Luke Bertels Tao Yang updated

11/23/2015 11/25/2015

**Update 11/23**

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| Reactants | | | | | | | | |
| CH3CCH | | | |  | SiH | | | |
|  | | | |  |  | | | |
| 0 | | | |  | 0 | | | |
| C3v – 1A1 | | | |  | C∞v – 2Π | | | |
| C | -1.919449 | 1.519750 | 0.000000 |  | Si | -7.063060 | 1.620720 | 0.000000 |
| C | -0.721221 | 1.524736 | 0.000000 |  | H | -5.534020 | 1.620720 | 0.000000 |
| C | -3.382029 | 1.513693 | 0.000000 |  |  |  |  |  |
| H | 0.343441 | 1.529181 | 0.000000 |  |  |  |  |  |
| H | -3.768514 | 1.986640 | -0.905294 |  |  |  |  |  |
| H | -3.768812 | 2.058826 | 0.863618 |  |  |  |  |  |
| H | -3.762327 | 0.490833 | 0.041676 |  |  |  |  |  |
| Products | | | | | | | | |
| [p1] | | | |  | [p2] | | | |
|  | | | |  |  | | | |
| -1.006119 (CCSD(T)/CBS) | | | |  | 24.048742 (CCSD(T)/CBS) | | | |
| Cs – 1A’ | | | |  | C1 – 1A | | | |
| Si | -0.000450 | 0.531770 | 0.121220 |  | Si | -0.072960 | 0.286450 | 0.168280 |
| C | -0.005400 | -0.185320 | 1.787230 |  | C | 1.806770 | 0.067770 | 1.262120 |
| C | -1.250430 | 0.124280 | 1.390180 |  | C | 0.621320 | 0.399290 | 1.860830 |
| C | -2.625670 | 0.038020 | 1.952780 |  | C | 1.844640 | 0.652470 | -0.101170 |
| H | 0.423160 | -0.619410 | 2.684520 |  | H | 2.539840 | -0.653500 | 1.631710 |
| H | -3.259180 | -0.565900 | 1.297380 |  | H | 0.336770 | 0.169040 | 2.880320 |
| H | -2.641320 | -0.394260 | 2.957330 |  | H | 2.043320 | 1.720800 | -0.106230 |
| H | -3.075620 | 1.033970 | 1.988990 |  | H | 2.419310 | 0.133330 | -0.867810 |

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| Intermediates | | | | | | | | |
| [i1] | | | |  | [i2] | | | |
|  | | | |  |  | | | |
| -69.957432 | | | |  | -74.446724 | | | |
| Cs – 2A’ | | | |  | Cs – 2A’ | | | |
| Si | -3.099616 | 1.777048 | 0.368214 |  | Si | -3.288845 | 1.750474 | 0.225591 |
| C | -2.292693 | 0.168058 | -0.167340 |  | C | -2.220009 | 0.260966 | -0.201448 |
| C | -1.005191 | 0.040901 | 0.076063 |  | C | -0.909275 | 0.406367 | -0.174923 |
| C | 0.119095 | -0.893165 | -0.081825 |  | C | 0.102954 | 1.436230 | 0.101735 |
| H | -2.827406 | -0.652613 | -0.661588 |  | H | -2.647397 | -0.706243 | -0.466950 |
| H | -4.499773 | 1.404092 | -0.126904 |  | H | -4.623027 | 1.031867 | 0.039005 |
| H | -0.203833 | -1.820123 | -0.574586 |  | H | -0.362386 | 2.393623 | 0.374026 |
| H | 0.545419 | -1.144537 | 0.892960 |  | H | 0.734922 | 1.590427 | -0.777045 |
| H | 0.912711 | -0.436697 | -0.679282 |  | H | 0.753154 | 1.116481 | 0.920523 |
| [i3] | | | |  | [i4] | | | |
|  | | | |  |  | | | |
| -174.073234 | | | |  | -207.578238 | | | |
| C1 – 2A | | | |  | Cs – 2A’ | | | |
| Si | 0.010240 | -0.006660 | -0.004460 |  | Si | -4.574656 | -0.775380 | 0.551722 |
| C | 1.585020 | -0.006680 | -0.901020 |  | C | -1.755185 | -1.781490 | 0.147741 |
| C | 1.019150 | -1.221880 | -0.914150 |  | C | -2.864517 | -1.322249 | 0.298059 |
| C | 1.342930 | -2.563880 | -1.467010 |  | C | -0.408865 | -2.318025 | -0.028068 |
| H | -0.004880 | -0.001700 | 1.504720 |  | H | -5.117662 | -0.122556 | -0.668157 |
| H | 2.502850 | 0.407370 | -1.303060 |  | H | -4.687941 | 0.104244 | 1.744418 |
| H | 1.392460 | -3.303440 | -0.663460 |  | H | -0.352169 | -3.341436 | 0.350611 |
| H | 2.293320 | -2.562500 | -2.008170 |  | H | -0.132438 | -2.325130 | -1.084804 |
| H | 0.551010 | -2.888040 | -2.148160 |  | H | 0.317799 | -1.709744 | 0.515472 |

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| [i5] | | | | | | |  | | [i6] | | | | | | |
|  | | | | | | |  | |  | | | | | | |
| -126.595364 | | | | | | |  | | -232.359393 | | | | | | |
| Cs – 2A’ | | | | | | |  | | Cs – 2A’ | | | | | | |
| Si | | -1.206506 | | 0.407411 | 0.088330 | |  | | Si | | -1.206506 | | 0.407411 | | 0.088330 |
| C | | -1.915619 | | -1.279068 | 0.015734 | |  | | C | | -1.915619 | | -1.279068 | | 0.015734 |
| C | | -0.624589 | | -1.394307 | 0.025073 | |  | | C | | -0.624589 | | -1.394307 | | 0.025073 |
| C | | 0.580168 | | -2.263943 | 0.004420 | |  | | C | | 0.580168 | | -2.263943 | | 0.004420 |
| H | | 0.279908 | | -3.313471 | -0.038984 | |  | | H | | 0.279908 | | -3.313471 | | -0.038984 |
| H | | 1.183808 | | -2.106204 | 0.900578 | |  | | H | | 1.183808 | | -2.106204 | | 0.900578 |
| H | | 1.202381 | | -2.038534 | -0.864145 | |  | | H | | 1.202381 | | -2.038534 | | -0.864145 |
| H | | -1.177438 | | 1.184414 | 1.348680 | |  | | H | | -1.177438 | | 1.184414 | | 1.348680 |
| H | | -1.151065 | | 1.279148 | -1.107516 | |  | | H | | -1.151065 | | 1.279148 | | -1.107516 |
| Transition States | | | | | | | | | | | | | | | |
| [i1-i3] | | | | | | |  | [i1-i5] | | | | | | | |
|  | | | | | | |  |  | | | | | | | |
| -15.088822 | | | | | | |  | -68.535317 | | | | | | | |
| C1 – 2A | | | | | | |  | C1 – 2A | | | | | | | |
| Si | -2.305052 | | 1.635707 | | | -0.354388 |  | Si | | -1.465132 | | 1.510126 | | 1.401211 | |
| C | 0.307434 | | 0.035992 | | | -0.007836 |  | C | | -0.111646 | | 1.081633 | | 0.179018 | |
| C | -0.734532 | | 0.707471 | | | -0.042306 |  | C | | -0.314922 | | -0.167795 | | -0.166199 | |
| C | 1.521459 | | -0.764976 | | | 0.036880 |  | C | | 0.280378 | | -1.366729 | | -0.774511 | |
| H | -2.806168 | | 1.415732 | | | 1.059314 |  | H | | -0.584405 | | 2.435478 | | 2.250363 | |
| H | -1.936253 | | 0.081710 | | | -0.723547 |  | H | | 0.830447 | | 1.602981 | | -0.019233 | |
| H | 1.349777 | | -1.738677 | | | -0.433857 |  | H | | 0.311337 | | -2.186085 | | -0.052069 | |
| H | 2.326396 | | -0.268956 | | | -0.511892 |  | H | | 1.304655 | | -1.165000 | | -1.115944 | |
| H | 1.846705 | | -0.932674 | | | 1.065876 |  | H | | -0.315707 | | -1.699817 | | -1.627899 | |

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| [i2-i3] | | | |  | [i2-i5] | | | |
|  | | | |  |  | | | |
| -15.097954 | | | |  | -66.144167 | | | |
| C1 – 2A | | | |  | C1 – 2A | | | |
| Si | -2.800580 | -0.339288 | 0.355061 |  | Si | -0.955919 | 0.780311 | 1.538849 |
| C | 0.218443 | 0.222305 | 0.080439 |  | C | -0.158467 | 1.320646 | -0.082204 |
| C | -1.010119 | 0.054092 | 0.096608 |  | C | 0.272266 | 0.155495 | -0.464312 |
| C | 1.662717 | 0.399268 | 0.055129 |  | C | 0.196080 | -1.290763 | -0.683615 |
| H | -3.095476 | -0.339888 | -1.131638 |  | H | -0.191136 | 1.818189 | 2.363562 |
| H | -1.513126 | -1.354167 | 0.349001 |  | H | 0.224970 | 2.287968 | -0.402815 |
| H | 2.165016 | -0.558616 | 0.227967 |  | H | -0.773385 | -1.699716 | -0.371592 |
| H | 1.995907 | 0.795593 | -0.906666 |  | H | 0.985003 | -1.810431 | -0.135811 |
| H | 1.975801 | 1.084878 | 0.847113 |  | H | 0.332926 | -1.504639 | -1.749179 |
| [i3-i4] | | | |  | [i4-i5] | | | |
|  | | | |  |  | | | |
| -114.094481 | | | |  | 2.800178 | | | |
| Cs – 2A’ | | | |  | C1 – 2A | | | |
| Si | -1.488876 | 0.982966 | 0.120887 |  | Si | -0.945476 | 1.426076 | 0.563695 |
| C | -1.171498 | -0.824767 | 0.443969 |  | C | 1.042650 | 1.128109 | -0.283612 |
| C | 0.012337 | -0.594114 | 0.124952 |  | C | 0.130012 | 0.171407 | -0.198799 |
| C | 1.443804 | -0.588234 | -0.199098 |  | C | 0.157973 | -1.278245 | -0.561626 |
| H | 1.824836 | -1.606015 | -0.083589 |  | H | -1.208125 | 1.266393 | 2.032829 |
| H | 1.994410 | 0.070152 | 0.474317 |  | H | 0.245184 | 2.387836 | 0.304483 |
| H | 1.609932 | -0.267620 | -1.228486 |  | H | -0.056299 | -1.897723 | 0.311975 |
| H | -1.907726 | 1.690326 | 1.357368 |  | H | 1.132045 | -1.561438 | -0.964589 |
| H | -2.440617 | 1.175454 | -1.002407 |  | H | -0.606135 | -1.493008 | -1.312373 |