

# Supporting Information of

## **Stabilization of Cyclic and Acyclic Carbon(0) Compounds by Differential Coordination of Heterocyclic Carbenes : A Theoretical Assessment**

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**Table S1.** Energies of the  $\pi$  symmetric HOMO (eV) of the first protonated derivatives of **1–6** and second proton affinities ( $\text{kcal mol}^{-1}$ ) calculated at BP86/TZVP level of theory.

Entry	$E_{\text{HOMO}}$	$E_{\text{PA-2}}$
<b>1-H</b> <sup>1+</sup>	-6.7	183.6
<b>2-H</b> <sup>1+</sup>	-8.0	162.9
<b>3-H</b> <sup>1+</sup>	-7.4	170.6
<b>4-H</b> <sup>1+</sup>	-7.7	168.3
<b>5-H</b> <sup>1+</sup>	-8.5	150.3
<b>6-H</b> <sup>1+</sup>	-8.1	158.7

Cartesian coordinates of the optimized geometries of all the molecules at the BP86/TZVP level of theory along with the total energies (T. E.) including zero point vibrational correction.

1.	<b>1</b> , T. E. = -647.61548		
6	3.510457000	0.178731000	-0.075127000
7	3.030210000	-1.062379000	0.122508000
6	1.642573000	-1.035341000	0.142070000
6	1.192382000	0.312779000	-0.008597000
7	2.465793000	1.026513000	-0.172715000
1	1.084024000	-1.926565000	0.401230000
1	4.560668000	0.427162000	-0.178020000
6	-0.000004000	1.003697000	0.000080000
6	-1.192379000	0.312771000	0.008721000
6	-1.642555000	-1.035345000	-0.142069000
7	-3.030203000	-1.062356000	-0.122772000
6	-3.510468000	0.178729000	0.074973000
7	-2.465808000	1.026488000	0.172854000
1	-1.084016000	-1.926435000	-0.401734000
1	-4.560666000	0.427082000	0.178211000
6	-2.522015000	2.461981000	0.358525000
1	-3.110941000	2.946530000	-0.435663000
1	-2.936574000	2.724518000	1.344523000
1	-1.461875000	2.777157000	0.298048000
6	-3.850286000	-2.255604000	-0.257880000
1	-3.651988000	-2.743142000	-1.224262000
1	-3.625421000	-2.964157000	0.553660000
1	-4.911014000	-1.976999000	-0.209983000
6	2.521979000	2.461983000	-0.358572000
1	2.936413000	2.724404000	-1.344654000
1	1.461851000	2.777176000	-0.298008000
1	3.111009000	2.946623000	0.435483000
6	3.850322000	-2.255561000	0.258029000
1	4.911004000	-1.977244000	0.207598000

1	3.653785000	-2.741604000	1.225533000
1	3.623761000	-2.965292000	-0.552004000
2.	<b>2</b> , T. E. = -613.17295		
6	-0.000322000	0.001228000	-0.006811000
6	1.332989000	0.010417000	0.003252000
6	2.151176000	-0.933136000	0.786012000
6	3.506008000	-0.887515000	0.784489000
7	4.226584000	0.064991000	0.067566000
6	3.504662000	0.959610000	-0.719158000
6	2.149887000	0.968936000	-0.762343000
1	4.111786000	-1.587358000	1.362940000
1	4.109754000	1.670568000	-1.284456000
6	-1.333635000	-0.008781000	-0.000499000
6	-2.152170000	0.758079000	0.955569000
6	-3.506773000	0.708093000	0.949246000
7	-4.227527000	-0.087566000	0.060978000
6	-3.504790000	-0.799670000	-0.894253000
6	-2.150127000	-0.794539000	-0.942885000
1	-4.112438000	1.274089000	1.659290000
1	-4.109074000	-1.383071000	-1.591295000
1	1.647565000	1.717815000	-1.375474000
1	1.650275000	-1.686125000	1.395140000
1	-1.651447000	1.378485000	1.699499000
1	-1.647788000	-1.399658000	-1.698188000
6	-5.662167000	0.099047000	-0.093117000
1	-6.113145000	-0.823395000	-0.485702000
1	-6.113212000	0.307738000	0.887404000
1	-5.910428000	0.931355000	-0.778649000
6	5.664800000	-0.071928000	-0.104661000
1	5.929653000	-0.725913000	-0.956657000
1	6.112007000	0.918475000	-0.272129000
1	6.105857000	-0.494031000	0.809420000

3.	<b>3</b> , T. E. = -630.38964		
6	3.628388000	0.298864000	-0.368836000
7	2.488375000	1.028174000	-0.365646000
6	1.396830000	0.273178000	0.215200000
6	2.006619000	-0.982048000	0.487766000
7	3.350310000	-0.909233000	0.154567000
1	4.592456000	0.605067000	-0.757312000
1	1.599086000	-1.853633000	0.984647000
6	0.201236000	0.882755000	0.550901000
6	-3.507116000	0.640356000	0.775840000
6	-2.232379000	1.055972000	0.988842000
6	-1.073363000	0.438234000	0.338290000
6	-1.465021000	-0.646844000	-0.573810000
6	-2.757185000	-1.021744000	-0.760527000
7	-3.812034000	-0.426012000	-0.071974000
1	-4.367422000	1.098641000	1.267063000
1	-2.050510000	1.880057000	1.681015000
1	-0.686400000	-1.174773000	-1.128648000
1	-3.047645000	-1.822812000	-1.443903000
6	2.333872000	2.422185000	-0.727892000
1	1.977455000	2.535249000	-1.763353000
1	1.551319000	2.815197000	-0.050394000
1	3.285024000	2.957818000	-0.600454000
6	4.312611000	-1.993426000	0.298085000
1	5.300803000	-1.649163000	-0.031881000
1	4.373267000	-2.303511000	1.351144000
1	4.006956000	-2.854243000	-0.314515000
6	-5.187196000	-0.673778000	-0.473474000
1	-5.296937000	-1.722414000	-0.785413000
1	-5.857765000	-0.500092000	0.380601000
1	-5.510017000	-0.024112000	-1.309534000
4.	<b>4</b> , T. E. = -646.41294		
6	2.927177000	-0.305878000	-0.009975000

7	2.443146000	0.958085000	0.027820000
6	1.034229000	0.936525000	0.052422000
6	0.696642000	-0.491579000	0.063703000
7	1.891354000	-1.198703000	-0.002663000
1	3.973089000	-0.586383000	0.036637000
6	-0.696599000	-0.491544000	-0.062890000
6	-1.034137000	0.936603000	-0.052185000
7	-1.891343000	-1.198639000	0.003081000
7	-2.443066000	0.958159000	-0.028785000
6	0.000091000	1.882273000	-0.000070000
6	-2.927139000	-0.305804000	0.009388000
1	-3.973033000	-0.586267000	-0.037866000
6	3.215908000	2.192226000	-0.022649000
1	2.496202000	3.003851000	0.156107000
1	3.994991000	2.198858000	0.753509000
1	3.676689000	2.331485000	-1.012288000
6	2.052576000	-2.641462000	-0.011573000
1	3.118314000	-2.893255000	-0.091653000
1	1.648971000	-3.081659000	0.914422000
1	1.520946000	-3.074996000	-0.873771000
6	-2.052642000	-2.641404000	0.011524000
1	-1.520814000	-3.075195000	0.873460000
1	-3.118372000	-2.893158000	0.091836000
1	-1.649293000	-3.081355000	-0.914701000
6	-3.216020000	2.192069000	0.022948000
1	-3.663847000	2.338179000	1.017582000
1	-2.499722000	3.003291000	-0.170474000
1	-4.005263000	2.192130000	-0.742837000
5.	<b>5, T. E. = -611.97061</b>		
6	1.664350000	-1.075315000	0.009558000
6	0.721890000	-0.082726000	0.000093000
6	1.096455000	1.350980000	0.005057000
6	2.499113000	1.609955000	0.024351000

6	3.404580000	0.580878000	0.031710000
7	3.002335000	-0.752745000	0.029082000
1	1.445353000	-2.146475000	0.008607000
1	2.856263000	2.641642000	0.036551000
1	4.483869000	0.732326000	0.044836000
6	-0.721903000	-0.082724000	0.000055000
6	-1.664364000	-1.075310000	-0.009629000
7	-3.002352000	-0.752732000	-0.029170000
6	-3.404591000	0.580885000	-0.031687000
6	-2.499120000	1.609963000	-0.024316000
6	-1.096466000	1.350986000	-0.005039000
1	-1.445377000	-2.146472000	-0.008921000
1	-4.483878000	0.732344000	-0.044765000
1	-2.856270000	2.641650000	-0.036557000
6	-0.000001000	2.257428000	-0.000089000
6	4.020030000	-1.801118000	-0.052137000
1	4.837154000	-1.585121000	0.650704000
1	3.571498000	-2.764644000	0.220401000
1	4.434687000	-1.876655000	-1.070601000
6	-4.019973000	-1.801166000	0.052188000
1	-3.571937000	-2.764356000	-0.222370000
1	-4.433135000	-1.878079000	1.071163000
1	-4.838109000	-1.584113000	-0.649131000

6. **6**, T. E. = -629.19759

6	-1.815686000	0.895384000	-0.014454000
6	-0.649400000	0.172732000	-0.005459000
6	-0.662887000	-1.362776000	-0.000953000
6	-1.967667000	-1.925823000	-0.010322000
6	-3.097241000	-1.144800000	-0.021144000
7	-3.026991000	0.252186000	-0.028316000
1	-1.872880000	1.986942000	-0.015346000
1	-2.076895000	-3.012710000	-0.013670000
1	-4.107919000	-1.550818000	-0.030214000

6	0.740013000	0.453424000	-0.006873000
6	1.397939000	-0.812241000	0.001377000
6	0.607753000	-1.980881000	0.003250000
7	2.773018000	-0.511587000	0.006995000
7	1.713259000	1.439043000	-0.004426000
6	2.934215000	0.834416000	0.003546000
1	3.880380000	1.363723000	0.004111000
6	-4.270739000	1.014448000	0.049582000
1	-4.067316000	2.069557000	-0.173645000
1	-4.992161000	0.634565000	-0.689105000
1	-4.721009000	0.944177000	1.053856000
6	3.816304000	-1.531709000	0.017389000
1	3.283754000	-2.494496000	0.013874000
1	4.451296000	-1.454470000	-0.876988000
1	4.435273000	-1.452716000	0.922789000
6	1.503769000	2.880968000	-0.011726000
1	0.935966000	3.181814000	0.880941000
1	2.473921000	3.394168000	-0.009360000
1	0.944355000	3.173912000	-0.912291000
7.	<b>1-H<sup>1+</sup></b> , T. E. = -648.11193		
6	-3.515199000	0.159356000	-0.022642000
7	-3.035097000	-1.086526000	0.037541000
6	-1.647287000	-1.048861000	0.051795000
6	-1.247271000	0.298481000	0.003034000
7	-2.467618000	1.018015000	-0.047272000
1	-1.074390000	-1.961361000	0.134208000
1	-4.562099000	0.437225000	-0.052342000
6	0.000000000	0.952819000	0.000027000
6	1.247271000	0.298480000	-0.003000000
6	1.647285000	-1.048863000	-0.051766000
7	3.035096000	-1.086526000	-0.037601000
6	3.515200000	0.159356000	0.022567000
7	2.467619000	1.018013000	0.047279000



1	1.074383000	-1.961365000	-0.134109000
1	4.562102000	0.437226000	0.052203000
6	2.578097000	2.469391000	0.114871000
1	2.065992000	2.843736000	1.013073000
1	3.637078000	2.748019000	0.163759000
1	2.128590000	2.926339000	-0.778784000
6	3.844789000	-2.305817000	-0.078357000
1	3.618580000	-2.930248000	0.796051000
1	3.627481000	-2.864136000	-0.998575000
1	4.906204000	-2.033902000	-0.063813000
6	-2.578092000	2.469393000	-0.114863000
1	-3.637068000	2.748018000	-0.163884000
1	-2.128698000	2.926341000	0.778849000
1	-2.065877000	2.843741000	-1.013000000
6	-3.844793000	-2.305813000	0.078380000
1	-4.906204000	-2.033920000	0.063152000
1	-3.618112000	-2.930580000	-0.795664000
1	-3.627962000	-2.863770000	0.998930000
1	0.000001000	2.040262000	0.000053000
8.	<b>1-H<sub>2</sub><sup>12+</sup></b> , T. E. = -648.40345		
6	3.437787000	0.023933000	-0.287181000
7	2.939246000	1.009204000	0.474674000
6	1.593769000	0.760530000	0.689632000
6	1.272234000	-0.406269000	0.035900000
7	2.452604000	-0.849703000	-0.570075000
1	0.986165000	1.421216000	1.298728000
1	4.466581000	-0.055992000	-0.625642000
6	0.000001000	-1.210824000	-0.000008000
6	-1.272234000	-0.406270000	-0.035906000
6	-1.593775000	0.760528000	-0.689638000
7	-2.939252000	1.009197000	-0.474677000
6	-3.437787000	0.023927000	0.287184000
7	-2.452598000	-0.849704000	0.570079000

1	-0.986174000	1.421216000	-1.298737000
1	-4.466579000	-0.056000000	0.625650000
6	-2.631923000	-2.069701000	1.379678000
1	-1.992439000	-2.027730000	2.270816000
1	-3.678275000	-2.124782000	1.699684000
1	-2.397903000	-2.957641000	0.778938000
6	-3.700019000	2.161435000	-0.999218000
1	-3.289568000	3.090604000	-0.584976000
1	-3.635146000	2.171097000	-2.094151000
1	-4.748449000	2.059820000	-0.698634000
6	2.631935000	-2.069703000	-1.379668000
1	3.678291000	-2.124787000	-1.699663000
1	2.397908000	-2.957641000	-0.778927000
1	1.992460000	-2.027735000	-2.270813000
6	3.700010000	2.161443000	0.999221000
1	4.748430000	2.059859000	0.698593000
1	3.289524000	3.090614000	0.585019000
1	3.635177000	2.171073000	2.094156000
1	-0.018500000	-1.880165000	0.877266000
1	0.018502000	-1.880154000	-0.877291000
9.	<b>2-H<sup>1+</sup></b> , T. E. = -613.63604		
6	-0.000027000	1.162273000	-0.001947000
6	-1.287051000	0.583843000	0.004276000
6	-1.621672000	-0.796261000	0.221952000
6	-2.923916000	-1.228552000	0.216429000
7	-3.972165000	-0.376931000	-0.002946000
6	-3.707668000	0.960501000	-0.182606000
6	-2.428265000	1.442324000	-0.173334000
1	-3.188293000	-2.270366000	0.395955000
1	-4.576120000	1.600949000	-0.335130000
6	1.287067000	0.583942000	-0.006729000
6	1.621984000	-0.795919000	-0.225482000
6	2.924199000	-1.228311000	-0.218158000

7	3.972060000	-0.376966000	0.003993000
6	3.707344000	0.960315000	0.184474000
6	2.427995000	1.442251000	0.173414000
1	3.188846000	-2.269936000	-0.398324000
1	4.575578000	1.600570000	0.339078000
1	-2.279015000	2.512265000	-0.324535000
1	-0.859449000	-1.537453000	0.448168000
1	0.860111000	-1.536705000	-0.454228000
1	2.278579000	2.512098000	0.325133000
6	5.365929000	-0.853346000	-0.023399000
1	5.913474000	-0.441738000	0.834213000
1	5.373532000	-1.946728000	0.044728000
1	5.857682000	-0.544936000	-0.957126000
6	-5.365844000	-0.853586000	0.027905000
1	-5.851405000	-0.556817000	0.968643000
1	-5.918876000	-0.431017000	-0.820745000
1	-5.374256000	-1.946039000	-0.054138000
1	-0.000092000	2.256290000	0.000207000

10. **2-H<sub>2</sub><sup>12+</sup>**, T. E. = -613.89563

6	0.000395000	1.570687000	-0.004859000
6	1.297720000	0.780951000	0.004812000
6	1.556885000	-0.238953000	-0.929510000
6	2.790022000	-0.871955000	-0.951931000
7	3.769835000	-0.524137000	-0.074832000
6	3.548028000	0.450378000	0.844646000
6	2.328106000	1.109843000	0.901840000
1	3.037255000	-1.656790000	-1.666920000
1	4.373818000	0.682343000	1.517374000
6	-1.297262000	0.781610000	-0.009288000
6	-1.562197000	-0.222300000	0.940758000
6	-2.795510000	-0.854736000	0.966623000
7	-3.770100000	-0.521741000	0.077921000
6	-3.542710000	0.437021000	-0.856540000

6	-2.322271000	1.095323000	-0.917719000
1	-3.047193000	-1.627239000	1.693419000
1	-4.364500000	0.657835000	-1.537859000
1	2.199287000	1.892052000	1.651824000
1	0.809650000	-0.544699000	-1.663343000
1	-0.819421000	-0.515455000	1.684219000
1	-2.189082000	1.864861000	-1.679952000
6	-5.106633000	-1.175376000	0.165218000
1	-5.579740000	-1.155161000	-0.822329000
1	-4.977411000	-2.214027000	0.488648000
1	-5.726008000	-0.628879000	0.889182000
6	5.105931000	-1.179121000	-0.158699000
1	5.723923000	-0.639922000	-0.889295000
1	5.581208000	-1.149681000	0.827602000
1	4.975639000	-2.220756000	-0.471869000
1	0.019174000	2.235131000	-0.885415000
1	-0.017778000	2.241299000	0.870974000

11. **3-H**<sup>1+</sup>, T. E. = -630.87842

6	-3.681293000	0.144288000	0.086997000
7	-2.657389000	1.024095000	0.091789000
6	-1.429262000	0.336583000	-0.066086000
6	-1.798965000	-1.009996000	-0.157584000
7	-3.179440000	-1.088256000	-0.060099000
1	-4.731047000	0.393489000	0.191225000
1	-1.209795000	-1.896709000	-0.348029000
6	-0.198072000	1.046071000	-0.128050000
6	3.515172000	0.967665000	-0.203349000
6	2.228691000	1.418584000	-0.239196000
6	1.098783000	0.535648000	-0.065104000
6	1.466489000	-0.837370000	0.184523000
6	2.775396000	-1.235081000	0.222136000
7	3.812216000	-0.362220000	0.012351000
1	4.371292000	1.626578000	-0.346530000

1	2.059960000	2.481065000	-0.420634000
1	0.712965000	-1.595024000	0.387552000
1	3.060650000	-2.267560000	0.423652000
6	-2.804472000	2.470519000	0.247747000
1	-2.205263000	2.813858000	1.101726000
1	-2.475812000	2.987448000	-0.664377000
1	-3.859906000	2.702844000	0.430057000
6	-3.964106000	-2.325716000	-0.120851000
1	-5.027410000	-2.081548000	-0.019425000
1	-3.797282000	-2.822233000	-1.085622000
1	-3.665443000	-2.993075000	0.697843000
6	5.211891000	-0.801173000	0.108666000
1	5.261180000	-1.886568000	-0.036518000
1	5.805260000	-0.316158000	-0.677144000
1	5.633323000	-0.548593000	1.093158000
1	-0.281902000	2.126715000	-0.254317000

12. **3-H<sub>2</sub><sup>12+</sup>**, T. E. = -631.15025

6	3.234717000	0.306497000	-0.835564000
7	2.074268000	0.925068000	-0.545579000
6	1.490407000	0.289721000	0.557602000
6	2.347343000	-0.728386000	0.906951000
7	3.419386000	-0.701543000	0.031773000
1	3.913508000	0.582321000	-1.637249000
1	2.290164000	-1.449434000	1.716657000
6	0.234276000	0.760395000	1.228120000
6	-3.506660000	0.634353000	0.530613000
6	-2.265181000	1.049655000	0.982799000
6	-1.104252000	0.331156000	0.639397000
6	-1.262898000	-0.796825000	-0.179859000
6	-2.526494000	-1.177424000	-0.611559000
7	-3.628919000	-0.469178000	-0.255853000
1	-4.429873000	1.158811000	0.778143000
1	-2.216960000	1.935536000	1.618836000

1	-0.409685000	-1.405915000	-0.481335000
1	-2.694164000	-2.050999000	-1.241582000
6	1.568763000	2.122840000	-1.238708000
1	0.537283000	1.954562000	-1.571123000
1	1.616180000	2.991480000	-0.568622000
1	2.196520000	2.315204000	-2.115810000
6	4.583380000	-1.611391000	0.062847000
1	5.267140000	-1.339498000	-0.748509000
1	5.098743000	-1.506631000	1.025619000
1	4.243160000	-2.644946000	-0.075339000
6	-4.973647000	-0.873746000	-0.755326000
1	-4.960816000	-1.943270000	-0.990064000
1	-5.717779000	-0.679982000	0.025251000
1	-5.212737000	-0.294019000	-1.656934000
1	0.247294000	1.859181000	1.315516000
1	0.260353000	0.396081000	2.270279000

13. **4-H<sup>1+</sup>**, T. E. = -646.91247

6	2.924480000	0.351755000	0.002414000
7	2.487766000	-0.931188000	-0.002881000
6	1.095572000	-0.928016000	-0.010754000
6	0.703403000	0.450111000	-0.010828000
7	1.872979000	1.205022000	0.001325000
1	3.965229000	0.655022000	0.000659000
6	-0.703407000	0.450109000	0.011238000
6	-1.095577000	-0.928015000	0.010631000
7	-1.872985000	1.205025000	-0.000804000
7	-2.487774000	-0.931184000	0.002339000
6	-0.000005000	-1.820166000	-0.000226000
6	-2.924483000	0.351758000	-0.002452000
1	-3.965232000	0.655027000	-0.000712000
6	3.340246000	-2.119790000	0.001143000
1	3.140402000	-2.721189000	-0.896117000
1	4.392411000	-1.813069000	0.004534000

1	3.134151000	-2.719344000	0.898326000
6	1.981052000	2.662490000	0.003091000
1	3.039529000	2.946345000	0.015934000
1	1.512427000	3.075258000	-0.901150000
1	1.491723000	3.073370000	0.897183000
6	-1.981049000	2.662492000	-0.003340000
1	-1.494095000	3.072839000	-0.898983000
1	-3.039555000	2.946351000	-0.013414000
1	-1.510018000	3.075788000	0.899399000
6	-3.340229000	-2.119802000	-0.000862000
1	-3.129437000	-2.722977000	-0.894497000
1	-3.145096000	-2.717567000	0.899879000
1	-4.392360000	-1.813121000	-0.011209000
1	-0.000001000	-2.904012000	-0.000012000
8.	<b>4-H<sub>2</sub><sup>12+</sup></b> , T. E. = -647.18063		
6	-2.928154000	0.387145000	0.000457000
7	-2.515075000	-0.901426000	0.000109000
6	-1.139282000	-0.895014000	-0.000681000
6	-0.726276000	0.427658000	-0.000488000
7	-1.858905000	1.220688000	0.000350000
1	-3.965352000	0.709554000	0.000620000
6	0.726276000	0.427658000	0.000519000
6	1.139282000	-0.895014000	0.000684000
7	1.858905000	1.220688000	-0.000341000
7	2.515076000	-0.901426000	-0.000161000
6	0.000000000	-1.887975000	-0.000010000
6	2.928154000	0.387144000	-0.000496000
1	3.965352000	0.709554000	-0.000682000
6	-3.404534000	-2.082365000	-0.000372000
1	-3.213133000	-2.682609000	0.897857000
1	-4.445072000	-1.740594000	0.006029000
1	-3.221681000	-2.675731000	-0.904959000
6	-1.946060000	2.694280000	0.000024000

1	-3.002773000	2.983098000	0.004460000
1	-1.464526000	3.092491000	0.901727000
1	-1.472055000	3.091792000	-0.905992000
6	1.946060000	2.694280000	-0.000013000
1	1.472101000	3.091789000	0.906029000
1	3.002774000	2.983098000	-0.004500000
1	1.464482000	3.092495000	-0.901690000
6	3.404533000	-2.082366000	0.000415000
1	3.222382000	-2.675153000	0.905527000
1	3.212434000	-2.683183000	-0.897277000
1	4.445066000	-1.740602000	-0.007041000
1	-0.000613000	-2.539140000	0.890520000
1	0.000613000	-2.539104000	-0.890566000

9. **5-H**<sup>+</sup>, T. E. = -612.46787

6	-1.667202000	-1.085474000	-0.001626000
6	-0.723582000	-0.081851000	-0.000345000
6	-1.137194000	1.315267000	-0.000951000
6	-2.529723000	1.586625000	-0.003088000
6	-3.417081000	0.540334000	-0.004646000
7	-2.995564000	-0.776608000	-0.004416000
1	-1.427262000	-2.148816000	-0.000747000
1	-2.913811000	2.607030000	-0.004535000
1	-4.496959000	0.682172000	-0.006307000
6	0.723579000	-0.081852000	0.000303000
6	1.667199000	-1.085476000	0.001500000
7	2.995560000	-0.776611000	0.004266000
6	3.417078000	0.540333000	0.004604000
6	2.529722000	1.586624000	0.003146000
6	1.137191000	1.315266000	0.001001000
1	1.427257000	-2.148818000	0.000574000
1	4.496957000	0.682166000	0.006248000
1	2.913810000	2.607029000	0.004617000
6	-0.000001000	2.146058000	0.000011000



6	-4.015713000	-1.844297000	0.007765000
1	-4.685979000	-1.727769000	-0.853993000
1	-3.518823000	-2.818314000	-0.055848000
1	-4.597223000	-1.796590000	0.938404000
6	4.015725000	-1.844288000	-0.007587000
1	3.518733000	-2.818379000	0.054027000
1	4.598653000	-1.795442000	-0.937271000
1	4.684678000	-1.728817000	0.855343000
1	0.000000000	3.233463000	0.000011000

10. **5-H<sub>2</sub><sup>12+</sup>**, T. E. = -612.70743

6	1.667235000	-1.100046000	0.006656000
6	0.735810000	-0.067654000	0.000576000
6	1.178350000	1.279808000	0.001957000
6	2.545018000	1.556816000	0.006867000
6	3.433680000	0.488742000	0.012553000
7	2.993991000	-0.801901000	0.012066000
1	1.414599000	-2.159956000	0.005866000
1	2.937766000	2.574688000	0.009817000
1	4.515413000	0.625087000	0.016224000
6	-0.735821000	-0.067654000	-0.000587000
6	-1.667245000	-1.100040000	-0.006710000
7	-2.994007000	-0.801889000	-0.012120000
6	-3.433690000	0.488749000	-0.012570000
6	-2.545021000	1.556824000	-0.006849000
6	-1.178359000	1.279814000	-0.001942000
1	-1.414622000	-2.159954000	-0.005949000
1	-4.515420000	0.625102000	-0.016240000
1	-2.937769000	2.574696000	-0.009785000
6	-0.000002000	2.218901000	0.000008000
6	4.001992000	-1.902499000	-0.020466000
1	4.808521000	-1.668838000	0.684069000
1	3.519778000	-2.839849000	0.275223000
1	4.402296000	-1.991472000	-1.039127000

6	-4.001949000	-1.902537000	0.020534000
1	-3.520143000	-2.839529000	-0.276966000
1	-4.400831000	-1.992708000	1.039652000
1	-4.809469000	-1.668051000	-0.682579000
1	0.001566000	2.885973000	-0.881114000
1	-0.001567000	2.885990000	0.881116000

11. **6-H**<sup>1+</sup>, T. E. = -629.69393

6	-1.818093000	0.883032000	-0.002748000
6	-0.653280000	0.141695000	-0.000697000
6	-0.719159000	-1.343071000	0.000058000
6	-2.010942000	-1.923223000	-0.001341000
6	-3.124210000	-1.120872000	-0.003668000
7	-3.028218000	0.261811000	-0.004929000
1	-1.844601000	1.972399000	-0.002836000
1	-2.143791000	-3.005740000	-0.001805000
1	-4.138469000	-1.516079000	-0.004959000
6	0.739443000	0.433789000	-0.000948000
6	1.444279000	-0.788158000	0.000357000
6	0.570782000	-1.901701000	0.000811000
7	2.796952000	-0.467688000	0.001062000
7	1.682961000	1.453788000	-0.000753000
6	2.908846000	0.885714000	0.000353000
1	3.845468000	1.432503000	0.000514000
6	1.422218000	2.894747000	-0.001710000
1	0.853878000	3.168859000	0.897355000
1	2.375682000	3.434832000	-0.001403000
1	0.855001000	3.167886000	-0.901777000
6	3.912785000	-1.416983000	0.002465000
1	3.860348000	-2.047077000	0.900341000
1	3.861559000	-2.048304000	-0.894616000
1	4.859071000	-0.864255000	0.002720000
6	-4.274836000	1.050380000	0.008267000
1	-4.029768000	2.116064000	-0.057542000

1	-4.899313000	0.773921000	-0.851647000
1	-4.827219000	0.865017000	0.939653000
1	0.823297000	-2.957506000	0.001135000
12.	<b>6-H<sub>2</sub><sup>12+</sup></b> , T. E. = -629.94690		
6	-1.830789000	0.878674000	-0.011024000
6	-0.671318000	0.114079000	0.000301000
6	-0.765506000	-1.314395000	0.001300000
6	-2.016804000	-1.915502000	-0.002829000
6	-3.148272000	-1.100015000	-0.011100000
7	-3.043195000	0.253966000	-0.015376000
1	-1.852799000	1.967334000	-0.014158000
1	-2.146099000	-2.998904000	-0.003970000
1	-4.159906000	-1.505275000	-0.014268000
6	0.750204000	0.423074000	-0.001090000
6	1.479463000	-0.746838000	0.001457000
6	0.611251000	-1.965645000	0.003427000
7	2.813619000	-0.411590000	0.002436000
7	1.648231000	1.479556000	-0.001379000
6	2.888196000	0.942089000	0.000527000
1	3.812667000	1.513235000	0.000322000
1	0.750460000	-2.606554000	0.891597000
1	0.751505000	-2.610343000	-0.881777000
6	3.970969000	-1.332298000	0.004664000
1	3.937979000	-1.956185000	0.906572000
1	3.939670000	-1.958376000	-0.895785000
1	4.892978000	-0.741070000	0.004812000
6	1.352741000	2.925753000	-0.003835000
1	2.298099000	3.479301000	-0.000854000
1	0.790495000	3.184260000	-0.910195000
1	0.783969000	3.185849000	0.897982000
6	-4.283926000	1.082976000	0.023132000
1	-4.529615000	1.312549000	1.068663000
1	-4.115047000	2.007886000	-0.539062000

1	-5.102188000	0.521066000	-0.439217000
13.	<b>1-AuCl</b> , T. E. = -1243.87934		
6	1.669040000	-3.448692000	0.075374000
7	2.812510000	-2.834841000	-0.252884000
6	2.608383000	-1.465979000	-0.275975000
6	1.238190000	-1.199071000	-0.001723000
7	0.708835000	-2.512221000	0.256025000
1	3.366382000	-0.806965000	-0.680535000
1	1.545686000	-4.514518000	0.224560000
6	0.488420000	0.000007000	0.000079000
6	1.238162000	1.199098000	0.001810000
6	2.608398000	1.466028000	0.275848000
7	2.812478000	2.834896000	0.252822000
6	1.668941000	3.448738000	-0.075221000
7	0.708736000	2.512248000	-0.255792000
1	3.366480000	0.807010000	0.680247000
1	1.545538000	4.514568000	-0.224340000
6	-0.651358000	2.871937000	-0.647237000
1	-1.364368000	2.643498000	0.158245000
1	-0.666154000	3.947880000	-0.873606000
1	-0.953712000	2.297818000	-1.533137000
6	4.083368000	3.502127000	0.504737000
1	4.462527000	3.219353000	1.496899000
1	4.819213000	3.215928000	-0.260580000
1	3.934257000	4.588347000	0.477023000
6	-0.651132000	-2.871901000	0.647916000
1	-0.666040000	-3.948004000	0.873508000
1	-0.952921000	-2.298392000	1.534407000
1	-1.364489000	-2.642714000	-0.157049000
6	4.083354000	-3.502062000	-0.505055000
1	3.934309000	-4.588283000	-0.477040000
1	4.462193000	-3.219498000	-1.497401000
1	4.819420000	-3.215650000	0.259969000

79	-1.559352000	-0.000019000	-0.000035000
17	-3.923530000	-0.000048000	-0.000170000

14. **1-(AuCl)<sub>2</sub>**, T. E. = -1840.10824

6	-2.141627000	1.681919000	-2.724902000
7	-2.019741000	2.842726000	-2.066897000
6	-1.170540000	2.651916000	-0.985755000
6	-0.777036000	1.311184000	-0.956020000
7	-1.403065000	0.747719000	-2.099334000
1	-1.024444000	3.438676000	-0.258183000
1	-2.725830000	1.523459000	-3.623625000
6	0.000008000	0.520821000	0.000047000
6	0.777118000	1.310954000	0.956246000
6	1.170735000	2.651647000	0.986219000
7	2.020010000	2.842174000	2.067352000
6	2.141758000	1.681252000	2.725180000
7	1.403131000	0.747222000	2.099435000
1	1.024699000	3.438549000	0.258789000
1	2.725953000	1.522580000	3.623871000
6	1.383514000	-0.658649000	2.505380000
1	1.824063000	-1.268862000	1.700538000
1	1.961313000	-0.759517000	3.432875000
1	0.340691000	-0.981969000	2.652413000
6	2.651554000	4.103971000	2.443043000
1	3.245095000	4.486631000	1.601708000
1	1.887012000	4.842864000	2.720798000
1	3.315731000	3.933488000	3.298464000
6	-1.383543000	-0.658072000	-2.505558000
1	-1.961328000	-0.758713000	-3.433086000
1	-0.340744000	-0.981453000	-2.652623000
1	-1.824167000	-1.268399000	-1.700843000
6	-2.651076000	4.104672000	-2.442436000
1	-3.315383000	3.934376000	-3.297792000
1	-3.244451000	4.487378000	-1.601006000

1	-1.886427000	4.843445000	-2.720217000
79	-1.429981000	-0.764223000	0.890650000
79	1.429899000	-0.764179000	-0.890766000
17	-3.069879000	-2.122321000	1.866824000
17	3.069710000	-2.122231000	-1.867148000
15.	<b>2-AuCl</b> , T. E. = -1209.41446		
6	0.001564000	-0.399894000	-0.001362000
6	-1.238528000	-1.088098000	-0.027938000
6	-1.465323000	-2.420898000	0.482786000
6	-2.708808000	-2.990906000	0.505545000
7	-3.817811000	-2.338030000	0.012695000
6	-3.661203000	-1.047479000	-0.459978000
6	-2.443935000	-0.431864000	-0.475804000
1	-2.892809000	-3.981598000	0.922567000
1	-4.570381000	-0.563423000	-0.817090000
6	1.244487000	-1.082717000	0.025975000
6	1.476235000	-2.416480000	-0.480101000
6	2.721951000	-2.981628000	-0.501581000
7	3.828741000	-2.322508000	-0.012073000
6	3.667384000	-1.030701000	0.455677000
6	2.447697000	-0.419918000	0.470150000
1	2.909524000	-3.973252000	-0.914783000
1	4.574939000	-0.541629000	0.810082000
1	-2.364887000	0.594726000	-0.839927000
1	-0.644839000	-2.984017000	0.926929000
1	0.657750000	-2.984631000	-0.921507000
1	2.364815000	0.607732000	0.830447000
6	5.165743000	-2.904119000	-0.136666000
1	5.788579000	-2.573680000	0.705092000
1	5.092440000	-3.998747000	-0.107141000
1	5.648523000	-2.601254000	-1.080088000
6	-5.152466000	-2.924662000	0.139056000
1	-5.633662000	-2.626613000	1.084820000

1	-5.778604000	-2.593209000	-0.699789000
1	-5.075747000	-4.018971000	0.105397000
79	-0.003854000	1.643706000	-0.000437000
17	-0.010379000	3.990924000	0.002978000

16. **2-(AuCl)<sub>2</sub>**, T. E. = -1805.62197

6	-0.011066000	0.661159000	-0.027135000
6	1.202198000	1.360301000	-0.365002000
6	1.537379000	2.669398000	0.122265000
6	2.747128000	3.253719000	-0.149126000
7	3.693549000	2.629980000	-0.923887000
6	3.420143000	1.367547000	-1.409476000
6	2.235312000	0.740144000	-1.146987000
1	3.026546000	4.231220000	0.244341000
1	4.204696000	0.912332000	-2.013449000
6	-1.224120000	1.368703000	0.289945000
6	-1.555120000	2.667696000	-0.226816000
6	-2.761903000	3.263284000	0.033018000
7	-3.710015000	2.660927000	0.822494000
6	-3.442489000	1.406764000	1.332746000
6	-2.261391000	0.767844000	1.081919000
1	-3.037071000	4.233672000	-0.380584000
1	-4.229112000	0.967503000	1.945741000
1	2.058479000	-0.258673000	-1.550099000
1	0.849840000	3.204373000	0.776766000
1	-0.865515000	3.186384000	-0.892175000
1	-2.089742000	-0.223205000	1.505629000
6	-5.027319000	3.274553000	1.020246000
1	-5.396487000	3.030596000	2.024652000
1	-4.938029000	4.364435000	0.934091000
1	-5.747567000	2.909646000	0.271595000
6	5.014802000	3.232181000	-1.130844000
1	5.731045000	2.878090000	-0.373264000
1	5.384879000	2.966139000	-2.129284000

1	4.931599000	4.324039000	-1.066570000
79	-0.593544000	-0.996732000	-1.256235000
79	0.598592000	-0.922299000	1.291701000
17	-1.315619000	-2.406182000	-2.956144000
17	1.350419000	-2.203183000	3.077440000
17.	<b>3-AuCl</b> , T. E. = -1226.65556		
6	1.340514000	3.516975000	0.516525000
7	1.128700000	2.229425000	0.849311000
6	0.070022000	1.689788000	0.065487000
6	-0.337690000	2.765197000	-0.727276000
7	0.456817000	3.862034000	-0.436942000
1	2.095744000	4.168600000	0.940310000
1	-1.074591000	2.794054000	-1.520618000
6	-0.320156000	0.306260000	0.083661000
6	-3.410706000	-1.781839000	-0.115758000
6	-2.101510000	-1.419764000	-0.094233000
6	-1.669408000	-0.038583000	0.069612000
6	-2.786555000	0.879481000	0.256496000
6	-4.084450000	0.466587000	0.240085000
7	-4.438296000	-0.854223000	0.018844000
1	-3.729965000	-2.815565000	-0.252934000
1	-1.333456000	-2.186257000	-0.216505000
1	-2.597646000	1.937862000	0.441739000
1	-4.918144000	1.152646000	0.397487000
6	1.868748000	1.507972000	1.883132000
1	1.187382000	1.229005000	2.697928000
1	2.278383000	0.581767000	1.444026000
1	2.670982000	2.154403000	2.260485000
6	0.387501000	5.164369000	-1.095203000
1	1.135537000	5.832594000	-0.652159000
1	0.595071000	5.053660000	-2.168313000
1	-0.611400000	5.600348000	-0.958106000
6	-5.821185000	-1.293542000	0.157952000



1	-6.496977000	-0.488891000	-0.162639000
1	-5.996440000	-2.165945000	-0.486738000
1	-6.066373000	-1.568746000	1.199246000
79	1.191951000	-1.061759000	-0.100989000
17	2.932732000	-2.625800000	-0.320380000
18.	<b>3-(AuCl)<sub>2</sub></b> , T. E. = -1822.86561		
6	2.044275000	3.104663000	1.442467000
7	1.641779000	1.836918000	1.237891000
6	0.482741000	1.827506000	0.422633000
6	0.223692000	3.177776000	0.183525000
7	1.198217000	3.934516000	0.812313000
1	2.905770000	3.405385000	2.026892000
1	-0.524714000	3.640900000	-0.446841000
6	-0.134748000	0.622531000	-0.116079000
6	-3.331195000	-0.228034000	-1.920118000
6	-2.033809000	-0.257866000	-1.502120000
6	-1.508321000	0.691221000	-0.552224000
6	-2.479615000	1.658356000	-0.103788000
6	-3.778028000	1.636967000	-0.536546000
7	-4.225169000	0.718131000	-1.453289000
1	-3.729263000	-0.937693000	-2.645097000
1	-1.359377000	-1.016175000	-1.904631000
1	-2.210749000	2.397109000	0.650507000
1	-4.526415000	2.340204000	-0.169693000
6	2.379914000	0.672398000	1.733362000
1	1.709723000	0.040184000	2.334983000
1	2.731724000	0.080177000	0.873530000
1	3.225465000	1.029454000	2.334828000
6	1.288256000	5.393224000	0.798838000
1	2.192242000	5.702419000	1.336321000
1	1.347297000	5.751518000	-0.237572000
1	0.408388000	5.829880000	1.290727000
6	-5.635268000	0.659810000	-1.846065000

1	-6.094913000	1.645297000	-1.701462000
1	-5.711076000	0.391388000	-2.908206000
1	-6.182225000	-0.084351000	-1.246053000
79	-0.408231000	-1.000536000	1.272167000
79	1.233493000	-0.501441000	-1.242573000
17	2.786134000	-1.581026000	-2.610381000
17	-0.714886000	-2.580023000	2.955800000

19. **4-AuCl**, T. E. = -1242.69568

6	2.333437000	-2.925759000	-0.020823000
7	1.061525000	-2.467077000	0.003859000
6	1.076572000	-1.070593000	0.041067000
6	2.475874000	-0.699206000	0.045593000
7	3.208324000	-1.882496000	-0.011037000
1	2.623680000	-3.969784000	-0.006984000
6	2.475826000	0.699250000	-0.045239000
6	1.076512000	1.070546000	-0.040405000
7	3.208227000	1.882604000	0.010884000
7	1.061385000	2.467030000	-0.003692000
6	0.156802000	-0.000039000	0.000439000
6	2.333272000	2.925803000	0.020618000
1	2.623418000	3.969849000	0.006421000
6	-0.146220000	-3.290139000	0.023234000
1	-0.871629000	-2.866874000	-0.684825000
1	0.108790000	-4.319379000	-0.259183000
1	-0.598237000	-3.272396000	1.024744000
6	4.656282000	-2.012992000	-0.035890000
1	4.927081000	-3.074817000	-0.084628000
1	5.066958000	-1.501149000	-0.919875000
1	5.095310000	-1.574285000	0.873194000
6	4.656191000	2.013236000	0.034759000
1	5.094662000	1.574757000	-0.874706000
1	4.926917000	3.075078000	0.083546000
1	5.067503000	1.501261000	0.918367000

6	-0.146425000	3.289975000	-0.021795000
1	-0.604420000	3.264434000	-1.020387000
1	-0.867754000	2.872598000	0.693861000
1	0.110530000	4.321329000	0.250973000
79	-1.856127000	-0.000029000	0.000049000
17	-4.207868000	0.000042000	-0.000814000

20. **4-(AuCl)<sub>2</sub>**, T. E. = -1838.91415

6	2.642751000	0.199101000	2.920683000
7	1.370266000	0.161792000	2.467734000
6	1.390651000	0.059246000	1.086344000
6	2.762119000	0.031451000	0.707055000
7	3.510932000	0.125825000	1.874632000
1	2.936551000	0.264928000	3.961608000
6	2.761901000	-0.036240000	-0.707114000
6	1.390313000	-0.062562000	-1.086073000
7	3.510342000	-0.130101000	-1.874963000
7	1.369496000	-0.164129000	-2.467530000
6	0.443909000	-0.001180000	0.000293000
6	2.641833000	-0.202128000	-2.920824000
1	2.935312000	-0.267564000	-3.961866000
6	0.152178000	0.218295000	3.278456000
1	-0.431034000	-0.697793000	3.107918000
1	0.423886000	0.312531000	4.336412000
1	-0.448727000	1.080088000	2.953999000
6	4.963775000	0.141009000	1.995596000
1	5.237659000	0.218127000	3.054429000
1	5.388197000	-0.787110000	1.586208000
1	5.378978000	1.005834000	1.457983000
6	4.963142000	-0.145923000	-1.996356000
1	5.378115000	-1.011254000	-1.459385000
1	5.236681000	-0.222506000	-3.055318000
1	5.388100000	0.781762000	-1.586539000
6	0.151179000	-0.219524000	-3.278020000

1	-0.448025000	-1.083888000	-2.957345000
1	-0.433638000	0.694722000	-3.103108000
1	0.422665000	-0.308175000	-4.336521000
79	-1.048100000	1.479552000	-0.080525000
79	-1.051273000	-1.478388000	0.080566000
17	-2.496675000	3.304453000	-0.169267000
17	-2.504736000	-3.299431000	0.169205000

21. **5-AuCl**, T. E. = -1208.25303

6	3.286982000	-1.665231000	-0.007311000
6	2.288850000	-0.723587000	-0.001398000
6	0.882001000	-1.121010000	-0.004599000
6	0.608566000	-2.515421000	-0.016048000
6	1.643424000	-3.412946000	-0.022571000
7	2.971754000	-3.000146000	-0.021754000
1	4.353004000	-1.433030000	-0.003453000
1	-0.423820000	-2.868853000	-0.022887000
1	1.496735000	-4.492333000	-0.031272000
6	2.288851000	0.723584000	0.001391000
6	3.286984000	1.665226000	0.007297000
7	2.971759000	3.000141000	0.021722000
6	1.643429000	3.412943000	0.022541000
6	0.608570000	2.515420000	0.016027000
6	0.882003000	1.121008000	0.004591000
1	4.353006000	1.433021000	0.003441000
1	1.496742000	4.492331000	0.031234000
1	-0.423816000	2.868853000	0.022861000
6	0.009319000	0.000000000	0.000003000
6	4.028395000	-4.016262000	0.037518000
1	3.833795000	-4.801119000	-0.706258000
1	4.993962000	-3.549334000	-0.190367000
1	4.077474000	-4.471133000	1.038839000
6	4.028391000	4.016270000	-0.037467000
1	4.994012000	3.549251000	0.190001000

1	4.077215000	4.471473000	-1.038648000
1	3.833999000	4.800882000	0.706625000
79	-1.993147000	0.000001000	0.000003000
17	-4.336638000	0.000001000	0.000000000

22. **5-(AuCl)<sub>2</sub>**, T. E. = -1804.45985

6	3.684621000	-1.651528000	-0.184211000
6	2.678245000	-0.720025000	-0.079842000
6	1.285050000	-1.126835000	-0.127329000
6	1.013311000	-2.508400000	-0.284526000
6	2.054180000	-3.394831000	-0.384792000
7	3.377120000	-2.976064000	-0.338883000
1	4.748187000	-1.412646000	-0.154321000
1	-0.015144000	-2.868675000	-0.328109000
1	1.912006000	-4.467695000	-0.506181000
6	2.678246000	0.720044000	0.079701000
6	3.684623000	1.651544000	0.184076000
7	3.377123000	2.976080000	0.338761000
6	2.054184000	3.394851000	0.384657000
6	1.013314000	2.508420000	0.284383000
6	1.285050000	1.126856000	0.127189000
1	4.748189000	1.412662000	0.154190000
1	1.912010000	4.467714000	0.506046000
1	-0.015140000	2.868698000	0.327969000
6	0.404499000	0.000010000	-0.000069000
6	4.440950000	-3.988169000	-0.397135000
1	4.253682000	-4.675766000	-1.232723000
1	5.404851000	-3.491982000	-0.558858000
1	4.482352000	-4.558921000	0.542529000
6	4.440968000	3.988177000	0.396894000
1	5.404799000	3.492038000	0.559181000
1	4.482704000	4.558506000	-0.543014000
1	4.253431000	4.676157000	1.232104000
79	-1.212716000	0.162790000	-1.368336000

79	-1.212588000	-0.162797000	1.368391000
17	-2.398912000	0.399995000	-3.348169000
17	-2.398503000	-0.400015000	3.348389000
23.	<b>6-AuCl</b> , T. E. = -1225.47985		
6	-3.690766000	-0.837170000	-0.008748000
6	-2.507394000	-0.137382000	-0.012204000
6	-1.191186000	-0.864333000	-0.015537000
6	-1.270028000	-2.279741000	-0.017324000
6	-2.484012000	-2.916761000	-0.015141000
7	-3.685643000	-2.204077000	-0.013458000
1	-4.677328000	-0.371148000	-0.003346000
1	-0.352673000	-2.871116000	-0.022102000
1	-2.591471000	-4.000083000	-0.016345000
6	-2.128492000	1.232284000	-0.015195000
6	-0.714613000	1.278954000	-0.014956000
6	-0.080646000	0.007294000	-0.016799000
7	-0.367371000	2.630400000	0.003822000
7	-2.586967000	2.541156000	0.003778000
6	-1.507200000	3.364358000	0.012782000
1	-1.557723000	4.447255000	0.023143000
6	-4.942190000	-2.954978000	0.037443000
1	-5.784435000	-2.265891000	-0.098153000
1	-4.967417000	-3.703495000	-0.767774000
1	-5.052382000	-3.466340000	1.006418000
6	0.999658000	3.161501000	-0.016218000
1	1.678258000	2.316879000	0.184387000
1	1.233976000	3.578076000	-1.005642000
1	1.116412000	3.930916000	0.758202000
6	-3.977051000	2.982402000	0.020429000
1	-4.479663000	2.602299000	0.921360000
1	-4.012117000	4.078379000	0.025642000
1	-4.497424000	2.610615000	-0.873709000
79	1.895777000	-0.351732000	-0.001740000

17 4.213000000 -0.711202000 0.024424000

24. **6-(AuCl)<sub>2</sub>**, T. E. = -1821.69053

6 -4.057012000 -0.000040000 -0.740536000

6 -2.859346000 -0.002224000 -0.059484000

6 -1.573518000 -0.006222000 -0.803681000

6 -1.660076000 -0.008069000 -2.212593000

6 -2.884911000 -0.005104000 -2.833408000

7 -4.070519000 0.001485000 -2.105353000

1 -5.034597000 0.001964000 -0.257771000

1 -0.751435000 -0.008975000 -2.816185000

1 -3.004964000 -0.005675000 -3.915174000

6 -2.468308000 0.003642000 1.312308000

6 -1.066517000 0.001278000 1.360631000

6 -0.433180000 -0.003822000 0.069116000

7 -0.708905000 0.003893000 2.700549000

7 -2.926984000 0.007124000 2.623814000

6 -1.842812000 0.007289000 3.439288000

1 -1.883939000 0.010621000 4.522667000

6 -5.342007000 -0.040225000 -2.838371000

1 -6.170531000 0.122045000 -2.139189000

1 -5.360622000 0.753109000 -3.598363000

1 -5.471903000 -1.016278000 -3.329296000

6 0.665650000 0.003755000 3.209736000

1 1.183922000 -0.889655000 2.833734000

1 1.185134000 0.895088000 2.830454000

1 0.645042000 0.005804000 4.305979000

6 -4.316767000 0.008807000 3.071637000

1 -4.828729000 -0.891535000 2.704033000

1 -4.344973000 0.013735000 4.167537000

1 -4.829048000 0.905664000 2.696082000

79 1.117924000 1.408474000 -0.228589000

79 1.125101000 -1.407700000 -0.220288000

17 2.412418000 3.332903000 -0.390154000

17 2.437309000 -3.321077000 -0.370091000