

Supporting Information for:

New Dihexadecyldithiophosphate SAMs on Gold
Provide Insight into the Unusual Dependence of
Adsorbate Chelation on Substrate Morphology in
SAMs of Dialkyldithiophosphinic Acids

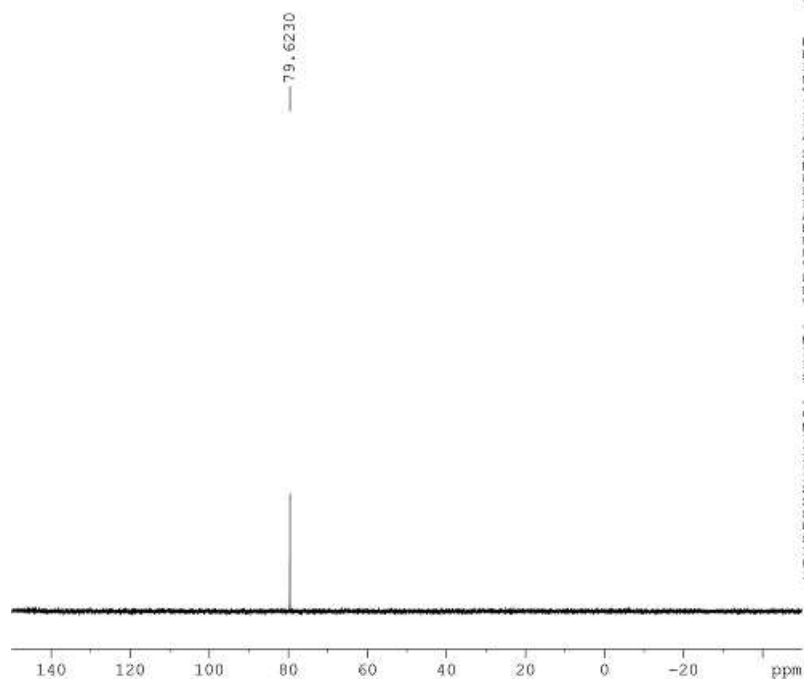
Ronan R. San Juan, Christopher J. Allan, Muhammad Iqbal, S. Holger Eichhorn, Charles L.B.

Macdonald and Tricia Breen Carmichael**

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N9B 3P4

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(C16)2DDP in CDC13
31P
Bruker 300 US

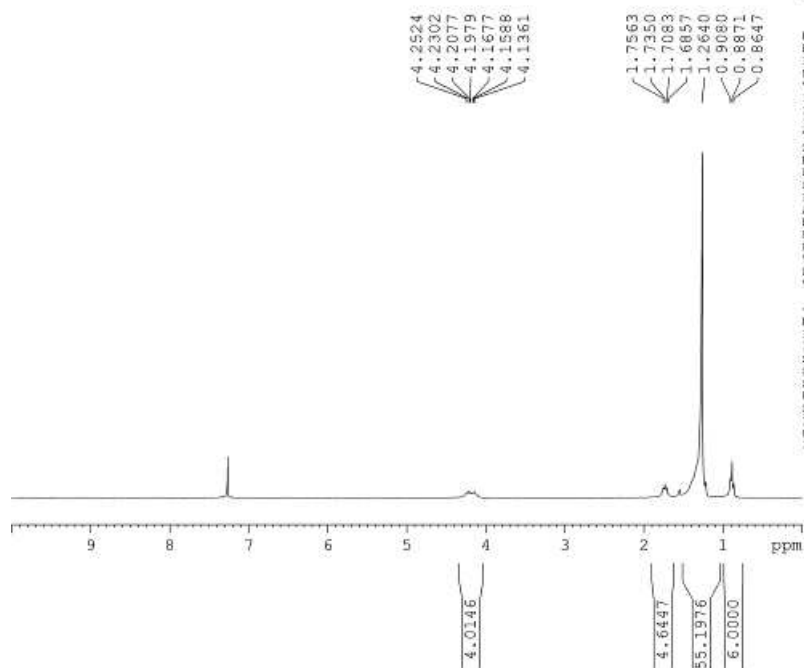


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(C16)2DDP in CDC13
1H
Bruker 300 US



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13C
Bruker 300 US

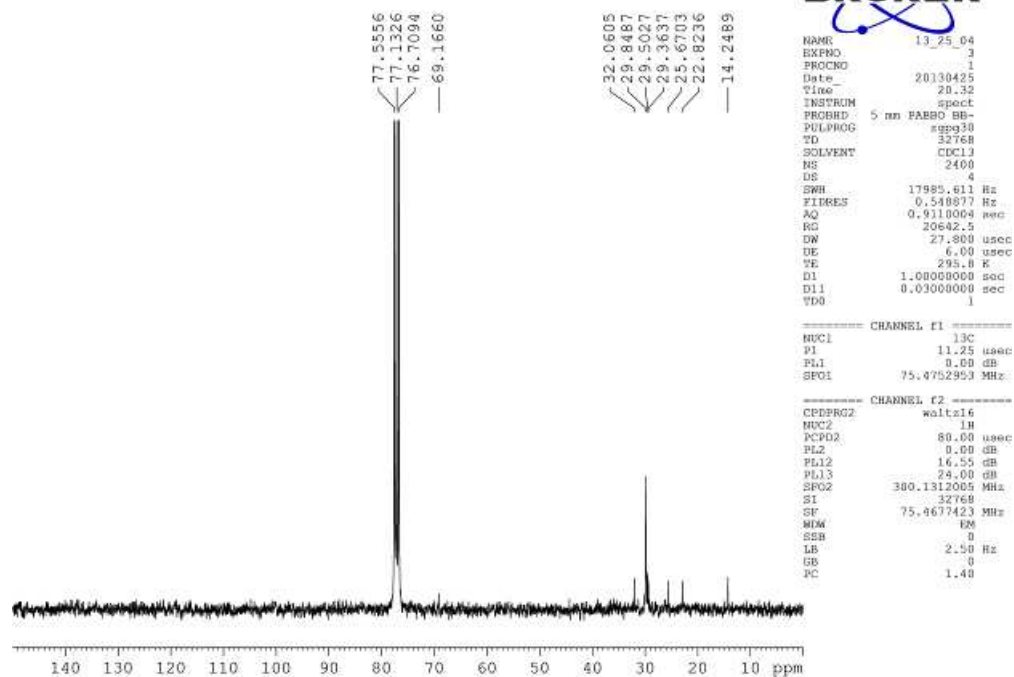


Figure S1. ^{31}P , ^1H and ^{13}C NMR spectra of $(\text{C}_{16})_2\text{DDP}$.

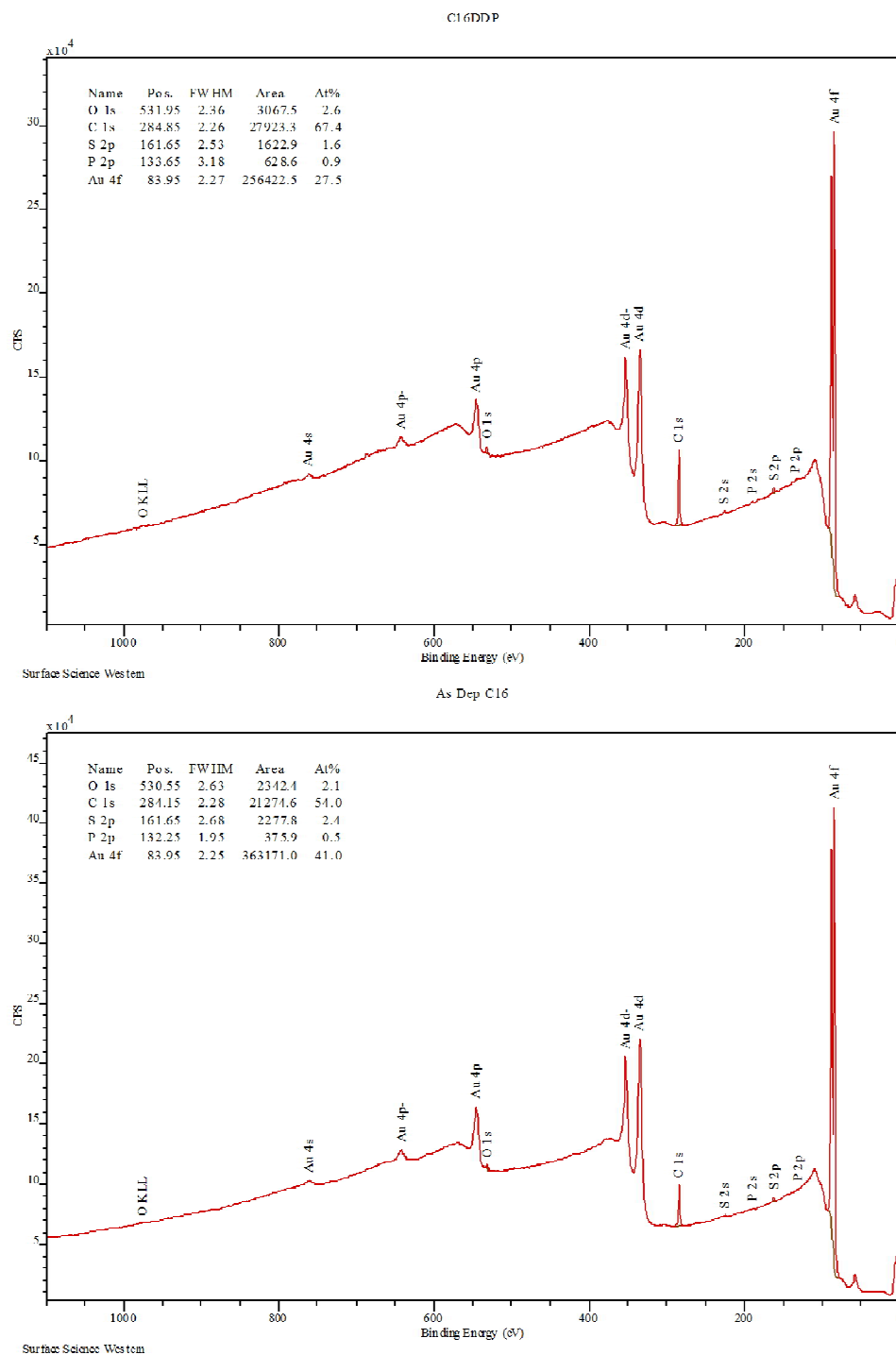


Figure S2. Survey scans of $(C_{16})_2DDP$ and $(C_{16})_2DTPA$ SAMs.

All density functional theory (DFT) calculations were performed using the B3PW91 method using the Gaussian 09 suites¹ using the SHARCNET high-performance computing network (www.sharcnet.ca). Where applicable, the Stuttgart group (SDD) effective core potentials (ECP)^{2,3} and corresponding basis sets were used for gold atoms and the 6-31+G(d) basis set was used for all lighter atoms. Natural bond order (NBO)⁴ analyses to determine orbital contributions, Wiberg Bond Indices and HOMO/LUMO energies were obtained using the routine included in the Gaussian distributions. All stationary points were confirmed to be minima exhibiting no imaginary frequencies. The anions DDP and DTPA were calculated with C₂ symmetry. Molecular orbital pictures and electrostatic potential plots were calculated using Molden.⁵ Molecular orbital diagrams were generated using POV-Ray for Windows.⁶ Proton and gold(I) ion affinities were calculated using energies in the following formula: Affinity = $\Delta E_{\text{Rxn}}^{\text{elec}}$ - $\Delta \text{ZPE} + 5/2RT$, where $\Delta E_{\text{Rxn}}^{\text{elec}}$ is the change in the electronic energy upon reaction (at 298.15K); ΔZPE is the change in zero point energy; R=8.314 J/molK and T=298.15K

Exo AuDDP

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Exo HDTPA

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 0.5466866034\H,-0.3630826176,-2.3565768891,-0.200920298\H,-0.9492944553,-
 1.5428448094,-1.644753861\C,-2.3995605844,-1.6035139531,-0.0200317651\H,-
 2.4000536907,-1.5487428872,1.0773843885\H,-2.9952296913,-0.7529822876,-
 0.3800423751\C,-3.0853434798,-2.9051468509,-0.4477632\H,-3.0792581613,-2.9743672256,-
 1.5446406442\H,-2.496480756,-3.7582304837,-0.0833130289\C,-4.5202314139,-
 3.0149266834,0.0646232678\H,-5.1423181792,-2.1934157237,-0.3124213655\H,-
 4.9843743938,-3.9550586245,-0.2543902831\H,-4.5557523417,-
 2.9829423857,1.1607199216\H,-2.7551941415,3.987989473,-4.113465424\H,-
 1.2284263674,0.1731314274,2.2413387733\\Version=AM64L-G09RevC.01\State=1-A\HF=-
 1453.8346017\RMSD=8.369e-09\RMSF=7.896e-06\Dipole=-2.2673439,0.0111243,-
 0.0932624\Quadrupole=-7.3773593,5.5202157,1.8571436,0.835391,-1.4357969,-
 0.925682\PG=C01 [X(C8H19P1S2)]\\@

Chelated HDTPA

1\1\GINC-ORC87\FOpt\RB3PW91\6-31+G(d)\C8H19P1S2\ALLANC\05-Sep-
 2012\0\#B3PW91/6-31+G(d) opt freq pop=(full,nboread) test\\Optimization and Freq Calc on
 HDTPA_close\\0,1\P,0.0262162534,0.0213219154,-0.0883828144\S,-
 0.0783186151,0.1380168385,2.0517210615\S,1.8415908993,-0.0070389853,-0.8215096531\C,-
 0.9883452656,1.4862158226,-0.5390195811\H,-1.9217874276,1.4541958076,0.0396923222\H,-
 0.4169925355,2.3525002626,-0.183205654\C,-1.2694149517,1.6026047959,-2.0389371319\H,-

0.3217480791,1.5424978048,-2.5897726625\H,-1.8820274456,0.7538390951,-
 2.3742738614\C,-1.986623317,2.9087279821,-2.3920100789\H,-1.3651528043,3.7569716377,-
 2.0726621273\H,-2.9220435091,2.9798667947,-1.8183576374\C,-
 2.2910893143,3.0301708972,-3.8840079884\H,-1.3718521122,2.9931938173,-
 4.4812828949\H,-2.9417420922,2.215166196,-4.2251843896\C,-0.9521117922,-
 1.4707742311,-0.5427426505\H,-0.3616463435,-2.3205022184,-0.1765121689\H,-
 0.9138058034,-1.5188088701,-1.6394525091\C,-2.3922623482,-1.5450155687,-
 0.0332015021\H,-2.4061534916,-1.420582469,1.0578742571\H,-2.9849852245,-
 0.7201098864,-0.4527402247\C,-3.0641680049,-2.8729148782,-0.396936508\H,-
 3.0386873085,-3.0076985971,-1.4876052842\H,-2.4789531418,-
 3.7004526419,0.0279301461\C,-4.5074217037,-2.959847344,0.0963072235\H,-5.125971107,-
 2.1646554169,-0.3385448746\H,-4.9626723979,-3.9193233427,-0.1747187636\H,-
 4.5612654563,-2.8628310877,1.1877198925\H,-2.7971516696,3.9757223191,-
 4.1102098095\H,1.14222493,-0.406607698,2.2202525418\\Version=AM64L-
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 1.6083544,-0.1443395,-0.0749362\Quadrupole=-5.8986653,4.8194192,1.079246,-
 0.2689254,2.9274056,-2.2877574\PG=C01 [X(C8H19P1S2)]\\@

DDP anion

1\1\GINC-ORC296\FOpt\RB3PW91\6-31+G(d)\C8H18O2P1S2(1-)\ALLANC\04-Sep-
 2012\0\#B3PW91/6-31+G(d) opt freq pop=(full,nboread) test\\Optimization and Freq Calc on
 on DDP_c2\1,1\1\P,-0.268183837,0.,-0.1896346097\S,-

0.4747226208,0.316887038,1.753512977\S,1.4949870155,-0.316887038,-1.0320771049\C,-
 1.0757951216,1.3774168882,-2.342746156\H,-0.0783962861,1.1373845685,-2.7372259123\H,-
 1.7871907517,0.6499072119,-2.7662542593\C,-1.4792604256,2.7967482168,-
 2.7145281315\H,-0.7545215993,3.4913992108,-2.2684698306\H,-
 2.4531424354,3.0246708598,-2.2576779081\C,-1.5500287891,3.0123512583,-
 4.2267566247\H,-2.2671001409,2.3022714353,-4.6654460367\C,-2.567360632,-1.377416888,-
 0.2333539821\H,-2.6068134344,-1.1373845684,0.8384959102\H,-3.2037797776,-
 0.6499072116,-0.7628948465\C,-3.0523684749,-2.7967482165,-0.4898173936\H,-
 2.9462732903,-3.0246708595,-1.5602855657\H,-2.3902410669,-
 3.4913992106,0.0447868242\C,-4.5017006257,-3.0123512579,-0.0524622822\H,-
 5.1543247536,-2.3022714348,-0.582293832\H,-4.5989545494,-
 2.7739444937,1.0165908973\H,-0.5745337602,2.7739444941,-4.6747995632\C,-
 1.9502009705,4.4365303108,-4.6113884401\H,-1.2317525066,5.1677145619,-
 4.2189005589\H,-1.9952971277,4.564591126,-5.7008014074\H,-2.9363854326,4.6943955772,-
 4.2035142029\C,-4.9977257061,-4.4365303103,-0.301537628\H,-4.3882017618,-
 5.1677145615,0.2449927859\H,-6.0398661542,-4.5645911254,0.0190829631\H,-
 4.9419063416,-4.6943955767,-1.3672793345\O,-1.067799636,1.2706276823,-
 0.9258784589\O,-1.2288597946,-1.2706276821,-0.6981049985\\Version=AM64L-
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 3.4140553,0.,-2.4141017\Quadrupole=-4.8396137,5.9932759,-1.1536622,1.321883,-5.2127225,-
 1.8694248\PG=C02 [C2(P1),X(C8H18O2S2)]\\@

DTPA anion

1\1\GINC-ORC8\FOpt\RB3PW91\6-31+G(d)\C8H18P1S2(1-)\ALLANC\04-Sep-
 2012\0\#B3PW91\6-31+G(d) opt freq pop=(full,nboread) test\Optimization and Freq Calc on
 on DTPA_c2\ -1,1\ P,0.079319244,0.0000000001,0.0560871753\S,-
 0.1171018699,0.1071049469,2.0576748844\S,1.900960529,-0.1071049468,-0.7962963298\C,-
 0.8301693302,1.4612649541,-0.6556727347\H,-1.8215151059,1.4858190912,-
 0.1829297139\H,-0.2768464457,2.3291123222,-0.2732001863\C,-
 0.9308191088,1.5206734232,-2.1780725467\H,0.0708297032,1.3641599738,-2.6013237068\H,-
 1.5568399441,0.6930209326,-2.5453330957\C,-1.5102532409,2.843650428,-2.6873870157\H,-
 0.8704584598,3.6697109008,-2.3440727714\H,-2.4975441234,3.013832448,-2.231494147\C,-
 1.6374568496,2.8975661826,-4.2102275665\H,-0.6607406976,2.7581184796,-
 4.6911052702\H,-2.3006575764,2.1039335419,-4.5794628805\C,-0.8948972927,-
 1.4612649539,-0.5641335723\H,-0.3498577544,-2.3291123221,-0.1699466034\H,-
 0.7796394902,-1.4858190911,-1.6563643399\C,-2.3637795265,-1.520673423,-
 0.1515604896\H,-2.4289416098,-1.3641599737,0.9338867868\H,-2.9187097046,-
 0.6930209324,-0.6193584103\C,-3.0371105236,-2.8436504278,-0.5280847386\H,-
 2.9363875658,-3.0138324479,-1.6108757989\H,-2.5001658229,-3.6697109007,-
 0.0393185158\C,-4.5152595667,-2.8975661824,-0.1403999341\H,-5.0844448681,-
 2.1039335418,-0.6425931378\H,-4.9728638628,-3.8585528902,-0.4110856835\H,-
 4.643063363,-2.7581184795,0.9407494529\H,-2.0451965869,3.8585528904,-
 4.5514324512\Version=AM64L-G09RevC.01\State=1-A\HF=-1453.319185\RMSD=2.404e-
 09\RMSF=2.978e-06\Dipole=-3.3981559,0.,-2.4028591\Quadrupole=-7.0148508,11.1888872,-
 4.1740364,-0.1420766,-4.0175182,0.2009266\PG=C02 [C2(P1),X(C8H18S2)]\ \@

Au Cation

1\1\GINC-ORC202\FOpt\RB3PW91\Gen\Au1(1+)\ALLANC\12-Sep-2012\0\#B3PW91/gen

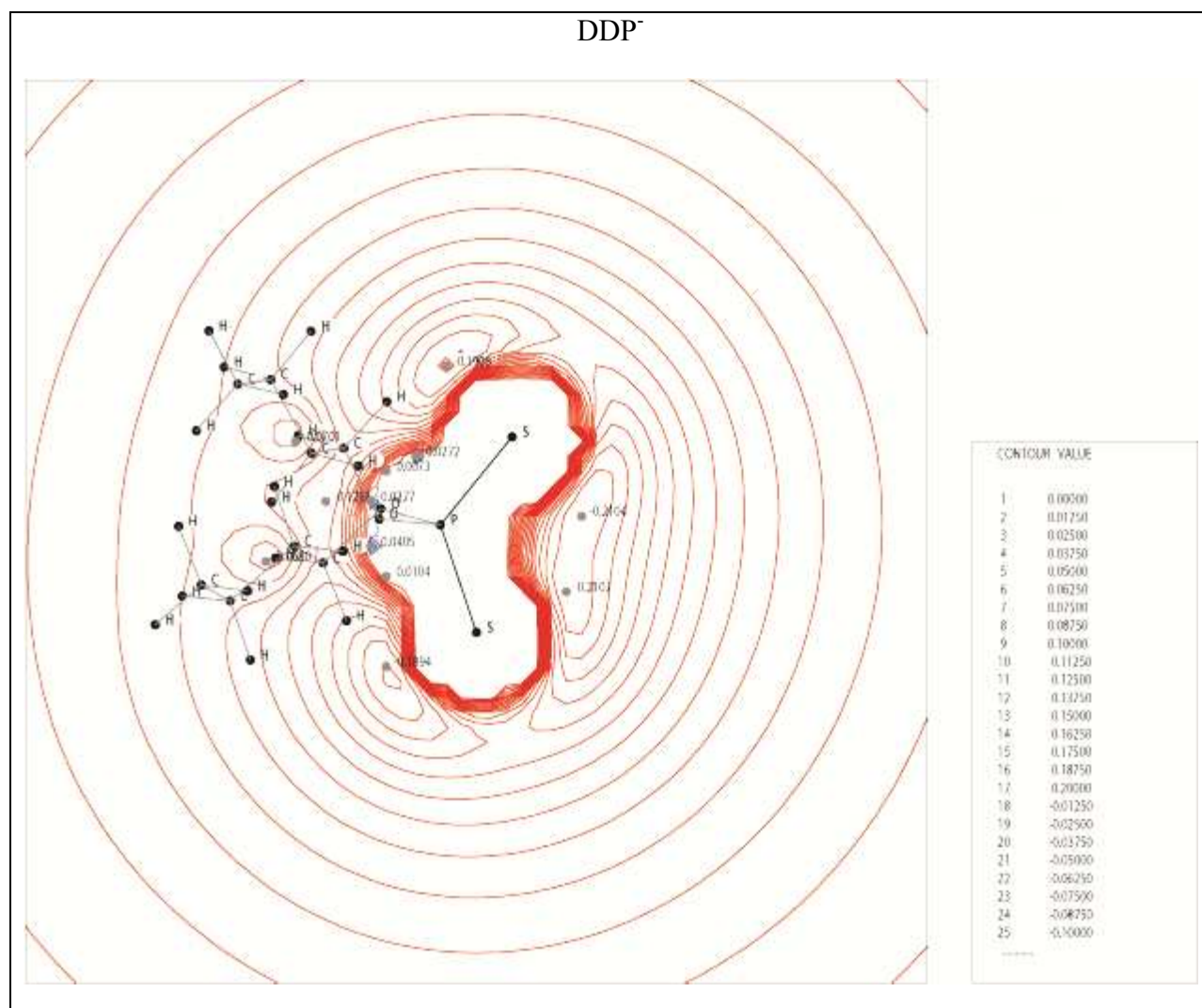
pseudo=read opt freq pop=(full,nboread) test\Optimization and Freq Calc on

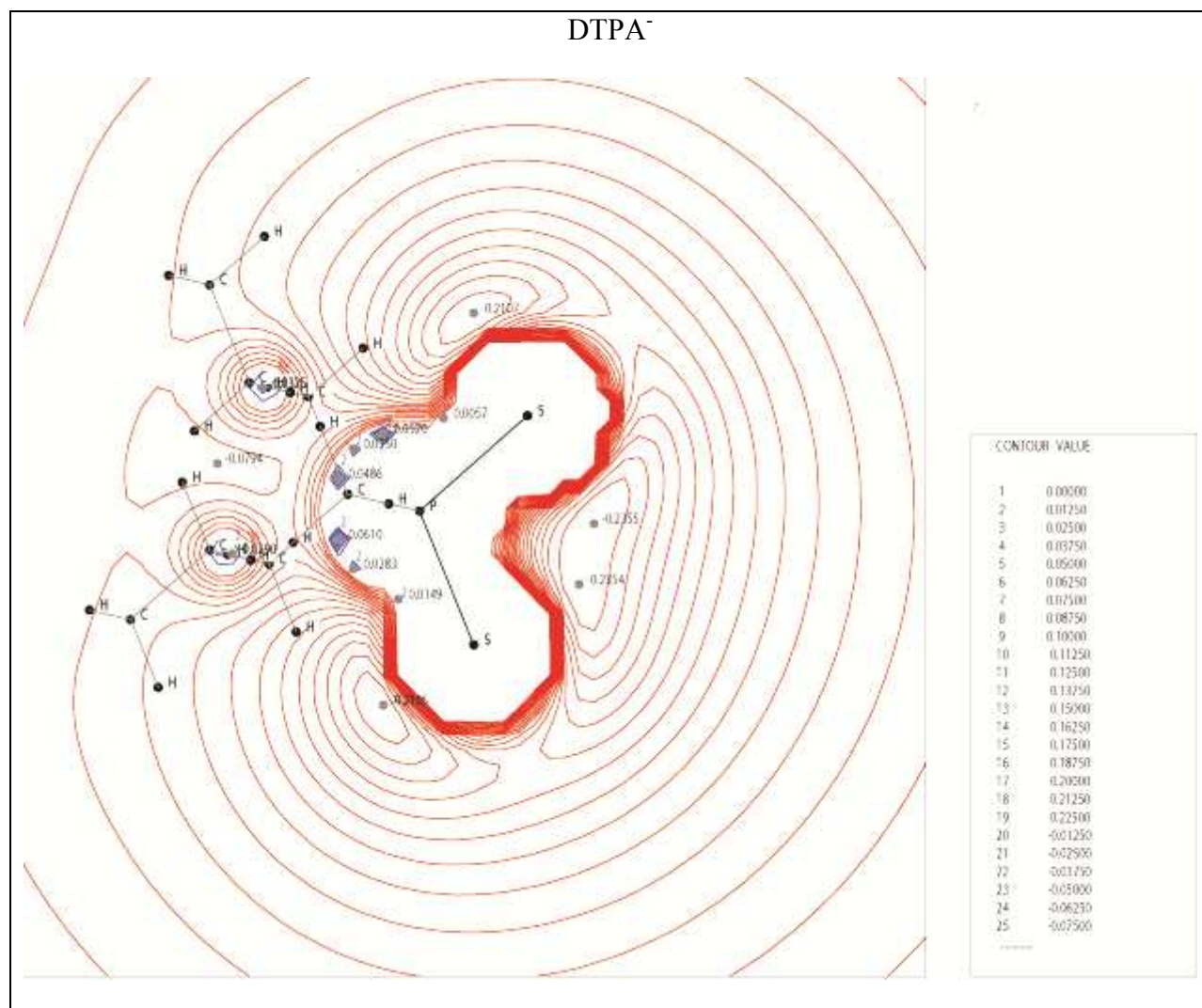
Au_cat\1,1\Au,0.,0.,0.\Version=AM64L-G09RevC.01\State=1-

A1G\HF=135.452234\RMSD=7.604e-10\RMSF=0.000e+00\Dipole=0.,0.,0.\Quadru

pole=0.,0.,0.,0.,0.,0.\PG=OH [O(Au1)]\@

Electrostatic Potentials:





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