Supporting information

Coordination Modes in Dithizonato-Metal Complexes

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Optimized Cartesian coordinates (Å)

DFT calculations: PW91 (Perdew-Wang 1991)[1] GGA (Generalized Gradient Approximation) functional as implemented in the ADF (Amsterdam Density Functional) 2013 program system[2] with the STO (Slater Type Orbital) QZ4P (quadruple-ζ plus 4 polarization functions) basis set on Sb and Sn and TZ2P (triple-ζ plus 2 polarization functions) on the other atoms. Geometries of the neutral complexes were optimized in gas phase.

1 H_2Dz

C	0.000010000	0.631554000	0.000028000
N	-1.111096000	-0.156210000	0.000040000
N	1.111173000	-0.156120000	0.000037000
N	2.212746000	0.527284000	0.000020000
N	-2.212728000	0.527105000	0.000025000
H	-2.082860000	1.566374000	0.000021000
H	2.082809000	1.566515000	0.000013000
C	3.479062000	-0.048660000	0.000008000
C	4.589352000	0.808868000	-0.000004000
C	3.654111000	-1.439421000	0.000005000
H	4.437419000	1.887524000	-0.000001000
H	2.778152000	-2.081594000	0.000013000
C	5.871050000	0.272796000	-0.000020000
C	4.942565000	-1.958273000	-0.000013000
H	6.730758000	0.939133000	-0.000030000
H	5.082760000	-3.037344000	-0.000018000
C	6.054442000	-1.111136000	-0.000025000
H	7.058961000	-1.528631000	-0.000039000
C	-3.479027000	-0.048892000	0.000011000
C	-4.589283000	0.808706000	-0.000001000
C	-3.654177000	-1.439667000	0.000005000
H	-4.437265000	1.887355000	0.000004000
H	-2.778336000	-2.082034000	0.000014000
C	-5.871012000	0.272724000	-0.000021000
C	-4.942669000	-1.958425000	-0.000016000
H	-6.730682000	0.939117000	-0.000030000
H	-5.082840000	-3.037526000	-0.000022000
C	-6.054498000	-1.111208000	-0.000029000
H	-7.059067000	-1.528579000	-0.000045000
S	-0.000006000	2.349213000	-0.000022000

2 HCl

H	-1.223126000	0.006360000	-4.829467000
Cl	-1.247028000	-0.687918000	-3.739911000

3 $CuCl_2$

Cu	-0.000001000	0.000000000	0.000000000

Cl	0.000000000	0.000000000	-2.069112000
Cl	0.000000000	0.000000000	2.069112000

4 Cu(HDz)Cl

Cu	-1.866589000	-1.498785000	0.000190000
Cl	-3.291687000	-3.051606000	0.000143000
S	0.343236000	-1.758995000	0.000280000
N	1.871247000	0.518417000	0.000139000
N	2.878517000	-0.316849000	0.000046000
H	2.680091000	-1.326297000	0.000004000
N	-0.338151000	0.900811000	0.000159000
N	-1.532302000	0.426914000	0.000124000
C	0.656486000	-0.018717000	0.000205000
C	4.209182000	0.102461000	-0.000023000
C	-2.589921000	1.364431000	-0.000004000
C	5.208974000	-0.880508000	-0.000171000
H	4.933085000	-1.934893000	-0.000230000
C	-3.904511000	0.878299000	-0.000236000
H	-4.087106000	-0.197168000	-0.000376000
C	-2.354170000	2.749836000	0.000112000
H	-1.329616000	3.109058000	0.000286000
C	-3.430036000	3.625992000	0.000046000
H	-3.245718000	4.698672000	0.000163000
C	5.890614000	1.822556000	-0.000021000
H	6.156887000	2.877749000	0.000040000
C	-4.973542000	1.768084000	-0.000309000
H	-5.990591000	1.382615000	-0.000478000
C	4.548465000	1.461559000	0.000048000
H	3.757576000	2.206117000	0.000162000
C	-4.742537000	3.143076000	-0.000156000
H	-5.579630000	3.838205000	-0.000196000
C	6.894188000	0.850282000	-0.000169000
H	7.941238000	1.144911000	-0.000223000
C	6.546006000	-0.501373000	-0.000246000
H	7.319097000	-1.266488000	-0.000365000

5 $Cu(HDz)_2$

Cu	0.011581000	-0.000449000	0.004546000
S	-1.363044000	-1.407164000	1.149129000
N	-2.075182000	-0.791050000	3.713000000
N	-2.703174000	-1.941496000	3.659417000
H	-2.655878000	-2.472093000	2.777194000
N	-0.843291000	0.787292000	2.709149000
N	-0.269608000	1.230268000	1.651498000
C	-1.430906000	-0.434865000	2.605120000
C	-3.443384000	-2.451886000	4.723309000
C	0.327591000	2.510444000	1.827500000
C	-4.084083000	-3.687443000	4.549089000
H	-3.992558000	-4.214046000	3.599299000

C	0.164388000	3.482268000	0.836224000
H	-0.416240000	3.247296000	-0.051100000
C	1.046023000	2.807524000	2.992714000
H	1.154052000	2.039017000	3.754096000
C	1.608053000	4.068536000	3.153369000
H	2.175484000	4.293251000	4.054494000
C	-4.308464000	-2.318774000	6.965701000
H	-4.397231000	-1.782967000	7.908801000
C	0.718872000	4.747138000	1.013513000
H	0.574300000	5.506406000	0.247646000
C	-3.555943000	-1.762226000	5.938045000
H	-3.054761000	-0.805251000	6.050728000
C	1.446517000	5.042899000	2.165709000
H	1.884712000	6.030396000	2.296850000
C	-4.949411000	-3.549374000	6.800666000
H	-5.536738000	-3.974458000	7.611490000
C	-4.832578000	-4.228876000	5.587155000
H	-5.328160000	-5.186888000	5.445872000
S	1.380545000	1.405611000	-1.147924000
N	2.068405000	0.791787000	-3.718970000
N	2.687930000	1.947005000	-3.674162000
H	2.639801000	2.482762000	-2.795262000
N	0.854206000	-0.791716000	-2.702236000
N	0.290952000	-1.235056000	-1.639547000
C	1.436519000	0.433797000	-2.604868000
C	3.412188000	2.460639000	-4.747720000
C	-0.301941000	-2.518530000	-1.806327000
C	4.044628000	3.702044000	-4.584446000
H	3.960452000	4.230242000	-3.634843000
C	-0.125023000	-3.486170000	-0.813130000
H	0.463346000	-3.245522000	0.067565000
C	-1.030331000	-2.822684000	-2.963360000
H	-1.148425000	-2.057572000	-3.726818000
C	-1.588648000	-4.086587000	-3.113953000
H	-2.163481000	-4.317087000	-4.008819000
C	4.251713000	2.329218000	-7.000167000
H	4.333945000	1.791381000	-7.942704000
C	-0.675714000	-4.754012000	-0.980444000
H	-0.520381000	-5.510022000	-0.213464000
C	3.516095000	1.769040000	-5.961956000
H	3.021984000	0.807609000	-6.066432000
C	-1.413559000	-5.056691000	-2.124365000
H	-1.849236000	-6.046390000	-2.247587000
C	4.883724000	3.565681000	-6.846140000
H	5.457399000	3.993868000	-7.665207000
C	4.775536000	4.247185000	-5.632923000
H	5.264579000	5.209811000	-5.500007000

6 $SbCl_3$

Sb	0.000134000	-0.000048000	-0.582226000

Cl	-1.321296000	1.576777000	0.581240000
Cl	2.025734000	0.355866000	0.582401000
Cl	-0.704743000	-1.932510000	0.581619000

7 $Sb(HDz)Cl_2$

Sb	1.910377000	-1.344564000	-0.331955000
Cl	1.678818000	-3.781609000	-0.323835000
S	-0.564671000	-1.371468000	-0.167700000
Cl	2.535002000	-1.258522000	1.979434000
N	-3.189431000	-0.134391000	-0.081711000
H	-2.937666000	-1.128747000	-0.106856000
N	1.150904000	1.067936000	-0.043794000
N	-0.086757000	1.371338000	-0.060558000
N	-2.241474000	0.768652000	-0.067160000
C	-5.479821000	-0.843769000	-0.060440000
H	-5.137941000	-1.877929000	-0.097107000
C	-4.545109000	0.200237000	-0.047421000
C	-0.985799000	0.354334000	-0.093284000
C	-4.968531000	1.533682000	0.002491000
H	-4.226461000	2.326436000	0.013759000
C	-6.837850000	-0.550775000	-0.023048000
H	-7.560543000	-1.362998000	-0.030999000
C	3.392769000	1.907893000	0.230211000
H	3.697998000	0.912754000	0.546225000
C	2.049193000	2.155549000	-0.083074000
C	4.319580000	2.944658000	0.187434000
H	5.358618000	2.746336000	0.441135000
C	-7.270086000	0.775055000	0.027102000
H	-8.332847000	1.002430000	0.057590000
C	-6.329927000	1.808367000	0.039731000
H	-6.661644000	2.843704000	0.080064000
C	1.643131000	3.453299000	-0.441583000
H	0.599451000	3.628148000	-0.688346000
C	3.917625000	4.230557000	-0.169837000
H	4.644125000	5.039194000	-0.206619000
C	2.577271000	4.478590000	-0.481958000
H	2.262080000	5.480607000	-0.766290000

8 $Sb(HDz)_2Cl$

Sb	-0.155979000	-0.499598000	-0.779199000
S	-2.902206000	-0.853496000	-0.904312000
N	-4.490470000	1.102880000	0.147211000
N	-5.371425000	0.143944000	0.198537000
H	-5.052350000	-0.799097000	-0.089031000
N	-2.442714000	1.815929000	-0.328978000
N	-1.228296000	1.652352000	-0.702532000
C	-3.280499000	0.749543000	-0.310086000
C	-6.687409000	0.341549000	0.611842000

C	-0.459975000	2.844531000	-0.762255000
C	-7.539427000	-0.771217000	0.652351000
H	-7.158891000	-1.753509000	0.374185000
C	0.497320000	2.968049000	-1.774525000
H	0.623957000	2.165417000	-2.497337000
C	-0.657941000	3.888856000	0.150579000
H	-1.407259000	3.770889000	0.928867000
C	0.107930000	5.043450000	0.047280000
H	-0.038290000	5.849706000	0.763432000
C	-8.487044000	1.753624000	1.358935000
H	-8.857470000	2.739413000	1.633223000
C	1.252394000	4.133299000	-1.875487000
H	1.985752000	4.228885000	-2.673322000
C	-7.161613000	1.611313000	0.966889000
H	-6.483899000	2.459060000	0.924850000
C	1.063207000	5.172038000	-0.965115000
H	1.656258000	6.081095000	-1.043142000
C	-9.343722000	0.650728000	1.400628000
H	-10.379580000	0.774086000	1.707254000
C	-8.862534000	-0.610911000	1.045616000
H	-9.520687000	-1.476090000	1.074390000
S	2.169303000	0.663474000	-0.436624000
N	4.469062000	-0.574992000	0.306304000
N	4.922389000	0.654482000	0.357989000
H	4.259706000	1.423308000	0.181425000
N	2.800692000	-2.028460000	0.001244000
N	1.569227000	-2.285741000	-0.211308000
C	3.188698000	-0.726824000	-0.014845000
C	6.240095000	0.960258000	0.690569000
C	1.222489000	-3.652186000	-0.253157000
C	6.609110000	2.312465000	0.743373000
H	5.868005000	3.083012000	0.531636000
C	-0.138245000	-3.984013000	-0.191920000
H	-0.884752000	-3.200778000	-0.063070000
C	2.181869000	-4.672002000	-0.373709000
H	3.232283000	-4.398113000	-0.423540000
C	1.774155000	-5.997426000	-0.433979000
H	2.519519000	-6.783748000	-0.534129000
C	8.483102000	0.323987000	1.288491000
H	9.213996000	-0.453069000	1.502792000
C	-0.536073000	-5.315507000	-0.250375000
H	-1.593823000	-5.562544000	-0.194174000
C	7.181222000	-0.040743000	0.964730000
H	6.873885000	-1.081528000	0.921043000
C	0.416373000	-6.326867000	-0.374055000
H	0.103902000	-7.367746000	-0.424354000
C	8.859444000	1.668407000	1.342515000
H	9.880582000	1.941857000	1.597572000
C	7.914897000	2.659038000	1.068249000
H	8.195302000	3.709318000	1.108764000
Cl	-0.474120000	-0.554766000	1.604871000

9 $Sb(HDz)_3$

Sb	-0.363843000	0.124909000	0.675207000
S	1.196504000	-1.176981000	-0.880684000
S	-2.016334000	0.087115000	-1.285322000
S	0.687611000	2.207670000	-0.405510000
N	1.971472000	-3.774055000	-0.662726000
N	2.970707000	-3.391687000	-1.426847000
H	3.041365000	-2.398893000	-1.682015000
N	0.100807000	-3.351846000	0.494773000
N	-0.803882000	-2.531466000	0.860528000
N	-4.561238000	1.034206000	-1.395352000
N	-4.617718000	0.347573000	-2.515613000
H	-3.797368000	-0.201711000	-2.798715000
N	-3.479147000	1.752043000	0.425479000
N	-2.411927000	1.829082000	1.118958000
N	3.350092000	2.761524000	-0.519567000
N	3.041645000	3.325149000	-1.666414000
H	2.075359000	3.237275000	-2.007009000
N	2.810956000	1.583060000	1.308028000
N	1.932980000	0.958060000	1.988131000
C	1.083618000	-2.858280000	-0.314026000
C	3.957099000	-4.272280000	-1.867085000
C	4.996423000	-3.760643000	-2.658168000
H	5.015674000	-2.699368000	-2.905410000
C	5.994630000	-4.610423000	-3.120934000
H	6.797461000	-4.207040000	-3.734325000
C	5.968283000	-5.969223000	-2.802712000
H	6.749907000	-6.632448000	-3.166549000
C	4.929598000	-6.470445000	-2.013973000
H	4.901583000	-7.528920000	-1.762112000
C	3.922878000	-5.634813000	-1.542949000
H	3.108909000	-6.011193000	-0.930153000
C	-1.777537000	-3.046960000	1.738311000
C	-1.646242000	-4.279380000	2.401737000
H	-0.755070000	-4.875823000	2.225111000
C	-2.645961000	-4.704347000	3.266444000
H	-2.541001000	-5.657044000	3.782683000
C	-3.782204000	-3.916735000	3.482032000
H	-4.560840000	-4.256767000	4.162220000
C	-3.913383000	-2.694305000	2.823478000
H	-4.796337000	-2.078373000	2.980491000
C	-2.915821000	-2.258657000	1.957678000
H	-3.021131000	-1.318264000	1.420395000
C	-3.424274000	1.006111000	-0.717226000
C	-5.749209000	0.333734000	-3.329965000
C	-6.891557000	1.080713000	-3.013506000
H	-6.895510000	1.682702000	-2.109400000
C	-7.989431000	1.036202000	-3.865483000
H	-8.875767000	1.617755000	-3.619533000

C	-7.965735000	0.259878000	-5.026794000
H	-8.829941000	0.233642000	-5.686571000
C	-6.823566000	-0.480837000	-5.334702000
H	-6.791840000	-1.088991000	-6.235872000
C	-5.717234000	-0.448164000	-4.494188000
H	-4.824691000	-1.026098000	-4.733193000
C	-2.513841000	2.564427000	2.317081000
C	-3.737210000	3.021122000	2.840411000
H	-4.652270000	2.808985000	2.293726000
C	-3.752996000	3.726861000	4.035760000
H	-4.700536000	4.076501000	4.441429000
C	-2.561920000	3.988425000	4.722215000
H	-2.582893000	4.541715000	5.659172000
C	-1.348658000	3.537997000	4.202179000
H	-0.417204000	3.742550000	4.726333000
C	-1.321902000	2.827714000	3.006314000
H	-0.375590000	2.495185000	2.582672000
C	2.376100000	2.171410000	0.153067000
C	3.985509000	3.974526000	-2.459779000
C	3.566429000	4.501430000	-3.690140000
H	2.527500000	4.390335000	-4.000210000
C	4.478087000	5.161969000	-4.505152000
H	4.145994000	5.568112000	-5.457858000
C	5.808102000	5.304245000	-4.106145000
H	6.519495000	5.822700000	-4.745160000
C	6.217380000	4.776723000	-2.879022000
H	7.252229000	4.884993000	-2.560208000
C	5.318909000	4.112737000	-2.051585000
H	5.623299000	3.699728000	-1.094338000
C	2.393395000	0.337996000	3.164995000
C	3.752492000	0.221679000	3.506501000
H	4.498692000	0.630617000	2.830799000
C	4.111090000	-0.413894000	4.687421000
H	5.163575000	-0.509806000	4.948450000
C	3.132225000	-0.936034000	5.540564000
H	3.423226000	-1.434414000	6.463276000
C	1.783902000	-0.820303000	5.203278000
H	1.017047000	-1.223920000	5.860926000
C	1.414268000	-0.189346000	4.020019000
H	0.365411000	-0.087448000	3.748084000

10 $SnCl_2$

Sn	0.000000000	0.629022000	0.000000000
Cl	1.816170000	-0.923124000	0.000000000
Cl	-1.816170000	-0.923120000	0.000000000

11 $Sn(HDz)_2Cl_2$

Sn	0.000897000	1.889099000	0.091279000
S	2.490525000	1.598623000	-0.181860000

S	-2.490594000	1.619222000	0.357418000
Cl	0.381686000	3.438717000	1.904233000
Cl	-0.356947000	3.526517000	-1.648367000
N	0.240687000	0.107831000	-1.495784000
N	1.356880000	-0.508098000	-1.582249000
N	3.532308000	-0.724186000	-1.149312000
N	4.639821000	-0.297293000	-0.601045000
H	4.609084000	0.568816000	-0.046804000
N	-0.265448000	0.032574000	1.586702000
N	-1.381262000	-0.589742000	1.610321000
N	-3.541675000	-0.785266000	1.087228000
N	-4.628683000	-0.325154000	0.524280000
H	-4.578783000	0.580023000	0.037403000
C	2.456295000	0.042344000	-1.001438000
C	5.842794000	-0.998789000	-0.681968000
C	6.957659000	-0.471708000	-0.015211000
H	6.863638000	0.457420000	0.546702000
C	8.175727000	-1.138044000	-0.077934000
H	9.038775000	-0.725361000	0.439829000
C	8.291104000	-2.326724000	-0.800802000
H	9.245434000	-2.846566000	-0.849624000
C	7.174605000	-2.843298000	-1.462929000
H	7.259954000	-3.767966000	-2.030127000
C	5.949162000	-2.189937000	-1.410850000
H	5.072957000	-2.577700000	-1.922353000
C	-0.843446000	-0.535239000	-2.148291000
C	-0.908562000	-1.933096000	-2.246447000
H	-0.115223000	-2.529490000	-1.802937000
C	-1.981702000	-2.525499000	-2.899767000
H	-2.040132000	-3.609936000	-2.964875000
C	-2.984259000	-1.735159000	-3.468508000
H	-3.821678000	-2.203820000	-3.981687000
C	-2.908468000	-0.345289000	-3.377584000
H	-3.677159000	0.274770000	-3.834558000
C	-1.847490000	0.261145000	-2.711153000
H	-1.764503000	1.344383000	-2.654409000
C	-2.469301000	-0.000559000	1.044552000
C	-5.821209000	-1.047754000	0.475174000
C	-5.946911000	-2.299516000	1.090397000
H	-5.094387000	-2.718787000	1.616829000
C	-7.160599000	-2.972277000	1.012265000
H	-7.261034000	-3.944721000	1.491087000
C	-8.246237000	-2.415924000	0.331785000
H	-9.191197000	-2.951465000	0.278222000
C	-8.112010000	-1.167175000	-0.277128000
H	-8.951182000	-0.723327000	-0.808042000
C	-6.905712000	-0.480388000	-0.208767000
H	-6.797163000	0.495402000	-0.681877000
C	0.810143000	-0.647333000	2.214389000
C	0.872508000	-2.048677000	2.240406000
H	0.081698000	-2.619934000	1.760833000

C	1.940404000	-2.675652000	2.869565000
H	1.997176000	-3.762244000	2.878774000
C	2.940120000	-1.917393000	3.485309000
H	3.773328000	-2.413497000	3.979271000
C	2.867005000	-0.524438000	3.465924000
H	3.633851000	0.070092000	3.958342000
C	1.811593000	0.116970000	2.824588000
H	1.731244000	1.201562000	2.822005000

12 $Sn(HDz)_3Cl$

Sn	-0.208943000	-0.920558000	-0.677273000
S	0.286531000	-2.689386000	1.035119000
S	-2.611196000	-1.731133000	-0.548618000
Cl	0.460175000	-2.226600000	-2.646454000
N	1.312772000	-1.304213000	3.438070000
N	2.281054000	-1.816755000	2.791923000
N	3.021441000	-2.910699000	0.964719000
N	2.841227000	-3.499293000	-0.193290000
H	1.882498000	-3.553580000	-0.567542000
N	-1.445285000	0.581731000	-2.073848000
N	-2.713144000	0.663844000	-1.940269000
N	-4.671496000	-0.059255000	-1.162842000
N	-5.390923000	-0.913252000	-0.483029000
H	-4.908797000	-1.685858000	-0.004404000
C	1.975418000	-2.431057000	1.601994000
C	3.892704000	-4.066687000	-0.913131000
C	3.605183000	-4.639922000	-2.160657000
H	2.584856000	-4.613338000	-2.541698000
C	4.625722000	-5.221647000	-2.903580000
H	4.395385000	-5.664174000	-3.870429000
C	5.934974000	-5.237445000	-2.418085000
H	6.731114000	-5.695387000	-3.000976000
C	6.212806000	-4.660905000	-1.176402000
H	7.230375000	-4.669657000	-0.789193000
C	5.203859000	-4.076075000	-0.418668000
H	5.405595000	-3.628467000	0.550251000
C	1.685052000	-0.697163000	4.655267000
C	2.992958000	-0.669225000	5.173515000
H	3.788873000	-1.145174000	4.606231000
C	3.240878000	-0.040797000	6.386355000
H	4.253589000	-0.019880000	6.786796000
C	2.199772000	0.565955000	7.098786000
H	2.403371000	1.056885000	8.048993000
C	0.902143000	0.539415000	6.587746000
H	0.089145000	1.011810000	7.135670000
C	0.645440000	-0.089196000	5.373323000
H	-0.357028000	-0.117892000	4.951270000
C	-3.366003000	-0.301380000	-1.239665000
C	-6.771563000	-0.784483000	-0.331214000
C	-7.483374000	0.249782000	-0.952119000

H	-6.946227000	0.969838000	-1.562634000
C	-8.859739000	0.324948000	-0.774173000
H	-9.414913000	1.126214000	-1.257731000
C	-9.533040000	-0.613834000	0.011484000
H	-10.610745000	-0.546097000	0.142429000
C	-8.815136000	-1.641187000	0.625938000
H	-9.329168000	-2.378465000	1.238429000
C	-7.438384000	-1.731268000	0.458803000
H	-6.874317000	-2.532704000	0.935691000
C	-0.862691000	1.627903000	-2.836754000
C	-1.411799000	2.918261000	-2.838607000
H	-2.292684000	3.116250000	-2.233225000
C	-0.820850000	3.914527000	-3.605397000
H	-1.238410000	4.919129000	-3.597014000
C	0.306453000	3.631418000	-4.381538000
H	0.764577000	4.414366000	-4.982740000
C	0.842009000	2.343436000	-4.384065000
H	1.708907000	2.113269000	-5.000237000
C	0.269649000	1.339940000	-3.607743000
H	0.663287000	0.326419000	-3.621092000
S	1.945314000	0.383963000	-0.786129000
N	-0.500219000	0.888003000	0.865355000
N	0.224322000	1.932259000	0.743772000
N	1.970758000	3.024569000	-0.115861000
N	3.042764000	3.065644000	-0.864163000
H	3.316646000	2.213750000	-1.371682000
C	1.347670000	1.855791000	-0.020919000
C	3.774398000	4.234819000	-1.073268000
C	4.877889000	4.174807000	-1.936326000
H	5.137973000	3.232475000	-2.417756000
C	5.633271000	5.318202000	-2.168606000
H	6.489273000	5.267182000	-2.837832000
C	5.297800000	6.521709000	-1.547133000
H	5.890811000	7.415163000	-1.729387000
C	4.197045000	6.571382000	-0.687670000
H	3.932167000	7.506763000	-0.198767000
C	3.430540000	5.437804000	-0.444220000
H	2.573071000	5.460202000	0.221970000
C	-1.642595000	1.039032000	1.692872000
C	-2.340558000	2.252932000	1.758744000
H	-1.995882000	3.093007000	1.160820000
C	-3.458805000	2.355624000	2.577351000
H	-4.011589000	3.292035000	2.619320000
C	-3.875162000	1.261886000	3.341209000
H	-4.750420000	1.348164000	3.982426000
C	-3.165992000	0.061512000	3.282339000
H	-3.474973000	-0.786283000	3.891034000
C	-2.054457000	-0.061409000	2.453203000
H	-1.465565000	-0.976751000	2.424074000

13 $Sn(HDz)_4$

Sn	-0.132528000	-0.067898000	-0.776187000
S	-0.093143000	-2.561216000	-1.300746000
S	0.952417000	0.337015000	-3.040106000
N	-2.904515000	-3.274015000	-0.833453000
N	-2.201250000	-3.723243000	0.126009000
N	-0.174077000	-3.873248000	1.111695000
N	1.122667000	-3.652679000	1.144704000
H	1.535649000	-3.145450000	0.349654000
N	2.380625000	2.923913000	-3.136278000
N	3.189744000	2.003276000	-2.801533000
N	3.576119000	-0.173226000	-2.386052000
N	3.207420000	-1.430138000	-2.300728000
H	2.221913000	-1.662105000	-2.492455000
C	-0.859395000	-3.420848000	0.084722000
C	1.918156000	-3.987945000	2.236021000
C	3.292159000	-3.706144000	2.164627000
H	3.707723000	-3.261673000	1.260063000
C	4.117229000	-4.011710000	3.241647000
H	5.182070000	-3.797888000	3.171171000
C	3.590562000	-4.596849000	4.395414000
H	4.239232000	-4.838604000	5.234842000
C	2.223336000	-4.878499000	4.456290000
H	1.803320000	-5.338151000	5.349040000
C	1.382620000	-4.579468000	3.389291000
H	0.317616000	-4.790179000	3.427367000
C	-4.270541000	-3.612194000	-0.766905000
C	-4.852355000	-4.424724000	0.223472000
H	-4.216013000	-4.829189000	1.006770000
C	-6.213281000	-4.693972000	0.180749000
H	-6.663720000	-5.324472000	0.945983000
C	-7.011230000	-4.162014000	-0.839095000
H	-8.077732000	-4.378894000	-0.864494000
C	-6.437259000	-3.356459000	-1.822490000
H	-7.053747000	-2.940466000	-2.616920000
C	-5.073507000	-3.083843000	-1.788989000
H	-4.599883000	-2.459371000	-2.544033000
C	2.669429000	0.735656000	-2.669605000
C	4.093123000	-2.443662000	-1.939513000
C	5.414000000	-2.167322000	-1.559941000
H	5.757464000	-1.136892000	-1.560751000
C	6.251350000	-3.216457000	-1.195038000
H	7.277756000	-2.998593000	-0.904939000
C	5.793331000	-4.536392000	-1.197559000
H	6.456078000	-5.349120000	-0.908771000
C	4.476683000	-4.803187000	-1.577261000
H	4.105468000	-5.825686000	-1.585208000
C	3.626714000	-3.767657000	-1.949300000
H	2.598763000	-3.973133000	-2.245939000
C	2.977866000	4.193662000	-3.283241000
C	4.334658000	4.476596000	-3.042908000

H	4.985030000	3.670303000	-2.713177000
C	4.813622000	5.765599000	-3.231625000
H	5.864050000	5.984245000	-3.045679000
C	3.957347000	6.786883000	-3.659881000
H	4.342014000	7.794854000	-3.805649000
C	2.611137000	6.509692000	-3.898338000
H	1.941198000	7.300532000	-4.230045000
C	2.123426000	5.220368000	-3.709946000
H	1.077805000	4.977264000	-3.887372000
S	1.886447000	-0.222069000	0.740873000
N	0.276834000	2.195971000	-0.030791000
N	0.959385000	2.375514000	1.033164000
N	2.275815000	1.636368000	2.685699000
N	2.940999000	0.668053000	3.265188000
H	2.919946000	-0.265920000	2.832165000
C	1.694280000	1.343887000	1.527189000
C	3.606553000	0.822369000	4.481076000
C	4.188312000	-0.316850000	5.056580000
H	4.092668000	-1.283904000	4.561978000
C	4.871267000	-0.203620000	6.261432000
H	5.319511000	-1.089735000	6.705853000
C	4.977999000	1.033727000	6.898666000
H	5.513886000	1.119204000	7.841594000
C	4.392082000	2.161834000	6.318370000
H	4.472692000	3.128952000	6.810311000
C	3.706168000	2.068365000	5.112588000
H	3.249076000	2.936662000	4.646795000
C	-0.515839000	3.299575000	-0.431941000
C	-0.995993000	4.231933000	0.502064000
H	-0.740862000	4.104491000	1.550610000
C	-1.793821000	5.283078000	0.072611000
H	-2.177768000	5.997420000	0.798025000
C	-2.112089000	5.421089000	-1.281933000
H	-2.738601000	6.247630000	-1.612304000
C	-1.624357000	4.497931000	-2.206380000
H	-1.855694000	4.607925000	-3.264272000
C	-0.830259000	3.433295000	-1.789292000
H	-0.400373000	2.737611000	-2.508445000
S	-1.682145000	-0.094907000	1.259738000
N	-2.284196000	0.368727000	-1.646794000
N	-3.239689000	0.721772000	-0.876413000
N	-4.153074000	1.043312000	1.128438000
N	-4.100595000	0.975700000	2.432474000
H	-3.240272000	0.616919000	2.868793000
C	-3.083614000	0.604215000	0.467494000
C	-5.149514000	1.387372000	3.255130000
C	-4.966180000	1.310261000	4.642666000
H	-4.023334000	0.940138000	5.044600000
C	-5.989504000	1.706713000	5.495113000
H	-5.843665000	1.644959000	6.571132000
C	-7.195176000	2.179717000	4.974741000

H	-7.995641000	2.488278000	5.643412000
C	-7.368519000	2.252272000	3.590226000
H	-8.307713000	2.617691000	3.179519000
C	-6.355737000	1.859804000	2.723191000
H	-6.476590000	1.905592000	1.645036000
C	-2.569701000	0.471568000	-3.034932000
C	-3.389017000	1.494626000	-3.531428000
H	-3.796857000	2.225191000	-2.837849000
C	-3.650202000	1.559810000	-4.894381000
H	-4.275192000	2.361075000	-5.284233000
C	-3.112182000	0.605468000	-5.762878000
H	-3.319577000	0.661724000	-6.829770000
C	-2.312502000	-0.419487000	-5.259271000
H	-1.904435000	-1.174199000	-5.927792000
C	-2.034208000	-0.490166000	-3.897055000
H	-1.449130000	-1.311199000	-3.487351000

14 H_2

H	0.000000000	0.000000000	0.374311000
H	0.000000000	0.000000000	-0.374311000

Crystallographic supplementary material

Complex **1:** Bond lengths [Å] and angles [°]

Cu(1)-N(1)#1	2.0282(8)
Cu(1)-N(1)	2.0282(8)
Cu(1)-S(1)	2.2890(3)
Cu(1)-S(1)#1	2.2890(3)
S(1)-C(1)	1.7391(10)
N(1)-N(2)	1.2792(12)
N(1)-C(8)	1.4365(13)
N(2)-C(1)	1.3694(13)
N(3)-N(4)	1.3184(12)
N(3)-C(1)	1.3217(13)
N(4)-C(2)	1.3990(12)
N(4)-HN4	0.8800
C(2)-C(7)	1.3916(14)
C(2)-C(3)	1.3922(14)
C(3)-C(4)	1.3871(15)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3918(17)
C(4)-H(4)	0.9500
C(5)-C(6)	1.3847(18)
C(5)-H(5)	0.9500
C(6)-C(7)	1.3883(15)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-C(9)	1.3896(14)
C(8)-C(13)	1.3948(14)
C(9)-C(10)	1.3914(15)
C(9)-H(9)	0.9500
C(10)-C(11)	1.3872(17)
C(10)-H(10)	0.9500
C(11)-C(12)	1.3916(17)
C(11)-H(11)	0.9500
C(12)-C(13)	1.3891(15)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500

N(1)#1-Cu(1)-N(1)	180.00(5)
N(1)#1-Cu(1)-S(1)	95.93(2)
N(1)-Cu(1)-S(1)	84.07(2)
N(1)#1-Cu(1)-S(1)#1	84.07(2)
N(1)-Cu(1)-S(1)#1	95.93(2)
S(1)-Cu(1)-S(1)#1	180.0
C(1)-S(1)-Cu(1)	94.74(3)
N(2)-N(1)-C(8)	111.28(8)
N(2)-N(1)-Cu(1)	121.52(7)
C(8)-N(1)-Cu(1)	126.96(6)
N(1)-N(2)-C(1)	115.92(8)
N(4)-N(3)-C(1)	116.45(8)
N(3)-N(4)-C(2)	120.76(8)
N(3)-N(4)-HN4	119.6
C(2)-N(4)-HN4	119.6
N(3)-C(1)-N(2)	110.89(8)
N(3)-C(1)-S(1)	125.91(8)
N(2)-C(1)-S(1)	123.18(7)
C(7)-C(2)-C(3)	120.55(9)
C(7)-C(2)-N(4)	118.19(9)
C(3)-C(2)-N(4)	121.27(9)
C(4)-C(3)-C(2)	119.52(10)
C(4)-C(3)-H(3)	120.2
C(2)-C(3)-H(3)	120.2
C(3)-C(4)-C(5)	120.20(10)
C(3)-C(4)-H(4)	119.9
C(5)-C(4)-H(4)	119.9
C(6)-C(5)-C(4)	119.85(10)
C(6)-C(5)-H(5)	120.1
C(4)-C(5)-H(5)	120.1
C(5)-C(6)-C(7)	120.55(10)
C(5)-C(6)-H(6)	119.7
C(7)-C(6)-H(6)	119.7
C(6)-C(7)-C(2)	119.31(10)
C(6)-C(7)-H(7)	120.3
C(2)-C(7)-H(7)	120.3
C(9)-C(8)-C(13)	120.90(9)
C(9)-C(8)-N(1)	118.82(9)

C(13)-C(8)-N(1)	120.24(9)
C(8)-C(9)-C(10)	119.12(10)
C(8)-C(9)-H(9)	120.4
C(10)-C(9)-H(9)	120.4
C(11)-C(10)-C(9)	120.54(10)
C(11)-C(10)-H(10)	119.7
C(9)-C(10)-H(10)	119.7
C(10)-C(11)-C(12)	119.88(10)
C(10)-C(11)-H(11)	120.1
C(12)-C(11)-H(11)	120.1
C(13)-C(12)-C(11)	120.27(10)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(8)	119.26(10)
C(12)-C(13)-H(13)	120.4
C(8)-C(13)-H(13)	120.4

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z

Complex **2:** Bond lengths [Å] and angles [°]

Sb(1)-N(1)	2.3642(12)
Sb(1)-Cl(2)	2.3749(4)
Sb(1)-S(1)	2.4297(4)
Sb(1)-Cl(1)	2.5460(4)
S(1)-C(1)	1.7620(14)
N(1)-N(2)	1.2760(17)
N(1)-C(8)	1.4180(18)
N(2)-C(1)	1.3629(18)
N(3)-N(4)	1.3096(18)
N(3)-C(1)	1.3186(18)
N(4)-C(2)	1.4082(18)
N(4)-HN4	0.8800
C(2)-C(3)	1.392(2)
C(2)-C(7)	1.395(2)
C(3)-C(4)	1.386(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.381(2)

C(4)-H(4)	0.9500
C(5)-C(6)	1.392(2)
C(5)-H(5)	0.9500
C(6)-C(7)	1.389(2)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-C(9)	1.394(2)
C(8)-C(13)	1.395(2)
C(9)-C(10)	1.389(2)
C(9)-H(9)	0.9500
C(10)-C(11)	1.385(2)
C(10)-H(10)	0.9500
C(11)-C(12)	1.388(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.385(2)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500

N(1)-Sb(1)-Cl(2)	83.31(3)
N(1)-Sb(1)-S(1)	75.64(3)
Cl(2)-Sb(1)-S(1)	97.476(14)
N(1)-Sb(1)-Cl(1)	157.36(3)
Cl(2)-Sb(1)-Cl(1)	92.329(14)
S(1)-Sb(1)-Cl(1)	82.970(13)
C(1)-S(1)-Sb(1)	100.15(5)
N(2)-N(1)-C(8)	116.07(12)
N(2)-N(1)-Sb(1)	122.07(9)
C(8)-N(1)-Sb(1)	121.08(9)
N(1)-N(2)-C(1)	116.46(12)
N(4)-N(3)-C(1)	119.35(12)
N(3)-N(4)-C(2)	119.83(12)
N(3)-N(4)-HN4	120.1
C(2)-N(4)-HN4	120.1
N(3)-C(1)-N(2)	112.09(12)
N(3)-C(1)-S(1)	123.67(11)
N(2)-C(1)-S(1)	124.24(11)
C(3)-C(2)-C(7)	120.91(13)
C(3)-C(2)-N(4)	117.75(13)
C(7)-C(2)-N(4)	121.30(13)

C(4)-C(3)-C(2)	119.28(14)
C(4)-C(3)-H(3)	120.4
C(2)-C(3)-H(3)	120.4
C(5)-C(4)-C(3)	120.76(15)
C(5)-C(4)-H(4)	119.6
C(3)-C(4)-H(4)	119.6
C(4)-C(5)-C(6)	119.47(14)
C(4)-C(5)-H(5)	120.3
C(6)-C(5)-H(5)	120.3
C(7)-C(6)-C(5)	120.98(14)
C(7)-C(6)-H(6)	119.5
C(5)-C(6)-H(6)	119.5
C(6)-C(7)-C(2)	118.58(14)
C(6)-C(7)-H(7)	120.7
C(2)-C(7)-H(7)	120.7
C(9)-C(8)-C(13)	120.31(13)
C(9)-C(8)-N(1)	117.56(12)
C(13)-C(8)-N(1)	122.13(13)
C(10)-C(9)-C(8)	119.77(14)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(11)-C(10)-C(9)	119.90(15)
C(11)-C(10)-H(10)	120.0
C(9)-C(10)-H(10)	120.0
C(10)-C(11)-C(12)	120.23(14)
C(10)-C(11)-H(11)	119.9
C(12)-C(11)-H(11)	119.9
C(13)-C(12)-C(11)	120.49(15)
C(13)-C(12)-H(12)	119.8
C(11)-C(12)-H(12)	119.8
C(12)-C(13)-C(8)	119.26(15)
C(12)-C(13)-H(13)	120.4
C(8)-C(13)-H(13)	120.4

Symmetry transformations used to generate equivalent atoms:

Complex **3:** Bond lengths [Å] and angles [°]

Sn(1)-N(5)	2.317(3)
Sn(1)-N(1)	2.331(3)
Sn(1)-Cl(2)	2.3918(10)
Sn(1)-Cl(1)	2.3958(10)
Sn(1)-S(1)	2.4626(11)
Sn(1)-S(2)	2.4676(11)
Sn(2)-N(13)	2.331(3)
Sn(2)-N(9)	2.335(3)
Sn(2)-Cl(4)	2.3964(10)
Sn(2)-Cl(3)	2.4022(10)
Sn(2)-S(3)	2.4612(10)
Sn(2)-S(4)	2.4630(10)
S(1)-C(1)	1.755(4)
S(2)-C(14)	1.751(4)
S(3)-C(27)	1.758(4)
S(4)-C(40)	1.752(4)
N(1)-N(2)	1.288(4)
N(1)-C(8)	1.426(5)
N(2)-C(1)	1.364(5)
N(3)-N(4)	1.306(4)
N(3)-C(1)	1.321(5)
N(4)-C(2)	1.411(5)
N(4)-HN4	0.8800
N(5)-N(6)	1.274(4)
N(5)-C(21)	1.431(4)
N(6)-C(14)	1.373(5)
N(7)-N(8)	1.306(4)
N(7)-C(14)	1.323(5)
N(8)-C(15)	1.407(5)
N(8)-H(8)	0.8800
N(9)-N(10)	1.284(4)
N(9)-C(34)	1.428(4)
N(10)-C(27)	1.360(5)
N(11)-C(27)	1.320(4)
N(11)-N(12)	1.314(4)
N(12)-C(28)	1.405(5)

N(12)-HN12	0.8800
N(13)-N(14)	1.278(4)
N(13)-C(47)	1.421(5)
N(14)-C(40)	1.363(5)
N(15)-N(16)	1.306(5)
N(15)-C(40)	1.325(5)
N(16)-C(41)	1.409(5)
N(16)-HN16	0.8800
C(2)-C(3)	1.384(5)
C(2)-C(7)	1.388(6)
C(3)-C(4)	1.383(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.384(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.394(7)
C(5)-H(5)	0.9500
C(6)-C(7)	1.381(6)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-C(13)	1.392(5)
C(8)-C(9)	1.390(5)
C(9)-C(10)	1.390(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.384(6)
C(10)-H(10)	0.9500
C(11)-C(12)	1.391(6)
C(11)-H(11)	0.9500
C(12)-C(13)	1.385(5)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
C(15)-C(20)	1.383(5)
C(15)-C(16)	1.397(5)
C(16)-C(17)	1.384(6)
C(16)-H(16)	0.9500
C(17)-C(18)	1.387(7)
C(17)-H(17)	0.9500
C(18)-C(19)	1.382(6)
C(18)-H(18)	0.9500
C(19)-C(20)	1.389(6)

C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-C(22)	1.387(5)
C(21)-C(26)	1.388(5)
C(22)-C(23)	1.385(5)
C(22)-H(22)	0.9500
C(23)-C(24)	1.388(6)
C(23)-H(23)	0.9500
C(24)-C(25)	1.382(6)
C(24)-H(24)	0.9500
C(25)-C(26)	1.386(5)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(28)-C(29)	1.387(5)
C(28)-C(33)	1.390(5)
C(29)-C(30)	1.384(6)
C(29)-H(29)	0.9500
C(30)-C(31)	1.385(6)
C(30)-H(30)	0.9500
C(31)-C(32)	1.384(6)
C(31)-H(31)	0.9500
C(32)-C(33)	1.388(6)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(35)	1.392(5)
C(34)-C(39)	1.396(5)
C(35)-C(36)	1.390(5)
C(35)-H(35)	0.9500
C(36)-C(37)	1.394(6)
C(36)-H(36)	0.9500
C(37)-C(38)	1.384(6)
C(37)-H(37)	0.9500
C(38)-C(39)	1.391(5)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(41)-C(46)	1.381(5)
C(41)-C(42)	1.388(5)
C(42)-C(43)	1.394(6)
C(42)-H(42)	0.9500

C(43)-C(44)	1.385(7)
C(43)-H(43)	0.9500
C(44)-C(45)	1.393(7)
C(44)-H(44)	0.9500
C(45)-C(46)	1.380(6)
C(45)-H(45)	0.9500
C(46)-H(46)	0.9500
C(47)-C(52)	1.390(5)
C(47)-C(48)	1.401(5)
C(48)-C(49)	1.381(5)
C(48)-H(48)	0.9500
C(49)-C(50)	1.392(5)
C(49)-H(49)	0.9500
C(50)-C(51)	1.387(6)
C(50)-H(50)	0.9500
C(51)-C(52)	1.383(5)
C(51)-H(51)	0.9500
C(52)-H(52)	0.9500

N(5)-Sn(1)-N(1)	78.34(11)
N(5)-Sn(1)-Cl(2)	163.71(8)
N(1)-Sn(1)-Cl(2)	96.31(8)
N(5)-Sn(1)-Cl(1)	93.19(8)
N(1)-Sn(1)-Cl(1)	162.68(8)
Cl(2)-Sn(1)-Cl(1)	95.70(4)
N(5)-Sn(1)-S(1)	97.08(8)
N(1)-Sn(1)-S(1)	76.01(8)
Cl(2)-Sn(1)-S(1)	96.51(4)
Cl(1)-Sn(1)-S(1)	90.27(4)
N(5)-Sn(1)-S(2)	75.92(8)
N(1)-Sn(1)-S(2)	95.56(8)
Cl(2)-Sn(1)-S(2)	89.44(4)
Cl(1)-Sn(1)-S(2)	96.98(4)
S(1)-Sn(1)-S(2)	170.13(3)
N(13)-Sn(2)-N(9)	77.89(11)
N(13)-Sn(2)-Cl(4)	163.32(8)
N(9)-Sn(2)-Cl(4)	95.15(8)
N(13)-Sn(2)-Cl(3)	93.76(8)
N(9)-Sn(2)-Cl(3)	162.42(8)

Cl(4)-Sn(2)-Cl(3)	96.74(4)
N(13)-Sn(2)-S(3)	97.51(8)
N(9)-Sn(2)-S(3)	75.87(8)
Cl(4)-Sn(2)-S(3)	95.40(4)
Cl(3)-Sn(2)-S(3)	90.13(4)
N(13)-Sn(2)-S(4)	76.08(8)
N(9)-Sn(2)-S(4)	95.67(8)
Cl(4)-Sn(2)-S(4)	89.73(4)
Cl(3)-Sn(2)-S(4)	97.29(4)
S(3)-Sn(2)-S(4)	170.44(3)
C(1)-S(1)-Sn(1)	95.68(13)
C(14)-S(2)-Sn(1)	95.24(12)
C(27)-S(3)-Sn(2)	95.50(12)
C(40)-S(4)-Sn(2)	95.25(13)
N(2)-N(1)-C(8)	113.5(3)
N(2)-N(1)-Sn(1)	117.9(2)
C(8)-N(1)-Sn(1)	123.6(2)
N(1)-N(2)-C(1)	116.8(3)
N(4)-N(3)-C(1)	117.2(3)
N(3)-N(4)-C(2)	121.1(3)
N(3)-N(4)-HN4	119.4
C(2)-N(4)-HN4	119.4
N(6)-N(5)-C(21)	114.2(3)
N(6)-N(5)-Sn(1)	118.1(2)
C(21)-N(5)-Sn(1)	122.7(2)
N(5)-N(6)-C(14)	117.2(3)
N(8)-N(7)-C(14)	116.7(3)
N(7)-N(8)-C(15)	121.4(3)
N(7)-N(8)-H(8)	119.3
C(15)-N(8)-H(8)	119.3
N(10)-N(9)-C(34)	113.9(3)
N(10)-N(9)-Sn(2)	117.7(2)
C(34)-N(9)-Sn(2)	124.2(2)
N(9)-N(10)-C(27)	117.2(3)
C(27)-N(11)-N(12)	117.2(3)
N(11)-N(12)-C(28)	121.3(3)
N(11)-N(12)-HN12	119.4
C(28)-N(12)-HN12	119.4
N(14)-N(13)-C(47)	114.5(3)

N(14)-N(13)-Sn(2)	117.3(2)
C(47)-N(13)-Sn(2)	123.4(2)
N(13)-N(14)-C(40)	117.5(3)
N(16)-N(15)-C(40)	117.7(3)
N(15)-N(16)-C(41)	121.0(3)
N(15)-N(16)-HN16	119.5
C(41)-N(16)-HN16	119.5
N(3)-C(1)-N(2)	111.4(3)
N(3)-C(1)-S(1)	124.2(3)
N(2)-C(1)-S(1)	124.3(3)
C(3)-C(2)-C(7)	121.5(4)
C(3)-C(2)-N(4)	117.3(3)
C(7)-C(2)-N(4)	121.2(4)
C(2)-C(3)-C(4)	118.7(4)
C(2)-C(3)-H(3)	120.6
C(4)-C(3)-H(3)	120.6
C(5)-C(4)-C(3)	120.9(4)
C(5)-C(4)-H(4)	119.6
C(3)-C(4)-H(4)	119.6
C(4)-C(5)-C(6)	119.6(4)
C(4)-C(5)-H(5)	120.2
C(6)-C(5)-H(5)	120.2
C(7)-C(6)-C(5)	120.3(4)
C(7)-C(6)-H(6)	119.9
C(5)-C(6)-H(6)	119.9
C(6)-C(7)-C(2)	119.1(4)
C(6)-C(7)-H(7)	120.5
C(2)-C(7)-H(7)	120.5
C(13)-C(8)-C(9)	120.6(3)
C(13)-C(8)-N(1)	121.4(3)
C(9)-C(8)-N(1)	117.9(3)
C(10)-C(9)-C(8)	119.4(4)
C(10)-C(9)-H(9)	120.3
C(8)-C(9)-H(9)	120.3
C(11)-C(10)-C(9)	120.2(4)
C(11)-C(10)-H(10)	119.9
C(9)-C(10)-H(10)	119.9
C(10)-C(11)-C(12)	120.1(4)
C(10)-C(11)-H(11)	120.0

C(12)-C(11)-H(11)	120.0
C(13)-C(12)-C(11)	120.2(4)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(8)	119.4(3)
C(12)-C(13)-H(13)	120.3
C(8)-C(13)-H(13)	120.3
N(7)-C(14)-N(6)	111.6(3)
N(7)-C(14)-S(2)	124.8(3)
N(6)-C(14)-S(2)	123.6(3)
C(20)-C(15)-C(16)	121.0(4)
C(20)-C(15)-N(8)	117.6(3)
C(16)-C(15)-N(8)	121.4(3)
C(17)-C(16)-C(15)	118.6(4)
C(17)-C(16)-H(16)	120.7
C(15)-C(16)-H(16)	120.7
C(16)-C(17)-C(18)	120.6(4)
C(16)-C(17)-H(17)	119.7
C(18)-C(17)-H(17)	119.7
C(19)-C(18)-C(17)	120.4(4)
C(19)-C(18)-H(18)	119.8
C(17)-C(18)-H(18)	119.8
C(18)-C(19)-C(20)	119.8(4)
C(18)-C(19)-H(19)	120.1
C(20)-C(19)-H(19)	120.1
C(15)-C(20)-C(19)	119.6(4)
C(15)-C(20)-H(20)	120.2
C(19)-C(20)-H(20)	120.2
C(22)-C(21)-C(26)	120.7(3)
C(22)-C(21)-N(5)	121.0(3)
C(26)-C(21)-N(5)	118.3(3)
C(21)-C(22)-C(23)	119.5(4)
C(21)-C(22)-H(22)	120.3
C(23)-C(22)-H(22)	120.3
C(24)-C(23)-C(22)	120.2(4)
C(24)-C(23)-H(23)	119.9
C(22)-C(23)-H(23)	119.9
C(25)-C(24)-C(23)	119.9(4)
C(25)-C(24)-H(24)	120.1

C(23)-C(24)-H(24)	120.1
C(24)-C(25)-C(26)	120.5(4)
C(24)-C(25)-H(25)	119.7
C(26)-C(25)-H(25)	119.7
C(25)-C(26)-C(21)	119.3(3)
C(25)-C(26)-H(26)	120.4
C(21)-C(26)-H(26)	120.4
N(11)-C(27)-N(10)	112.1(3)
N(11)-C(27)-S(3)	123.9(3)
N(10)-C(27)-S(3)	124.0(3)
C(29)-C(28)-C(33)	121.5(3)
C(29)-C(28)-N(12)	117.4(3)
C(33)-C(28)-N(12)	121.1(3)
C(30)-C(29)-C(28)	118.9(3)
C(30)-C(29)-H(29)	120.5
C(28)-C(29)-H(29)	120.5
C(31)-C(30)-C(29)	120.2(4)
C(31)-C(30)-H(30)	119.9
C(29)-C(30)-H(30)	119.9
C(30)-C(31)-C(32)	120.5(4)
C(30)-C(31)-H(31)	119.8
C(32)-C(31)-H(31)	119.8
C(31)-C(32)-C(33)	120.2(4)
C(31)-C(32)-H(32)	119.9
C(33)-C(32)-H(32)	119.9
C(32)-C(33)-C(28)	118.7(4)
C(32)-C(33)-H(33)	120.6
C(28)-C(33)-H(33)	120.6
C(35)-C(34)-C(39)	121.3(3)
C(35)-C(34)-N(9)	121.6(3)
C(39)-C(34)-N(9)	117.1(3)
C(34)-C(35)-C(36)	119.1(4)
C(34)-C(35)-H(35)	120.5
C(36)-C(35)-H(35)	120.5
C(35)-C(36)-C(37)	119.9(4)
C(35)-C(36)-H(36)	120.0
C(37)-C(36)-H(36)	120.0
C(38)-C(37)-C(36)	120.6(4)
C(38)-C(37)-H(37)	119.7

C(36)-C(37)-H(37)	119.7
C(37)-C(38)-C(39)	120.1(4)
C(37)-C(38)-H(38)	120.0
C(39)-C(38)-H(38)	120.0
C(38)-C(39)-C(34)	119.0(4)
C(38)-C(39)-H(39)	120.5
C(34)-C(39)-H(39)	120.5
N(15)-C(40)-N(14)	111.4(3)
N(15)-C(40)-S(4)	124.4(3)
N(14)-C(40)-S(4)	124.2(3)
C(46)-C(41)-C(42)	121.1(4)
C(46)-C(41)-N(16)	118.1(3)
C(42)-C(41)-N(16)	120.8(4)
C(41)-C(42)-C(43)	118.6(4)
C(41)-C(42)-H(42)	120.7
C(43)-C(42)-H(42)	120.7
C(44)-C(43)-C(42)	120.8(4)
C(44)-C(43)-H(43)	119.6
C(42)-C(43)-H(43)	119.6
C(43)-C(44)-C(45)	119.4(4)
C(43)-C(44)-H(44)	120.3
C(45)-C(44)-H(44)	120.3
C(46)-C(45)-C(44)	120.3(4)
C(46)-C(45)-H(45)	119.9
C(44)-C(45)-H(45)	119.9
C(45)-C(46)-C(41)	119.8(4)
C(45)-C(46)-H(46)	120.1
C(41)-C(46)-H(46)	120.1
C(52)-C(47)-C(48)	120.0(3)
C(52)-C(47)-N(13)	118.7(3)
C(48)-C(47)-N(13)	121.3(3)
C(49)-C(48)-C(47)	119.8(3)
C(49)-C(48)-H(48)	120.1
C(47)-C(48)-H(48)	120.1
C(48)-C(49)-C(50)	120.2(3)
C(48)-C(49)-H(49)	119.9
C(50)-C(49)-H(49)	119.9
C(49)-C(50)-C(51)	119.7(3)
C(49)-C(50)-H(50)	120.2

C(51)-C(50)-H(50)	120.2
C(52)-C(51)-C(50)	120.7(3)
C(52)-C(51)-H(51)	119.6
C(50)-C(51)-H(51)	119.6
C(51)-C(52)-C(47)	119.6(3)
C(51)-C(52)-H(52)	120.2
C(47)-C(52)-H(52)	120.2

Symmetry transformations used to generate equivalent atoms:

[1] J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, C. Fiolhais, *Phys. Rev. B*, **1992**, *46*, 6671. *Erratum*: J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Perderson, D. J. Singh, C. Fiolhais, *Phys. Rev. B*, **1993**, *48*, 4978.

[2] *ADF2013*, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, The ADF program system uses methods described in: G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. F. Guerra, S. J. A. van Gisbergen, J. G. Snijders, T. Ziegler, *J. Comput. Chem*. **2001**, *22*, 931-967.