

Supporting Information to

Understanding the electronic structure of metal/SAM/organic-semiconductor heterojunctions

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Cartesian coordinates of the three component systems:

The metal/SAM systems were optimized using a damped molecular dynamics strategy as implemented in the VASP code. The isolated biphenyl monolayers were optimized with the same strategy, keeping the lowermost hydrogens fixed. For further details, see methods section in the main text. The Cartesian coordinates and lattice vectors of the complete three component systems as they were used are listed below.

System (1), Au|Pyr|2P|N(CH₃)₂||2P:

x: +5.1135503988 +0.0000000000 +0.0000000000
y: +0.0000000000 +8.8569290977 +0.0000000000
z: +0.0000000000 +0.0000000000 +60.0000000000

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H +3.5508738606 +8.2817969124 +28.3519070462
H +1.0209144684 +0.7535442485 +29.3714759138

System (2), Au|Pyr|2P|NH₂||2P:

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Au +5.0858883015 +8.8208226106 +9.5915271478
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Au +5.0901468311 +5.8782020417 +9.7215788767
Au +2.5515357179 +1.4504317942 +9.7214656825
Au +2.5556278621 +4.3930177519 +9.5976208346
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System (3), Au|CN|2P|NH₂||2P:

x: +5.1135503988 +0.0000000000 +0.0000000000
y: +0.0000000000 +8.8569300817 +0.0000000000
z: +0.0000000000 +0.0000000000 +60.0000000000

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C +1.5250089958 +3.9974880335 +20.6700039762
H +0.6361145256 +2.3711999957 +14.1547106993
H +2.5281473064 +8.4130931976 +13.4941831359
H +0.5803075344 +1.8859711756 +16.5500450781
H +2.4660707741 +7.9110363623 +15.8884405020
H +4.9867578354 +6.7951183710 +14.0718631545
H +3.2202293811 +4.1087286509 +13.5086731009
H +4.9228974621 +6.2335854484 +16.4494450366
H +3.1853292458 +3.5569106170 +15.8920758128
H +2.3804810045 +7.5738907051 +17.8399959163
H +0.6237227334 +1.3997913448 +18.4432430432
H +2.3479798814 +7.0873651946 +20.2192034489
H +0.5763217190 +0.9199733285 +20.8215104237
H +5.0065990434 +5.9312750361 +18.3912667372
H +3.0790514867 +3.0458481995 +17.7938979567
H +5.0307513135 +5.4582698461 +20.7725217089
H +3.1050197536 +2.5842147699 +20.1789985375
H +3.4859751809 +7.2942354872 +22.3797315798
H +4.8122352341 +8.3345618147 +22.6177449478
H +0.7185384292 +3.9728753714 +22.5736899573
H +2.0099781546 +2.8890090474 +22.3463486339
N +3.9369197142 +8.1744084155 +22.1090218454
N +1.5886675978 +3.7810238007 +22.0668755997
C +1.6910304599 +6.0792762421 +29.7780281224
C +4.2632745264 +2.1011904454 +28.3565344793
C +4.2507353342 +1.6507773341 +29.7779916326
C +1.6785124648 +6.5296624517 +28.3565661185
C +0.7491571685 +6.5632691904 +30.7135034266
C +3.3117309425 +1.6302978892 +27.4239150789
C +2.6301409455 +6.0588816264 +27.4239810306
C +0.0790185243 +2.1347838847 +30.7134943235
C +0.7708147633 +6.1545004336 +32.0510691751
C +3.3160571075 +2.0631752537 +26.0938446574
C +0.0572956248 +1.7260144675 +32.0510619573
C +2.6257141418 +6.4916771667 +26.0938799165
C +4.2732070228 +2.9841388191 +25.6506580205
C +1.7355935617 +5.2441132796 +32.5009107035
C +1.6684381541 +7.4124980562 +25.6506708102
C +4.2060917303 +0.8155874215 +32.5008557769
C +0.1155783733 +3.4610461877 +26.5557990026
C +2.6744363586 +4.7450354537 +31.5890951032

C +0.7124546007 +7.8893281839 +26.5557895072
C +3.2672318667 +0.3165344959 +31.5890236766
C +0.1099496596 +3.0246944675 +27.8847754081
C +2.6510285262 +5.1565892808 +30.2519983583
C +0.7181355049 +7.4529956175 +27.8847779382
C +3.2906912507 +0.7281109514 +30.2519376453
H +2.5436709040 +0.9138735894 +27.7239681231
H +5.0916622612 +7.2752510748 +30.4107322589
H +0.8500569315 +2.8467720507 +30.4107183524
H +3.3983519392 +5.3426352833 +27.7240840374
H +0.0177910178 +6.5503752848 +32.7393316632
H +2.5531872523 +1.6830675648 +25.4075373767
H +3.3886524071 +6.1116977212 +25.4075842171
H +0.8102713424 +2.1219025463 +32.7393615388
H +1.7533662477 +4.9229706395 +33.5475322990
H +4.2699137052 +3.3361719477 +24.6155890448
H +1.6716361023 +7.7644788163 +24.6155890448
H +4.1883690267 +0.4943828447 +33.5474581386
H +0.8738457197 +4.1810150834 +26.2342536037
H +3.4367069051 +4.0300056726 +31.9119957284
H +2.5049293904 +8.4584417930 +31.9118907337
H +5.0676294233 +8.6091856579 +26.2342383192
H +3.4058813542 +4.7473219039 +29.5762933229
H +0.8757857214 +3.4189457588 +28.5566873011
H +5.0657711780 +7.8471386199 +28.5566660910
H +2.5358117858 +0.3188859560 +29.5762349586

System (4), Au|Pyr|2P|H||2P:

x: +5.1135503988 +0.0000000000 +0.0000000000
y: +0.0000000000 +8.8569290977 +0.0000000000
z: +0.0000000000 +0.0000000000 +60.0000000000

Au +5.0829005601 +8.8288694075 +9.5938403968
Au +5.1084023934 +2.9245993470 +9.6036410067
Au +5.0883221129 +5.8851194730 +9.7218177824
Au +2.5466382427 +1.4553730626 +9.7249819191
Au +2.5539347110 +4.3985304864 +9.5972680755
Au +2.5279513101 +7.3520154442 +9.5990727956
Au +3.3870524711 +0.0018674146 +7.2112612156
Au +3.3958332491 +2.9217572360 +7.2127717249
Au +3.4196171966 +5.8908586693 +7.2121153017
Au +0.8627045200 +1.4624584065 +7.2150735878
Au +0.8377196853 +4.4304754506 +7.2164343678
Au +0.8331024678 +7.3517480651 +7.2118260818
Au +1.7044997544 +0.0000000000 +4.8211660106
Au +1.7044997544 +2.9522801761 +4.8211660106
Au +1.7044997544 +5.9046489216 +4.8211660106

Au +4.2612749538 +1.4761843727 +4.8211660106
Au +4.2612749538 +4.4284645489 +4.8211660106
Au +4.2612749538 +7.3807447250 +4.8211660106
Au +0.0000000000 +0.0000000000 +2.4105830053
Au +0.0000000000 +2.9522801761 +2.4105830053
Au +0.0000000000 +5.9046489216 +2.4105830053
Au +2.5567751994 +1.4761843727 +2.4105830053
Au +2.5567751994 +4.4284645489 +2.4105830053
Au +2.5567751994 +7.3807447250 +2.4105830053
Au +3.4090506443 +0.0000000000 +0.0000000000
Au +3.4090506443 +2.9522801761 +0.0000000000
Au +3.4090506443 +5.9046489216 +0.0000000000
Au +0.8522754450 +1.4761843727 +0.0000000000
Au +0.8522754450 +4.4284645489 +0.0000000000
Au +0.8522754450 +7.3807447250 +0.0000000000
N +2.4829617998 +1.2782039386 +12.3273729500
N +5.1133595827 +5.7232076634 +12.3197536645
C +3.3439081113 +1.9168533325 +13.1593607390
C +1.6273992022 +0.3863579746 +12.8886792667
C +3.3754493108 +1.6958351805 +14.5392899135
C +1.6035230012 +0.1105170057 +14.2563574790
C +2.4916143980 +0.7678580297 +15.1369378517
C +4.2008929308 +6.3134386536 +13.1328385197
C +0.8888060488 +4.8766685537 +12.8988944928
C +4.1472170244 +6.0849365446 +14.5109710409
C +0.8996810995 +4.6042434779 +14.2670433910
C +5.0688757075 +5.2074873409 +15.1274643772
C +2.4914106639 +0.4973135237 +16.5989932758
C +1.5781011274 +8.4427636626 +17.1788386553
C +3.3999311635 +1.1418751318 +17.4696200251
C +1.5716797690 +8.1898294782 +18.5542203623
C +3.3934888517 +0.8924072220 +18.8457524722
C +2.4787298643 +8.8431750733 +19.3996562504
C +5.0547020051 +4.9328707998 +16.5882449764
C +4.1913685493 +5.6294285659 +17.4647012539
C +0.7993639860 +3.9645443311 +17.1598546062
C +4.1897140062 +5.3737734400 +18.8400649709
C +0.8029609067 +3.7111720544 +18.5350872336
C +5.0545413652 +4.4155590883 +19.3866806211
H +4.0289397615 +2.6268930149 +12.6802227400
H +0.9475178984 +8.7368657483 +12.1893148115
H +4.1009693654 +2.2575992321 +15.1332819848
H +0.8810004320 +8.2297210196 +14.6138404223
H +3.4902279372 +6.9867777741 +12.6382733608
H +1.6089945810 +4.4080397477 +12.2137948581
H +3.3705003773 +6.5938538924 +15.0874731422
H +1.6613141782 +3.9173310314 +14.6431489961
H +0.8496139008 +7.9178812137 +16.5559677113

H +4.1308186019 +1.8549412502 +17.0810034126
H +0.8490691734 +7.4750978810 +18.9592103974
H +4.1156689731 +1.4119279490 +19.4830710689
H +2.4732502610 +8.6464770936 +20.4771266873
H +3.5095121451 +6.3936177131 +17.0826293394
H +1.4807697704 +3.3887063754 +16.5285379559
H +3.5042328668 +5.9341158169 +19.4834736860
H +1.4846310829 +2.9535067087 +18.9340590286
H +5.0557990000 +4.2181780000 +20.4639550000
C +5.0090618019 +6.4795198283 +26.3976392918
C +2.4677554696 +2.5014340316 +24.9761456487
C +2.4552162774 +2.0510209203 +26.3976028020
C +4.9965438068 +6.9299060379 +24.9761772879
C +4.0671885105 +6.9635127766 +27.3331145960
C +1.5162118857 +2.0305414754 +24.0435262483
C +0.8346218887 +6.4591252126 +24.0435922000
C +3.3970498663 +2.5350274709 +27.3331054929
C +4.0888461053 +6.5547440198 +28.6706803445
C +1.5205380507 +2.4634188399 +22.7134558268
C +3.3753269668 +2.1262580537 +28.6706731267
C +0.8301950850 +6.8919207529 +22.7134910859
C +2.4776879660 +3.3843824053 +22.2702691899
C +5.0536249037 +5.6443568658 +29.1205218729
C +4.9864694961 +7.8127416424 +22.2702819796
C +2.4105726735 +1.2158310077 +29.1204669463
C +3.4336097153 +3.8612897739 +23.1754101720
C +0.8789173018 +5.1452790399 +28.2087062726
C +4.0304859427 +8.2895717701 +23.1754006766
C +1.4717128099 +0.7167780821 +28.2086348460
C +3.4279810016 +3.4249380537 +24.5043865775
C +0.8555094694 +5.5568328670 +26.8716095277
C +4.0361668469 +7.8532392037 +24.5043891076
C +1.4951721939 +1.1283545376 +26.8715488147
H +0.7481518472 +1.3141171756 +24.3435792925
H +3.2961432044 +7.6754946610 +27.0303434283
H +4.1680882735 +3.2470156369 +27.0303295218
H +1.6028328824 +5.7428788695 +24.3436952068
H +3.3358223598 +6.9506188710 +29.3589428326
H +0.7576681955 +2.0833111510 +22.0271485461
H +1.5931333503 +6.5119413074 +22.0271953865
H +4.1283026844 +2.5221461325 +29.3589727082
H +5.0713975897 +5.3232142257 +30.1671434684
H +2.4743946484 +3.7364155339 +21.2352002142
H +4.9896674443 +8.1647224025 +21.2352002142
H +2.3928499699 +0.8946264309 +30.1670693080
H +4.1918770617 +4.5812586696 +22.8538647731
H +1.6411878483 +4.4302492588 +28.5316068978
H +0.7094103336 +0.0017562815 +28.5315019031

H +3.2721103665 +0.1525001464 +22.8538494886
H +1.6103622974 +5.1475654901 +26.1959044923
H +4.1938170634 +3.8191893450 +25.1762984705
H +3.2702521212 +8.2473822061 +25.1762772604
H +0.7402927290 +0.7191295422 +26.1958461280

System (5), Au₁Si₂P₁NH₂||2P:

x: +5.1135503988 +0.0000000000 +0.0000000000
y: +0.0000000000 +8.8569300817 +0.0000000000
z: +0.0000000000 +0.0000000000 +60.0000000000

Au +0.0744766025 +8.6915997760 +9.6895315301
Au +0.0961857162 +3.0667841533 +9.5240724774
Au +4.9567386450 +5.8770236523 +9.6697550074
Au +2.3944329751 +1.4348079849 +9.6843184863
Au +2.6501393155 +4.2567347151 +9.7237318043
Au +2.6356701378 +7.4834750428 +9.5066572883
Au +3.4316124487 +0.0438919496 +7.1824603744
Au +3.3954268835 +2.9628316541 +7.2630370731
Au +3.4223235422 +5.8909210758 +7.2315569038
Au +0.8674812695 +1.4678449395 +7.2365692773
Au +0.8772834101 +4.4667503417 +7.1918480991
Au +0.8369913514 +7.3888926083 +7.2398698175
Au +1.7044997544 +0.0000000000 +4.8211658864
Au +1.7044997544 +2.9522805041 +4.8211658864
Au +1.7044997544 +5.9046495776 +4.8211658864
Au +4.2612749538 +1.4761845367 +4.8211658864
Au +4.2612749538 +4.4284650409 +4.8211658864
Au +4.2612749538 +7.3807455450 +4.8211658864
Au +0.0000000000 +0.0000000000 +2.4105829432
Au +0.0000000000 +2.9522805041 +2.4105829432
Au +0.0000000000 +5.9046495776 +2.4105829432
Au +2.5567751994 +1.4761845367 +2.4105829432
Au +2.5567751994 +4.4284650409 +2.4105829432
Au +2.5567751994 +7.3807455450 +2.4105829432
Au +3.4090506443 +0.0000000000 +0.0000000000
Au +3.4090506443 +2.9522805041 +0.0000000000
Au +3.4090506443 +5.9046495776 +0.0000000000
Au +0.8522754450 +1.4761845367 +0.0000000000
Au +0.8522754450 +4.4284650409 +0.0000000000
Au +0.8522754450 +7.3807455450 +0.0000000000
S +4.2419913314 +1.3958272429 +11.4102515298
S +1.6780078946 +5.7927950674 +11.4235612530
C +4.1988537007 +0.9268137311 +13.1270577425
C +5.1026853497 +1.5611191649 +14.0000793550
C +3.2882850367 +8.8475690598 +13.6492864943
C +5.0878922278 +1.2671273898 +15.3628837322

C +3.2870705640 +8.5624903551 +15.0173266567
C +4.1804893208 +0.3347347466 +15.9174987131
C +1.5897595092 +5.3006704328 +13.1290085857
C +0.6379937069 +5.8983640938 +13.9768858042
C +2.5286078037 +4.4095737229 +13.6805545585
C +0.6397196743 +5.6170736407 +15.3437652029
C +2.5239736459 +4.1462193913 +15.0512995706
C +1.5867377909 +4.7425459532 +15.9276062189
C +4.1612818186 +0.0516515961 +17.3750175724
C +3.2235166153 +8.0247217846 +17.9568535691
C +5.0736277611 +0.6648002262 +18.2646820874
C +3.1850673647 +7.7810253726 +19.3301536122
C +5.0406728794 +0.4336162759 +19.6402681462
C +4.0877057154 +8.4196558254 +20.1993503126
C +1.6067439282 +4.4740762559 +17.3873553181
C +0.7596487953 +5.1615359675 +18.2866160426
C +2.4852106094 +3.5247162189 +17.9594822508
C +0.7974652767 +4.9318683661 +19.6628553228
C +2.5328830728 +3.2879275359 +19.3335562139
C +1.6930947918 +3.9958366566 +20.2122858533
H +0.7033778213 +2.2925563458 +13.6113847733
H +2.5779304147 +8.3452841428 +12.9856598227
H +0.6930497756 +1.7920364435 +15.9971361372
H +2.5587286437 +7.8297350911 +15.3751765630
H +5.0091767098 +6.5890255327 +13.5668342505
H +3.2757002367 +3.9369664841 +13.0357776291
H +4.9859482617 +6.0961197353 +15.9575066676
H +3.2888758122 +3.4648321543 +15.4320338028
H +2.4899369115 +7.5072378396 +17.3336330263
H +0.7291313115 +1.3452291482 +17.8925724161
H +2.4376511804 +7.0850470857 +19.7258150491
H +0.6631999938 +0.9315189631 +20.2820630188
H +0.0485669515 +5.9072778839 +17.9222532281
H +3.1573329713 +2.9405562474 +17.3258531787
H +0.1166665033 +5.4904034224 +20.3158336367
H +3.2342480995 +2.5404395540 +19.7210083034
H +3.5480146926 +7.3618431234 +21.8923792589
H +4.8661737449 +8.4164644157 +22.1160344327
H +0.9359015107 +4.0326142018 +22.1366863466
H +2.2039611934 +2.9216797287 +21.9025364606
N +3.9998060000 +8.2344670000 +21.5994700000
N +1.7888849921 +3.8132757489 +21.6122556831
C +1.7465372643 +6.1115271129 +29.3178009674
C +4.3187813308 +2.1334413162 +27.8963073243
C +4.3062421386 +1.6830282049 +29.3177644776
C +1.7340192692 +6.5619133225 +27.8963389635
C +0.8046639729 +6.5955200612 +30.2532762716
C +3.3672377469 +1.6625487600 +26.9636879239

C +2.6856477499 +6.0911324972 +26.9637538756
C +0.1345253287 +2.1670347555 +30.2532671685
C +0.8263215677 +6.1867513044 +31.5908420201
C +3.3715639119 +2.0954261245 +25.6336175024
C +0.1128024292 +1.7582653383 +31.5908348023
C +2.6812209462 +6.5239280375 +25.6336527615
C +4.3287138272 +3.0163896899 +25.1904308655
C +1.7911003661 +5.2763641504 +32.0406835485
C +1.7239449585 +7.4447489270 +25.1904436552
C +4.2615985347 +0.8478382923 +32.0406286219
C +0.1710851777 +3.4932970585 +26.0955718476
C +2.7299431630 +4.7772863245 +31.1288679482
C +0.7679614051 +7.9215790547 +26.0955623522
C +3.3227386711 +0.3487853667 +31.1287965216
C +0.1654564640 +3.0569453383 +27.4245482531
C +2.7065353306 +5.1888401516 +29.7917712033
C +0.7736423093 +7.4852464883 +27.4245507832
C +3.3461980551 +0.7603618222 +29.7917104903
H +2.5991777084 +0.9461244602 +27.2637409681
H +0.0336186668 +7.3075019456 +29.9505051039
H +0.9055637359 +2.8790229215 +29.9504911974
H +3.4538587436 +5.3748861541 +27.2638568824
H +0.0732978222 +6.5826261556 +32.2791045082
H +2.6086940567 +1.7153184356 +24.9473102217
H +3.4441592115 +6.1439485920 +24.9473570621
H +0.8657781468 +2.1541534171 +32.2791343838
H +1.8088730521 +4.9552215103 +33.0873051440
H +4.3254205096 +3.3684228185 +24.1553618898
H +1.7271429067 +7.7967296871 +24.1553618898
H +4.2438758311 +0.5266337155 +33.0872309836
H +0.9293525241 +4.2132659542 +25.7740264487
H +3.4922137095 +4.0622565434 +31.4517685734
H +2.5604361948 +8.4906926638 +31.4516635787
H +0.0095858289 +8.6414365287 +25.7740111642
H +3.4613881586 +4.7795727747 +29.1160661679
H +0.9312925258 +3.4511966296 +28.0964601461
H +0.0077275836 +7.8793894907 +28.0964389360
H +2.5913185902 +0.3511368268 +29.1160078036

System (6), Au|CN|2P|H||2P:

x: +5.1135503988 +0.0000000000 +0.0000000000
y: +0.0000000000 +8.8569300817 +0.0000000000
z: +0.0000000000 +0.0000000000 +60.0000000000

Au +0.0044794701 +8.7136869515 +9.6833533384
Au +5.0535991339 +2.9200678494 +9.7510434492
Au +4.9837838303 +5.7912188740 +9.6915938736

Au +2.4197269351 +1.4177730828 +9.7234240729
Au +2.4964966673 +4.2875069986 +9.6750675255
Au +2.5707403055 +7.3699135195 +9.7528998335
Au +3.3720541072 +8.8040364953 +7.2436115782
Au +3.3888112119 +2.9066496004 +7.2181202522
Au +3.3822812080 +5.8642796903 +7.2318846627
Au +0.8316473827 +1.4378074587 +7.2357332643
Au +0.8204180260 +4.3771037033 +7.2193880268
Au +0.8238645589 +7.3415624863 +7.2310243870
Au +1.7044997544 +0.0000000000 +4.8211658864
Au +1.7044997544 +2.9522805041 +4.8211658864
Au +1.7044997544 +5.9046495776 +4.8211658864
Au +4.2612749538 +1.4761845367 +4.8211658864
Au +4.2612749538 +4.4284650409 +4.8211658864
Au +4.2612749538 +7.3807455450 +4.8211658864
Au +0.0000000000 +0.0000000000 +2.4105829432
Au +0.0000000000 +2.9522805041 +2.4105829432
Au +0.0000000000 +5.9046495776 +2.4105829432
Au +2.5567751994 +1.4761845367 +2.4105829432
Au +2.5567751994 +4.4284650409 +2.4105829432
Au +2.5567751994 +7.3807455450 +2.4105829432
Au +3.4090506443 +0.0000000000 +0.0000000000
Au +3.4090506443 +2.9522805041 +0.0000000000
Au +3.4090506443 +5.9046495776 +0.0000000000
Au +0.8522754450 +1.4761845367 +0.0000000000
Au +0.8522754450 +4.4284650409 +0.0000000000
Au +0.8522754450 +7.3807455450 +0.0000000000
N +4.1832472883 +1.2432738464 +12.3189210045
N +1.5920885760 +5.8313673381 +12.3020324350
C +4.1771008007 +1.2911544104 +11.0865534885
C +1.6307061086 +5.9135950770 +11.0717476917
C +4.1371077230 +0.9777785102 +13.6554271524
C +5.0201002652 +1.6322170740 +14.5461746776
C +3.2127209903 +0.0416807130 +14.1818252985
C +4.9828378235 +1.3437822889 +15.9075835420
C +3.1946292490 +8.6265259026 +15.5479430401
C +4.0774019086 +0.4033445959 +16.4568016318
C +1.5483881743 +5.4906766656 +13.6211972369
C +0.5855322020 +6.0732500986 +14.4786656775
C +2.4721203725 +4.5657120294 +14.1662497814
C +0.5626950859 +5.7465799464 +15.8313812299
C +2.4357476885 +4.2625393127 +15.5251230964
C +1.4909885711 +4.8444661899 +16.4056378691
C +4.0614834262 +0.0978247928 +17.9114372106
C +3.1217662694 +8.0588763967 +18.4742838779
C +4.9900223618 +0.6913099637 +18.7990605769
C +3.1096318143 +7.7747815074 +19.8442049435
C +4.9766453139 +0.4123520938 +20.1690721977

C +4.0353225023 +8.3801261077 +20.7046164324
C +1.4807512432 +4.5362450230 +17.8591867839
C +0.6022432847 +5.1989648164 +18.7486665345
C +2.3594586301 +3.5794397232 +18.4204940106
C +0.6059506087 +4.9249756843 +20.1199912077
C +2.3688829035 +3.3082848088 +19.7929959031
C +1.4923794568 +3.9807206544 +20.6550826657
H +0.6237304234 +2.3583170590 +14.1547039765
H +2.5193440105 +8.3924018128 +13.5048789127
H +0.5760977015 +1.8718324604 +16.5522016743
H +2.4674568146 +7.8906124390 +15.9014257794
H +4.9704783721 +6.7770749045 +14.0685405779
H +3.2183101009 +4.1061347844 +13.5127572266
H +4.9023914486 +6.2107273673 +16.4476102656
H +3.1806334616 +3.5555791536 +15.8988902301
H +2.3731169233 +7.5714795343 +17.8446073754
H +0.6351950034 +1.3848075891 +18.4299570428
H +2.3658965901 +7.0732949311 +20.2336381496
H +0.6050761916 +0.8921851379 +20.8147769940
H +4.0254482365 +8.1586497141 +21.7771537870
H +5.0145878579 +5.9530349866 +18.3827777147
H +3.0587928962 +3.0296369315 +17.7853841882
H +5.0203406021 +5.4617056473 +20.7688201629
H +3.0700938426 +2.5636472691 +20.1822932763
H +1.4993389989 +3.7711391179 +21.7298839036
C +1.4826531425 +6.0139345346 +27.6829590776
C +4.0548972090 +2.0358487379 +26.2614654345
C +4.0423580168 +1.5854356266 +27.6829225878
C +1.4701351474 +6.4643207442 +26.2614970737
C +0.5407798511 +6.4979274829 +28.6184343818
C +3.1033536251 +1.5649561817 +25.3288460341
C +2.4217636281 +5.9935399189 +25.3289119858
C -0.1293587931 +2.0694421772 +28.6184252787
C +0.5624374459 +6.0891587261 +29.9560001303
C +3.1076797901 +1.9978335462 +23.9987756126
C +4.9624687062 +1.6606727600 +29.9559929125
C +2.4173368244 +6.4263354592 +23.9988108717
C +4.0648297054 +2.9187971116 +23.5555889757
C +1.5272162443 +5.1787715721 +30.4058416587
C +1.4600608367 +7.3471563487 +23.5556017654
C +3.9977144129 +0.7502457140 +30.4057867321
C -0.0927989441 +3.3957044802 +24.4607299578
C +2.4660590412 +4.6796937462 +29.4940260584
C +0.5040772833 +7.8239864764 +24.4607204624
C +3.0588545493 +0.2511927884 +29.4939546318
C -0.0984276578 +2.9593527600 +25.7897063633
C +2.4426512088 +5.0912475733 +28.1569293135
C +0.5097581875 +7.3876539100 +25.7897088934

C +3.0823139333 +0.6627692439 +28.1568686005
H +2.3352935866 +0.8485318819 +25.6288990783
H +4.8832849438 +7.2099093673 +28.3156632141
H +0.6416796141 +2.7814303432 +28.3156493076
H +3.1899746218 +5.2772935758 +25.6290149926
H +4.9229640992 +6.4850335773 +30.6442626184
H +2.3448099349 +1.6177258573 +23.3124683319
H +3.1802750897 +6.0463560137 +23.3125151723
H +0.6018940250 +2.0565608388 +30.6442924940
H +1.5449889303 +4.8576289320 +31.4524632542
H +4.0615363878 +3.2708302402 +22.5205200000
H +1.4632587849 +7.6991371088 +22.5205200000
H +3.9799917093 +0.4290411372 +31.4523890938
H +0.6654684023 +4.1156733759 +24.1391845589
H +3.2283295877 +3.9646639651 +29.8169266836
H +2.2965520730 +8.3931000855 +29.8168216889
H +4.8592521059 +8.5438439504 +24.1391692744
H +3.1975040368 +4.6819801964 +27.4812242781
H +0.6674084040 +3.3536040513 +26.4616182563
H +4.8573938606 +7.7817969124 +26.4615970462
H +2.3274344684 +0.2535442485 +27.4811659138

System (7), AuSI2PIHII2P:

x: +5.1135503988 +0.0000000000 +0.0000000000
y: +0.0000000000 +8.8569300817 +0.0000000000
z: +0.0000000000 +0.0000000000 +60.0000000000

Au +0.0754299819 +8.6944142716 +9.6879716603
Au +0.0982722116 +3.0712467890 +9.5261945593
Au +4.9562013394 +5.8810458589 +9.6676872659
Au +2.3947472414 +1.4379757403 +9.6827194511
Au +2.6522451853 +4.2587751174 +9.7209338012
Au +2.6361426151 +7.4873918401 +9.5096682112
Au +3.4312587937 +0.0444883598 +7.1833017269
Au +3.3965275594 +2.9647510617 +7.2623565320
Au +3.4220237217 +5.8937555536 +7.2310243870
Au +0.8674166677 +1.4705515292 +7.2363218739
Au +0.8770659373 +4.4680466614 +7.1922214272
Au +0.8377836431 +7.3907981606 +7.2397629766
Au +1.7044997544 +0.0000000000 +4.8211658864
Au +1.7044997544 +2.9522805041 +4.8211658864
Au +1.7044997544 +5.9046495776 +4.8211658864
Au +4.2612749538 +1.4761845367 +4.8211658864
Au +4.2612749538 +4.4284650409 +4.8211658864
Au +4.2612749538 +7.3807455450 +4.8211658864
Au +0.0000000000 +0.0000000000 +2.4105829432
Au +0.0000000000 +2.9522805041 +2.4105829432

Au +0.0000000000 +5.9046495776 +2.4105829432
Au +2.5567751994 +1.4761845367 +2.4105829432
Au +2.5567751994 +4.4284650409 +2.4105829432
Au +2.5567751994 +7.3807455450 +2.4105829432
Au +3.4090506443 +0.0000000000 +0.0000000000
Au +3.4090506443 +2.9522805041 +0.0000000000
Au +3.4090506443 +5.9046495776 +0.0000000000
Au +0.8522754450 +1.4761845367 +0.0000000000
Au +0.8522754450 +4.4284650409 +0.0000000000
Au +0.8522754450 +7.3807455450 +0.0000000000
S +4.2436229778 +1.4021406012 +11.4049007589
S +1.6804200456 +5.7980564240 +11.4167635074
C +4.1993754262 +0.9384625976 +13.1234145758
C +5.0977188467 +1.5805191731 +13.9964585335
C +3.2932236143 +8.8539984379 +13.6439719029
C +5.0821736535 +1.2872130765 +15.3598143375
C +3.2930957755 +8.5687698615 +15.0122629725
C +4.1814779998 +0.3474307963 +15.9123829746
C +1.6002446889 +5.3145477539 +13.1254520707
C +0.6442766689 +5.9076520769 +13.9718274832
C +2.5467526406 +4.4316092510 +13.6771151545
C +0.6471760520 +5.6263471205 +15.3390771664
C +2.5440117776 +4.1706486631 +15.0486662160
C +1.6003571870 +4.7589613869 +15.9228873931
C +4.1707395440 +0.0552229591 +17.3715915977
C +3.2208208542 +8.0380626110 +17.9482932308
C +5.1085544600 +0.6503555190 +18.2473069378
C +3.2075307367 +7.7755609172 +19.3226515077
C +5.0943081086 +0.3935754020 +19.6216199369
C +4.1421650244 +8.3823049125 +20.1718341354
C +1.6120109684 +4.4801098002 +17.3840882335
C +0.7707092025 +5.1824643556 +18.2776429740
C +2.4701516556 +3.5038812527 +17.9417279692
C +0.7853339567 +4.9213177722 +19.6519106955
C +2.4925848012 +3.2468265709 +19.3167654111
C +1.6486239892 +3.9538752994 +20.1833799402
H +0.6946451404 +2.3159366486 +13.6077497700
H +2.5873951392 +8.3466203412 +12.9791599316
H +0.6805624226 +1.8177431884 +15.9969616549
H +2.5726885682 +7.8284367898 +15.3707262550
H +5.0102362265 +6.5921422044 +13.5605704420
H +3.2969820738 +3.9635027824 +13.0324517446
H +4.9882837546 +6.0958264134 +15.9537667614
H +3.3143579181 +3.4974599784 +15.4328924906
H +2.4632330219 +7.5547753642 +17.3262233763
H +0.7605536915 +1.3297263409 +17.8663406552
H +2.4545246456 +7.0919033412 +19.7247171826
H +0.7281184413 +0.8760123836 +20.2590389203

H +4.1288851340 +8.1802606235 +21.2480842586
H +0.0919058413 +5.9574280239 +17.9121163756
H +3.1389887071 +2.9237611893 +17.3007320502
H +0.1139452435 +5.4864607668 +20.3061729707
H +3.1754176402 +2.4839526122 +19.7035725126
H +1.6628703406 +3.7525927063 +21.2595847858
C +1.6161331425 +6.0139345346 +27.1832690776
C +4.1883772090 +2.0358487379 +25.7617754345
C +4.1758380168 +1.5854356266 +27.1832325878
C +1.6036151474 +6.4643207442 +25.7618070737
C +0.6742598511 +6.4979274829 +28.1187443818
C +3.2368336251 +1.5649561817 +24.8291560341
C +2.5552436281 +5.9935399189 +24.8292219858
C +0.0041212069 +2.0694421772 +28.1187352787
C +0.6959174459 +6.0891587261 +29.4563101303
C +3.2411597901 +1.9978335462 +23.4990856126
C +5.0959487062 +1.6606727600 +29.4563029125
C +2.5508168244 +6.4263354592 +23.4991208717
C +4.1983097054 +2.9187971116 +23.0558989757
C +1.6606962443 +5.1787715721 +29.9061516587
C +1.5935408367 +7.3471563487 +23.0559117654
C +4.1311944129 +0.7502457140 +29.9060967321
C +0.0406810559 +3.3957044802 +23.9610399578
C +2.5995390412 +4.6796937462 +28.9943360584
C +0.6375572833 +7.8239864764 +23.9610304624
C +3.1923345493 +0.2511927884 +28.9942646318
C +0.0350523422 +2.9593527600 +25.2900163633
C +2.5761312088 +5.0912475733 +27.6572393135
C +0.6432381875 +7.3876539100 +25.2900188934
C +3.2157939333 +0.6627692439 +27.6571786005
H +2.4687735866 +0.8485318819 +25.1292090783
H +5.0167649438 +7.2099093673 +27.8159732141
H +0.7751596141 +2.7814303432 +27.8159593076
H +3.3234546218 +5.2772935758 +25.1293249926
H +5.0564440992 +6.4850335773 +30.1445726184
H +2.4782899349 +1.6177258573 +22.8127783319
H +3.3137550897 +6.0463560137 +22.8128251723
H +0.7353740250 +2.0565608388 +30.1446024940
H +1.6784689303 +4.8576289320 +30.9527732542
H +4.1950163878 +3.2708302402 +22.0208300000
H +1.5967387849 +7.6991371088 +22.0208300000
H +4.1134717093 +0.4290411372 +30.9526990938
H +0.7989484023 +4.1156733759 +23.6394945589
H +3.3618095877 +3.9646639651 +29.3172366836
H +2.4300320730 +8.3931000855 +29.3171316889
H +4.9927321059 +8.5438439504 +23.6394792744
H +3.3309840368 +4.6819801964 +26.9815342781
H +0.8008884040 +3.3536040513 +25.9619282563

H +4.9908738606 +7.7817969124 +25.9619070462
H +2.4609144684 +0.2535442485 +26.9814759138

System (8), Au|S|2P|F||2P:

x: +5.1135503988 +0.0000000000 +0.0000000000
y: +0.0000000000 +8.8569300817 +0.0000000000
z: +0.0000000000 +0.0000000000 +60.0000000000

Au +0.0739419388 +8.6937854296 +9.6882433263
Au +0.0970040511 +3.0696436846 +9.5254248390
Au +4.9557206657 +5.8799475996 +9.6682305979
Au +2.3941898644 +1.4367180563 +9.6829458394
Au +2.6508594132 +4.2581551323 +9.7222015759
Au +2.6347005939 +7.4856470249 +9.5079023822
Au +3.4309622078 +0.0446920692 +7.1829395056
Au +3.3956787100 +2.9645473523 +7.2626734756
Au +3.4217373629 +5.8928698606 +7.2308432764
Au +0.8669973566 +1.4699758287 +7.2361407633
Au +0.8767795785 +4.4678340951 +7.1920855942
Au +0.8368274092 +7.3903730280 +7.2393101999
Au +1.7044997544 +0.0000000000 +4.8211658864
Au +1.7044997544 +2.9522805041 +4.8211658864
Au +1.7044997544 +5.9046495776 +4.8211658864
Au +4.2612749538 +1.4761845367 +4.8211658864
Au +4.2612749538 +4.4284650409 +4.8211658864
Au +4.2612749538 +7.3807455450 +4.8211658864
Au +0.0000000000 +0.0000000000 +2.4105829432
Au +0.0000000000 +2.9522805041 +2.4105829432
Au +0.0000000000 +5.9046495776 +2.4105829432
Au +2.5567751994 +1.4761845367 +2.4105829432
Au +2.5567751994 +4.4284650409 +2.4105829432
Au +2.5567751994 +7.3807455450 +2.4105829432
Au +3.4090506443 +0.0000000000 +0.0000000000
Au +3.4090506443 +2.9522805041 +0.0000000000
Au +3.4090506443 +5.9046495776 +0.0000000000
Au +0.8522754450 +1.4761845367 +0.0000000000
Au +0.8522754450 +4.4284650409 +0.0000000000
Au +0.8522754450 +7.3807455450 +0.0000000000
S +4.2423292496 +1.4000326519 +11.4075721412
S +1.6779911091 +5.7960281871 +11.4195707227
C +4.1975447752 +0.9356992354 +13.1260859581
C +5.0989818937 +1.5732299196 +13.9993563041
C +3.2878237050 +8.8554332605 +13.6480921705
C +5.0825367156 +1.2810486532 +15.3629837741
C +3.2858754423 +8.5721089241 +15.0167454614
C +4.1765689914 +0.3472890854 +15.9174540732
C +1.5936891173 +5.3094461622 +13.1272631774

C +0.6407738869 +5.9058806909 +13.9748158091
C +2.5357789614 +4.4218931987 +13.6791073718
C +0.6438726985 +5.6255145691 +15.3422918807
C +2.5327210583 +4.1609060400 +15.0506131557
C +1.5937453663 +4.7546037773 +15.9266907171
C +4.1641481775 +0.0543195522 +17.3760288090
C +3.2215316377 +8.0240863753 +17.9460746252
C +5.0924979118 +0.6584507531 +18.2572680243
C +3.2050557783 +7.7431799809 +19.3164031897
C +5.0922882562 +0.3979064409 +19.6317621341
C +4.1459695059 +8.3646707647 +20.1318086785
C +1.6064065171 +4.4765050296 +17.3876198915
C +0.7517941796 +5.1653173390 +18.2807671330
C +2.4799492182 +3.5136150189 +17.9458029592
C +0.7560077452 +4.9098569047 +19.6567101281
C +2.5064885448 +3.2448337617 +19.3181690187
C +1.6371236144 +3.9490659863 +20.1459805880
H +0.7000910715 +2.3043340701 +13.6102853193
H +2.5798986743 +8.3497734083 +12.9841404748
H +0.6867804999 +1.8069643045 +15.9975049869
H +2.5608251313 +7.8356906156 +15.3738504140
H +5.0087686375 +6.5930810390 +13.5643284882
H +3.2831652606 +3.9492519819 +13.0343534065
H +4.9871792277 +6.1002105938 +15.9558042564
H +3.2991860140 +3.4813669364 +15.4315341606
H +2.4696965496 +7.5359278170 +17.3212881107
H +0.7344950386 +1.3515143889 +17.8810558967
H +2.4723300281 +7.0558910635 +19.7459976857
H +0.7020649020 +0.8680854312 +20.3033204777
H +0.0612705609 +5.9287492843 +17.9136105386
H +3.1623627460 +2.9468954906 +17.3077500885
H +0.0905098421 +5.4432743758 +20.3409914959
H +3.1889992300 +2.5013830506 +19.7380740941
F +4.1445837337 +8.0751465773 +21.4949833719
F +1.6458780126 +3.6751831374 +21.5115097200
C +1.6161331425 +5.8639345346 +28.0532690776
C +4.1883772090 +1.8858487379 +26.6317754345
C +4.1758380168 +1.4354356266 +28.0532325878
C +1.6036151474 +6.3143207442 +26.6318070737
C +0.6742598511 +6.3479274829 +28.9887443818
C +3.2368336251 +1.4149561817 +25.6991560341
C +2.5552436281 +5.8435399189 +25.6992219858
C +0.0041212069 +1.9194421772 +28.9887352787
C +0.6959174459 +5.9391587261 +30.3263101303
C +3.2411597901 +1.8478335462 +24.3690856126
C +5.0959487062 +1.5106727600 +30.3263029125
C +2.5508168244 +6.2763354592 +24.3691208717
C +4.1983097054 +2.7687971116 +23.9258989757

C +1.6606962443 +5.0287715721 +30.7761516587
C +1.5935408367 +7.1971563487 +23.9259117654
C +4.1311944129 +0.6002457140 +30.7760967321
C +0.0406810559 +3.2457044802 +24.8310399578
C +2.5995390412 +4.5296937462 +29.8643360584
C +0.6375572833 +7.6739864764 +24.8310304624
C +3.1923345493 +0.1011927884 +29.8642646318
C +0.0350523422 +2.8093527600 +26.1600163633
C +2.5761312088 +4.9412475733 +28.5272393135
C +0.6432381875 +7.2376539100 +26.1600188934
C +3.2157939333 +0.5127692439 +28.5271786005
H +2.4687735866 +0.6985318819 +25.9992090783
H +5.0167649438 +7.0599093673 +28.6859732141
H +0.7751596141 +2.6314303432 +28.6859593076
H +3.3234546218 +5.1272935758 +25.9993249926
H +5.0564440992 +6.3350335773 +31.0145726184
H +2.4782899349 +1.4677258573 +23.6827783319
H +3.3137550897 +5.8963560137 +23.6828251723
H +0.7353740250 +1.9065608388 +31.0146024940
H +1.6784689303 +4.7076289320 +31.8227732542
H +4.1950163878 +3.1208302402 +22.8908300000
H +1.5967387849 +7.5491371088 +22.8908300000
H +4.1134717093 +0.2790411372 +31.8226990938
H +0.7989484023 +3.9656733759 +24.5094945589
H +3.3618095877 +3.8146639651 +30.1872366836
H +2.4300320730 +8.2431000855 +30.1871316889
H +4.9927321059 +8.3938439504 +24.5094792744
H +3.3309840368 +4.5319801964 +27.8515342781
H +0.8008884040 +3.2036040513 +26.8319282563
H +4.9908738606 +7.6317969124 +26.8319070462
H +2.4609144684 +0.1035442485 +27.8514759138

System (9), AulPyrI2PICNI2P:

x: +5.1135503988 +0.0000000000 +0.0000000000
y: +0.0000000000 +8.8569290977 +0.0000000000
z: +0.0000000000 +0.0000000000 +60.0000000000

Au +5.0852786949 +8.8220062445 +9.5908205042
Au +5.1111917601 +2.9202974354 +9.6018225200
Au +5.0898780164 +5.8793693087 +9.7347946764
Au +2.5508449729 +1.4515185512 +9.7353122193
Au +2.5552765377 +4.3943127440 +9.5963650838
Au +2.5292200145 +7.3456320795 +9.5977661576
Au +3.3859507809 -0.0005699906 +7.2139409371
Au +3.3950985616 +2.9167734991 +7.2151661451
Au +3.4213944870 +5.8869114955 +7.2142317555
Au +0.8640365671 +1.4586123199 +7.2174903456

Au +0.8373175481 +4.4283511744 +7.2183240176
Au +0.8325734473 +7.3461859213 +7.2130019775
Au +1.7044997544 +0.0000000000 +4.8211660106
Au +1.7044997544 +2.9522801761 +4.8211660106
Au +1.7044997544 +5.9046489216 +4.8211660106
Au +4.2612749538 +1.4761843727 +4.8211660106
Au +4.2612749538 +4.4284645489 +4.8211660106
Au +4.2612749538 +7.3807447250 +4.8211660106
Au +0.0000000000 +0.0000000000 +2.4105830053
Au +0.0000000000 +2.9522801761 +2.4105830053
Au +0.0000000000 +5.9046489216 +2.4105830053
Au +2.5567751994 +1.4761843727 +2.4105830053
Au +2.5567751994 +4.4284645489 +2.4105830053
Au +2.5567751994 +7.3807447250 +2.4105830053
Au +3.4090506443 +0.0000000000 +0.0000000000
Au +3.4090506443 +2.9522801761 +0.0000000000
Au +3.4090506443 +5.9046489216 +0.0000000000
Au +0.8522754450 +1.4761843727 +0.0000000000
Au +0.8522754450 +4.4284645489 +0.0000000000
Au +0.8522754450 +7.3807447250 +0.0000000000
N +2.4945935124 +1.2793008131 +12.3058984871
N +5.1101897960 +5.7220842256 +12.3156195310
C +3.3630891316 +1.9078716925 +13.1389968214
C +1.6243156045 +0.4018765315 +12.8688203336
C +3.3878800295 +1.6908380514 +14.5193146487
C +1.5931343994 +0.1316330984 +14.2360776065
C +2.4882263692 +0.7784650133 +15.1189385717
C +4.1934638518 +6.3094668263 +13.1269920755
C +0.8920804362 +4.8850595518 +12.8999186234
C +4.1415095312 +6.0874334559 +14.5058481711
C +0.9035977774 +4.6182585086 +14.2682455945
C +5.0682368948 +5.2180915435 +15.1275736698
C +2.4771884732 +0.5095629531 +16.5776896424
C +1.5515309847 +8.4598137881 +17.1475052903
C +3.3830494637 +1.1439582059 +17.4613935260
C +1.5330660620 +8.1935197530 +18.5144297850
C +3.3744151336 +0.8887156411 +18.8329313894
C +5.0545360273 +4.9448933411 +16.5855306784
C +4.1788097149 +5.6241791554 +17.4660235961
C +2.4488293058 +8.8305474066 +19.3795944580
C +5.0476301596 +4.4066858185 +19.3863771927
C +2.4436541193 +8.5207967063 +20.7729865476
C +5.0375407404 +4.1017980226 +20.7808887152
C +0.8144205059 +3.9887551117 +17.1565497991
C +4.1693121288 +5.3658960397 +18.8372989497
C +0.8179603203 +3.7228958689 +18.5237576056
H +4.0603068819 +2.6053255371 +12.6597933918
H +0.9380512216 +8.7597694850 +12.1708441894

H +4.1217614499 +2.2412468846 +15.1133817228
H +0.8588037736 +8.2626428576 +14.5927439191
H +3.4773906649 +6.9746923541 +12.6299199627
H +1.6173040808 +4.4192132653 +12.2188912317
H +3.3612296576 +6.5932646837 +15.0800059342
H +1.6693783190 +3.9374170136 +14.6462462410
H +0.8209892337 +7.9447240692 +16.5195117448
H +4.1202020716 +1.8558048349 +17.0821296547
H +0.8082489869 +7.4863217579 +18.9254089025
H +4.0851978478 +1.3900496831 +19.4956273688
H +3.4869223453 +6.3803446339 +17.0857971191
H +1.5103092057 +3.4283550628 +16.5278559086
H +3.4842231192 +5.9032677475 +19.4989236572
H +1.5042236532 +2.9784059876 +18.9359798177
N +2.4355256898 +8.2146939937 +21.9242047953
N +5.0333527990 +3.8013883313 +21.9335773417
C +5.0417089759 +6.0051562750 +28.6536538478
C +2.5004026436 +2.0270704783 +27.2321602047
C +2.4878634514 +1.5766573670 +28.6536173580
C +5.0291909808 +6.4555424846 +27.2321918439
C +4.0998356845 +6.4891492233 +29.5891291520
C +1.5488590597 +1.5561779221 +26.2995408043
C +0.8672690627 +5.9847616593 +26.2996067560
C +3.4296970403 +2.0606639176 +29.5891200489
C +4.1214932793 +6.0803804665 +30.9266949005
C +1.5531852247 +1.9890552866 +24.9694703828
C +3.4079741408 +1.6518945004 +30.9266876827
C +0.8628422590 +6.4175571996 +24.9695056419
C +2.5103351400 +2.9100188520 +24.5262837459
C +5.0862720777 +5.1699933125 +31.3765364289
C +5.0191166701 +7.3383780891 +24.5262965356
C +2.4432198475 +0.7414674544 +31.3764815023
C +3.4662568893 +3.3869262206 +25.4314247280
C +0.9115644758 +4.6709154866 +30.4647208286
C +4.0631331167 +7.8152082168 +25.4314152326
C +1.5043599839 +0.2424145288 +30.4646494020
C +3.4606281756 +2.9505745004 +26.7604011335
C +0.8881566434 +5.0824693137 +29.1276240837
C +4.0688140209 +7.3788756504 +26.7604036636
C +1.5278193679 +0.6539909843 +29.1275633707
H +0.7807990212 +0.8397536223 +26.5995938485
H +3.3287903784 +7.2011311077 +29.2863579843
H +4.2007354475 +2.7726520836 +29.2863440778
H +1.6354800564 +5.2685153162 +26.5997097628
H +3.3684695338 +6.4762553177 +31.6149573886
H +0.7903153695 +1.6089475977 +24.2831631021
H +1.6257805243 +6.0375777541 +24.2832099425
H +4.1609498584 +2.0477825792 +31.6149872642

H +5.1040447637 +4.8488506724 +32.4231580244
H +2.5070418224 +3.2620519806 +23.4912147702
H +5.0223146183 +7.6903588492 +23.4912147702
H +2.4254971439 +0.4202628776 +32.4230838640
H +4.2245242357 +4.1068951163 +25.1098793291
H +1.6738350223 +3.9558857055 +30.7876214538
H +0.7420575076 -0.4726072718 +30.7875164591
H +3.3047575405 -0.3218634069 +25.1098640446
H +1.6430094714 +4.6732019368 +28.4519190483
H +4.2264642374 +3.3448257917 +27.4323130265
H +3.3028992952 +7.7730186528 +27.4322918164
H +0.7729399030 +0.2447659889 +28.4518606840

System (10), Au|CN|2P|CN||2P:

x: +5.1135503988 +0.0000000000 +0.0000000000
y: +0.0000000000 +8.8569300817 +0.0000000000
z: +0.0000000000 +0.0000000000 +60.0000000000

Au +0.0073511838 +8.7059910454 +9.6849823366
Au +5.0566627199 +2.9177047681 +9.7489604034
Au +4.9808468370 +5.7845466555 +9.6991911797
Au +2.4253686941 +1.4097371958 +9.7208000650
Au +2.4936734221 +4.2826936271 +9.6738288178
Au +2.5734127134 +7.3653567203 +9.7569426374
Au +3.3685130273 +8.7937016993 +7.2455307755
Au +3.3836973400 +2.8967725725 +7.2178756400
Au +3.3788861837 +5.8548413339 +7.2346104493
Au +0.8273754791 +1.4273121139 +7.2352206963
Au +0.8151449673 +4.3679250016 +7.2213615028
Au +0.8205444665 +7.3309639530 +7.2324031899
Au +1.7044997544 +0.0000000000 +4.8211658864
Au +1.7044997544 +2.9522805041 +4.8211658864
Au +1.7044997544 +5.9046495776 +4.8211658864
Au +4.2612749538 +1.4761845367 +4.8211658864
Au +4.2612749538 +4.4284650409 +4.8211658864
Au +4.2612749538 +7.3807455450 +4.8211658864
Au +0.0000000000 +0.0000000000 +2.4105829432
Au +0.0000000000 +2.9522805041 +2.4105829432
Au +0.0000000000 +5.9046495776 +2.4105829432
Au +2.5567751994 +1.4761845367 +2.4105829432
Au +2.5567751994 +4.4284650409 +2.4105829432
Au +2.5567751994 +7.3807455450 +2.4105829432
Au +3.4090506443 +0.0000000000 +0.0000000000
Au +3.4090506443 +2.9522805041 +0.0000000000
Au +3.4090506443 +5.9046495776 +0.0000000000
Au +0.8522754450 +1.4761845367 +0.0000000000
Au +0.8522754450 +4.4284650409 +0.0000000000

Au +0.8522754450 +7.3807455450 +0.0000000000
N +4.2102833224 +1.2656815645 +12.3135252512
N +1.5873288986 +5.8410344579 +12.3071355008
C +4.1987075949 +1.3049228775 +11.0806476676
C +1.6208972125 +5.9216360632 +11.0767982324
C +4.1565458392 +1.0065776775 +13.6506474735
C +5.0377970968 +1.6599676356 +14.5441073898
C +3.2248878536 +0.0767083002 +14.1747254272
C +4.9926526635 +1.3757050839 +15.9059247669
C +3.1984063084 +8.6657721699 +15.5406239704
C +4.0797990392 +0.4406418087 +16.4531540784
C +1.5549444810 +5.5112596687 +13.6290195398
C +0.6041617805 +6.1045836570 +14.4929446831
C +2.4778893153 +4.5833260564 +14.1704374483
C +0.5891796017 +5.7824188277 +15.8467461198
C +2.4483815238 +4.2828202499 +15.5292060291
C +1.5127469980 +4.8715846720 +16.4161230416
C +4.0556115227 +0.1335234355 +17.9043228464
C +3.1141509792 +8.0883174890 +18.4559936862
C +4.9756682063 +0.7244622315 +18.8046449545
C +3.0966548092 +7.7851507089 +19.8161644740
C +4.9674885962 +0.4332584006 +20.1685055541
C +1.5055711370 +4.5547635667 +17.8650631940
C +0.6140596926 +5.1897548923 +18.7643382069
C +2.4007565584 +3.6071633539 +18.4175967071
C +0.6106256498 +4.9006737960 +20.1291365130
C +2.4101645980 +3.3103092987 +19.7790085713
C +4.0280292259 +8.3784068065 +20.6945557397
C +1.5112989121 +3.9516735956 +20.6575977512
C +4.0304399854 +8.0290399639 +22.0787869939
C +1.5063480432 +3.6157355233 +22.0452306352
H +0.6467066572 +2.3815852142 +14.1544419129
H +2.5330563173 +8.4292732549 +13.4949741966
H +0.5857479373 +1.9005197379 +16.5533406741
H +2.4660544175 +7.9343030629 +15.8914676784
H +4.9912680480 +6.8125784035 +14.0865912966
H +3.2162631429 +4.1168127899 +13.5131275286
H +4.9389984512 +6.2559409151 +16.4684099842
H +3.1890216627 +3.5688984542 +15.8974514359
H +2.3672522669 +7.6066859460 +17.8203533785
H +0.6160864103 +1.4288870855 +18.4462097601
H +2.3587525751 +7.0820898357 +20.2108751371
H +0.5782535369 +0.9023103554 +20.8403782385
H +5.0131864602 +5.9350921995 +18.4062234832
H +3.1149801514 +3.0805296158 +17.7801505670
H +5.0247850181 +5.4060988356 +20.8010408785
H +3.1162364552 +2.5750258906 +20.1738356874
N +4.0365170011 +7.6919821184 +23.2212051545

N +1.5032664385 +3.2904649406 +23.1911099526
C +1.5291495771 +5.4624442750 +29.9206548478
C +4.1013936436 +1.4843584783 +28.4991612047
C +4.0888544514 +1.0339453670 +29.9206183580
C +1.5166315820 +5.9128304846 +28.4991928439
C +0.5872762857 +5.9464372233 +30.8561301520
C +3.1498500597 +1.0134659221 +27.5665418043
C +2.4682600627 +5.4420496593 +27.5666077560
C -0.0828623585 +1.5179519176 +30.8561210489
C +0.6089338805 +5.5376684665 +32.1936959005
C +3.1541762247 +1.4463432866 +26.2364713828
C +5.0089651408 +1.1091825004 +32.1936886827
C +2.4638332590 +5.8748451996 +26.2365066419
C +4.1113261400 +2.3673068520 +25.7932847459
C +1.5737126789 +4.6272813125 +32.6435374289
C +1.5065572713 +6.7956660891 +25.7932975356
C +4.0442108475 +0.1987554544 +32.6434825023
C -0.0463025095 +2.8442142206 +26.6984257280
C +2.5125554758 +4.1282034866 +31.7317218286
C +0.5505737179 +7.2724962168 +26.6984162326
C +3.1053509839 -0.3002974712 +31.7316504020
C -0.0519312232 +2.4078625004 +28.0274021335
C +2.4891476434 +4.5397573137 +30.3946250837
C +0.5562546221 +6.8361636504 +28.0274046636
C +3.1288103679 +0.1112789843 +30.3945643707
H +2.3817900212 +0.2970416223 +27.8665948485
H +4.9297813784 +6.6584191077 +30.5533589843
H +0.6881760487 +2.2299400836 +30.5533450778
H +3.2364710564 +4.7258033162 +27.8667107628
H +4.9694605338 +5.9335433177 +32.8819583886
H +2.3913063695 +1.0662355977 +25.5501641021
H +3.2267715243 +5.4948657541 +25.5502109425
H +0.6483904596 +1.5050705792 +32.8819882642
H +1.5914853649 +4.3061386724 +33.6901590244
H +4.1080328224 +2.7193399806 +24.7582157702
H +1.5097552195 +7.1476468492 +24.7582157702
H +4.0264881439 -0.1224491224 +33.6900848640
H +0.7119648369 +3.5641831163 +26.3768803291
H +3.2748260223 +3.4131737055 +32.0546224538
H +2.3430485076 +7.8416098259 +32.0545174591
H +4.9057485405 +7.9923536908 +26.3768650446
H +3.2440004714 +4.1304899368 +29.7189200483
H +0.7139048386 +2.8021137917 +28.6993140265
H +4.9038902952 +7.2303066528 +28.6992928164
H +2.3739309030 -0.2979460111 +29.7188616840

System (11), Au|S|2P|CN||2P:

x: +5.1135503988 +0.0000000000 +0.0000000000
y: +0.0000000000 +8.8569300817 +0.0000000000
z: +0.0000000000 +0.0000000000 +60.0000000000

Au +0.0723107162 +8.6948748320 +9.6889224913
Au +0.0969171207 +3.0692805505 +9.5262851147
Au +4.9558280503 +5.8805144431 +9.6694983726
Au +2.3951256442 +1.4361600697 +9.6844852800
Au +2.6505986221 +4.2587219758 +9.7255521232
Au +2.6327318770 +7.4842564869 +9.5081740482
Au +3.4306656219 +0.0450197756 +7.1832111716
Au +3.3953003073 +2.9651407666 +7.2641676386
Au +3.4216197512 +5.8927635774 +7.2313866083
Au +0.8670945140 +1.4703832475 +7.2365482623
Au +0.8767284430 +4.4681352307 +7.1927647592
Au +0.8361473070 +7.3908424453 +7.2394007552
Au +1.7044997544 +0.0000000000 +4.8211658864
Au +1.7044997544 +2.9522805041 +4.8211658864
Au +1.7044997544 +5.9046495776 +4.8211658864
Au +4.2612749538 +1.4761845367 +4.8211658864
Au +4.2612749538 +4.4284650409 +4.8211658864
Au +4.2612749538 +7.3807455450 +4.8211658864
Au +0.0000000000 +0.0000000000 +2.4105829432
Au +0.0000000000 +2.9522805041 +2.4105829432
Au +0.0000000000 +5.9046495776 +2.4105829432
Au +2.5567751994 +1.4761845367 +2.4105829432
Au +2.5567751994 +4.4284650409 +2.4105829432
Au +2.5567751994 +7.3807455450 +2.4105829432
Au +3.4090506443 +0.0000000000 +0.0000000000
Au +3.4090506443 +2.9522805041 +0.0000000000
Au +3.4090506443 +5.9046495776 +0.0000000000
Au +0.8522754450 +1.4761845367 +0.0000000000
Au +0.8522754450 +4.4284650409 +0.0000000000
Au +0.8522754450 +7.3807455450 +0.0000000000
S +4.2431780989 +1.4000592227 +11.4119187971
S +1.6746417336 +5.7937696699 +11.4253662640
C +4.1993294043 +0.9346984023 +13.1299345597
C +5.1054096265 +1.5674817720 +14.0024804631
C +3.2844334211 +0.0023382295 +13.6523029935
C +5.0882076430 +1.2761419139 +15.3661079331
C +3.2804653060 +8.5779722119 +15.0210015621
C +4.1752445819 +0.3491224700 +15.9213026748
C +1.5873585419 +5.3071610743 +13.1326059420
C +0.6369898596 +5.9079089278 +13.9807019057
C +2.5264518455 +4.4156756338 +13.6839068044
C +0.6411574032 +5.6298101802 +15.3484949210
C +2.5233530340 +4.1553616018 +15.0551409223
C +1.5884988636 +4.7551617638 +15.9324409807

C +4.1582675946 +0.0596159964 +17.3784285253
C +3.2147357292 +8.0286654082 +17.9467990678
C +5.0809310608 +0.6653768724 +18.2655991149
C +3.1952582157 +7.7545611360 +19.3135506968
C +5.0713431538 +0.4032825974 +19.6355201804
C +4.1269880068 +8.3644227707 +20.1799841153
C +1.6038037200 +4.4791886794 +17.3920118251
C +0.7395421129 +5.1535021943 +18.2881021149
C +2.4914393659 +3.5297169177 +17.9520059994
C +0.7489561592 +4.8932058761 +19.6591098445
C +2.5161173602 +3.2636990227 +19.3199348477
C +1.6389133570 +3.9384465272 +20.1953332441
C +4.1233727266 +8.0493729107 +21.5727251246
C +1.6446916690 +3.6299685093 +21.5895684163
H +0.7100982897 +2.2943877377 +13.6122775366
H +2.5737521867 +8.3572929419 +12.9885324084
H +0.6959081873 +1.7960525666 +16.0015346991
H +2.5505417814 +7.8476828989 +15.3803251202
H +5.0073930925 +6.5975980733 +13.5699429188
H +3.2710256920 +3.9395447865 +13.0384736741
H +4.9896490726 +6.1096697951 +15.9644070129
H +3.2855328345 +3.4712346084 +15.4361072049
H +2.4668227343 +7.5372563565 +17.3196581147
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H +2.4547240741 +7.0626666150 +19.7225891323
H +0.6841009994 +0.8840013345 +20.2969363268
H +0.0375692548 +5.9072180873 +17.9221227398
H +3.1850362285 +2.9747948204 +17.3155378471
H +0.0682812385 +5.4256048002 +20.3295815241
H +3.2154720804 +2.5256156113 +19.7218194120
N +4.1235005654 +7.7434722596 +22.7238192298
N +1.6496722670 +3.3281686168 +22.7417039079
C +1.6161331425 +5.5139345346 +29.5032690776
C +4.1883772090 +1.5358487379 +28.0817754345
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C +3.2411597901 +1.4978335462 +25.8190856126
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C +4.1311944129 +0.2502457140 +32.2260967321

C +0.0406810559 +2.8957044802 +26.2810399578
C +2.5995390412 +4.1796937462 +31.3143360584
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