Supporting information

A Theoretical Study of Intrinsic Reactivities of Various Allyl-metals towards Carbonyls and Water

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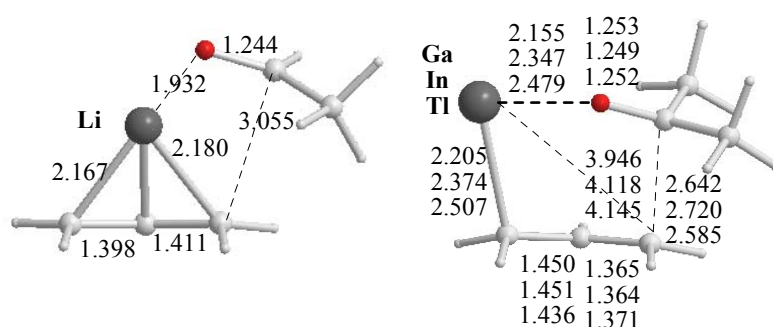
Figure S1. The calculated allylation transition structures for allyl-lithium, gallium(I), indium(I) and thallium(I) by the MP2 method.
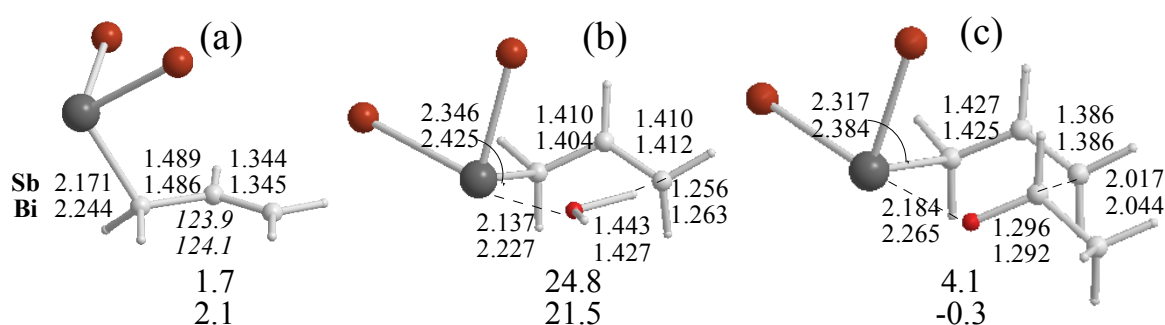

Figure S2. The calculated (a) allyl-M(XV) complexes, (b) hydrolysis and (c) allylation transition structures by the MP2 method. The values are the relative energy (in kcal/mol).
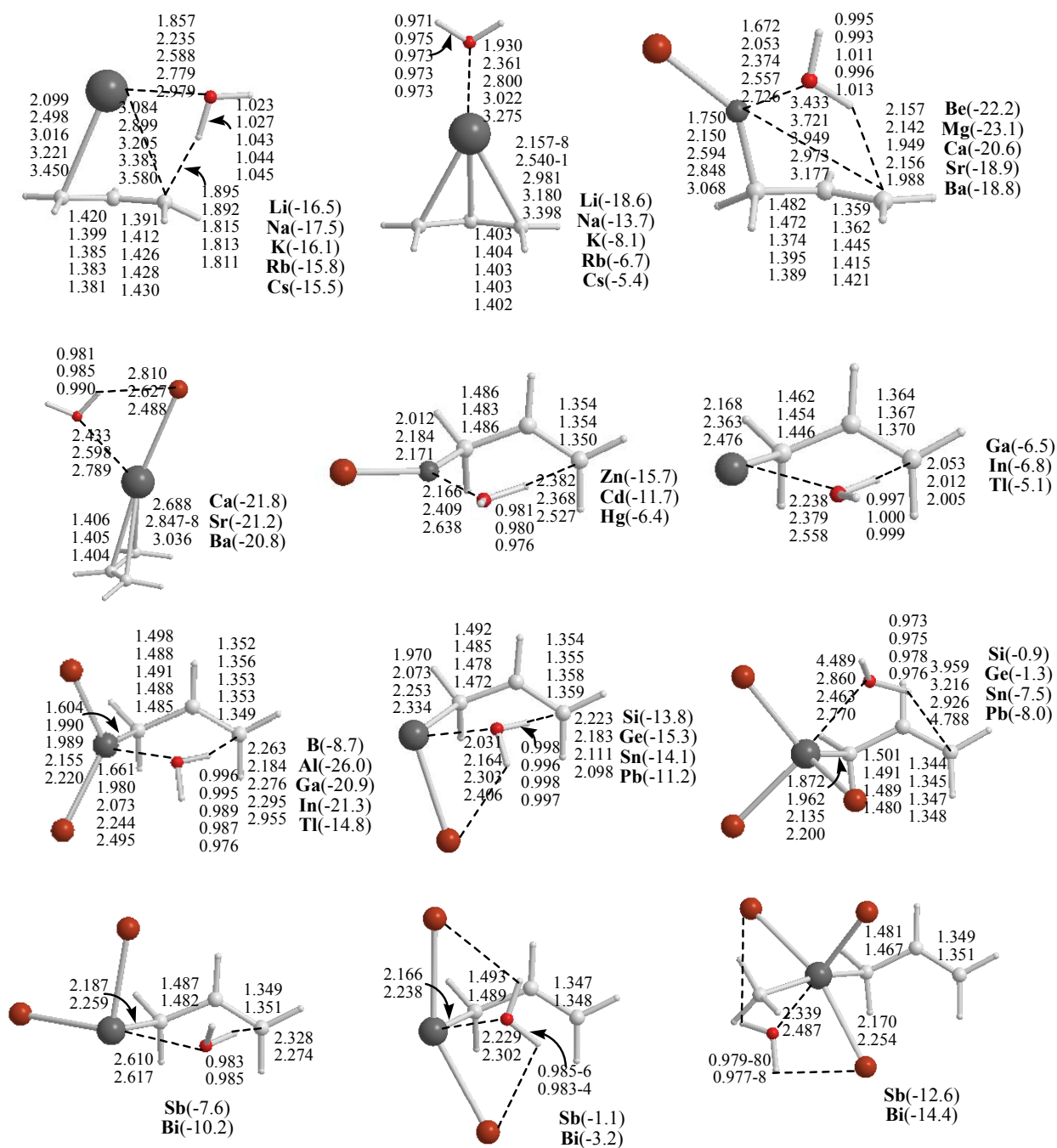
Figure S3. The calculated allyl-metal-water adducts by the MP2 method. The values are the relative energy of the adducts (in kcal/mol).
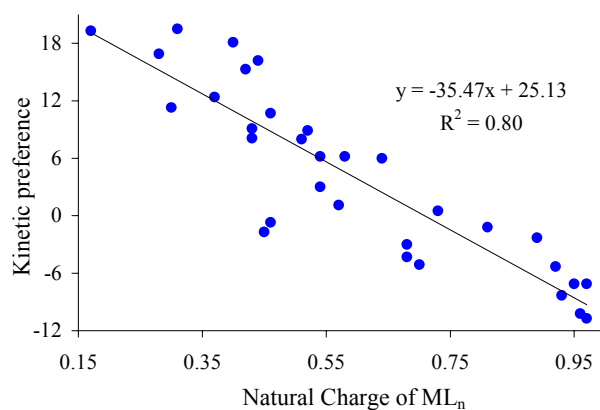
Figure S4. Plots of correlations of the calculated kinetic preference ($\Delta\Delta E^{\ddagger}$) against (a) the natural charge on the $C_{\gamma}H_2$ of allyl-metals (top) and (b) the natural charge on the ML_n of allyl-metals (bottom).
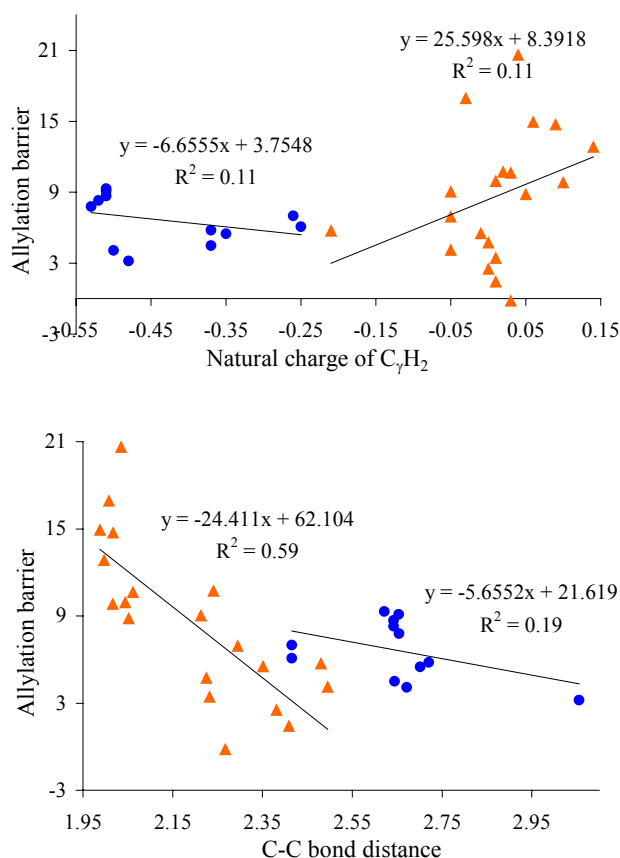

Figure S5. Plots of correlation between the calculated activation energy of allylation against (a) calculated natural charge of $C_{\gamma}H_2$ of allyl-metals (top) and against (b) forming C--C bond distances in the allylation transition structures for π-allyl-metals (blue circle) and σ-allyl-metals (orange triangle) .
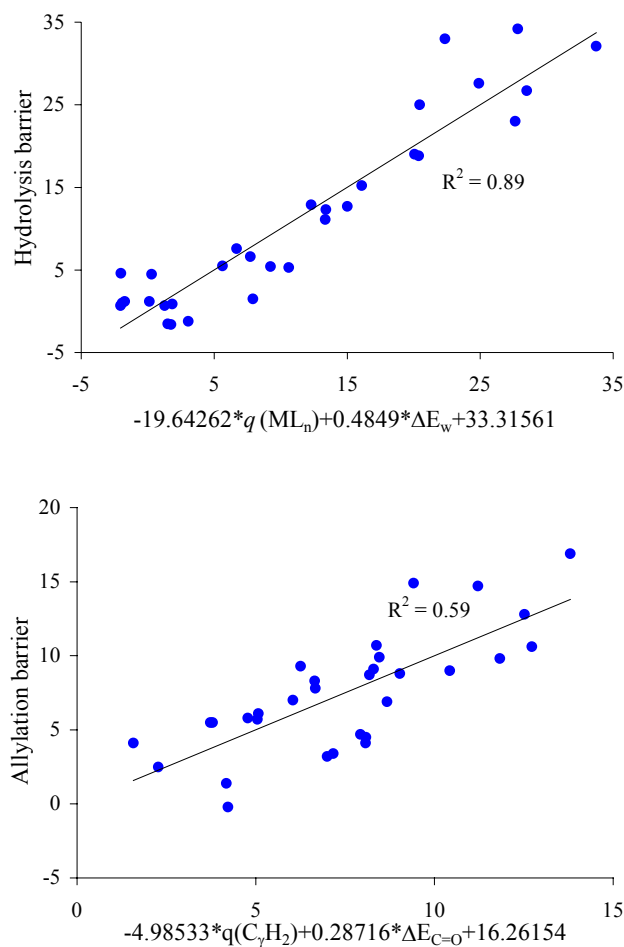
Figure S6. Plot of correlation between (a) the activation energy of hydrolysis and a combination of the calculated natural charge of ML_n and hydrolysis reaction energy and between (b) the activation energy of allylation and a combination of the calculated natural charge of $C_\gamma H_2$ and allylation reaction energy for all allyl-metals except allyl-$SiBr_3$
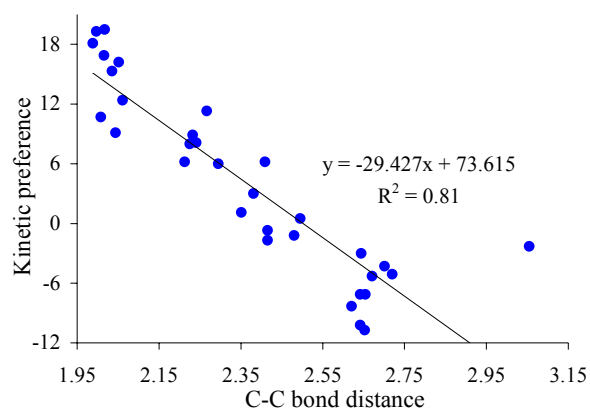
Figure S7. Plots of correlations between calculated intrinsic kinetic preferences and the forming C--C

bond distances in the allylation transition structures.

AllylLi

Li,0,-0.9705251496,0.1501499147,-1.2956984034
C,0,-0.9467243929,0.1502326959,0.8268970357
C,0,1.0597088634,0.1502308345,-0.6760575151
C,0,0.2279018174,-0.4159177571,0.3042596799
H,0,-1.0521260974,1.2401529083,0.8377008063
H,0,-1.5174634869,-0.3814935172,1.5808641567
H,0,1.0998027668,1.2401553772,-0.7740759849
H,0,1.9437505046,-0.3815059376,-1.0117245711
H,0,0.3922940339,-1.4750332146,0.5237356003

AllylLi+h2o (Mode B complex)

H,0,-3.0932819708,-0.6803928613,0.6102203578
O,0,-2.4324609817,-0.7872924039,-0.094413069
Li,0,-0.6017063809,-0.1812440138,-0.0272982123
C,0,1.2657120561,0.7816204314,-0.0466309428
C,0,0.9621279948,0.4991970406,1.2940083269
C,0,1.2579666024,-0.1223754402,-1.1198018626
H,0,1.5144483832,0.2164776389,-2.1183445565
H,0,1.4172097967,-1.1872418082,-0.9251622571
H,0,1.317840029,1.8420596847,-0.3133608728
H,0,1.0989695245,-0.5184134508,1.6720812001
H,0,1.0052378952,1.2871611662,2.0389596026
H,0,-2.9104565808,-1.068231287,-0.8926474138

AllylLi+h2o (Mode A complex)

Li,0,-1.2198711375,0.4839484211,-1.016919652
C,0,-1.2044209849,0.4381392967,1.0819475183
C,0,0.2150189083,0.4245579338,1.0393786859
C,0,1.07650189,-0.6199340527,0.7203837594
H,0,-1.7070633902,-0.5170895185,1.2640837761
H,0,-1.674861783,1.289107525,1.5717426564
H,0,0.6941375348,1.402501472,1.1660524535
H,0,2.1463179339,-0.4793744439,0.8494697597
H,0,0.7164403733,-1.6492203002,0.7631461328
H,0,0.7658077076,-0.4220672507,-1.1384003518
O,0,0.2094367851,-0.2188614639,-1.9720485039
H,0,0.520741875,-0.7813901026,-2.6992072215

AllylLi+h2o (TS)

Li,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,2.172702
C,0,1.387755,0.000000,2.057208
C,0,2.239249,-1.054921,1.640221
H,0,-0.531789,-0.950275,2.266738
H,0,-0.504319,0.872223,2.581362
H,0,1.867865,0.978969,2.165733
H,0,3.303388,-0.909303,1.818029
H,0,1.889941,-2.073313,1.828319
H,0,1.946958,-0.952437,0.110734
O,0,1.373682,-0.771065,-0.853008
H,0,1.780454,-1.247340,-1.594057

AllylLi+CH3CHO (TS)

O,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.243855
C,0,3.049380,0.000000,1.428294
C,0,3.791837,-0.642985,0.415498
C,0,3.962148,-0.216635,-0.904564
Li,0,1.865337,-0.337501,-0.371125
C,0,-0.272253,1.212457,2.068823
H,0,0.126286,-0.949924,1.785218
H,0,3.077844,-0.408489,2.435045
H,0,2.919898,1.085674,1.368775
H,0,4.109196,-1.667695,0.633118
H,0,3.845987,0.840717,-1.156925
H,0,4.535980,-0.813701,-1.605325
H,0,-0.256108,2.110871,1.449819
H,0,-1.259871,1.104378,2.535661
H,0,0.466406,1.283352,2.872707

AllylLi+Me2CO (TS)

O,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.265932
C,0,2.538037,0.000000,1.855424
C,0,3.345251,-0.932990,1.148416
C,0,3.976523,-0.731762,-0.070745
Li,0,1.827171,-0.241488,-0.162741
C,0,-0.199607,1.293841,2.009945
C,0,-0.310786,-1.279245,2.001916
H,0,2.275290,-0.241606,2.881218
H,0,2.726155,1.064825,1.677793
H,0,3.325742,-1.962976,1.517103
H,0,4.164979,0.278924,-0.441368
H,0,4.506977,-1.536280,-0.568403
H,0,0.211539,2.126692,1.436749

H,0,-1.282980,1.450509,2.116984
H,0,0.241594,1.265895,3.008023
H,0,0.127289,-2.134064,1.482831
H,0,0.031656,-1.252305,3.037809
H,0,-1.403599,-1.402264,1.999118

AllylNa
Na,0,-0.783009975,0.1346447957,-1.3247551881
C,0,-0.7676386361,0.1083902148,1.191833609
C,0,1.4142676665,0.1083862948,-0.0978187719
C,0,0.4315694839,-0.4598870029,0.7301631403
H,0,-0.8596621109,1.1975460416,1.242844717
H,0,-1.3816746226,-0.4440599786,1.8967500178
H,0,1.5033358954,1.1975417565,-0.153835811
H,0,2.3279017327,-0.4440666145,-0.2958513737
H,0,0.5540177441,-1.5293909976,0.9373316544

AllylNa +h2o (Mode B complex) (-4.9742 cm^{-1})
C,0,-1.0105099984,-1.471854862,-0.9305610374
C,0,-1.0147891314,-1.4703223276,0.4735049352
C,0,0.0719979404,-1.4731018766,1.3622988088
Na,0,0.2404744752,0.5843532552,-0.119428363
O,0,1.1774417638,2.7101828904,-0.5379196673
H,0,1.064178238,3.2580546674,-1.336136528
H,0,-0.111849301,-1.5579116638,2.4293902081
H,0,1.0461117292,-1.8362092652,1.0218123655
H,0,-1.9976179006,-1.3244950446,0.9376107932
H,0,-0.1288588949,-1.8354084324,-1.4664902972
H,0,-1.9513561219,-1.5564419272,-1.4666041919
H,0,1.7344460506,3.2347371323,0.0660307425

AllylNa +h2o (Mode A complex)
C,0,-0.841956,0.178358,1.772004
C,0,0.482550,0.236502,1.326727
C,0,1.219415,-0.701269,0.571104
Na,0,-1.140628,0.406319,-0.697636
O,0,0.486953,-0.104707,-2.142004
H,0,-1.347451,-0.788327,1.839391
H,0,-1.217477,0.955134,2.432337
H,0,0.991099,1.191597,1.506047
H,0,2.300302,-0.568337,0.555034
H,0,0.891852,-1.744529,0.601748
H,0,0.969449,-0.364099,-1.273707
H,0,0.903450,-0.594834,-2.869827

AllylNa +h2o (TS)
Na,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,2.575660
C,0,1.346879,0.000000,2.274842
C,0,2.139490,-1.045026,1.688243
H,0,-0.561213,-0.936070,2.614054
H,0,-0.463538,0.863202,3.045218
H,0,1.858130,0.960565,2.407162
H,0,3.208814,-0.944003,1.883729
H,0,1.777777,-2.059932,1.886655
H,0,2.068540,-0.946677,0.154863
O,0,1.751253,-0.801464,-0.945709
H,0,2.396398,-1.235153,-1.527589

allylNa +Me2CO (TS)
O,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.257799
C,0,2.577658,0.000000,1.958340
C,0,3.377176,-0.999897,1.384908
C,0,4.232386,-0.921519,0.275765
Na,0,2.043843,-0.429367,-0.756774
C,0,-0.182647,1.297503,2.000073
C,0,-0.290102,-1.280258,2.000380
H,0,2.184035,-0.174860,2.955170
H,0,2.779998,1.047153,1.714193
H,0,3.242939,-2.004885,1.802583
H,0,4.633071,0.048331,-0.029452
H,0,4.828294,-1.785329,-0.003859
H,0,0.253729,2.120030,1.430758
H,0,-1.263701,1.477919,2.093116
H,0,0.245941,1.263640,3.002891
H,0,0.166200,-2.128784,1.486976
H,0,0.051268,-1.244110,3.036023
H,0,-1.380485,-1.424229,1.998345

allylK
C,0,-0.6548024403,0.6779742118,-1.0957427525
C,0,-0.6542262469,0.665182596,0.3077764695
C,0,0.426419271,0.6775934567,1.2033429003
K,0,0.7437103219,-1.8170767574,-0.3499543327
H,0,-1.6001332168,0.7959855331,-1.6190778412
H,0,0.2210002935,1.072139397,-1.6200060216
H,0,-1.6348126683,0.4923508198,0.7688129292
H,0,0.2273700099,0.7975610704,2.2651690868
H,0,1.3888391811,1.0711524095,0.8624311367

allylK +h2o (Mode B complex) (-11.6898 cm^{-1})
C,0,2.0094795252,1.2719048888,0.1905354358
C,0,2.2496640149,0.0024785759,-0.3569009652
C,0,2.0137603294,-1.2694177549,0.1866567954
K,0,-0.6770749685,-0.0030427399,-0.0149401471
O,0,-3.4775247746,0.0015885271,-0.0291422385
H,0,-4.0660509801,0.7762115707,-0.0336514398
H,0,2.3883307695,-2.1440282839,-0.3392109045
H,0,1.9345245915,-1.3749457041,1.2727100018
H,0,2.5497469797,0.0045973921,-1.4125386791
H,0,1.9298618997,1.3738484588,1.2769027092
H,0,2.3811003231,2.1493759725,-0.332652944
H,0,-4.0703142029,-0.7697498222,-0.0363056369

allylK +h2o (Mode A complex)
C,0,-0.8385365179,0.4029117794,2.0027366317
C,0,0.4935199435,0.3599038945,1.6264612492
C,0,1.2323197091,-0.694011957,1.0119768167
K,0,-1.0855449953,0.2325476796,-0.9978348367
O,0,1.280087833,-0.4203556995,-1.8188716218
H,0,-1.4094057943,-0.5218768535,2.1122764089
H,0,-1.2374632073,1.2776721467,2.5089899581
H,0,1.0352004152,1.3085496644,1.7242645925
H,0,2.3118021253,-0.6447163645,1.1704926366
H,0,0.8298372803,-1.7028514997,1.1602690277
H,0,1.3978226601,-0.5381635692,-0.7888872339
H,0,2.1330399594,-0.6469961416,-2.2246187036

allylK +h2o (TS)
K,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,3.086058
C,0,1.345582,0.000000,2.808408
C,0,2.149085,-1.035412,2.204451
H,0,-0.572377,-0.929431,3.075044
H,0,-0.476661,0.860143,3.548630
H,0,1.862696,0.950979,2.980810
H,0,3.191918,-1.010483,2.534597
H,0,1.725658,-2.042267,2.312516
H,0,2.374426,-0.821704,0.687914
O,0,2.394429,-0.649379,-0.449409
H,0,3.286548,-0.882657,-0.756688

allylK +Me2CO (TS)
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,2.642200

C,0,1.202206,0.000000,3.386199
C,0,1.783026,1.020347,4.134036
K,0,1.846061,2.268899,1.471006
O,0,0.618231,1.016357,-0.404470
C,0,-1.508543,0.019630,0.034830
C,0,0.678460,-1.348368,-0.065639
H,0,-0.448176,-0.971672,2.455030
H,0,-0.725473,0.795793,2.847457
H,0,1.807992,-0.909207,3.288169
H,0,2.697100,0.833387,4.690537
H,0,1.171792,1.855663,4.483001
H,0,-1.863264,1.018236,0.297778
H,0,-1.867828,-0.216605,-0.977952
H,0,-1.921275,-0.717059,0.725998
H,0,0.632135,-1.693417,-1.109439
H,0,1.729544,-1.256591,0.215781
H,0,0.190644,-2.092686,0.566176

allylRb
C,0,-0.9984196603,1.6653772839,-0.9400417139
C,0,-1.0048708272,1.6629706197,0.4631654945
C,0,0.0664978234,1.6656673711,1.3693651949
Rb,0,0.3989645214,-1.0583404453,-0.1838424065
H,0,-1.938044513,1.8071714564,-1.4684779486
H,0,-0.1097468902,2.0307299781,-1.4633904953
H,0,-1.9929186403,1.5179210028,0.9187936878
H,0,-0.1417286219,1.8076451896,2.4270651333
H,0,1.0415073565,2.0310372025,1.0332448116

allylRb +h2o (Mode B complex) (-7.1921 cm^{-1})
C,0,-1.2229153638,-2.2478358504,-0.8377007153
C,0,-1.2299036802,-2.2391017899,0.5651700527
C,0,-0.1611080649,-2.2471507767,1.4738950927
Rb,0,0.1908633844,0.4998051413,-0.0882740641
O,0,1.2485928518,3.2892788538,-0.5719522079
H,0,1.1325208357,3.8358764477,-1.3681843532
H,0,-0.3721615216,-2.3813149648,2.5321791631
H,0,0.8148126328,-2.6131310592,1.1415845676
H,0,-2.217572355,-2.0839148536,1.0188000446
H,0,-0.3348938862,-2.6138896421,-1.3613566007
H,0,-2.1632279002,-2.3824516445,-1.367039287
H,0,1.7733968102,3.8363351609,0.0375879218

allylRb +h2o (Mode A complex)
C,0,-0.4296190429,0.3846704261,2.3792211473

C,0,0.8809255047,0.3386373572,1.9399520689
C,0,1.5951956074,-0.722398429,1.3050534796
Rb,0,-0.911320861,0.1426742699,-0.7962987444
O,0,1.7002144084,-0.4605314717,-1.5299629701
H,0,-0.9992667005,-0.5368399938,2.5175047304
H,0,-0.8110061136,1.2679733286,2.8844817401
H,0,1.4259494779,1.2884665302,2.0037183732
H,0,2.6787480074,-0.6798939822,1.4409538945
H,0,1.1927619324,-1.7279837888,1.4770530029
H,0,1.7616236094,-0.5625039166,-0.493083451
H,0,2.5893339629,-0.6493705162,-1.8732311597

allylRb +h2o (TS)

Rb,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,3.291584
C,0,1.349168,0.000000,3.041346
C,0,2.164487,-1.029937,2.439404
H,0,-0.578084,-0.924713,3.245734
H,0,-0.487638,0.857591,3.747706
H,0,1.866545,0.945245,3.242326
H,0,3.189048,-1.034468,2.825565
H,0,1.721258,-2.032689,2.504260
H,0,2.495228,-0.766669,0.956664
O,0,2.642201,-0.569753,-0.171262
H,0,3.578093,-0.751903,-0.362186

allylRb +Me2CO (TS)

C,0,0.000000,0.000000,0.000000
O,0,0.000000,0.000000,1.255565
C,0,2.498161,0.000000,-0.893574
C,0,3.381340,1.072335,-0.626388
C,0,4.519685,1.111741,0.171681
Rb,0,2.451176,0.426464,2.428707
C,0,-0.222235,-1.299860,-0.735176
C,0,-0.312304,1.282258,-0.735997
H,0,1.940859,0.063217,-1.823918
H,0,2.839034,-1.012843,-0.647235
H,0,3.076540,2.037718,-1.049501
H,0,5.114093,2.019470,0.228697
H,0,5.032175,0.185266,0.439428
H,0,0.259080,-2.119015,-0.196966
H,0,-1.305670,-1.490992,-0.752766
H,0,0.138143,-1.268293,-1.764594
H,0,0.158563,2.128902,-0.232116
H,0,0.003026,1.252790,-1.780478

H,0,-1.402712,1.427715,-0.705194

allylCs

C,0,-1.1244683722,2.0721261656,-0.8838350946
C,0,-1.1323211628,2.0713491956,0.5186837653
C,0,-0.0652267707,2.0720541206,1.4288653313
Cs,0,0.3219821952,-0.8821788514,-0.1475006106
H,0,-2.0622092553,2.2227619812,-1.4138541648
H,0,-0.230929386,2.4240327212,-1.4080022849
H,0,-2.1226735932,1.9332927742,0.9722701696
H,0,-0.2764421018,2.2226020797,2.4851289048
H,0,0.9153314361,2.4239703772,1.0947069487
]

allylCs +h2o (Mode B complex) (-1.3996 cm^{-1})

C,0,0.00985,0.01299,-0.01329
C,0,0.00228,0.02193,1.38899
C,0,1.06758,0.01379,2.30093
Cs,0,1.48965,2.98583,0.7082
O,0,2.63547,6.01719,0.23752
H,0,2.53147,6.57566,-0.55211
H,0,0.85374,-0.12648,3.35818
H,0,2.04741,-0.34313,1.97038
H,0,-0.98695,0.17377,1.84107
H,0,0.90109,-0.34397,-0.53769
H,0,-0.92949,-0.12778,-0.54339
H,0,3.15129,6.55581,0.86208

allylCs +h2o (Mode A complex)

C,0,-1.1824973324,-2.2046294131,-1.0316599523
C,0,-1.2090186583,-2.1810259995,0.3487203643
C,0,-0.1291967547,-2.1774964249,1.2858314649
Cs,0,0.2741178648,0.8819822176,-0.5284321188
O,0,0.4351419037,0.3846729386,2.4040139615
H,0,-0.2714612275,-2.4827531029,-1.5656957286
H,0,-2.1061359573,-2.2326822224,-1.603821539
H,0,-2.2044889826,-2.0558678476,0.7923912667
H,0,-0.3823312995,-2.6045980716,2.2602501088
H,0,0.822858271,-2.5648083611,0.9019282887
H,0,0.214432937,-0.5760078941,2.0580452534
H,0,0.4937849383,0.3092230466,3.3712059326

allylCs +Me2CO (TS)

C,0,0.000000,0.000000,0.000000
O,0,0.000000,0.000000,1.255399
C,0,2.482644,0.000000,-0.935921

C,0,3.310185,1.140403,-0.774322
C,0,4.497396,1.289579,-0.072423
Cs,0,2.597670,0.402595,2.567510
C,0,-0.243846,-1.299663,-0.730827
C,0,-0.302087,1.284856,-0.735767
H,0,1.888631,-0.023222,-1.845413
H,0,2.912064,-0.974834,-0.671340
H,0,2.909541,2.064633,-1.209557
H,0,5.022875,2.240682,-0.077216
H,0,5.088000,0.414691,0.206784
H,0,0.261664,-2.117651,-0.213217
H,0,-1.326180,-1.496196,-0.706537
H,0,0.077030,-1.265884,-1.773147
H,0,0.168085,2.127471,-0.224515
H,0,0.022479,1.257796,-1.777603
H,0,-1.392362,1.434712,-0.714424

allylBeBr

C,0,-1.308515208,2.0121256297,-2.431423891
C,0,-1.3176785519,1.9935791279,-1.0847577645
C,0,-0.1032617205,2.0351846311,-0.2005950946
Be,0,0.226664383,0.4450562317,0.2829988652
Br,0,0.5679578422,-1.4032497027,0.7953573505
H,0,-0.3819414603,2.1048454831,-2.9943150765
H,0,-2.2287740551,1.9437292027,-3.0033828183
H,0,0.7554423783,2.4402884645,-0.754603351
H,0,-0.2718684557,2.6926923419,0.6624149742
H,0,-2.2813075339,1.906622842,-0.5789559572

allylBeBr +h2o (complex)

C,0,-1.7828998297,2.2869966175,-2.003365418
C,0,-1.716402012,1.9828797647,-0.6809770471
C,0,-0.486571204,1.7994731419,0.1252040556
Be,0,0.0629438961,0.1480327992,-0.0535349588
O,0,-0.3022547938,-0.316390249,-1.6177030463
Br,0,0.9742518238,-1.2776469079,1.0504082709
H,0,-0.8949901078,2.5836059554,-2.5615256886
H,0,-2.7371482114,2.3685273782,-2.5159831017
H,0,0.3234647238,2.446029106,-0.2456559101
H,0,-0.6577456217,2.0442394283,1.1785131788
H,0,-2.6613083246,1.7581317936,-0.1785428304
H,0,-0.998210913,0.2777203375,-2.0089682746
H,0,-0.3913743388,-1.2377185716,-1.9215321907

allylBeBr +h2o (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.396283
C,0,1.151272,0.000000,2.226250
Be, 0,1.768204,-1.711483,1.965740
Br,0,2.933841,-2.767549,3.234134
H,0,0.824272,0.488400,-0.521776
H,0,-0.955160,0.002096,-0.517886
H,0,2.015334,0.557829,1.846505
H,0,0.983654,0.145137,3.292381
H,0,-0.946672,-0.255850,1.880743
H,0,0.592632,-1.327533,0.075537
O,0,1.320294,-2.169060,0.542348
H,0,1.573165,-2.949032,0.021993

allylBeBr +Me2CO (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.367455
C,0,1.177153,0.000000,2.216938
Be,0,1.810687,-1.676678,2.266725
Br,0,2.486559,-2.831156,3.776271
H,0,0.902504,0.247095,-0.554702
H,0,-0.932001,-0.020947,-0.559128
H,0,2.009562,0.581472,1.799815
H,0,0.975853,0.311659,3.245557
H,0,-0.962622,-0.156790,1.862456
C,0,0.788557,-2.366814,-0.001959
O,0,1.795390,-2.192392,0.746259
C,0,-0.452134,-3.008025,0.551873
C,0,1.021476,-2.416578,-1.482212
H,0,0.127322,-2.131491,-2.040193
H,0,1.862389,-1.777216,-1.755730
H,0,1.272430,-3.453194,-1.748525
H,0,-1.336068,-2.750139,-0.034758
H,0,-0.307442,-4.097169,0.501900
H,0,-0.606162,-2.738269,1.598655

allylMgBr

C,0,-1.0942201611,1.7986903406,-1.7668196892
C,0,-1.1731325497,2.4280225073,-0.5541365635
C,0,-0.0406992738,2.7080727999,0.3411200129
Mg,0,0.0633394978,0.5924048854,0.2528493474
Br,0,0.4806143776,-1.7402430259,0.358442245
H,0,-0.1330786616,1.6432351723,-2.2650380567
H,0,-1.9815873312,1.5522833419,-2.3394240344
H,0,0.8448433256,3.1044999595,-0.1684982179

H,0,-0.2876037016,3.2983916062,1.221361042
H,0,-2.1758389129,2.5925233156,-0.1490540376

allylMgBr +h2o (complex)
C,0,-1.9297374845,2.5065461344,-2.103492058
C,0,-1.8959284851,2.2991059533,-0.7580929295
C,0,-0.7148197607,2.2759305741,0.1196189089
Mg,0,0.0368243235,0.2612494565,0.118009365
Br,0,1.1784123664,-1.6081697403,1.0955580158
H,0,-1.0400714487,2.818056779,-2.6504471791
H,0,-2.8709107108,2.5124741223,-2.6459615746
H,0,0.0915965358,2.9136913898,-0.2683213829
H,0,-0.961272385,2.6014904226,1.1357876489
H,0,-2.8497360831,2.0579775889,-0.2786730435
H,0,-1.2222089558,0.4854333509,-2.1296213637
O,0,-0.6154340649,-0.2132868838,-1.7704049982
H,0,-0.6673347556,-1.0213771207,-2.3083695823

allylMgBr +h2o (TS)
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.405798
C,0,1.118874,0.000000,2.259184
Mg,0,1.701782,-2.158780,2.014050
Br,0,2.936402,-3.652302,3.407234
H,0,0.848562,0.463953,-0.506452
H,0,-0.959153,0.124151,-0.497004
H,0,2.037683,0.462912,1.884737
H,0,0.940942,0.148787,3.323661
H,0,-0.965023,-0.194265,1.884940
H,0,0.423994,-1.392277,-0.060019
O,0,0.990479,-2.412789,0.218708
H,0,1.063039,-3.042704,-0.516509

allylMgBr +Me2CO (TS)
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.371059
C,0,1.154947,0.000000,2.233476
Mg,0,1.814224,-2.079558,2.403921
Br,0,2.708412,-3.659140,3.967099
H,0,0.913543,0.215381,-0.550103
H,0,-0.933504,0.060467,-0.552362
H,0,2.028791,0.511074,1.813100
H,0,0.952869,0.340548,3.253036
H,0,-0.971174,-0.114329,1.863109
C,0,0.443571,-2.426094,-0.261051

O,0,1.427607,-2.591810,0.513330
C,0,-0.919672,-2.908683,0.159140
C,0,0.717296,-2.276550,-1.731788
H,0,-0.095386,-1.767287,-2.252999
H,0,1.660750,-1.751509,-1.889974
H,0,0.812996,-3.288325,-2.151727
H,0,-0.958044,-3.991068,-0.031193
H,0,-1.081159,-2.747077,1.227301
H,0,-1.717402,-2.429836,-0.411737

allylCaBr
C,0,-1.089875858,-1.2615523968,-0.9150337145
C,0,-1.1211503541,-1.2650776056,0.491623372
C,0,-0.018119864,-1.3261084943,1.3629901491
Ca,0,0.422027156,0.7999896321,-0.1758722165
Br,0,1.8384650369,3.2053708188,-0.7741340648
H,0,-0.2735037426,-1.8015976152,-1.4085667788
H,0,-2.0307531869,-1.2709340934,-1.4559527132
H,0,-2.0791901848,-0.9968976117,0.9499575529
H,0,0.8707308213,-1.8705285094,1.0235215178
H,0,-0.2019340686,-1.3811032421,2.4312222007

allylCaBr +h2o (Mode B complex)
C,0,-0.9351170215,3.0528303588,-0.4773508564
C,0,-1.1465462885,2.9438980318,0.908578523
C,0,-0.2050804705,2.6045601663,1.896415363
Ca,0,-0.2258305419,0.5430976304,0.171999542
O,0,-1.9167279358,-1.1954835057,0.3636849778
Br,0,1.1848704957,-1.8469246268,-0.7131771066
H,0,-2.8388804871,-1.3782978319,0.6127368808
H,0,-2.1941759663,2.9397280902,1.2299855628
H,0,0.0607014032,3.3441350206,-0.8290887447
H,0,0.8454349496,2.862237431,1.7224935035
H,0,-0.5121735282,2.6220413723,2.9374598006
H,0,-1.7555590636,3.3855802078,-1.1054749399
H,0,-1.5049176505,-2.0388782565,0.0777578299

allylCaBr +h2o (Mode A complex)
H,0,2.441327994,1.4960948987,0.0351659391
C,0,4.0566820553,0.4125953294,-0.0938785765
C,0,3.3446169338,-0.6389050622,0.4319592201
C,0,2.3897353018,-1.5040262387,-0.2219008254
Ca,0,0.1549186821,-0.1968015001,-0.0570476265
Br,0,-2.7068027411,-0.021220884,0.022674849
O,0,1.4726714856,1.7775570103,-0.0258640636

H,0,4.7930970123,0.9320600231,0.5128444199
H,0,4.1135067785,0.5616684146,-1.172644028
H,0,3.4515936913,-0.7888703026,1.5124075638
H,0,2.5832177413,-1.6349811645,-1.2938762736
H,0,2.290630415,-2.4743311536,0.2725283554
H,0,1.4387710357,2.7486799713,-0.0092595608

allylCaBr +h2o (TS)

Ca,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,2.681839
C,0,1.393144,0.000000,2.813956
C,0,2.284531,-1.085661,2.680628
H,0,-0.528539,-0.937689,2.875656
H,0,-0.534883,0.899917,2.983216
H,0,1.859910,0.988923,2.890115
H,0,3.306512,-0.917024,3.014667
H,0,1.891014,-2.079846,2.905367
H,0,2.287360,-1.161829,1.162509
O,0,1.985221,-1.159980,0.048490
H,0,2.668130,-1.625507,-0.462446
Br,0,-1.720031,0.901755,-2.100947

allylCaBr +MeCHO (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,2.621471
C,0,1.380841,0.000000,2.937316
C,0,2.113897,0.992044,3.584978
Ca,0,1.048960,2.386237,1.555106
O,0,0.645464,1.030400,-0.317906
H,0,0.550273,-0.932997,0.180152
C,0,-1.476512,-0.105409,-0.212852
H,0,-0.447725,-0.958471,2.376282
H,0,-0.657962,0.629067,3.235782
H,0,1.971300,-0.801583,2.481377
H,0,3.174285,0.844546,3.761297
H,0,1.610824,1.669417,4.281810
Br,0,0.544463,5.202806,1.632813
H,0,-1.963568,0.864009,-0.089115
H,0,-1.631992,-0.433957,-1.250421
H,0,-1.925767,-0.845148,0.451918

allylSrBr

C,0,-1.8310153184,-2.6259434572,-0.5484642082
C,0,-1.84532735,-2.6102196694,0.8570955371
C,0,-0.7396897364,-2.6512510581,1.7242818552

Sr,0,-0.2557874044,-0.3777588204,0.1187778851
Br,0,1.2450586068,2.1644646639,-0.5739787773
H,0,-1.0107517132,-3.1594897243,-1.0427532268
H,0,-2.7794173148,-2.670025281,-1.0755772746
H,0,-2.8031999709,-2.3476409499,1.3199707734
H,0,0.1542389996,-3.186611235,1.3835322544
H,0,-0.9218054448,-2.7131757635,2.7930459424

allylSrBr +h2o (Mode B complex)

C,0,-0.8280294957,3.2201742238,-0.4346005509
C,0,-1.032636118,3.1076952939,0.9509076671
C,0,-0.0991086085,2.7376791841,1.9336691901
Sr,0,-0.1643213563,0.5147072925,0.1554884548
O,0,-1.8891563636,-1.4236630596,0.2916888428
Br,0,1.1498781493,-2.1310373449,-0.7881807795
H,0,-2.7842778691,-1.7382655478,0.5032813496
H,0,-2.0784182844,3.1333993882,1.2780161718
H,0,0.176084558,3.481557048,-0.7869019998
H,0,0.9572673555,2.9645584295,1.7512363175
H,0,-0.3985659851,2.7777670408,2.9768325325
H,0,-1.6382803202,3.5982931436,-1.0510323665
H,0,-1.3634368974,-2.1938672801,-0.0270345865

allylSrBr +h2o (Mode A complex)

Br,0,2.6983251139,-0.1367642895,0.0873293299
Sr,0,-0.3292288666,0.0047892644,-0.110400439
O,0,-1.3734710624,2.3304977752,-0.3128752369
C,0,-3.1304740555,0.2239382285,0.8615307268
C,0,-3.1515705654,-0.7473444708,-0.1672305371
C,0,-2.4151117139,-1.9296382404,-0.2521611473
H,0,-2.0854703163,-2.4119197232,0.6737541756
H,0,-2.586541002,-2.6010702251,-1.0878974471
H,0,-3.6893945443,-0.4596489389,-1.0773558456
H,0,-3.95218787,0.9402053624,0.8654024044
H,0,-2.8643802426,-0.1220666953,1.867212333
H,0,-2.2147181392,2.0334664314,0.130502542
H,0,-1.3672834312,3.3000765676,-0.382760385

allylSrBr +h2o (TS)

Sr,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,2.929967
C,0,1.355749,0.000000,2.686966
C,0,2.137025,-1.005573,2.013311
H,0,-0.560026,-0.939080,2.919412
H,0,-0.468065,0.829936,3.450568

H,0,1.881824,0.932874,2.915259
H,0,3.184119,-1.017327,2.325001
H,0,1.706303,-2.014663,2.061809
H,0,2.483612,-0.582998,0.511459
O,0,2.390836,-0.197251,-0.538930
H,0,3.236397,-0.263466,-1.012647
Br,0,-2.466825,0.104783,-1.760715

allylSrBr +MeCHO (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,2.641801
C,0,1.335381,0.000000,3.116813
C,0,1.985246,0.977989,3.863652
Sr,0,1.223263,2.506477,1.583741
O,0,0.623199,1.032246,-0.348747
H,0,0.565262,-0.923370,0.183202
C,0,-1.481243,-0.124699,-0.170132
H,0,-0.409327,-0.965883,2.360267
H,0,-0.723534,0.621653,3.186175
H,0,1.974857,-0.798406,2.724584
H,0,3.014244,0.820871,4.171543
H,0,1.399532,1.644797,4.502977
Br,0,1.089172,5.537345,1.447210
H,0,-1.972396,0.843033,-0.049007
H,0,-1.663763,-0.472149,-1.196862
H,0,-1.905771,-0.855707,0.519921

allylBaBr

C,0,-0.7986579704,0.2398939932,3.2873336214
C,0,0.5307702222,-0.1952403939,3.4104133273
C,0,1.105204483,-1.3700851458,2.8989036792
Ba,0,0.0672740587,-0.0195331097,0.4101901224
H,0,-1.5790880033,-0.524568318,3.1966343663
H,0,-1.1033581297,1.1300546681,3.8307758807
H,0,1.238850468,0.5505361284,3.7899023253
H,0,0.4562306534,-2.2457143916,2.781402036
H,0,2.1306186274,-1.6047216768,3.1709866339
Br,0,-0.2838428946,0.3354530576,-2.7805786247

allylBaBr +h2o (Mode B complex)

C,0,-0.8190406951,3.4023322233,-0.3689092673
C,0,-1.0145494987,3.2798581969,1.0158243306
C,0,-0.0822056283,2.898556175,1.9936039455
Ba,0,-0.1326549204,0.4903995364,0.1459514829
O,0,-1.8473651745,-1.7081213446,0.2118795619

allylBaBr +h2o (Mode A complex)

Br,0,2.9420128374,-0.2469258842,0.183121235
Ba,0,-0.2639394655,0.0350982287,-0.0916412172
O,0,-1.5375251841,2.4343568103,-0.3166631762
C,0,-3.3377625843,0.3460773998,0.6501042695
C,0,-3.3076216873,-0.7181268252,-0.2916511343
C,0,-2.6220667681,-1.9232065617,-0.2127684187
H,0,-2.3561586445,-2.3239982666,0.7700391723
H,0,-2.7396998673,-2.6600469274,-1.0018018618
H,0,-3.765776792,-0.4990196999,-1.2626856714
H,0,-4.1779986104,1.0345965125,0.5450971198
H,0,-3.159254708,0.07015296,1.6967882717
H,0,-2.3632435361,1.9673601596,0.0376137404
H,0,-1.7227993739,3.3845418424,-0.4031887214

allylBaBr +h2o (TS)

Ba,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,3.148954
C,0,1.353503,0.000000,2.908782
C,0,2.139621,-1.002018,2.230509
H,0,-0.565957,-0.934664,3.117317
H,0,-0.470526,0.826677,3.673046
H,0,1.881018,0.928812,3.150467
H,0,3.174731,-1.037771,2.580969
H,0,1.694673,-2.006587,2.258743
H,0,2.573512,-0.572813,0.753318
O,0,2.609144,-0.205361,-0.308654
H,0,3.520405,-0.256609,-0.642553
Br,0,-2.499296,0.132733,-2.038585

allylBaBr +MeCHO (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,2.654348
C,0,1.122933,0.000000,3.525608
C,0,1.584247,1.023651,4.340802
Ba,0,1.861412,2.342686,1.598812

O,0,0.730200,0.942695,-0.388353
H,0,0.445525,-0.993804,0.139104
C,0,-1.493275,0.076710,-0.055437
H,0,-0.358635,-0.987015,2.373364
H,0,-0.812117,0.694865,2.904722
H,0,1.781212,-0.872130,3.442214
H,0,2.443773,0.858770,4.983483
H,0,0.897297,1.811441,4.662187
Br,0,3.157145,5.254270,1.051014
H,0,-1.835966,1.104997,0.078526
H,0,-1.802275,-0.258120,-1.055556
H,0,-1.958699,-0.578300,0.683116

allylZnBr

C,0,-1.4029180352,-2.1999771134,-2.7734644046
C,0,-1.4127404232,-2.1801175033,-1.427047679
C,0,-0.2028490317,-2.2062704452,-0.5507425584
Zn,0,0.1465577633,-0.3864902567,0.1430884012
H,0,-0.4733372465,-2.260070458,-3.3358473619
H,0,-2.3247357917,-2.162954511,-3.3455225979
H,0,-2.3778017574,-2.1233134089,-0.919564861
H,0,0.6742243339,-2.548916045,-1.1132075208
H,0,-0.3450220574,-2.8886214375,0.2954471492
Br,0,0.5303138446,1.8027649695,0.9323877431

allylZnBr +h2o (complex)

C,0,-1.8982366548,2.5817717271,-1.9751291174
C,0,-1.8337658296,2.2549391105,-0.6632204446
C,0,-0.6093440425,2.1887932924,0.1753358479
Zn,0,0.0715221605,0.2957741965,0.1701243557
O,0,-0.4790436086,-0.2547275252,-1.8506041941
Br,0,1.0497015511,-1.743025439,0.9473817453
H,0,-1.0157540426,2.9096594828,-2.5227548892
H,0,-2.8474634296,2.6100186151,-2.5029019918
H,0,0.1759508444,2.8440023512,-0.2217673075
H,0,-0.8254847727,2.5033251358,1.2015890077
H,0,-2.7671137255,1.9690540573,-0.1710757841
H,0,-1.1614614818,0.3324080878,-2.2403615196
H,0,-0.5634644645,-1.1510078397,-2.2219034357

allylZnBr +h2o (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.406316
C,0,1.132289,0.000000,2.248966
Zn,0,1.651097,-2.060256,1.991306

Br,0,2.943533,-3.544262,3.316408
H,0,0.846807,0.475340,-0.499041
H,0,-0.960215,0.130173,-0.493709
H,0,2.025545,0.505848,1.872579
H,0,0.950955,0.148849,3.312183
H,0,-0.958150,-0.213255,1.889778
H,0,0.372403,-1.340929,-0.086663
O,0,0.887988,-2.435589,0.233258
H,0,1.211500,-3.008502,-0.482879

allylZnBr +MeCHO (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.373959
C,0,1.169615,0.000000,2.211788
Zn,0,1.746524,-1.994727,2.356602
Br,0,2.551380,-3.623967,3.890745
H,0,0.902214,0.272194,-0.543234
H,0,-0.938135,0.065364,-0.543924
H,0,2.030624,0.522240,1.784771
H,0,0.980373,0.315439,3.240644
H,0,-0.961083,-0.152370,1.873634
C,0,0.440037,-2.231956,-0.303207
O,0,1.432712,-2.508275,0.435263
H,0,-0.568989,-2.474649,0.055111
C,0,0.638672,-2.146228,-1.788527
H,0,-0.200455,-1.656059,-2.287266
H,0,1.572377,-1.629086,-2.020163
H,0,0.716421,-3.173131,-2.169727

allylCdBr

C,0,-1.4837359921,-2.2639899918,-2.8969208686
C,0,-1.4898307237,-2.238629546,-1.5497089864
C,0,-0.2810686198,-2.2900010065,-0.6785222184
Cd,0,0.1204197259,-0.3277391381,0.1150718338
H,0,-0.5564396019,-2.3367108248,-3.4615590935
H,0,-2.4064969799,-2.2157063116,-3.4667051604
H,0,-2.4527351375,-2.1691137271,-1.0395515642
H,0,0.6025403002,-2.6168989427,-1.2383293278
H,0,-0.4218498857,-2.9665189274,0.1714023251
Br,0,0.5423613278,1.965490018,0.9789202068

allylCdBr +h2o (complex)

C,0,-1.96055419,2.6121538847,-2.0901383599
C,0,-1.8871054119,2.3149932849,-0.7714893229
C,0,-0.6665780099,2.3303120111,0.0710249827

Cd,0,0.0947140509,0.2893867824,0.2342498059
O,0,-0.4939287839,-0.2313462933,-2.0427553115
Br,0,1.0253582729,-1.9452836149,0.8995386319
H,0,-1.0884824471,2.9555216006,-2.6445685872
H,0,-2.9085515751,2.5904479359,-2.6205229529
H,0,0.1235648367,2.9458118712,-0.3743684919
H,0,-0.8800162881,2.7066867158,1.0761566269
H,0,-2.8105290216,2.0109626757,-0.2716464097
H,0,-1.1742424065,0.3954422136,-2.3669968018
H,0,-0.6587011506,-1.1044967856,-2.4402374889

allylHgBr

C,0,-0.9736900695,-1.1928060763,-2.2109641445
C,0,-0.9887722089,-1.211587975,-0.8645643638
C,0,0.2253906388,-1.2529572251,-0.002299059
Hg,0,0.5561758444,0.6810027189,0.8958817201
H,0,-0.0409109796,-1.2074454414,-2.7705905162
H,0,-1.8944685406,-1.163536705,-2.7850956924
H,0,-1.9518218485,-1.1959268341,-0.35211195
H,0,1.1250567251,-1.4996172098,-0.5757094202
H,0,0.1236303788,-1.9630162455,0.8244912219
Br,0,0.9124048528,2.9716596382,1.9107715884

allylCdBr +h2o (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.410566
C,0,1.121833,0.000000,2.261333
Cd,0,1.565400,-2.271466,1.994123
Br,0,2.873194,-3.987536,3.268221
H,0,0.867237,0.446676,-0.491381
H,0,-0.953123,0.204171,-0.483597
H,0,2.044752,0.446909,1.885104
H,0,0.948122,0.141866,3.326373
H,0,-0.966129,-0.178428,1.893008
H,0,0.247122,-1.353398,-0.149124
O,0,0.613949,-2.536721,0.068894
H,0,1.001025,-2.992493,-0.699822

allylHgBr +h2o (complex)

C,0,-1.3383486577,2.1465593062,-2.9667687102
C,0,-1.343883856,2.2258688027,-1.6188894782
C,0,-0.1376712001,2.2470070548,-0.7509528052
Hg,0,0.1371067617,0.3017904967,0.1731116996
O,0,-0.4848897855,-0.8925191638,-2.0956719465
Br,0,0.4612276409,-1.9013026581,1.4049343615
H,0,-0.4077277444,2.1106971327,-3.5301447797
H,0,-2.2636048772,2.161741138,-3.536266369
H,0,0.7722688892,2.4573003476,-1.3227942699
H,0,-0.2310650041,2.9786760845,0.0569263336
H,0,-2.3083159597,2.2785072783,-1.1093454622
H,0,-1.0860857947,-0.3457017449,-2.6359000307
H,0,-0.7884373096,-1.8153246066,-2.1590725114

allylHgBr +h2o (TS)

H,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.325379
C,0,1.402417,0.000000,1.506533
C,0,2.257174,1.116611,1.453194
Hg,0,2.328671,1.162023,-0.898030
O,0,0.357646,0.107898,-1.268730
H,0,-0.520115,-0.905825,1.631989
H,0,-0.520372,0.927194,1.575976
H,0,1.890595,-0.978525,1.538070
H,0,3.296043,0.979468,1.746050
H,0,1.835851,2.096437,1.683139
Br,0,3.746322,2.102709,-2.787176
H,0,-0.297958,0.556750,-1.835638

allylHgBr +MeCHO (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.390034

allylCdBr +MeCHO (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.378827
C,0,1.163444,0.000000,2.211156
Cd,0,1.723342,-2.190073,2.394481
Br,0,2.502878,-4.093541,3.831712
H,0,0.904203,0.281326,-0.535134
H,0,-0.938404,0.120059,-0.533675
H,0,2.050845,0.467348,1.778049
H,0,0.995218,0.301553,3.246780
H,0,-0.962501,-0.135736,1.880683
C,0,0.306435,-2.150623,-0.422885
O,0,1.305787,-2.559544,0.250304
H,0,-0.703985,-2.389305,-0.059039
C,0,0.462638,-1.991539,-1.912291
H,0,1.411938,-1.504237,-2.146870
H,0,0.481497,-2.997515,-2.351291
H,0,-0.366101,-1.435783,-2.357879

C,0,1.170777,0.000000,2.189231
Hg,0,1.729221,-2.229805,2.311804
Br,0,2.537193,-4.297911,3.555306
H,0,0.893959,0.352730,-0.510699
H,0,-0.940332,0.191227,-0.510295
H,0,2.064939,0.440884,1.746521
H,0,1.041095,0.234497,3.246436
H,0,-0.953323,-0.157059,1.901669
C,0,0.224667,-1.929671,-0.508809
O,0,1.259865,-2.441282,0.063900
H,0,-0.765943,-2.257108,-0.147290
C,0,0.316676,-1.737821,-2.009952
H,0,1.255549,-1.242951,-2.271622
H,0,0.317274,-2.731929,-2.472214
H,0,-0.529017,-1.169300,-2.408285

allylBBr2 +h2o (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.392140
C,0,1.214088,0.000000,2.159082
B,0,1.742176,1.607407,2.029539
H,0,0.789695,-0.536506,-0.527764
H,0,-0.943374,0.105689,-0.528336
H,0,-0.916541,0.307580,1.897164
H,0,2.008939,-0.607138,1.717590
H,0,1.082597,-0.206120,3.221393
Br,0,0.460787,2.883540,3.005492
Br,0,3.623788,1.709859,2.743396
H,0,0.662108,1.139243,0.120446
O,0,1.713284,1.902046,0.577149
H,0,1.635708,2.853624,0.371535

allylBBr2

C,0,-0.5827173109,-0.6059365748,-2.2066943886
C,0,-0.8482773258,-0.7388855618,-0.8956544953
C,0,0.2015805262,-1.0046568323,0.1613751417
B,0,0.4103269396,0.3614412187,0.8982386649
H,0,0.4267106939,-0.7065158822,-2.5981543099
H,0,-1.3733438485,-0.3981730012,-2.9214790671
H,0,-1.8741999781,-0.6301286109,-0.544553368
H,0,1.1239315512,-1.3532408765,-0.314708499
H,0,-0.1537681226,-1.7786417681,0.8522263696
Br,0,-0.8086201579,0.9051749228,2.286850534
Br,0,1.8336943964,1.5457347714,0.3819091808

allylBBr2 +MeCHO (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.369951
C,0,1.225375,0.000000,2.159005
B,0,1.752961,1.573712,2.251038
H,0,0.883041,-0.313601,-0.552053
H,0,-0.931360,0.063513,-0.557755
H,0,-0.939245,0.211332,1.882460
H,0,2.025868,-0.580607,1.690532
H,0,1.071935,-0.339755,3.187538
Br,0,0.422292,2.772983,3.230114
Br,0,3.606164,1.692461,3.006063
C,0,0.796578,2.121616,0.072719
O,0,1.847780,1.971642,0.792863
C,0,0.995557,2.339473,-1.389434
H,0,-0.103170,2.515628,0.548077
H,0,0.081647,2.135437,-1.951385
H,0,1.252728,3.397859,-1.530237
H,0,1.820800,1.732374,-1.766516

allylBBr2 +h2o (complex)

C,0,-1.2176685738,-1.4111090676,-3.0537715535
C,0,-1.3177600161,-1.5118311666,-1.7097099881
C,0,-0.144594581,-1.5274117633,-0.7786052773
B,0,0.0897597706,-0.0804349911,-0.1263609468
O,0,0.0561706822,0.9629931938,-1.4181818248
H,0,-0.2527060016,-1.464059441,-3.5577134668
H,0,-2.0988644034,-1.3554072481,-3.6864777202
H,0,-2.3104423447,-1.49876604,-1.2597871732
H,0,0.7550699317,-1.8354782099,-1.3291324586
H,0,-0.2983371961,-2.255592758,0.0265803087
Br,0,-1.3969629602,0.560504462,1.0488489398
Br,0,1.937323998,0.1869054075,0.634956378
H,0,-0.4829525665,0.5193611839,-2.12835112
H,0,0.9575709711,1.1309384684,-1.768524247

allylAlBr2

C,0,-1.4630411359,-2.2274681465,-1.6642040223
C,0,-1.4718481374,-2.1964295716,-0.3128547418
C,0,-0.2459103813,-2.2218426004,0.5618586216
Al,0,0.1429354821,-0.3288049742,0.3091876652
H,0,-0.5438940682,-2.364807416,-2.2303639934
H,0,-2.3852815966,-2.148087721,-2.2312149353
H,0,-2.4284019451,-2.0591316174,0.1931862227
H,0,0.5388876033,-2.8634043097,0.147435912

H,0,-0.478824314,-2.536538519,1.5819988968
Br,0,-1.0432430278,1.2604181261,1.4200174158
Br,0,1.6867901987,0.3430354784,-1.2197111556

allylAlBr2 +h2o (complex)

C,0,-1.8787002769,-2.4459406134,-2.1753168261
C,0,-1.7985269118,-2.1500941091,-0.8547866406
C,0,-0.5474268488,-2.0733194835,-0.0529877893
Al,0,0.0336740355,-0.1715659012,0.0196732389
O,0,-0.4973059713,0.3121842678,-1.8254497415
H,0,-1.0080516688,-2.7904593351,-2.7330891126
H,0,-2.8337737483,-2.4591144445,-2.6924206036
H,0,-2.7218870902,-1.8708921045,-0.3426397938
H,0,0.2479305801,-2.6785106032,-0.5083683878
H,0,-0.7180810307,-2.444845128,0.9646740392
Br,0,-1.2441916785,1.2114245001,1.3321562662
Br,0,2.2951095261,0.2707220438,-0.1086792685
H,0,-1.0613819588,-0.4203713843,-2.1936394447
H,0,0.201729783,0.5380717727,-2.4698182559

allylAlBr2 +h2o (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.395896
C,0,1.165257,0.000000,2.213083
Al,0,1.718221,2.011736,2.106579
H,0,0.829913,-0.483812,-0.517706
H,0,-0.955660,-0.016897,-0.516814
H,0,-0.944064,0.247108,1.888348
H,0,2.027476,-0.533143,1.802101
H,0,0.994412,-0.204654,3.271346
Br,0,0.457783,3.265233,3.559087
Br,0,4.006963,2.244926,2.167973
H,0,0.513359,1.303815,0.030674
O,0,1.163946,2.329156,0.374309
H,0,1.775337,2.665259,-0.306801

allylAlBr +MeCHO (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.367672
C,0,1.190841,0.000000,2.206109
Al,0,1.693552,1.943330,2.467726
H,0,0.904835,-0.238393,-0.554868
H,0,-0.935479,-0.004898,-0.553022
H,0,-0.958628,0.142872,1.871055
H,0,2.047537,-0.505208,1.747392

H,0,1.003000,-0.408681,3.205568
Br,0,-0.017976,3.186406,3.409394
Br,0,3.819934,2.373273,3.207023
C,0,0.620368,2.325424,-0.096161
O,0,1.661355,2.364396,0.629316
C,0,0.771283,2.376610,-1.578961
H,0,-0.343415,2.595386,0.345937
H,0,1.655072,1.821528,-1.898644
H,0,-0.121278,2.010173,-2.089155
H,0,0.912463,3.432128,-1.850758

allylGa

C,0,-0.606655904,-0.0421811662,-1.1023865212
C,0,-0.445403871,-0.3202883581,0.269058752
C,0,0.7908618627,-0.2693907743,0.9420255552
Ga,0,0.6099578441,1.7765838105,-0.2204671327
H,0,0.1726152348,-0.3414704642,-1.806936863
H,0,-1.6079084636,-0.0004836599,-1.5202532184
H,0,-1.3383663676,-0.2142510603,0.891292171
H,0,1.6983590387,-0.5887891277,0.4246885094
H,0,0.8126144991,-0.3935953279,2.0204240832

allylGa +h2o (complex)

C,0,-0.9971557734,-1.3569869641,-2.0322037505
C,0,-1.0131063563,-1.4692920738,-0.6730780548
C,0,0.1236082119,-1.3554799367,0.2392470736
Ga,0,0.5327467942,0.6391751691,0.9847503555
O,0,-0.1534448106,1.3041003001,-1.0395288318
H,0,-0.059649373,-1.3453643533,-2.5869376182
H,0,-1.9125784613,-1.4429201524,-2.6110306814
H,0,-1.9972594023,-1.5565127156,-0.2034864733
H,0,1.0702187718,-1.6443542296,-0.2421206527
H,0,-0.0157626266,-1.9680225254,1.1376536826
H,0,-0.6457019822,0.6095749208,-1.5589241936
H,0,-0.406935554,2.1909202606,-1.3499760402

allylGa +h2o (TS)

O,0,0.000000,0.000000,0.000000
H,0,0.000000,0.000000,1.143560
C,0,0.600555,0.000000,2.546788
C,0,1.620582,0.858929,2.119859
C,0,2.673538,0.539214,1.237383
Ga,0,1.742343,0.500013,-0.908026
H,0,-0.110719,0.374608,3.279307
H,0,0.810684,-1.069409,2.603621

H,0,1.464212,1.924219,2.315902
H,0,3.477023,1.269384,1.149817
H,0,3.029604,-0.495894,1.252697
H,0,-0.844327,-0.282641,-0.397396

allylGa +MeCHO (TS)

O,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.246352
C,0,2.684737,0.000000,1.538888
C,0,2.846353,0.994750,0.621084
C,0,2.618506,0.903050,-0.813792
Ga,0,0.639021,1.604535,-1.403371
H,0,0.036216,0.952217,1.792639
C,0,-0.258650,-1.241174,2.038512
H,0,2.864223,0.177961,2.596290
H,0,2.537611,-1.032284,1.227975
H,0,3.081994,1.989662,1.011210
H,0,3.284586,1.564397,-1.381040
H,0,2.701547,-0.122925,-1.195178
H,0,0.002053,-2.126114,1.454722
H,0,0.294678,-1.226196,2.980739
H,0,-1.330522,-1.279180,2.276486

allylGa +Me2CO (TS)

O,0,-0.840512,-0.702970,-0.074551
C,0,-0.840512,-0.702970,1.178844
C,0,1.795196,-0.702970,1.360991
C,0,1.903305,0.368158,0.521717
C,0,1.688633,0.371307,-0.912251
Ga,0,-0.371926,0.740507,-1.604209
C,0,-1.055094,0.571895,1.950636
C,0,-1.002634,-2.007199,1.909001
H,0,1.974089,-0.597779,2.428245
H,0,1.714625,-1.715004,0.970219
H,0,2.070474,1.344175,0.987673
H,0,2.247646,1.164611,-1.420847
H,0,1.905913,-0.597757,-1.381924
H,0,-0.671662,-2.833037,1.277073
H,0,-0.455618,-2.008881,2.854701
H,0,-2.069624,-2.143940,2.135878
H,0,-0.629323,1.426482,1.422662
H,0,-2.139982,0.727484,2.046290
H,0,-0.626097,0.512356,2.953269

allylGaBr2

C,0,-1.125991993,-1.8821044184,-2.9901135612
C,0,-1.4254875376,-1.8903776758,-1.6778397424
C,0,-0.4298903275,-2.1108349198,-0.5757088774
Ga,0,0.045390677,-0.3419652583,0.1323204835
H,0,-0.1161599647,-2.0715198861,-3.3476188237
H,0,-1.8899068118,-1.6973070066,-3.7388135385
H,0,-2.4542727183,-1.6969744625,-1.3719057195
H,0,0.4702943497,-2.6059077971,-0.9560931364
H,0,-0.8595692589,-2.7291870937,0.2205228275
Br,0,-1.4828011449,0.9078596572,1.4271387671
Br,0,2.0922503611,0.7121895238,-0.382740296

allylGaBr2 +h2o (complex)

C,0,-1.4267153031,-1.9465869182,-2.982252139
C,0,-1.5360524093,-1.9784077897,-1.634280767
C,0,-0.3962666714,-2.0269520064,-0.6747361751
Ga,0,0.0128240414,-0.1995267112,-0.0057051134
O,0,-0.5250509989,0.8251453492,-1.7251205168
H,0,-0.4622893315,-2.057003529,-3.4766382167
H,0,-2.306762541,-1.9041071158,-3.6175016116
H,0,-2.5351457373,-1.9082254076,-1.1995793199
H,0,0.5009848283,-2.4349464135,-1.1558516346
H,0,-0.6439099801,-2.6678962705,0.1789304739
Br,0,-1.4310776075,0.7446315725,1.633386434
Br,0,2.2928402237,0.53305656,0.067942599
H,0,-0.910620217,0.1851732411,-2.3730940354
H,0,0.1531204205,1.363766397,-2.1773446778

allylGaBr2 +h2o (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.398488
C,0,1.166831,0.000000,2.210544
Ga,0,1.747726,2.021767,2.054728
H,0,0.829112,-0.491300,-0.512264
H,0,-0.958403,-0.036749,-0.511324
H,0,-0.941419,0.253239,1.892812
H,0,2.020781,-0.550525,1.807758
H,0,0.996600,-0.179421,3.272390
Br,0,0.557999,3.353198,3.626426
Br,0,4.125540,2.221234,1.979535
H,0,0.468725,1.280805,-0.006635
O,0,1.107466,2.367551,0.315402
H,0,1.728723,2.675366,-0.371314

allylGaBr2 +MeCHO (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.374902
C,0,1.189388,0.000000,2.195478
Ga,0,1.728399,1.979482,2.323846
H,0,0.890835,-0.302507,-0.545557
H,0,-0.941844,-0.031566,-0.540997
H,0,-0.951613,0.176462,1.880524
H,0,2.041392,-0.526665,1.757040
H,0,1.007849,-0.327419,3.223342
Br,0,-0.052964,3.324331,3.235189
Br,0,3.930439,2.491040,3.036547
C,0,0.544536,2.153377,-0.221225
O,0,1.639947,2.282884,0.430998
C,0,0.620370,2.170385,-1.716171
H,0,-0.385018,2.495520,0.246457
H,0,1.479558,1.595886,-2.068154
H,0,-0.299808,1.803914,-2.175637
H,0,0.763019,3.216838,-2.016992

allylGaBr2 +Me2CO (TS)
O,0-0.840512,-0.702970,-0.074551
C,0-0.840512,-0.702970,1.178844
C,01.795196,-0.702970,1.360991
C,01.903305,0.368158,0.521717
C,01.688633,0.371307,-0.912251
Ga,0-0.371926,0.740507,-1.604209
C,0-1.055094,0.571895,1.950636
C,0-1.002634,-2.007199,1.909001
H,01.974089,-0.597779,2.428245
H,01.714625,-1.715004,0.970219
H,02.070474,1.344175,0.987673
H,02.247646,1.164611,-1.420847
H,01.905913,-0.597757,-1.381924
H,0-0.671662,-2.833037,1.277073
H,0-0.455618,-2.008881,2.854701
H,0-2.069624,-2.143940,2.135878
H,0-0.629323,1.426482,1.422662
H,0-2.139982,0.727484,2.046290
H,0-0.626097,0.512356,2.953269

allylIn
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.406973
C,0,1.143515,0.000000,2.226646
In,0,1.429606,1.993907,0.672454

H,0,-0.946955,0.051119,-0.528833
H,0,0.803524,-0.507201,-0.538393
H,0,-0.933013,0.311629,1.886233
H,0,2.049673,-0.506253,1.887032
H,0,1.022171,0.050989,3.304435

allylIn +h2o (σ-complex)
O,0,0.000000,0.000000,0.000000
H,0,0.000000,0.000000,1.000429
C,0,0.834439,0.000000,2.831209
C,0,1.612526,0.984132,2.287235
C,0,2.680118,0.837877,1.310821
In,0,1.972351,0.939983,-0.941902
H,0,0.062424,0.238411,3.557603
H,0,1.087502,-1.052284,2.705192
H,0,1.336532,2.012424,2.540900
H,0,3.431564,1.629981,1.397087
H,0,3.172644,-0.143284,1.363639
H,0,-0.891682,-0.215695,-0.323533

allylIn +h2o (π-complex)
C,0,-0.8820199054,-1.5136133674,-0.8619523896
C,0,-0.7977633225,-1.5715373057,0.5510956827
C,0,0.3832450155,-1.6378982971,1.2962173467
In,0,0.5712906229,0.4409459169,-0.2690005005
H,0,-1.8672703583,-1.4587118372,-1.3191182799
H,0,-0.1431784934,-2.0533896479,-1.4571931658
H,0,-1.6897617956,-1.2668034097,1.1032989711
H,0,1.277578563,-2.0963677615,0.8720317171
H,0,0.3374343829,-1.6086810277,2.3805376534
O,0,-1.7278198565,1.4478594462,0.600232935
H,0,-2.4905235696,1.2511218606,0.0265877397
H,0,-1.8157311262,2.3819001455,0.8608525673

allylIn +h2o (TS)
O,0,0.000000,0.000000,0.000000
H,0,0.000000,0.000000,1.145437
C,0,0.527122,0.000000,2.571106
C,0,1.576463,0.873972,2.242865
C,0,2.721846,0.577947,1.486043
In,0,1.908480,0.577485,-0.917535
H,0,-0.235066,0.363805,3.256942
H,0,0.751739,-1.065228,2.651700
H,0,1.389161,1.936169,2.430973
H,0,3.513441,1.325263,1.464772

H,0,3.083159,-0.454138,1.502138
H,0,-0.854054,-0.288961,-0.370453

allylIn +Me2CO (TS)

O,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.248715
C,0,2.710750,0.000000,1.470913
C,0,2.855903,1.051821,0.614404
C,0,2.732618,1.029647,-0.830791
In,0,0.581859,1.471982,-1.732316
C,0,-0.134012,-1.301691,1.990420
H,0,2.833010,0.129172,2.543413
H,0,2.635693,-1.020198,1.099717
H,0,3.002099,2.037254,1.068739
H,0,3.340713,1.802128,-1.315499
H,0,2.960552,0.047451,-1.266209
C,0,-0.191964,1.277992,2.022583
H,0,0.188468,-2.127669,1.354415
H,0,0.435755,-1.293437,2.922371
H,0,-1.193922,-1.444827,2.244271
H,0,0.231035,2.125734,1.481374
H,0,-1.273124,1.442323,2.139662
H,0,0.255946,1.218581,3.016742

allylInBr2

C,0,-0.9580237878,-1.2508211725,-2.0607780491
C,0,-0.9418135849,-1.263341161,-0.7142387473
C,0,0.2960198603,-1.2708454361,0.1260158086
In,0,0.6016631856,0.7079731683,0.8747317874
H,0,-0.0397426506,-1.2697152615,-2.6440889769
H,0,-1.893611237,-1.2335699164,-2.6108554084
H,0,-1.8926739175,-1.2487540143,-0.1795164037
H,0,1.1737582426,-1.5652729104,-0.4592667961
H,0,0.1945526409,-1.957179918,0.9740997241
Br,0,-1.1218209835,1.8389827744,2.3364278965
Br,0,2.5897684747,2.1411056732,0.2620633071

allylInBr2 +h2o (complex)

C,0,-3.8931812239,-0.1985821953,-0.3807592875
C,0,-3.0236289432,0.3465725849,0.5009121842
C,0,-1.9708149465,-0.3855571665,1.256428149
In,0,-0.0987890134,-0.1446540481,0.215585092
H,0,-3.9364118957,-1.2739456166,-0.5481823344
H,0,-4.6369500986,0.4119376736,-0.8848896618
H,0,-3.0587164672,1.4278403197,0.649367184

H,0,-2.1985186736,-1.4548990585,1.3332456889
H,0,-1.8701871372,0.0185604889,2.2692645274
Br,0,0.6946570666,2.248214946,-0.2355344005
Br,0,1.7374052896,-1.8909380507,0.1492041044
O,0,-1.0668962214,-0.3856335703,-1.7947231939
H,0,-2.014916843,-0.128774955,-1.6978087717
H,0,-0.704899244,0.093107392,-2.5648065032

allylInBr2 +h2o (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.401941
C,0,1.148810,0.000000,2.231295
In,0,1.714708,2.206768,2.054916
H,0,0.842621,-0.475085,-0.506073
H,0,-0.960163,-0.095494,-0.501151
H,0,-0.951289,0.225950,1.891766
H,0,2.029144,-0.515381,1.839980
H,0,0.967667,-0.172507,3.291999
Br,0,0.412219,3.599789,3.721897
Br,0,4.227655,2.509143,1.840711
H,0,0.390958,1.313059,-0.072136
O,0,0.940701,2.449543,0.169105
H,0,1.487882,2.769450,-0.572407

allylInBr2 +MeCHO (TS)

O,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.280292
C,0,2.139482,0.000000,1.892330
C,0,2.539900,1.136239,1.225779
C,0,2.829738,1.213630,-0.182819
In,0,0.823891,1.570836,-1.096564
C,0,-0.377999,-1.271220,1.978780
H,0,2.013967,0.029241,2.970979
H,0,2.297358,-0.977528,1.442310
H,0,2.494217,2.081633,1.771279
H,0,3.433102,2.081011,-0.462830
H,0,3.212385,0.291635,-0.627130
H,0,-0.200178,0.943019,1.802918
H,0,0.086000,-2.132844,1.494180
H,0,-0.123393,-1.247028,3.040279
H,0,-1.467258,-1.374995,1.886971
Br,0,-0.296292,3.618359,-0.027861
Br,0,0.444832,1.149751,-3.561959

allylTl

C,0,-2.0506218219,-0.2198415284,-0.7353401037
C,0,-1.1129762727,-0.7208956927,-1.6552856182
C,0,-0.0169799904,-0.0199117712,-2.1885398294
Tl,0,0.3051975122,0.0872393957,0.4387257801
H,0,-2.8413697299,-0.872687115,-0.3774868542
H,0,-2.2872951802,0.8460925438,-0.733076409
H,0,-1.0834041331,-1.8097950509,-1.7636672323
H,0,-0.0784789256,1.0631786584,-2.3125778338
H,0,0.653017988,-0.5292861306,-2.8749865525

allylTl +h2o (complex)

O,0,0.8255303699,1.9098802577,0.0907248237
H,0,1.7536087662,1.5531164543,-0.006851933
C,0,1.3254071753,-1.3351003801,0.248577418
C,0,2.428067421,-0.6628191446,-0.4021343351
C,0,3.2845272542,0.2655813365,0.1286125434
H,0,1.1008101663,-2.3116071989,-0.1917833396
H,0,1.4388956717,-1.4166187261,1.3370713602
H,0,2.5305582151,-0.8515080461,-1.4759238413
H,0,3.320032496,0.4497031964,1.201973079
H,0,4.0888925728,0.6835820547,-0.4705605228
Tl,0,-0.7889052856,-0.0720812428,-0.0098600592
H,0,0.836276187,2.8468999974,-0.1713923526

allylTl +h2o (TS)

H,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.476432
C,0,1.404200,0.000000,1.633407
C,0,2.281493,-1.068979,1.448796
Tl,0,2.511031,-1.053623,-1.197249
O,0,0.290688,-0.238460,-1.108185
H,0,-0.528851,0.882879,1.832485
H,0,-0.523199,-0.941826,1.655247
H,0,1.870932,0.985116,1.741228
H,0,3.320496,-0.937591,1.745676
H,0,1.893662,-2.084824,1.552662
H,0,-0.352135,0.136341,-1.740051

allylTl +MeCHO (TS)

O,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.245134
C,0,2.603446,0.000000,1.703824
C,0,2.974039,0.954586,0.794637
C,0,3.006017,0.828487,-0.639946
Tl,0,0.898108,1.754772,-1.579480

H,0,0.018551,0.953232,1.793627
C,0,-0.272939,-1.239545,2.041848
H,0,2.632523,0.206787,2.770676
H,0,2.484248,-1.038790,1.403137
H,0,3.186418,1.952182,1.194540
H,0,3.746035,1.475660,-1.122325
H,0,3.074136,-0.201496,-1.005612
H,0,0.050117,-2.123693,1.488265
H,0,0.216769,-1.199740,3.017747
H,0,-1.357170,-1.308725,2.205473

allylTl +Me2CO (TS)

O,0,-0.859634,-1.105135,0.586340
C,0,-0.859634,-1.105135,1.837938
C,0,1.700480,-1.105135,2.192598
C,0,1.977160,-0.014980,1.408756
C,0,2.035815,0.032157,-0.025243
Tl,0,-0.158432,0.548075,-1.122323
C,0,-1.111915,0.171478,2.603065
C,0,-1.040006,-2.407372,2.574540
H,0,1.726166,-1.028816,3.276584
H,0,1.683223,-2.106523,1.767549
H,0,2.072812,0.946420,1.924707
H,0,2.646165,0.851583,-0.417410
H,0,2.287942,-0.921522,-0.502465
H,0,-0.662060,-3.232151,1.967715
H,0,-0.549011,-2.397853,3.550317
H,0,-2.116824,-2.559677,2.737280
H,0,-0.660432,1.023630,2.091475
H,0,-2.200009,0.328318,2.647027
H,0,-0.729310,0.117549,3.624731

allylTlBr2

C,0,-1.1885228956,-1.5241570668,-2.1998751379
C,0,-1.1266261576,-1.4517627776,-0.8564857016
C,0,0.1385751041,-1.4782924011,-0.0773816179
Tl,0,0.5253221764,0.5748069743,0.6743154612
H,0,-0.291937538,-1.6135028765,-2.8096174745
H,0,-2.1410465316,-1.503432087,-2.719821725
H,0,-2.0521008725,-1.361417379,-0.2872359836
H,0,1.0010938122,-1.7700641953,-0.6839869947
H,0,0.0754748614,-2.1163193545,0.8098836105
Br,0,-1.3582787127,1.984840129,1.8386550286
Br,0,2.7352460941,1.9605196852,0.4080781593

allylTlBr2 +h2o (complex)

C,0,-1.603304232,-2.0274947452,-2.9540647509
C,0,-1.5355685764,-2.1819316844,-1.6159285207
C,0,-0.2742944346,-2.3129031325,-0.8434635451
Tl,0,0.1322331724,-0.3300971005,0.0681868076
O,0,-0.0661151431,0.8435286155,-2.1251329051
H,0,-0.7077760875,-2.0088926172,-3.5719521617
H,0,-2.5604257265,-1.9478540806,-3.4614183418
H,0,-2.4622888191,-2.1949802911,-1.0409161371
H,0,0.5860920594,-2.558418633,-1.4731749091
H,0,-0.3552357589,-3.0349071206,-0.0259338323
Br,0,-1.9138937527,1.011688679,1.1015833536
Br,0,2.3860752918,0.9387590777,0.560912585
H,0,-0.9460456614,0.8249807984,-2.5474413473
H,0,0.2163637645,1.7780140506,-2.1078483973

allylTlBr2 +h2o (TS)

H,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.326412
C,0,1.399263,0.000000,1.491866
C,0,2.250181,-1.113084,1.333138
Tl,0,2.345883,-1.011641,-1.048145
O,0,0.302518,-0.159229,-1.289010
H,0,-0.526712,0.899650,1.638367
H,0,-0.521130,-0.934927,1.543954
H,0,1.887514,0.976179,1.559723
H,0,3.288327,-0.989271,1.637760
H,0,1.828354,-2.101838,1.519886
Br,0,4.068317,0.771352,-1.847140
Br,0,2.160161,-3.407366,-2.081970
H,0,-0.345895,-0.744778,-1.729533

allylTlBr2 +MeCHO (TS)

O,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.291555
C,0,1.953518,0.000000,1.948951
C,0,2.476512,1.152022,1.379431
C,0,2.930439,1.249497,0.034417
Tl,0,0.917263,1.763102,-1.058591
C,0,-0.436057,-1.283755,1.953858
H,0,-0.291838,0.929247,1.802534
H,0,2.189583,-0.961486,1.498050
H,0,1.766156,-0.004151,3.019211
H,0,2.389301,2.083513,1.943018
H,0,3.271257,0.328016,-0.439219

H,0,3.545699,2.119478,-0.201736

H,0,3.545699,2.119478,-0.201736
Br,0,0.606680,1.515329,-3.639223
Br,0,-0.297144,3.761507,0.196411
H,0,0.060123,-2.142375,1.495159
H,0,-0.254221,-1.273791,3.031496
H,0,-1.515013,-1.384038,1.784647

allylSiBr

C,0,-2.1822041566,-0.896268429,-2.8747933059
C,0,-2.1906014362,-0.9061959289,-1.5292836483
C,0,-0.9661159013,-0.9386211983,-0.6682317671
Si,0,-0.5819986744,0.8044759648,0.0324984761
Br,0,1.3961134213,0.3073693449,1.1130086272
H,0,-3.1037784838,-0.836544565,-3.4455503474
H,0,-1.2544931397,-0.9609906096,-3.4394729922
H,0,-3.1513451961,-0.847213937,-1.0157645593
H,0,-0.093648134,-1.2840143274,-1.244312087
H,0,-1.0791943866,-1.6453138017,0.1686716976

allylSiBr +h2o (complex)

O,0,-1.482716,1.012430,-0.268931
H,0,-1.482716,1.012430,0.965862
C,0,-0.969700,1.012430,2.292517
C,0,0.065717,1.806565,1.807311
C,0,1.103393,1.347819,0.938876
Si,0,0.238156,0.882358,-0.926573
H,0,-1.702876,1.460204,2.958899
H,0,-0.805229,-0.059211,2.409163
H,0,-0.080788,2.887578,1.874309
H,0,1.874828,2.089682,0.733762
H,0,1.528098,0.377274,1.202850
H,0,-2.088897,0.319337,-0.607193
Br,0,0.288247,-1.529732,-0.704183

allylSiBr +h2o (TS)

O,0,0.000000,0.000000,0.000000
H,0,0.000000,0.000000,1.234793
C,0,0.513016,0.000000,2.561449
C,0,1.548434,0.794134,2.076243
C,0,2.586110,0.335389,1.207808
Si,0,1.720873,-0.130073,-0.657641
H,0,-0.220159,0.447774,3.227831
H,0,0.677487,-1.071642,2.678094
H,0,1.401929,1.875148,2.143240
H,0,3.357544,1.077251,1.002693

H,0,3.010815,-0.635156,1.471781
H,0,-0.606180,-0.693093,-0.338262
Br,0,1.770964,-2.542163,-0.435252

allylSiBr +MeCHO (TS)
O,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.272256
C,0,2.341496,0.000000,1.704247
C,0,2.515627,1.111494,0.924695
C,0,2.377632,1.117402,-0.518325
Si,0,0.444333,1.587941,-0.938378
H,0,-0.125840,0.950408,1.801185
C,0,-0.315198,-1.266408,1.996645
H,0,2.422245,0.062308,2.786722
H,0,2.370350,-0.993861,1.264425
H,0,2.593430,2.077483,1.429105
H,0,2.936828,1.925280,-1.003353
H,0,2.611891,0.157212,-0.985403
Br,0,0.348118,0.566356,-3.063598
H,0,0.087735,-2.129535,1.463381
H,0,0.057562,-1.243135,3.022890
H,0,-1.409187,-1.363077,2.032654

allylSiBr3
Br,0,2.0794006411,0.3823061109,2.0528381846
Si,0,0.3543733694,0.473148736,0.6133617452
Br,0,-1.4962456357,1.0933962708,1.7264464824
C,0,0.1097032204,-1.2217858533,-0.1461884221
C,0,-1.0769737412,-1.2921379941,-1.0619325554
C,0,-0.9919052798,-1.375571776,-2.4004150898
Br,0,0.8073279111,1.9837655431,-0.9804419787
H,0,-1.8838294519,-1.414501373,-3.0179624928
H,0,-0.0329188466,-1.4065739014,-2.9119894538
H,0,-2.0596598862,-1.2657271543,-0.5925418196
H,0,1.030106839,-1.4795610746,-0.6873036706
H,0,0.0067485614,-1.9370205334,0.6820505899

allylSiBr3 +h2o (complex)
C,0,-0.442834312,-0.5164243406,1.8768901632
C,0,-1.935282394,-0.3610878733,1.8412598083
C,0,-2.7957944171,-1.3912138031,1.9177584497
Si,0,0.3715059379,-0.0549167296,0.2562324463
Br,0,0.078155117,2.1281750598,-0.1718979442
Br,0,2.5724290796,-0.4936313243,0.3738416605
Br,0,-0.5191122715,-1.2628863264,-1.423694574

O,0,-4.0200476182,0.6125121485,-0.3941220034
H,0,-2.4527728472,-2.417839522,2.0275420203
H,0,-3.8670631802,-1.2208181749,1.8752943834
H,0,-2.3319729488,0.6470681891,1.7305230514
H,0,-0.168654195,-1.5539586632,2.1114497243
H,0,0.0030774493,0.1233284547,2.6523246569
H,0,-4.3293006587,1.0240966811,-1.2184802061
H,0,-3.4520664426,-0.1287931555,-0.6671023592

allylSiBr3 +h2o (TS)
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.393912
C,0,1.190815,0.000000,2.193758
Si,0,2.142164,1.775616,2.215456
H,0,0.858291,-0.418407,-0.525217
H,0,-0.948959,-0.007906,-0.528782
H,0,-0.938969,0.253739,1.890477
H,0,1.972843,-0.661683,1.805957
H,0,0.992296,-0.211948,3.243764
Br,0,1.305429,3.421614,3.570002
Br,0,3.549227,0.798598,3.968505
H,0,0.373595,1.192585,0.207698
O,0,1.061146,2.306978,0.869460
H,0,1.338498,3.089324,0.356491
Br,0,3.980609,2.171373,0.849870

allylSiBr3 +MeCHO (TS)
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.380010
C,0,1.215434,0.000000,2.148242
Si,0,1.740809,1.919701,2.479903
H,0,0.849362,-0.429184,-0.524720
H,0,-0.942321,0.019123,-0.542517
H,0,-0.935051,0.198806,1.907130
H,0,2.070319,-0.445652,1.630373
H,0,1.089930,-0.418255,3.145264
Br,0,0.068459,3.507600,2.615137
Br,0,1.842147,1.553047,4.861700
C,0,0.696970,1.903025,-0.187330
O,0,1.714337,2.025749,0.605823
C,0,1.029952,1.884532,-1.655343
H,0,-0.227822,2.416017,0.095464
Br,0,3.905556,2.624125,2.294602
H,0,1.900050,1.252964,-1.846431
H,0,0.182184,1.560653,-2.264078

H,0,1.285567,2.913722,-1.935638

allylGeBr

C,0,-2.1173346716,-1.0898953011,-2.8845459978
C,0,-2.1314869683,-1.1532936988,-1.5392068798
C,0,-0.9199837046,-1.1448509784,-0.6697984356
Ge,0,-0.4988372652,0.7286253829,-0.0559996674
Br,0,1.5820675881,0.1038884437,1.180040693
H,0,-3.038057689,-1.0613846592,-3.4589611901
H,0,-1.1850664676,-1.0897688887,-3.4459220132
H,0,-3.0988962749,-1.1622699371,-1.0344151854
H,0,-0.0386415619,-1.5135075154,-1.2154454488
H,0,-1.0360790362,-1.7969369125,0.2066168157

allylGeBr +h2o (complex)

C,0,-1.1384097741,0.579009943,2.6209627883
C,0,-0.372630893,1.5221226327,2.0211379146
C,0,0.8185063885,1.2601370226,1.1730908397
Ge,0,0.4470648354,0.8258566423,-0.8191175756
Br,0,0.2269045512,-1.7277178704,-0.4467587826
O,0,-1.6783967834,0.9241896658,-0.4221279619
H,0,-1.8127445756,0.7803982886,0.5545150346
H,0,-1.9953052326,0.8593907687,3.2276432987
H,0,-0.8726838314,-0.4751051635,2.5836446949
H,0,-0.687986896,2.5636799204,2.1112843361
H,0,1.4745357575,2.1387780575,1.1722840087
H,0,1.391611436,0.4101806411,1.5602570248
H,0,-2.1627807416,0.2042554821,-0.875434147

allylGeBr +h2o (TS)

O,0,0.000000,0.000000,0.000000
H,0,0.000000,0.000000,1.247074
C,0,0.460921,0.000000,2.567752
C,0,1.507188,0.843019,2.184527
C,0,2.623114,0.446889,1.405589
Ge,0,1.845084,0.071294,-0.666516
H,0,-0.318291,0.404528,3.209494
H,0,0.666269,-1.065498,2.679894
H,0,1.324176,1.916999,2.275827
H,0,3.393984,1.206451,1.281659
H,0,3.024109,-0.544847,1.619382
H,0,-0.497552,-0.788687,-0.304857
Br,0,2.040639,-2.506376,-0.475886

allylGeBr +MeCHO (TS)

O,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.269707
C,0,2.306716,0.000000,1.725377
C,0,2.542389,1.126094,0.978862
C,0,2.485849,1.172238,-0.461903
Ge,0,0.479581,1.672948,-1.042537
H,0,-0.124692,0.947378,1.807116
C,0,-0.333516,-1.263137,1.996598
H,0,2.355311,0.038080,2.810867
H,0,2.349302,-0.983731,1.264559
H,0,2.620478,2.077436,1.511691
H,0,3.068627,1.990322,-0.897648
H,0,2.717314,0.223911,-0.951149
Br,0,0.601601,0.422155,-3.242299
H,0,0.072048,-2.128457,1.468778
H,0,0.026710,-1.240647,3.027448
H,0,-1.428109,-1.354474,2.016898

allylGeBr3

Br,0,0.4237263513,0.5258521091,-3.1919149572
Ge,0,0.4278128959,0.4963882887,-0.7888619607
Br,0,2.7006276355,0.480700263,-0.0154174796
C,0,-0.509919567,-1.0966105077,-0.1632595123
C,0,-0.423754917,-1.2709922712,1.318999838
C,0,-1.4235277714,-0.975011639,2.1671195518
Br,0,-0.6641295404,2.4746532842,0.0119670958
H,0,-1.307890193,-1.1088780576,3.2380283485
H,0,-2.380325645,-0.5971756987,1.8148704926
H,0,0.5209776724,-1.6418010057,1.7142510982
H,0,-1.5533080425,-0.9999905229,-0.488335613
H,0,-0.0690629673,-1.9504609572,-0.6929683618

allylGeBr3 +h2o (complex)

Br,0,1.6327108821,-0.5784846881,1.8560630915
Ge,0,-0.0761042036,-0.1402400604,0.1671915682
O,0,-2.1125407824,0.5348225357,-1.7239802405
Br,0,1.1721939616,0.1813237563,-1.8711328131
C,0,-1.1357433005,-1.7909182401,0.2184544594
C,0,-1.9954039442,-2.1314612121,-0.9506878802
C,0,-1.6254974039,-2.9856299184,-1.9220820411
Br,0,-1.0911104555,1.9020478934,0.9572730263
H,0,-0.6537664065,-3.4741178691,-1.9178714366
H,0,-2.2945459336,-3.2256937507,-2.7432105947
H,0,-2.9722828557,-1.657685028,-0.993652035
H,0,-0.3821705597,-2.5730152645,0.3747819863

H,0,-1.7284920685,-1.7226057749,1.1399794169
H,0,-2.125980127,1.4986053519,-1.8687420439
H,0,-1.9500369707,0.1406265497,-2.6007964457

allylGeBr3 +h2o (TS)
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.399763
C,0,1.182596,0.000000,2.192689
Ge,0,2.091237,1.898935,2.177068
H,0,0.843445,-0.461520,-0.514683
H,0,-0.955031,-0.033867,-0.517677
H,0,-0.936609,0.257292,1.899296
H,0,1.991450,-0.623841,1.799650
H,0,1.009591,-0.177242,3.252890
Br,0,0.908632,3.538756,3.521902
Br,0,3.545143,1.001235,4.144030
H,0,0.381086,1.191908,0.108466
O,0,1.062587,2.378581,0.654759
H,0,1.509080,2.950505,0.000793
Br,0,4.114574,2.370628,0.818622

allylGeBr3 +MeCHO (TS)
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.384802
C,0,1.204690,0.000000,2.154238
Ge,0,1.808404,2.005379,2.379671
H,0,0.855521,-0.422761,-0.520904
H,0,-0.949129,-0.036175,-0.529501
H,0,-0.936590,0.201393,1.908267
H,0,2.063492,-0.475691,1.672852
H,0,1.075686,-0.319416,3.187270
Br,0,-0.018934,3.642521,2.596789
Br,0,2.125931,1.675889,4.904585
C,0,0.559543,1.889449,-0.263198
O,0,1.646648,2.082795,0.421786
C,0,0.755604,1.870785,-1.758856
H,0,-0.352212,2.381919,0.094130
Br,0,4.072300,2.788325,1.975721
H,0,1.624063,1.265188,-2.026411
H,0,-0.133965,1.516733,-2.285583
H,0,0.953020,2.905499,-2.063040

allylSnBr
C,0,-2.2030350882,-0.1311437056,0.2926828293
C,0,-2.087970617,1.2010862811,-0.1618602631

C,0,-0.960545196,2.0229007426,0.0350160648
Sn,0,-0.0957525206,-0.0679641033,-0.953978176
H,0,-3.0665649323,-0.7045704311,-0.0298886556
H,0,-1.7780101588,-0.4184262696,1.2533548126
H,0,-2.7378415079,1.4767352394,-0.9974052739
H,0,-0.3886933816,1.958704165,0.9594600422
H,0,-0.9308881939,2.9810285143,-0.4743632795
Br,0,1.291397989,-0.5843521703,1.3140776962

allylSnBr +h2o (complex)
O,0,-1.8570788732,0.6936461431,-0.1855460843
H,0,-1.9187127843,0.6192914562,0.8081203757
C,0,-1.2858299722,0.4533518628,2.8148163476
C,0,-0.45886317,1.3842119212,2.2740459137
C,0,0.7538586961,1.1104277984,1.4739151061
Sn,0,0.3807875404,0.7753817177,-0.7221283963
H,0,-2.1550881639,0.7486779071,3.3962486155
H,0,-1.0468100493,-0.6076296694,2.772605717
H,0,-0.7479293513,2.4328581153,2.3785273332
H,0,1.4563917238,1.94784566,1.5522722478
H,0,1.2565062756,0.1995357219,1.8181452115
H,0,-2.3051969739,-0.1002493472,-0.5417245263
Br,0,0.2063742847,-1.9213295534,-0.3991448769

allylSnBr +h2o (TS)
O,0,0.000000,0.000000,0.000000
H,0,0.000000,0.000000,1.235090
C,0,0.414995,0.000000,2.581176
C,0,1.458544,0.886812,2.291313
C,0,2.651590,0.559839,1.608388
Sn,0,1.986901,0.240229,-0.694271
H,0,-0.409269,0.365112,3.189676
H,0,0.654827,-1.058440,2.693738
H,0,1.232614,1.951489,2.399936
H,0,3.406874,1.344229,1.580751
H,0,3.056527,-0.437075,1.790293
H,0,-0.449653,-0.821265,-0.290190
Br,0,2.282544,-2.450661,-0.482906

allylSnBr +MeCHO (TS)
O,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.263137
C,0,2.369084,0.000000,1.734143
C,0,2.638719,1.108393,0.975596
C,0,2.648981,1.146141,-0.467992

Sn,0,0.550618,1.720257,-1.247727
H,0,-0.092057,0.949037,1.805887
C,0,-0.313216,-1.259107,2.005394
H,0,2.394749,0.055118,2.819535
H,0,2.390437,-0.991594,1.288503
H,0,2.728929,2.063899,1.500222
H,0,3.283632,1.941231,-0.873461
H,0,2.875607,0.187710,-0.941255
Br,0,0.778929,0.140065,-3.391935
H,0,0.086067,-2.125347,1.474352
H,0,0.065888,-1.227750,3.029066
H,0,-1.406991,-1.355492,2.046504

allylSnBr3

C,0,-1.0466194245,-1.2897278911,-2.3126138119
C,0,-1.0536198084,-1.3593619612,-0.9695778449
C,0,0.176218432,-1.3324431992,-0.1224338548
Sn,0,0.473767572,0.5778907535,0.7559327395
Br,0,1.132039726,2.2779329001,-1.0268249242
H,0,-1.972533656,-1.3031356728,-2.8787685247
H,0,-0.1201888926,-1.2220293012,-2.8782812183
H,0,-2.007045301,-1.4200977747,-0.4453846875
H,0,1.0716771093,-1.5557940178,-0.7147416481
H,0,0.1197298781,-2.0576717949,0.6979854383
Br,0,2.3276662569,0.5008915065,2.5115958829
Br,0,-1.6657895,1.3835132872,1.8899737202

allylSnBr3 +h2o (complex)

Br,0,1.717899,-1.799619,0.650139
Sn,0,-0.025888,0.091362,0.211195
Br,0,-1.285920,-0.847010,-1.831258
C,0,-1.106323,-0.036395,2.048623
C,0,-2.411700,0.675499,2.136387
C,0,-3.605938,0.100345,1.895383
Br,0,1.581515,2.008913,-0.401042
O,0,-1.551637,1.981515,-0.193445
H,0,-3.689914,-0.947091,1.614228
H,0,-4.531196,0.659760,1.998863
H,0,-2.376975,1.727233,2.417331
H,0,-1.240958,-1.116093,2.188275
H,0,-0.412255,0.305181,2.826045
H,0,-1.344644,2.533966,-0.972549
H,0,-2.503521,1.763093,-0.244373

allylSnBr3 +h2o (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.401333
C,0,1.167964,0.000000,2.204692
Sn,0,1.972898,2.138212,2.211035
H,0,0.827878,-0.496755,-0.508649
H,0,-0.959695,-0.043301,-0.508646
H,0,-0.940447,0.245667,1.900415
H,0,2.018789,-0.558478,1.802087
H,0,1.000438,-0.187212,3.264252
Br,0,0.229364,3.747801,3.186667
Br,0,3.196101,1.556315,4.506366
H,0,0.424199,1.209547,0.016700
O,0,1.126970,2.383260,0.357786
H,0,1.702813,2.709075,-0.360998
Br,0,4.207147,2.790504,1.038230

allylSnBr3 +MeCHO (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.382319
C,0,1.194345,0.000000,2.169986
Sn,0,1.792757,2.163128,2.456238
H,0,0.873382,-0.376831,-0.526502
H,0,-0.947405,-0.061931,-0.529213
H,0,-0.944867,0.180120,1.899440
H,0,2.062241,-0.469412,1.699487
H,0,1.055120,-0.322239,3.202920
Br,0,-0.269933,3.735413,2.640473
Br,0,2.184230,1.820169,5.051829
C,0,0.491374,1.967991,-0.307700
O,0,1.567496,2.215281,0.363637
C,0,0.654995,1.910779,-1.803808
H,0,-0.447189,2.396357,0.063678
Br,0,4.097994,3.167755,1.940979
H,0,1.543730,1.336706,-2.074489
H,0,-0.228897,1.503838,-2.300554
H,0,0.800425,2.943700,-2.143147

allylPbBr

C,0,-1.7771727325,-1.4075661152,-0.4987261001
C,0,-1.7852358196,-1.4299310743,0.9101856734
C,0,-0.6400099854,-1.4079403937,1.730908201
Pb,0,-0.399905513,0.6044310684,0.2039465548
Br,0,1.8550020159,-0.4717357123,-0.9458487477
H,0,-2.7273909895,-1.3331465498,-1.0189802817
H,0,-0.9697850181,-1.8893675862,-1.0488066491

H,0,-2.7235968121,-1.1339749686,1.388892941
H,0,0.2792957056,-1.889706466,1.400205166
H,0,-0.776830151,-1.3337766037,2.8055708516

allylPbBr +h2o (complex)
C,0,-1.4213000206,0.2266404703,3.021921827
C,0,-0.5456921381,1.1401673746,2.5254488356
C,0,0.6748433526,0.8484048318,1.7567095509
Pb,0,0.2890839082,0.6526548633,-0.537295126
Br,0,0.1883569062,-2.107305575,-0.3984914949
O,0,-2.0380976964,0.44206494,0.0369155434
H,0,-2.0635844718,0.3948708328,1.0319742732
H,0,-2.2942795483,0.5389436067,3.588704111
H,0,-1.213347213,-0.8407026701,2.9682263291
H,0,-0.803642103,2.1954731717,2.6485638567
H,0,1.4164206601,1.6456303402,1.8818542922
H,0,1.1181069606,-0.1118198477,2.0407823403
H,0,-2.3993720629,-0.4121946831,-0.2745081801

allylPbBr +h2o (TS)
O,0,0.000000,0.000000,0.000000
H,0,0.000000,0.000000,1.227236
C,0,0.392592,0.000000,2.583994
C,0,1.461885,0.881932,2.361858
C,0,2.691077,0.558947,1.759120
Pb,0,2.079514,0.346770,-0.668110
H,0,-0.447239,0.365540,3.171053
H,0,0.624781,-1.059258,2.707560
H,0,1.241659,1.947206,2.480261
H,0,3.458499,1.331835,1.778734
H,0,3.064109,-0.457131,1.893159
H,0,-0.379575,-0.857579,-0.286429
Br,0,2.490888,-2.375931,-0.610159

allylPbBr +MeCHO (TS)
O,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.260681
C,0,2.364507,0.000000,1.753120
C,0,2.676580,1.114393,1.016402
C,0,2.755874,1.173370,-0.419108
Pb,0,0.622190,1.776934,-1.324520
H,0,-0.084360,0.949096,1.806882
C,0,-0.318849,-1.255896,2.010587
H,0,2.359574,0.043231,2.839279
H,0,2.394301,-0.986852,1.297333

H,0,2.759150,2.061728,1.557998
H,0,3.393620,1.980481,-0.794073
H,0,2.981704,0.224185,-0.909961
Br,0,0.975881,0.194039,-3.513516
H,0,0.085492,-2.124593,1.487196
H,0,0.054869,-1.218716,3.036182
H,0,-1.412514,-1.354910,2.045566

allylPbBr3
C,0,-1.415841785,-2.2003464658,-2.9774977522
C,0,-1.4219464297,-2.2731544284,-1.6324543718
C,0,-0.1958280255,-2.2196499836,-0.799762418
Pb,0,0.0670455347,-0.2026402319,0.0358214726
Br,0,0.7340610822,1.4601315207,-1.8591721277
H,0,-2.3405813161,-2.2395354483,-3.5445012564
H,0,-0.490840894,-2.1059721405,-3.5418803826
H,0,-2.372243247,-2.3558944586,-1.106019282
H,0,0.7159882256,-2.411033293,-1.3763045711
H,0,-0.2324118655,-2.885205856,0.0692060851
Br,0,1.9237983006,-0.135381473,1.8717415568
Br,0,-2.1600293059,0.6401941088,1.1022998826

allylPbBr3 +h2o (complex)
C,0,-0.9526438267,0.5035765644,2.1117659989
C,0,-2.423102355,0.4886586342,1.9421246931
C,0,-3.2054870884,-0.5461197457,2.3072114059
Pb,0,0.0388635048,0.0663703155,0.1968675729
O,0,-1.0086586528,2.6182416,-0.0565239911
Br,0,0.9704600466,-2.3974290104,0.4393571024
Br,0,-1.5098544553,-0.1112782383,-1.9180859538
Br,0,2.1795095556,1.4888690915,-0.3627591222
H,0,-2.7924724405,-1.4428766024,2.7641364301
H,0,-4.2808079291,-0.5143861975,2.1618174613
H,0,-2.8682570806,1.367818474,1.4797675852
H,0,-0.5954355603,-0.2754211595,2.7938368571
H,0,-0.5616506057,1.4838653789,2.3983307397
H,0,-0.3371828492,3.3164683446,-0.1730057657
H,0,-1.5983622287,2.6938758778,-0.8303658738

allylPbBr3 +h2o (TS)
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.407464
C,0,1.160890,0.000000,2.204824
Pb,0,1.843491,2.284363,2.145706
H,0,0.818606,-0.524607,-0.497180

H,0,-0.964156,-0.074247,-0.497993
H,0,-0.941530,0.236848,1.908980
H,0,2.050537,-0.484449,1.794003
H,0,1.025461,-0.141260,3.275410
Br,0,-0.122374,3.865174,2.838572
Br,0,2.897393,1.975907,4.633188
H,0,0.406899,1.206811,-0.076150
O,0,1.082715,2.433635,0.133800
H,0,1.782219,2.545286,-0.542916
Br,0,4.194178,2.801911,1.026438

allylSbBr2 +h2o (complex)

C,0,-1.6656890633,-1.9990021607,-2.9311071622
C,0,-1.6101752662,-1.5450447497,-1.6616258827
C,0,-0.434958284,-1.6668610827,-0.7586898813
Sb,0,0.6973807495,0.1567042237,-0.34180249
H,0,-0.8228387126,-2.5079976943,-3.3945802906
H,0,-2.5760185843,-1.9141845542,-3.5182279556
H,0,-2.4909127607,-1.0604405427,-1.2401477122
H,0,0.2912347323,-2.3894039867,-1.1536887006
H,0,-0.7571187921,-2.0215380772,0.2259039925
Br,0,-1.4853346254,1.5502230503,0.3617359718
Br,0,1.3453433596,-0.8314503519,2.1098914063
H,0,-0.8296970774,0.1723597825,-3.0197357664
O,0,-0.0975326837,0.769874544,-2.7506913182
H,0,-0.4361755773,1.6786968257,-2.860486707

allylPbBr3 +MeCHO (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.389749
C,0,1.188843,0.000000,2.159273
Pb,0,1.724777,2.303151,2.421128
H,0,0.873381,-0.390704,-0.517087
H,0,-0.949399,-0.102485,-0.519762
H,0,-0.943485,0.178469,1.909339
H,0,2.086157,-0.404978,1.686995
H,0,1.091288,-0.247497,3.216507
Br,0,-0.512551,3.717244,2.571352
Br,0,2.220949,1.949545,5.055243
C,0,0.408843,1.930862,-0.415213
O,0,1.483995,2.273385,0.216582
C,0,0.556242,1.792252,-1.913216
H,0,-0.539629,2.357396,-0.061625
Br,0,3.908821,3.621935,1.821736
H,0,1.462503,1.235440,-2.162015
H,0,-0.317398,1.322888,-2.372392
H,0,0.658605,2.807089,-2.315514

allylSbBr2 +h2o (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.395957
C,0,1.179086,0.000000,2.204224
Sb,0,2.052539,2.113508,1.969261
H,0,0.861501,-0.407760,-0.529847
H,0,-0.958994,-0.072038,-0.508267
H,0,-0.935304,0.254327,1.894175
H,0,1.989849,-0.632549,1.842373
H,0,0.973135,-0.107097,3.270154
Br,0,-0.497671,3.046984,3.050892
Br,0,3.889752,0.953707,0.223595
H,0,0.342044,1.268076,0.006013
O,0,1.018781,2.438317,0.246239
H,0,0.294704,3.097628,0.367660

allylSbBr2

C,0,-1.4158712869,-1.4990921638,-3.4168629059
C,0,-1.4270899901,-1.4925140054,-2.0709002459
C,0,-0.2033544498,-1.4805820708,-1.2169414464
Sb,0,0.2079627195,0.5235372401,-0.5318941414
H,0,-0.4864008007,-1.532417781,-3.9817842724
H,0,-2.3396438831,-1.4921313066,-3.9869800036
H,0,-2.3839921737,-1.4690233207,-1.5499192972
H,0,0.6760680585,-1.8119698614,-1.7833931565
H,0,-0.3101606227,-2.1261259909,-0.3386363753
Br,0,-1.8203919884,0.5095564071,1.187719526
Br,0,2.177989848,-0.2648593084,1.069295957

allylSbBr2 +MeCHO (TS1)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.385632
C,0,1.187583,0.000000,2.176688
Sb,0,1.933954,2.172718,2.478741
H,0,0.873238,-0.376698,-0.527698
H,0,-0.949572,-0.086016,-0.523026
H,0,-0.943891,0.183764,1.900195
H,0,2.051209,-0.486979,1.716646
H,0,1.038685,-0.302553,3.213561
Br,0,-0.516212,3.266240,2.798254
Br,0,2.195484,1.480585,5.207256
C,0,0.442966,1.942056,-0.319846

O,0,1.542167,2.162670,0.330334
C,0,0.544349,1.942587,-1.823062
H,0,-0.479758,2.359463,0.100026
H,0,1.415861,1.372409,-2.152882
H,0,-0.362590,1.554558,-2.294192
H,0,0.677567,2.985283,-2.136474

allylSbBr2 +MeCHO (TS2)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.371845
C,0,1.208473,0.000000,2.182978
Sb,0,2.090660,2.057618,2.331041
H,0,0.913164,-0.201343,-0.556270
H,0,-0.940215,-0.082889,-0.538834
H,0,-0.950501,0.124906,1.887819
H,0,2.018772,-0.597429,1.759837
H,0,0.999419,-0.287578,3.217927
Br,0,-0.591598,2.999001,3.054586
Br,0,4.397479,1.104829,1.070745
C,0,0.302044,2.218041,-0.115002
O,0,1.491314,2.325532,0.361107
C,0,0.159044,2.401491,-1.588200
H,0,-0.546523,2.431054,0.538110
H,0,0.980551,1.924939,-2.126710
H,0,-0.805861,2.034947,-1.944434
H,0,0.204620,3.482837,-1.776371

allylSbMeBr3

C,0,-1.6027652235,-0.0951600344,-2.4502215432
C,0,-1.5979287515,-0.6136595769,-1.2068554337
C,0,-0.4303118413,-1.3354221284,-0.6274908681
Sb,0,0.5792290863,0.0607224957,0.6514446856
H,0,-0.7415211048,-0.1769184181,-3.108477226
H,0,-2.4809487308,0.4132805666,-2.8369642372
H,0,-2.4754730289,-0.5110475828,-0.5697487381
H,0,0.282218136,-1.6525853164,-1.3926169351
H,0,-0.7336237273,-2.1747486623,0.0040879476
Br,0,-1.2605820812,-0.5698978231,2.604745459
Br,0,2.2782069019,0.6642807797,-1.4220340388
Br,0,2.5652385972,-0.637697539,2.1859013686
C,0,0.026571676,2.0960129541,0.7541581697
H,0,0.9253216812,2.7058494596,0.6471461921
H,0,-0.6385155212,2.2893730434,-0.0930835136
H,0,-0.4870422195,2.2957592207,1.6946016123

allylSbMeBr3 +h2o (complex)

C,0,-2.9793774286,-2.2796028591,-0.7778693732
C,0,-1.9466380958,-2.1637124889,0.0815321401
C,0,-0.5716977859,-1.8081984743,-0.3369400715
Sb,0,0.064095228,0.2262158387,0.0704410594
Br,0,0.3128470597,-0.5295262576,2.737109782
Br,0,2.5261116095,-0.1971691334,-0.8195670734
H,0,-2.8599717217,-2.0854125057,-1.8406320281
H,0,-3.9608348076,-2.5960336545,-0.4353656412
H,0,-2.0956530641,-2.3807360904,1.1389298799
H,0,-0.4343647116,-1.9106371585,-1.417938587
H,0,0.1779337944,-2.40535329,0.1922880305
C,0,0.3637266514,2.2455081422,0.6504939457
H,0,-0.5732143889,2.614813262,1.0686826923
H,0,0.6399620163,2.8114537722,-0.2411922655
H,0,1.1618007554,2.266684638,1.3944740015
O,0,-2.1379215321,0.6453730494,0.9260218158
H,0,-2.8724341577,0.3183618715,0.3666522925
H,0,-2.2937820129,0.310518665,1.8337060755
Br,0,-1.1889874154,1.0236206026,-2.2250733615

allylSbMeBr3 +h2o (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.401143
C,0,1.175353,0.000000,2.196416
Sb,0,2.076638,2.158002,2.065379
H,0,0.850602,-0.444021,-0.518222
H,0,-0.959128,-0.058037,-0.509942
H,0,-0.934574,0.266792,1.897742
H,0,2.013775,-0.586799,1.820102
H,0,1.006698,-0.098638,3.267733
Br,0,-0.090136,2.990294,3.421367
Br,0,3.889731,1.106236,0.263323
H,0,0.324725,1.225531,0.059924
O,0,0.973898,2.504130,0.359121
Br,0,3.538338,1.413318,4.254938
C,0,2.962224,4.084980,2.009560
H,0,4.022497,3.979795,1.771092
H,0,2.444901,4.677314,1.251194
H,0,2.836713,4.540879,2.994117
H,0,1.533187,2.646028,-0.434315

allylSbMeBr3 +MeCHO (TS)

C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.384949

C,0,1.199126,0.000000,2.162960
Sb,0,2.154125,2.088929,2.217189
H,0,0.903384,-0.287291,-0.534827
H,0,-0.941995,-0.132780,-0.525600
H,0,-0.945015,0.168322,1.901243
H,0,2.028678,-0.574683,1.747023
H,0,1.040219,-0.179643,3.227431
Br,0,-0.303651,3.039816,3.095978
Br,0,4.333743,1.053627,0.941570
C,0,0.211837,1.994517,-0.204163
O,0,1.370068,2.323233,0.278743
C,0,0.127013,2.060370,-1.708988
H,0,-0.673535,2.314496,0.357426
Br,0,3.079150,1.591716,4.704458
C,0,2.936643,4.053521,2.080977
H,0,3.999156,4.010529,2.328230
H,0,2.796395,4.388225,1.050563
H,0,2.397868,4.698304,2.777495
H,0,0.977880,1.554729,-2.170272
H,0,-0.813712,1.652597,-2.085870
H,0,0.175943,3.123360,-1.974462

allylBiBr2
C,0,-1.4851575757,-1.723368879,-3.2318632991
C,0,-1.4890201833,-1.7266988461,-1.8839976577
C,0,-0.2663864635,-1.7118715872,-1.0355505943
Bi,0,0.1522531172,0.3987531207,-0.4638877304
H,0,-0.5586584243,-1.7643118288,-3.8018340278
H,0,-2.4115572275,-1.7091423692,-3.7976539107
H,0,-2.4448720027,-1.6982755896,-1.3605599473
H,0,0.6126423921,-2.0753185123,-1.582402525
H,0,-0.3811939701,-2.2966539423,-0.1176523888
Br,0,-1.8797515035,0.4660585417,1.315115048
Br,0,2.2223233847,-0.2540919962,1.14406363

allylBiBr2 +h2o (complex)
C,0,-1.7869312908,-2.0176015501,-2.9017464269
C,0,-1.7523571731,-1.6071786995,-1.6147348944
C,0,-0.5938095855,-1.7449277373,-0.7002380426
Bi,0,0.5644434571,0.1486583556,-0.2821148619
Br,0,1.3342071547,-0.8807630759,2.1626739732
Br,0,-1.6731134428,1.5243930742,0.4414236431
O,0,-0.2059657889,0.7217156897,-2.7169071578
H,0,-0.9405772295,-2.5219392272,-3.3646580689
H,0,-2.6880937673,-1.9135191519,-3.4998782176

H,0,-2.639335368,-1.1298048858,-1.1972306955
H,0,0.1391861014,-2.4673714432,-1.0826755489
H,0,-0.9188327716,-2.076278315,0.2912629827
H,0,-0.9092002106,0.0795001252,-2.9679604177
H,0,-0.5839190058,1.6082418444,-2.8711696218

allylBiBr2 +h2o (TS)
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.398670
C,0,1.168797,0.000000,2.208682
Bi,0,1.981844,2.226162,1.986793
O,0,0.921508,2.472394,0.174745
Br,0,-0.593247,3.109852,3.066643
Br,0,3.974249,1.120981,0.323230
H,0,0.863968,-0.409578,-0.524964
H,0,-0.958801,-0.099511,-0.504473
H,0,-0.938614,0.247617,1.895272
H,0,2.013160,-0.577703,1.832829
H,0,0.973832,-0.116869,3.275630
H,0,0.314783,1.283031,-0.033231
H,0,0.165418,3.098086,0.272744

allylBiBr2 +MeCHO (TS1)
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.385558
C,0,1.177590,0.000000,2.187358
Bi,0,1.928079,2.241276,2.498134
H,0,0.881112,-0.353130,-0.531174
H,0,-0.948322,-0.103607,-0.521720
H,0,-0.948339,0.176083,1.894887
H,0,2.053824,-0.478337,1.742164
H,0,1.024939,-0.284522,3.229259
Br,0,-0.592347,3.219082,2.933254
Br,0,2.556582,1.466104,5.163498
C,0,0.392425,1.976764,-0.341626
O,0,1.502387,2.218048,0.273727
C,0,0.434972,1.966863,-1.847741
H,0,-0.530509,2.360663,0.111136
H,0,1.302591,1.408470,-2.207009
H,0,-0.482471,1.559807,-2.280884
H,0,0.538333,3.008782,-2.175444

allylBiBr2 +MeCHO (TS2)
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.373249

C,0,1.200245,0.000000,2.184457
Bi,0,2.008635,2.164845,2.407868
H,0,0.909869,-0.218801,-0.554936
H,0,-0.941249,-0.081559,-0.537190
H,0,-0.951624,0.130690,1.886454
H,0,2.046432,-0.531070,1.743574
H,0,1.009658,-0.320759,3.213432
Br,0,-0.745359,3.062829,2.974822
Br,0,4.507997,1.305503,1.417719
C,0,0.327346,2.217333,-0.183850
O,0,1.500495,2.343852,0.321365
C,0,0.215097,2.349391,-1.666631
H,0,-0.542419,2.441875,0.438270
H,0,1.052384,1.861362,-2.169632
H,0,-0.737676,1.960323,-2.031783
H,0,0.255380,3.423366,-1.893649

allylBiMeBr3
C,0,-0.5348187241,-0.0082575203,-2.2422905459
Bi,0,-0.0620551421,0.0186427866,-0.1085754301
Br,0,2.5495011054,0.022160995,0.3607045806
C,0,-1.5650719889,0.0735603436,1.5428169343
C,0,-2.8691342071,0.2481490316,0.8709444451
C,0,-3.6996617082,-0.7826404822,0.6029100889
Br,0,-0.2270335542,2.8232526712,-0.131170644
Br,0,-0.236807982,-2.7761446736,-0.0512550344
H,0,-3.4464700644,-1.8057472012,0.8696147917
H,0,-4.6580617037,-0.6132667659,0.1209235562
H,0,-3.1435608523,1.2617763647,0.5823504759
H,0,-1.460209267,-0.8815077566,2.0629490124
H,0,-1.2689754231,0.9268462204,2.1580194821
H,0,-0.0913887085,-0.91015216,-2.6661434796
H,0,-1.6250672962,-0.0427482172,-2.3185373235
H,0,-0.1416550426,0.9081652445,-2.683462923

allylBiMeBr3 +h2o (complex)
C,0,-2.9648280291,-2.3426481352,-0.8033428195
C,0,-1.9294075493,-2.2484010839,0.0588539484
C,0,-0.5653469494,-1.9244668237,-0.3727732468
Bi,0,0.0822305962,0.1906221753,0.0600201793
Br,0,0.2768001022,-0.5732368429,2.7759719952
Br,0,2.5842134785,-0.2285327836,-0.8847933016
H,0,-2.8409533154,-2.1428421465,-1.8645427145
H,0,-3.9526671664,-2.6406178114,-0.4626801329
H,0,-2.0774972849,-2.4563393322,1.1173565111

H,0,-0.4228553603,-1.9821181661,-1.4561049786
H,0,0.207802315,-2.4780445341,0.1686775612
C,0,0.3914298555,2.2798347586,0.648448224
H,0,-0.5535381454,2.6161397716,1.074881322
H,0,0.6519290702,2.8233107692,-0.261360295
H,0,1.2003921531,2.2776265427,1.3807728457
O,0,-2.1873989754,0.6562856444,0.9627927352
H,0,-2.9645240317,0.6033286971,0.3726552636
H,0,-2.437044028,0.3051418706,1.8402332097
Br,0,-1.3103871766,1.0136718075,-2.2277793219

allylBiMeBr3 +h2o (TS)
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.409743
C,0,1.162661,0.000000,2.196078
Bi,0,1.982627,2.335733,1.973580
H,0,0.843930,-0.472797,-0.505364
H,0,-0.962730,-0.104001,-0.497899
H,0,-0.936108,0.259587,1.906642
H,0,2.053667,-0.492130,1.806816
H,0,1.034921,-0.038556,3.276642
Br,0,-0.352685,3.125359,3.163932
Br,0,3.939001,1.245631,0.282133
H,0,0.293132,1.225774,-0.051573
O,0,0.909304,2.540209,0.110946
Br,0,3.393777,1.803615,4.318148
C,0,2.758185,4.378932,1.790962
H,0,3.827294,4.302654,1.581225
H,0,2.208552,4.861168,0.980522
H,0,2.566043,4.862843,2.751529
H,0,1.517153,2.547904,-0.661005

allylBiMeBr3 +MeCHO (TS)
C,0,0.000000,0.000000,0.000000
C,0,0.000000,0.000000,1.393896
C,0,1.191299,0.000000,2.151806
Bi,0,2.064814,2.261897,2.199141
H,0,0.901437,-0.313060,-0.524293
H,0,-0.942289,-0.166783,-0.516114
H,0,-0.942988,0.173506,1.911520
H,0,2.072810,-0.466468,1.709557
H,0,1.084918,-0.144406,3.227998
Br,0,-0.529433,3.128233,2.916453
Br,0,4.377952,1.252247,1.024562
C,0,0.162370,1.958751,-0.353464

O,0,1.286458,2.371397,0.142035
C,0,0.123777,1.909546,-1.863894
H,0,-0.754228,2.282182,0.156845
Br,0,2.899863,1.910351,4.789861
C,0,2.761658,4.321365,1.933506
H,0,3.808870,4.333869,2.242783
H,0,2.652089,4.548703,0.871230
H,0,2.135870,4.962492,2.557083
H,0,1.011608,1.411149,-2.259528
H,0,-0.783963,1.428561,-2.236300
H,0,0.132723,2.949648,-2.211015