1	5.557693	1.087231	2.029241
6	2.315297	-2.455481	-2.454073
1	3.241584	-3.002357	-2.222964
1	2.076740	-2.623585	-3.517101
1	1.503676	-2.878802	-1.846127
6	3.624792	-0.386067	-3.035867
1	3.863873	0.647496	-2.744663
1	3.292747	-0.375832	-4.086176
1	4.542653	-0.984110	-2.986742
6	-2.950888	-3.668552	-0.056888
1	-2.235073	-3.509079	0.764820
1	-2.803343	-4.686995	-0.451351
1	-3.970142	-3.610203	0.352436
6	-3.725369	-2.864943	-2.322152
1	-4.761756	-2.971043	-1.979113
1	-3.451153	-3.797017	-2.841405
1	-3.681761	-2.040667	-3.050154
6	4.637173	-2.197386	2.754029
1	3.683241	-2.736840	2.862506
1	5.221011	-2.335156	3.679020
1	5.202827	-2.653579	1.929450
6	-5.592640	1.729703	0.818191
1	-6.000796	2.624884	1.312866
1	-6.375325	0.961634	0.827099
1	-5.372334	1.990523	-0.227867
6	-4.676558	0.746844	2.948954
1	-3.773607	0.463679	3.508854
1	-5.322717	-0.139193	2.861334
1	-5.218933	1.508132	3.532488
6	2.494107	3.700780	0.201531
1	3.389454	4.297243	0.402155
6	1.472243	4.178307	-0.590161
6	1.278382	5.483457	-1.339196
1	2.118240	5.689923	-2.023108

1	1.233076	6.335498	-0.639655
1	-0.789779	6.111339	-1.875450
1	0.077605	5.334711	-3.201544

Table S15

B3LYP-D3/def2-SVP

TS-C (with Ph_2CO)

1st frequency = -795.8 cm^{-1}

G = -2502.039222 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.297809	0.133402	-0.176731
6	-0.849118	-1.129531	-0.288004
8	0.062167	-1.938986	-1.719464
7	-2.526493	-0.000771	1.309435
6	-0.519237	-1.923452	0.891560
6	1.337700	-0.424947	0.665861
7	-2.237063	-1.080458	-0.703893
7	0.307619	1.419518	-0.540204
6	0.750284	-1.525349	1.335996
7	2.390892	2.490392	-0.602360
6	1.337994	-1.645833	-1.885151
6	2.336090	-2.485600	-1.249851
6	3.733811	-2.226082	-1.310406
1	4.105888	-1.397300	-1.911751
6	1.659352	-0.746138	-3.024598
6	1.417721	-2.217051	2.338844
6	-3.066395	-0.377878	0.215053
6	2.743027	-1.921105	2.691258
6	2.704816	-0.161798	0.981677
1	3.268884	0.586241	0.440936
6	-1.135690	-2.988108	1.575764
1	-2.151812	-3.287923	1.325898
6	3.381031	-0.905453	1.977383
1	4.436744	-0.679787	2.151105
6	2.570529	0.322666	-2.962690
1	3.064019	0.549558	-2.022030
6	0.849769	-3.330140	2.976313
6	1.357252	2.292830	0.082282
6	-4.449995	0.011447	-0.228154
6	-0.633914	2.168617	-1.484743
6	-0.445904	-3.688301	2.603349
1	-0.953414	-4.528729	3.086678
6	-5.587232	-0.407513	0.479129
1	-5.470328	-1.078139	1.331105
6	4.646800	-3.023566	-0.623732
1	5.713034	-2.785729	-0.682262
6	2.120297	0.918961	-5.274248
1	2.295951	1.566063	-6.137523
6	1.008753	2.913301	1.409225
6	1.224191	-0.154302	-5.361784
1	0.701639	-0.356882	-6.300911
6	2.791574	1.147151	-4.069666
1	3.485565	1.987954	-3.985657
6	-3.040820	0.726843	2.472228

6	-4.621512	0.847927	-1.340268
1	-3.753681	1.163647	-1.914213
6	-1.792982	2.747653	-0.660546
1	-2.308620	1.960810	-0.107278
1	-2.512952	3.240138	-1.330553
1	-1.446442	3.490052	0.067087
6	1.000849	-0.972016	-4.255382
1	0.309711	-1.813014	-4.330349
6	1.256870	2.268811	2.631236
1	1.642805	1.252309	2.640121
6	-1.810879	1.419207	3.081290
1	-0.999308	0.692572	3.220875
1	-2.047672	1.881724	4.052322
1	-1.447082	2.208431	2.410659
6	4.216733	-4.114105	0.141212
1	4.937651	-4.732475	0.682195
6	3.572594	3.320057	-0.309785
6	2.847543	-4.418078	0.174662
1	2.490896	-5.279965	0.745629
6	0.111064	3.312249	-2.198761
1	0.432284	4.116284	-1.525720
1	-0.590461	3.752887	-2.922423
1	0.987733	2.936409	-2.740346
6	-1.136397	1.226487	-2.571103
1	-0.311797	0.872639	-3.196156
1	-1.843180	1.771820	-3.214468
1	-1.651699	0.367985	-2.146733
6	1.928394	-3.624695	-0.498493
1	0.868282	-3.866094	-0.446726
6	-2.792779	-2.179778	-1.663374
6	1.909718	-3.889884	3.917008
6	3.149916	-2.918377	3.765512
6	-7.023592	0.838814	-1.019736
1	-8.022478	1.157189	-1.328235
6	-5.897659	1.265157	-1.729026
1	-6.011184	1.920015	-2.596767
6	-2.130501	-3.562264	-1.436485
1	-1.043606	-3.517946	-1.401453
1	-2.416048	-4.210203	-2.279314
1	-2.507159	-4.036445	-0.521349
6	-6.862690	-0.005568	0.085035
1	-7.736893	-0.353983	0.640757
6	3.325703	4.689806	-0.972057
1	3.064677	4.570159	-2.033968
1	4.235566	5.305895	-0.902602
1	2.509427	5.228616	-0.468955
6	1.038334	2.936316	3.838191
1	1.242126	2.418063	4.778181
6	3.943935	3.509469	1.175234
1	3.240754	4.155933	1.713261
1	4.939492	3.976109	1.233490
1	3.990032	2.543322	1.698075
6	4.750152	2.622996	-1.022465
1	4.936677	1.625498	-0.595511
1	5.670995	3.216142	-0.913938
1	4.538178	2.498554	-2.092740
6	0.534511	4.236916	1.429943
1	0.358282	4.766538	0.493000
6	-4.117101	1.812831	2.239106
1	-3.831110	2.484206	1.416571

1	-4.209797	2.422313	3.151877
1	-5.107906	1.405958	2.011437
6	0.301032	4.896052	2.638142
1	-0.071658	5.923248	2.630523
6	-2.601703	-1.724946	-3.118508
1	-3.173531	-0.806884	-3.317716
1	-2.975997	-2.503568	-3.801459
1	-1.546471	-1.546298	-3.336441
6	0.556745	4.246817	3.849865
1	0.382640	4.762493	4.797440
6	-3.549215	-0.327031	3.478850
1	-4.446857	-0.840438	3.104993
1	-3.806050	0.151891	4.437425
1	-2.771813	-1.085236	3.657543
6	-4.295720	-2.478435	-1.468850
1	-4.543415	-2.703852	-0.422907
1	-4.508541	-3.385598	-2.053626
1	-4.966088	-1.697739	-1.837741
1	4.062124	-3.467308	3.483229
1	3.373380	-2.409061	4.719474
1	1.561897	-3.940918	4.962566
1	2.184550	-4.919757	3.630548

Table S16
B3LYP-D3/def2-SVP
TS-Si (with Ph_2CO)
1st frequency = -86.6 cm^{-1}
G = -3004.958877 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.758307	0.025218	-0.382584
14	-1.507351	-0.673749	0.085712
8	-0.314639	-2.238434	-2.361935
7	-2.745262	0.338819	1.055626
6	-1.079941	-2.173345	1.093771
6	1.119707	-0.892909	1.300345
7	-3.158505	-0.731407	-0.772466
7	0.893974	1.866902	-0.080504
6	0.237403	-1.990466	1.634551
7	3.139795	1.378329	-0.198059
6	0.869357	-1.845315	-2.428381
6	1.941173	-2.661275	-1.750976
6	3.308933	-2.591879	-2.071759
1	3.653938	-1.909820	-2.848293
6	1.242320	-0.891943	-3.547543
6	0.666186	-2.943723	2.582839
6	-3.686412	0.110275	0.133290
6	1.890009	-2.859005	3.281027
6	2.296761	-0.811162	2.051433
1	2.981052	0.010492	1.858005
6	-1.825288	-3.292052	1.454739
1	-2.828523	-3.423937	1.039150
6	2.691531	-1.763249	3.035763
1	3.641549	-1.621658	3.559897
6	2.245459	0.091935	-3.463075
1	2.764586	0.250464	-2.515628
6	-0.087826	-4.084459	2.935625
6	2.233385	2.179381	0.229358
6	-5.015986	0.776422	0.086592
6	0.118296	2.910904	-0.843700
6	-1.330855	-4.274298	2.358479
1	-1.944609	-5.146297	2.601173
6	-6.125846	0.230819	0.742628
1	-6.029780	-0.719806	1.271418
6	4.239053	-3.400543	-1.413802
1	5.298244	-3.322483	-1.673566
6	1.806242	0.784377	-5.748421
1	2.022626	1.438332	-6.597479
6	2.446057	3.343822	1.160605
6	0.802647	-0.182745	-5.839913
1	0.230825	-0.293421	-6.765586
6	2.525590	0.916794	-4.552677
1	3.299388	1.684258	-4.460484
6	-2.788450	1.000965	2.375768
6	-5.138047	1.990118	-0.605825
1	-4.266930	2.410644	-1.112783
6	-0.366173	4.055628	0.073126
1	-0.889922	3.648708	0.949449
1	-1.064622	4.706652	-0.477884

1	0.454000	4.684469	0.437116
6	0.524401	-1.013159	-4.749068
1	-0.258704	-1.771201	-4.810294
6	1.974069	3.205401	2.475428
1	1.467496	2.281020	2.759880
6	-1.329810	1.153254	2.838273
1	-0.852456	0.174090	2.982205
1	-1.296131	1.692556	3.796743
1	-0.734323	1.706925	2.098748
6	3.823606	-4.302066	-0.429606
1	4.555130	-4.924327	0.092791
6	4.593753	1.375259	0.027327
6	2.459607	-4.411378	-0.133089
1	2.115434	-5.121747	0.623257
6	0.980086	3.475341	-1.992413
1	1.878638	3.983861	-1.617903
1	0.407447	4.209426	-2.581777
1	1.303134	2.664925	-2.661753
6	-1.131370	2.283706	-1.484118
1	-0.879636	1.438406	-2.140685
1	-1.640181	3.041179	-2.100315
1	-1.840322	1.947784	-0.716800
6	1.530739	-3.615106	-0.798036
1	0.467020	-3.708039	-0.583946
6	-3.666461	-1.280521	-2.057862
6	0.705527	-4.892658	3.947206
6	2.016809	-4.066129	4.191690
6	-7.474930	2.108228	0.018735
1	-8.435548	2.628395	-0.007082
6	-6.365961	2.653042	-0.638386
1	-6.457774	3.598744	-1.177811
6	-3.344252	-2.786601	-2.053580
1	-2.269967	-2.963070	-1.923004
1	-3.644464	-3.232969	-3.014445
1	-3.903931	-3.292525	-1.250404
6	-7.353635	0.897258	0.707374
1	-8.218691	0.467760	1.218205
6	5.234962	2.278094	-1.048017
1	4.881060	1.989843	-2.050019
1	6.332169	2.179886	-1.026188
1	4.984930	3.335611	-0.884688
6	2.162769	4.226829	3.407824
1	1.802534	4.100484	4.432194
6	5.079682	1.805510	1.429301
1	4.942918	2.876407	1.620331
1	6.154316	1.583342	1.523178
1	4.553757	1.252343	2.221482
6	5.053585	-0.074068	-0.230279
1	4.586458	-0.776370	0.473753
1	6.148130	-0.160123	-0.138219
1	4.761691	-0.391138	-1.239700
6	3.095091	4.530086	0.792518
1	3.458862	4.656646	-0.228075
6	-3.445778	2.391493	2.308818
1	-2.978371	3.008458	1.527463
1	-3.312302	2.903091	3.274298
1	-4.523205	2.335182	2.107385
6	3.267014	5.561651	1.720021
1	3.765431	6.485947	1.416639
6	-2.933394	-0.565472	-3.206059

1	-3.148974	0.514731	-3.187030
1	-3.266034	-0.966980	-4.176249
1	-1.850793	-0.729204	-3.124636
6	2.805576	5.411639	3.031478
1	2.945430	6.216207	3.757957
6	-3.546892	0.095242	3.364441
1	-4.604837	-0.003442	3.079083
1	-3.508505	0.521336	4.379448
1	-3.093458	-0.907489	3.388436
6	-5.184097	-1.111564	-2.227739
1	-5.741475	-1.548637	-1.386721
1	-5.482889	-1.644578	-3.142684
1	-5.488845	-0.063366	-2.339438
1	2.916908	-4.655904	3.950627
1	2.116110	-3.767505	5.248901
1	0.134162	-5.042476	4.878419
1	0.928670	-5.900000	3.557159

Table S17
B3LYP-D3/def2-SVP
TS-Ge (with Ph_2CO)
1st frequency = -83.9 cm^{-1}
G = -6579.720784 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	1.230658	0.116682	0.054928
32	-1.580535	-0.259621	0.262082
8	-0.731549	-1.218402	2.194418
7	-3.051741	-0.175165	-1.243778
6	-1.607366	1.748709	0.510360
6	0.695475	1.928261	-0.626184
7	-3.489729	-0.696459	0.841595
7	2.283467	-0.713404	-1.465641
6	-0.543175	2.472960	-0.135084
7	3.292755	0.486061	0.068421
6	0.527451	-1.254751	2.338616
6	1.125510	-0.293219	3.323854
6	2.224987	-0.605060	4.144283
1	2.715602	-1.574317	4.056156
6	1.243671	-2.486758	1.862368
6	-0.759234	3.857008	-0.361845
6	-3.976654	-0.621133	-0.406905
6	0.123333	4.684228	-1.094211
6	1.536269	2.750809	-1.369461
1	2.473543	2.336159	-1.751897
6	-2.721487	2.460036	0.944057
1	-3.549978	1.907108	1.394488
6	1.264691	4.123378	-1.631087
1	1.968105	4.714232	-2.225204
6	2.641971	-2.583448	1.695852
1	3.271179	-1.719123	1.899083
6	-1.895317	4.562945	0.097724
6	3.462471	-0.259000	-1.016040
6	-5.354997	-1.035825	-0.816468
6	1.974104	-1.690461	-2.530987
6	-2.873572	3.866956	0.777005
1	-3.774147	4.364085	1.150012
6	-6.411550	-0.115091	-0.826136
1	-6.221425	0.920869	-0.537552
6	2.681024	0.302049	5.107873
1	3.538269	0.035572	5.732016
6	2.434586	-4.851559	0.856870
1	2.896306	-5.762675	0.468205
6	4.779966	-0.542314	-1.661222
6	1.048315	-4.765882	1.003853
1	0.415449	-5.613847	0.728587
6	3.226700	-3.748889	1.205153
1	4.312276	-3.797663	1.083026
6	-3.076258	0.084697	-2.689201
6	-5.595235	-2.365036	-1.191175
1	-4.772477	-3.083664	-1.179922
6	1.811719	-0.941011	-3.867948
1	1.064845	-0.139037	-3.772324
1	1.484171	-1.629856	-4.663363

1	2.764085	-0.489170	-4.181838
6	0.459950	-3.598978	1.499438
1	-0.621944	-3.528177	1.605744
6	5.143007	0.135737	-2.833704
1	4.461235	0.874681	-3.259680
6	-1.800089	0.885581	-3.007501
1	-1.814295	1.862102	-2.504062
1	-1.709510	1.049550	-4.092258
1	-0.900013	0.354541	-2.668494
6	2.044181	1.531760	5.281380
1	2.406072	2.241327	6.029685
6	4.236686	1.321520	0.836593
6	0.928422	1.841574	4.490626
1	0.414212	2.797803	4.617343
6	3.029897	-2.805503	-2.673715
1	3.969357	-2.450150	-3.113920
1	2.632410	-3.591745	-3.334390
1	3.245523	-3.259137	-1.694902
6	0.643607	-2.365048	-2.155899
1	0.738620	-2.920487	-1.211747
1	0.339354	-3.066604	-2.947973
1	-0.159794	-1.629124	-2.026396
6	0.471804	0.940526	3.533740
1	-0.393331	1.190881	2.917954
6	-4.078551	-1.238236	2.087672
6	-1.767475	6.019968	-0.306903
6	-0.444517	6.090473	-1.142759
6	-7.931878	-1.849189	-1.567309
1	-8.936853	-2.166018	-1.857224
6	-6.879816	-2.770319	-1.564840
1	-7.059570	-3.809255	-1.852452
6	-3.527962	-0.409033	3.266171
1	-2.432160	-0.417794	3.279829
1	-3.888530	-0.830222	4.217919
1	-3.877159	0.633059	3.203489
6	-7.694342	-0.520300	-1.198553
1	-8.513437	0.203190	-1.200326
6	5.066764	0.459214	1.808254
1	4.409351	-0.058132	2.521390
1	5.751817	1.095952	2.390429
1	5.671152	-0.283835	1.270446
6	6.375055	-0.117661	-3.440901
1	6.652539	0.419630	-4.351120
6	5.183113	2.135036	-0.069362
1	5.926983	1.504182	-0.572689
1	5.728445	2.872002	0.540733
1	4.613797	2.683660	-0.834627
6	3.388480	2.304705	1.663426
1	2.820545	2.983743	1.012925
1	4.037726	2.906361	2.317447
1	2.677775	1.765762	2.303227
6	5.662143	-1.479174	-1.105884
1	5.367445	-2.025452	-0.208845
6	-3.058286	-1.241199	-3.476330
1	-2.188460	-1.849588	-3.186465
1	-2.999111	-1.048287	-4.559901
1	-3.970204	-1.825083	-3.285007
6	6.891297	-1.736602	-1.716824
1	7.569384	-2.475084	-1.281963
6	-3.649407	-2.710790	2.240204

1	-4.018103	-3.307571	1.390413
1	-4.058795	-3.143244	3.167523
1	-2.554031	-2.777105	2.278409
6	7.251337	-1.055404	-2.884437
1	8.214109	-1.255927	-3.361043
6	-4.285856	0.938600	-3.120693
1	-5.228320	0.378494	-3.078987
1	-4.146241	1.279083	-4.159094
1	-4.374362	1.826623	-2.475934
6	-5.616407	-1.147465	2.148942
1	-5.965025	-0.125854	1.937926
1	-5.938467	-1.410647	3.168284
1	-6.118406	-1.834457	1.457215
1	0.264122	6.827377	-0.729680
1	-0.639802	6.399846	-2.183491
1	-2.640811	6.358026	-0.888904
1	-1.717177	6.672148	0.581439

Table S18
B3LYP-D3/def2-SVP
Prod-C (with C_2H_4)
1st frequency = 19.3 cm^{-1}
G = -2004.577252 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.022278	0.418776	-0.098725
6	-0.707233	0.900605	0.110012
6	0.800858	2.774705	-0.083127
6	-0.587407	0.217975	1.489842
1	-1.087053	0.744333	2.311649
1	-0.971283	-0.811486	1.461279
6	1.713137	1.747069	-0.390078
6	3.022207	2.124118	-0.661127
1	3.770474	1.354051	-0.846316
6	1.206155	4.102153	-0.013769
7	1.478302	-0.829262	-0.732614
7	-1.871123	0.476079	-0.680202
6	2.528119	-1.501816	-0.020524
6	3.208475	-3.958349	-0.074072
1	4.152047	-3.674043	-0.541623
6	0.774624	-4.698110	1.072658
1	-0.180338	-4.976430	1.525754
6	1.043911	-3.354643	0.798441
1	0.303920	-2.592274	1.034958
6	2.266197	-2.963787	0.232753
6	4.557604	-1.099674	1.385154
6	-4.302837	0.269145	2.178026
6	-2.389781	1.207869	-1.908895
6	1.418619	-1.068171	-2.224237
6	-3.833864	1.145033	3.362612
1	-2.830093	0.841601	3.696818
1	-4.521157	1.049503	4.218321
1	-3.785516	2.201963	3.062042
7	3.506924	-0.810183	0.407282
6	-1.350502	3.392754	0.759853
1	-2.354615	3.118384	1.088194
7	-3.393148	0.604695	1.076042
6	-0.925834	4.761871	0.836433
1	-1.627359	5.505004	1.226638
6	1.848061	0.186245	-3.012763
1	1.291785	1.082156	-2.732981
1	1.695978	0.012415	-4.089746
1	2.913195	0.398620	-2.846144
6	-0.507246	2.402859	0.271677
6	0.351072	5.125581	0.431416
6	-3.325916	-1.498363	-0.265326
6	1.149378	6.422475	0.396617
6	0.932574	0.223462	1.463998
1	1.399454	-0.681647	1.862411
1	1.375755	1.076300	1.993811
6	-4.654354	-1.865890	-0.532013
1	-5.438538	-1.108464	-0.499516
6	-2.330964	-2.481435	-0.357803
1	-1.293229	-2.198242	-0.203282

6	-2.936517	-0.096272	0.116538
6	-2.652734	-3.805343	-0.663359
1	-1.857375	-4.553525	-0.714172
6	-4.979712	-3.182565	-0.863088
1	-6.017941	-3.446197	-1.080517
6	-3.980647	-4.161034	-0.918337
1	-4.236255	-5.193234	-1.171153
6	1.719974	-5.679188	0.758473
1	1.508471	-6.732542	0.959258
6	2.937343	-5.303907	0.178432
1	3.677707	-6.064728	-0.081715
6	-1.245904	1.748641	-2.775924
1	-0.566509	2.402355	-2.217753
1	-1.680546	2.347778	-3.590314
1	-0.670127	0.940947	-3.233658
6	4.776462	0.240513	2.125105
1	4.994193	1.044385	1.407514
1	5.608290	0.165251	2.843952
1	3.866253	0.525722	2.674983
6	5.843856	-1.454282	0.614802
1	5.744157	-2.416946	0.091905
1	6.697268	-1.529124	1.307293
1	6.069970	-0.679182	-0.133593
6	0.004165	-1.527374	-2.599085
1	-0.166638	-2.548837	-2.229401
1	-0.141245	-1.533315	-3.691412
1	-0.746640	-0.885301	-2.135066
6	2.391018	-2.178988	-2.676641
1	3.430417	-1.969462	-2.382764
1	2.359193	-2.225110	-3.775796
1	2.107957	-3.168794	-2.301817
6	-3.204403	0.223115	-2.781575
1	-2.680477	-0.728838	-2.932458
1	-3.380800	0.683021	-3.765970
1	-4.189519	0.004268	-2.350468
6	-3.329971	2.391544	-1.572596
1	-4.089576	2.112579	-0.830849
1	-3.848697	2.707554	-2.492006
1	-2.777314	3.256727	-1.190756
6	4.247093	-2.179655	2.443954
1	3.259023	-2.007174	2.898022
1	5.000793	-2.129687	3.245451
1	4.258048	-3.198267	2.039636
6	-5.724238	0.717094	1.785174
1	-6.404240	0.623002	2.646505
1	-6.128570	0.105975	0.966291
1	-5.719747	1.768761	1.459540
6	-4.297866	-1.201216	2.645318
1	-3.265008	-1.556801	2.783499
1	-4.797360	-1.879449	1.944558
1	-4.816250	-1.277424	3.614070
6	3.425142	3.503526	-0.644967
1	4.469455	3.740544	-0.869133
6	2.522138	4.500963	-0.308648
6	2.587554	6.009907	-0.112355
1	2.840089	6.527515	-1.053129
1	3.367528	6.291772	0.614337
1	1.196572	6.890862	1.393910
1	0.684836	7.166258	-0.272174

Table S19

B3LYP-D3/def2-SVP

Prod-Si (with C_2H_4)

1st frequency = 16.3 cm^{-1}

G = -2507.420987 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	1.248099	0.322668	-0.001526
14	-1.127632	0.334463	0.051125
6	0.124079	2.858361	-0.249247
6	-0.707968	-0.388611	1.768163
1	-1.284984	-0.012600	2.624269
1	-0.865896	-1.480857	1.720677
6	1.388281	2.174622	-0.341127
6	2.528296	2.925967	-0.613206
1	3.489061	2.407619	-0.667614
6	0.133007	4.260315	-0.417030
7	2.375018	-0.870317	-0.749974
7	-2.520409	-0.466874	-0.744477
6	3.541639	-0.888780	0.012306
6	5.676521	-2.241596	-0.294850
1	6.169065	-1.364638	-0.718138
6	4.397213	-4.501599	0.738470
1	3.894661	-5.382612	1.145810
6	3.693693	-3.304137	0.594655
1	2.640991	-3.240936	0.879254
6	4.331150	-2.160921	0.088245
6	4.630593	0.425220	1.847310
6	-4.521532	0.015131	2.351586
6	-2.859922	-0.411655	-2.205904
6	2.165560	-1.442215	-2.115491
6	-3.969385	1.117585	3.280169
1	-2.916423	0.924131	3.531832
1	-4.545012	1.168150	4.218265
1	-4.016254	2.096779	2.780724
7	3.712056	0.166560	0.730695
6	-2.277979	3.041260	0.093314
1	-3.239290	2.558847	0.291460
7	-3.729011	0.116099	1.117324
6	-2.235915	4.457325	-0.066015
1	-3.159701	5.037747	0.014621
6	1.886685	-0.256973	-3.063994
1	1.067115	0.374286	-2.696175
1	1.617379	-0.611335	-4.071576
1	2.780252	0.381180	-3.142455
6	-1.146518	2.231094	0.008460
6	-1.024142	5.066558	-0.327855
6	-4.201309	-2.093010	0.053886
6	-0.626506	6.513726	-0.556107
6	0.814526	-0.057284	1.834002
1	1.427094	-0.865079	2.266912
1	0.999862	0.845213	2.436008
6	-5.565953	-2.256705	-0.220158
1	-6.196094	-1.379229	-0.371803

6	-3.396445	-3.234255	0.203350
1	-2.327429	-3.106449	0.386555
6	-3.546984	-0.745289	0.188487
6	-3.951601	-4.511147	0.117598
1	-3.316334	-5.390691	0.250355
6	-6.119995	-3.535984	-0.327692
1	-7.183599	-3.649093	-0.552670
6	-5.316898	-4.666308	-0.150262
1	-5.751461	-5.666155	-0.227800
6	5.741620	-4.574341	0.357346
1	6.292122	-5.512508	0.463217
6	6.376961	-3.443058	-0.165713
1	7.423150	-3.497706	-0.477228
6	-1.725222	0.295348	-2.961276
1	-1.515939	1.295288	-2.552632
1	-2.007670	0.417895	-4.017954
1	-0.804843	-0.297094	-2.933672
6	3.992325	1.581395	2.645809
1	3.776623	2.431992	1.983170
1	4.662952	1.917036	3.452945
1	3.043575	1.259997	3.098370
6	5.985871	0.911643	1.294689
1	6.521002	0.105855	0.774283
1	6.628847	1.268227	2.115350
1	5.835848	1.743602	0.588976
6	0.974002	-2.417492	-2.066625
1	1.217112	-3.273242	-1.417731
1	0.735463	-2.801004	-3.071518
1	0.074676	-1.932961	-1.661893
6	3.383647	-2.188794	-2.684973
1	4.288357	-1.564158	-2.666434
1	3.170134	-2.437254	-3.736167
1	3.598999	-3.125969	-2.158398
6	-3.029249	-1.815164	-2.824941
1	-2.151431	-2.440027	-2.603588
1	-3.126297	-1.729692	-3.919373
1	-3.919491	-2.335593	-2.452219
6	-4.147643	0.413632	-2.395097
1	-5.009908	-0.062950	-1.907375
1	-4.386684	0.515809	-3.465621
1	-4.023977	1.418586	-1.964334
6	4.838606	-0.767886	2.802911
1	3.867037	-1.181749	3.114940
1	5.370184	-0.429623	3.706598
1	5.426355	-1.577607	2.352187
6	-5.999542	0.337288	2.052905
1	-6.557550	0.472978	2.993062
1	-6.482686	-0.471572	1.489940
1	-6.078580	1.267194	1.468155
6	-4.398198	-1.342442	3.071615
1	-3.337805	-1.608159	3.204375
1	-4.889942	-2.155977	2.523130
1	-4.862379	-1.279051	4.068744
6	2.503304	4.339420	-0.799600
1	3.434722	4.872363	-1.012046
6	1.299858	5.008638	-0.692213
6	0.920517	6.473803	-0.810500
1	1.178552	6.872241	-1.806087
1	1.469609	7.090411	-0.079485
1	-0.877729	7.137784	0.317888

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          1       -1.169811    6.948157   -1.411835
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Table S20
B3LYP-D3/def2-SVP
Prod-Ge (with C_2H_4)
1st frequency = 10.2 cm^{-1}
G = -6082.133102 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	1.286257	0.148645	0.090016
32	-1.196671	0.132974	0.109617
6	0.060070	2.722406	-0.343522
6	-0.723417	-0.503424	1.952420
1	-1.273137	0.018970	2.745603
1	-0.982329	-1.573336	2.009616
6	1.345589	2.077067	-0.313581
6	2.484732	2.832352	-0.567159
1	3.455298	2.331567	-0.533973
6	0.052345	4.111181	-0.615958
7	2.613561	-0.997333	-0.699499
7	-2.685898	-0.753789	-0.712663
6	3.757536	-0.868986	0.064950
6	6.076989	-1.803395	-0.401583
1	6.372225	-0.844052	-0.829741
6	5.300185	-4.277385	0.640396
1	4.993753	-5.242918	1.050951
6	4.381909	-3.227863	0.572334
1	3.355859	-3.365730	0.921231
6	4.766417	-1.978700	0.060839
6	4.667076	0.507090	1.954514
6	-4.495801	0.196358	2.372492
6	-2.922655	-0.824284	-2.189345
6	2.429368	-1.610254	-2.044790
6	-3.889968	1.386418	3.145049
1	-2.824192	1.215501	3.352733
1	-4.411090	1.543320	4.103062
1	-3.964007	2.307750	2.547716
7	3.763278	0.155423	0.852340
6	-2.364678	2.883855	-0.163178
1	-3.327872	2.399218	0.016099
7	-3.716569	0.106701	1.128773
6	-2.337541	4.284403	-0.427313
1	-3.274269	4.849056	-0.446596
6	1.963463	-0.489170	-2.999371
1	1.068822	0.020385	-2.619117
1	1.722629	-0.893635	-3.995120
1	2.754812	0.268302	-3.108308
6	-1.216550	2.099129	-0.113110
6	-1.122153	4.897230	-0.656899
6	-4.701628	-1.938321	0.090747
6	-0.738892	6.333961	-0.960817
6	0.802514	-0.268646	1.998895
1	1.382360	-1.129535	2.366352
1	1.066300	0.601295	2.615502
6	-6.044946	-1.788734	-0.278515
1	-6.435087	-0.796229	-0.508652
6	-4.210894	-3.226002	0.363493
1	-3.158213	-3.344777	0.629403

6	-3.744513	-0.782211	0.200364
6	-5.050987	-4.337398	0.288928
1	-4.658095	-5.332489	0.512929
6	-6.883815	-2.903874	-0.371392
1	-7.926707	-2.773722	-0.671479
6	-6.391289	-4.179700	-0.082993
1	-7.048468	-5.050285	-0.151674
6	6.609099	-4.094584	0.180264
1	7.327465	-4.916842	0.228017
6	6.992627	-2.857073	-0.347007
1	8.009815	-2.712126	-0.719648
6	-1.637110	-0.406045	-2.917299
1	-1.310854	0.603642	-2.624132
1	-1.814628	-0.393779	-4.003430
1	-0.822964	-1.113366	-2.721196
6	3.889922	1.522406	2.818632
1	3.507002	2.342842	2.193908
1	4.535406	1.942490	3.606390
1	3.030497	1.037536	3.303387
6	5.921721	1.211902	1.398066
1	6.549473	0.519411	0.821538
1	6.533463	1.614261	2.221556
1	5.633735	2.049402	0.743552
6	1.364685	-2.718482	-1.932869
1	1.735095	-3.530851	-1.288670
1	1.124162	-3.140115	-2.921939
1	0.436190	-2.331596	-1.488540
6	3.703573	-2.215752	-2.658795
1	4.520392	-1.481608	-2.703716
1	3.471857	-2.523678	-3.690290
1	4.061314	-3.100140	-2.118956
6	-3.276810	-2.249436	-2.663532
1	-2.536729	-2.970506	-2.284490
1	-3.266196	-2.287660	-3.764796
1	-4.270482	-2.572708	-2.331179
6	-4.034803	0.167578	-2.585051
1	-4.994762	-0.095305	-2.120328
1	-4.184076	0.167891	-3.676759
1	-3.766120	1.186857	-2.268205
6	5.078275	-0.677908	2.853344
1	4.189124	-1.248654	3.164669
1	5.575225	-0.300352	3.761325
1	5.771380	-1.367810	2.355172
6	-5.983144	0.511200	2.108163
1	-6.475090	0.821605	3.043848
1	-6.524148	-0.361645	1.722575
1	-6.078304	1.334869	1.382869
6	-4.369144	-1.078339	3.229970
1	-3.309443	-1.322474	3.401448
1	-4.848670	-1.941914	2.748458
1	-4.849223	-0.926036	4.210031
6	2.441996	4.229251	-0.848145
1	3.373209	4.771455	-1.036572
6	1.219213	4.869427	-0.866440
6	0.821013	6.313524	-1.110520
1	1.137581	6.649659	-2.112165
1	1.308620	6.990279	-0.389217
1	-1.059962	7.010656	-0.151310
1	-1.232810	6.694194	-1.878679

Table S21
B3LYP-D3/def2-SVP
Prod-C (with Ph_2CO)
1st frequency = 25.8 cm^{-1}
G = -2502.109496 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.567652	0.274829	0.285584
6	-0.993098	1.211070	0.120574
8	-0.355425	2.199185	0.913285
7	-2.500476	-0.588061	-1.040061
6	-0.994451	1.558293	-1.360438
6	1.089094	0.366730	-1.159669
7	-2.372828	0.996918	0.623657
7	0.781227	-1.036526	0.887984
6	0.169314	1.071989	-1.962250
7	3.100552	-1.310153	0.886301
6	0.961827	1.669041	1.050044
6	1.963385	2.549657	0.286472
6	3.339392	2.290258	0.355624
1	3.694382	1.461569	0.961769
6	1.370681	1.699409	2.519850
6	0.429370	1.351272	-3.302011
6	-3.070416	-0.044786	-0.036393
6	1.625325	0.975744	-3.935128
6	2.299591	0.050532	-1.775093
1	3.105145	-0.398103	-1.211327
6	-1.884720	2.281630	-2.140836
1	-2.822357	2.635894	-1.714975
6	2.566595	0.331250	-3.153932
1	3.542354	0.044236	-3.555627
6	2.311687	0.816934	3.063876
1	2.733774	0.035861	2.429468
6	-0.459574	2.081870	-4.111303
6	1.970365	-1.795284	0.560484
6	-4.353415	-0.559110	0.558869
6	-0.039349	-1.681138	1.989252
6	-1.626151	2.544445	-3.523391
1	-2.360127	3.119914	-4.094602
6	-5.572866	-0.443534	-0.125070
1	-5.608914	0.103883	-1.068106
6	4.252785	3.062427	-0.361028
1	5.319677	2.830909	-0.298445
6	2.155682	1.925874	5.218767
1	2.452940	2.007025	6.267607
6	1.781816	-3.119128	-0.153841
6	1.240870	2.831801	4.671739
1	0.824653	3.632160	5.289422
6	2.694717	0.926829	4.404476
1	3.420608	0.218199	4.813828
6	-2.916578	-1.649493	-1.960208
6	-4.326084	-1.253404	1.775947
1	-3.387624	-1.351482	2.317385
6	-1.019817	-2.696224	1.370127
1	-1.662546	-2.191398	0.642552
1	-1.654684	-3.148370	2.148855

1	-0.496932	-3.509111	0.851967
6	0.858477	2.723840	3.332976
1	0.158792	3.444381	2.908786
6	1.404573	-3.117394	-1.504084
1	1.195777	-2.172165	-1.997665
6	-1.603069	-2.238492	-2.502759
1	-0.955029	-1.435299	-2.883033
1	-1.791998	-2.964063	-3.310348
1	-1.068542	-2.754743	-1.697133
6	3.807091	4.125982	-1.153663
1	4.521027	4.734604	-1.714835
6	4.463926	-1.839603	0.687291
6	2.440142	4.404668	-1.213701
1	2.075099	5.234730	-1.824516
6	0.869540	-2.392681	3.015811
1	1.416514	-3.242952	2.601618
1	0.237953	-2.787187	3.826228
1	1.591984	-1.695045	3.456457
6	-0.828506	-0.651611	2.793372
1	-0.174343	0.034094	3.338417
1	-1.444982	-1.180460	3.536428
1	-1.493394	-0.075320	2.156895
6	1.525329	3.623818	-0.499184
1	0.459664	3.838727	-0.564896
6	-3.056305	2.132369	1.424690
6	0.167356	2.195844	-5.493156
6	1.561688	1.468006	-5.372199
6	-6.705104	-1.690150	1.614551
1	-7.618561	-2.127443	2.025400
6	-5.492802	-1.819905	2.297733
1	-5.452377	-2.363235	3.245308
6	-2.717871	3.543257	0.868263
1	-1.650634	3.734146	0.758596
1	-3.125180	4.288332	1.568358
1	-3.208980	3.711300	-0.099680
6	-6.740959	-0.995194	0.400049
1	-7.684456	-0.884019	-0.140417
6	4.821323	-2.655944	1.946173
1	4.643202	-2.061707	2.855715
1	5.884583	-2.942393	1.921047
1	4.222379	-3.573888	2.012013
6	1.313493	-4.308717	-2.228032
1	1.021981	-4.273698	-3.280641
6	4.725365	-2.676538	-0.585443
1	4.275663	-3.674368	-0.548059
1	5.812079	-2.804201	-0.709593
1	4.342049	-2.168451	-1.482237
6	5.389401	-0.604568	0.639326
1	5.168292	0.021919	-0.237396
1	6.444397	-0.913932	0.581083
1	5.258217	0.011435	1.541048
6	2.059110	-4.357203	0.451527
1	2.372579	-4.398455	1.493633
6	-3.750549	-2.819505	-1.387584
1	-3.304067	-3.205715	-0.460246
1	-3.763290	-3.640561	-2.121883
1	-4.791071	-2.550670	-1.174661
6	1.949399	-5.551552	-0.262722
1	2.161897	-6.500233	0.236736
6	-2.663613	2.034010	2.908719

1	-3.030687	1.092292	3.341296
1	-3.123220	2.862116	3.470789
1	-1.581339	2.082461	3.047284
6	1.579077	-5.533038	-1.610877
1	1.498836	-6.466176	-2.174162
6	-3.667294	-0.980227	-3.130783
1	-4.628619	-0.560035	-2.802420
1	-3.871724	-1.717377	-3.924012
1	-3.061362	-0.164484	-3.552933
6	-4.599535	2.103133	1.366150
1	-4.976145	2.088575	0.335122
1	-4.948311	3.039109	1.827286
1	-5.054874	1.282327	1.925973
1	2.394958	2.154688	-5.595635
1	1.645819	0.634697	-6.089511
1	-0.465563	1.724574	-6.263675
1	0.288873	3.249531	-5.794373

Table S22
B3LYP-D3/def2-SVP
Prod-Si (with Ph_2CO)
1st frequency = 12.0 cm^{-1}
G = -3005.023236 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.723005	0.061254	-0.260607
14	-1.524949	-0.507491	-0.286189
8	-0.944337	-1.139034	-1.838047
7	-2.563095	0.729503	0.956414
6	-1.269445	-1.928489	0.935458
6	1.165979	-1.128950	1.150507
7	-3.299438	-0.268003	-0.820430
7	1.513392	1.648021	-0.242389
6	0.061167	-2.004562	1.481681
7	3.677909	0.829446	-0.392796
6	0.485066	-1.056864	-1.897172
6	1.101204	-2.447037	-1.723223
6	2.492489	-2.611388	-1.640660
1	3.133909	-1.735808	-1.706789
6	0.918731	-0.435615	-3.219638
6	0.303192	-3.019067	2.434465
6	-3.619501	0.579694	0.184824
6	1.541570	-3.202471	3.091533
6	2.369924	-1.324842	1.818222
1	3.213061	-0.683037	1.574519
6	-2.214168	-2.861154	1.349852
1	-3.227176	-2.803883	0.937516
6	2.576923	-2.342172	2.793873
1	3.555570	-2.434917	3.273413
6	2.162614	0.200729	-3.366890
1	2.822569	0.307534	-2.502638
6	-0.667847	-3.962714	2.841540
6	2.885694	1.685172	0.130268
6	-4.934697	1.258400	0.365848
6	0.895121	2.901845	-0.826694
6	-1.932722	-3.891143	2.293556
1	-2.717338	-4.599396	2.575115
6	-5.984665	0.639022	1.055509
1	-5.846647	-0.366390	1.458560
6	3.060568	-3.868538	-1.437829
1	4.147926	-3.963012	-1.366260
6	1.703280	0.643755	-5.709699
1	2.005736	1.064023	-6.672608
6	3.214446	2.670017	1.221151
6	0.461785	0.014463	-5.571164
1	-0.210773	-0.064403	-6.430066
6	2.551425	0.729520	-4.601833
1	3.522451	1.225355	-4.691681
6	-2.454558	1.285844	2.319317
6	-5.116480	2.542343	-0.168569
1	-4.294641	3.023797	-0.703507
6	0.558927	3.956204	0.249883
1	-0.050415	3.514237	1.049752
1	-0.020440	4.774954	-0.206468

1	1.450468	4.397909	0.709172
6	0.075186	-0.520848	-4.339541
1	-0.887619	-1.020936	-4.233907
6	2.661110	2.434240	2.489895
1	2.020560	1.562487	2.637758
6	-0.972225	1.219398	2.722880
1	-0.620960	0.181827	2.781211
1	-0.831661	1.684470	3.710309
1	-0.340004	1.751490	2.000753
6	2.244372	-4.998529	-1.311994
1	2.686094	-5.984720	-1.145495
6	5.112532	0.607339	-0.126369
6	0.858307	-4.848051	-1.396080
1	0.205114	-5.719419	-1.295428
6	1.859010	3.500619	-1.867557
1	2.818974	3.789148	-1.418938
1	1.419173	4.407344	-2.311789
1	2.056607	2.778448	-2.670861
6	-0.419364	2.556244	-1.552703
1	-0.287504	1.755365	-2.294370
1	-0.769098	3.449254	-2.092763
1	-1.207886	2.267847	-0.843840
6	0.291806	-3.585243	-1.600393
1	-0.790305	-3.471944	-1.645202
6	-4.009584	-0.566547	-2.095780
6	-0.044295	-4.898272	3.861130
6	1.427553	-4.387785	4.031288
6	-7.386691	2.577593	0.674180
1	-8.343767	3.091297	0.793637
6	-6.339850	3.197958	-0.016249
1	-6.476465	4.197077	-0.437146
6	-3.685902	-2.021957	-2.484778
1	-2.606413	-2.165641	-2.603195
1	-4.187029	-2.273212	-3.432272
1	-4.051994	-2.712855	-1.708482
6	-7.206156	1.298800	1.210768
1	-8.021904	0.809968	1.748915
6	5.903269	1.521309	-1.085244
1	5.556293	1.383104	-2.120874
1	6.977331	1.279730	-1.043418
1	5.782352	2.580790	-0.819658
6	2.935356	3.295787	3.553140
1	2.507785	3.093393	4.538501
6	5.597940	0.819466	1.324963
1	5.622833	1.874017	1.620333
1	6.619823	0.421464	1.424337
1	4.958912	0.284857	2.042927
6	5.395165	-0.857674	-0.518164
1	4.807144	-1.553708	0.097276
1	6.462839	-1.094352	-0.388711
1	5.130111	-1.031396	-1.571035
6	4.030849	3.793332	1.032804
1	4.459258	3.996108	0.050349
6	-2.913886	2.756094	2.382196
1	-2.392652	3.357335	1.621338
1	-2.675876	3.176347	3.371963
1	-3.994889	2.862647	2.226397
6	4.290072	4.667167	2.092319
1	4.919756	5.545442	1.928919
6	-3.503890	0.413076	-3.171382

1	-3.767076	1.448086	-2.898374
1	-3.961108	0.191003	-4.148947
1	-2.413092	0.342372	-3.269200
6	3.746683	4.418890	3.356584
1	3.952969	5.100154	4.185956
6	-3.266220	0.425220	3.308067
1	-4.345788	0.508494	3.120605
1	-3.079470	0.754946	4.342567
1	-2.971055	-0.631432	3.219458
6	-5.542074	-0.458445	-1.986397
1	-5.929946	-1.067228	-1.156771
1	-5.979328	-0.842987	-2.920316
1	-5.897964	0.570644	-1.858503
1	2.161303	-5.169288	3.773124
1	1.640432	-4.094913	5.073044
1	-0.596596	-4.876952	4.815461
1	-0.072514	-5.943198	3.510058

Table S23
B3LYP-D3/def2-SVP
Prod-Ge (with Ph_2CO)
G = -6579.725521 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	0.976343	0.060130	0.054222
32	-1.466557	0.024574	0.539076
8	-0.633692	-0.306787	2.258019
7	-2.800659	-0.272694	-1.194424
6	-1.600354	1.992380	0.419786
6	0.738038	1.919806	-0.633820
7	-3.292419	-0.646718	0.922996
7	1.864550	-1.149208	-1.211944
6	-0.484453	2.584487	-0.262743
7	3.270751	0.206844	-0.150504
6	0.745477	-0.407647	2.140979
6	1.426051	0.627520	3.022212
6	2.561397	0.356261	3.804456
1	2.989489	-0.645731	3.815779
6	1.222132	-1.841767	2.333931
6	-0.632033	3.931409	-0.669689
6	-3.722876	-0.693696	-0.361953
6	0.305807	4.617088	-1.474328
6	1.626868	2.594846	-1.461339
1	2.538860	2.087121	-1.779416
6	-2.708108	2.777509	0.709806
1	-3.567838	2.313599	1.204516
6	1.426314	3.935021	-1.902703
1	2.168928	4.405052	-2.553857
6	2.512939	-2.272095	1.976170
1	3.210390	-1.558231	1.542232
6	-1.759554	4.726179	-0.357104
6	3.149457	-0.707436	-1.076525
6	-5.079876	-1.177049	-0.766055
6	1.387899	-2.401079	-1.875147
6	-2.796907	4.155652	0.353043
1	-3.692421	4.727541	0.613290
6	-6.171708	-0.299621	-0.818185
1	-6.028641	0.750926	-0.557453
6	3.150208	1.351205	4.593398
1	4.034988	1.109415	5.188883
6	2.019498	-4.534738	2.700183
1	2.326657	-5.574706	2.837890
6	4.258746	-1.178644	-1.963240
6	0.734583	-4.120494	3.061529
1	0.028425	-4.836618	3.491187
6	2.909061	-3.598249	2.162339
1	3.919597	-3.904138	1.876306
6	-2.870529	0.032538	-2.633451
6	-5.264670	-2.527231	-1.094674
1	-4.412842	-3.210036	-1.060789
6	1.237248	-2.184787	-3.393427
1	0.588094	-1.323026	-3.603152
1	0.787724	-3.075060	-3.861947
1	2.210899	-2.012101	-3.871063

6	0.344641	-2.789547	2.883401
1	-0.648665	-2.457773	3.180137
6	4.341201	-0.686426	-3.273546
1	3.574415	0.001716	-3.635663
6	-1.523389	0.674706	-3.010817
1	-1.399363	1.647447	-2.518635
1	-1.464589	0.827304	-4.099425
1	-0.680608	0.040911	-2.706920
6	2.613882	2.639199	4.626891
1	3.077563	3.417757	5.238096
6	4.451388	1.014118	0.242364
6	1.463900	2.914832	3.876663
1	1.019129	3.913416	3.900928
6	2.323720	-3.598777	-1.611333
1	3.269157	-3.525070	-2.160500
1	1.827286	-4.524541	-1.941029
1	2.538020	-3.691544	-0.537141
6	0.014206	-2.771322	-1.286163
1	0.080297	-2.937883	-0.200310
1	-0.339831	-3.702298	-1.754827
1	-0.738635	-1.996284	-1.469991
6	0.874788	1.922637	3.094951
1	-0.029978	2.147278	2.530698
6	-3.902663	-1.224682	2.150963
6	-1.556137	6.112221	-0.942257
6	-0.198849	6.026571	-1.721944
6	-7.616691	-2.118628	-1.505268
1	-8.605948	-2.485299	-1.790207
6	-6.529262	-2.996599	-1.460590
1	-6.664996	-4.051522	-1.711513
6	-3.378125	-0.428225	3.361243
1	-2.284755	-0.458179	3.431149
1	-3.809828	-0.838087	4.287514
1	-3.684776	0.627116	3.278906
6	-7.433888	-0.768533	-1.186357
1	-8.280247	-0.078077	-1.221087
6	5.310947	0.210612	1.240358
1	4.729379	-0.038574	2.138416
1	6.179791	0.808833	1.557691
1	5.686351	-0.717913	0.789518
6	5.407742	-1.051395	-4.098466
1	5.468443	-0.654132	-5.114689
6	5.334084	1.474257	-0.938036
1	5.928276	0.661228	-1.372583
1	6.035680	2.244155	-0.580835
1	4.726985	1.922085	-1.739151
6	3.932491	2.270781	0.967312
1	3.411201	2.948812	0.280198
1	4.777685	2.816885	1.413814
1	3.237174	2.004016	1.769763
6	5.250296	-2.051444	-1.493560
1	5.176253	-2.456062	-0.482811
6	-3.065169	-1.248602	-3.468868
1	-2.270864	-1.977960	-3.248693
1	-3.023086	-1.010085	-4.543718
1	-4.036082	-1.721084	-3.266999
6	6.311836	-2.422943	-2.321200
1	7.076603	-3.108326	-1.947640
6	-3.494252	-2.706013	2.255334
1	-3.928311	-3.283734	1.424068

1	-3.848797	-3.147727	3.200574
1	-2.401957	-2.809157	2.209354
6	6.396027	-1.919737	-3.623975
1	7.230183	-2.206101	-4.269298
6	-3.980445	1.055091	-2.953509
1	-4.983235	0.618163	-2.864874
1	-3.866766	1.420965	-3.986597
1	-3.905793	1.917018	-2.272261
6	-5.442043	-1.119471	2.188897
1	-5.774467	-0.091450	1.982457
1	-5.780122	-1.385923	3.201994
1	-5.945009	-1.795830	1.488634
1	0.524209	6.780737	-1.369631
1	-0.338385	6.212404	-2.800171
1	-2.391504	6.400226	-1.601618
1	-1.514311	6.874041	-0.145659

Table S21-S28. Geometrical coordinates of the reactants and products for the reaction of Rea-E (E = Sn and Pb) with C_2H_4 and Ph_2CO at B3LYP-D3/def2-SVP level of theory.

Table S24
B3LYP-D3/def2-SVP
Rea-Sn(Singlet)
E = -2279.60880002 Hartree
G = -2278.834171 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
50	-1.568273	-0.786620	-0.633930
7	-3.223954	-0.839602	0.929488
7	-3.767489	-0.579187	-1.209357
6	-4.783774	-2.208277	-2.776645
1	-3.872085	-2.822706	-2.712166
1	-5.215730	-2.333775	-3.783040
1	-5.511842	-2.590599	-2.046417
6	-0.000032	2.054399	0.000256
6	-5.740793	0.120214	-2.615591
1	-6.559216	-0.277351	-2.002689
1	-6.084225	0.130829	-3.662295
1	-5.549325	1.159687	-2.307453
6	-3.459283	-0.222014	-3.562584
1	-3.200580	0.832392	-3.379472
1	-3.886306	-0.307946	-4.573564
1	-2.528593	-0.813096	-3.541377
6	-4.054980	-1.828080	3.077382
1	-5.129572	-1.754382	2.865324
1	-3.925289	-1.776594	4.170454
1	-3.699887	-2.812609	2.734135
6	-1.138369	4.283265	-0.262393
6	-1.789113	-0.791744	2.865218
1	-1.336031	-1.749225	2.564028
1	-1.727708	-0.713531	3.961557
1	-1.195154	0.030233	2.435398
6	-1.257920	1.424102	-0.328205
6	-3.804187	0.679223	2.808783
1	-3.269389	1.475918	2.269309
1	-3.670879	0.836531	3.891392
1	-4.876927	0.765925	2.590303
6	-6.276231	-2.100508	0.522993
1	-5.677446	-3.004820	0.394380
6	-0.000079	3.482998	0.000432
6	-4.209283	-0.751142	0.039474
6	-5.664633	-0.845697	0.391555
6	-4.455990	-0.726875	-2.501101
6	-3.253070	-0.701366	2.395612
6	-2.363459	2.239996	-0.575687
1	-3.316080	1.765667	-0.826211
6	-8.396501	-1.035587	1.011235
1	-9.459950	-1.109161	1.252206
6	-2.333928	3.661235	-0.541926
1	-3.244614	4.231856	-0.748559
6	-7.636958	-2.195393	0.826831
1	-8.104325	-3.178527	0.924045
6	-0.761897	5.749062	-0.173031
1	-1.356985	6.266720	0.598036
1	-0.965607	6.272510	-1.122274
6	-6.431921	0.313630	0.575482

1	-5.960483	1.292109	0.462441
6	-7.789999	0.218972	0.887977
1	-8.378442	1.128667	1.031295
50	1.568322	-0.786646	0.633629
7	3.224043	-0.839182	-0.929676
7	3.767513	-0.579367	1.209265
6	4.783924	-2.209221	2.775740
1	3.872310	-2.823726	2.710917
1	5.215866	-2.335200	3.782079
1	5.512058	-2.591071	2.045331
6	5.740618	0.119505	2.615991
1	6.559133	-0.277631	2.002936
1	6.083990	0.129640	3.662720
1	5.549001	1.159105	2.308370
6	3.459124	-0.223568	3.562682
1	3.200092	0.830829	3.379976
1	3.886210	-0.309743	4.573614
1	2.528618	-0.814930	3.541281
6	4.054859	-1.826826	-3.078025
1	5.129473	-1.753371	-2.865992
1	3.925119	-1.774870	-4.171070
1	3.699638	-2.811443	-2.735167
6	1.138159	4.283273	0.263458
6	1.789179	-0.790195	-2.865373
1	1.335892	-1.747668	-2.564465
1	1.727801	-0.711666	-3.961691
1	1.195395	0.031791	-2.435333
6	1.257898	1.424112	0.328571
6	3.804496	0.680407	-2.808309
1	3.269778	1.476953	-2.268534
1	3.671259	0.838187	-3.890857
1	4.877239	0.766876	-2.589743
6	6.276066	-2.100367	-0.523926
1	5.677109	-3.004644	-0.395864
6	4.209351	-0.750968	-0.039602
6	5.664698	-0.845526	-0.391698
6	4.455954	-0.727718	2.500979
6	3.253154	-0.700273	-2.395743
6	2.363382	2.240012	0.576276
1	3.316028	1.765677	0.826710
6	8.396524	-1.035530	-1.011526
1	9.459958	-1.109148	-1.252552
6	2.333756	3.661257	0.542861
1	3.244399	4.231891	0.749648
6	7.636773	-2.195313	-0.827834
1	8.103962	-3.178471	-0.925658
6	0.761595	5.749068	0.174441
1	1.356651	6.266943	-0.596505
1	0.965273	6.272306	1.123806
6	6.432197	0.313774	-0.574908
1	5.960927	1.292266	-0.461282
6	7.790255	0.219063	-0.887480
1	8.378861	1.128740	-1.030246

Table S25
B3LYP-D3/def2-SVP
Rea-Sn(Triplet)
E = -2279.52382610 Hartree
G = -2278.748753 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
50	-1.322359	-0.772718	-0.692823
7	-2.959169	-0.789825	0.907913
7	-3.649858	-0.837323	-1.224291
6	-4.618433	-2.762159	-2.420761
1	-3.655593	-3.287102	-2.319519
1	-5.096989	-3.090894	-3.357857
1	-5.267392	-3.063228	-1.585300
6	-0.000020	2.056869	-0.000043
6	-5.753341	-0.513586	-2.588607
1	-6.503979	-0.858234	-1.866736
1	-6.147879	-0.705302	-3.599211
1	-5.632275	0.573764	-2.467841
6	-3.511710	-0.857729	-3.626165
1	-3.331495	0.228276	-3.650471
1	-3.995427	-1.151686	-4.570589
1	-2.534640	-1.361596	-3.565649
6	-3.957580	-1.146505	3.199712
1	-5.000978	-0.879227	2.995038
1	-3.764284	-0.930363	4.262371
1	-3.838880	-2.229803	3.041925
6	-1.017608	4.271571	-0.583333
6	-1.548998	-0.623477	2.873534
1	-1.266806	-1.679962	2.746733
1	-1.501907	-0.378699	3.945514
1	-0.803437	0.009513	2.367821
6	-1.100819	1.422765	-0.680419
6	-3.242360	1.155645	2.429737
1	-2.549365	1.719993	1.788190
1	-3.117088	1.498852	3.469638
1	-4.270307	1.390958	2.121790
6	-6.080359	-1.981579	0.830832
1	-5.523551	-2.921032	0.826806
6	-0.000034	3.479586	-0.000070
6	-3.990076	-0.809848	0.055296
6	-5.425839	-0.789441	0.488059
6	-4.398308	-1.235972	-2.422594
6	-2.960680	-0.357690	2.324291
6	-2.096668	2.218760	-1.244107
1	-2.942050	1.733061	-1.739686
6	-8.134550	-0.757763	1.224169
1	-9.188809	-0.745441	1.511736
6	-2.078073	3.641307	-1.200046
1	-2.891639	4.209159	-1.661427
6	-7.429121	-1.965625	1.193447
1	-7.930535	-2.899787	1.459001
6	-0.684660	5.737789	-0.379484
1	-1.471325	6.247079	0.202451
1	-0.619289	6.271388	-1.342384
6	-6.138906	0.417782	0.512620

1	-5.636353	1.342983	0.223233
6	-7.484842	0.433961	0.885047
1	-8.030877	1.380506	0.903863
50	1.322373	-0.772665	0.692849
7	2.959178	-0.789788	-0.907896
7	3.649873	-0.837188	1.224309
6	4.618492	-2.761953	2.420837
1	3.655655	-3.286916	2.319657
1	5.097093	-3.090643	3.357926
1	5.267419	-3.063044	1.585359
6	5.753371	-0.513360	2.588560
1	6.503979	-0.857998	1.866651
1	6.147963	-0.705063	3.599146
1	5.632280	0.573987	2.467792
6	3.511765	-0.857488	3.626192
1	3.331537	0.228515	3.650457
1	3.995504	-1.151400	4.570619
1	2.534699	-1.361369	3.565717
6	3.957541	-1.146557	-3.199714
1	5.000941	-0.879226	-2.995124
1	3.764174	-0.930499	-4.262377
1	3.838890	-2.229848	-3.041842
6	1.017524	4.271614	0.583161
6	1.548970	-0.623542	-2.873488
1	1.266796	-1.680027	-2.746638
1	1.501846	-0.378808	-3.945477
1	0.803413	0.009456	-2.367780
6	1.100792	1.422813	0.680356
6	3.242315	1.155621	-2.429820
1	2.549332	1.719988	-1.788277
1	3.117004	1.498779	-3.469733
1	4.270268	1.390967	-2.121918
6	6.080352	-1.981644	-0.830683
1	5.523515	-2.921080	-0.826606
6	3.990088	-0.809795	-0.055279
6	5.425859	-0.789461	-0.488019
6	4.398343	-1.235771	2.422618
6	2.960663	-0.357713	-2.324294
6	2.096625	2.218849	1.244013
1	2.942017	1.733185	1.739611
6	8.134595	-0.757922	-1.224040
1	9.188864	-0.745654	-1.511574
6	2.078002	3.641394	1.199898
1	2.891557	4.209280	1.661257
6	7.429126	-1.965759	-1.193259
1	7.930518	-2.899955	-1.458732
6	0.684547	5.737817	0.379257
1	1.471201	6.247100	-0.202698
1	0.619165	6.271452	1.342137
6	6.138970	0.417735	-0.512624
1	5.636441	1.342970	-0.223305
6	7.484919	0.433845	-0.885010
1	8.030986	1.380370	-0.903867

Table S26
B3LYP-D3/def2-SVP
Rea-Pb(Singlet)
E = -2236.72748575 Hartree
G = -2235.957274 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
82	-1.615263	-0.877766	-0.671875
7	-3.349850	-0.799747	0.974931
7	-3.922806	-0.555600	-1.174255
6	-5.166513	-2.110748	-2.642013
1	-4.319954	-2.813476	-2.587717
1	-5.649389	-2.224518	-3.626553
1	-5.899070	-2.392505	-1.871723
6	0.000013	2.059296	-0.000137
6	-5.874591	0.307770	-2.534619
1	-6.707961	0.016370	-1.883687
1	-6.250571	0.319825	-3.570101
1	-5.568860	1.331231	-2.268841
6	-3.680967	-0.299837	-3.548111
1	-3.301184	0.724641	-3.410412
1	-4.157697	-0.365479	-4.538233
1	-2.820800	-0.990587	-3.548758
6	-4.274708	-1.615117	3.155832
1	-5.331246	-1.393954	2.956541
1	-4.120815	-1.560067	4.245647
1	-4.068412	-2.646815	2.829522
6	-1.127532	4.289888	-0.306844
6	-1.889424	-0.918920	2.881889
1	-1.581732	-1.932250	2.577277
1	-1.794330	-0.846883	3.976169
1	-1.196246	-0.186191	2.437832
6	-1.246262	1.433582	-0.372668
6	-3.673409	0.825005	2.836520
1	-3.052521	1.530333	2.263490
1	-3.483633	0.980672	3.910968
1	-4.730387	1.056265	2.649587
6	-6.591093	-1.588158	0.663653
1	-6.164784	-2.587541	0.551767
6	0.000026	3.489377	-0.000249
6	-4.329453	-0.618803	0.096679
6	-5.772188	-0.464562	0.484961
6	-4.678364	-0.663285	-2.430129
6	-3.335604	-0.626223	2.435608
6	-2.341723	2.246554	-0.664100
1	-3.287140	1.773150	-0.943406
6	-8.481408	-0.154473	1.155341
1	-9.535997	-0.033745	1.415545
6	-2.311586	3.668651	-0.632378
1	-3.213203	4.239912	-0.874806
6	-7.940705	-1.433911	0.993367
1	-8.570971	-2.316579	1.128271
6	-0.754716	5.755787	-0.202579
1	-1.378094	6.272980	0.546182
1	-0.922712	6.280066	-1.158347
6	-6.320714	0.816163	0.647625

1	-5.686679	1.692466	0.496777
6	-7.667040	0.970327	0.984850
1	-8.083912	1.972867	1.109705
82	1.615255	-0.877698	0.672033
7	3.349838	-0.799985	-0.974836
7	3.922800	-0.555489	1.174307
6	5.166625	-2.110175	2.642449
1	4.320124	-2.812985	2.588310
1	5.649493	-2.223669	3.627025
1	5.899218	-2.392059	1.872240
6	5.874511	0.308375	2.534458
1	6.707895	0.016891	1.883581
1	6.250505	0.320703	3.569931
1	5.568692	1.331749	2.268446
6	3.680935	-0.299162	3.548102
1	3.301088	0.725261	3.410172
1	4.157666	-0.364549	4.538240
1	2.820813	-0.989968	3.548903
6	4.274835	-1.615631	-3.155586
1	5.331342	-1.394298	-2.956323
1	4.120947	-1.560783	-4.245412
1	4.068674	-2.647303	-2.829110
6	1.127598	4.289916	0.306220
6	1.889454	-0.919719	-2.881782
1	1.581932	-1.933064	-2.577052
1	1.794345	-0.847818	-3.976069
1	1.196161	-0.187056	-2.437799
6	1.246280	1.433627	0.372495
6	3.673201	0.824462	-2.836711
1	3.052223	1.529810	-2.263802
1	3.483399	0.979919	-3.911186
1	4.730150	1.055898	-2.649822
6	6.591125	-1.588278	-0.663290
1	6.164849	-2.587647	-0.551143
6	4.329440	-0.618881	-0.096617
6	5.772169	-0.464662	-0.484922
6	4.678362	-0.662803	2.430210
6	3.335589	-0.626741	-2.435541
6	2.341757	2.246622	0.663801
1	3.287165	1.773243	0.943181
6	8.481389	-0.154649	-1.155336
1	9.535978	-0.033951	-1.415551
6	2.311644	3.668715	0.631853
1	3.213267	4.240004	0.874189
6	7.940733	-1.434067	-0.993024
1	8.571039	-2.316744	-1.127681
6	0.754809	5.755805	0.201721
1	1.378198	6.272867	-0.547122
1	0.922813	6.280233	1.157406
6	6.320644	0.816036	-0.647929
1	5.686571	1.692354	-0.497335
6	7.666974	0.970163	-0.985169
1	8.083805	1.972686	-1.110286

Table S27
B3LYP-D3/def2-SVP
Rea-Pb(Triplet)
E = -2236.64026086 Hartree
G = -2235.877014 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
82	-1.671893	-0.751409	-0.795894
7	-3.483596	-1.117131	0.745197
7	-4.001028	-0.150082	-1.203824
6	-5.738945	-0.444569	-2.975830
1	-5.264264	-1.402489	-3.241635
1	-6.140610	0.009160	-3.896590
1	-6.585864	-0.651036	-2.308166
6	-0.000234	1.982310	-0.002119
6	-5.392189	1.814950	-1.891629
1	-6.250546	1.633941	-1.232173
1	-5.761626	2.355525	-2.778059
1	-4.673149	2.461361	-1.365336
6	-3.628581	0.841204	-3.359443
1	-2.875576	1.519584	-2.926870
1	-4.072415	1.338329	-4.235936
1	-3.119027	-0.071145	-3.710167
6	-4.331521	-3.034591	2.100464
1	-5.398349	-2.885577	1.886996
1	-4.251628	-3.522697	3.085583
1	-3.917217	-3.717606	1.341963
6	-1.134585	4.204230	0.268492
6	-2.104528	-1.978972	2.518898
1	-1.615103	-2.674489	1.817917
1	-2.070214	-2.432776	3.521442
1	-1.521753	-1.044668	2.545072
6	-1.278012	1.357410	0.143886
6	-4.167955	-0.727498	3.127899
1	-3.671607	0.253529	3.064200
1	-4.026420	-1.120902	4.147459
1	-5.244872	-0.584394	2.975011
6	-6.730919	-1.674397	0.059123
1	-6.319812	-2.541383	-0.462505
6	0.000030	3.419060	-0.002994
6	-4.441015	-0.619746	-0.040745
6	-5.892286	-0.590074	0.356437
6	-4.710252	0.496900	-2.315610
6	-3.559352	-1.698804	2.093501
6	-2.407299	2.175012	0.537881
1	-3.344508	1.669584	0.779940
6	-8.608359	-0.537063	1.084952
1	-9.663680	-0.516394	1.368229
6	-2.360374	3.556690	0.577666
1	-3.249994	4.135602	0.844115
6	-8.080595	-1.648822	0.420916
1	-8.722299	-2.500783	0.182307
6	-0.749086	5.664440	0.223236
1	-0.868669	6.142233	1.213170
1	-1.393311	6.236874	-0.466934
6	-6.430103	0.521490	1.022187

1	-5.783621	1.368776	1.259663
6	-7.778830	0.548528	1.384626
1	-8.183216	1.421083	1.903777
82	1.672319	-0.748436	0.799628
7	3.482575	-1.119515	-0.742313
7	4.002091	-0.146291	1.203097
6	5.741830	-0.435697	2.974132
1	5.267372	-1.392915	3.242848
1	6.144194	0.020504	3.893363
1	6.588245	-0.643946	2.306380
6	5.394233	1.820617	1.883538
1	6.251803	1.637488	1.223658
1	5.764764	2.363729	2.767953
1	4.674719	2.465599	1.356147
6	3.632052	0.851546	3.356112
1	2.878506	1.528450	2.922162
1	4.076820	1.351588	4.230478
1	3.122950	-0.059675	3.710397
6	4.326562	-3.043133	-2.090922
1	5.393637	-2.895376	-1.877790
1	4.245885	-3.534498	-3.074355
1	3.910821	-3.722679	-1.330099
6	1.134966	4.203617	-0.275463
6	2.101642	-1.984509	-2.512999
1	1.610879	-2.676532	-1.809504
1	2.066328	-2.441822	-3.513913
1	1.520764	-1.049125	-2.542379
6	1.277691	1.357030	-0.147092
6	4.167553	-0.739443	-3.126594
1	3.673671	0.243024	-3.065925
1	4.024470	-1.135891	-4.144755
1	5.244900	-0.598457	-2.974805
6	6.730385	-1.675383	-0.058199
1	6.319640	-2.540795	0.466316
6	4.440837	-0.619812	0.041108
6	5.891731	-0.591652	-0.357585
6	4.712572	0.503953	2.312177
6	3.557046	-1.705802	-2.088686
6	2.406937	2.173759	-0.543533
1	3.343667	1.667616	-0.785981
6	8.607032	-0.541380	-1.089180
1	9.662050	-0.521782	-1.373657
6	2.360450	3.555336	-0.584689
1	3.250035	4.133702	-0.852439
6	8.079682	-1.651165	-0.421526
1	8.721419	-2.502636	-0.181260
6	0.749910	5.663966	-0.231740
1	0.869666	6.140687	-1.222179
1	1.394305	6.236947	0.457826
6	6.429145	0.517943	-1.026944
1	5.782606	1.364697	-1.266145
6	7.777477	0.543627	-1.390909
1	8.181533	1.414641	-1.912897

Table S28
B3LYP-D3/def2-SVP
Prod-Sn (with C_2H_4)
G = -2357.328199 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
50	1.595745	-0.844433	1.119173
50	-1.852803	-0.120309	1.359037
6	0.274383	1.670297	-0.392102
6	-1.316482	4.576834	1.213315
1	-1.484630	4.031234	0.280684
1	-2.106882	5.263784	1.534111
6	1.423440	1.277966	0.384937
6	2.559643	2.085046	0.343083
1	3.438424	1.785543	0.919975
6	0.462590	2.779724	-1.265810
7	2.989027	-1.202698	-0.658270
7	-3.101307	-1.534345	0.059779
6	4.089187	-0.958156	0.042528
6	6.025350	0.246569	-0.999462
1	5.440251	1.166165	-0.929155
6	7.519761	-2.111700	-1.139620
1	8.100986	-3.035628	-1.194134
6	6.224800	-2.135872	-0.614556
1	5.788869	-3.076604	-0.271312
6	5.471233	-0.956657	-0.538792
6	4.731593	-0.627737	2.492971
6	-4.993788	1.323396	1.320608
6	-2.795106	-2.704318	-0.776959
6	2.769265	-1.275311	-2.112987
6	-4.168900	2.572815	1.680666
1	-3.387931	2.337391	2.421700
1	-4.810533	3.357170	2.110967
1	-3.670727	2.975741	0.787440
7	3.838652	-0.666338	1.325107
6	-1.960609	1.517773	-1.339921
1	-2.959493	1.074150	-1.353344
7	-4.026804	0.342899	0.806638
6	-1.712676	2.575092	-2.261199
1	-2.490998	2.874141	-2.969841
6	1.293507	-1.676290	-2.295636
1	1.092452	-2.651998	-1.827198
1	1.037767	-1.749213	-3.363642
1	0.623430	-0.926084	-1.846308
6	-1.035729	1.061277	-0.400286
6	-0.502823	3.231033	-2.197413
6	-5.525060	-1.210108	-0.443637
6	0.055515	4.414661	-2.962849
6	-0.202868	4.402790	1.927079
1	-0.031447	4.943585	2.864246
1	0.579585	3.710544	1.603032
6	-5.855610	-0.846473	-1.756493
1	-5.152256	-0.250552	-2.342015
6	-6.436767	-1.959605	0.312495
1	-6.174755	-2.257363	1.330072
6	-4.208861	-0.798969	0.144740

6	-7.664122	-2.338517	-0.236443
1	-8.368568	-2.923716	0.360065
6	-7.081227	-1.228781	-2.306852
1	-7.330497	-0.939731	-3.330920
6	-7.988828	-1.974947	-1.547687
1	-8.948554	-2.272655	-1.977424
6	8.068295	-0.909611	-1.598331
1	9.080548	-0.891176	-2.009951
6	7.317197	0.268805	-1.529552
1	7.741387	1.210649	-1.886487
6	-1.520243	-3.330135	-0.184563
1	-0.695699	-2.602631	-0.169675
1	-1.192007	-4.193445	-0.783588
1	-1.695645	-3.667393	0.848877
6	3.898121	-0.021060	3.637921
1	3.573462	1.000545	3.384810
1	4.483076	0.022230	4.569284
1	3.000270	-0.629987	3.836688
6	5.981604	0.255335	2.293399
1	6.704748	-0.194830	1.601987
1	6.489777	0.398087	3.260355
1	5.702446	1.246247	1.903799
6	3.650710	-2.341826	-2.793407
1	4.709451	-2.053360	-2.811945
1	3.325462	-2.484499	-3.836315
1	3.562483	-3.306755	-2.269757
6	2.988726	0.099179	-2.777397
1	2.377667	0.869336	-2.286374
1	2.709059	0.055828	-3.842449
1	4.042335	0.404212	-2.719407
6	-3.893358	-3.788529	-0.780916
1	-4.198903	-4.036916	0.247074
1	-3.501696	-4.703158	-1.253791
1	-4.785547	-3.483292	-1.341330
6	-2.506806	-2.242818	-2.220708
1	-3.416033	-1.835927	-2.686982
1	-2.154058	-3.083530	-2.840213
1	-1.738448	-1.456244	-2.222919
6	5.161773	-2.056556	2.881990
1	4.277645	-2.695132	3.035486
1	5.752476	-2.051482	3.812617
1	5.780062	-2.506194	2.091311
6	-6.062903	1.745210	0.290414
1	-6.606370	2.626216	0.667043
1	-6.801181	0.956132	0.100787
1	-5.592313	2.016636	-0.666964
6	-5.678946	0.781794	2.591366
1	-4.924449	0.490040	3.338764
1	-6.295294	-0.099159	2.359560
1	-6.334498	1.545797	3.040612
6	2.674160	3.255834	-0.458261
1	3.590459	3.853219	-0.425609
6	1.629416	3.580147	-1.295830
6	1.435885	4.708583	-2.289240
1	2.256965	4.759890	-3.022718
1	1.422379	5.678950	-1.764534
1	-0.620546	5.284025	-2.920911
1	0.175271	4.164592	-4.031030

Table S29

B3LYP-D3/def2-SVP

Prod-Sn (with Ph_2CO)

G = -2854.920458 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
50	-1.652608	0.111032	-0.560248
50	1.835467	0.355079	-1.082194
8	0.824190	3.173197	-0.013350
7	3.421983	-1.321439	-1.057580
6	1.627125	-0.086542	1.128815
6	-0.691652	-1.233397	0.985420
7	4.048638	0.804867	-0.851017
7	-2.975564	-1.538194	-1.400131
6	0.561191	-0.917364	1.631018
7	-3.757299	-0.294881	0.260240
6	-0.299137	3.583273	0.251538
6	-0.805299	3.516695	1.660933
6	-1.755065	4.413254	2.183443
1	-2.161264	5.208445	1.555940
6	-1.163023	4.132307	-0.845352
6	0.776829	-1.511590	2.908909
6	4.431863	-0.479263	-0.896198
6	-0.091241	-2.459193	3.502402
6	-1.514192	-2.188966	1.581195
1	-2.458090	-2.449098	1.093926
6	2.703866	0.185211	1.971948
1	3.516334	0.813284	1.598094
6	-1.228028	-2.831550	2.818561
1	-1.922147	-3.575948	3.220968
6	-2.565205	4.032806	-0.832501
1	-3.070605	3.573747	0.017416
6	1.889139	-1.231902	3.738939
6	-4.035857	-1.222089	-0.650607
6	5.858057	-0.909416	-0.715443
6	-2.856615	-2.426099	-2.566699
6	2.843422	-0.347672	3.284818
1	3.714929	-0.081855	3.891370
6	6.363866	-1.085591	0.580837
1	5.710503	-0.904698	1.437225
6	-2.164416	4.305906	3.514588
1	-2.896759	5.011099	3.915629
6	-2.674001	5.031074	-3.035412
1	-3.261854	5.381719	-3.887758
6	-5.394277	-1.839741	-0.808818
6	-1.277294	5.127916	-3.059869
1	-0.773580	5.554044	-3.931138
6	-3.315260	4.475387	-1.923928
1	-4.403608	4.376425	-1.908817
6	3.352717	-2.782299	-0.894354
6	6.698043	-1.127554	-1.815778
1	6.302301	-1.009452	-2.826770
6	-3.145644	-3.897342	-2.202656
1	-2.553859	-4.192687	-1.322299
1	-2.871587	-4.557095	-3.041576
1	-4.207909	-4.064395	-1.983065

6	-0.527068	4.669774	-1.977552
1	0.563695	4.712265	-1.990774
6	-5.692548	-3.061836	-0.188700
1	-4.920345	-3.569163	0.393285
6	1.922220	-3.181038	-1.302981
1	1.178513	-2.700816	-0.647392
1	1.781992	-4.269917	-1.221848
1	1.720367	-2.883254	-2.343767
6	-1.640547	3.298252	4.331768
1	-1.976248	3.207145	5.368168
6	-4.577982	0.331996	1.303730
6	-0.684071	2.412157	3.822905
1	-0.268248	1.621131	4.451554
6	-3.762718	-1.975159	-3.729715
1	-4.826443	-2.090715	-3.480683
1	-3.561425	-2.576225	-4.631445
1	-3.573915	-0.917228	-3.971674
6	-1.387174	-2.330495	-3.017335
1	-1.129218	-1.299099	-3.308703
1	-1.199124	-2.981356	-3.884885
1	-0.715123	-2.639489	-2.203682
6	-0.256823	2.531613	2.501828
1	0.492866	1.852323	2.097177
6	4.847336	2.034248	-1.000291
6	1.764893	-2.022120	5.027789
6	0.476252	-2.889359	4.841665
6	8.528701	-1.682071	-0.328762
1	9.568962	-1.981644	-0.178223
6	8.028910	-1.508618	-1.623405
1	8.676539	-1.674743	-2.488026
6	3.891415	3.205073	-0.710349
1	3.038936	3.208458	-1.406286
1	4.417659	4.166904	-0.812943
1	3.477003	3.139464	0.306297
6	7.691881	-1.472990	0.772810
1	8.076861	-1.607546	1.786834
6	-5.460401	1.441068	0.694705
1	-4.842550	2.134870	0.103868
1	-5.973670	2.014727	1.483731
1	-6.226898	1.015393	0.031076
6	-6.968107	-3.618918	-0.300534
1	-7.190193	-4.569293	0.191231
6	-5.456503	-0.666526	2.084824
1	-6.301144	-1.037986	1.491192
1	-5.869482	-0.172589	2.978653
1	-4.856222	-1.527899	2.415818
6	-3.582567	0.963505	2.295023
1	-2.935932	0.192317	2.739447
1	-4.110047	1.490692	3.103971
1	-2.932656	1.697414	1.794777
6	-6.391420	-1.185959	-1.546421
1	-6.160835	-0.238708	-2.038756
6	4.344251	-3.530076	-1.808931
1	4.256504	-3.170984	-2.846571
1	4.123361	-4.609539	-1.797640
1	5.384717	-3.400688	-1.484680
6	-7.667667	-1.744574	-1.661264
1	-8.436312	-1.227568	-2.241261
6	5.369877	2.162933	-2.445560
1	6.085649	1.362271	-2.681023

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          1        5.883346    3.127474   -2.591853
          1        4.534428    2.103015   -3.160711
          6       -7.959479   -2.961064   -1.036500
          1       -8.958020   -3.396689   -1.123478
          6        3.572603   -3.196334    0.576096
          1        4.601907   -2.988887    0.898788
          1        3.394290   -4.277300    0.697482
          1        2.884372   -2.652741    1.238548
          6        6.027741    2.129663   -0.009497
          1        5.688700    1.931642    1.018966
          1        6.451199    3.146205   -0.039641
          1        6.836035    1.427444   -0.247564
          1       -0.247819   -2.735818    5.659066
          1        0.713306   -3.966935    4.838162
          1        2.657525   -2.642461    5.211838
          1        1.674030   -1.347381    5.896203
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Table S30
B3LYP-D3/def2-SVP
Prod-Pb (with C_2H_4)
1st frequency = 5.8 cm^{-1}
G = -2314.453718 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
82	-1.651210	-0.865103	-1.082610
82	1.904886	-0.034256	-1.322894
6	-0.318054	1.768062	0.471822
6	1.392914	4.309000	-1.421250
1	1.489037	3.918779	-0.403941
1	2.238965	4.884452	-1.811604
6	-1.456770	1.354096	-0.306516
6	-2.607529	2.138887	-0.274473
1	-3.480097	1.818277	-0.849461
6	-0.520062	2.894878	1.321283
7	-3.063191	-1.185791	0.827769
7	3.174731	-1.510210	0.099728
6	-4.182157	-0.891411	0.178607
6	-5.975516	0.473101	1.283523
1	-5.342033	1.350642	1.136170
6	-7.594460	-1.780306	1.621741
1	-8.224415	-2.663740	1.753081
6	-6.337291	-1.906282	1.023671
1	-5.979551	-2.885987	0.699417
6	-5.521525	-0.780636	0.847389
6	-4.993779	-0.598297	-2.222200
6	5.190094	1.301093	-1.093482
6	2.808479	-2.638926	0.967629
6	-2.772845	-1.221711	2.271497
6	4.432408	2.560930	-1.552315
1	3.701282	2.323156	-2.342428
1	5.125190	3.314331	-1.958215
1	3.881747	3.004677	-0.710318
7	-4.015785	-0.648299	-1.126430
6	1.924308	1.669683	1.418281
1	2.930796	1.242408	1.432959
7	4.159654	0.374896	-0.602820
6	1.664529	2.749693	2.310862
1	2.441196	3.080718	3.007147
6	-1.289647	-1.621413	2.387097
1	-1.110409	-2.599652	1.914230
1	-0.980294	-1.690152	3.441135
1	-0.644098	-0.870122	1.904174
6	0.998257	1.177912	0.499536
6	0.443668	3.383618	2.236376
6	5.534950	-1.147110	0.802351
6	-0.128206	4.577511	2.976224
6	0.298056	4.087605	-2.151426
1	0.201259	4.475152	-3.171605
1	-0.543665	3.511439	-1.756243
6	5.762666	-0.699801	2.111498
1	5.021581	-0.061053	2.596715
6	6.497346	-1.949494	0.174379
1	6.315340	-2.312842	-0.839343

6	4.273598	-0.761440	0.085968
6	7.673034	-2.296852	0.844446
1	8.417856	-2.922472	0.346014
6	6.934939	-1.052195	2.784201
1	7.103002	-0.698380	3.804518
6	7.894049	-1.850357	2.151633
1	8.812776	-2.123928	2.676530
6	-8.042190	-0.528517	2.055533
1	-9.024295	-0.430102	2.524906
6	-7.228185	0.597242	1.887965
1	-7.573182	1.577805	2.225624
6	1.549717	-3.261768	0.336482
1	0.737388	-2.521876	0.277587
1	1.181483	-4.106694	0.938272
1	1.763398	-3.623176	-0.681719
6	-4.221862	-0.068792	-3.446823
1	-3.823242	0.938852	-3.248642
1	-4.873821	-0.014583	-4.332154
1	-3.377778	-0.733375	-3.697447
6	-6.185164	0.351807	-1.970158
1	-6.884213	-0.042618	-1.222568
1	-6.747086	0.495140	-2.906911
1	-5.833882	1.336738	-1.626945
6	-3.619534	-2.275359	3.013922
1	-4.678327	-1.990559	3.065027
1	-3.254493	-2.391555	4.047061
1	-3.546475	-3.252145	2.509961
6	-2.950416	0.164003	2.925850
1	-2.382763	0.927014	2.374872
1	-2.587598	0.142034	3.966237
1	-4.006455	0.463914	2.947235
6	3.880803	-3.745534	1.061739
1	4.227742	-4.037178	0.058321
1	3.449917	-4.634729	1.549162
1	4.752573	-3.435971	1.650932
6	2.458380	-2.123858	2.379184
1	3.354467	-1.735491	2.884111
1	2.041280	-2.932020	3.002197
1	1.720437	-1.311174	2.316195
6	-5.518564	-2.014730	-2.533431
1	-4.679237	-2.699806	-2.732255
1	-6.178562	-2.007620	-3.416480
1	-6.093785	-2.411859	-1.684504
6	6.216122	1.737308	-0.024871
1	6.806304	2.585006	-0.407831
1	6.918276	0.936421	0.236887
1	5.704451	2.062696	0.893596
6	5.927943	0.683315	-2.298577
1	5.207270	0.380001	-3.074587
1	6.499491	-0.205242	-1.992277
1	6.633277	1.404299	-2.743811
6	-2.743806	3.315772	0.515940
1	-3.672930	3.893205	0.480318
6	-1.702533	3.672631	1.344578
6	-1.535119	4.810197	2.333176
1	-2.339196	4.816246	3.087400
1	-1.584494	5.784176	1.817607
1	0.521275	5.463001	2.879764
1	-0.208252	4.367482	4.056376

Table S31

B3LYP-D3/def2-SVP

Prod-Pb (with Ph_2CO)

G = -2812.043821 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
82	1.695178	0.266284	0.445780
82	-1.819932	0.513200	0.967983
8	-0.821581	3.276424	-0.214129
7	-3.431438	-1.283165	1.127300
6	-1.624966	-0.210506	-1.283468
6	0.753798	-1.225702	-1.132023
7	-4.155748	0.788191	0.673134
7	3.010140	-1.445755	1.466196
6	-0.538565	-1.036330	-1.744896
7	3.918814	-0.309577	-0.230665
6	0.305552	3.658374	-0.507833
6	0.850368	3.411856	-1.880883
6	1.820952	4.232012	-2.485394
1	2.204194	5.107150	-1.957814
6	1.149684	4.333670	0.533046
6	-0.767976	-1.751345	-2.958670
6	-4.463135	-0.505128	0.835719
6	0.144642	-2.675092	-3.523158
6	1.631566	-2.142512	-1.707439
1	2.618770	-2.284714	-1.259754
6	-2.750458	-0.080102	-2.093808
1	-3.578263	0.542970	-1.745459
6	1.344705	-2.892668	-2.883561
1	2.083047	-3.600455	-3.273321
6	2.550684	4.214486	0.570221
1	3.072892	3.652251	-0.204701
6	-1.932564	-1.619406	-3.753535
6	4.082448	-1.244082	0.704158
6	-5.859524	-1.020993	0.635339
6	2.684489	-2.524913	2.406919
6	-2.919258	-0.752808	-3.337749
1	-3.831329	-0.597520	-3.922857
6	-6.300428	-1.335101	-0.658837
1	-5.617780	-1.203681	-1.501325
6	2.280341	3.942666	-3.771934
1	3.028309	4.588167	-4.238951
6	2.619840	5.476243	2.635676
1	3.191801	5.921487	3.453892
6	5.363366	-2.006424	0.877639
6	1.224886	5.597044	2.608534
1	0.706985	6.137790	3.404626
6	3.279601	4.777228	1.620190
1	4.365991	4.661635	1.647311
6	-3.293155	-2.747320	1.089687
6	-6.738169	-1.176373	1.715878
1	-6.392418	-0.948800	2.726664
6	2.270235	-3.791267	1.628584
1	1.460408	-3.558074	0.921379
1	1.923701	-4.579971	2.316420
1	3.120428	-4.190297	1.056481

6	0.494491	5.017831	1.571758
1	-0.595292	5.079346	1.548315
6	5.572559	-3.206866	0.184451
1	4.800596	-3.576928	-0.493737
6	-1.853199	-3.039613	1.556539
1	-1.119766	-2.585368	0.870283
1	-1.656170	-4.122689	1.577161
1	-1.685681	-2.642096	2.570076
6	1.790731	2.825655	-4.458626
1	2.170305	2.590066	-5.456288
6	4.877173	0.357421	-1.117151
6	0.813926	2.014648	-3.870013
1	0.424855	1.138482	-4.394042
6	3.813820	-2.863691	3.402754
1	4.651424	-3.386150	2.924066
1	3.421622	-3.520174	4.195866
1	4.202901	-1.947939	3.874110
6	1.472938	-2.023506	3.216876
1	1.732301	-1.114203	3.781839
1	1.128907	-2.789630	3.928655
1	0.627017	-1.792378	2.550447
6	0.331473	2.319161	-2.598457
1	-0.442936	1.703162	-2.140675
6	-5.013537	1.982115	0.665755
6	-1.814688	-2.515279	-4.971947
6	-0.448559	-3.255970	-4.792733
6	-8.477769	-1.942640	0.213489
1	-9.497552	-2.299953	0.049184
6	-8.043199	-1.631027	1.505738
1	-8.721650	-1.746280	2.354943
6	-4.105634	3.153089	0.242439
1	-3.259607	3.277335	0.936326
1	-4.669610	4.098828	0.228036
1	-3.684494	2.983534	-0.760221
6	-7.601642	-1.797171	-0.867773
1	-7.935450	-2.040037	-1.879832
6	5.657520	1.434744	-0.334860
1	4.958302	2.116519	0.175429
1	6.297694	2.029770	-1.006918
1	6.300643	0.973245	0.429085
6	6.764858	-3.916535	0.345836
1	6.918538	-4.851123	-0.199527
6	5.867363	-0.597950	-1.816204
1	6.617204	-1.004571	-1.126387
1	6.404123	-0.055647	-2.611039
1	5.328388	-1.439597	-2.276917
6	4.030728	1.037317	-2.211515
1	3.451692	0.289300	-2.773352
1	4.666658	1.593561	-2.917130
1	3.314070	1.755547	-1.781585
6	6.364451	-1.523753	1.731970
1	6.197769	-0.596359	2.284504
6	-4.266408	-3.460522	2.050888
1	-4.203233	-3.019157	3.058255
1	-4.008358	-4.529371	2.125273
1	-5.306923	-3.392491	1.708103
6	7.558833	-2.230874	1.890159
1	8.333047	-1.847393	2.559669
6	-5.555805	2.255414	2.083786
1	-6.227860	1.447921	2.409454

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           1       -6.121816    3.201103    2.116008
           1       -4.724692    2.324430    2.803458
           6        7.761514   -3.429790    1.198327
           1        8.695010   -3.984162    1.323500
           6       -3.457392   -3.301647   -0.340928
           1       -4.490127   -3.187574   -0.696195
           1       -3.211398   -4.375942   -0.364177
           1       -2.790216   -2.774938   -1.037704
           6       -6.189060    1.912112   -0.333713
           1       -5.835138    1.605055   -1.329679
           1       -6.652794    2.907177   -0.427245
           1       -6.969845    1.210460   -0.015590
           1        0.218648   -3.107439   -5.658171
           1       -0.590264   -4.345913   -4.696774
           1       -2.659609   -3.220661   -5.037761
           1       -1.834462   -1.922660   -5.902456
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