Tiling, Propensity for Planarity of the Group-XIV Pentatomic Dihydrides $XYZH_2$(X,Y,Z=C, Si, Ge), and Beyond

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C3H2

5
RCCSD(T)/VTZ ENERGY=-115.13495363
C 0.0000000000 -0.2648083342 -0.1595472786
C 0.0000000000 -0.2618586472 1.2698017063
H 0.0000000000 1.9897701540 0.4066952493
H 0.0000000000 -0.8383439987 -1.0716488129
C 0.0000000000 0.9134745395 0.4563945430

5
RCCSD(T)/VTZ ENERGY=-115.11378855
C 0.0943908736 0.0104113294 -0.2099904828
C -0.6327700484 -0.0702688442 0.9055843439
H 0.2995255250 0.9667533478 -0.6816467453
H 0.5043214658 -0.8776885286 -0.6815469661
C -1.3384008681 -0.1485683704 1.9893681721

5
RCCSD(T)/VTZ ENERGY=-115.08049646
H 0.0000000000 0.0017714265 -0.7822851628
H 0.0000000000 -0.0041124951 2.2806144902
C 0.0000000000 0.8558467919 1.3531815349
C 0.0000000000 -0.8767171640 1.3455506638
C 0.0000000000 -0.0063841513 0.2904819481

5
RCCSD(T)/VTZ ENERGY=-115.05327613
C -0.0433852230 -0.0053549451 -0.2328144309
C -0.3043577050 0.5397034453 1.1982145621
H 0.6272796830 0.7782428719 -0.5820834160
H -0.2160868752 -0.7645534936 -0.9941414290
C -0.9275979798 -0.6041839183 0.8940158238

5
RCCSD(T)/VTZ ENERGY=-115.09393927
C -0.0574863658 -0.7286830288 -0.7932947956
H -0.0108840281 -0.0909799210 2.8033642150
H 0.7509499706 -0.2359037693 -1.3517898413
C -0.1045045276 -0.3317604995 1.7702141950
C 0.0200497609 -0.4453075514 0.5411808668

5
RCCSD(T)/AVTZ ENERGY=-115.14244038
C 0.0000000000 -0.2651494769 -0.1598522185
C 0.0000000000 -0.2609149335 1.2679969714
H 0.0000000000 1.9909518739 0.4085856064
H 0.0000000000 -0.8405740026 -1.0715371081
C 0.0000000000 0.9139202525 0.4565021559

5
RCCSD(T)/AVTZ ENERGY=-115.12088874
C -0.0666647085 0.0436416521 -0.1597053698
C -0.0623014494 0.0068245311 1.1743335009
H 0.1319136061 0.9654437671 -0.6991834709
H -0.2684289553 -0.8473404196 -0.7476227528
C -0.0623412488 -0.0308067293 2.4688693455

5
RCCSD(T)/AVTZ ENERGY=-115.12088897 (accurate)
C -0.0667471512 0.0433743096 -0.1595945383
C -0.0639500804 0.0061421888 1.1743389008
H 0.1322246607 0.9654091413 -0.6986160126
H -0.2680863564 -0.8471811397 -0.7483692472
C -0.0612638286 -0.0299816986 2.4689321503

5
RCCSD(T)/AVTZ ENERGY=-115.10122081
C -0.0576984928 -0.7276558621 -0.7925499441
H -0.0156831096 -0.0949475885 2.8066465898
H 0.7499689656 -0.2384353939 -1.3560163884
C -0.1003419643 -0.3278458501 1.7704773777
C 0.0218794110 -0.4437500754 0.5411170050

5
RCCSD(T)/AVTZ ENERGY=-115.10122109 (accurate)
C -0.0583132311 -0.7267961271 -0.7925293211
H -0.0171946473 -0.0948646514 2.8069595565
H 0.7494823038 -0.2387630662 -1.3567197581
C -0.0994219946 -0.3276009176 1.7705538002
C 0.0235723792 -0.4446100078 0.5414103625

5
RCCSD(T)/AVTZ ENERGY=-115.08766076
H 0.0000000000 -0.0009466258 -0.7835381607
H 0.0000000000 -0.0100728581 2.2823409811
C 0.0000000000 0.8579453879 1.3520373149
C 0.0000000000 -0.8724221353 1.3469180371
C 0.0000000000 -0.0040993607 0.2897853018

5
RCCSD(T)/AVTZ ENERGY=-115.06089012
C -0.0435278770 -0.0051833894 -0.2321388391
C -0.3043554376 0.5390612618 1.1988160899
H 0.6274873919 0.7784981562 -0.5833324546
H -0.2154697139 -0.7647131077 -0.9947079610
C -0.9282824633 -0.6038089609 0.8945542748

Si3H2

5
RCCSD(T)/VTZ ENERGY=-868.27479579
Si -0.0022307110 0.0615135137 -0.5014029975
Si 0.0046277753 0.0325084987 1.6431377414
H -0.0120387217 0.8257250292 2.9020138002
H -0.0264775342 0.8890290089 -1.7376947889
Si 0.0527738643 -2.0070175371 0.5432373151

5
RCCSD(T)/VTZ ENERGY=-868.27419934
Si 0.0000000000 -0.2657773140 -0.1301378207
Si 0.0000000000 -0.0940302505 2.0563411205
H 0.0000000000 1.2891750772 -0.7606430600
H 0.0000000000 -0.8588833331 -1.4920915942
Si 0.0000000000 1.9333679702 0.7794938105

5
RCCSD(T)/VTZ ENERGY=-868.27259796
Si -0.0135146272 -0.4038228223 -0.6368789246
Si 0.0132567603 -0.2395401962 2.1712126961
H -0.0071098588 2.8814802070 0.5798126257
H 0.0019508553 -1.2328013939 0.8200974510
Si -0.0038070911 1.4074850369 0.6659023453

5
RCCSD(T)/VTZ ENERGY=-868.26870517
Si 0.0000000000 -0.2217573725 -0.4153052591
Si 0.0000000000 -0.2291432427 2.0084193322
H 0.0000000000 1.5596557174 -0.6436810510
H 0.0000000000 -1.4025044616 0.9379960721
Si 0.0000000000 1.7964505573 0.9268318223

5
RCCSD(T)/VTZ ENERGY=-868.26713201
Si -0.0661383250 0.1612400237 -0.0802524556
Si 1.1099507932 0.6631339746 1.8040890623
H 0.3567415776 0.8669712704 -1.3153227355
H -1.2090214888 -0.7097021370 -0.5011324771
Si -0.5193553129 -0.8438803302 2.1293098589

5
RCCSD(T)/AVTZ ENERGY=-868.28097629
Si -0.0022642978 0.0623263279 -0.5016547619
Si 0.0046609848 0.0332461360 1.6434181538
H -0.0119463661 0.8238886278 2.9042705463
H -0.0264384737 0.8873936630 -1.7399456404
Si 0.0526428255 -2.0050962415 0.5432027725

5
RCCSD(T)/AVTZ ENERGY=-868.28077774
Si 0.0000000000 -0.2674196064 -0.1293902837
Si 0.0000000000 -0.0927362412 2.0573173434
H 0.0000000000 1.2865094836 -0.7598529152
H 0.0000000000 -0.8556025236 -1.4934999197
Si 0.0000000000 1.9331010373 0.7783882313

5
RCCSD(T)/AVTZ ENERGY=-868.27913332
Si -0.0133499870 -0.4044495429 -0.6378870854
Si 0.0131272930 -0.2398939032 2.1724470663
H -0.0073317168 2.8812046369 0.5796423645
H 0.0021931582 -1.2308185030 0.8200156669
Si -0.0038627088 1.4067581437 0.6659281812

5
RCCSD(T)/AVTZ ENERGY=-868.27547994
Si 0.0000000000 -0.2222144498 -0.4161611926
Si 0.0000000000 -0.2292029196 2.0094736170
H 0.0000000000 1.5576474809 -0.6430811554
H 0.0000000000 -1.4008887703 0.9366609276
Si 0.0000000000 1.7973598567 0.9273687199

5
RCCSD(T)/AVTZ ENERGY=-868.27352421
Si -0.0659148944 0.1617046701 -0.0811588987
Si 1.1097900575 0.6626293457 1.8037332724

H 0.3578358111 0.8684777963 -1.3157796830
H -1.2093073029 -0.7113084377 -0.4981339426
Si -0.5202264272 -0.8437405729 2.1280305050

5
RCCSD(T)/AUG-CC-PV(T+D)Z,H=AUG-CC-PVTZ
ENERGY=-868.28574172
Si -0.0022712857 0.0643723557 -0.4982452317
Si 0.0044304885 0.0352328964 1.6404223164
H -0.0117047814 0.8180361164 2.9032892516
H -0.0262800969 0.8812409841 -1.7392158047
Si 0.0524803482 -1.9971238395 0.5430405387

5
RCCSD(T)/AUG-CC-PV(T+D)Z,H=AUG-CC-PVTZ
ENERGY=-868.28547261
Si 0.0000000000 -0.2634450664 -0.1286001209
Si 0.0000000000 -0.0920936652 2.0517552787
H 0.0000000000 1.2850680366 -0.7587003794
H 0.0000000000 -0.8541508300 -1.4889625217
Si 0.0000000000 1.9284736748 0.7774701994

5
RCCSD(T)/AUG-CC-PV(T+D)Z,H=AUG-CC-PVTZ
ENERGY=-868.28312799
Si -0.0132412190 -0.4023207295 -0.6349824082
Si 0.0131757501 -0.2381709247 2.1689437124
H -0.0073245379 2.8765427965 0.5799824232
H 0.0020748611 -1.2274801537 0.8201197522
Si -0.0039088158 1.4042298428 0.6660827139

5
RCCSD(T)/AUG-CC-PV(T+D)Z,H=AUG-CC-PVTZ
ENERGY=-868.27982642
Si 0.0000000000 -0.2198725177 -0.4117751276
Si 0.0000000000 -0.2279847696 2.0051884398
H 0.0000000000 1.5549477255 -0.6408231324
H 0.0000000000 -1.3975105589 0.9356735085
Si 0.0000000000 1.7931213186 0.9259972282

5
RCCSD(T)/AUG-CC-PV(T+D)Z,H=AUG-CC-PVTZ
ENERGY=-868.27796054
Si -0.0537590901 0.1723321504 -0.0796725212
Si 1.1039845433 0.6552105963 1.8046261765
H 0.3475369144 0.8643672849 -1.3267766818
H -1.1966934847 -0.7089618832 -0.4761145867
Si -0.5288916388 -0.8451853470 2.1146288663

Ge3H2

5
RCCSD(T)/VTZ ENERGY=-6227.70486720
Ge 0.0000000000 -0.2621201382 -0.4967651094
Ge 0.0000000000 -0.2747804902 2.1089037610
H 0.0000000000 1.6258549866 -0.6836676839
H 0.0000000000 -1.4818589507 0.9563750257
Ge 0.0000000000 1.8961315514 0.9632414463

5
RCCSD(T)/VTZ ENERGY=-6227.70467152
Ge 0.0212919014 -0.4516040107 -0.7284270850
Ge -0.0005224569 -0.2875452688 2.2649943936
H -0.0176771753 2.9927969222 0.5782537966
H 0.0083454803 -1.3019340280 0.8172484875
Ge -0.0206617110 1.4610872168 0.6680766008

5
RCCSD(T)/VTZ ENERGY=-6227.70179981
Ge 0.0000000000 -0.3473708391 -0.1547414675
Ge 0.0000000000 -0.3591452627 2.1826432127
H 0.0000000000 1.4050971787 -0.6038309692
H 0.0000000000 -0.6930231010 -1.6652580366
Ge 0.0000000000 1.9384698056 1.0441458805

5
RCCSD(T)/VTZ ENERGY=-6227.69483754
Ge -0.0413851959 -0.0115217944 -0.2255247233
Ge -0.1068617065 0.8923518500 2.1345227228
H 0.9664202232 0.9947097686 -0.8345540218
H -0.4334518207 -0.9808176501 -1.3680986669
Ge -1.4576545522 -1.0140832403 1.6154230111

5
RCCSD(T)/VTZ ENERGY=-6227.69331512
Ge -0.0013998512 -0.2643299338 -0.2295863068
Ge 0.0212048448 -0.3575748318 2.2400682675
H -0.0986272064 3.2593426912 0.7100669420
H 0.0052260763 -0.8723547305 -1.6548025480
Ge -0.0513576136 1.7232821650 0.9083732853

5
RCCSD(T)/AVTZ ENERGY=-6227.71178443
Ge 0.0000000000 -0.2629277950 -0.4982962740
Ge 0.0000000000 -0.2750438915 2.1105843544
H 0.0000000000 1.6250277842 -0.6837944565
H 0.0000000000 -1.4814965546 0.9556210945
Ge 0.0000000000 1.8976674158 0.9639727213

5
RCCSD(T)/AVTZ ENERGY=-6227.71127075
Ge 0.0000000000 -0.3488527512 -0.1544518122
Ge 0.0000000000 -0.3590037073 2.1842206122
H 0.0000000000 1.4031888405 -0.6049571891

H 0.0000000000 -0.6902469701 -1.6657321431
Ge 0.0000000000 1.9389423695 1.0438791521

5
RCCSD(T)/AVTZ ENERGY=-6227.70849015
Ge 0.0000000000 -0.3488527512 -0.1544518122
Ge 0.0000000000 -0.3590037073 2.1842206122
H 0.0000000000 1.4031888405 -0.6049571891
H 0.0000000000 -0.6902469701 -1.6657321431
Ge 0.0000000000 1.9389423695 1.0438791521

5
RCCSD(T)/AVTZ ENERGY=-6227.70113704
Ge -0.0384187715 -0.0138182435 -0.2248216910
Ge -0.1097714593 0.8949000304 2.1332677962
H 0.9681906787 0.9940351141 -0.8334349862
H -0.4375627208 -0.9785795829 -1.3691309462
Ge -1.4553707792 -1.0158983843 1.6158881490

5
RCCSD(T)/AVTZ ENERGY=-6227.69950146
Ge -0.0014131188 -0.2646108582 -0.2301815689
Ge 0.0212152881 -0.3575882052 2.2400916384
H -0.0986322366 3.2601283307 0.7109329206
H 0.0052699649 -0.8735009541 -1.6550409334
Ge -0.0513936476 1.7239370468 0.9083175833

CSiGeH2

5
RCCSD(T)/VTZ ENERGY=-2403.73878294
C -0.0061376234 -0.2405159880 -0.3263504946
Ge 0.0307024778 -0.3491692832 1.5537714866
H -0.0346289909 1.4388157320 1.3958098394
H 0.0061288050 -0.9858555919 -1.1071400113
Si -0.0684900137 1.5459241629 -0.2901756640

5
RCCSD(T)/VTZ ENERGY=-2403.71847889
C 0.0000000000 -0.3478475796 -0.0730584771
Ge 0.0000000000 -0.3463326982 1.8781219266
H 0.0000000000 2.4449284846 -0.7827522192
H 0.0000000000 -1.1220817107 -0.8296791677
Si 0.0000000000 1.3751856537 0.2603303935

5
RCCSD(T)/VTZ ENERGY=-2403.70846418
C 0.0000000000 0.3109593126 0.0088601085
Ge 0.0000000000 -0.4067481575 2.0139623524
H 0.0000000000 0.9196528667 -0.8951416148
H 0.0000000000 1.1131164097 0.8137331467
Si 0.0000000000 -1.5283535180 -0.0640524731

5
RCCSD(T)/VTZ ENERGY=-2403.70679563
C 0.0000000000 -0.0826770772 -0.3359936068
Ge 0.0000000000 -0.0586021102 1.6850561566
H 0.0000000000 0.8274913495 -0.9151892377
H 0.0000000000 1.5159085839 1.5909738372
Si 0.0000000000 -1.7929749677 -0.1375811283

5
RCCSD(T)/VTZ ENERGY=-2403.69268818 (accurate)
C 0.2313990777 0.0342463961 0.1983194386
Ge 0.3855758400 -0.4313300142 1.9097427262
H 1.0648105548 0.1410423761 -2.4989348856
H -1.0434993670 1.2611429674 -2.0040575626
Si 0.0836139644 0.4807500045 -1.4419535367

5
RCCSD(T)/VTZ ENERGY=-2403.67132489
C 0.0132232773 -0.0136433893 0.6203870471
Si 0.4877516218 -0.7609129931 2.0608779812
H 0.3375477197 1.8344478320 -1.6484860596
H -1.8054319032 0.4532753110 -1.6469354274
Ge -0.4897902855 0.7658717294 -0.9073990313

5
RCCSD(T)/VTZ ENERGY=-2403.64277308
Ge -0.0701911987 -0.5964600128 -1.1677690822
H 0.3652523148 0.1618811893 3.2336702160
H 0.7228384088 0.7431548893 -1.5076827622
Si -0.2314957665 -0.8518602268 2.3016773116
C 0.0783334673 -0.3352292380 0.6847454193

5
RCCSD(T)/VQZ ENERGY=-2403.76728887
C -0.0046830378 -0.2378029715 -0.3253094385
Ge 0.0311058637 -0.3477033527 1.5510037059
H -0.0355919110 1.4378323180 1.3928093039
H 0.0048033855 -0.9833627978 -1.1054149450
Si -0.0680596455 1.5402358359 -0.2871734700

5
RCCSD(T)/VQZ ENERGY=-2403.74768202
C 0.0000000000 -0.3451380542 -0.0751591963
Ge 0.0000000000 -0.3412364688 1.8739953765
H 0.0000000000 2.4447746620 -0.7758019345
H 0.0000000000 -1.1235032924 -0.8268613238
Si 0.0000000000 1.3689553032 0.2567895342

5
RCCSD(T)/VQZ ENERGY=-2403.73663187

C 0.0000000000 0.3071975707 0.0091627391
Ge 0.0000000000 -0.4036155070 2.0092277492
H 0.0000000000 0.9181018713 -0.8928322206
H 0.0000000000 1.1103432105 0.8134353372
Si 0.0000000000 -1.5234002321 -0.0616320851

5
RCCSD(T)/VQZ ENERGY=-2403.73545367
C 0.0000000000 -0.0842849703 -0.3364384136
Ge 0.0000000000 -0.0592017483 1.6788163036
H 0.0000000000 0.8258313136 -0.9149501401
H 0.0000000000 1.5136099431 1.5911425865
Si 0.0000000000 -1.7868087597 -0.1313043153

5
RCCSD(T)/VQZ ENERGY=-2403.72335765
C 0.2800624928 -0.4309577550 0.2338677439
Ge 0.2209157100 -0.3444525755 2.0112889011
H 0.2520952178 1.8438075871 -1.4479434229
H -1.7781373502 0.5177441083 -1.4595118046
Si -0.4340314042 0.6718894020 -0.8579492399

5
RCCSD(T)/VQZ ENERGY=-2403.72279977
C 0.2126143261 0.0043101219 0.1863838642
Ge 0.3958921077 -0.4097818615 1.9045818550
H 1.0695939557 0.1470399386 -2.4907985012
H -1.0382409729 1.2669021325 -1.9961194124
Si 0.0820406534 0.4773813986 -1.4409316255

5
RCCSD(T)/VQZ ENERGY=-2403.70035124
C 0.0123875911 -0.0133976332 0.6194908988 Si 0.4858187231 -0.7568221669 2.0533576195 H 0.3395356081 1.8329616004 -1.6446817496 H -1.8049656291 0.4512122497 -1.6437269253 Ge -0.4894758631 0.7650844399 -0.9059953334

5
RCCSD(T)/VQZ ENERGY=-2403.67133467
Ge -0.0695996028 -0.5959108594 -1.1612196418
H 0.3649820433 0.1611061567 3.2258410944
H 0.7222967454 0.7421721850 -1.5036468073
Si -0.2304910181 -0.8504225344 2.2964333437
C 0.0775490582 -0.3354583469 0.6872331135

5
RCCSD(T)/AVTZ ENERGY=-2403.74574621
C -0.0058189241 -0.2405298399 -0.3264398942
Ge 0.0307594955 -0.3502503426 1.5552657782
H -0.0348982613 1.4395014427 1.3955197008
H 0.0058526615 -0.9865006409 -1.1078745536
Si -0.0683203167 1.5469784125 -0.2905558751

5
RCCSD(T)/AVTZ ENERGY=-2403.72533493
C 0.0000000000 -0.3472297400 -0.0732465183
Ge 0.0000000000 -0.3478963830 1.8790161845
H 0.0000000000 2.4448723880 -0.7839117032
H 0.0000000000 -1.1224592416 -0.8299193651
Si 0.0000000000 1.3765651264 0.2610238582

5
RCCSD(T)/AVTZ ENERGY=-2403.71551628
C 0.0000000000 0.3114629569 0.0100981027
Ge 0.0000000000 -0.4081796999 2.0156663437
H 0.0000000000 0.9183511986 -0.8962723604
H 0.0000000000 1.1163825066 0.8128579505
Si 0.0000000000 -1.5293900487 -0.0649885167

5
RCCSD(T)/AVTZ ENERGY=-2403.71386842
C 0.0000000000 -0.0837112533 -0.3370493651
Ge 0.0000000000 -0.0591560349 1.6873577323
H 0.0000000000 0.8301520289 -0.9119896940
H 0.0000000000 1.5162625604 1.5869027593
Si 0.0000000000 -1.7944015228 -0.1379554115

5
RCCSD(T)/AVTZ ENERGY=-2403.69985737
C 0.2085840652 -0.0045368035 0.1895389555
Ge 0.3994968657 -0.4074972452 1.9144892550
H 1.0722435819 0.1511438532 -2.4960711174
H -1.0399020110 1.2693726103 -2.0014598648
Si 0.0814775683 0.4773693152 -1.4433810483

5
RCCSD(T)/AVTZ ENERGY=-2403.70025974
C -0.0739982849 -0.4909785426 0.0843052362
Ge 0.5420386913 -0.0427655107 1.6995762953
H 1.1465497240 0.2481269312 -2.3710966790
H -0.9552157825 1.3621174955 -1.8789370499
Si 0.0625257222 0.4093513567 -1.3707316226

5
RCCSD(T)/AVTZ ENERGY=-2403.70025974
C -0.0739982849 -0.4909785426 0.0843052362
Ge 0.5420386913 -0.0427655107 1.6995762953
H 1.1465497240 0.2481269312 -2.3710966790
H -0.9552157825 1.3621174955 -1.8789370499
Si 0.0625257222 0.4093513567 -1.3707316226

5
RCCSD(T)/AVTZ ENERGY=-2403.67838504

C 0.0132012454 -0.0134984986 0.6204574847
Si 0.4879095601 -0.7612791898 2.0614128111
H 0.3389785868 1.8351206796 -1.6482580480
H -1.8066256689 0.4522076424 -1.6466347610
Ge -0.4901632934 0.7664878565 -0.9085329768

5
RCCSD(T)/AVTZ ENERGY=-2403.64976606
Ge -0.0703075770 -0.5966517368 -1.1673057921
H 0.3660767836 0.1665173614 3.2259200663
H 0.7226993824 0.7455868344 -1.5030438324
Si -0.2334592181 -0.8558712774 2.3032678759
C 0.0797278550 -0.3380945806 0.6858027847

5
RCCSD(T)/AVTZ ENERGY=-2403.71386798
C 0.0000000000 -0.0829235220 -0.3379958954
Ge 0.0000000000 -0.0623948555 1.6883398285
H 0.0000000000 0.8345177483 -0.9066703010
H 0.0000000000 1.5132354904 1.5869941297
Si 0.0000000000 -1.7932890829 -0.1434017407

5
RCCSD(T)/AVTZ ENERGY=-2403.70025964
C 0.2798618007 -0.4250786565 0.2426424410
Ge 0.2257058600 -0.3605252768 2.0265439284
H 0.2529229788 1.8467209722 -1.4612067039
H -1.7823635624 0.5208110612 -1.4653567650
Si -0.4352224110 0.6761026669 -0.8628707228

5
RCCSD(T)/VTZ ENERGY=-2403.67132503
C 0.0115086116 -0.0155789814 0.6199241105
Si 0.4896952914 -0.7591018595 2.0611434123
H 0.3381935074 1.8340620852 -1.6469695655
H -1.8057145317 0.4542868137 -1.6481502190
Ge -0.4903824486 0.7653704320 -0.9075032283

4
RCCSD(T)/AVQZ ENERGY=-77.06506641
C 0.9202021038 0.6184492854 0.0306932431
C -0.1890877114 -0.0993557095 0.0089181599
H 0.8923115079 1.6939956945 -0.1352292780
H 1.8850330897 0.1492222196 0.2151800349

4
RCCSD(T)/AVTZ ENERGY=-77.03838319
C -0.0335578733 -0.0793002862 -0.5920008734
C 0.0080881581 -0.5986928799 0.6470818945
H -0.4379703046 0.8520662907 -0.9684290597
H 0.4125726998 -1.5300093545 1.0235546485

4
RCCSD(T)/AVTZ ENERGY=-151.60885234
C 2.3006307258 -0.8455433405 0.3722472934
O 2.9895130023 0.2234932618 0.0223881150
H 2.6539150750 -1.7977414971 0.7367449918
C 1.3366079070 0.0385180258 0.0006747797

4
RCCSD(T)/AVTZ ENERGY=-151.60510989
H 0.0654521032 0.7646263436 2.4259602813
C 2.3464294422 0.7230286201 4.5081060407
O 0.0141397279 0.6945097041 3.3929521907
C 1.2007687667 0.7130531123 3.9027347372

4
RCCSD(T)/AVTZ ENERGY=-151.69085770
C 2.2231296814 -0.9602643225 0.2249039081
O 0.9394379635 1.1344996641 -0.0494678696
H 2.0872450712 -1.9991275629 -0.0156727641
C 1.4553785938 0.0810824613 0.0253186257

C2H2

4
RCCSD(T)/AVTZ ENERGY=-77.19219737
C 0.8676658405 0.5989583116 0.0001434597
C -0.1138937041 -0.1090491999 0.0000582232
H 1.7307845040 1.2210660660 0.0002167230
H -0.9766528204 -0.7316555079 -0.0000203160

4
RCCSD(T)/AVTZ ENERGY=-77.12199860
C 0.9225687030 0.6200579455 0.0307175732
C -0.1743477784 -0.0899278319 0.0092282850
H 0.8806525773 1.6934519626 -0.1365141989
H 1.8795852981 0.1387293038 0.2161304908

C3H (gs)

4
RCCSD(T)/AVTZ ENERGY=-114.46551638
H 0.0000000000 -0.1467884790 -0.2816155881
C 0.0000000000 -0.0113471958 2.0801485241
C 0.0000000000 1.3018537981 1.6318562299
C 0.0000000000 0.1556307020 0.7536756803

C3H (linear,sp)

4
RCCSD(T)/AVTZ ENERGY=-114.46268456
C 0.8923200726 0.6166348746 0.0001459461
C -0.1197520269 -0.1128828760 0.0000622835

H 1.7570011017 1.2399573211 0.0002174189
C -1.2131732874 -0.9010548596 -0.0000275585

Si2H2

4
RCCSD(T)/AVTZ ENERGY=-579.22698751
Si -0.2429229973 0.3038671663 -0.4987869587
Si 0.2486714853 0.1173625054 1.6662843908
H -0.6698180874 1.2389419792 0.8250676116
H 1.1590004194 0.6355700791 0.3578784663

4
RCCSD(T)/AVTZ ENERGY=-579.21099224
Si -0.4734545585 0.5346253690 -0.6978729099
Si 0.0805144844 -0.9757308342 0.7056448976
H -1.2414638898 1.6603365473 -1.3040330593
H -1.2493724761 0.1177163080 0.6879821515

4
RCCSD(T)/AVTZ ENERGY=-579.20704429
Si -0.2798553812 0.7109500946 -0.9643294495
Si -0.2521511365 -0.7613143088 0.6970848089
H -1.3977791592 1.6592801807 -1.2102976980
H 0.8176027171 0.8596399635 -1.9558242615

4
RCCSD(T)/AVTZ ENERGY=-579.19857461
Si -0.2835132561 0.5302913900 -0.9967011938
Si -0.1148968025 -0.8032334082 0.6467021144
H -1.3070417464 1.6091691307 -1.1191802681
H 0.9088383549 -1.8819061526 0.7692568976

4
RCCSD(T)/VQZ ENERGY=-579.21290414
Si -0.2821437261 0.5263250511 -0.9929029874
Si -0.1162163467 -0.7992149904 0.6429391737
H -1.3029816086 1.6021931883 -1.1149963463
H 0.9047282313 -1.8749822891 0.7650377100

4
RCCSD(T)/AVQZ ENERGY=-579.21448739
Si -0.2818681121 0.5261938196 -0.9931709882
Si -0.1165329723 -0.7991264529 0.6431740025
H -1.3031461113 1.6023333268 -1.1148939242
H 0.9049337456 -1.8750797336 0.7649684599

Si3H

4
RCCSD(T)/AVTZ ENERGY=-867.66806203
H -0.0008784010 -0.0000020635 -0.5592127071
Si -0.0019110675 -0.8252319289 0.8844216010
Si -0.0004326800 0.9053014885 2.4292390259
Si 0.0005524385 1.4879474339 0.1825350202

4 RCCSD(T)/AVTZ ENERGY=-867.66546168
H 0.0000000000 -0.2773561791 -0.9183527007
Si 0.0000000000 -0.2838792887 2.7086831855
Si 0.0000000000 1.9110560078 1.8410258156
Si 0.0000000000 -0.0504717148 0.5527085458

Ge2H2

4
RCCSD(T)/AVTZ ENERGY=-4152.17968086
Ge -0.2653708584 0.2988947968 -0.5804089511
Ge 0.2675762478 0.1032665028 1.7496198686
H -0.7139582566 1.2665760287 0.8376177758
H 1.2121830172 0.6322504617 0.3438011368

4
RCCSD(T)/AVTZ ENERGY=-4152.16355361
Ge -0.4551918479 0.5588291612 -0.7396885370
Ge 0.1234362086 -1.0584412939 0.7499147044
H -1.2853796274 1.7217428723 -1.3491293204
H -1.2666411732 0.1148166504 0.7306242330

4
RCCSD(T)/AVTZ ENERGY=-4152.16074433
Ge -0.2797903545 0.7143863056 -0.9675497821
Ge -0.2519701171 -0.8423903312 0.7802915029
H -1.4317294072 1.7103950768 -1.2378136658
H 0.8513069187 0.8861648788 -2.0082946550

4
RCCSD(T)/AVTZ ENERGY=-4152.15060775
Ge -0.2842903031 0.5670642681 -1.0451393718
Ge -0.1141252079 -0.8399593008 0.6955553402
H -1.3617488069 1.6846201961 -1.1632692072
H 0.9635507279 -1.9574041334 0.8129305589

Ge3H

4
RCCSD(T)/AVTZ ENERGY=-6227.11004397
H 0.0000000000 -0.0155454063 -0.6280486227
Ge 0.0000000000 -0.9277329604 0.8724394369
Ge 0.0000000000 0.9264848477 2.5337989090
Ge 0.0000000000 1.5690852790 0.1287234468

4
RCCSD(T)/AVTZ ENERGY=-6227.10040414
H 0.0437237253 -0.1576620722 -1.0613830170

Ge 0.0486739732 0.3204143575 0.4134557311
Ge 0.0687225756 1.1035041866 2.5888157042
Ge -0.3208000441 -1.3939033819 2.2474921618

4
RCCSD(T)/AVTZ ENERGY=-6227.07108368
H -1.2323723682 -0.1362326901 4.7741084333
Ge -0.0065758543 0.0142618518 -0.0032402635
Ge -0.0017873606 -0.0286921102 2.3337453056
Ge 0.3671394931 0.0085559485 4.7035061045

CSiH2

4
RCCSD(T)/AVTZ ENERGY=-328.20624289
C 1.1094555893 0.3530517917 0.0765254289
Si -0.5568305261 -0.0883079013 -0.0101875807
H 1.4499134151 1.3867729761 0.1457207795
H 1.9220433017 -0.3741075065 0.0675290723

CSiH2

4
RCCSD(T)/AVTZ ENERGY=-328.14879139
C 1.1340121717 0.5809598879 0.0181444418
Si -0.4943957057 0.2299517041 -0.0525982780
H 1.9379494590 1.3008880000 0.0062159287
H -1.0696621050 -1.1324799222 0.0286359975

4
RCCSD(T)/AVTZ ENERGY=-328.06701354
C 1.1438101980 0.6131717585 0.0013127290
Si -0.6011722131 0.1740761679 0.0197085630
H -1.6504271686 1.2172225856 0.0596608631
H -1.0323052163 -1.2416392020 -0.0040246351

CGeH2

4
RCCSD(T)/AVTZ ENERGY=-2114.67930740
C 1.1338297925 0.3598580635 0.0779314672
Ge -0.6210744401 -0.1061644519 -0.0135298321
H 1.4693649418 1.3945324839 0.1467850772
H 1.9424618958 -0.3708165354 0.0684010178

4
RCCSD(T)/AVTZ ENERGY=-2114.60945783
C 1.2168880738 0.5660093622 0.0245732482
Ge -0.4912589655 0.2133384139 -0.0509760300
H 1.9431725812 1.3680660025 0.0007667148
H -1.1608976995 -1.1680941286 0.0260341569

4
RCCSD(T)/AVTZ ENERGY=-2114.52488925
C 1.2200170700 0.6318263528 -0.0104592221
Ge -0.5948368350 0.1757774151 0.0201611553
H -1.7005070479 1.2433281654 0.0628038221
H -1.0647675872 -1.2881006234 0.0041517648

GeSiH2

4
RCCSD(T)/AVTZ ENERGY=-2365.70301134
Si -0.2286738487 0.3196560638 -0.5033529071
Ge 0.2525336552 0.0808530848 1.7477834932
H -0.7069754222 1.2512264102 0.7867129598
H 1.1780463758 0.6440059210 0.3192998243

4
RCCSD(T)/AVTZ ENERGY=-2365.69388323
Si -0.2787665937 0.7227811297 -0.9735551685
Ge -0.2531262584 -0.8031986785 0.7357992084
H -1.3951889579 1.6731782473 -1.2253041078
H 0.8148986799 0.8757954115 -1.9703067721

4
RCCSD(T)/AVTZ ENERGY=-2365.68157780
Ge -0.1502788278 -0.4495102682 0.4739475210
H -0.3750491207 0.3458209953 1.7876429133
H 0.3250377448 0.6955908177 -0.7716241933
Si 0.3772804937 -0.7589037147 -1.6381391510

HSiGeH

4
RCCSD(T)/AVTZ ENERGY=-2365.68157780
Ge -0.1502788278 -0.4495102682 0.4739475210
H -0.3750491207 0.3458209953 1.7876429133
H 0.3250377448 0.6955908177 -0.7716241933
Si 0.3772804937 -0.7589037147 -1.6381391510

4
RCCSD(T)/AVTZ ENERGY=-2365.67424107
Ge -0.3382415999 0.5733945815 -0.9831909460
Si -0.2199011355 -0.7667131699 0.7349102163
H -1.3418966966 1.7276773653 -1.2489037341
H 0.8344429120 -1.8244839069 0.7972617937

SiGeH2

4
RCCSD(T)/AVTZ ENERGY=-2365.67300377
Ge -0.2796024786 0.7044735719 -0.9564422699
Si -0.2528940486 -0.8047867142 0.7381798290

H -1.4335672567 1.6970794076 -1.2220099594
H 0.8538808240 0.8717896646 -1.9930941997

CSiGeH

4
RCCSD(T)/AVTZ ENERGY=-2403.11989870
H 0.0000000000 -0.1401830040 -0.3505730949
Si 0.0000000000 -0.5288011642 2.3469240495
Ge 0.0000000000 1.8719512158 1.4799778523
C 0.0000000000 0.0963819025 0.7077364831

4
RCCSD(T)/AVTZ ENERGY=-2403.05522176
H -0.1954338320 0.7072972546 0.0584640195
C -0.3273392700 -0.2651276555 2.1838960792
Ge -0.3641099607 1.5486604904 1.7121124731
Si -0.1657771473 -0.9153168395 0.5232430882

C3O (singlet)
4

RCCSD(T)/AVTZ ENERGY=-188.92604599
C 0.8429991246 0.4999075672 -0.0326401107
C 0.1504356751 -0.5667915588 -0.0127366724
O 1.3218645274 1.7248883288 0.0495878280
C 1.7678836329 2.8116418228 0.1153511050

C3O (triplet)

4
RCCSD(T)/AVTZ ENERGY=-188.98337355
C 0.9397931471 0.7494375182 -0.0082149890
C 0.3101657315 -0.5888440506 0.0249031880
O 0.8955849369 1.9287786998 -0.1344244491
C 1.6671564344 -0.5151994076 0.2372984000

C3O- (doublet)

4
RCCSD(T)/AVTZ ENERGY=-189.11998895
C 1.2799953600 0.5687789754 0.0077751752
C 0.3877008631 -0.5712162160 -0.0075217493
O 1.4887590316 1.7688844162 -0.0252950455
C 1.7353455154 -0.8029030957 0.0922690597

hc3 (quartet)

4
RCCSD(T)/AVTZ ENERGY=-114.41384729
H 0.0000000000 -0.0010901619 -0.8059503276
C 0.0000000000 -0.0037520028 0.2579254329
C 0.0000000000 0.0042451194 1.5069845114
C 0.0000000000 0.0098685467 2.8206403962

4
RCCSD(T)/AVTZ ENERGY=-114.35423630
H 0.0000000000 -0.2183851303 -0.6492434251
C 0.0000000000 -0.1758424268 1.7150188675
C 0.0000000000 1.2201584429 1.4393043759
C 0.0000000000 0.0256556826 0.3949707928