

Figure S1. Comparison of powder patterns for $[Co(NCS)_2(pia)_2]$ (1): calculated - blue, experimantal - red.



Figure S2. Comparison of powder patterns for [Ni(NCS)₂(pia)₂] (2): calculated - blue, experimantal - red.



Figure S3. Comparison of powder patterns for $[Cu(SCN)_2(pia)_2]$ (3): calculated - blue, experimantal - red.



Figure S4. TG/DTA curve for the compound [Co(NCS)₂(pia)₂] (1).



Figure S5. TG/DTA curve for the compound [Ni(NCS)₂(pia)₂] (2).



Figure S6. TG/DTA curve for the compound [Cu(SCN)₂(pia)₂] (**3**).

Table S1. The π - π interactions in compounds [Co(NCS)₂(pia)₂] (1) and [Ni(NCS)₂(pia)₂] (2).

Compound	$R(i) \rightarrow R(j)^{a}$	Dihedral angle between planes i and j (°)	Distance between ring centroids (Å)	Perpendicular distance between ring planes (Å)	Slippage (Å)
1	$R(1) \rightarrow R(1)^i$	0.00	3.740(1)	3.433	1.483
2	$R(1) \rightarrow R(1)^i$	0.02	3.743(1)	3.436	1.487

^a R(*i*) and R(*j*) denote the centroids of the *i*th and *j*th ring: R(1) N2, C2, C3, C4, C5, C6. Symmetry operator: (*i*) 1–*x*,1–*y*,–*z*.



Figure S7. Optimized structures of four isomers of $[Ni(NCS)_2(pia)_2]$ (2), with their relative energies (kcal mol⁻¹).



Figure S8. Optimized structures of three isomers of $[Cu(SNC)_2(pia)_2]$ (3), with their relative energies (kcal mol⁻¹). The cis,S isomer could not be calculated.



Figure S9. Optimized structures of four isomers of $[Zn(NCS)_2(pia)_2]$ (4), with their relative energies (kcal mol⁻¹).

Coordinates of Optimized Structures

[Co(NCS)2(pia)2] cis. N

CIS , 1			
Co	7.421413000	1.620501000	3.243006000
S	3.423167000	-0.860109000	2.737175000
0	6.130574000	3.347609000	2.619979000
Ν	5.889181000	0.471175000	2.948871000
Ν	7.869660000	1.932285000	1.197297000
Ν	5.215220000	4.348368000	0.799892000
С	4.844414000	-0.091280000	2.848238000
С	7.165356000	2.881922000	0.540450000
С	7.428818000	3.224137000	-0.788012000
С	8.436644000	2.545969000	-1.470972000
С	9.144661000	1.549511000	-0.798494000
С	8.835528000	1.278642000	0.532833000
С	6.126729000	3.530869000	1.395439000
Н	6.879992000	4.026795000	-1.278973000
Η	8.668193000	2.796070000	-2.505314000
Н	9.937409000	0.989612000	-1.291554000
Η	9.371410000	0.525507000	1.108183000
Н	5.030901000	4.271499000	-0.192094000
Н	4.451431000	4.667318000	1.386217000
S	11.423061000	-0.855461000	3.740819000
0	8.712683000	3.347388000	3.866275000
Ν	8.954041000	0.471532000	3.536802000
Ν	6.972251000	1.933006000	5.288293000
Ν	9.628252000	4.347079000	5.686851000
С	10.000338000	-0.088734000	3.633858000
С	7.676643000	2.882444000	5.945342000
С	7.412564000	3.225082000	7.273569000
С	6.403955000	2.547595000	7.956052000
С	5.695790000	1.551366000	7.283360000
С	6.005576000	1.280054000	5.952257000
С	8.716206000	3.530534000	5.090831000
Н	7.961545000	4.027532000	7.764692000
Н	6.172023000	2.797948000	8.990255000
Н	4.902471000	0.991976000	7.776083000
Н	5.469699000	0.527100000	5.376650000
Н	9.812148000	4.270020000	6.678904000
Н	10.392564000	4.665419000	5.100876000

[Co(NCS)2(pia)2]		
tran	s, N		
Co	1.839500000	2.799038000	4.793473000
Ν	1.078861000	4.166549000	5.989318000
0	0.309725000	3.068300000	3.213487000
S	0.700267000	5.739707000	8.291616000
Ν	2.654314000	4.316747000	3.555508000
Ν	0.233364000	3.562013000	0.996099000
С	0.912497000	4.831052000	6.963677000
С	2.002624000	4.520354000	2.392364000
С	2.407709000	5.491763000	1.474442000
С	3.530628000	6.264968000	1.766524000
С	4.205889000	6.043899000	2.966434000
С	3.730263000	5.062277000	3.834678000
С	0.793903000	3.649851000	2.231068000
Η	1.841065000	5.669408000	0.561526000
Н	3.865673000	7.034188000	1.072328000
Н	5.085101000	6.627095000	3.234844000
Η	4.214610000	4.857042000	4.788241000
Η	0.795400000	3.759018000	0.177298000
Н	-0.491427000	2.860377000	0.888246000
Ν	2.602390000	1.431110000	3.600614000
0	3.370711000	2.531311000	6.376294000
S	3.013282000	-0.151919000	1.311019000
Ν	1.025961000	1.280619000	6.032816000
Ν	3.434687000	2.052885000	8.597694000
С	2.783979000	0.763233000	2.631301000
С	1.675837000	1.081468000	7.197680000
С	1.271809000	0.110919000	8.117045000
С	0.151704000	-0.666384000	7.824553000
С	-0.522006000	-0.449778000	6.623032000
С	-0.047437000	0.531470000	5.753553000
С	2.882056000	1.955596000	7.359843000
Η	1.837541000	-0.062977000	9.031257000
Η	-0.182246000	-1.435501000	8.519727000
Н	-1.399022000	-1.036405000	6.354096000
Н	-0.530522000	0.733050000	4.798558000
Н	2.866452000	1.862412000	9.413919000
Н	4.156000000	2.758240000	8.705251000

[Co(NCS)2(pia)2]		
cis, S	5		
Co	-0.924031000	3.158352000	6.006068000
Ν	-4.503055000	3.588459000	8.210382000
0	-2.053257000	1.723929000	7.342857000
0	0.426475000	1.706197000	4.909025000
S	-2.365950000	4.875352000	6.825541000
S	0.250125000	4.908528000	4.891624000
Ν	0.374296000	2.708627000	7.598870000
Ν	-2.442913000	1.736042000	9.581560000
Ν	-2.122601000	2.249279000	4.531155000
Ν	0.828577000	1.400473000	2.693281000
С	-3.625631000	4.124521000	7.633104000
С	1.617965000	4.232896000	4.203404000
С	1.682413000	3.002967000	7.609692000
Н	2.077883000	3.453999000	6.701171000
С	2.492938000	2.742441000	8.714907000
Η	3.552005000	2.990483000	8.674677000
С	1.927115000	2.161682000	9.847950000
Η	2.536750000	1.938784000	10.722809000
С	0.564392000	1.858781000	9.840570000
Η	0.095265000	1.379505000	10.698777000
С	-0.177223000	2.145356000	8.696259000
С	-1.632759000	1.844790000	8.502207000
С	-3.460315000	2.332461000	4.492816000
Η	-3.929870000	2.865972000	5.317634000
С	-4.210125000	1.764727000	3.462443000
Η	-5.295192000	1.849714000	3.478088000
С	-3.550174000	1.092729000	2.435888000
Н	-4.109352000	0.631750000	1.622783000
С	-2.156943000	1.009581000	2.471078000
Η	-1.611020000	0.468842000	1.699087000
С	-1.479831000	1.598684000	3.536533000
С	0.002889000	1.563628000	3.753181000
Н	-3.430999000	1.904149000	9.366921000
Н	-2.119503000	2.110045000	10.467236000
Н	1.775597000	1.754782000	2.858311000
Н	0.458951000	1.567145000	1.763636000
Ν	2.569981000	3.745694000	3.706940000

[Co(NCS)2(pia)2]		
tran	s, S		
Co	1.847975000	2.802926000	4.803189000
S	0.642126000	4.633843000	5.903120000
0	0.419058000	2.874410000	3.180845000
Ν	0.824981000	3.979115000	8.666971000
Ν	2.667499000	4.202549000	3.526762000
Ν	0.210746000	3.452985000	0.985424000
С	0.728888000	4.268713000	7.527141000
С	2.046745000	4.366242000	2.337115000
С	2.480534000	5.301900000	1.395573000
С	3.602334000	6.073405000	1.683646000
С	4.253882000	5.885840000	2.904588000
С	3.753011000	4.944898000	3.798264000
С	0.847260000	3.491549000	2.186695000
Η	1.941802000	5.438613000	0.460018000
Η	3.961150000	6.813038000	0.969408000
Η	5.134641000	6.468192000	3.169357000
Η	4.214168000	4.769339000	4.768353000
Η	0.796889000	3.536811000	0.160556000
Η	-0.498299000	2.728263000	0.917900000
S	3.039146000	0.961644000	3.692698000
0	3.276481000	2.737205000	6.426756000
Ν	2.860797000	1.647066000	0.936119000
Ν	1.032602000	1.402420000	6.081876000
Ν	3.476980000	2.175233000	8.627600000
С	2.955049000	1.345653000	2.073221000
С	1.646788000	1.250883000	7.276241000
С	1.205893000	0.326754000	8.225703000
С	0.083133000	-0.444361000	7.940518000
С	-0.561788000	-0.268609000	6.714303000
С	-0.053485000	0.660316000	5.812733000
С	2.845905000	2.126695000	7.423747000
Н	1.739680000	0.198341000	9.165263000
Н	-0.281511000	-1.175094000	8.660795000
Н	-1.443123000	-0.851041000	6.451772000
Н	-0.508225000	0.824859000	4.837707000
Н	2.885792000	2.096960000	9.449417000
Н	4.183073000	2.902853000	8.693886000

[Ni(]	NCS)2(pia)2]		
cis, l	N		
Ni	7.408647000	1.690104000	3.237172000
S	3.369582000	-0.557467000	3.297290000
0	6.045993000	3.296063000	2.613893000
Ν	5.953960000	0.446225000	2.806793000
Ν	7.933457000	1.991017000	1.249209000
Ν	5.039604000	4.086954000	0.742545000
С	4.859605000	0.026938000	3.011505000
С	7.143110000	2.839972000	0.557960000
С	7.389549000	3.163753000	-0.776415000
С	8.477142000	2.573783000	-1.421427000
С	9.275321000	1.683154000	-0.709013000
С	8.973541000	1.419450000	0.628232000
С	6.029623000	3.412517000	1.381162000
Н	6.766902000	3.886072000	-1.302235000
Н	8.697621000	2.813382000	-2.460641000
Н	10.133024000	1.196245000	-1.169734000
Н	9.580290000	0.740418000	1.226887000
Н	4.882023000	3.952959000	-0.247894000
Н	4.238784000	4.350439000	1.307072000
S	11.441776000	-0.566620000	3.163546000
0	8.770585000	3.297457000	3.860956000
Ν	8.864660000	0.448041000	3.668983000
Ν	6.882626000	1.991706000	5.224634000
Ν	9.774987000	4.089045000	5.733089000
С	9.955771000	0.023819000	3.457336000
С	7.671647000	2.841734000	5.916038000
С	7.423518000	3.166284000	7.249874000
С	6.335518000	2.576093000	7.894104000
С	5.538582000	1.684547000	7.181423000
С	5.842122000	1.420004000	5.844766000
С	8.785712000	3.414312000	5.093633000
Н	8.045222000	3.889295000	7.775880000
Н	6.113732000	2.816341000	8.932840000
Н	4.680531000	1.197540000	7.641512000
Н	5.236612000	0.740240000	5.245701000
Н	9.931295000	3.955810000	6.723627000
Η	10.576345000	4.352575000	5.169288000

[Ni	(NCS)2(pia)2]		
trai	ns, N		
Ni	1.835805000	2.793607000	4.783728000
Ν	0.946250000	4.223845000	5.909268000
0	0.359762000	2.930475000	3.244041000
S	0.730736000	4.950852000	8.626924000
Ν	2.667656000	4.215969000	3.575344000
Ν	0.204700000	3.482194000	1.045093000
С	0.854680000	4.534344000	7.056047000
С	2.023605000	4.404380000	2.406459000
С	2.444874000	5.355299000	1.476811000
С	3.577045000	6.117406000	1.763659000
С	4.244947000	5.905573000	2.968079000
С	3.752987000	4.945727000	3.852082000
С	0.810126000	3.535626000	2.257267000
Η	1.887824000	5.522898000	0.556595000
Η	3.926425000	6.870328000	1.058650000
Η	5.131390000	6.480361000	3.230436000
Η	4.225892000	4.747593000	4.812162000
Η	0.769108000	3.647718000	0.219669000
Η	-0.504254000	2.761634000	0.949199000
Ν	2.724814000	1.363150000	3.658116000
0	3.311307000	2.657726000	6.323137000
S	2.938482000	0.635840000	0.940472000
Ν	1.004113000	1.371284000	5.992512000
Ν	3.468150000	2.104878000	8.522148000
С	2.815519000	1.052763000	2.511261000
С	1.648816000	1.182440000	7.160977000
С	1.228248000	0.231059000	8.090454000
С	0.095889000	-0.530957000	7.804044000
С	-0.572842000	-0.318519000	6.600182000
С	-0.081484000	0.641643000	5.716239000
С	2.861958000	2.051606000	7.310025000
Η	1.785846000	0.063036000	9.010255000
Η	-0.252991000	-1.284259000	8.508885000
Η	-1.459556000	-0.893095000	6.338169000
Η	-0.555028000	0.840082000	4.756520000
Η	2.905569000	1.937065000	9.348264000
Н	4.176811000	2.825877000	8.618618000

[Ni(]	NCS)2(pia)2]		
cis, S	8		
Ni	-0.902321000	2.841525000	6.033358000
Ν	-4.458772000	3.185263000	8.190867000
0	-1.840682000	1.411772000	7.323039000
0	0.260129000	1.373955000	4.991863000
S	-2.287747000	4.600904000	7.002812000
S	0.208090000	4.601161000	4.760521000
Ν	0.400161000	2.796852000	7.623199000
Ν	-2.271854000	1.396045000	9.552951000
Ν	-2.163390000	2.326603000	4.492717000
Ν	0.715948000	1.048269000	2.792177000
С	-3.569156000	3.777999000	7.691619000
С	1.607633000	3.878932000	4.201077000
С	1.638977000	3.304216000	7.670744000
Н	1.981181000	3.808889000	6.768930000
С	2.441798000	3.197301000	8.807595000
Η	3.444073000	3.621645000	8.797932000
С	1.943319000	2.542881000	9.930857000
Η	2.550623000	2.434765000	10.828678000
С	0.650928000	2.016564000	9.884562000
Η	0.239488000	1.474635000	10.735024000
С	-0.089299000	2.165554000	8.714094000
С	-1.468754000	1.626829000	8.490493000
С	-3.464774000	2.621869000	4.377099000
Η	-3.891907000	3.213666000	5.184859000
С	-4.227223000	2.201291000	3.286306000
Η	-5.282805000	2.462130000	3.237784000
С	-3.620062000	1.449936000	2.283596000
Η	-4.192296000	1.098970000	1.425651000
С	-2.262861000	1.143920000	2.400578000
Η	-1.762432000	0.535087000	1.648788000
С	-1.569099000	1.601810000	3.518235000
С	-0.126171000	1.328314000	3.810626000
Η	-3.267891000	1.383815000	9.321443000
Н	-2.039983000	1.840474000	10.434371000
Н	1.698907000	1.231530000	3.008915000
Н	0.428491000	1.293017000	1.850621000
Ν	2.582593000	3.352982000	3.794510000

[Ni(NCS)2(pia)2]		
trar	ns, S		
Ni	1.847919000	2.794406000	4.800612000
S	0.540990000	4.646874000	5.905921000
0	0.447109000	2.792986000	3.234356000
Ν	0.912170000	4.017460000	8.654072000
Ν	2.668359000	4.156588000	3.585554000
Ν	0.202476000	3.406482000	1.053375000
С	0.740332000	4.302338000	7.520110000
С	2.045571000	4.320978000	2.397227000
С	2.470160000	5.268487000	1.464969000
С	3.585092000	6.047418000	1.761358000
С	4.238206000	5.855692000	2.980085000
С	3.746070000	4.903624000	3.867571000
С	0.855968000	3.431843000	2.243497000
Н	1.931538000	5.406380000	0.529671000
Н	3.937743000	6.796291000	1.053751000
Н	5.113456000	6.443932000	3.249718000
Н	4.204955000	4.723180000	4.837203000
Н	0.782624000	3.500810000	0.224861000
Н	-0.495456000	2.670931000	0.983735000
S	3.125973000	0.925301000	3.663892000
0	3.247616000	2.800591000	6.361871000
Ν	2.827770000	1.678302000	0.939225000
Ν	1.028195000	1.436960000	6.023377000
Ν	3.493066000	2.211678000	8.549213000
С	2.970135000	1.339301000	2.062297000
С	1.642959000	1.291368000	7.218576000
С	1.204821000	0.366523000	8.167010000
С	0.086383000	-0.410413000	7.878933000
С	-0.556224000	-0.240093000	6.651390000
С	-0.051818000	0.690439000	5.748528000
С	2.837341000	2.175578000	7.361046000
Η	1.735106000	0.243509000	9.109124000
Η	-0.276999000	-1.141201000	8.599654000
Η	-1.433301000	-0.828265000	6.387486000
Η	-0.502962000	0.854528000	4.772351000
Η	2.915824000	2.120251000	9.380085000
Η	4.189412000	2.949353000	8.613574000

[Cu(NCS)2(pia)2]		
cis, ľ	N		
Cu	7.395351000	1.355924000	3.230613000
S	3.817544000	-1.128598000	4.018677000
0	6.196188000	2.770014000	2.543151000
Ν	6.026069000	0.060162000	2.737055000
Ν	8.187453000	1.933203000	0.926530000
Ν	5.116761000	3.812146000	0.858832000
С	5.102133000	-0.436074000	3.304996000
С	7.322366000	2.828308000	0.427485000
С	7.497534000	3.438863000	-0.819079000
С	8.611932000	3.081944000	-1.579123000
С	9.499908000	2.137419000	-1.069553000
С	9.250789000	1.590324000	0.194276000
С	6.175223000	3.120934000	1.351547000
Η	6.807929000	4.197700000	-1.187715000
Η	8.784142000	3.541371000	-2.551831000
Η	10.379349000	1.829646000	-1.633756000
Η	9.922814000	0.852203000	0.640148000
Η	4.968864000	3.886148000	-0.138986000
Η	4.303524000	3.887461000	1.460377000
S	10.980426000	-1.114591000	2.440349000
0	8.593860000	2.769296000	3.920694000
Ν	8.764804000	0.060528000	3.722998000
Ν	6.599832000	1.932654000	5.534374000
Ν	9.671941000	3.808773000	5.607807000
С	9.691874000	-0.429903000	3.154774000
С	7.463958000	2.828219000	6.034329000
С	7.285649000	3.441477000	7.279214000
С	6.168800000	3.086613000	8.036628000
С	5.282124000	2.141024000	7.526551000
С	5.534469000	1.591238000	6.264455000
С	8.613284000	3.119352000	5.112541000
Η	7.974334000	4.201214000	7.647988000
Н	5.993710000	3.548650000	9.007685000
Н	4.401071000	1.834621000	8.088917000
Н	4.863421000	0.852544000	5.817887000
Н	9.818800000	3.879119000	6.606085000
Η	10.486769000	3.882075000	5.008080000

[Cu(NCS)2(pia)2]		
trans	s, N		
Cu	1.837618000	2.795533000	4.784787000
Ν	0.936826000	4.263125000	5.723752000
0	0.696173000	3.030292000	3.187255000
S	1.100406000	5.699659000	8.140956000
Ν	2.996821000	4.481359000	3.374537000
Ν	0.470489000	3.532411000	0.996419000
С	1.023871000	4.865589000	6.749504000
С	2.221936000	4.650449000	2.293912000
С	2.435718000	5.670147000	1.360702000
С	3.512664000	6.533926000	1.557397000
С	4.328232000	6.348925000	2.671375000
С	4.025854000	5.310551000	3.556308000
С	1.085968000	3.669912000	2.196993000
Н	1.761630000	5.816991000	0.517711000
Н	3.703323000	7.344389000	0.855229000
Н	5.179393000	7.001075000	2.861298000
Н	4.628942000	5.137465000	4.447810000
Н	0.960488000	3.801973000	0.152716000
Н	-0.172534000	2.750749000	0.916196000
Ν	2.738674000	1.329173000	3.843448000
0	2.980869000	2.560497000	6.380976000
S	2.516462000	-0.146888000	1.455425000
Ν	0.680592000	1.111398000	6.191411000
Ν	3.213900000	2.047171000	8.568122000
С	2.626413000	0.708946000	2.830957000
С	1.454914000	0.939377000	7.271799000
С	1.238442000	-0.080985000	8.203730000
С	0.159295000	-0.941595000	8.006043000
С	-0.655775000	-0.753209000	6.892302000
С	-0.350536000	0.285137000	6.008553000
С	2.593161000	1.916980000	7.369537000
Η	1.911913000	-0.230566000	9.046699000
Н	-0.033787000	-1.752202000	8.707381000
Н	-1.508696000	-1.402881000	6.701768000
Η	-0.952933000	0.461005000	5.117145000
Η	2.726260000	1.775967000	9.412448000
Н	3.860516000	2.825650000	8.649197000

[Cu((NCS)2(pia)2]		
tran	s, S		
Cu	1.856037000	2.745637000	4.749274000
S	0.424244000	4.856679000	6.103349000
0	0.502920000	2.793750000	3.308023000
Ν	0.965827000	3.833912000	8.691230000
Ν	2.737108000	4.067094000	3.580486000
Ν	0.184947000	3.385867000	1.120271000
С	0.719466000	4.294549000	7.626383000
С	2.101896000	4.254138000	2.400959000
С	2.545980000	5.192788000	1.469903000
С	3.687173000	5.933795000	1.761314000
С	4.348368000	5.717298000	2.972899000
С	3.839834000	4.775481000	3.861650000
С	0.886660000	3.400837000	2.283571000
Н	2.001718000	5.347707000	0.540824000
Η	4.055802000	6.675637000	1.054525000
Η	5.244159000	6.276983000	3.234804000
Η	4.302650000	4.571655000	4.824480000
Η	0.756986000	3.385161000	0.278618000
Η	-0.551328000	2.684889000	1.102610000
S	3.193288000	0.688722000	3.446289000
0	3.173275000	2.761476000	6.224081000
Ν	2.694521000	1.725290000	0.853853000
Ν	0.947442000	1.472529000	5.950103000
Ν	3.468242000	2.212821000	8.426065000
С	2.925118000	1.256190000	1.917591000
С	1.566470000	1.315961000	7.142524000
С	1.112226000	0.398200000	8.089411000
С	-0.023310000	-0.352100000	7.800553000
С	-0.668608000	-0.166191000	6.575156000
С	-0.149371000	0.754141000	5.670525000
С	2.778932000	2.174085000	7.256293000
Η	1.643689000	0.268156000	9.029575000
Η	-0.400410000	-1.077098000	8.520275000
Η	-1.560158000	-0.733445000	6.315107000
Η	-0.598881000	0.932983000	4.696444000
Η	2.883282000	2.241641000	9.258993000
Н	4.206808000	2.911783000	8.434988000

[Zn(NCS)2(pia)2]					
cis,]	N				
Zn	-0.869018000	3.188487000	5.891807000		
S	-4.664657000	4.063868000	8.332833000		
Ο	-1.652818000	1.511114000	7.075711000		
Ο	0.207324000	1.545968000	4.905334000		
Ν	-2.358078000	4.240706000	6.727928000		
Ν	0.342909000	4.424908000	4.931816000		
Ν	0.497817000	2.966205000	7.654360000		
Ν	-1.998867000	0.938596000	9.248410000		
Ν	-2.199746000	2.461003000	4.250038000		
Ν	0.419182000	0.333129000	2.999596000		
С	-3.329601000	4.164557000	7.413119000		
С	1.436310000	4.776449000	4.620958000		
С	1.677855000	3.572144000	7.819787000		
Η	1.992741000	4.239422000	7.016770000		
С	2.470393000	3.352247000	8.949423000		
Η	3.429374000	3.858448000	9.043184000		
С	2.016180000	2.475387000	9.930871000		
Η	2.617931000	2.270704000	10.815614000		
С	0.779575000	1.850227000	9.760500000		
Η	0.414452000	1.136735000	10.497992000		
С	0.050020000	2.128266000	8.604530000		
С	-1.274249000	1.508200000	8.251708000		
С	-3.457075000	2.867724000	4.054639000		
Η	-3.801437000	3.662758000	4.715724000		
С	-4.276868000	2.295682000	3.079112000		
Η	-5.298396000	2.649608000	2.952732000		
С	-3.767559000	1.263710000	2.294994000		
Η	-4.386770000	0.782018000	1.539280000		
С	-2.452030000	0.843818000	2.498428000		
Η	-2.045671000	0.017279000	1.917117000		
С	-1.697201000	1.477855000	3.486552000		
С	-0.278365000	1.130475000	3.849738000		
Η	-2.962688000	0.718925000	9.013156000		
Η	-1.830030000	1.222060000	10.206189000		
Н	1.406911000	0.214931000	3.198511000		
Н	0.121679000	0.214527000	2.040073000		
S	2.926473000	5.274862000	4.215463000		

[Zn(NCS)2(pia)2]					
trar	ns, N				
Zn	1.831913000	2.788535000	4.773169000		
Ν	0.915158000	4.170490000	5.898826000		
0	0.380590000	3.021675000	3.139587000		
S	0.316839000	4.909715000	8.548360000		
Ν	2.709635000	4.356805000	3.445370000		
Ν	0.176577000	3.633444000	0.967926000		
С	0.664712000	4.487142000	7.019164000		
С	2.045582000	4.515438000	2.288035000		
С	2.466186000	5.424694000	1.314421000		
С	3.621218000	6.170076000	1.546125000		
С	4.313489000	5.987592000	2.740882000		
С	3.816323000	5.071206000	3.667483000		
С	0.813429000	3.652029000	2.167363000		
Н	1.899423000	5.575426000	0.397373000		
Н	3.971358000	6.885803000	0.803675000		
Н	5.219529000	6.549585000	2.960369000		
Η	4.312366000	4.901022000	4.622337000		
Η	0.679550000	3.877308000	0.124234000		
Н	-0.560077000	2.942881000	0.870792000		
Ν	2.750746000	1.404484000	3.649442000		
0	3.279788000	2.553584000	6.409543000		
S	3.344963000	0.691773000	0.991598000		
Ν	0.953924000	1.214660000	6.098720000		
Ν	3.481078000	1.940360000	8.581010000		
С	3.000947000	1.099582000	2.525637000		
С	1.616814000	1.054975000	7.256339000		
С	1.196496000	0.143546000	8.228248000		
С	0.043652000	-0.604149000	7.993414000		
С	-0.646923000	-0.421490000	6.797579000		
С	-0.150598000	0.497804000	5.873504000		
С	2.846734000	1.921216000	7.380263000		
Η	1.762293000	-0.007245000	9.145903000		
Η	-0.306380000	-1.321766000	8.734140000		
Η	-1.551205000	-0.985474000	6.575638000		
Η	-0.645767000	0.668796000	4.918331000		
Η	2.977285000	1.694061000	9.423352000		
Η	4.215411000	2.633048000	8.680366000		

[Zn(NCS)2(pia)2]					
cis, S	5				
Zn	-0.925572000	3.154417000	5.992115000		
Ν	-4.422418000	3.224444000	8.293735000		
0	-1.839254000	1.619620000	7.272264000		
0	0.227992000	1.580902000	4.980913000		
S	-2.531691000	4.825114000	6.880080000		
S	0.415069000	4.875502000	4.811629000		
Ν	0.471884000	2.866761000	7.691488000		
Ν	-2.276365000	1.476616000	9.494321000		
Ν	-2.241285000	2.370864000	4.384963000		
Ν	0.711036000	1.131154000	2.809560000		
С	-3.645154000	3.883252000	7.701863000		
С	1.669193000	3.989718000	4.144390000		
С	1.727215000	3.318361000	7.775566000		
Η	2.078755000	3.901523000	6.924269000		
С	2.533290000	3.059518000	8.885887000		
Η	3.554575000	3.434696000	8.912481000		
С	2.008937000	2.314298000	9.939033000		
Η	2.616301000	2.085078000	10.813915000		
С	0.692480000	1.856688000	9.856808000		
Н	0.261235000	1.253975000	10.655046000		
С	-0.042642000	2.155618000	8.710884000		
С	-1.458005000	1.719578000	8.447447000		
С	-3.550011000	2.602905000	4.242112000		
Н	-3.998217000	3.261845000	4.985922000		
С	-4.292229000	2.037322000	3.203383000		
Н	-5.358741000	2.240514000	3.127235000		
С	-3.645755000	1.213303000	2.285553000		
Н	-4.199245000	0.747605000	1.471019000		
С	-2.275599000	0.984672000	2.426585000		
Н	-1.746375000	0.328444000	1.736862000		
С	-1.610274000	1.583815000	3.495026000		
С	-0.148497000	1.420540000	3.810628000		
Η	-3.271405000	1.585996000	9.264623000		
Н	-2.003043000	1.822465000	10.407437000		
Н	1.674323000	1.430067000	3.003651000		
Η	0.399628000	1.270282000	1.854598000		
Ν	2.545683000	3.367189000	3.662033000		

[Zn(NCS)2(pia)2]						
trans, S						
Zn	1.821602000	2.821300000	4.802533000			
S	0.551874000	4.693724000	6.000142000			
0	0.373459000	2.926713000	3.153039000			
Ν	0.858324000	3.879820000	8.709369000			
Ν	2.678229000	4.258987000	3.498460000			
Ν	0.242366000	3.465913000	0.943881000			
С	0.722292000	4.235381000	7.591241000			
С	2.055021000	4.390530000	2.312497000			
С	2.493263000	5.303464000	1.350790000			
С	3.619192000	6.075160000	1.623672000			
С	4.273093000	5.913938000	2.845725000			
С	3.766548000	4.994757000	3.759616000			
С	0.841721000	3.515132000	2.163398000			
Η	1.956827000	5.422364000	0.412177000			
Η	3.980162000	6.797164000	0.892612000			
Η	5.155816000	6.499253000	3.096297000			
Η	4.226203000	4.837900000	4.733927000			
Η	0.871015000	3.485246000	0.145151000			
Η	-0.477100000	2.750850000	0.876098000			
S	3.088025000	0.925507000	3.599505000			
0	3.282541000	2.717017000	6.440779000			
Ν	2.786056000	1.725329000	0.885812000			
Ν	0.992668000	1.356590000	6.096859000			
Ν	3.428349000	2.165162000	8.645969000			
С	2.924367000	1.375205000	2.005683000			
С	1.626899000	1.221116000	7.276531000			
С	1.212831000	0.287984000	8.229364000			
С	0.099237000	-0.501035000	7.954359000			
С	-0.566494000	-0.335992000	6.739399000			
С	-0.083604000	0.604374000	5.833903000			
С	2.826559000	2.114835000	7.427776000			
Н	1.759452000	0.165829000	9.161780000			
Η	-0.242422000	-1.239684000	8.678072000			
Η	-1.439859000	-0.934585000	6.487299000			
Η	-0.552801000	0.764253000	4.864581000			
Η	2.803593000	2.127705000	9.446866000			
Н	4.137206000	2.890296000	8.717455000			