Structural and electronic features of triphenylstibine-functionalized Fischer carbene complexes of Molybdenum(0)

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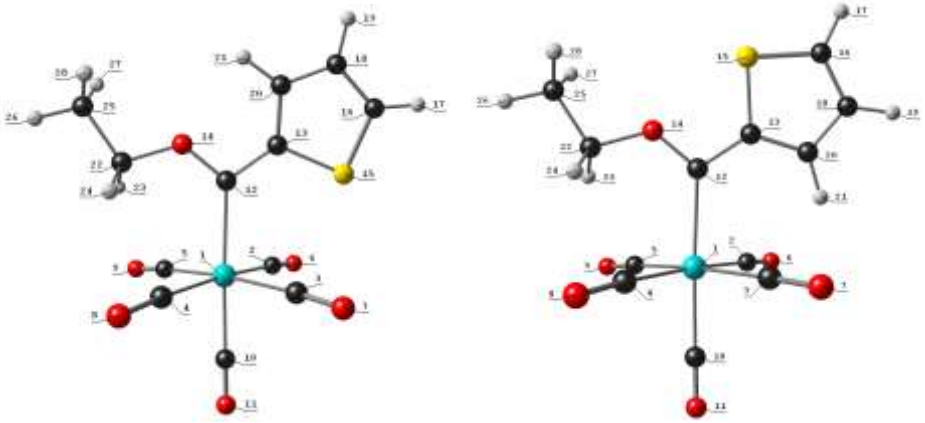

Figure S 1. DFT atom numbering of *anti* [(CO)$_5$MoC(OEt)(C$_4$H$_3$S)] (left) and *syn* [(CO)$_5$MoC(OEt)(C$_4$H$_3$S)] (right). Colour code: Mo (light blue), C (black), S (yellow), O (red), H (white).

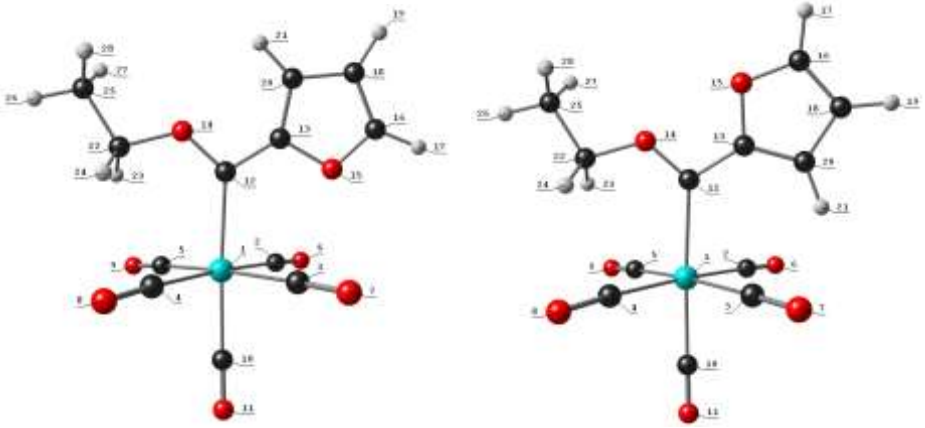

Figure S 2. DFT atom numbering of *anti* [(CO)$_5$MoC(OEt)(C$_4$H$_3$O)] (left) and *syn* [(CO)$_5$MoC(OEt)(C$_4$H$_3$O)]. Colour code: Mo (light blue), C (black), O (red), H (white).

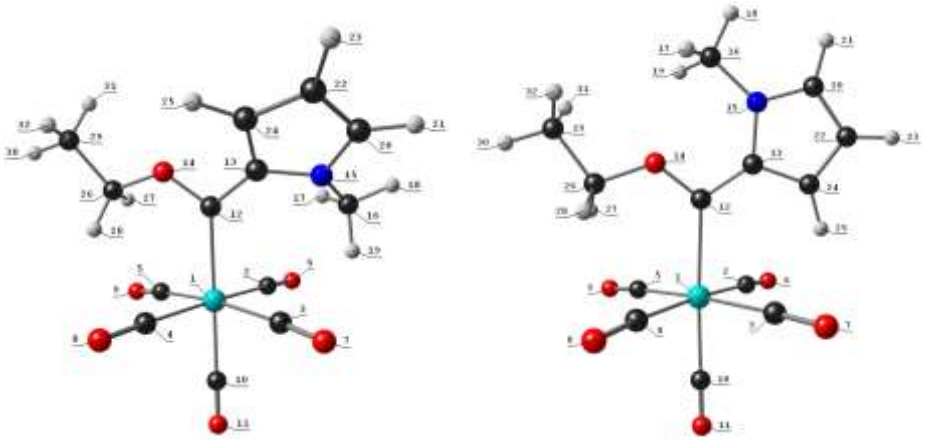

Figure S 3. DFT atom numbering of *anti* [(CO)$_5$MoC(OEt)(C$_4$H$_3$NMe)] (left) and *syn* [(CO)$_5$MoC(OEt)(C$_4$H$_3$NMe)]. Colour code: Mo (light blue), C (black), N (dark blue), O (red), H (white).

Optimized Cartesian coordinates (Å)

All compounds were optimized B3LYP as implemented in the Gaussian 09 program package. Geometries of the neutral complexes were optimized in gas phase with the triple-ζ basis set 6-311G(d,p) on all atoms except Mo and Sb, where def2-TZVPP was used. The coordinates of the lowest energy conformations of each complex are provided.

1. [$(SbPh_3)(CO)_4MoC(OEt)(C_4H_3S)$] (1) cis-syn 1

Mo	1.142252000	-1.473464000	-0.722891000
C	1.314374000	-0.546511000	-2.546619000
O	1.393642000	-0.118557000	-3.609666000
C	2.651614000	-2.664220000	-1.249886000
O	3.505216000	-3.376234000	-1.556829000
C	0.866954000	-2.606624000	0.955121000
O	0.664438000	-3.327465000	1.831494000
C	-0.118899000	-2.757584000	-1.664946000
O	-0.802885000	-3.495939000	-2.222618000
C	2.589541000	-0.021834000	0.162315000
O	3.502315000	-0.244944000	1.109457000
C	3.642872000	-1.500341000	1.813427000
H	3.710692000	-2.307513000	1.085008000
H	2.752110000	-1.647217000	2.425026000
C	4.893212000	-1.402146000	2.664293000
H	5.023761000	-2.330396000	3.226138000
H	4.819714000	-0.576776000	3.375550000
H	5.777779000	-1.249263000	2.042724000
C	2.803828000	1.352699000	-0.278031000
C	2.026431000	2.159165000	-1.091047000
H	1.096415000	1.833259000	-1.529911000
C	2.547559000	3.458131000	-1.279408000
H	2.068654000	4.216041000	-1.884018000
C	3.730907000	3.649351000	-0.613381000
H	4.343956000	4.538536000	-0.598900000
S	4.221779000	2.258213000	0.269905000
Sb	-1.134751000	0.034249000	0.084888000
C	-1.170058000	1.026636000	2.015620000
C	-2.339533000	1.102691000	2.781942000
H	-3.257035000	0.651271000	2.421849000
C	-2.335592000	1.749729000	4.017178000
H	-3.247934000	1.797839000	4.601771000
C	-1.164504000	2.329074000	4.501038000
H	-1.162719000	2.830587000	5.462476000
C	0.004920000	2.258241000	3.747152000
H	0.920427000	2.705751000	4.118342000
C	0.002536000	1.608762000	2.513475000
H	0.923600000	1.561513000	1.942808000

C	-3.020937000	-1.020796000	0.247357000
C	-4.219778000	-0.485501000	-0.237990000
H	-4.228187000	0.485367000	-0.720310000
C	-5.413592000	-1.195923000	-0.112629000
H	-6.334702000	-0.771191000	-0.496807000
C	-5.423308000	-2.446642000	0.500319000
H	-6.351558000	-2.999019000	0.595095000
C	-4.235178000	-2.988537000	0.986109000
H	-4.234680000	-3.963939000	1.459847000
C	-3.041055000	-2.282139000	0.856575000
H	-2.126820000	-2.726946000	1.235065000
C	-1.805561000	1.685609000	-1.155080000
C	-1.870966000	1.498251000	-2.542304000
H	-1.597159000	0.543984000	-2.981022000
C	-2.287124000	2.530875000	-3.380952000
H	-2.334456000	2.369017000	-4.452127000
C	-2.635834000	3.768108000	-2.842539000
H	-2.956163000	4.573551000	-3.494042000
C	-2.569353000	3.967108000	-1.465140000
H	-2.838633000	4.928568000	-1.041330000
C	-2.158068000	2.932192000	-0.625111000
H	-2.112068000	3.102504000	0.444570000

2. [$(SbPh_3)(CO)_4MoC(OEt)(C_4H_3S)$] (1) cis-syn 2

Sb	-1.197037000	0.029728000	0.102049000
Mo	1.122791000	-1.508427000	-0.522531000
S	4.593052000	1.898221000	0.354082000
O	-0.717542000	-4.101171000	-0.498770000
O	1.434843000	-1.902329000	2.636238000
O	3.576635000	-3.425712000	-0.959779000
O	0.619404000	-1.548171000	-3.677135000
O	2.530985000	1.307781000	-1.345281000
C	-0.070313000	-3.147403000	-0.502474000
C	1.336175000	-1.718638000	1.506456000
C	2.682288000	-2.714465000	-0.812566000
C	0.813323000	-1.473181000	-2.544381000
C	2.526428000	0.232905000	-0.555499000
C	3.679626000	0.381976000	0.323768000
C	4.263755000	-0.526177000	1.189705000
H	3.897628000	-1.531989000	1.317620000
C	5.397493000	-0.026854000	1.867191000
H	5.975558000	-0.601217000	2.578202000
C	5.684680000	1.269438000	1.524093000
H	6.484858000	1.889809000	1.900331000
C	1.555611000	1.561852000	-2.378299000
H	0.563002000	1.324511000	-1.995721000
H	1.778271000	0.903125000	-3.218991000
C	1.671122000	3.022618000	-2.764703000
H	0.961804000	3.244151000	-3.566184000

H	1.442455000	3.667222000	-1.914029000
H	2.676889000	3.253189000	-3.121961000
C	-2.254664000	-0.494504000	1.919256000
C	-2.512447000	-1.844615000	2.190677000
H	-2.183360000	-2.618841000	1.505602000
C	-3.196601000	-2.216595000	3.346206000
H	-3.389631000	-3.265440000	3.542462000
C	-3.624727000	-1.244861000	4.248498000
H	-4.152591000	-1.535084000	5.150100000
C	-3.368195000	0.099565000	3.990674000
H	-3.695745000	0.860111000	4.691190000
C	-2.687771000	0.474004000	2.831968000
H	-2.493302000	1.524247000	2.646767000
C	-2.896138000	0.075161000	-1.246393000
C	-4.209222000	0.191135000	-0.773424000
H	-4.402203000	0.246167000	0.292063000
C	-5.281609000	0.224379000	-1.663787000
H	-6.293797000	0.309599000	-1.283566000
C	-5.055683000	0.141559000	-3.036342000
H	-5.890984000	0.163237000	-3.727391000
C	-3.754100000	0.021117000	-3.517383000
H	-3.571656000	-0.053784000	-4.583702000
C	-2.681642000	-0.014567000	-2.627217000
H	-1.678404000	-0.128665000	-3.022461000
C	-0.998549000	2.164772000	0.459469000
C	0.112220000	2.620703000	1.181331000
H	0.853773000	1.917564000	1.548003000
C	0.286201000	3.980220000	1.436182000
H	1.148911000	4.316658000	2.000531000
C	-0.644362000	4.903028000	0.961602000
H	-0.508499000	5.961174000	1.155841000
C	-1.748293000	4.461725000	0.234909000
H	-2.474059000	5.176074000	-0.138606000
C	-1.926209000	3.100540000	-0.013365000
H	-2.791052000	2.772230000	-0.578706000

3. [$(SbPh_3)(CO)_4MoC(OEt)(C_4H_3O)$] (2) cis-anti (1)

Mo	1.541300000	-1.136477000	-0.705660000
C	1.509115000	-0.132754000	-2.504068000
O	1.493889000	0.349931000	-3.544748000
C	3.235133000	-2.029452000	-1.254053000
O	4.196901000	-2.578372000	-1.579108000
C	1.513408000	-2.281389000	0.985940000
O	1.474296000	-2.998405000	1.887339000
C	0.543371000	-2.631925000	-1.663825000
O	0.014478000	-3.483127000	-2.228565000
C	2.646789000	0.559608000	0.186575000
O	3.640526000	0.569060000	1.078228000
C	4.143087000	-0.637319000	1.695874000

H	4.354991000	-1.370757000	0.918821000
H	3.367433000	-1.033047000	2.352945000
C	5.389560000	-0.260490000	2.471517000
H	5.793067000	-1.146719000	2.967563000
H	5.164928000	0.487734000	3.234860000
H	6.157391000	0.139457000	1.805858000
C	2.466868000	1.952769000	-0.185289000
C	3.171591000	3.102328000	0.105169000
H	4.060399000	3.147727000	0.712060000
C	2.510538000	4.173190000	-0.547703000
H	2.784138000	5.216198000	-0.546426000
C	1.441137000	3.616669000	-1.190503000
H	0.650255000	4.021176000	-1.800069000
O	1.400778000	2.285536000	-0.986098000
Sb	-0.992121000	-0.088676000	0.084348000
C	-1.238904000	0.761889000	2.067848000
C	-2.454406000	0.685462000	2.759131000
H	-3.304619000	0.182476000	2.312393000
C	-2.582000000	1.241429000	4.031374000
H	-3.528428000	1.171457000	4.556593000
C	-1.496889000	1.879372000	4.629350000
H	-1.596765000	2.309118000	5.619934000
C	-0.281454000	1.955924000	3.953297000
H	0.568835000	2.445427000	4.415683000
C	-0.153417000	1.397784000	2.681965000
H	0.804427000	1.452961000	2.175906000
C	-2.653168000	-1.481145000	0.150370000
C	-3.932340000	-1.145955000	-0.309055000
H	-4.122095000	-0.163238000	-0.725675000
C	-4.973631000	-2.071781000	-0.243220000
H	-5.958814000	-1.799740000	-0.606484000
C	-4.749652000	-3.341541000	0.283555000
H	-5.559296000	-4.061222000	0.332190000
C	-3.479732000	-3.686427000	0.741528000
H	-3.296547000	-4.675348000	1.146974000
C	-2.438196000	-2.763539000	0.671696000
H	-1.454999000	-3.056203000	1.025632000
C	-1.952789000	1.468566000	-1.083059000
C	-1.945603000	1.359498000	-2.479542000
H	-1.472074000	0.510598000	-2.961529000
C	-2.540162000	2.338815000	-3.273420000
H	-2.527739000	2.237566000	-4.353063000
C	-3.144819000	3.445661000	-2.679898000
H	-3.606662000	4.209102000	-3.296221000
C	-3.153922000	3.566667000	-1.291844000
H	-3.623575000	4.425402000	-0.824116000
C	-2.562655000	2.583668000	-0.497288000
H	-2.578745000	2.693918000	0.581203000

4. [$(SbPh_3)(CO)_4MoC(OEt)(C_4H_3O)$] (2) cis-anti (2)

Mo	1.409854000	-1.142820000	-0.735520000
C	1.066006000	-0.731364000	-2.705727000
O	0.847849000	-0.606735000	-3.830287000
C	3.132304000	-2.038239000	-1.211904000
O	4.119796000	-2.568363000	-1.472538000
C	1.652617000	-1.787772000	1.202817000
O	1.746043000	-2.240130000	2.254195000
C	0.454189000	-2.901246000	-1.109961000
O	-0.046473000	-3.910560000	-1.343631000
C	2.590901000	0.691666000	-0.367629000
O	2.546793000	1.900438000	-0.940007000
C	1.593039000	2.242820000	-1.967386000
H	0.615596000	1.840984000	-1.699533000
H	1.916890000	1.775532000	-2.898845000
C	1.567154000	3.753754000	-2.083870000
H	0.869894000	4.046075000	-2.872728000
H	2.555669000	4.143906000	-2.335857000
H	1.237832000	4.212878000	-1.149214000
C	3.698406000	0.768495000	0.570023000
C	4.565397000	1.788403000	0.907491000
H	4.547728000	2.780701000	0.489007000
C	5.455804000	1.274587000	1.882366000
H	6.265966000	1.789232000	2.373800000
C	5.082220000	-0.025244000	2.078473000
H	5.454651000	-0.812770000	2.712527000
O	4.031932000	-0.345412000	1.300429000
Sb	-1.070044000	-0.039133000	0.106867000
C	-1.112051000	1.227595000	1.870078000
C	-2.181172000	1.206322000	2.773895000
H	-3.018707000	0.536878000	2.612479000
C	-2.176441000	2.034460000	3.895848000
H	-3.009204000	2.004034000	4.590151000
C	-1.104825000	2.894100000	4.127948000
H	-1.101474000	3.535699000	5.002135000
C	-0.033940000	2.920586000	3.237218000
H	0.807358000	3.581194000	3.416243000
C	-0.036410000	2.089239000	2.118090000
H	0.814187000	2.111691000	1.444855000
C	-2.656768000	-1.403608000	0.668830000
C	-3.995053000	-1.171266000	0.330891000
H	-4.268927000	-0.290580000	-0.238858000
C	-4.988219000	-2.071436000	0.716253000
H	-6.020892000	-1.881622000	0.444200000
C	-4.655669000	-3.211489000	1.444371000
H	-5.428255000	-3.911904000	1.741530000
C	-3.326115000	-3.452758000	1.784081000
H	-3.059655000	-4.341283000	2.345632000
C	-2.332495000	-2.556485000	1.395192000
H	-1.302177000	-2.768154000	1.661984000

C	-2.215693000	1.232338000	-1.233821000
C	-2.345833000	0.851810000	-2.576490000
H	-1.879908000	-0.058748000	-2.938624000
C	-3.072219000	1.636486000	-3.470676000
H	-3.166019000	1.326466000	-4.505607000
C	-3.672106000	2.816732000	-3.035490000
H	-4.235265000	3.428999000	-3.731070000
C	-3.543704000	3.208270000	-1.704604000
H	-4.007342000	4.126730000	-1.361013000
C	-2.820579000	2.420936000	-0.808197000
H	-2.729561000	2.738233000	0.224498000

5. [($SbPh_3$)$(CO)_4$MoC(OEt)(C_4H_3NMe)] (3) cis-syn (1)

Mo	1.126515000	-1.412674000	-0.761562000
C	1.286869000	-0.459579000	-2.575566000
O	1.347650000	-0.029596000	-3.638935000
C	2.672495000	-2.554469000	-1.277209000
O	3.557308000	-3.235347000	-1.571171000
C	0.830463000	-2.585571000	0.879707000
O	0.612763000	-3.335631000	1.729285000
C	-0.085186000	-2.701880000	-1.741559000
O	-0.741773000	-3.448052000	-2.324356000
C	2.593844000	0.050315000	0.140954000
O	3.474982000	-0.190881000	1.120447000
C	3.495898000	-1.425541000	1.871290000
H	3.580927000	-2.261549000	1.177627000
H	2.554024000	-1.510636000	2.413486000
C	4.675446000	-1.367524000	2.822228000
H	4.704798000	-2.283206000	3.418010000
H	4.590039000	-0.519864000	3.506158000
H	5.619228000	-1.286660000	2.278407000
C	2.857078000	1.381892000	-0.362038000
C	1.989903000	2.200726000	-1.101883000
H	1.006012000	1.920561000	-1.434309000
C	2.597763000	3.443788000	-1.297971000
H	2.189561000	4.294400000	-1.819435000
C	3.843483000	3.375289000	-0.694483000
H	4.633445000	4.109649000	-0.652235000
N	4.007729000	2.157489000	-0.118185000
Sb	-1.165658000	0.047016000	0.076724000
C	-1.200102000	0.937122000	2.058679000
C	-2.347340000	0.920261000	2.860858000
H	-3.256166000	0.451143000	2.501424000
C	-2.333297000	1.497106000	4.130578000
H	-3.228673000	1.472170000	4.742298000
C	-1.174059000	2.100261000	4.613372000
H	-1.164072000	2.547459000	5.601239000
C	-0.026699000	2.123479000	3.823200000
H	0.879176000	2.591468000	4.193346000

C	-0.038680000	1.542641000	2.555868000
H	0.866288000	1.565235000	1.957730000
C	-3.052257000	-1.017557000	0.174950000
C	-4.266817000	-0.409442000	-0.165299000
H	-4.286147000	0.622206000	-0.498246000
C	-5.462170000	-1.123577000	-0.088748000
H	-6.395068000	-0.641010000	-0.359647000
C	-5.458568000	-2.452433000	0.329401000
H	-6.388240000	-3.007812000	0.385352000
C	-4.255548000	-3.067506000	0.668764000
H	-4.244203000	-4.103418000	0.989128000
C	-3.059902000	-2.355714000	0.588554000
H	-2.133885000	-2.857806000	0.847384000
C	-1.852051000	1.762635000	-1.065024000
C	-1.915253000	1.652950000	-2.460573000
H	-1.628232000	0.728726000	-2.952225000
C	-2.344366000	2.725924000	-3.239668000
H	-2.389333000	2.624549000	-4.318391000
C	-2.708938000	3.926209000	-2.632521000
H	-3.039427000	4.763101000	-3.237741000
C	-2.644743000	4.048139000	-1.246133000
H	-2.925782000	4.980814000	-0.768883000
C	-2.219978000	2.972640000	-0.465816000
H	-2.175155000	3.082322000	0.611856000
C	5.260886000	1.766388000	0.522920000
H	5.137155000	1.662594000	1.599720000
H	5.619380000	0.820338000	0.120428000
H	5.998670000	2.541511000	0.314367000

6. [$(SbPh_3)(CO)_4MoC(OEt)(C_4H_3NMe)$] (3) cis-syn (2)

Mo	1.125635000	-1.575717000	-0.486793000
N	4.408885000	1.531178000	0.627653000
O	-0.746293000	-4.134649000	-0.427516000
O	0.641960000	-1.699872000	-3.638913000
O	3.561108000	-3.519345000	-0.903047000
O	1.374595000	-1.964958000	2.679555000
O	2.539459000	1.262607000	-1.308653000
Sb	-1.158862000	0.017661000	0.092054000
C	-0.083132000	-3.189848000	-0.447099000
C	0.833223000	-1.588495000	-2.507163000
C	2.674284000	-2.797215000	-0.759326000
C	1.306811000	-1.776417000	1.548214000
C	2.544141000	0.199350000	-0.495138000
C	3.640241000	0.363591000	0.432528000
C	4.215729000	-0.616400000	1.258259000
H	3.888084000	-1.638012000	1.320515000
C	5.302544000	-0.059162000	1.934777000
H	5.958579000	-0.551180000	2.634633000
C	5.383449000	1.265027000	1.532109000

H	6.067879000	2.040826000	1.840169000
C	1.611634000	1.419990000	-2.400985000
H	0.601874000	1.214367000	-2.045225000
H	1.867114000	0.690946000	-3.170740000
C	1.735612000	2.839291000	-2.919366000
H	1.057915000	2.975247000	-3.765991000
H	1.466612000	3.564471000	-2.148762000
H	2.751851000	3.046265000	-3.262475000
C	4.222429000	2.866355000	0.064233000
H	3.193277000	3.198147000	0.189384000
H	4.885055000	3.547921000	0.598491000
H	4.467027000	2.881640000	-0.996873000
C	-2.824996000	0.142810000	-1.295080000
C	-4.133884000	0.372737000	-0.852456000
H	-4.340380000	0.477557000	0.206830000
C	-5.185770000	0.455201000	-1.763486000
H	-6.194859000	0.628998000	-1.405757000
C	-4.944021000	0.307155000	-3.128036000
H	-5.763739000	0.366821000	-3.835372000
C	-3.647583000	0.071879000	-3.579135000
H	-3.453588000	-0.055719000	-4.638432000
C	-2.595426000	-0.012226000	-2.667688000
H	-1.597842000	-0.217470000	-3.039607000
C	-0.909588000	2.146089000	0.483804000
C	0.127494000	2.548187000	1.336632000
H	0.783043000	1.808329000	1.786333000
C	0.332552000	3.897084000	1.623662000
H	1.129762000	4.190447000	2.298422000
C	-0.488651000	4.865881000	1.047974000
H	-0.329475000	5.915603000	1.268640000
C	-1.516121000	4.479095000	0.190694000
H	-2.158635000	5.227904000	-0.259974000
C	-1.728190000	3.127709000	-0.086553000
H	-2.538356000	2.843104000	-0.748590000
C	-2.284061000	-0.477450000	1.878468000
C	-2.551549000	-1.824265000	2.156448000
H	-2.193139000	-2.606272000	1.495499000
C	-3.281533000	-2.182671000	3.288098000
H	-3.480896000	-3.229344000	3.489571000
C	-3.747079000	-1.200607000	4.159980000
H	-4.310822000	-1.480252000	5.043056000
C	-3.481613000	0.140917000	3.895789000
H	-3.838168000	0.909797000	4.572758000
C	-2.754925000	0.501556000	2.761081000
H	-2.553829000	1.549819000	2.571654000

7. [$(SbPh_3)(CO)_4MoC(OEt)(C_8H_5S_2)$ (4) cis-syn-anti (1)

Mo	0.950574000	1.986564000	-0.820137000

C	0.156107000	1.352206000	-2.600199000
O	-0.214166000	1.050044000	-3.645566000
C	0.620188000	3.861920000	-1.407587000
O	0.461806000	4.951632000	-1.750967000
C	1.964503000	2.701005000	0.804431000
O	2.625473000	3.129889000	1.645591000
C	2.716754000	2.053232000	-1.815660000
O	3.702831000	2.120450000	-2.405721000
C	-1.069231000	1.910869000	0.149484000
O	-1.561403000	2.732756000	1.080842000
C	-0.807121000	3.800416000	1.696702000
H	-0.341139000	4.399911000	0.915817000
H	-0.028163000	3.353022000	2.314919000
C	-1.777621000	4.615111000	2.528650000
H	-1.239693000	5.427971000	3.022928000
H	-2.249490000	3.998063000	3.296161000
H	-2.558469000	5.050511000	1.901777000
C	-2.149732000	0.996958000	-0.179000000
C	-2.165200000	-0.117117000	-1.003292000
H	-1.302228000	-0.454297000	-1.554658000
C	-3.402804000	-0.776261000	-1.061918000
H	-3.582426000	-1.649681000	-1.674499000
C	-4.380968000	-0.183393000	-0.281142000
S	-3.747193000	1.203032000	0.559902000
Sb	1.651649000	-0.621668000	0.090886000
C	1.121370000	-1.264828000	2.096386000
C	2.050612000	-1.870070000	2.950450000
H	3.067901000	-2.039919000	2.616789000
C	1.681037000	-2.255774000	4.239008000
H	2.412712000	-2.719946000	4.891434000
C	0.379233000	-2.045380000	4.687596000
H	0.093692000	-2.345591000	5.689720000
C	-0.554353000	-1.445659000	3.844645000
H	-1.569822000	-1.278724000	4.186917000
C	-0.184259000	-1.054304000	2.559095000
H	-0.923672000	-0.586175000	1.918562000
C	3.764682000	-1.097942000	0.159302000
C	4.248374000	-2.366401000	-0.182774000
H	3.562428000	-3.142853000	-0.501759000
C	5.613758000	-2.642824000	-0.123512000
H	5.975208000	-3.628540000	-0.395860000
C	6.511005000	-1.656664000	0.280731000
H	7.572906000	-1.871832000	0.323931000
C	6.040163000	-0.391081000	0.623419000
H	6.733303000	0.382851000	0.933902000
C	4.676056000	-0.112435000	0.559331000
H	4.332606000	0.882247000	0.822452000
C	0.977597000	-2.373551000	-1.002125000
C	1.033829000	-2.351603000	-2.402011000
H	1.406889000	-1.475432000	-2.922954000
C	0.612904000	-3.451258000	-3.148091000

H	0.665487000	-3.420099000	-4.230774000
C	0.122720000	-4.584884000	-2.502336000
H	-0.208440000	-5.439734000	-3.081488000
C	0.058091000	-4.615666000	-1.110916000
H	-0.323375000	-5.495351000	-0.603824000
C	0.484011000	-3.517191000	-0.363906000
H	0.428806000	-3.555766000	0.718148000
C	-5.760055000	-0.587138000	-0.122331000
C	-6.822552000	0.140290000	0.367793000
H	-6.726723000	1.167114000	0.695213000
C	-8.046757000	-0.576322000	0.371236000
H	-8.986139000	-0.163339000	0.713251000
C	-7.917678000	-1.846842000	-0.115163000
H	-8.678370000	-2.603921000	-0.227229000
S	-6.288824000	-2.195765000	-0.580498000

8. [$(SbPh_3)(CO)_4MoC(OEt)(C_8H_5S_2)$] (4) cis-syn-anti (2)

Mo	0.296244000	-1.933521000	-0.250363000
Sb	2.045570000	0.278065000	0.184663000
S	-3.946789000	0.492121000	-1.007035000
S	-7.460492000	0.296261000	1.615840000
O	2.604835000	-3.821299000	0.847134000
O	-0.604162000	-1.545266000	2.794062000
O	-1.525501000	-4.491797000	-0.400211000
O	1.466229000	-2.685039000	-3.126695000
O	-1.482290000	0.070375000	-2.111099000
C	1.782606000	-3.116425000	0.451677000
C	-0.302896000	-1.645810000	1.689876000
C	-0.861687000	-3.550703000	-0.361768000
C	1.020429000	-2.361872000	-2.115045000
C	-1.418280000	-0.713868000	-1.030356000
C	-2.732913000	-0.657973000	-0.419846000
C	-3.276658000	-1.418531000	0.603130000
H	-2.732266000	-2.208629000	1.094343000
C	-4.608081000	-1.102657000	0.912910000
H	-5.183555000	-1.620735000	1.668511000
C	-5.128299000	-0.081533000	0.135466000
C	-0.385243000	0.280879000	-3.023790000
H	-0.291964000	-0.610024000	-3.647011000
H	0.533675000	0.409061000	-2.452178000
C	-0.706859000	1.510275000	-3.849501000
H	0.095755000	1.684934000	-4.570588000
H	-0.795317000	2.391855000	-3.211957000
H	-1.640528000	1.377111000	-4.400013000
C	-6.452973000	0.494862000	0.193921000
C	-7.116774000	1.236257000	-0.758872000
H	-6.686807000	1.466123000	-1.724835000
C	-8.418687000	1.635240000	-0.360847000
H	-9.088046000	2.214960000	-0.982044000

C	-8.746303000	1.198405000	0.891909000
H	-9.663608000	1.352666000	1.438814000
C	1.372726000	2.301362000	-0.242321000
C	0.057048000	2.648494000	0.091635000
H	-0.603047000	1.917464000	0.548254000
C	-0.427039000	3.931473000	-0.159491000
H	-1.446536000	4.184884000	0.109555000
C	0.397097000	4.882139000	-0.759255000
H	0.021212000	5.879504000	-0.958835000
C	1.704449000	4.545475000	-1.104198000
H	2.349124000	5.280649000	-1.573753000
C	2.190766000	3.263643000	-0.846154000
H	3.210544000	3.018441000	-1.120612000
C	3.982201000	0.354949000	-0.788923000
C	5.090176000	0.955390000	-0.177669000
H	5.000884000	1.383130000	0.814685000
C	6.321560000	0.998239000	-0.829907000
H	7.172198000	1.462567000	-0.342867000
C	6.461906000	0.440802000	-2.099330000
H	7.421259000	0.471227000	-2.603799000
C	5.368452000	-0.164805000	-2.713750000
H	5.473183000	-0.610335000	-3.696860000
C	4.137121000	-0.209616000	-2.061141000
H	3.304909000	-0.703987000	-2.550119000
C	2.709311000	0.596510000	2.222627000
C	2.742540000	1.868255000	2.805991000
H	2.425480000	2.737026000	2.240342000
C	3.176875000	2.031180000	4.121519000
H	3.194394000	3.021783000	4.562982000
C	3.584154000	0.927142000	4.866547000
H	3.919796000	1.055000000	5.889668000
C	3.554472000	-0.343083000	4.294552000
H	3.866571000	-1.207595000	4.869919000
C	3.116325000	-0.508030000	2.982169000
H	3.094852000	-1.506779000	2.558833000

9. [(CO)$_5$MoC(OEt)(C$_4$H$_3$S) ***anti***

Mo	1.901100000	3.643351000	6.040919000
C	0.404517000	3.721310000	7.463162000
C	3.397683000	3.721310000	7.463162000
C	3.363280000	3.755902000	4.597421000
C	0.438920000	3.755902000	4.597421000
O	-0.442280000	3.839900000	8.224051000
O	4.244480000	3.839900000	8.224051000
O	4.177401000	3.897202000	3.801496000
O	-0.375201000	3.897202000	3.801496000
C	1.901100000	5.682847000	6.068376000
O	1.901100000	6.830192000	6.086968000
C	1.901100000	1.391217000	6.091815000

C	1.901100000	0.561865000	7.293373000
O	1.901100000	0.546288000	5.068007000
S	1.901100000	1.240437000	8.907609000
C	1.901100000	-0.318831000	9.622676000
H	1.901100000	-0.413947000	10.698371000
C	1.901100000	-1.324035000	8.685019000
H	1.901100000	-2.375607000	8.938497000
C	1.901100000	-0.825689000	7.368415000
H	1.901100000	-1.445086000	6.483796000
C	1.901100000	0.963451000	3.682278000
H	1.013649000	1.569200000	3.502208000
H	2.788551000	1.569200000	3.502208000
C	1.901100000	-0.293157000	2.835319000
H	1.901100000	-0.019091000	1.777478000
H	1.013745000	-0.898221000	3.032707000
H	2.788455000	-0.898221000	3.032707000

10. [(CO)$_5$MoC(OEt)(C$_4$H$_3$S) ***syn***

Mo	-0.239711000	-1.202778000	0.000000000
C	-1.595514000	-0.735396000	1.481003000
C	-1.595514000	-0.735396000	-1.481003000
C	1.076183000	-1.805933000	-1.465084000
C	1.076183000	-1.805933000	1.465084000
O	-2.357510000	-0.513853000	2.306712000
O	-2.357510000	-0.513853000	-2.306712000
O	1.775310000	-2.206250000	-2.281537000
O	1.775310000	-2.206250000	2.281537000
C	-0.983296000	-3.102032000	0.000000000
O	-1.408707000	-4.167809000	0.000000000
C	0.487283000	0.927356000	0.000000000
C	-0.368479000	2.101272000	0.000000000
O	1.738334000	1.372068000	0.000000000
S	0.330362000	3.725696000	0.000000000
C	-1.230386000	4.443507000	0.000000000
H	-1.325560000	5.519456000	0.000000000
C	-2.239886000	3.513516000	0.000000000
H	-3.290601000	3.768984000	0.000000000
C	-1.751162000	2.190978000	0.000000000
H	-2.394847000	1.325833000	0.000000000
C	2.904682000	0.513721000	0.000000000
H	2.869220000	-0.116834000	0.887775000
H	2.869220000	-0.116834000	-0.887775000
C	4.123953000	1.413285000	0.000000000
H	5.027879000	0.799218000	0.000000000
H	4.140329000	2.049799000	0.886899000
H	4.140329000	2.049799000	-0.886899000

11. [(CO)$_5$MoC(OEt)(C$_4$H$_3$O) ***anti***

Mo	0.942909000	0.326536000	0.000000000
C	1.181308000	-1.117328000	1.462460000
C	1.181308000	-1.117328000	-1.462460000
C	0.829532000	1.769456000	-1.459910000
C	0.829532000	1.769456000	1.459910000
O	1.353662000	-1.906545000	2.272303000
O	1.353662000	-1.906545000	-2.272303000
O	0.829532000	2.577489000	-2.275026000
O	0.829532000	2.577489000	2.275026000
C	2.970889000	0.588838000	0.000000000
O	4.109600000	0.729784000	0.000000000
C	-1.246389000	-0.081104000	0.000000000
C	-1.815457000	-1.413102000	0.000000000
O	-2.282463000	0.750714000	0.000000000
O	-0.966032000	-2.494225000	0.000000000
C	-1.723310000	-3.605796000	0.000000000
H	-1.187129000	-4.540481000	0.000000000
C	-3.053886000	-3.291276000	0.000000000
H	-3.876312000	-3.988466000	0.000000000
C	-3.115641000	-1.876984000	0.000000000
H	-3.995412000	-1.255389000	0.000000000
C	-2.127208000	2.189566000	0.000000000
H	-1.563261000	2.476980000	0.887377000
H	-1.563261000	2.476980000	-0.887377000
C	-3.517591000	2.791736000	0.000000000
H	-3.443118000	3.881923000	0.000000000
H	-4.076071000	2.485934000	0.887187000
H	-4.076071000	2.485934000	-0.887187000

12. [(CO)$_5$MoC(OEt)(C$_4$H$_3$O) ***syn***

Mo	1.901100000	3.522227000	6.093225000
C	0.425742000	3.447829000	7.528950000
C	3.376458000	3.447829000	7.528950000
C	3.366843000	3.727375000	4.659952000
C	0.435357000	3.727375000	4.659952000
O	-0.394041000	3.440498000	8.329088000
O	4.196241000	3.440498000	8.329088000
O	4.183911000	3.910762000	3.876213000
O	-0.381711000	3.910762000	3.876213000
C	1.901100000	5.554253000	6.273360000
O	1.901100000	6.696598000	6.383540000
C	1.901100000	1.274964000	5.998964000
C	1.901100000	0.427149000	7.174331000
O	1.901100000	0.476656000	4.946095000
O	1.901100000	-0.947471000	7.007149000
C	1.901100000	-1.502566000	8.228754000
H	1.901100000	-2.580356000	8.257824000

C	1.901100000	-0.547537000	9.206661000
H	1.901100000	-0.714540000	10.271453000
C	1.901100000	0.694310000	8.529240000
H	1.901100000	1.668993000	8.983737000
C	1.901100000	0.960412000	3.582054000
H	1.013498000	1.574923000	3.432424000
H	2.788702000	1.574923000	3.432424000
C	1.901100000	-0.256441000	2.679391000
H	1.901100000	0.063474000	1.634475000
H	1.014841000	-0.869810000	2.853308000
H	2.787359000	-0.869810000	2.853308000

13. [(CO)$_5$MoC(OEt)(C$_4$H$_3$NMe) ***anti***

Mo	-1.041612000	-0.297682000	0.065192000
C	-1.014300000	-1.420247000	-1.661266000
C	-0.072919000	-1.747525000	1.162464000
C	-1.211725000	0.826710000	1.784866000
C	-2.217373000	1.042451000	-0.958485000
O	-1.060349000	-2.045244000	-2.621730000
O	0.391592000	-2.579395000	1.799708000
O	-1.341662000	1.436751000	2.746268000
O	-2.959382000	1.728157000	-1.503449000
C	-2.766915000	-1.231741000	0.589143000
O	-3.736710000	-1.763599000	0.898910000
C	0.967763000	0.726243000	-0.266963000
C	2.286224000	0.147151000	-0.089154000
O	1.178536000	2.039076000	-0.352634000
N	2.707297000	-1.145504000	-0.413886000
C	2.085778000	-2.095424000	-1.333782000
H	1.688743000	-1.575896000	-2.203544000
H	2.852305000	-2.793851000	-1.667438000
H	1.286710000	-2.656722000	-0.854219000
C	3.978973000	-1.313524000	0.039720000
H	4.509253000	-2.232096000	-0.157980000
C	4.400236000	-0.165491000	0.690613000
H	5.352271000	-0.027632000	1.177986000
C	3.354409000	0.757745000	0.587605000
H	3.317644000	1.752202000	1.000361000
C	0.123489000	3.019926000	-0.466305000
H	-0.419571000	2.829588000	-1.392548000
H	-0.561208000	2.912110000	0.374704000
C	0.781685000	4.385301000	-0.479272000
H	0.017135000	5.158374000	-0.589619000
H	1.482675000	4.471566000	-1.311877000
H	1.322517000	4.568109000	0.451597000

14. [(CO)$_5$MoC(OEt)(C$_4$H$_3$NMe) ***syn***

Mo	-1.217026000	-0.164201000	-0.002596000
C	-0.885251000	-1.578717000	-1.466632000
C	-0.929977000	-1.536742000	1.510137000
C	-1.712875000	1.218505000	1.434066000
C	-1.644467000	1.181827000	-1.495578000
O	-0.753425000	-2.366442000	-2.287784000
O	-0.815793000	-2.300668000	2.356094000
O	-2.066418000	1.962405000	2.234493000
O	-1.951324000	1.907230000	-2.331304000
C	-3.176303000	-0.693267000	-0.034081000
O	-4.283564000	-1.000031000	-0.052480000
C	1.013977000	0.332764000	0.021190000
C	2.069510000	-0.646093000	0.015337000
O	1.563710000	1.548810000	0.029632000
N	3.459955000	-0.395778000	-0.010824000
C	4.173760000	0.878182000	-0.062871000
H	3.961666000	1.480106000	0.819067000
H	5.240778000	0.658703000	-0.101679000
H	3.891727000	1.445568000	-0.948156000
C	4.114765000	-1.580387000	0.003478000
H	5.193676000	-1.607479000	-0.016640000
C	3.202409000	-2.625677000	0.041775000
H	3.441986000	-3.676476000	0.062484000
C	1.935186000	-2.045721000	0.047258000
H	0.999056000	-2.572527000	0.076030000
C	0.790775000	2.771352000	0.050261000
H	0.131979000	2.784838000	-0.816852000
H	0.185267000	2.783894000	0.955756000
C	1.764667000	3.933010000	0.022216000
H	1.206593000	4.872339000	0.041126000
H	2.372630000	3.918230000	-0.885056000
H	2.427509000	3.915034000	0.890147000

Crystallographic supplementary material

Complex **1:** Crystal data and structure refinement

Table 1. Crystal data and structure refinement for Complex **1**.

Empirical formula	C_{29} H_{23} Mo O_5 S Sb	
Formula weight	701.22	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	a = 10.310(2) Å	α= 90.00(3)°.
	b = 28.081(6) Å	β= 116.13(3)°.
	c = 10.917(2) Å	γ = 90.00(3)°.
Volume	2837.5(12) $Å^3$	
Z	4	
Density (calculated)	1.641 Mg/m^3	
Absorption coefficient	1.503 mm^{-1}	
F(000)	1384	
Crystal size	0.258 x 0.236 x 0.030 mm^3	
Theta range for data collection	2.201 to 25.347°.	
Index ranges	-12<=h<=12, -33<=k<=33, -13<=l<=13	
Reflections collected	73897	
Independent reflections	5194 [R(int) = 0.0395]	
Completeness to theta = 25.242°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5194 / 1 / 335	
Goodness-of-fit on F^2	1.268	
Final R indices [I>2sigma(I)]	R1 = 0.0391, wR2 = 0.0864	
R indices (all data)	R1 = 0.0420, wR2 = 0.0878	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.852 and -1.042 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Sb(1)	2746(1)	6510(1)	5431(1)	19(1)
Mo(1)	1985(1)	5842(1)	6848(1)	22(1)
S(1)	6220(2)	5634(1)	11236(2)	42(1)
O(1)	-1149(4)	6052(2)	4539(5)	56(1)
O(2)	1571(4)	6753(1)	8376(4)	38(1)
O(3)	557(5)	5180(2)	8214(5)	55(1)
O(4)	1999(5)	4967(2)	5021(4)	55(1)
O(6)	5346(4)	5531(1)	8467(4)	36(1)
C(1)	-19(6)	5974(2)	5372(6)	35(1)
C(2)	1766(5)	6421(2)	7872(5)	27(1)
C(3)	1108(6)	5417(2)	7729(6)	36(1)
C(4)	2064(6)	5282(2)	5701(5)	34(1)
C(6)	4136(5)	5680(2)	8511(5)	24(1)
C(7)	4489(5)	5711(2)	9947(5)	24(1)
C(8)	3572(5)	5813(2)	10545(5)	26(1)
C(9)	4288(7)	5832(2)	11989(6)	38(1)
C(10)	5686(7)	5751(2)	12474(6)	45(2)
C(11)	5419(6)	5464(2)	7171(7)	43(1)
C(12)	7045(8)	5432(3)	7595(9)	69(2)
C(20)	1954(5)	7202(2)	5532(5)	22(1)
C(21)	469(6)	7266(2)	4998(6)	37(1)
C(22)	-90(7)	7697(2)	5112(7)	45(2)
C(23)	801(7)	8067(2)	5776(7)	46(2)
C(24)	2275(7)	8013(2)	6307(7)	49(2)
C(25)	2851(6)	7579(2)	6190(6)	33(1)
C(30)	1711(5)	6427(2)	3246(4)	22(1)
C(31)	1611(5)	6808(2)	2397(5)	26(1)
C(32)	918(6)	6754(2)	995(5)	31(1)
C(33)	296(6)	6323(2)	431(5)	33(1)
C(34)	357(6)	5948(2)	1271(5)	35(1)
C(35)	1067(5)	5999(2)	2681(5)	29(1)
C(40)	4898(5)	6703(2)	5823(5)	23(1)
C(41)	5892(5)	6763(2)	7186(5)	30(1)
C(42)	7300(6)	6903(2)	7502(6)	38(1)

C(43)	7715(6)	6973(2)	6477(7)	43(2)
C(44)	6739(6)	6909(2)	5123(7)	46(2)
C(45)	5327(6)	6775(2)	4793(6)	32(1)

Table 3. Bond lengths [Å] and angles [°] for Complex 1.

Sb(1)-C(20)	2.130(5)
Sb(1)-C(40)	2.135(5)
Sb(1)-C(30)	2.153(4)
Sb(1)-Mo(1)	2.7552(9)
Mo(1)-C(3)	1.985(6)
Mo(1)-C(1)	2.017(5)
Mo(1)-C(4)	2.035(6)
Mo(1)-C(2)	2.039(6)
Mo(1)-C(6)	2.208(5)
S(1)-C(10)	1.700(7)
S(1)-C(7)	1.733(4)
O(1)-C(1)	1.140(6)
O(2)-C(2)	1.145(6)
O(3)-C(3)	1.145(7)
O(4)-C(4)	1.138(7)
O(6)-C(6)	1.337(6)
O(6)-C(11)	1.462(7)
C(6)-C(7)	1.447(7)
C(7)-C(8)	1.394(7)
C(8)-C(9)	1.417(7)
C(8)-H(8)	0.9500
C(9)-C(10)	1.318(9)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
C(11)-C(12)	1.533(8)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(20)-C(25)	1.380(7)
C(20)-C(21)	1.389(7)
C(21)-C(22)	1.368(8)
C(21)-H(21)	0.9500
C(22)-C(23)	1.365(9)
C(22)-H(22)	0.9500
C(23)-C(24)	1.376(9)

C(23)-H(23)	0.9500
C(24)-C(25)	1.386(8)
C(24)-H(24)	0.9500
C(25)-H(25)	0.9500
C(30)-C(35)	1.383(7)
C(30)-C(31)	1.388(7)
C(31)-C(32)	1.383(7)
C(31)-H(31)	0.9500
C(32)-C(33)	1.381(7)
C(32)-H(32)	0.9500
C(33)-C(34)	1.381(7)
C(33)-H(33)	0.9500
C(34)-C(35)	1.390(7)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500
C(40)-C(45)	1.393(7)
C(40)-C(41)	1.397(7)
C(41)-C(42)	1.393(7)
C(41)-H(41)	0.9500
C(42)-C(43)	1.376(9)
C(42)-H(42)	0.9500
C(43)-C(44)	1.386(9)
C(43)-H(43)	0.9500
C(44)-C(45)	1.390(7)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500

C(20)-Sb(1)-C(40)	98.41(18)
C(20)-Sb(1)-C(30)	98.12(18)
C(40)-Sb(1)-C(30)	102.35(18)
C(20)-Sb(1)-Mo(1)	112.41(12)
C(40)-Sb(1)-Mo(1)	125.98(13)
C(30)-Sb(1)-Mo(1)	115.07(13)
C(3)-Mo(1)-C(1)	88.4(2)
C(3)-Mo(1)-C(4)	89.0(2)
C(1)-Mo(1)-C(4)	87.4(2)
C(3)-Mo(1)-C(2)	91.7(2)
C(1)-Mo(1)-C(2)	88.3(2)
C(4)-Mo(1)-C(2)	175.6(2)

C(3)-Mo(1)-C(6)	89.08(19)
C(1)-Mo(1)-C(6)	177.5(2)
C(4)-Mo(1)-C(6)	92.8(2)
C(2)-Mo(1)-C(6)	91.53(18)
C(3)-Mo(1)-Sb(1)	170.16(16)
C(1)-Mo(1)-Sb(1)	82.67(15)
C(4)-Mo(1)-Sb(1)	94.72(15)
C(2)-Mo(1)-Sb(1)	83.92(13)
C(6)-Mo(1)-Sb(1)	99.83(12)
C(10)-S(1)-C(7)	92.5(3)
C(6)-O(6)-C(11)	121.4(4)
O(1)-C(1)-Mo(1)	179.4(5)
O(2)-C(2)-Mo(1)	175.8(4)
O(3)-C(3)-Mo(1)	177.6(5)
O(4)-C(4)-Mo(1)	174.9(5)
O(6)-C(6)-C(7)	105.3(4)
O(6)-C(6)-Mo(1)	130.6(4)
C(7)-C(6)-Mo(1)	124.1(3)
C(8)-C(7)-C(6)	128.4(4)
C(8)-C(7)-S(1)	108.2(4)
C(6)-C(7)-S(1)	123.4(4)
C(7)-C(8)-C(9)	113.6(5)
C(7)-C(8)-H(8)	123.2
C(9)-C(8)-H(8)	123.2
C(10)-C(9)-C(8)	112.5(6)
C(10)-C(9)-H(9)	123.8
C(8)-C(9)-H(9)	123.8
C(9)-C(10)-S(1)	113.2(5)
C(9)-C(10)-H(10)	123.4
S(1)-C(10)-H(10)	123.4
O(6)-C(11)-C(12)	103.3(5)
O(6)-C(11)-H(11A)	111.1
C(12)-C(11)-H(11A)	111.1
O(6)-C(11)-H(11B)	111.1
C(12)-C(11)-H(11B)	111.1
H(11A)-C(11)-H(11B)	109.1
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5

C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(25)-C(20)-C(21)	118.8(5)
C(25)-C(20)-Sb(1)	122.8(4)
C(21)-C(20)-Sb(1)	118.2(4)
C(22)-C(21)-C(20)	120.4(5)
C(22)-C(21)-H(21)	119.8
C(20)-C(21)-H(21)	119.8
C(23)-C(22)-C(21)	120.7(6)
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(22)-C(23)-C(24)	119.9(5)
C(22)-C(23)-H(23)	120.0
C(24)-C(23)-H(23)	120.0
C(23)-C(24)-C(25)	119.8(6)
C(23)-C(24)-H(24)	120.1
C(25)-C(24)-H(24)	120.1
C(20)-C(25)-C(24)	120.4(5)
C(20)-C(25)-H(25)	119.8
C(24)-C(25)-H(25)	119.8
C(35)-C(30)-C(31)	119.5(4)
C(35)-C(30)-Sb(1)	119.6(3)
C(31)-C(30)-Sb(1)	120.8(3)
C(32)-C(31)-C(30)	120.4(4)
C(32)-C(31)-H(31)	119.8
C(30)-C(31)-H(31)	119.8
C(33)-C(32)-C(31)	120.0(5)
C(33)-C(32)-H(32)	120.0
C(31)-C(32)-H(32)	120.0
C(32)-C(33)-C(34)	119.8(5)
C(32)-C(33)-H(33)	120.1
C(34)-C(33)-H(33)	120.1
C(33)-C(34)-C(35)	120.3(5)
C(33)-C(34)-H(34)	119.9
C(35)-C(34)-H(34)	119.9
C(30)-C(35)-C(34)	119.9(5)
C(30)-C(35)-H(35)	120.0
C(34)-C(35)-H(35)	120.0

C(45)-C(40)-C(41)	119.9(4)
C(45)-C(40)-Sb(1)	123.1(4)
C(41)-C(40)-Sb(1)	117.0(4)
C(42)-C(41)-C(40)	119.6(5)
C(42)-C(41)-H(41)	120.2
C(40)-C(41)-H(41)	120.2
C(43)-C(42)-C(41)	120.2(5)
C(43)-C(42)-H(42)	119.9
C(41)-C(42)-H(42)	119.9
C(42)-C(43)-C(44)	120.6(5)
C(42)-C(43)-H(43)	119.7
C(44)-C(43)-H(43)	119.7
C(43)-C(44)-C(45)	119.8(6)
C(43)-C(44)-H(44)	120.1
C(45)-C(44)-H(44)	120.1
C(44)-C(45)-C(40)	120.0(5)
C(44)-C(45)-H(45)	120.0
C(40)-C(45)-H(45)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Complex **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Sb(1)	18(1)	17(1)	20(1)	0(1)	7(1)	-1(1)
Mo(1)	18(1)	21(1)	22(1)	4(1)	4(1)	-5(1)
S(1)	28(1)	41(1)	46(1)	4(1)	5(1)	3(1)
O(1)	24(2)	56(3)	60(3)	16(2)	-7(2)	-9(2)
O(2)	44(2)	40(2)	37(2)	-3(2)	25(2)	1(2)
O(3)	50(3)	57(3)	54(3)	22(2)	19(2)	-20(2)
O(4)	78(3)	28(2)	38(2)	-9(2)	6(2)	-3(2)
O(6)	26(2)	32(2)	51(2)	-2(2)	18(2)	3(2)
C(1)	26(3)	32(3)	41(3)	5(2)	9(3)	-11(2)
C(2)	19(2)	36(3)	25(2)	9(2)	7(2)	-4(2)
C(3)	23(3)	38(3)	35(3)	6(2)	4(2)	-6(2)
C(4)	38(3)	25(3)	26(3)	4(2)	4(2)	-6(2)
C(6)	20(2)	17(2)	35(3)	-2(2)	13(2)	-3(2)
C(7)	17(2)	15(2)	27(2)	3(2)	-2(2)	1(2)
C(8)	28(3)	27(2)	19(2)	5(2)	7(2)	3(2)
C(9)	49(4)	31(3)	30(3)	1(2)	13(3)	-2(3)
C(10)	45(4)	39(3)	37(3)	4(3)	6(3)	-6(3)
C(11)	40(3)	27(3)	74(4)	-7(3)	36(3)	1(2)
C(12)	58(5)	64(5)	117(7)	-10(5)	69(5)	4(4)
C(20)	28(2)	21(2)	21(2)	5(2)	15(2)	3(2)
C(21)	24(3)	32(3)	53(4)	7(3)	15(3)	4(2)
C(22)	35(3)	39(3)	65(4)	14(3)	27(3)	14(3)
C(23)	58(4)	28(3)	56(4)	7(3)	29(3)	19(3)
C(24)	58(4)	25(3)	53(4)	-10(3)	16(3)	1(3)
C(25)	32(3)	24(3)	39(3)	-3(2)	11(2)	3(2)
C(30)	26(2)	26(2)	14(2)	-4(2)	9(2)	-1(2)
C(31)	31(3)	20(2)	28(3)	-1(2)	15(2)	1(2)
C(32)	37(3)	27(3)	28(3)	7(2)	15(2)	5(2)
C(33)	32(3)	40(3)	19(2)	0(2)	5(2)	-1(2)
C(34)	37(3)	31(3)	28(3)	-5(2)	8(2)	-12(2)
C(35)	31(3)	24(2)	26(3)	3(2)	6(2)	-4(2)
C(40)	18(2)	18(2)	32(3)	-2(2)	9(2)	1(2)
C(41)	26(3)	27(3)	33(3)	1(2)	9(2)	3(2)
C(42)	22(3)	30(3)	46(3)	-3(2)	0(2)	2(2)

C(43)	17(2)	38(3)	72(4)	-9(3)	17(3)	-2(2)
C(44)	32(3)	55(4)	59(4)	-10(3)	29(3)	-5(3)
C(45)	28(3)	39(3)	34(3)	-9(2)	17(2)	-4(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex **1**.

	x	y	z	U(eq)
H(8)	2564	5864	10033	31
H(9)	3813	5895	12545	46
H(10)	6330	5758	13419	53
H(11A)	4981	5737	6551	51
H(11B)	4920	5168	6712	51
H(12A)	7204	5346	6802	103
H(12B)	7475	5190	8306	103
H(12C)	7495	5742	7950	103
H(21)	-163	7010	4551	44
H(22)	-1107	7739	4725	53
H(23)	403	8362	5871	55
H(24)	2897	8272	6754	58
H(25)	3869	7540	6564	40
H(31)	2020	7107	2782	31
H(32)	870	7014	419	37
H(33)	-173	6285	-531	39
H(34)	-88	5653	884	41
H(35)	1110	5739	3255	35
H(41)	5610	6709	7894	36
H(42)	7976	6950	8427	46
H(43)	8678	7067	6701	52
H(44)	7036	6957	4422	55
H(45)	4654	6732	3865	38

Table 6. Torsion angles [°] for Complex **1**.

C(11)-O(6)-C(6)-C(7)	-178.9(4)
C(11)-O(6)-C(6)-Mo(1)	2.4(6)
O(6)-C(6)-C(7)-C(8)	-174.2(5)
Mo(1)-C(6)-C(7)-C(8)	4.5(7)
O(6)-C(6)-C(7)-S(1)	7.1(5)
Mo(1)-C(6)-C(7)-S(1)	-174.1(2)
C(10)-S(1)-C(7)-C(8)	-1.5(4)
C(10)-S(1)-C(7)-C(6)	177.4(4)
C(6)-C(7)-C(8)-C(9)	-177.9(5)
S(1)-C(7)-C(8)-C(9)	0.9(5)
C(7)-C(8)-C(9)-C(10)	0.3(7)
C(8)-C(9)-C(10)-S(1)	-1.5(7)
C(7)-S(1)-C(10)-C(9)	1.8(5)
C(6)-O(6)-C(11)-C(12)	164.6(5)
C(25)-C(20)-C(21)-C(22)	0.7(8)
Sb(1)-C(20)-C(21)-C(22)	176.0(4)
C(20)-C(21)-C(22)-C(23)	-1.4(9)
C(21)-C(22)-C(23)-C(24)	1.7(10)
C(22)-C(23)-C(24)-C(25)	-1.3(10)
C(21)-C(20)-C(25)-C(24)	-0.3(8)
Sb(1)-C(20)-C(25)-C(24)	-175.4(4)
C(23)-C(24)-C(25)-C(20)	0.6(9)
C(35)-C(30)-C(31)-C(32)	-2.4(7)
Sb(1)-C(30)-C(31)-C(32)	-178.7(4)
C(30)-C(31)-C(32)-C(33)	1.3(8)
C(31)-C(32)-C(33)-C(34)	0.6(8)
C(32)-C(33)-C(34)-C(35)	-1.3(9)
C(31)-C(30)-C(35)-C(34)	1.6(8)
Sb(1)-C(30)-C(35)-C(34)	177.9(4)
C(33)-C(34)-C(35)-C(30)	0.2(8)
C(45)-C(40)-C(41)-C(42)	1.2(7)
Sb(1)-C(40)-C(41)-C(42)	-178.1(4)
C(40)-C(41)-C(42)-C(43)	-1.1(8)
C(41)-C(42)-C(43)-C(44)	0.4(9)
C(42)-C(43)-C(44)-C(45)	0.4(9)
C(43)-C(44)-C(45)-C(40)	-0.3(9)
C(41)-C(40)-C(45)-C(44)	-0.4(8)

Sb(1)-C(40)-C(45)-C(44)	178.7(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for Complex **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(10)-H(10)...O(1)#1	0.95	2.48	3.157(7)	128.5
C(12)-H(12A)...O(4)#2	0.98	2.62	3.587(9)	170.3

Symmetry transformations used to generate equivalent atoms:

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

Complex **2:** Crystal data and structure refinement

Table 1. Crystal data and structure refinement for Complex **2**.

Empirical formula	$C_{29}\,H_{23}\,Mo\,O_6\,Sb$	
Formula weight	685.16	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.48(3) Å	α= 101.33(12)°.
	b = 10.84(4) Å	β= 91.72(14)°.
	c = 14.09(5) Å	γ = 118.44(8)°.
Volume	1366(8) $Å^3$	
Z	2	
Density (calculated)	1.666 Mg/m^3	
Absorption coefficient	1.488 mm^{-1}	
F(000)	676	
Crystal size	0.610 x 0.243 x 0.149 mm^3	
Theta range for data collection	2.202 to 25.678°.	
Index ranges	-12<=h<=12, -13<=k<=13, -17<=l<=17	
Reflections collected	40058	
Independent reflections	5195 [R(int) = 0.0438]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5195 / 0 / 334	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0268, wR2 = 0.0588	
R indices (all data)	R1 = 0.0385, wR2 = 0.0627	
Largest diff. peak and hole	1.608 and -0.632 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2380(1)	7385(1)	1704(1)	18(1)
Sb(1)	3451(1)	6429(1)	3040(1)	16(1)
O(1)	-730(3)	5045(3)	2061(2)	45(1)
O(2)	2019(3)	4923(3)	-122(2)	36(1)
O(3)	765(3)	8314(3)	338(2)	37(1)
O(4)	2546(3)	9610(3)	3629(2)	35(1)
O(6)	5141(3)	10191(3)	1325(2)	39(1)
O(7)	5252(3)	6963(3)	1158(2)	46(1)
C(1)	385(4)	5907(4)	1940(3)	27(1)
C(2)	2191(4)	5819(4)	542(3)	24(1)
C(3)	1390(4)	7999(4)	842(3)	24(1)
C(4)	2506(4)	8853(4)	2920(3)	24(1)
C(6)	4545(4)	8824(4)	1384(2)	22(1)
C(7)	5639(4)	8431(5)	1180(3)	37(1)
C(8)	7057(5)	9068(6)	1058(4)	53(1)
C(9)	7540(5)	8059(5)	926(3)	48(1)
C(10)	6434(6)	6811(7)	986(4)	57(1)
C(11)	4252(5)	10907(4)	1414(3)	46(1)
C(12)	5446(6)	12507(5)	1392(4)	57(1)
C(13)	5691(4)	7031(4)	3421(2)	22(1)
C(14)	6137(4)	6023(4)	3434(3)	30(1)
C(15)	7614(4)	6468(5)	3669(3)	39(1)
C(16)	8643(4)	7922(5)	3889(3)	42(1)
C(17)	8202(4)	8931(5)	3890(3)	39(1)
C(18)	6733(4)	8501(4)	3656(3)	30(1)
C(19)	2950(4)	6938(4)	4478(2)	21(1)
C(20)	1532(4)	6614(5)	4594(3)	35(1)
C(21)	1166(5)	6967(5)	5511(3)	43(1)
C(22)	2209(5)	7650(5)	6311(3)	45(1)
C(23)	3619(6)	7993(6)	6206(3)	62(2)
C(24)	3995(5)	7630(5)	5290(3)	45(1)
C(25)	2461(4)	4143(3)	2830(2)	20(1)
C(26)	1759(4)	3239(4)	1917(3)	34(1)
C(27)	1098(5)	1742(4)	1773(3)	38(1)

C(28)	1121(4)	1160(4)	2550(3)	32(1)
C(29)	1820(4)	2054(4)	3466(3)	29(1)
C(30)	2485(4)	3543(4)	3608(3)	24(1)

Table 3. Bond lengths [Å] and angles [°] for Complex **2**.

Mo(1)-C(3)	1.974(6)
Mo(1)-C(1)	2.028(6)
Mo(1)-C(2)	2.042(7)
Mo(1)-C(4)	2.050(7)
Mo(1)-C(6)	2.180(7)
Mo(1)-Sb(1)	2.761(6)
Sb(1)-C(25)	2.132(8)
Sb(1)-C(13)	2.135(8)
Sb(1)-C(19)	2.142(7)
O(1)-C(1)	1.141(5)
O(2)-C(2)	1.147(5)
O(3)-C(3)	1.153(5)
O(4)-C(4)	1.146(5)
O(6)-C(6)	1.327(6)
O(6)-C(11)	1.464(6)
O(7)-C(10)	1.348(7)
O(7)-C(7)	1.436(8)
C(6)-C(7)	1.421(6)
C(7)-C(8)	1.342(7)
C(8)-C(9)	1.393(8)
C(8)-H(8)	0.9500
C(9)-C(10)	1.318(8)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
C(11)-C(12)	1.591(7)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.381(6)
C(13)-C(18)	1.397(7)
C(14)-C(15)	1.391(7)
C(14)-H(14)	0.9500
C(15)-C(16)	1.382(8)
C(15)-H(15)	0.9500
C(16)-C(17)	1.376(7)

C(16)-H(16)	0.9500
C(17)-C(18)	1.387(7)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(24)	1.369(7)
C(19)-C(20)	1.378(7)
C(20)-C(21)	1.393(7)
C(20)-H(20)	0.9500
C(21)-C(22)	1.357(8)
C(21)-H(21)	0.9500
C(22)-C(23)	1.363(8)
C(22)-H(22)	0.9500
C(23)-C(24)	1.398(7)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-C(30)	1.385(6)
C(25)-C(26)	1.385(7)
C(26)-C(27)	1.394(7)
C(26)-H(26)	0.9500
C(27)-C(28)	1.371(7)
C(27)-H(27)	0.9500
C(28)-C(29)	1.385(7)
C(28)-H(28)	0.9500
C(29)-C(30)	1.387(7)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500

C(3)-Mo(1)-C(1)	88.8(3)
C(3)-Mo(1)-C(2)	89.4(3)
C(1)-Mo(1)-C(2)	86.7(3)
C(3)-Mo(1)-C(4)	92.8(3)
C(1)-Mo(1)-C(4)	90.4(3)
C(2)-Mo(1)-C(4)	176.24(13)
C(3)-Mo(1)-C(6)	92.9(3)
C(1)-Mo(1)-C(6)	175.29(14)
C(2)-Mo(1)-C(6)	89.0(3)
C(4)-Mo(1)-C(6)	93.9(3)
C(3)-Mo(1)-Sb(1)	172.46(10)
C(1)-Mo(1)-Sb(1)	84.6(3)

C(2)-Mo(1)-Sb(1)	93.8(3)
C(4)-Mo(1)-Sb(1)	83.6(3)
C(6)-Mo(1)-Sb(1)	93.9(3)
C(25)-Sb(1)-C(13)	99.89(17)
C(25)-Sb(1)-C(19)	98.7(2)
C(13)-Sb(1)-C(19)	98.7(2)
C(25)-Sb(1)-Mo(1)	116.0(2)
C(13)-Sb(1)-Mo(1)	126.40(16)
C(19)-Sb(1)-Mo(1)	112.6(2)
C(6)-O(6)-C(11)	119.4(4)
C(10)-O(7)-C(7)	107.9(4)
O(1)-C(1)-Mo(1)	178.0(4)
O(2)-C(2)-Mo(1)	176.9(3)
O(3)-C(3)-Mo(1)	177.6(3)
O(4)-C(4)-Mo(1)	175.9(3)
O(6)-C(6)-C(7)	105.0(4)
O(6)-C(6)-Mo(1)	130.4(3)
C(7)-C(6)-Mo(1)	124.7(4)
C(8)-C(7)-C(6)	138.6(5)
C(8)-C(7)-O(7)	104.6(4)
C(6)-C(7)-O(7)	116.6(3)
C(7)-C(8)-C(9)	109.9(5)
C(7)-C(8)-H(8)	125.1
C(9)-C(8)-H(8)	125.1
C(10)-C(9)-C(8)	107.8(5)
C(10)-C(9)-H(9)	126.1
C(8)-C(9)-H(9)	126.1
C(9)-C(10)-O(7)	109.7(5)
C(9)-C(10)-H(10)	125.1
O(7)-C(10)-H(10)	125.1
O(6)-C(11)-C(12)	100.8(5)
O(6)-C(11)-H(11A)	111.6
C(12)-C(11)-H(11A)	111.6
O(6)-C(11)-H(11B)	111.6
C(12)-C(11)-H(11B)	111.6
H(11A)-C(11)-H(11B)	109.4
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5

C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	119.5(4)
C(14)-C(13)-Sb(1)	122.3(3)
C(18)-C(13)-Sb(1)	118.2(3)
C(13)-C(14)-C(15)	120.2(4)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
C(16)-C(15)-C(14)	120.2(4)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(17)-C(16)-C(15)	119.8(5)
C(17)-C(16)-H(16)	120.1
C(15)-C(16)-H(16)	120.1
C(16)-C(17)-C(18)	120.5(4)
C(16)-C(17)-H(17)	119.7
C(18)-C(17)-H(17)	119.7
C(17)-C(18)-C(13)	119.8(4)
C(17)-C(18)-H(18)	120.1
C(13)-C(18)-H(18)	120.1
C(24)-C(19)-C(20)	118.2(4)
C(24)-C(19)-Sb(1)	122.7(4)
C(20)-C(19)-Sb(1)	119.1(3)
C(19)-C(20)-C(21)	121.1(4)
C(19)-C(20)-H(20)	119.5
C(21)-C(20)-H(20)	119.5
C(22)-C(21)-C(20)	120.3(5)
C(22)-C(21)-H(21)	119.8
C(20)-C(21)-H(21)	119.8
C(21)-C(22)-C(23)	119.3(4)
C(21)-C(22)-H(22)	120.4
C(23)-C(22)-H(22)	120.4
C(22)-C(23)-C(24)	120.8(4)
C(22)-C(23)-H(23)	119.6
C(24)-C(23)-H(23)	119.6
C(19)-C(24)-C(23)	120.4(5)
C(19)-C(24)-H(24)	119.8
C(23)-C(24)-H(24)	119.8

C(30)-C(25)-C(26)	119.2(4)
C(30)-C(25)-Sb(1)	120.5(3)
C(26)-C(25)-Sb(1)	120.3(3)
C(25)-C(26)-C(27)	120.8(4)
C(25)-C(26)-H(26)	119.6
C(27)-C(26)-H(26)	119.6
C(28)-C(27)-C(26)	119.5(4)
C(28)-C(27)-H(27)	120.2
C(26)-C(27)-H(27)	120.2
C(27)-C(28)-C(29)	120.2(4)
C(27)-C(28)-H(28)	119.9
C(29)-C(28)-H(28)	119.9
C(28)-C(29)-C(30)	120.3(4)
C(28)-C(29)-H(29)	119.8
C(30)-C(29)-H(29)	119.8
C(25)-C(30)-C(29)	120.0(4)
C(25)-C(30)-H(30)	120.0
C(29)-C(30)-H(30)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Complex **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	15(1)	17(1)	18(1)	6(1)	1(1)	5(1)
Sb(1)	15(1)	16(1)	16(1)	4(1)	2(1)	6(1)
O(1)	19(1)	49(2)	44(2)	20(2)	1(1)	-2(1)
O(2)	44(2)	30(2)	26(1)	0(1)	1(1)	15(1)
O(3)	30(2)	41(2)	42(2)	19(1)	-3(1)	16(1)
O(4)	48(2)	32(2)	32(2)	2(1)	5(1)	26(1)
O(6)	34(2)	33(2)	31(2)	12(1)	4(1)	0(1)
O(7)	43(2)	55(2)	52(2)	6(2)	9(2)	35(2)
C(1)	24(2)	32(2)	22(2)	6(2)	-2(2)	11(2)
C(2)	22(2)	22(2)	25(2)	11(2)	2(1)	6(2)
C(3)	18(2)	22(2)	28(2)	8(2)	3(1)	6(2)
C(4)	21(2)	23(2)	32(2)	14(2)	3(2)	12(2)
C(6)	19(2)	23(2)	17(2)	3(1)	-1(1)	6(2)
C(7)	14(2)	53(3)	24(2)	-11(2)	3(2)	7(2)
C(8)	35(2)	61(3)	50(3)	14(2)	10(2)	12(2)
C(9)	28(2)	60(3)	55(3)	6(2)	12(2)	25(2)
C(10)	53(3)	82(4)	54(3)	14(3)	21(2)	46(3)
C(11)	60(3)	17(2)	48(3)	6(2)	-26(2)	13(2)
C(12)	84(4)	27(2)	48(3)	10(2)	-14(3)	20(2)
C(13)	17(2)	29(2)	18(2)	7(1)	3(1)	8(2)
C(14)	23(2)	36(2)	31(2)	5(2)	5(2)	16(2)
C(15)	31(2)	57(3)	40(2)	15(2)	9(2)	31(2)
C(16)	19(2)	68(3)	37(2)	17(2)	6(2)	18(2)
C(17)	21(2)	42(2)	38(2)	13(2)	3(2)	2(2)
C(18)	25(2)	31(2)	31(2)	11(2)	4(2)	10(2)
C(19)	24(2)	21(2)	18(2)	7(1)	5(1)	10(2)
C(20)	28(2)	52(3)	28(2)	8(2)	7(2)	22(2)
C(21)	42(2)	55(3)	41(3)	16(2)	22(2)	29(2)
C(22)	62(3)	41(2)	26(2)	5(2)	20(2)	20(2)
C(23)	47(3)	85(4)	20(2)	-5(2)	2(2)	13(3)
C(24)	29(2)	64(3)	25(2)	3(2)	1(2)	12(2)
C(25)	17(2)	18(2)	25(2)	6(1)	3(1)	9(1)
C(26)	43(2)	21(2)	30(2)	9(2)	-5(2)	9(2)
C(27)	48(3)	20(2)	33(2)	4(2)	-10(2)	8(2)

C(28)	31(2)	20(2)	39(2)	9(2)	4(2)	7(2)
C(29)	36(2)	28(2)	34(2)	17(2)	13(2)	20(2)
C(30)	29(2)	25(2)	21(2)	5(1)	3(1)	14(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex **2**.

	x	y	z	U(eq)
H(8)	7644	10060	1060	64
H(9)	8495	8238	814	57
H(10)	6465	5936	917	69
H(11A)	3835	10878	2036	55
H(11B)	3449	10471	859	55
H(12A)	4988	13117	1447	85
H(12B)	6235	12896	1941	85
H(12C)	5852	12492	775	85
H(14)	5434	5022	3281	36
H(15)	7916	5771	3678	46
H(16)	9653	8223	4040	50
H(17)	8909	9930	4051	47
H(18)	6435	9203	3657	36
H(20)	793	6142	4039	42
H(21)	181	6730	5577	51
H(22)	1959	7886	6938	54
H(23)	4356	8486	6762	74
H(24)	4980	7864	5230	54
H(26)	1727	3643	1382	41
H(27)	635	1131	1142	46
H(28)	656	141	2459	38
H(29)	1843	1646	3999	35
H(30)	2956	4152	4239	29

Table 6. Torsion angles [°] for Complex **2**.

C(11)-O(6)-C(6)-C(7)	174.7(3)
C(11)-O(6)-C(6)-Mo(1)	-4.8(5)
O(6)-C(6)-C(7)-C(8)	8.7(7)
Mo(1)-C(6)-C(7)-C(8)	-171.7(5)
O(6)-C(6)-C(7)-O(7)	-177.6(3)
Mo(1)-C(6)-C(7)-O(7)	2.0(5)
C(10)-O(7)-C(7)-C(8)	-2.5(5)
C(10)-O(7)-C(7)-C(6)	-178.2(4)
C(6)-C(7)-C(8)-C(9)	176.3(5)
O(7)-C(7)-C(8)-C(9)	2.2(5)
C(7)-C(8)-C(9)-C(10)	-1.1(6)
C(8)-C(9)-C(10)-O(7)	-0.5(6)
C(7)-O(7)-C(10)-C(9)	1.9(5)
C(6)-O(6)-C(11)-C(12)	175.3(3)
C(18)-C(13)-C(14)-C(15)	-0.7(5)
Sb(1)-C(13)-C(14)-C(15)	178.7(3)
C(13)-C(14)-C(15)-C(16)	-0.1(6)
C(14)-C(15)-C(16)-C(17)	0.9(6)
C(15)-C(16)-C(17)-C(18)	-0.9(6)
C(16)-C(17)-C(18)-C(13)	0.2(6)
C(14)-C(13)-C(18)-C(17)	0.7(5)
Sb(1)-C(13)-C(18)-C(17)	-178.8(3)
C(24)-C(19)-C(20)-C(21)	-0.6(6)
Sb(1)-C(19)-C(20)-C(21)	-177.9(3)
C(19)-C(20)-C(21)-C(22)	0.4(7)
C(20)-C(21)-C(22)-C(23)	0.4(7)
C(21)-C(22)-C(23)-C(24)	-1.1(8)
C(20)-C(19)-C(24)-C(23)	-0.1(7)
Sb(1)-C(19)-C(24)-C(23)	177.1(4)
C(22)-C(23)-C(24)-C(19)	0.9(8)
C(30)-C(25)-C(26)-C(27)	-0.9(6)
Sb(1)-C(25)-C(26)-C(27)	-179.5(3)
C(25)-C(26)-C(27)-C(28)	1.3(7)
C(26)-C(27)-C(28)-C(29)	-1.2(7)
C(27)-C(28)-C(29)-C(30)	0.9(6)
C(26)-C(25)-C(30)-C(29)	0.5(5)
Sb(1)-C(25)-C(30)-C(29)	179.1(3)

C(28)-C(29)-C(30)-C(25)	-0.5(6)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for Complex **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

Complex **4:** Crystal data and structure refinement

Table 1. Crystal data and structure refinement for Complex **4**.

Empirical formula	C_{33} H_{25} Mo O_5 S_2 Sb	
Formula weight	783.34	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.6033(15) Å	α= 71.439(4)°.
	b = 11.9518(17) Å	β= 75.642(4)°.
	c = 15.980(2) Å	γ = 67.086(4)°.
Volume	1585.3(4) $Å^3$	
Z	2	
Density (calculated)	1.641 Mg/m^3	
Absorption coefficient	1.418 mm^{-1}	
F(000)	776	
Crystal size	0.171 x 0.144 x 0.048 mm^3	
Theta range for data collection	2.326 to 25.348°.	
Index ranges	-11<=h<=11, -14<=k<=14, -19<=l<=19	
Reflections collected	35775	
Independent reflections	5799 [R(int) = 0.0547]	
Completeness to theta = 25.242°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5799 / 0 / 380	
Goodness-of-fit on F^2	1.127	
Final R indices [I>2sigma(I)]	R1 = 0.0469, wR2 = 0.0991	
R indices (all data)	R1 = 0.0646, wR2 = 0.1096	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.774 and -1.248 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2769(1)	-1331(1)	-3073(1)	22(1)
Sb(1)	5645(1)	-3096(1)	-2867(1)	24(1)
S(1)	1408(2)	-1583(2)	107(1)	30(1)
S(2)	-1950(2)	-3188(2)	1864(1)	42(1)
O(1)	3178(5)	-1613(5)	-5036(3)	39(1)
O(2)	1598(6)	-3660(5)	-2379(4)	49(1)
O(3)	-641(6)	352(4)	-3227(3)	42(1)
O(4)	3982(5)	944(4)	-4163(3)	40(1)
O(6)	3170(5)	-618(4)	-1375(3)	31(1)
C(1)	3053(7)	-1547(6)	-4314(4)	28(1)
C(2)	2028(7)	-2829(6)	-2594(5)	33(2)
C(3)	624(8)	-247(6)	-3177(4)	29(1)
C(4)	3571(7)	148(6)	-3733(4)	29(1)
C(6)	2412(7)	-1061(5)	-1726(4)	25(1)
C(7)	1257(7)	-1400(5)	-1007(4)	26(1)
C(8)	-27(7)	-1628(6)	-1036(4)	32(2)
C(9)	-849(8)	-1950(6)	-197(4)	35(2)
C(10)	-213(7)	-1989(6)	498(4)	31(1)
C(11)	4421(7)	-211(6)	-1888(5)	32(2)
C(12)	5284(9)	-175(7)	-1235(5)	48(2)
C(13)	-701(7)	-2346(6)	1448(4)	30(1)
C(14)	-296(8)	-2152(6)	2145(4)	35(2)
C(15)	-961(8)	-2676(7)	2982(5)	42(2)
C(16)	-1879(9)	-3263(7)	2933(5)	47(2)
C(20)	6476(7)	-3685(5)	-1627(4)	27(1)
C(21)	5436(8)	-3582(6)	-843(4)	34(2)
C(22)	5945(8)	-3974(6)	-21(5)	38(2)
C(23)	7483(8)	-4491(7)	42(5)	40(2)
C(24)	8515(9)	-4595(8)	-733(5)	44(2)
C(25)	8048(8)	-4169(7)	-1565(4)	38(2)
C(30)	7672(7)	-2899(6)	-3733(4)	25(1)
C(31)	8804(8)	-3916(6)	-4011(4)	34(2)
C(32)	10131(8)	-3763(7)	-4565(5)	40(2)
C(33)	10325(8)	-2618(7)	-4839(4)	36(2)

C(34)	9202(8)	-1607(7)	-4557(5)	37(2)
C(35)	7871(8)	-1736(6)	-4010(4)	33(2)
C(40)	5840(7)	-4884(5)	-2981(4)	26(1)
C(41)	6405(7)	-5994(6)	-2344(5)	32(2)
C(42)	6467(8)	-7125(6)	-2442(5)	39(2)
C(43)	6043(8)	-7181(6)	-3176(5)	39(2)
C(44)	5481(9)	-6100(7)	-3808(5)	47(2)
C(45)	5361(9)	-4954(7)	-3711(5)	43(2)

Table 3. Bond lengths [Å] and angles [°] for Complex **4**.

Mo(1)-C(3)	1.976(7)
Mo(1)-C(1)	2.020(7)
Mo(1)-C(2)	2.037(7)
Mo(1)-C(4)	2.073(7)
Mo(1)-C(6)	2.202(6)
Mo(1)-Sb(1)	2.7674(7)
Sb(1)-C(20)	2.124(6)
Sb(1)-C(40)	2.134(6)
Sb(1)-C(30)	2.139(6)
S(1)-C(10)	1.721(7)
S(1)-C(7)	1.758(6)
S(2)-C(16)	1.699(8)
S(2)-C(13)	1.737(7)
O(1)-C(1)	1.153(7)
O(2)-C(2)	1.143(8)
O(3)-C(3)	1.152(7)
O(4)-C(4)	1.129(8)
O(6)-C(6)	1.347(7)
O(6)-C(11)	1.437(8)
C(6)-C(7)	1.461(9)
C(7)-C(8)	1.377(9)
C(8)-C(9)	1.397(9)
C(8)-H(8)	0.9500
C(9)-C(10)	1.374(9)
C(9)-H(9)	0.9500
C(10)-C(13)	1.448(9)
C(11)-C(12)	1.505(9)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.375(9)
C(14)-C(15)	1.395(10)
C(14)-H(14)	0.9500
C(15)-C(16)	1.352(11)
C(15)-H(15)	0.9500

C(16)-H(16)	0.9500
C(20)-C(21)	1.402(9)
C(20)-C(25)	1.408(9)
C(21)-C(22)	1.390(9)
C(21)-H(21)	0.9500
C(22)-C(23)	1.377(10)
C(22)-H(22)	0.9500
C(23)-C(24)	1.387(10)
C(23)-H(23)	0.9500
C(24)-C(25)	1.383(9)
C(24)-H(24)	0.9500
C(25)-H(25)	0.9500
C(30)-C(31)	1.390(8)
C(30)-C(35)	1.393(9)
C(31)-C(32)	1.400(9)
C(31)-H(31)	0.9500
C(32)-C(33)	1.370(10)
C(32)-H(32)	0.9500
C(33)-C(34)	1.385(9)
C(33)-H(33)	0.9500
C(34)-C(35)	1.391(9)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500
C(40)-C(45)	1.393(9)
C(40)-C(41)	1.394(9)
C(41)-C(42)	1.386(9)
C(41)-H(41)	0.9500
C(42)-C(43)	1.362(10)
C(42)-H(42)	0.9500
C(43)-C(44)	1.371(10)
C(43)-H(43)	0.9500
C(44)-C(45)	1.385(10)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500

C(3)-Mo(1)-C(1)	90.4(2)
C(3)-Mo(1)-C(2)	87.9(3)
C(1)-Mo(1)-C(2)	88.6(3)
C(3)-Mo(1)-C(4)	92.4(2)

C(1)-Mo(1)-C(4)	83.4(2)
C(2)-Mo(1)-C(4)	172.0(3)
C(3)-Mo(1)-C(6)	88.4(2)
C(1)-Mo(1)-C(6)	178.8(2)
C(2)-Mo(1)-C(6)	91.7(2)
C(4)-Mo(1)-C(6)	96.3(2)
C(3)-Mo(1)-Sb(1)	172.94(18)
C(1)-Mo(1)-Sb(1)	88.85(17)
C(2)-Mo(1)-Sb(1)	85.04(18)
C(4)-Mo(1)-Sb(1)	94.46(17)
C(6)-Mo(1)-Sb(1)	92.39(15)
C(20)-Sb(1)-C(40)	98.5(2)
C(20)-Sb(1)-C(30)	98.5(2)
C(40)-Sb(1)-C(30)	99.0(2)
C(20)-Sb(1)-Mo(1)	120.11(16)
C(40)-Sb(1)-Mo(1)	112.94(16)
C(30)-Sb(1)-Mo(1)	123.23(16)
C(10)-S(1)-C(7)	92.2(3)
C(16)-S(2)-C(13)	91.8(4)
C(6)-O(6)-C(11)	122.0(5)
O(1)-C(1)-Mo(1)	176.8(5)
O(2)-C(2)-Mo(1)	175.7(6)
O(3)-C(3)-Mo(1)	177.9(6)
O(4)-C(4)-Mo(1)	173.7(6)
O(6)-C(6)-C(7)	106.1(5)
O(6)-C(6)-Mo(1)	130.1(4)
C(7)-C(6)-Mo(1)	123.8(4)
C(8)-C(7)-C(6)	130.4(6)
C(8)-C(7)-S(1)	109.5(5)
C(6)-C(7)-S(1)	120.1(5)
C(7)-C(8)-C(9)	113.7(6)
C(7)-C(8)-H(8)	123.2
C(9)-C(8)-H(8)	123.2
C(10)-C(9)-C(8)	113.9(6)
C(10)-C(9)-H(9)	123.0
C(8)-C(9)-H(9)	123.0
C(9)-C(10)-C(13)	129.1(6)
C(9)-C(10)-S(1)	110.7(5)
C(13)-C(10)-S(1)	120.2(5)

O(6)-C(11)-C(12)	106.9(6)
O(6)-C(11)-H(11A)	110.3
C(12)-C(11)-H(11A)	110.3
O(6)-C(11)-H(11B)	110.3
C(12)-C(11)-H(11B)	110.3
H(11A)-C(11)-H(11B)	108.6
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(10)	130.0(6)
C(14)-C(13)-S(2)	109.5(5)
C(10)-C(13)-S(2)	120.5(5)
C(13)-C(14)-C(15)	113.8(7)
C(13)-C(14)-H(14)	123.1
C(15)-C(14)-H(14)	123.1
C(16)-C(15)-C(14)	112.5(7)
C(16)-C(15)-H(15)	123.7
C(14)-C(15)-H(15)	123.7
C(15)-C(16)-S(2)	112.4(6)
C(15)-C(16)-H(16)	123.8
S(2)-C(16)-H(16)	123.8
C(21)-C(20)-C(25)	118.4(6)
C(21)-C(20)-Sb(1)	119.4(5)
C(25)-C(20)-Sb(1)	122.1(5)
C(22)-C(21)-C(20)	120.8(6)
C(22)-C(21)-H(21)	119.6
C(20)-C(21)-H(21)	119.6
C(23)-C(22)-C(21)	120.6(6)
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(22)-C(23)-C(24)	118.7(6)
C(22)-C(23)-H(23)	120.7
C(24)-C(23)-H(23)	120.7
C(25)-C(24)-C(23)	122.1(7)
C(25)-C(24)-H(24)	118.9
C(23)-C(24)-H(24)	118.9

C(24)-C(25)-C(20)	119.2(6)
C(24)-C(25)-H(25)	120.4
C(20)-C(25)-H(25)	120.4
C(31)-C(30)-C(35)	119.5(6)
C(31)-C(30)-Sb(1)	121.2(5)
C(35)-C(30)-Sb(1)	119.3(4)
C(30)-C(31)-C(32)	119.8(6)
C(30)-C(31)-H(31)	120.1
C(32)-C(31)-H(31)	120.1
C(33)-C(32)-C(31)	120.6(6)
C(33)-C(32)-H(32)	119.7
C(31)-C(32)-H(32)	119.7
C(32)-C(33)-C(34)	119.5(6)
C(32)-C(33)-H(33)	120.2
C(34)-C(33)-H(33)	120.2
C(33)-C(34)-C(35)	120.8(6)
C(33)-C(34)-H(34)	119.6
C(35)-C(34)-H(34)	119.6
C(34)-C(35)-C(30)	119.7(6)
C(34)-C(35)-H(35)	120.2
C(30)-C(35)-H(35)	120.2
C(45)-C(40)-C(41)	118.0(6)
C(45)-C(40)-Sb(1)	119.1(5)
C(41)-C(40)-Sb(1)	122.8(5)
C(42)-C(41)-C(40)	120.2(6)
C(42)-C(41)-H(41)	119.9
C(40)-C(41)-H(41)	119.9
C(43)-C(42)-C(41)	120.9(7)
C(43)-C(42)-H(42)	119.6
C(41)-C(42)-H(42)	119.6
C(42)-C(43)-C(44)	119.8(7)
C(42)-C(43)-H(43)	120.1
C(44)-C(43)-H(43)	120.1
C(43)-C(44)-C(45)	120.4(7)
C(43)-C(44)-H(44)	119.8
C(45)-C(44)-H(44)	119.8
C(44)-C(45)-C(40)	120.6(7)
C(44)-C(45)-H(45)	119.7
C(40)-C(45)-H(45)	119.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Complex **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	19(1)	18(1)	27(1)	-9(1)	-4(1)	-2(1)
Sb(1)	21(1)	19(1)	30(1)	-10(1)	-4(1)	-1(1)
S(1)	26(1)	31(1)	32(1)	-13(1)	-5(1)	-5(1)
S(2)	44(1)	41(1)	40(1)	-14(1)	3(1)	-16(1)
O(1)	43(3)	45(3)	32(3)	-18(2)	-1(2)	-16(2)
O(2)	46(3)	35(3)	67(4)	-16(3)	0(3)	-18(2)
O(3)	41(3)	33(3)	41(3)	-12(2)	-13(2)	8(2)
O(4)	41(3)	32(3)	46(3)	-5(2)	0(2)	-17(2)
O(6)	31(2)	33(2)	32(2)	-12(2)	-9(2)	-8(2)
C(1)	21(3)	27(3)	38(4)	-10(3)	-5(3)	-7(3)
C(2)	27(3)	24(3)	43(4)	-14(3)	-2(3)	-3(3)
C(3)	33(4)	26(3)	30(3)	-12(3)	-3(3)	-10(3)
C(4)	24(3)	29(3)	32(3)	-11(3)	-6(3)	-3(3)
C(6)	25(3)	15(3)	29(3)	-4(2)	-8(3)	2(2)
C(7)	23(3)	22(3)	30(3)	-10(3)	-7(3)	1(2)
C(8)	35(4)	37(4)	28(3)	-12(3)	-8(3)	-11(3)
C(9)	27(3)	40(4)	37(4)	-15(3)	-3(3)	-8(3)
C(10)	23(3)	28(3)	38(4)	-14(3)	-3(3)	-1(3)
C(11)	30(4)	25(3)	45(4)	-12(3)	-4(3)	-11(3)
C(12)	53(5)	48(5)	55(5)	-8(4)	-22(4)	-23(4)
C(13)	26(3)	22(3)	35(4)	-12(3)	-1(3)	1(3)
C(14)	30(4)	30(4)	40(4)	-12(3)	-8(3)	1(3)
C(15)	37(4)	45(4)	36(4)	-15(3)	-10(3)	2(3)
C(16)	51(5)	41(4)	31(4)	-4(3)	6(3)	-9(4)
C(20)	25(3)	21(3)	35(4)	-11(3)	-6(3)	-4(3)
C(21)	26(3)	30(4)	38(4)	-5(3)	-2(3)	-5(3)
C(22)	40(4)	35(4)	33(4)	-11(3)	1(3)	-9(3)
C(23)	49(4)	42(4)	34(4)	-10(3)	-15(3)	-13(3)
C(24)	36(4)	64(5)	42(4)	-17(4)	-12(3)	-20(4)
C(25)	30(4)	56(5)	26(3)	-18(3)	-2(3)	-8(3)
C(30)	21(3)	26(3)	25(3)	-10(3)	-5(2)	-2(2)
C(31)	38(4)	25(3)	38(4)	-11(3)	2(3)	-10(3)
C(32)	30(4)	41(4)	44(4)	-17(3)	-1(3)	-4(3)
C(33)	28(4)	47(4)	34(4)	-14(3)	-1(3)	-15(3)

C(34)	35(4)	34(4)	44(4)	-8(3)	-3(3)	-16(3)
C(35)	37(4)	23(3)	38(4)	-13(3)	-5(3)	-6(3)
C(40)	20(3)	21(3)	39(4)	-12(3)	-2(3)	-4(2)
C(41)	25(3)	31(4)	41(4)	-13(3)	-6(3)	-8(3)
C(42)	43(4)	27(4)	45(4)	-6(3)	-11(3)	-11(3)
C(43)	36(4)	28(4)	52(4)	-20(3)	-2(3)	-5(3)
C(44)	63(5)	38(4)	47(4)	-23(4)	-17(4)	-7(4)
C(45)	59(5)	29(4)	41(4)	-10(3)	-19(4)	-7(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex **4**.

	x	y	z	U(eq)
H(8)	-327	-1572	-1576	38
H(9)	-1764	-2126	-114	41
H(11A)	4035	632	-2291	39
H(11B)	5096	-802	-2255	39
H(12A)	6192	40	-1557	73
H(12B)	5595	-999	-814	73
H(12C)	4626	458	-907	73
H(14)	374	-1703	2063	42
H(15)	-788	-2625	3527	50
H(16)	-2423	-3672	3439	56
H(21)	4371	-3242	-874	41
H(22)	5225	-3884	503	46
H(23)	7830	-4771	605	48
H(24)	9575	-4971	-691	53
H(25)	8781	-4202	-2088	45
H(31)	8677	-4713	-3826	41
H(32)	10904	-4460	-4753	48
H(33)	11224	-2518	-5220	43
H(34)	9342	-815	-4740	45
H(35)	7102	-1034	-3826	39
H(41)	6748	-5975	-1842	38
H(42)	6810	-7870	-1990	46
H(43)	6137	-7967	-3249	46
H(44)	5172	-6138	-4317	57
H(45)	4949	-4209	-4147	52

Table 6. Torsion angles [°] for Complex **4**.

C(11)-O(6)-C(6)-C(7)	178.8(5)
C(11)-O(6)-C(6)-Mo(1)	0.8(8)
O(6)-C(6)-C(7)-C(8)	163.7(6)
Mo(1)-C(6)-C(7)-C(8)	-18.2(9)
O(6)-C(6)-C(7)-S(1)	-16.7(6)
Mo(1)-C(6)-C(7)-S(1)	161.4(3)
C(10)-S(1)-C(7)-C(8)	1.2(5)
C(10)-S(1)-C(7)-C(6)	-178.5(5)
C(6)-C(7)-C(8)-C(9)	179.0(6)
S(1)-C(7)-C(8)-C(9)	-0.6(7)
C(7)-C(8)-C(9)-C(10)	-0.6(8)
C(8)-C(9)-C(10)-C(13)	-176.5(6)
C(8)-C(9)-C(10)-S(1)	1.5(7)
C(7)-S(1)-C(10)-C(9)	-1.5(5)
C(7)-S(1)-C(10)-C(13)	176.7(5)
C(6)-O(6)-C(11)-C(12)	-162.5(5)
C(9)-C(10)-C(13)-C(14)	-164.8(7)
S(1)-C(10)-C(13)-C(14)	17.4(9)
C(9)-C(10)-C(13)-S(2)	17.1(9)
S(1)-C(10)-C(13)-S(2)	-160.7(4)
C(16)-S(2)-C(13)-C(14)	-0.5(5)
C(16)-S(2)-C(13)-C(10)	178.0(5)
C(10)-C(13)-C(14)-C(15)	-177.7(6)
S(2)-C(13)-C(14)-C(15)	0.5(7)
C(13)-C(14)-C(15)-C(16)	-0.4(9)
C(14)-C(15)-C(16)-S(2)	0.0(8)
C(13)-S(2)-C(16)-C(15)	0.3(6)
C(25)-C(20)-C(21)-C(22)	-1.3(10)
Sb(1)-C(20)-C(21)-C(22)	179.2(5)
C(20)-C(21)-C(22)-C(23)	-1.1(10)
C(21)-C(22)-C(23)-C(24)	1.0(11)
C(22)-C(23)-C(24)-C(25)	1.6(12)
C(23)-C(24)-C(25)-C(20)	-4.1(12)
C(21)-C(20)-C(25)-C(24)	3.8(10)
Sb(1)-C(20)-C(25)-C(24)	-176.7(5)
C(35)-C(30)-C(31)-C(32)	0.0(10)
Sb(1)-C(30)-C(31)-C(32)	-178.8(5)

C(30)-C(31)-C(32)-C(33)	-0.2(11)
C(31)-C(32)-C(33)-C(34)	0.6(11)
C(32)-C(33)-C(34)-C(35)	-0.9(11)
C(33)-C(34)-C(35)-C(30)	0.7(10)
C(31)-C(30)-C(35)-C(34)	-0.3(9)
Sb(1)-C(30)-C(35)-C(34)	178.5(5)
C(45)-C(40)-C(41)-C(42)	-0.6(10)
Sb(1)-C(40)-C(41)-C(42)	178.3(5)
C(40)-C(41)-C(42)-C(43)	2.9(10)
C(41)-C(42)-C(43)-C(44)	-3.0(11)
C(42)-C(43)-C(44)-C(45)	0.9(12)
C(43)-C(44)-C(45)-C(40)	1.4(12)
C(41)-C(40)-C(45)-C(44)	-1.5(11)
Sb(1)-C(40)-C(45)-C(44)	179.6(6)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for Complex **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)