

Supplementary Information

Formation of a Stannastannylene via Intramolecular Carbene Insertion Reaction of Stannaacetylene (RSn≡CR')

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1. An NMR Study of Photoreaction of Diazomethylstannylene (1)

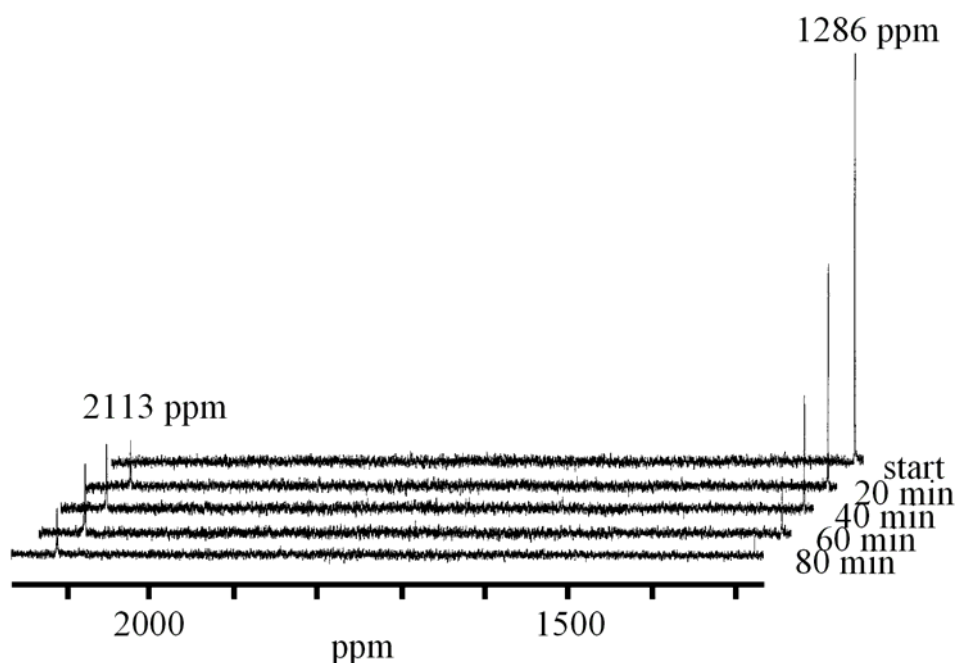


Figure S1. Time course of ^{119}Sn NMR spectra obtained during irradiation of diazomethylstannylene **1** in benzene- d_6 .

2. Theoretical Calculations of Relative Energies of Intermediates

Relative energies of possible reaction intermediates **8-14** during the rearrangement of stannaacetylene **2** were calculated at the RHF/3-21G* level.^{S1} The results are shown in Figure S2. Because the theoretical level of the present preliminary calculations is low, the absolute relative energies are not reliable enough but the relative stability among the intermediates suggests an interesting feature of the rearrangement: (1) Symmetry allowed consecutive [1,5]sigmatropic rearrangements from **9** to **11** may not be feasible, because the relative energies of highly strained intermediates **13** and **14** are very high compared with those of **9**, **10**, and **11**. (2) On the other hand, a short-cut pathway from **9** to **10** that is more energetically favorable is allowed not only by photochemical [1,3]sigmatropic rearrangement but thermal suprafacial [1,3]sigmatropic rearrangement of tin. See ref. 10 in text.

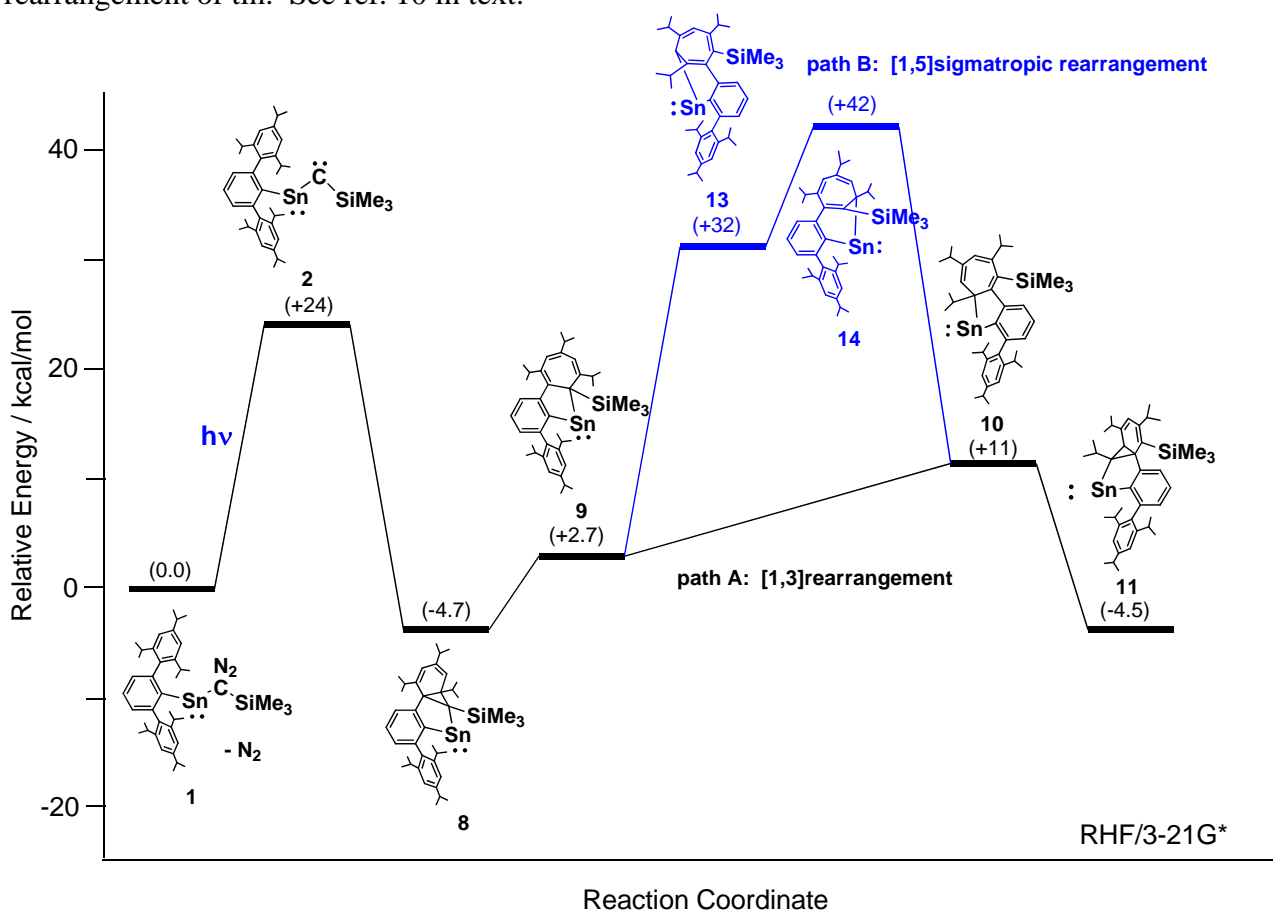


Figure S2. Relative energies of possible reaction intermediates in the photoreaction of **1** calculated at the RHF/3-21G* level.

Optimized Structures

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H,4.8280201089,-3.3464912131,0.3811995684
H,4.0446444655,-1.7772983964,0.3452487232
H,1.5291666028,7.3302030705,-0.648305932
H,1.1310626825,8.4452538001,-1.9445649739

H,2.4521946736,7.3098296407,-2.1428468999
H,4.0811196433,1.6384088428,1.320883403
H,2.8357815483,1.149913558,2.4663011476
H,3.7790723666,2.5904650644,2.7584821043

Compound 9 HF=-7824.198076

C,0.6752175306,-1.4718060672,5.8903915431
C,-3.6899687401,4.4093093093,1.6326198932
C,-4.8651699523,1.7765541607,0.6697345376
C,-2.9221861594,1.8934018615,3.0424329318
C,-1.5507661831,-1.9040905542,4.7625932982
C,1.0884493089,6.148976909,1.0149601304
Si,-3.283675158,2.5945959868,1.3064934543
C,-0.1157504235,-1.3680494612,4.5675446709
C,2.1407699713,2.181152799,3.2468128112
C,1.2541296974,2.8706698438,2.4463315614
C,2.2034062486,0.79730715,3.2085940106
C,0.6299990289,-2.0986858475,3.4497754227
C,1.0774464755,4.8532227625,0.1715728099
C,0.6516490334,-3.4867245102,3.4462223036
C,0.4221349647,2.1898453083,1.5519092141
C,1.3109955377,0.0964036365,2.4168337833
C,-1.8011280581,2.1175318467,0.214915578
C,-0.5206004315,2.9039847952,0.6199965688
C,-0.2877219318,4.1421342327,0.1426377249
C,1.5134377007,5.1718356604,-1.278553922
C,0.4029628355,0.7866924902,1.6036342357
C,1.3131558388,-1.4073037006,2.4441932397
C,-3.1849827852,0.1313271107,-2.3116260189
C,2.7492250359,-6.2888502303,2.6659835237
C,-1.8291397678,0.8462464907,-2.1269865453
C,1.3243758034,-4.2052766805,2.4762499507
C,-1.3112558233,4.9676480987,-0.5302614323
C,1.3203506133,-5.7284935312,2.5018085035
C,-1.9780716629,2.1528311431,-1.3215356888
C,-3.2908267886,6.9628564303,-1.3957457818
C,2.0066568953,-2.1193239421,1.4565110377
Sn,-1.4405894762,-0.0488721567,0.8216608658
C,-1.1468279973,1.0216210247,-3.5010994875
C,1.9968443183,-3.5038941029,1.4895858447
C,-2.1923369959,4.6235627635,-1.4621591167
C,0.6511203867,-6.3042009435,1.2355176694
C,4.3029326375,-1.7274519317,0.4717735446
C,-3.1070190477,5.6363998854,-2.1580070153
C,-2.2250116683,3.2655977139,-1.9990632509
C,2.7964883434,-1.4083558056,0.3568871725
C,-2.5621936483,5.9541584657,-3.5738343838
C,2.2665385592,-1.7783872859,-1.0445171912
H,0.1627768278,-0.9325168453,6.6806376675
H,0.7736696696,-2.5087440853,6.1909861897
H,1.6680957385,-1.0537253494,5.7782978895
H,-4.4099393568,4.462075478,2.4489839468
H,-4.131343151,4.8912713626,0.7687357436
H,-2.8117935921,4.9766491521,1.9242710022
H,-5.7039201302,2.0455456037,1.3096547452
H,-5.1001487685,2.1082926525,-0.3389485599
H,-4.8026350796,0.690898945,0.6560540615
H,-3.7124195373,2.2042391989,3.7236063086
H,-1.9828612138,2.2766008967,3.4340259671
H,-2.8869032692,0.8043283996,3.1011483841
H,-2.0778476412,-1.2877063767,5.4834085394
H,-1.5447003882,-2.9206859143,5.1366483096
H,-2.1013438579,-1.8899573938,3.8293276525
H,0.7082279726,5.9806181723,2.0158925804
H,2.1024124978,6.5278650182,1.0937269888
H,0.4861167935,6.9219160097,0.5533882308
H,-0.1837716724,-0.323669029,4.3010806653
H,2.7800791772,2.7243776882,3.9153632273
H,1.1947070968,3.9319016472,2.5379784976
H,2.9081067932,0.269244649,3.8199487136
H,1.8125061884,4.1759053109,0.5710648878
H,0.1315776934,-4.0209468627,4.2164089713
H,2.5192116931,5.5808311765,-1.2797866506
H,0.8490191327,5.8925084346,-1.7375437883
H,1.5070495547,4.2704217706,-1.879974321
H,-3.6693944597,-0.0672926319,-1.3656338644
H,-3.0510363054,-0.8126209599,-2.8293028512
H,-3.8400378424,0.7621853934,-2.9009608619

H,3.2143105506,-5.8955429429,3.5622337577
H,2.7241747811,-7.3714317092,2.7363145409
H,3.3655818514,-6.0196921657,1.8160641929
H,-1.1614343483,0.1847195137,-1.5736993795
H,-1.2738733859,5.9974756988,-0.2331410598
H,0.7367346417,-6.0412121751,3.3609758052
H,-3.6263622657,6.7977415122,-0.3804597701
H,-2.3645529533,7.5257887637,-1.3677527846
H,-4.030426379,7.5713487194,-1.9048826815
H,-0.9204334922,0.0463905307,-3.9191605045
H,-0.2263908656,1.5831462783,-3.4043646595
H,-1.7954949334,1.5348288258,-4.2000267511
H,2.5286018103,-4.0449256828,0.7326062691
H,-0.3564080427,-5.9204985428,1.1272981425
H,0.6049968251,-7.3869335048,1.2918727398
H,1.2150609805,-6.0353654504,0.3498053696
H,4.677798075,-1.4463886945,1.4489567994
H,4.4881184029,-2.7853661367,0.3266508298
H,4.8605140234,-1.1788045368,-0.2804932327
H,-4.0823666741,5.1701538218,-2.2632725725
H,-2.3852930462,3.2017016332,-3.0581981333
H,2.6724030294,-0.3448569357,0.4868857764
H,-1.5859125789,6.417564851,-3.4896474321
H,-3.2278261887,6.6398060732,-4.087700669
H,-2.4654402644,5.0639346828,-4.1820670428
H,2.3835799389,-2.8374801435,-1.2410191282
H,1.2139332429,-1.5331088998,-1.1313201845
H,2.8090646357,-1.2296820232,-1.8073905025

Compound 10 HF=-7824.185363

C,1.1342391106,-2.3849206765,3.9477259564
C,-1.3963614535,2.203439726,2.8087249289
C,2.224066239,4.4926947153,3.0481578258
C,-3.3347836787,2.4702508497,1.2169826917
C,-1.8091834328,2.6198119524,1.3808346979
C,2.0433801194,-2.6640122872,2.7321710534
C,3.210112119,1.803107012,2.2938258124
C,3.3272709364,-3.401582471,3.1703358821
C,0.8234883292,-4.723567977,1.9584038238
Sn,-1.3101196981,-0.401222441,0.7798756786
C,-1.8829094701,-6.9646133156,1.259825372
Si,2.6303861812,3.4283770701,1.5157981993
C,1.3016815763,-3.455934857,1.6552704877
C,-0.2812157726,6.6186760424,1.2020549413
C,-0.3470966667,-6.8857172186,1.392496368
C,-1.0349013376,1.7863683303,0.3167322792
C,0.1658938375,-5.4995657195,1.0232818617
C,1.0350681843,3.2749178388,0.4634252565
C,4.0996981248,4.2068165316,0.6129526029
C,0.3312772043,-7.9783710072,0.5389119289
C,0.8120568305,5.8716645168,0.4076685309
C,0.4756703839,2.0331682545,0.2951347081
C,0.3285717577,4.4704876382,-0.018514078
C,0.8188882294,-0.4467546622,0.3002118809
C,1.1067897354,-2.947835584,0.3685793175
C,-1.4015879524,2.1146126631,-1.1159723132
C,1.3064092768,0.8329086251,-0.0089166248
C,1.6016443386,-1.5708989814,0.0237570836
C,-0.0093510286,-4.9834329711,-0.2502908295
C,-0.6293167399,4.4494012023,-0.9739496171
C,-1.2489478596,3.3319910269,-1.650480341
C,0.4472581708,-3.7225520288,-0.5958818758
C,1.2900432465,6.7289002972,-0.7855611648
C,-2.9449811748,4.5784735499,-3.0779511451
C,2.8372536449,-1.4176023961,-0.5893371631
C,2.5090162766,0.9597066977,-0.7002317098
C,-1.7573859088,3.5911896939,-3.0729499803
C,3.2719570854,-0.1590611396,-0.9727850983
C,0.24433491,-3.2230098736,-2.0274928424
C,-1.234063433,-3.3030487805,-2.4652975609
C,-0.6269482993,4.0895266003,-3.9963132119
C,1.1376766373,-4.0189778036,-3.0042242861
H,1.6626773162,-1.7845810523,4.6810476327
H,0.2432596864,-1.8470034605,3.6434385516
H,0.8242937824,-3.30734848,4.4242396688
H,-1.844210068,2.8621240237,3.5455418911
H,-1.7409231228,1.1951384491,3.0416560075
H,-0.3214150302,2.2413204233,2.9319426038

H,2.6913191794,4.0498964805,3.9250885711
H,1.1555762478,4.5404934096,3.2400965558
H,2.5911178006,5.5126956533,2.9697775185
H,-3.8505216315,3.0914648024,1.9423910697
H,-3.6510873242,1.4435819662,1.3746119423
H,-3.6457109992,2.7758733169,0.2265712145
H,-1.5736575111,3.6641817893,1.2591256576
H,2.335482603,-1.7143528415,2.311883316
H,3.9295420465,2.0553116235,3.0723270067
H,2.3877011466,1.2731241515,2.7694515654
H,3.688053899,1.1199530233,1.6058553698
H,3.8722877323,-2.8047082177,3.894386876
H,3.0912416681,-4.3557385636,3.6267052038
H,3.9730780249,-3.5809899949,2.3187238911
H,0.9698167157,-5.1158445698,2.9457308755
H,-2.359633689,-6.2054987802,1.8676671617
H,-2.2398447993,-7.9384712884,1.5779535193
H,-2.1851776622,-6.8143137742,0.2290653404
H,-0.5993691772,6.1935942495,2.0604052581
H,0.0937603223,7.5744585911,1.5543365059
H,-1.1468346865,6.8011366561,0.5762871307
H,-0.0911189845,-7.0647736113,2.4312358796
H,4.9268332451,4.3505460051,1.3071170832
H,3.8606369388,5.1756491325,0.1825423592
H,4.4585145923,3.5696656315,-0.1920401589
H,-0.0039574613,-8.9623752849,0.8500722633
H,1.4088871723,-7.9320841181,0.6431475504
H,0.0844015793,-7.8533026025,-0.5090217816
H,1.6578697912,5.7607456001,1.0603652123
H,-1.8058542577,1.3384106606,-1.746609181
H,-0.5112621927,-5.5749682398,-0.9892685743
H,-0.9295166386,5.4059836898,-1.3554782712
H,1.7353324255,7.6496672384,-0.4219047362
H,0.4682775891,6.9945847158,-1.4384607859
H,2.0298881358,6.1948355867,-1.3699143955
H,-3.7417436473,4.2197595615,-2.4367470242
H,-2.641096113,5.559011461,-2.7309417423
H,-3.3359628479,4.6882861259,-4.0843273616
H,3.4369128414,-2.2816352699,-0.7983658721
H,2.827212317,1.9235925748,-1.0401560065
H,-2.1173194732,2.6461664601,-3.4649619258
H,4.2006615932,-0.0548595706,-1.4992535822
H,0.548719897,-2.1879770244,-2.0699726586
H,-1.8738948164,-2.7682377231,-1.7723291682
H,-1.5756184121,-4.3298695174,-2.5125723915
H,-1.3523862877,-2.8657651281,-3.4513300207
H,0.1960148097,3.3843425986,-4.0029180922
H,-0.2496173755,5.0476406579,-3.6597483639
H,-0.9915140323,4.2043452664,-5.0122755031
H,2.1809809925,-3.9330286613,-2.7249690272
H,0.8686936234,-5.0689639359,-2.9968906987
H,1.0207339471,-3.6425997546,-4.0153933512

Compound **11** HF=-7824.2095364

C,-0.4350894384,-1.5668779051,5.0671031054
C,-3.7300856776,-2.1481393869,0.2973991362
C,-5.6393256375,-1.3291517797,1.121415178
C,-2.696161948,-2.9083243133,-1.8743327494
C,-2.9949799824,-1.6908634546,-0.9777796597
C,0.4599825772,-0.3550224062,4.7321674437
C,-3.0433168891,1.1697505103,2.6203326343
C,0.7699995207,0.4601821363,6.006454712
C,2.6050307828,-1.6703997986,4.6887541437
Sn,-0.1982741781,-1.9181226082,0.6864740614
C,4.8852158347,-4.3624358967,4.0656453681
Si,-3.8360375505,1.9225322348,1.076081617
C,1.7540897325,-0.7845931571,4.04133595408
C,-5.8330919937,1.5739218665,-2.6931771368
C,4.7070640853,-3.0544098837,4.865696537
C,-1.7039927128,-0.965231973,-0.6160113719
C,3.7999092421,-2.0781890437,4.1274759112
C,-2.962557702,1.367231242,-0.5302287258
C,-3.8413974913,3.802871756,1.2968782397
C,6.0771494278,-2.416369997,5.1794788334
C,-4.712937193,2.4073432452,-2.0343696394
C,-1.6917363519,0.5588658825,-0.3922695172
C,-3.4661426308,1.5684861714,-1.7618998034
C,0.2003610211,0.1688661442,1.2161135125

C,2.1159247946,-0.2930901053,2.7849288374
C,-1.0635744703,-0.0207027233,-1.6644468548
C,-0.6348644231,1.0743674532,0.5472006331
C,1.2073734034,0.6574258931,2.0562539148
C,4.1454251601,-1.5747935371,2.8838576808
C,-2.8251821851,1.0191911047,-2.9690464833
C,-1.7134898192,0.2945270929,-2.9503141528
C,3.32680175,-0.6903102952,2.2020000638
C,-4.369410311,3.6425379757,-2.8975989242
C,-1.8788711249,-0.3426282967,-5.4321264405
C,1.3738945255,2.02436166,2.219352013
C,-0.4227699611,2.4411827653,0.6766089404
C,-0.9719658731,-0.1602986814,-4.2010088071
C,0.5670556796,2.9086145605,1.5208085564
C,3.778313355,-0.1504141795,0.8441924015
C,4.0808509227,-1.2884531473,-0.1538463124
C,0.1544021236,0.8508402441,-4.5261671149
C,5.0105046632,0.7653331204,1.0111164754
H,-1.3728695955,-1.230023019,5.4963717411
H,-0.6545017938,-2.1413619628,4.1738904704
H,0.0459033818,-2.2257274237,5.7801080131
H,-4.6740109214,-2.6237276113,0.050931018
H,-3.1322312322,-2.8699847074,0.8486069061
H,-3.9335139528,-1.3045577471,0.9426774243
H,-6.0491083011,1.5286286302,2.111018905
H,-5.7130579854,0.2582718619,0.9502517086
H,-6.2849978431,1.8206314494,0.4011322499
H,-3.6150689436,-3.420501012,-2.1418765726
H,-2.0546346563,-3.6157757784,-1.3584178947
H,-2.200907349,-2.6007064292,-2.7870227496
H,-3.6506007216,-1.0256745558,-1.5221880299
H,-0.0866762361,0.2831950077,4.0558860858
H,-3.7431639523,1.2613697114,3.4500053653
H,-2.8142133217,0.1149052383,2.499715081
H,-2.1249552086,1.6731572184,2.8999549748
H,-0.1514460141,0.7990978689,6.4688941953
H,1.3113820421,-0.1414638305,6.7273569589
H,1.3722707856,1.328361067,5.7656717451
H,2.3306241798,-2.049278641,5.6537759565
H,3.9241014851,-4.8165335635,3.8557354393
H,5.4869531215,-5.0695607369,4.6273548292
H,5.3832266655,-4.168652932,3.1226970907
H,-6.0841248952,0.7175556026,-2.0785772964
H,-6.7247492651,2.1798465089,-2.8185033792
H,-5.5318902731,1.2158967101,-3.6701772231
H,4.2281051883,-3.300026645,5.8074455949
H,-4.4402863778,4.069466947,2.1669175079
H,-4.2560889175,4.3291028924,0.4410406293
H,-2.8371175012,4.182557823,1.4647523333
H,6.6914532073,-3.1039618848,5.7516672192
H,5.9531159599,-1.5053426398,5.7529777263
H,6.6045839187,-2.173793977,4.2642055071
H,-5.0907100023,2.778557507,-1.0964650004
H,0.0116361138,0.0006193619,-1.7026204066
H,5.071647327,-1.8757047612,2.436800915
H,-3.2860494391,1.253782295,-3.9054555279
H,-5.249578997,4.2658496906,-3.0182603354
H,-4.0262085747,3.3541693026,-3.8833429562
H,-3.5924086385,4.2318959547,-2.4247037572
H,-2.7037785824,-1.0103920298,-5.2132379851
H,-2.2803955147,0.6074720082,-5.7648113902
H,-1.3039761267,-0.7627342363,-6.2502336088
H,2.1386771053,2.3929862788,2.8743525595
H,-1.0224398318,3.129470635,0.1153389704
H,-0.5152634748,-1.1191816231,-3.9757436923
H,0.7193183542,3.9651442688,1.6286457465
H,2.97639464,0.4457103568,0.4361582936
H,3.2211630614,-1.9391651051,-0.2693975091
H,4.9160333992,-1.8924312066,0.1795289369
H,4.3323524296,-0.8747225813,-1.1250620104
H,0.8210215912,0.9878636432,-3.6829610638
H,-0.2816329896,1.8112979106,-4.7742116163
H,0.7419026719,0.5056474989,-5.3705658885
H,4.7869888192,1.5856052405,1.6828724248
H,5.8484114114,0.2104983675,1.4172020093
H,5.3067115131,1.1779407535,0.0519751367

Compound **13** HF=-7824.1515041

C,1.2032121173,-3.069913486,-2.979665524
C,-4.7498638295,2.2445992909,1.6815404173
C,-4.5603099917,5.264038342,1.2154971331
C,-5.3142822151,3.4058096146,-1.0958881838
C,3.137626572,-1.8662642534,-1.8834631242
C,-0.2076586445,5.1847960814,2.4135610282
Si,-4.2229237052,3.5674112864,0.4449611942
C,1.6313484301,-2.1911323847,-1.7828631475
C,-2.5706650057,-0.601083317,-1.4760519263
C,-2.4472318346,0.6609708739,-0.9192702839
C,-1.7345433161,-1.6229796005,-1.0858104314
C,1.2696172968,-2.8857879185,-0.4698202758
C,-0.9601958946,3.8530765704,2.6013290882
C,2.0464344664,-3.9504452643,-0.0313974603
C,-1.4809589257,0.9373842674,0.0442744041
C,-0.7282341429,-1.3648484545,-0.1593925771
C,-2.3792311226,3.3316683248,0.1177604254
C,-1.5512341356,2.2452132554,0.7747735241
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Supplementary Material (ESI) for Chemical Communications
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Reference

- S1. *Gaussian 03*, revision A.11.4, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A., Jr.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Salvador, P.; Dannenberg, J. J.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Baboul, A. G.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A.; Gaussian, Inc.: Pittsburgh, PA, 2001.

3. Laser Flash Photolysis Experiment for Diazomethylstannylene

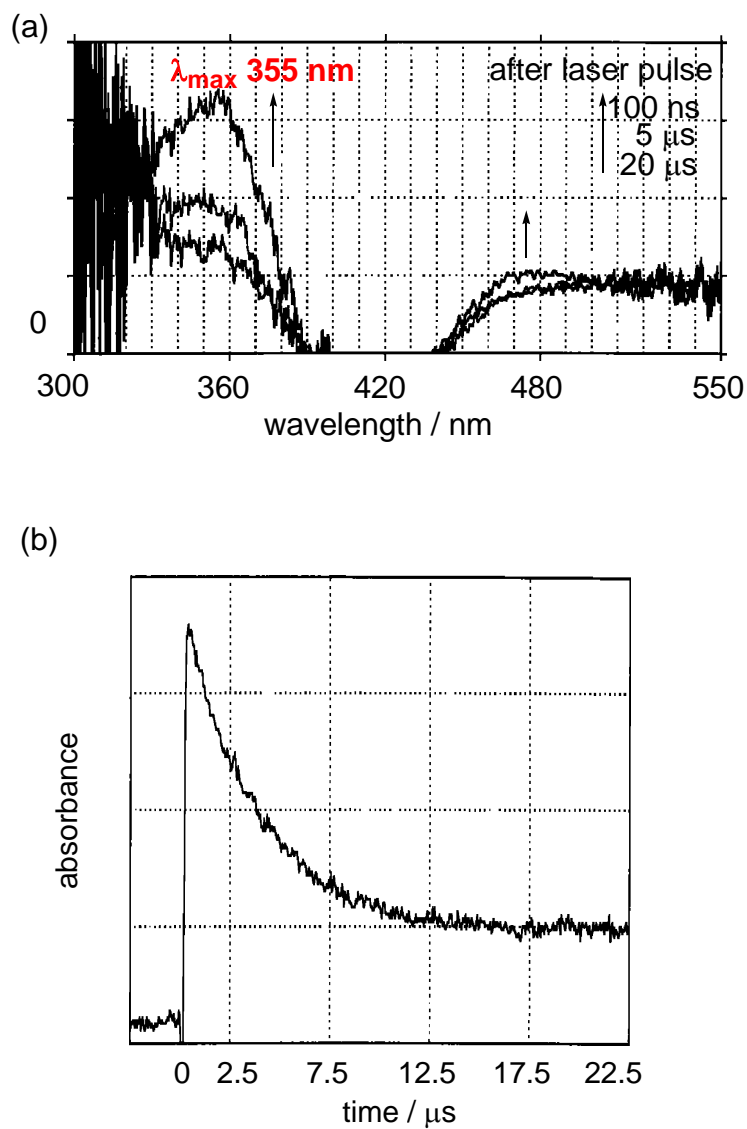


Figure S4. (a) Absorption spectra of the transient products formed by pulsed irradiation of diazomethylstannylene **1** in degassed benzene using a 308-nm excimer laser; (b) decay kinetics measured at 355 nm for stannaacetylene **2**.