# *E versus Z* isomers of Fischer aminocarbene complex $[Mo(CO)_4(PPh_3)\{C(NHCy)(2\text{-furyl})\}]$: N–H···O *versus* C–H···O intramolecular hydrogen bonds

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Supporting information

## Optimized Cartesian coordinates (Å)

DFT calculations: Geometries were optimized in gas phase with the B3LYP functional and the triple-ζ basis set 6-311G(d,p) on all atoms except tungsten, where def2-TZVPP [1] was used.

1 $[Mo(CO)_4(PPh_3)\{C(NC_6H_{12})(C_4H_3O)\}]$, trans-anti,Z

| | | | |
|---|---|---|---|
| C | 0.129423000 | 1.915503000 | -1.290320000 |
| C | 0.146954000 | 1.576528000 | 1.695186000 |
| C | 1.011612000 | -1.091130000 | 1.332945000 |
| C | 1.012666000 | -0.843650000 | -1.489230000 |
| C | 2.423994000 | 4.746901000 | 0.295988000 |
| C | 2.614547000 | 1.172936000 | 0.087234000 |
| C | 2.892836000 | 2.614381000 | 0.023120000 |
| C | 3.616306000 | 4.714440000 | -0.358697000 |
| C | 3.923914000 | 3.334838000 | -0.535778000 |
| C | 4.026088000 | -0.931065000 | 0.025477000 |
| C | 4.737637000 | -1.423328000 | 1.296355000 |
| C | 4.842104000 | -1.263258000 | -1.236076000 |
| C | 5.050125000 | -2.924532000 | 1.212006000 |
| C | 5.155170000 | -2.764932000 | -1.315744000 |
| C | 5.857602000 | -3.267566000 | -0.047215000 |
| C | -1.983582000 | -2.346425000 | 1.883477000 |
| C | -2.065927000 | -1.104156000 | -2.695657000 |
| C | -2.377897000 | -2.991478000 | 3.050932000 |
| C | -2.440367000 | -1.904840000 | -3.769621000 |
| C | -2.455472000 | -1.428500000 | -1.389008000 |
| C | -2.563442000 | -1.125953000 | 1.506698000 |
| C | -2.925668000 | 2.379259000 | 0.185543000 |
| C | -3.202659000 | -3.052198000 | -3.555899000 |
| C | -3.211788000 | 1.078051000 | -0.241194000 |
| C | -3.228705000 | -2.576803000 | -1.185975000 |
| C | -3.347590000 | -2.420541000 | 3.874173000 |
| C | -3.536933000 | -0.562771000 | 2.339065000 |
| C | -3.593625000 | -3.385280000 | -2.262733000 |
| C | -3.874628000 | 3.393437000 | 0.068344000 |
| C | -3.921427000 | -1.205022000 | 3.516057000 |
| C | -4.471434000 | 0.818744000 | -0.799275000 |
| C | -5.122064000 | 3.124000000 | -0.486999000 |
| C | -5.416869000 | 1.833255000 | -0.921849000 |
| H | 1.797587000 | 5.545080000 | 0.656877000 |
| H | 3.055454000 | -1.414622000 | -0.048577000 |
| H | 4.106786000 | -3.483514000 | 1.206238000 |
| H | 4.112278000 | -1.210099000 | 2.166658000 |

| | | | |
|---|---|---|---|
| H | 4.194500000 | 5.564228000 | -0.684598000 |
| H | 4.218274000 | -3.316665000 | -1.458463000 |
| H | 4.288360000 | -0.939339000 | -2.121237000 |
| H | 4.627883000 | 1.055719000 | 0.192819000 |
| H | 4.775396000 | 2.930757000 | -1.060859000 |
| H | 5.590496000 | -3.238971000 | 2.109986000 |
| H | 5.673320000 | -0.861071000 | 1.424634000 |
| H | 5.769908000 | -2.965882000 | -2.198408000 |
| H | 5.782436000 | -0.694577000 | -1.215640000 |
| H | 6.019010000 | -4.348219000 | -0.109158000 |
| H | 6.851920000 | -2.807348000 | 0.023228000 |
| H | -1.218108000 | -2.797537000 | 1.264237000 |
| H | -1.466177000 | -0.219851000 | -2.876809000 |
| H | -1.918317000 | -3.935248000 | 3.322166000 |
| H | -1.957927000 | 2.606381000 | 0.611078000 |
| H | -2.128872000 | -1.636023000 | -4.772674000 |
| H | -3.487530000 | -3.681337000 | -4.391748000 |
| H | -3.552055000 | -2.845686000 | -0.188750000 |
| H | -3.632330000 | 4.394896000 | 0.405931000 |
| H | -3.648223000 | -2.918387000 | 4.789217000 |
| H | -3.999527000 | 0.379342000 | 2.075011000 |
| H | -4.188737000 | -4.274480000 | -2.085584000 |
| H | -4.673616000 | -0.749732000 | 4.150799000 |
| H | -4.715884000 | -0.177615000 | -1.145439000 |
| H | -5.858249000 | 3.914102000 | -0.584815000 |
| H | -6.384305000 | 1.614016000 | -1.360105000 |
| Mo | 0.547816000 | 0.411033000 | 0.046928000 |
| N | 3.774597000 | 0.509459000 | 0.105064000 |
| O | 1.303490000 | -1.944225000 | 2.055127000 |
| O | 1.317191000 | -1.568585000 | -2.333013000 |
| O | 1.970152000 | 3.492161000 | 0.524873000 |
| O | -0.065992000 | 2.184385000 | 2.647211000 |
| O | -0.088222000 | 2.741333000 | -2.060073000 |
| P | -1.944170000 | -0.272769000 | -0.022896000 |

2 $[Mo(CO)_4(PPh_3)\{C(NC_6H_{12})(C_4H_3O)\}]$, trans-anti,E

| | | | |
|---|---|---|---|
| C | 2.472698000 | -2.606363000 | -1.431779000 |
| C | 2.591598000 | -0.419006000 | 2.787150000 |
| C | 2.813412000 | 2.409395000 | -0.915476000 |
| C | 2.920295000 | -1.280292000 | -1.338681000 |
| C | 2.921154000 | -3.438849000 | -2.451899000 |
| C | 2.979640000 | -0.949884000 | 1.549425000 |
| C | 3.123737000 | -0.914625000 | 3.972863000 |
| C | 3.288977000 | 1.331066000 | -0.159971000 |
| C | 3.589024000 | 3.553166000 | -1.092915000 |
| C | 3.813346000 | -2.956872000 | -3.408945000 |
| C | 3.818780000 | -0.808260000 | -2.301436000 |
| C | 3.914088000 | -1.991222000 | 1.530442000 |
| C | 4.046506000 | -1.959195000 | 3.943979000 |
| C | 4.257153000 | -1.640913000 | -3.331287000 |

| | | | |
|---|---|---|---|
| C | 4.438278000 | -2.495114000 | 2.721089000 |
| C | 4.559947000 | 1.431403000 | 0.421803000 |
| C | 4.849201000 | 3.642590000 | -0.507601000 |
| C | 5.331063000 | 2.578716000 | 0.251702000 |
| C | -0.051064000 | 1.931286000 | 0.937908000 |
| C | -0.265805000 | 0.920896000 | -1.873875000 |
| C | -0.581648000 | -0.798169000 | 1.824272000 |
| C | -0.655069000 | -1.700979000 | -0.822705000 |
| C | -2.492768000 | 0.477679000 | 0.007107000 |
| C | -2.980679000 | 3.956526000 | -0.587269000 |
| C | -3.071551000 | 1.820003000 | -0.052480000 |
| C | -4.050946000 | 3.831108000 | 0.243716000 |
| C | -4.117586000 | 2.450059000 | 0.583765000 |
| C | -4.837575000 | -0.587959000 | -0.045490000 |
| C | -5.178922000 | -1.638571000 | -1.116375000 |
| C | -5.533721000 | -0.916055000 | 1.286817000 |
| C | -6.697006000 | -1.785596000 | -1.294952000 |
| C | -7.052344000 | -1.060053000 | 1.106857000 |
| C | -7.396968000 | -2.101810000 | 0.033696000 |
| H | 1.770462000 | -2.993983000 | -0.704375000 |
| H | 1.832524000 | 2.360018000 | -1.368807000 |
| H | 1.869401000 | 0.387897000 | 2.825679000 |
| H | 2.564642000 | -4.461476000 | -2.503792000 |
| H | 2.810533000 | -0.489623000 | 4.919828000 |
| H | 3.201762000 | 4.376380000 | -1.682843000 |
| H | 4.155397000 | -3.602673000 | -4.209931000 |
| H | 4.180621000 | 0.210591000 | -2.254713000 |
| H | 4.238034000 | -2.414273000 | 0.588379000 |
| H | 4.454603000 | -2.352232000 | 4.868435000 |
| H | 4.948849000 | -1.254794000 | -4.071915000 |
| H | 4.950306000 | 0.614736000 | 1.015694000 |
| H | 5.156372000 | -3.307162000 | 2.687289000 |
| H | 5.449646000 | 4.536010000 | -0.638134000 |
| H | 6.309513000 | 2.639771000 | 0.715414000 |
| H | -2.546642000 | 4.788547000 | -1.115721000 |
| H | -2.950085000 | -1.435634000 | 0.221989000 |
| H | -4.702717000 | -1.361108000 | -2.060936000 |
| H | -4.706120000 | 4.621072000 | 0.574401000 |
| H | -4.750596000 | -2.605035000 | -0.818147000 |
| H | -4.823824000 | 1.990504000 | 1.254854000 |
| H | -5.120302000 | -1.855063000 | 1.676634000 |
| H | -5.171260000 | 0.388356000 | -0.398898000 |
| H | -5.301289000 | -0.146756000 | 2.029082000 |
| H | -6.906637000 | -2.565744000 | -2.032663000 |
| H | -7.083988000 | -3.094788000 | 0.380526000 |
| H | -7.103478000 | -0.852943000 | -1.706184000 |
| H | -7.477540000 | -0.089716000 | 0.819301000 |
| H | -7.513195000 | -1.328689000 | 2.062103000 |
| H | -8.480428000 | -2.149811000 | -0.111977000 |
| Mo | -0.325411000 | 0.113507000 | 0.015092000 |
| N | -3.373806000 | -0.522367000 | 0.117900000 |

| | | | |
|---|---|---|---|
| O | 0.096511000 | 2.933143000 | 1.482261000 |
| O | -0.274098000 | 1.336836000 | -2.946058000 |
| O | -0.813866000 | -1.338819000 | 2.814559000 |
| O | -0.909359000 | -2.738461000 | -1.266353000 |
| O | -2.371548000 | 2.763403000 | -0.765055000 |
| P | 2.241118000 | -0.201104000 | 0.013913000 |

3 $[Mo(CO)_4(PPh_3)\{C(NC_6H_{12})(C_4H_3O)\}]$,trans-syn,Z

| | | | |
|---|---|---|---|
| C | 0.102424000 | 1.829573000 | -1.444990000 |
| C | 0.188943000 | 1.773674000 | 1.546398000 |
| C | 0.913875000 | -0.930384000 | -1.426395000 |
| C | 0.953739000 | -0.924580000 | 1.449333000 |
| C | 2.287102000 | 3.716715000 | 0.006503000 |
| C | 2.643381000 | 1.122942000 | -0.015061000 |
| C | 3.001140000 | 2.545473000 | -0.021538000 |
| C | 3.217263000 | 4.793691000 | -0.013734000 |
| C | 3.900425000 | -1.080586000 | -0.030293000 |
| C | 4.451919000 | 4.224939000 | -0.052827000 |
| C | 4.623300000 | -1.542391000 | -1.307731000 |
| C | 4.658276000 | -1.531476000 | 1.230804000 |
| C | 4.848168000 | -3.061532000 | -1.302082000 |
| C | 4.882509000 | -3.050661000 | 1.231712000 |
| C | 5.596153000 | -3.520625000 | -0.043058000 |
| C | -2.007818000 | -2.251161000 | 1.933632000 |
| C | -2.163086000 | -1.052517000 | -2.656108000 |
| C | -2.387133000 | -2.879855000 | 3.114879000 |
| C | -2.524179000 | -1.365452000 | -1.338447000 |
| C | -2.562031000 | -1.861295000 | -3.714964000 |
| C | -2.581121000 | -1.028255000 | 1.555027000 |
| C | -2.937958000 | 2.468505000 | 0.156438000 |
| C | -3.246032000 | 1.155742000 | -0.214025000 |
| C | -3.294665000 | -2.510588000 | -1.109398000 |
| C | -3.321135000 | -3.005644000 | -3.475310000 |
| C | -3.334636000 | -2.289433000 | 3.950106000 |
| C | -3.531738000 | -0.445086000 | 2.399890000 |
| C | -3.684320000 | -3.327292000 | -2.171273000 |
| C | -3.883041000 | 3.485930000 | 0.034696000 |
| C | -3.901012000 | -1.070770000 | 3.590546000 |
| C | -4.525283000 | 0.886833000 | -0.721094000 |
| C | -5.149847000 | 3.206775000 | -0.469246000 |
| C | -5.467428000 | 1.903648000 | -0.848009000 |
| H | 1.216402000 | 3.801675000 | 0.039176000 |
| H | 2.902190000 | -1.510230000 | -0.014402000 |
| H | 2.995743000 | 5.848608000 | -0.000772000 |
| H | 3.875766000 | -3.565894000 | -1.353590000 |
| H | 3.911478000 | -3.553851000 | 1.313338000 |
| H | 4.040027000 | -1.243813000 | -2.182381000 |
| H | 4.099231000 | -1.225258000 | 2.118487000 |
| H | 4.638809000 | 0.863020000 | -0.049861000 |
| H | 5.397147000 | -3.355451000 | -2.201847000 |

| | | | |
|---|---|---|---|
| H | 5.451686000 | 4.626094000 | -0.079939000 |
| H | 5.455212000 | -3.337540000 | 2.118873000 |
| H | 5.592542000 | -1.029110000 | -1.374717000 |
| H | 5.628926000 | -1.017826000 | 1.266708000 |
| H | 5.695562000 | -4.610542000 | -0.039821000 |
| H | 6.616041000 | -3.114345000 | -0.058568000 |
| H | -1.259420000 | -2.716977000 | 1.303759000 |
| H | -1.567253000 | -0.170231000 | -2.858465000 |
| H | -1.933329000 | -3.826011000 | 3.387436000 |
| H | -1.955522000 | 2.700216000 | 0.543120000 |
| H | -2.272560000 | -1.600825000 | -4.726785000 |
| H | -3.597462000 | -2.770286000 | -0.103392000 |
| H | -3.623246000 | 4.496656000 | 0.328959000 |
| H | -3.623706000 | -2.774616000 | 4.875587000 |
| H | -3.625352000 | -3.640992000 | -4.299552000 |
| H | -3.988342000 | 0.499618000 | 2.134528000 |
| H | -4.277056000 | -4.213812000 | -1.973863000 |
| H | -4.635642000 | -0.600361000 | 4.234746000 |
| H | -4.787685000 | -0.118796000 | -1.024769000 |
| H | -5.883689000 | 3.998553000 | -0.570836000 |
| H | -6.450269000 | 1.676761000 | -1.246233000 |
| Mo | 0.515562000 | 0.457144000 | 0.016705000 |
| N | 3.746851000 | 0.374883000 | -0.033956000 |
| O | 0.034009000 | 2.497609000 | 2.429543000 |
| O | 1.162359000 | -1.723215000 | -2.225267000 |
| O | 1.230162000 | -1.698376000 | 2.258851000 |
| O | 4.352747000 | 2.875866000 | -0.058152000 |
| O | -0.129221000 | 2.587241000 | -2.280849000 |
| P | -1.981011000 | -0.197387000 | 0.006124000 |

4 $[Mo(CO)_4(PPh_3)\{C(NC_6H_{12})(C_4H_3O)\}]$,trans-syn,E

| | | | |
|---|---|---|---|
| C | 2.486144000 | -0.618049000 | 2.784774000 |
| C | 2.533431000 | -2.472936000 | -1.589479000 |
| C | 2.914887000 | -1.066215000 | 1.527888000 |
| C | 2.928976000 | 2.494080000 | -0.626098000 |
| C | 2.951308000 | -1.216522000 | 3.950977000 |
| C | 2.985815000 | -1.162026000 | -1.379374000 |
| C | 3.009249000 | -3.227598000 | -2.656558000 |
| C | 3.354939000 | 1.333253000 | 0.029371000 |
| C | 3.736573000 | 3.628933000 | -0.665599000 |
| C | 3.821793000 | -2.130080000 | 1.469747000 |
| C | 3.846221000 | -2.283269000 | 3.882161000 |
| C | 3.916658000 | -0.624115000 | -2.274515000 |
| C | 3.934437000 | -2.680518000 | -3.544842000 |
| C | 4.278192000 | -2.737463000 | 2.639937000 |
| C | 4.382772000 | -1.377990000 | -3.351714000 |
| C | 4.610012000 | 1.340099000 | 0.653061000 |
| C | 4.980383000 | 3.624638000 | -0.040236000 |
| C | 5.413665000 | 2.476980000 | 0.620129000 |
| C | -0.043210000 | 1.885699000 | 1.048709000 |

| | | | |
|---|---|---|---|
| C | -0.116059000 | 1.170336000 | -1.854275000 |
| C | -0.595384000 | -1.522507000 | -1.127120000 |
| C | -0.618016000 | -0.901192000 | 1.628615000 |
| C | -2.482949000 | 0.541075000 | -0.112597000 |
| C | -2.564319000 | 3.073170000 | -0.604456000 |
| C | -3.068980000 | 1.872591000 | -0.164206000 |
| C | -3.563112000 | 4.063078000 | -0.402532000 |
| C | -4.618213000 | 3.420585000 | 0.169048000 |
| C | -4.789000000 | -0.641569000 | -0.146718000 |
| C | -5.098648000 | -1.869896000 | -1.017508000 |
| C | -5.435483000 | -0.771783000 | 1.242861000 |
| C | -6.611436000 | -2.112600000 | -1.124243000 |
| C | -6.948188000 | -1.014294000 | 1.134110000 |
| C | -7.265732000 | -2.234318000 | 0.258768000 |
| H | 1.784765000 | 0.205141000 | 2.853627000 |
| H | 1.805577000 | -2.909692000 | -0.916959000 |
| H | 1.961316000 | 2.515002000 | -1.108790000 |
| H | 2.607504000 | -0.854326000 | 4.913292000 |
| H | 2.648420000 | -4.240012000 | -2.799168000 |
| H | 3.387209000 | 4.517617000 | -1.179259000 |
| H | 4.177687000 | -2.489888000 | 0.513064000 |
| H | 4.201761000 | -2.756384000 | 4.790639000 |
| H | 4.282064000 | 0.385313000 | -2.137698000 |
| H | 4.298138000 | -3.265298000 | -4.382281000 |
| H | 4.961898000 | 0.458072000 | 1.172966000 |
| H | 4.975848000 | -3.565267000 | 2.575079000 |
| H | 5.099736000 | -0.941211000 | -4.038134000 |
| H | 5.605875000 | 4.510059000 | -0.062989000 |
| H | 6.379063000 | 2.464784000 | 1.114018000 |
| H | -1.589383000 | 3.223738000 | -1.032060000 |
| H | -2.854364000 | -1.390238000 | 0.036669000 |
| H | -3.500379000 | 5.113433000 | -0.636860000 |
| H | -4.621138000 | -2.753963000 | -0.572911000 |
| H | -4.657008000 | -1.737617000 | -2.009505000 |
| H | -4.964717000 | -1.610246000 | 1.771871000 |
| H | -5.180579000 | 0.246100000 | -0.640547000 |
| H | -5.227781000 | 0.130192000 | 1.821877000 |
| H | -5.578488000 | 3.752037000 | 0.528721000 |
| H | -6.798142000 | -3.013212000 | -1.716720000 |
| H | -6.896567000 | -3.141000000 | 0.754817000 |
| H | -7.072032000 | -1.280473000 | -1.671619000 |
| H | -7.374447000 | -1.140639000 | 2.133939000 |
| H | -7.426304000 | -0.125090000 | 0.703317000 |
| H | -8.348445000 | -2.355018000 | 0.154354000 |
| Mo | -0.284467000 | 0.185344000 | -0.072326000 |
| N | -3.320747000 | -0.496284000 | -0.044396000 |
| O | 0.083119000 | 2.828057000 | 1.696679000 |
| O | -0.063942000 | 1.708846000 | -2.872705000 |
| O | -0.838768000 | -2.493802000 | -1.702724000 |
| O | -0.885693000 | -1.535060000 | 2.551600000 |
| O | -4.354701000 | 2.102404000 | 0.313302000 |

| | | | |
|---|---|---|---|
| P | 2.265684000 | -0.180225000 | 0.025199000 |

5 $[Mo(CO)_4(PPh_3)\{C(NC_6H_{12})(C_4H_3O)\}]$, cis-anti,Z (1)

| | | | |
|---|---|---|---|
| C | 0.057756000 | -0.637330000 | 3.904671000 |
| C | 0.072386000 | -1.444396000 | -2.488080000 |
| C | 0.233744000 | -0.153798000 | 2.611227000 |
| C | 0.357152000 | -4.167994000 | 0.376437000 |
| C | 0.430738000 | 1.299828000 | -2.763520000 |
| C | 1.072888000 | -1.364259000 | 4.524328000 |
| C | 1.432210000 | -0.374481000 | 1.920469000 |
| C | 2.113520000 | 2.076807000 | 0.558141000 |
| C | 2.161047000 | 2.609717000 | 1.850620000 |
| C | 2.264439000 | -1.596983000 | 3.843287000 |
| C | 2.440050000 | 2.908550000 | -0.523332000 |
| C | 2.446075000 | -1.101947000 | 2.552404000 |
| C | 2.519401000 | 3.942305000 | 2.056210000 |
| C | 2.805607000 | 4.234148000 | -0.314454000 |
| C | 2.842513000 | 4.757832000 | 0.977076000 |
| C | 3.185433000 | -1.641363000 | -1.059028000 |
| C | 3.208684000 | -0.423445000 | -0.368372000 |
| C | 4.368830000 | -2.240783000 | -1.483486000 |
| C | 4.446981000 | 0.181159000 | -0.115320000 |
| C | 5.594711000 | -1.629749000 | -1.229819000 |
| C | 5.629652000 | -0.417775000 | -0.545057000 |
| C | -0.834690000 | -4.804363000 | 0.542444000 |
| C | -1.148395000 | 1.900219000 | -0.475399000 |
| C | -1.179384000 | -2.599781000 | 0.222452000 |
| C | -1.653251000 | -1.237138000 | -0.025471000 |
| C | -1.830517000 | -3.792660000 | 0.444471000 |
| C | -2.135571000 | 0.275842000 | -2.551551000 |
| C | -3.779424000 | 0.056164000 | 0.419033000 |
| C | -4.005663000 | 0.717853000 | 1.788031000 |
| C | -5.021169000 | 1.866311000 | 1.689743000 |
| C | -5.105569000 | -0.419202000 | -0.199434000 |
| C | -6.119118000 | 0.731266000 | -0.291789000 |
| C | -6.345523000 | 1.399445000 | 1.071014000 |
| H | 0.934399000 | -1.747139000 | 5.529253000 |
| H | 1.381401000 | -4.500642000 | 0.382319000 |
| H | 1.920146000 | 1.990945000 | 2.704910000 |
| H | 2.241189000 | -2.122583000 | -1.270946000 |
| H | 2.416134000 | 2.524833000 | -1.534834000 |
| H | 2.545735000 | 4.337995000 | 3.065562000 |
| H | 3.054613000 | 4.859242000 | -1.164571000 |
| H | 3.059618000 | -2.162913000 | 4.316119000 |
| H | 3.119718000 | 5.793549000 | 1.138257000 |
| H | 3.380672000 | -1.287762000 | 2.038802000 |
| H | 4.329003000 | -3.179190000 | -2.025310000 |
| H | 4.492206000 | 1.125385000 | 0.412176000 |
| H | 6.515215000 | -2.091300000 | -1.569330000 |
| H | 6.578366000 | 0.068272000 | -0.345940000 |

| | | | |
|---|---|---|---|
| H | -0.565565000 | 0.397904000 | 2.131797000 |
| H | -0.874394000 | -0.450295000 | 4.426481000 |
| H | -0.983188000 | -5.860452000 | 0.701074000 |
| H | -2.898387000 | -3.942832000 | 0.480578000 |
| H | -3.052229000 | 1.085460000 | 2.177255000 |
| H | -3.214663000 | -1.823005000 | 1.118367000 |
| H | -3.315774000 | 0.772592000 | -0.254397000 |
| H | -4.373400000 | -0.037779000 | 2.496365000 |
| H | -4.592855000 | 2.667501000 | 1.076234000 |
| H | -4.911263000 | -0.839630000 | -1.189322000 |
| H | -5.191758000 | 2.292702000 | 2.682884000 |
| H | -5.523220000 | -1.224331000 | 0.421685000 |
| H | -5.748638000 | 1.475026000 | -1.007075000 |
| H | -6.832028000 | 0.686115000 | 1.749301000 |
| H | -7.030717000 | 2.246103000 | 0.966274000 |
| H | -7.063903000 | 0.356171000 | -0.696330000 |
| Mo | -0.528273000 | 0.183925000 | -1.392662000 |
| N | -2.848753000 | -1.071212000 | 0.537575000 |
| O | 0.167961000 | -2.844710000 | 0.170386000 |
| O | 0.370122000 | -2.315305000 | -3.177782000 |
| O | 0.936782000 | 1.919466000 | -3.597583000 |
| O | -1.510569000 | 2.898536000 | -0.026387000 |
| O | -3.077752000 | 0.350991000 | -3.219718000 |
| P | 1.605780000 | 0.322126000 | 0.204808000 |

6 $[Mo(CO)_4(PPh_3)\{C(NC_6H_{12})(C_4H_3O)\}]$, cis-anti,E (1)

| | | | |
|---|---|---|---|
| C | 0.356246000 | -2.275979000 | -1.744348000 |
| C | 0.780071000 | -0.105091000 | 4.332667000 |
| C | 0.965534000 | 0.429504000 | 1.974010000 |
| C | 1.395326000 | -0.288328000 | 3.093634000 |
| C | 1.513358000 | -0.104582000 | -3.063112000 |
| C | 2.676062000 | 1.840960000 | 0.156056000 |
| C | 2.738474000 | -2.351395000 | 0.628449000 |
| C | 2.985334000 | 2.619276000 | 1.279684000 |
| C | 3.076375000 | -0.992281000 | 0.571233000 |
| C | 3.132263000 | 2.265057000 | -1.098456000 |
| C | 3.718104000 | -3.319600000 | 0.827277000 |
| C | 3.725117000 | 3.792748000 | 1.149057000 |
| C | 3.878640000 | 3.434042000 | -1.225655000 |
| C | 4.174224000 | 4.203768000 | -0.103353000 |
| C | 4.420745000 | -0.628345000 | 0.707618000 |
| C | 5.054764000 | -2.947154000 | 0.959915000 |
| C | 5.401772000 | -1.601041000 | 0.897352000 |
| C | -0.090711000 | 1.339434000 | 2.122510000 |
| C | -0.262406000 | 0.805623000 | 4.471878000 |
| C | -0.285419000 | 1.759923000 | -1.830761000 |
| C | -0.692611000 | 1.532479000 | 3.361830000 |
| C | -1.206579000 | -3.448735000 | 1.610393000 |
| C | -1.244601000 | -0.483668000 | -3.198222000 |

| | | | |
|---|---|---|---|
| C | -1.749081000 | -0.522010000 | -0.328565000 |
| C | -1.970603000 | -1.708749000 | 0.487126000 |
| C | -2.553204000 | -3.628757000 | 1.526914000 |
| C | -3.048926000 | -2.504787000 | 0.811276000 |
| C | -4.052205000 | 0.452629000 | 0.295201000 |
| C | -4.260591000 | 1.889874000 | 0.799838000 |
| C | -5.194864000 | 0.036165000 | -0.649574000 |
| C | -5.633904000 | 2.058253000 | 1.467154000 |
| C | -6.566790000 | 0.198391000 | 0.021495000 |
| C | -6.775668000 | 1.629159000 | 0.535795000 |
| H | 1.125005000 | -0.672436000 | 5.190194000 |
| H | 1.706056000 | -2.652171000 | 0.511642000 |
| H | 2.213851000 | -0.991270000 | 3.005284000 |
| H | 2.647147000 | 2.314756000 | 2.261736000 |
| H | 2.909106000 | 1.684198000 | -1.982488000 |
| H | 3.438036000 | -4.366524000 | 0.863315000 |
| H | 3.949235000 | 4.384645000 | 2.029694000 |
| H | 4.220776000 | 3.744368000 | -2.206427000 |
| H | 4.709814000 | 0.413391000 | 0.660271000 |
| H | 4.747924000 | 5.118285000 | -0.204381000 |
| H | 5.819710000 | -3.702071000 | 1.103112000 |
| H | 6.439466000 | -1.301201000 | 0.993000000 |
| H | -0.414260000 | -4.012647000 | 2.073447000 |
| H | -0.436375000 | 1.906219000 | 1.265848000 |
| H | -0.735130000 | 0.952051000 | 5.436587000 |
| H | -1.497306000 | 2.252674000 | 3.462702000 |
| H | -2.572734000 | 1.137142000 | -1.007902000 |
| H | -3.118786000 | -4.457085000 | 1.922465000 |
| H | -3.459426000 | 2.148895000 | 1.497641000 |
| H | -4.023059000 | -0.215503000 | 1.157522000 |
| H | -4.074571000 | -2.336322000 | 0.531654000 |
| H | -4.181030000 | 2.581762000 | -0.049494000 |
| H | -5.045978000 | -0.992422000 | -0.989696000 |
| H | -5.148891000 | 0.664255000 | -1.547867000 |
| H | -5.665911000 | 1.454059000 | 2.382637000 |
| H | -5.765567000 | 3.098697000 | 1.778515000 |
| H | -6.647716000 | -0.503914000 | 0.861401000 |
| H | -6.824168000 | 2.316172000 | -0.318378000 |
| H | -7.356543000 | -0.072697000 | -0.685242000 |
| H | -7.735646000 | 1.708644000 | 1.054741000 |
| Mo | 0.039974000 | -0.245043000 | -1.698935000 |
| N | -2.745478000 | 0.360951000 | -0.380775000 |
| O | 0.518001000 | -3.407533000 | -1.865642000 |
| O | 2.318557000 | -0.045524000 | -3.890491000 |
| O | -0.493480000 | 2.888342000 | -1.961599000 |
| O | -0.835112000 | -2.315540000 | 0.979768000 |
| O | -2.002384000 | -0.596884000 | -4.063536000 |
| P | 1.723086000 | 0.247841000 | 0.286885000 |

7 $[Mo(CO)_4(PPh_3)\{C(NC_6H_{12})(C_4H_3O)\}]$, cis-syn,Z (1)

| | | | |
|---|---|---|---|
| C | 0.117845000 | 3.226977000 | -0.573350000 |
| C | 0.271514000 | 4.600307000 | -0.238176000 |
| C | 1.078769000 | -1.969537000 | -0.101309000 |
| C | 1.266528000 | 2.574373000 | -0.204777000 |
| C | 1.506600000 | 4.714953000 | 0.321069000 |
| C | 1.712142000 | 1.186111000 | -0.275569000 |
| C | 2.061293000 | -0.846149000 | -2.470686000 |
| C | 3.779576000 | -0.127168000 | 0.349500000 |
| C | 3.981948000 | -0.526246000 | 1.820983000 |
| C | 4.922232000 | -1.734046000 | 1.947554000 |
| C | 5.125916000 | 0.134738000 | -0.347249000 |
| C | 6.062836000 | -1.074893000 | -0.216545000 |
| C | 6.265527000 | -1.482928000 | 1.248711000 |
| C | -0.024012000 | 0.924987000 | -2.761320000 |
| C | -0.393029000 | 2.105770000 | 3.392805000 |
| C | -0.489267000 | 1.139155000 | 2.397487000 |
| C | -0.542142000 | -1.789128000 | -2.416326000 |
| C | -1.413475000 | 3.041692000 | 3.560728000 |
| C | -1.617142000 | 1.073950000 | 1.566876000 |
| C | -2.000089000 | -1.776135000 | 1.218331000 |
| C | -2.135823000 | -2.981473000 | 0.514182000 |
| C | -2.142964000 | -1.792260000 | 2.609702000 |
| C | -2.405423000 | -2.986282000 | 3.282114000 |
| C | -2.406252000 | -4.168417000 | 1.186666000 |
| C | -2.529849000 | 2.995854000 | 2.732212000 |
| C | -2.537758000 | -4.176341000 | 2.574537000 |
| C | -2.635332000 | 2.015668000 | 1.744640000 |
| C | -3.306126000 | 0.047555000 | -0.558742000 |
| C | -3.380675000 | 0.697338000 | -1.794749000 |
| C | -4.496079000 | -0.371619000 | 0.053636000 |
| C | -4.613096000 | 0.936336000 | -2.400764000 |
| C | -5.726142000 | -0.136605000 | -0.554187000 |
| C | -5.788217000 | 0.519814000 | -1.782388000 |
| H | 0.319490000 | 0.430251000 | 2.260942000 |
| H | 0.482828000 | 2.134615000 | 4.031521000 |
| H | 2.062084000 | 5.547295000 | 0.721170000 |
| H | 3.011412000 | -0.749287000 | 2.273066000 |
| H | 3.266443000 | -0.929998000 | -0.172966000 |
| H | 3.374261000 | 1.899234000 | 0.610350000 |
| H | 4.403382000 | 0.327951000 | 2.368781000 |
| H | 4.436717000 | -2.610644000 | 1.503043000 |
| H | 4.948307000 | 0.369351000 | -1.399850000 |
| H | 5.078974000 | -1.968665000 | 3.004828000 |
| H | 5.600641000 | 1.016002000 | 0.106751000 |
| H | 5.637425000 | -1.916875000 | -0.775437000 |
| H | 6.805933000 | -0.685766000 | 1.775990000 |
| H | 6.893684000 | -2.377012000 | 1.307904000 |
| H | 7.024160000 | -0.846180000 | -0.686277000 |
| H | -0.440844000 | 5.394601000 | -0.391279000 |
| H | -0.744040000 | 2.772556000 | -1.027188000 |
| H | -1.335115000 | 3.801684000 | 4.330009000 |

| | | | |
|---|---|---|---|
| H | -2.034964000 | -2.998724000 | -0.563710000 |
| H | -2.054354000 | -0.875934000 | 3.178161000 |
| H | -2.475170000 | 1.004735000 | -2.298854000 |
| H | -2.507674000 | -5.089453000 | 0.623892000 |
| H | -2.508411000 | -2.979263000 | 4.361683000 |
| H | -2.741010000 | -5.103787000 | 3.098003000 |
| H | -3.327375000 | 3.720763000 | 2.852711000 |
| H | -3.515014000 | 1.989622000 | 1.114251000 |
| H | -4.462052000 | -0.891670000 | 1.003072000 |
| H | -4.648775000 | 1.435994000 | -3.362182000 |
| H | -6.636335000 | -0.472694000 | -0.069975000 |
| H | -6.746630000 | 0.696383000 | -2.257675000 |
| Mo | 0.484328000 | -0.448085000 | -1.335118000 |
| N | 2.926827000 | 1.059186000 | 0.249627000 |
| O | 1.434717000 | -2.876005000 | 0.513951000 |
| O | 2.127505000 | 3.514867000 | 0.355721000 |
| O | 2.974699000 | -1.107908000 | -3.130960000 |
| O | -0.265664000 | 1.630452000 | -3.640008000 |
| O | -1.098752000 | -2.560097000 | -3.074413000 |
| P | -1.653106000 | -0.228559000 | 0.243929000 |

8 $[Mo(CO)_4(PPh_3)\{C(NC_6H_{12})(C_4H_3O)\}]$, cis-syn,E (1)

| | | | |
|---|---|---|---|
| C | 0.268102000 | -2.452641000 | 0.012805000 |
| C | 0.477881000 | 2.153974000 | 3.062468000 |
| C | 1.095722000 | 2.620265000 | -1.072271000 |
| C | 1.267934000 | -1.899057000 | -2.523258000 |
| C | 1.780247000 | 0.211278000 | -0.533869000 |
| C | 1.810952000 | 3.841745000 | -1.161303000 |
| C | 1.990360000 | 1.627146000 | -0.747471000 |
| C | 3.111427000 | 3.532149000 | -0.898758000 |
| C | 4.086627000 | -0.171579000 | 0.589582000 |
| C | 4.363722000 | -1.081644000 | 1.795917000 |
| C | 5.169476000 | -0.342210000 | -0.490467000 |
| C | 5.768340000 | -0.839784000 | 2.368364000 |
| C | 6.572697000 | -0.097801000 | 0.083435000 |
| C | 6.853766000 | -0.997227000 | 1.294701000 |
| C | -0.038228000 | 1.174251000 | 2.221093000 |
| C | -0.137339000 | 3.403172000 | 3.144146000 |
| C | -0.253915000 | 0.377872000 | -2.879826000 |
| C | -1.193858000 | 1.415157000 | 1.463359000 |
| C | -1.273675000 | 3.658858000 | 2.383891000 |
| C | -1.503950000 | -2.033784000 | -2.182972000 |
| C | -1.803209000 | 2.670636000 | 1.552725000 |
| C | -2.490593000 | -1.177670000 | 1.534590000 |
| C | -2.510832000 | -0.985190000 | 2.920100000 |
| C | -3.032355000 | -2.360610000 | 1.011390000 |
| C | -3.051001000 | -1.956829000 | 3.763131000 |
| C | -3.369470000 | 0.790622000 | -0.349119000 |
| C | -3.389188000 | 1.305624000 | -1.649068000 |
| C | -3.578738000 | -3.323007000 | 1.853950000 |

| | | | |
|---|---|---|---|
| C | -3.586038000 | -3.126793000 | 3.234061000 |
| C | -4.544107000 | 0.847375000 | 0.414787000 |
| C | -4.548884000 | 1.876255000 | -2.171552000 |
| C | -5.702822000 | 1.413340000 | -0.109152000 |
| C | -5.708080000 | 1.931165000 | -1.403393000 |
| H | 0.039722000 | 2.480828000 | -1.216761000 |
| H | 0.269519000 | 4.170054000 | 3.793626000 |
| H | 0.459584000 | 0.214109000 | 2.150320000 |
| H | 1.364951000 | 1.945181000 | 3.650324000 |
| H | 1.417259000 | 4.816903000 | -1.397630000 |
| H | 2.537532000 | -1.483660000 | 0.121086000 |
| H | 3.602350000 | -0.917932000 | 2.564925000 |
| H | 4.017103000 | 4.116241000 | -0.875234000 |
| H | 4.075431000 | 0.864475000 | 0.923746000 |
| H | 4.277018000 | -2.130828000 | 1.481773000 |
| H | 4.965458000 | 0.341036000 | -1.317182000 |
| H | 5.106298000 | -1.361007000 | -0.892644000 |
| H | 5.817194000 | 0.173380000 | 2.787336000 |
| H | 5.949641000 | -1.527543000 | 3.199663000 |
| H | 6.662570000 | 0.954127000 | 0.383918000 |
| H | 6.889131000 | -2.043930000 | 0.967211000 |
| H | 7.322843000 | -0.262027000 | -0.695871000 |
| H | 7.837133000 | -0.769302000 | 1.717361000 |
| H | -1.758009000 | 4.627646000 | 2.437592000 |
| H | -2.107947000 | -0.077841000 | 3.350806000 |
| H | -2.502801000 | 1.250630000 | -2.265416000 |
| H | -2.694228000 | 2.884081000 | 0.976215000 |
| H | -3.032591000 | -2.534293000 | -0.057264000 |
| H | -3.053623000 | -1.792137000 | 4.835047000 |
| H | -3.992787000 | -4.230714000 | 1.429779000 |
| H | -4.005009000 | -3.881474000 | 3.890120000 |
| H | -4.544839000 | 2.264913000 | -3.183583000 |
| H | -4.558029000 | 0.441008000 | 1.418582000 |
| H | -6.604054000 | 1.444118000 | 0.493120000 |
| H | -6.613140000 | 2.366322000 | -1.812215000 |
| Mo | -0.030371000 | -0.958330000 | -1.347288000 |
| N | 2.744603000 | -0.495286000 | 0.054361000 |
| O | 0.472977000 | -3.342117000 | 0.717179000 |
| O | 2.022426000 | -2.465439000 | -3.190278000 |
| O | 3.249577000 | 2.215757000 | -0.637088000 |
| O | -0.355005000 | 1.050079000 | -3.810206000 |
| O | -2.325090000 | -2.668829000 | -2.692640000 |
| P | -1.800348000 | 0.068569000 | 0.337265000 |

9 $[Mo(CO)_4(PPh_3)\{C(NC_6H_{12})(C_4H_3O)\}]$, cis-anti,Z (2)

| | | | |
|---|---|---|---|
| C | 0.453889000 | -2.818578000 | -0.450819000 |
| C | 0.690189000 | -0.809863000 | 2.672867000 |
| C | 0.856635000 | -1.151893000 | 4.013970000 |
| C | 0.875919000 | 4.897974000 | 0.293110000 |
| C | 0.925522000 | 4.207244000 | -0.917569000 |

| | | | |
|---|---|---|---|
| C | 0.966625000 | -1.290009000 | -2.715903000 |
| C | 0.991044000 | 4.195628000 | 1.489135000 |
| C | 1.090956000 | 2.825516000 | -0.928616000 |
| C | 1.167852000 | 2.811572000 | 1.479902000 |
| C | 1.225813000 | 2.109890000 | 0.270637000 |
| C | 1.723831000 | -0.196663000 | 1.958921000 |
| C | 2.063378000 | -0.891924000 | 4.656828000 |
| C | 2.937989000 | 0.055378000 | 2.613817000 |
| C | 3.104492000 | -0.289177000 | 3.952118000 |
| C | 3.194291000 | 0.123042000 | -0.475562000 |
| C | 3.697984000 | -1.161614000 | -0.723506000 |
| C | 4.024222000 | 1.225250000 | -0.708305000 |
| C | 4.997145000 | -1.337039000 | -1.188150000 |
| C | 5.323361000 | 1.046825000 | -1.184135000 |
| C | 5.813858000 | -0.232524000 | -1.424216000 |
| C | -0.980721000 | 0.537743000 | -2.258596000 |
| C | -1.623972000 | -2.189265000 | -2.268709000 |
| C | -2.035698000 | -0.985548000 | 0.321738000 |
| C | -2.413620000 | -4.271638000 | 1.702214000 |
| C | -2.565642000 | -2.230835000 | 0.894385000 |
| C | -2.818503000 | 1.420905000 | 0.244255000 |
| C | -2.952490000 | 2.328742000 | 1.477635000 |
| C | -3.017393000 | 3.810958000 | 1.080261000 |
| C | -3.745608000 | -4.011707000 | 1.606563000 |
| C | -3.848644000 | -2.687578000 | 1.088971000 |
| C | -3.944882000 | 1.693406000 | -0.769155000 |
| C | -4.001835000 | 3.175350000 | -1.164727000 |
| C | -4.136726000 | 4.081505000 | 0.066028000 |
| H | 0.045707000 | -1.633136000 | 4.549248000 |
| H | 0.746087000 | 5.974376000 | 0.302005000 |
| H | 0.832682000 | 4.742261000 | -1.855922000 |
| H | 0.950562000 | 4.722701000 | 2.436045000 |
| H | 1.122469000 | 2.303389000 | -1.877058000 |
| H | 1.268724000 | 2.283405000 | 2.419265000 |
| H | 2.197209000 | -1.165102000 | 5.697620000 |
| H | 3.077921000 | -2.033195000 | -0.554948000 |
| H | 3.664579000 | 2.228806000 | -0.522341000 |
| H | 3.759566000 | 0.512801000 | 2.076391000 |
| H | 4.051209000 | -0.091959000 | 4.442778000 |
| H | 5.366609000 | -2.338779000 | -1.375652000 |
| H | 5.949529000 | 1.913616000 | -1.364824000 |
| H | 6.823043000 | -0.369786000 | -1.795890000 |
| H | -0.240443000 | -1.037555000 | 2.171422000 |
| H | -1.843403000 | -5.120016000 | 2.041045000 |
| H | -1.849896000 | 1.592772000 | -0.223385000 |
| H | -2.055246000 | 4.106328000 | 0.647845000 |
| H | -2.113205000 | 2.148919000 | 2.155418000 |
| H | -3.089677000 | 3.432436000 | -1.715145000 |
| H | -3.157012000 | 4.423616000 | 1.976380000 |
| H | -3.616841000 | -0.192405000 | 1.290726000 |
| H | -3.802112000 | 1.063394000 | -1.649805000 |

| | | | |
|---|---|---|---|
| H | -3.869056000 | 2.059594000 | 2.022443000 |
| H | -4.123752000 | 5.133496000 | -0.235464000 |
| H | -4.551005000 | -4.683692000 | 1.856415000 |
| H | -4.757919000 | -2.166425000 | 0.832961000 |
| H | -4.836152000 | 3.338408000 | -1.853555000 |
| H | -4.901549000 | 1.399612000 | -0.315301000 |
| H | -5.110461000 | 3.905557000 | 0.542043000 |
| Mo | -0.349055000 | -1.082806000 | -1.206992000 |
| N | -2.842592000 | 0.016755000 | 0.663098000 |
| O | 0.972000000 | -3.804316000 | -0.163529000 |
| O | 1.670220000 | -1.425993000 | -3.619683000 |
| O | -1.288516000 | 1.394768000 | -2.969820000 |
| O | -1.689540000 | -3.211041000 | 1.269695000 |
| O | -2.350197000 | -2.837020000 | -2.888835000 |
| P | 1.458200000 | 0.268634000 | 0.178417000 |

10 $[Mo(CO)_4(PPh_3)\{C(NC_6H_{12})(C_4H_3O)\}]$, cis-anti,E (2)

| | | | |
|---|---|---|---|
| C | 0.029309000 | 4.325506000 | 0.511997000 |
| C | 0.248752000 | 3.842963000 | -1.836044000 |
| C | 0.550630000 | 3.068852000 | 0.821695000 |
| C | 0.762007000 | 2.585787000 | -1.529089000 |
| C | 0.763453000 | -0.187411000 | 2.756845000 |
| C | 0.829550000 | -0.183174000 | 4.149323000 |
| C | 0.896322000 | -2.771167000 | 0.505159000 |
| C | 0.926623000 | 2.182925000 | -0.194567000 |
| C | 1.734630000 | 0.471916000 | 1.996209000 |
| C | 1.867532000 | -2.088800000 | -2.052623000 |
| C | 1.871474000 | 0.472609000 | 4.798894000 |
| C | 2.782987000 | 1.125139000 | 2.659315000 |
| C | 2.849820000 | 1.124478000 | 4.049788000 |
| C | 3.379774000 | 0.637498000 | -0.342979000 |
| C | 3.964616000 | 1.832238000 | -0.776161000 |
| C | 4.180602000 | -0.508465000 | -0.244381000 |
| C | 5.318137000 | 1.876163000 | -1.111202000 |
| C | 5.531970000 | -0.459406000 | -0.568381000 |
| C | 6.104749000 | 0.733286000 | -1.007551000 |
| C | -0.120942000 | 4.718011000 | -0.814761000 |
| C | -0.252121000 | -0.417137000 | -2.625091000 |
| C | -0.751035000 | -3.024841000 | -1.757721000 |
| C | -1.684505000 | -0.865968000 | -0.001818000 |
| C | -2.454752000 | -1.776544000 | 0.841732000 |
| C | -2.558397000 | -3.448002000 | 2.280548000 |
| C | -3.397289000 | 2.334313000 | 0.397664000 |
| C | -3.590704000 | 0.861082000 | 0.006637000 |
| C | -3.769725000 | -2.180622000 | 0.915895000 |
| C | -3.831667000 | -3.264595000 | 1.836375000 |
| C | -4.584100000 | 0.728102000 | -1.162573000 |
| C | -4.739213000 | 3.009681000 | 0.717034000 |
| C | -5.735409000 | 2.871905000 | -0.441988000 |
| C | -5.925955000 | 1.402370000 | -0.840666000 |

| | | | |
|---|---|---|---|
| H | 0.071508000 | -0.704879000 | 4.722805000 |
| H | 0.138737000 | 4.136625000 | -2.873941000 |
| H | 0.666994000 | 2.783959000 | 1.859296000 |
| H | 1.044132000 | 1.919901000 | -2.334833000 |
| H | 1.927807000 | 0.468664000 | 5.881779000 |
| H | 3.371339000 | 2.734224000 | -0.854516000 |
| H | 3.554058000 | 1.629026000 | 2.089644000 |
| H | 3.670291000 | 1.629349000 | 4.547685000 |
| H | 3.746795000 | -1.445607000 | 0.083676000 |
| H | 5.754396000 | 2.808838000 | -1.451618000 |
| H | 6.134253000 | -1.357136000 | -0.488763000 |
| H | 7.156016000 | 0.768710000 | -1.270284000 |
| H | -0.035221000 | -0.721811000 | 2.260166000 |
| H | -0.253839000 | 4.998387000 | 1.314018000 |
| H | -0.520581000 | 5.697271000 | -1.053414000 |
| H | -1.738573000 | 0.863518000 | -0.959579000 |
| H | -2.109384000 | -4.124053000 | 2.988754000 |
| H | -2.718541000 | 2.398662000 | 1.252193000 |
| H | -2.910020000 | 2.864656000 | -0.430630000 |
| H | -3.970717000 | 0.317998000 | 0.873274000 |
| H | -4.141138000 | 1.196187000 | -2.050559000 |
| H | -4.571283000 | 4.064826000 | 0.952593000 |
| H | -4.591823000 | -1.787026000 | 0.342603000 |
| H | -4.702067000 | -3.833160000 | 2.122267000 |
| H | -4.728585000 | -0.326691000 | -1.413096000 |
| H | -5.167943000 | 2.555667000 | 1.619517000 |
| H | -5.364119000 | 3.435289000 | -1.307399000 |
| H | -6.416315000 | 0.864959000 | -0.018565000 |
| H | -6.594089000 | 1.323502000 | -1.703361000 |
| H | -6.696868000 | 3.317363000 | -0.168930000 |
| Mo | 0.267321000 | -1.495390000 | -0.982184000 |
| N | -2.285483000 | 0.270991000 | -0.345911000 |
| O | 1.304032000 | -3.544553000 | 1.251442000 |
| O | 2.745959000 | -2.454076000 | -2.706006000 |
| O | -0.534961000 | 0.121701000 | -3.607247000 |
| O | -1.339035000 | -3.913373000 | -2.201529000 |
| O | -1.716789000 | -2.575316000 | 1.685167000 |
| P | 1.593953000 | 0.478999000 | 0.142840000 |

11 $[Mo(CO)_4(PPh_3)\{C(NC_6H_{12})(C_4H_3O)\}]$, cis-syn,Z (2)

| | | | |
|---|---|---|---|
| C | 0.041922000 | -2.854659000 | -0.149769000 |
| C | 0.141199000 | -0.584078000 | 4.110267000 |
| C | 0.191654000 | -0.426774000 | 2.726020000 |
| C | 1.028957000 | -1.668108000 | -2.513132000 |
| C | 1.305977000 | -0.494299000 | 4.866995000 |
| C | 1.404796000 | -0.167491000 | 2.079924000 |
| C | 1.570976000 | 2.453660000 | -1.238694000 |
| C | 1.585776000 | 1.911008000 | 0.054780000 |
| C | 1.729724000 | 3.822247000 | -1.439003000 |
| C | 1.742927000 | 2.777746000 | 1.142484000 |

| | | | |
|---|---|---|---|
| C | 1.892625000 | 4.675608000 | -0.348597000 |
| C | 1.893068000 | 4.149736000 | 0.940299000 |
| C | 2.522642000 | -0.247970000 | 4.233042000 |
| C | 2.573408000 | -0.086558000 | 2.851025000 |
| C | 3.152716000 | -0.504584000 | -0.163111000 |
| C | 3.445204000 | -1.869223000 | -0.025065000 |
| C | 4.163929000 | 0.356731000 | -0.600131000 |
| C | 4.715511000 | -2.355295000 | -0.313580000 |
| C | 5.435080000 | -0.135529000 | -0.898285000 |
| C | 5.715323000 | -1.490024000 | -0.755705000 |
| C | -0.811455000 | 0.391319000 | -2.464749000 |
| C | -1.664056000 | -2.250098000 | -2.333331000 |
| C | -2.059814000 | 4.165242000 | 0.886886000 |
| C | -2.236089000 | -0.716933000 | 0.118172000 |
| C | -2.383073000 | 2.708797000 | 1.251322000 |
| C | -2.411715000 | 1.805798000 | 0.005603000 |
| C | -3.000754000 | -1.805269000 | 0.732327000 |
| C | -3.021141000 | 4.715025000 | -0.175005000 |
| C | -3.035456000 | -3.167261000 | 0.569411000 |
| C | -3.047160000 | 3.814731000 | -1.417098000 |
| C | -3.382688000 | 2.361922000 | -1.052358000 |
| C | -4.058166000 | -3.678997000 | 1.416678000 |
| C | -4.592317000 | -2.604719000 | 2.056925000 |
| H | 1.269132000 | -0.624429000 | 5.942802000 |
| H | 1.443854000 | 1.805151000 | -2.096607000 |
| H | 1.723574000 | 4.219211000 | -2.447814000 |
| H | 1.754007000 | 2.387392000 | 2.151749000 |
| H | 2.014028000 | 4.805544000 | 1.795450000 |
| H | 2.014791000 | 5.741694000 | -0.503654000 |
| H | 2.683023000 | -2.559925000 | 0.312399000 |
| H | 3.436315000 | -0.186596000 | 4.813840000 |
| H | 3.527729000 | 0.093476000 | 2.371297000 |
| H | 3.970631000 | 1.415550000 | -0.710408000 |
| H | 4.920797000 | -3.413803000 | -0.200679000 |
| H | 6.204518000 | 0.547309000 | -1.241247000 |
| H | 6.702953000 | -1.871482000 | -0.989057000 |
| H | -0.714936000 | -0.520637000 | 2.143141000 |
| H | -0.808178000 | -0.788944000 | 4.592243000 |
| H | -1.033057000 | 4.218803000 | 0.509593000 |
| H | -1.408428000 | 1.737330000 | -0.413497000 |
| H | -1.652898000 | 2.321268000 | 1.967609000 |
| H | -2.069536000 | 3.842811000 | -1.912013000 |
| H | -2.092399000 | 4.783667000 | 1.789440000 |
| H | -2.417136000 | -3.740002000 | -0.097230000 |
| H | -2.731986000 | 5.733643000 | -0.451976000 |
| H | -3.359957000 | 1.725756000 | -1.939489000 |
| H | -3.365968000 | 2.666001000 | 1.741583000 |
| H | -3.673327000 | 0.435943000 | 0.931445000 |
| H | -3.774420000 | 4.186749000 | -2.145068000 |
| H | -4.032678000 | 4.781189000 | 0.246705000 |
| H | -4.352969000 | -4.709281000 | 1.533793000 |

| | | | |
|---|---|---|---|
| H | -4.403593000 | 2.313327000 | -0.649162000 |
| H | -5.367498000 | -2.494412000 | 2.797402000 |
| Mo | -0.426086000 | -1.172567000 | -1.211676000 |
| N | -2.810371000 | 0.451347000 | 0.392192000 |
| O | 0.336886000 | -3.838907000 | 0.372434000 |
| O | 1.812121000 | -1.974082000 | -3.302556000 |
| O | -1.000658000 | 1.201550000 | -3.263952000 |
| O | -2.359972000 | -2.897970000 | -2.989484000 |
| O | -3.980577000 | -1.463520000 | 1.662928000 |
| P | 1.426817000 | 0.067288000 | 0.236014000 |

12 $[Mo(CO)_4(PPh_3)\{C(NC_6H_{12})(C_4H_3O)\}]$, cis-syn,E (2)

| | | | |
|---|---|---|---|
| C | 0.050862000 | -0.612817000 | -2.693456000 |
| C | 0.346321000 | -3.221151000 | -1.783800000 |
| C | 0.356302000 | 4.237279000 | 0.225129000 |
| C | 0.408404000 | 4.565018000 | -1.126575000 |
| C | 1.592019000 | -1.055884000 | -0.117643000 |
| C | 2.168778000 | -3.274487000 | 1.056982000 |
| C | 2.320257000 | -1.935648000 | 0.780314000 |
| C | 3.135142000 | -3.626634000 | 2.036430000 |
| C | 3.568119000 | 0.590109000 | -0.366954000 |
| C | 3.675428000 | 1.647305000 | 0.743915000 |
| C | 3.814020000 | -2.481682000 | 2.323530000 |
| C | 4.002426000 | 1.166055000 | -1.724440000 |
| C | 5.092009000 | 2.237140000 | 0.815617000 |
| C | 5.418241000 | 1.756829000 | -1.650484000 |
| C | 5.538021000 | 2.806966000 | -0.537848000 |
| C | -0.130712000 | 3.688165000 | -2.067780000 |
| C | -0.233054000 | 3.042003000 | 0.639173000 |
| C | -0.380252000 | 0.008895000 | 4.114294000 |
| C | -0.453421000 | -0.049211000 | 2.723876000 |
| C | -0.712725000 | 2.491995000 | -1.657348000 |
| C | -0.776798000 | 2.154432000 | -0.296165000 |
| C | -1.041444000 | -2.727729000 | 0.623820000 |
| C | -1.346700000 | 0.703206000 | 4.837023000 |
| C | -1.488766000 | 0.593425000 | 2.036305000 |
| C | -2.183792000 | -2.072819000 | -1.890614000 |
| C | -2.386893000 | 1.340051000 | 4.162839000 |
| C | -2.458475000 | 1.286962000 | 2.773193000 |
| C | -3.338905000 | 0.799831000 | -0.145685000 |
| C | -3.874178000 | 2.036335000 | -0.522753000 |
| C | -4.206323000 | -0.287049000 | 0.027050000 |
| C | -5.246187000 | 2.179544000 | -0.728835000 |
| C | -5.575351000 | -0.138936000 | -0.168504000 |
| C | -6.099474000 | 1.094700000 | -0.551242000 |
| H | 0.291415000 | -0.606293000 | 2.171035000 |
| H | 0.426110000 | -0.500041000 | 4.630255000 |
| H | 0.770302000 | 4.912950000 | 0.965515000 |
| H | 0.862955000 | 5.495939000 | -1.446304000 |
| H | 1.452826000 | -3.930306000 | 0.594726000 |

| | | | |
|---|---|---|---|
| H | 1.603187000 | 0.676341000 | -1.063966000 |
| H | 2.952990000 | 2.446856000 | 0.539760000 |
| H | 3.295853000 | 1.951896000 | -2.023619000 |
| H | 3.296849000 | -4.597553000 | 2.476079000 |
| H | 3.395494000 | 1.195739000 | 1.698080000 |
| H | 3.949979000 | 0.384854000 | -2.488345000 |
| H | 4.212983000 | -0.252045000 | -0.121114000 |
| H | 4.606589000 | -2.247299000 | 3.015369000 |
| H | 4.912126000 | 3.672623000 | -0.789523000 |
| H | 5.130023000 | 3.012437000 | 1.587051000 |
| H | 5.685614000 | 2.191924000 | -2.618040000 |
| H | 5.795067000 | 1.454408000 | 1.128513000 |
| H | 6.136647000 | 0.948192000 | -1.465447000 |
| H | 6.567269000 | 3.173604000 | -0.474600000 |
| H | -0.098504000 | 3.932405000 | -3.123591000 |
| H | -0.269164000 | 2.805999000 | 1.694850000 |
| H | -1.125881000 | 1.822876000 | -2.402067000 |
| H | -1.295552000 | 0.741079000 | 5.919453000 |
| H | -3.148400000 | 1.875742000 | 4.718741000 |
| H | -3.226084000 | 2.892778000 | -0.657424000 |
| H | -3.277005000 | 1.779385000 | 2.263066000 |
| H | -3.811035000 | -1.254991000 | 0.310539000 |
| H | -5.644443000 | 3.143114000 | -1.026994000 |
| H | -6.230461000 | -0.991894000 | -0.033484000 |
| H | -7.165534000 | 1.206891000 | -0.713609000 |
| Mo | -0.455847000 | -1.590121000 | -0.975244000 |
| N | 2.185912000 | 0.074441000 | -0.494525000 |
| O | 0.322725000 | -0.134234000 | -3.707320000 |
| O | 0.803374000 | -4.178791000 | -2.241744000 |
| O | 3.354953000 | -1.451584000 | 1.578343000 |
| O | -1.406667000 | -3.421651000 | 1.466776000 |
| O | -3.141752000 | -2.384099000 | -2.454221000 |
| P | -1.532434000 | 0.522405000 | 0.179079000 |

## Crystallographic supplementary material

Table S1. Bond lengths [Å] and angles [°] for **1**

| | |
|---|---|
| Mo(1)-C(3) | 1.9812(18) |
| Mo(1)-C(1) | 1.9870(19) |
| Mo(1)-C(4) | 2.0285(18) |
| Mo(1)-C(2) | 2.0293(19) |
| Mo(1)-C(6) | 2.2693(17) |
| Mo(1)-P(1) | 2.5669(5) |
| P(1)-C(17) | 1.8311(17) |
| P(1)-C(29) | 1.8358(17) |
| P(1)-C(23) | 1.8374(16) |
| N(1)-C(6) | 1.310(2) |
| N(1)-C(11) | 1.459(2) |
| N(1)-H(1) | 0.8800 |
| O(1)-C(1) | 1.155(2) |
| O(2)-C(2) | 1.149(2) |
| O(3)-C(3) | 1.153(2) |
| O(4)-C(4) | 1.150(2) |
| O(6)-C(10) | 1.360(3) |
| O(6)-C(7) | 1.385(2) |
| C(6)-C(7) | 1.465(2) |
| C(7)-C(8) | 1.359(3) |
| C(8)-C(9) | 1.425(3) |
| C(8)-H(8) | 0.9500 |
| C(9)-C(10) | 1.345(4) |
| C(9)-H(9) | 0.9500 |
| C(10)-H(10) | 0.9500 |
| C(11)-C(12) | 1.521(3) |
| C(11)-C(16) | 1.533(2) |
| C(11)-H(11) | 1.0000 |
| C(12)-C(13) | 1.528(3) |
| C(12)-H(12A) | 0.9900 |
| C(12)-H(12B) | 0.9900 |
| C(13)-C(14) | 1.525(3) |
| C(13)-H(13A) | 0.9900 |
| C(13)-H(13B) | 0.9900 |
| C(14)-C(15) | 1.520(3) |
| C(14)-H(14A) | 0.9900 |

| | |
|---|---|
| C(14)-H(14B) | 0.9900 |
| C(15)-C(16) | 1.528(3) |
| C(15)-H(15A) | 0.9900 |
| C(15)-H(15B) | 0.9900 |
| C(16)-H(16A) | 0.9900 |
| C(16)-H(16B) | 0.9900 |
| C(17)-C(18) | 1.394(2) |
| C(17)-C(22) | 1.398(2) |
| C(18)-C(19) | 1.393(3) |
| C(18)-H(18) | 0.9500 |
| C(19)-C(20) | 1.387(3) |
| C(19)-H(19) | 0.9500 |
| C(20)-C(21) | 1.381(3) |
| C(20)-H(20) | 0.9500 |
| C(21)-C(22) | 1.390(3) |
| C(21)-H(21) | 0.9500 |
| C(22)-H(22) | 0.9500 |
| C(23)-C(28) | 1.389(2) |
| C(23)-C(24) | 1.395(2) |
| C(24)-C(25) | 1.385(3) |
| C(24)-H(24) | 0.9500 |
| C(25)-C(26) | 1.390(3) |
| C(25)-H(25) | 0.9500 |
| C(26)-C(27) | 1.376(3) |
| C(26)-H(26) | 0.9500 |
| C(27)-C(28) | 1.399(3) |
| C(27)-H(27) | 0.9500 |
| C(28)-H(28) | 0.9500 |
| C(29)-C(34) | 1.389(2) |
| C(29)-C(30) | 1.399(2) |
| C(30)-C(31) | 1.397(3) |
| C(30)-H(30) | 0.9500 |
| C(31)-C(32) | 1.383(3) |
| C(31)-H(31) | 0.9500 |
| C(32)-C(33) | 1.386(3) |
| C(32)-H(32) | 0.9500 |
| C(33)-C(34) | 1.395(3) |
| C(33)-H(33) | 0.9500 |
| C(34)-H(34) | 0.9500 |

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|---|---|
| C(3)-Mo(1)-C(1) | 90.24(8) |
| C(3)-Mo(1)-C(4) | 84.87(8) |
| C(1)-Mo(1)-C(4) | 83.15(8) |
| C(3)-Mo(1)-C(2) | 89.84(8) |
| C(1)-Mo(1)-C(2) | 86.20(8) |
| C(4)-Mo(1)-C(2) | 168.07(7) |
| C(3)-Mo(1)-C(6) | 87.33(7) |
| C(1)-Mo(1)-C(6) | 177.23(7) |
| C(4)-Mo(1)-C(6) | 97.96(7) |
| C(2)-Mo(1)-C(6) | 92.46(7) |
| C(3)-Mo(1)-P(1) | 176.36(6) |
| C(1)-Mo(1)-P(1) | 89.53(6) |
| C(4)-Mo(1)-P(1) | 98.71(5) |
| C(2)-Mo(1)-P(1) | 86.52(5) |
| C(6)-Mo(1)-P(1) | 92.81(4) |
| C(17)-P(1)-C(29) | 102.36(8) |
| C(17)-P(1)-C(23) | 101.31(8) |
| C(29)-P(1)-C(23) | 101.12(7) |
| C(17)-P(1)-Mo(1) | 117.29(6) |
| C(29)-P(1)-Mo(1) | 119.46(5) |
| C(23)-P(1)-Mo(1) | 112.62(6) |
| C(6)-N(1)-C(11) | 126.69(14) |
| C(6)-N(1)-H(1) | 116.7 |
| C(11)-N(1)-H(1) | 116.7 |
| C(10)-O(6)-C(7) | 107.06(19) |
| O(1)-C(1)-Mo(1) | 177.88(18) |
| O(2)-C(2)-Mo(1) | 173.18(18) |
| O(3)-C(3)-Mo(1) | 178.75(19) |
| O(4)-C(4)-Mo(1) | 170.48(18) |
| N(1)-C(6)-C(7) | 110.73(15) |
| N(1)-C(6)-Mo(1) | 128.36(12) |
| C(7)-C(6)-Mo(1) | 120.90(12) |
| C(8)-C(7)-O(6) | 108.56(16) |
| C(8)-C(7)-C(6) | 133.78(18) |
| O(6)-C(7)-C(6) | 117.62(16) |
| C(7)-C(8)-C(9) | 107.4(2) |
| C(7)-C(8)-H(8) | 126.3 |
| C(9)-C(8)-H(8) | 126.3 |

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|---|---|
| C(10)-C(9)-C(8) | 106.3(2) |
| C(10)-C(9)-H(9) | 126.9 |
| C(8)-C(9)-H(9) | 126.9 |
| C(9)-C(10)-O(6) | 110.7(2) |
| C(9)-C(10)-H(10) | 124.6 |
| O(6)-C(10)-H(10) | 124.6 |
| N(1)-C(11)-C(12) | 110.65(15) |
| N(1)-C(11)-C(16) | 109.35(14) |
| C(12)-C(11)-C(16) | 111.16(15) |
| N(1)-C(11)-H(11) | 108.5 |
| C(12)-C(11)-H(11) | 108.5 |
| C(16)-C(11)-H(11) | 108.5 |
| C(11)-C(12)-C(13) | 109.70(16) |
| C(11)-C(12)-H(12A) | 109.7 |
| C(13)-C(12)-H(12A) | 109.7 |
| C(11)-C(12)-H(12B) | 109.7 |
| C(13)-C(12)-H(12B) | 109.7 |
| H(12A)-C(12)-H(12B) | 108.2 |
| C(14)-C(13)-C(12) | 111.30(18) |
| C(14)-C(13)-H(13A) | 109.4 |
| C(12)-C(13)-H(13A) | 109.4 |
| C(14)-C(13)-H(13B) | 109.4 |
| C(12)-C(13)-H(13B) | 109.4 |
| H(13A)-C(13)-H(13B) | 108.0 |
| C(15)-C(14)-C(13) | 111.52(17) |
| C(15)-C(14)-H(14A) | 109.3 |
| C(13)-C(14)-H(14A) | 109.3 |
| C(15)-C(14)-H(14B) | 109.3 |
| C(13)-C(14)-H(14B) | 109.3 |
| H(14A)-C(14)-H(14B) | 108.0 |
| C(14)-C(15)-C(16) | 110.86(17) |
| C(14)-C(15)-H(15A) | 109.5 |
| C(16)-C(15)-H(15A) | 109.5 |
| C(14)-C(15)-H(15B) | 109.5 |
| C(16)-C(15)-H(15B) | 109.5 |
| H(15A)-C(15)-H(15B) | 108.1 |
| C(15)-C(16)-C(11) | 110.15(15) |
| C(15)-C(16)-H(16A) | 109.6 |
| C(11)-C(16)-H(16A) | 109.6 |

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|---|---|
| C(15)-C(16)-H(16B) | 109.6 |
| C(11)-C(16)-H(16B) | 109.6 |
| H(16A)-C(16)-H(16B) | 108.1 |
| C(18)-C(17)-C(22) | 118.64(15) |
| C(18)-C(17)-P(1) | 123.55(13) |
| C(22)-C(17)-P(1) | 117.79(13) |
| C(19)-C(18)-C(17) | 120.45(17) |
| C(19)-C(18)-H(18) | 119.8 |
| C(17)-C(18)-H(18) | 119.8 |
| C(20)-C(19)-C(18) | 120.11(19) |
| C(20)-C(19)-H(19) | 119.9 |
| C(18)-C(19)-H(19) | 119.9 |
| C(21)-C(20)-C(19) | 120.08(18) |
| C(21)-C(20)-H(20) | 120.0 |
| C(19)-C(20)-H(20) | 120.0 |
| C(20)-C(21)-C(22) | 119.90(19) |
| C(20)-C(21)-H(21) | 120.0 |
| C(22)-C(21)-H(21) | 120.0 |
| C(21)-C(22)-C(17) | 120.81(18) |
| C(21)-C(22)-H(22) | 119.6 |
| C(17)-C(22)-H(22) | 119.6 |
| C(28)-C(23)-C(24) | 118.67(16) |
| C(28)-C(23)-P(1) | 123.17(13) |
| C(24)-C(23)-P(1) | 118.16(13) |
| C(25)-C(24)-C(23) | 120.83(18) |
| C(25)-C(24)-H(24) | 119.6 |
| C(23)-C(24)-H(24) | 119.6 |
| C(24)-C(25)-C(26) | 119.94(19) |
| C(24)-C(25)-H(25) | 120.0 |
| C(26)-C(25)-H(25) | 120.0 |
| C(27)-C(26)-C(25) | 119.96(18) |
| C(27)-C(26)-H(26) | 120.0 |
| C(25)-C(26)-H(26) | 120.0 |
| C(26)-C(27)-C(28) | 120.1(2) |
| C(26)-C(27)-H(27) | 120.0 |
| C(28)-C(27)-H(27) | 120.0 |
| C(23)-C(28)-C(27) | 120.52(18) |
| C(23)-C(28)-H(28) | 119.7 |
| C(27)-C(28)-H(28) | 119.7 |

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|---|---|
| C(34)-C(29)-C(30) | 118.47(16) |
| C(34)-C(29)-P(1) | 119.61(12) |
| C(30)-C(29)-P(1) | 121.80(13) |
| C(31)-C(30)-C(29) | 120.45(17) |
| C(31)-C(30)-H(30) | 119.8 |
| C(29)-C(30)-H(30) | 119.8 |
| C(32)-C(31)-C(30) | 120.32(18) |
| C(32)-C(31)-H(31) | 119.8 |
| C(30)-C(31)-H(31) | 119.8 |
| C(31)-C(32)-C(33) | 119.71(18) |
| C(31)-C(32)-H(32) | 120.1 |
| C(33)-C(32)-H(32) | 120.1 |
| C(32)-C(33)-C(34) | 120.04(18) |
| C(32)-C(33)-H(33) | 120.0 |
| C(34)-C(33)-H(33) | 120.0 |
| C(29)-C(34)-C(33) | 121.01(16) |
| C(29)-C(34)-H(34) | 119.5 |
| C(33)-C(34)-H(34) | 119.5 |

[1] F. Weigend, R. Ahlrichs, Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy, Physical Chemistry Chemical Physics 7 (2005) 3297-3305.