Electrochemical behaviour and structure of novel phosphine- and phosphite substituted tungsten(0) Fischer carbene complexes

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Supporting information

DFT calculations:

Geometries were optimized in gas phase with the triple-ζ basis set 6-311G(d,p) on all atoms except tungsten, where def-TZSVPP [i] was used (this level is denoted B3LYP/def2-TZSVPP).

Optimized Cartesian coordinates (Å)

1 *cis*-[W(PPh$_3$)(CO)$_4${C(OEt)C$_4$H$_4$S}], (1*cis*)

W	0.598609000	-1.200136000	-0.663467000
C	0.870071000	-0.144047000	-2.411655000
O	1.004074000	0.364206000	-3.434846000
C	1.952540000	-2.533393000	-1.322600000
O	2.705047000	-3.325708000	-1.696566000
C	0.248285000	-2.416714000	0.947426000
O	0.008828000	-3.166588000	1.792708000
C	-0.803920000	-2.263772000	-1.711561000
O	-1.549951000	-2.879497000	-2.336554000
C	2.270529000	-0.060340000	0.247840000
O	3.181007000	-0.483776000	1.140511000
C	3.153409000	-1.782975000	1.768508000
H	3.039885000	-2.547492000	1.000688000
H	2.292768000	-1.823017000	2.437664000
C	4.455365000	-1.942382000	2.528927000
H	4.467341000	-2.912493000	3.032143000

H	4.567216000	-1.161010000	3.283708000
H	5.309972000	-1.895812000	1.850917000
C	2.705071000	1.278586000	-0.138871000
C	2.024412000	2.271615000	-0.819273000
H	1.009311000	2.155276000	-1.164033000
C	2.768016000	3.460058000	-0.995700000
H	2.390105000	4.335131000	-1.506670000
C	4.023539000	3.379444000	-0.451113000
H	4.796297000	4.134021000	-0.457183000
S	4.314909000	1.861676000	0.305647000
P	-1.385480000	0.314091000	0.219653000
C	-1.340079000	0.835404000	2.001771000
C	-2.513452000	1.042957000	2.739604000
H	-3.480222000	0.872025000	2.282957000
C	-2.448398000	1.460042000	4.066793000
H	-3.364978000	1.610598000	4.626207000
C	-1.214012000	1.679369000	4.674693000
H	-1.166047000	2.001884000	5.708738000
C	-0.042794000	1.475417000	3.949657000
H	0.922750000	1.639560000	4.414631000
C	-0.105638000	1.051158000	2.624111000
H	0.808882000	0.884573000	2.070425000
C	-3.060825000	-0.483986000	0.110027000
C	-4.163909000	0.146108000	-0.476307000
H	-4.065043000	1.136935000	-0.899633000
C	-5.402860000	-0.492830000	-0.522631000
H	-6.245069000	0.008554000	-0.986359000
C	-5.558652000	-1.763053000	0.022693000
H	-6.521505000	-2.259750000	-0.016008000
C	-4.467639000	-2.394737000	0.617126000
H	-4.576669000	-3.385076000	1.044248000
C	-3.228712000	-1.763718000	0.657560000
H	-2.394861000	-2.274275000	1.121410000
C	-1.637643000	1.916420000	-0.679744000
C	-1.770068000	1.884434000	-2.076060000
H	-1.747334000	0.936960000	-2.601188000
C	-1.931532000	3.061122000	-2.800456000
H	-2.033531000	3.016222000	-3.878674000
C	-1.952032000	4.290905000	-2.142864000
H	-2.071471000	5.208419000	-2.707880000
C	-1.815417000	4.333299000	-0.758530000
H	-1.828505000	5.284891000	-0.238892000
C	-1.662741000	3.154300000	-0.028618000
H	-1.560208000	3.204507000	1.047670000

2 *trans*-[W(PPh$_3$)(CO)$_4${C(OEt)C$_4$H$_4$S}], (1*trans*)

W	0.776485000	-0.257014000	0.011409000
C	0.640613000	-1.741094000	1.424445000
O	0.553641000	-2.582880000	2.208012000

C	0.910658000	1.097166000	1.555167000
O	0.993987000	1.827522000	2.441507000
C	0.880809000	1.175651000	-1.467345000
O	0.941610000	1.957865000	-2.308862000
C	0.564621000	-1.736333000	-1.399710000
O	0.407942000	-2.585302000	-2.163380000
C	2.945194000	-0.328172000	-0.027615000
O	3.766644000	-1.388602000	-0.080754000
C	3.329776000	-2.760691000	-0.140651000
H	2.774715000	-2.911239000	-1.066441000
H	2.671779000	-2.963156000	0.703234000
C	4.573953000	-3.627155000	-0.094702000
H	4.287639000	-4.680787000	-0.145569000
H	5.128126000	-3.464564000	0.832006000
H	5.233391000	-3.407891000	-0.936953000
C	3.832542000	0.838380000	-0.009442000
C	3.546731000	2.190358000	0.048864000
H	2.541411000	2.576810000	0.094538000
C	4.688437000	3.022979000	0.042887000
H	4.645960000	4.103071000	0.083583000
C	5.857133000	2.310132000	-0.019522000
H	6.866280000	2.694498000	-0.036540000
S	5.585314000	0.612417000	-0.072937000
P	-1.813643000	0.086710000	0.003038000
C	-2.656545000	-0.428847000	1.572575000
C	-2.602262000	-1.774251000	1.964709000
H	-2.108483000	-2.503800000	1.334681000
C	-3.175673000	-2.187928000	3.162473000
H	-3.125184000	-3.232727000	3.447089000
C	-3.798802000	-1.262006000	3.997901000
H	-4.237877000	-1.583338000	4.935601000
C	-3.846910000	0.077204000	3.624006000
H	-4.324585000	0.806167000	4.269082000
C	-3.283507000	0.492997000	2.418089000
H	-3.335206000	1.538002000	2.141432000
C	-2.459403000	1.817740000	-0.240838000
C	-3.755758000	2.045496000	-0.724748000
H	-4.388714000	1.209218000	-0.993946000
C	-4.239952000	3.341883000	-0.872402000
H	-5.243606000	3.499069000	-1.251575000
C	-3.438922000	4.432969000	-0.539537000
H	-3.816202000	5.442488000	-0.658304000
C	-2.150387000	4.219030000	-0.059841000
H	-1.516959000	5.060301000	0.197820000
C	-1.663864000	2.920703000	0.084722000
H	-0.659054000	2.770005000	0.453441000
C	-2.759874000	-0.806757000	-1.324918000
C	-2.320832000	-0.657718000	-2.647634000
H	-1.444376000	-0.058065000	-2.864315000
C	-3.000910000	-1.269359000	-3.695146000
H	-2.645734000	-1.141864000	-4.711381000

C	-4.127051000	-2.049707000	-3.438468000
H	-4.652631000	-2.533167000	-4.254196000
C	-4.571137000	-2.205086000	-2.129095000
H	-5.447885000	-2.807723000	-1.919082000
C	-3.896843000	-1.583539000	-1.077868000
H	-4.264663000	-1.704701000	-0.067365000

3 *cis*-[W(PPh$_3$)(CO)$_4${C(OEt)C$_4$H$_4$O}], (2*cis*)

W	0.952214000	-1.018822000	-0.658823000
C	1.024651000	0.076961000	-2.411247000
O	1.058969000	0.590692000	-3.438539000
C	2.544891000	-2.076783000	-1.281599000
O	3.441676000	-2.715617000	-1.631956000
C	0.809792000	-2.284455000	0.944257000
O	0.695651000	-3.069774000	1.783916000
C	-0.198209000	-2.333660000	-1.736318000
O	-0.791577000	-3.083309000	-2.377927000
C	2.308654000	0.443623000	0.275308000
O	3.268919000	0.262290000	1.199456000
C	3.537983000	-1.020257000	1.801824000
H	3.707129000	-1.754421000	1.013777000
H	2.665707000	-1.324386000	2.381937000
C	4.761534000	-0.855320000	2.681910000
H	4.998134000	-1.807852000	3.162644000
H	4.586726000	-0.110939000	3.462118000
H	5.626257000	-0.544404000	2.091788000
C	2.411889000	1.849668000	-0.078676000
C	3.291542000	2.844784000	0.295705000
H	4.125586000	2.715189000	0.964554000
C	2.886950000	4.029944000	-0.369006000
H	3.345079000	5.004788000	-0.316985000
C	1.786441000	3.689201000	-1.103409000
H	1.132352000	4.240221000	-1.758218000
O	1.487702000	2.386160000	-0.939917000
P	-1.266362000	0.129122000	0.210165000
C	-1.374014000	0.477362000	2.033008000
C	-2.593490000	0.422801000	2.721246000
H	-3.500189000	0.147073000	2.197846000
C	-2.651817000	0.713307000	4.082162000
H	-3.602737000	0.660399000	4.600499000
C	-1.496057000	1.066397000	4.775041000
H	-1.542862000	1.289417000	5.835060000
C	-0.279584000	1.124927000	4.099898000
H	0.626178000	1.395244000	4.631036000
C	-0.218158000	0.827426000	2.740168000
H	0.734131000	0.863325000	2.227969000
C	-2.801516000	-0.883473000	-0.057258000
C	-3.970077000	-0.360513000	-0.621566000
H	-4.007984000	0.674623000	-0.934445000

C	-5.097841000	-1.164545000	-0.786771000
H	-5.992575000	-0.744267000	-1.232497000
C	-5.077042000	-2.495306000	-0.381713000
H	-5.953546000	-3.119693000	-0.512907000
C	-3.920801000	-3.022022000	0.191400000
H	-3.892370000	-4.057985000	0.509210000
C	-2.791665000	-2.225315000	0.348858000
H	-1.901738000	-2.654946000	0.791780000
C	-1.712757000	1.761370000	-0.549696000
C	-1.789890000	1.851723000	-1.946333000
H	-1.606227000	0.977003000	-2.557997000
C	-2.099402000	3.059767000	-2.562802000
H	-2.159341000	3.108976000	-3.644186000
C	-2.323692000	4.201839000	-1.793639000
H	-2.562207000	5.144213000	-2.274114000
C	-2.241250000	4.123303000	-0.406512000
H	-2.413677000	5.005298000	0.200363000
C	-1.941372000	2.910400000	0.213653000
H	-1.885126000	2.866645000	1.293573000

4 *trans*-[W(PPh$_3$)(CO)$_4${C(OEt)C$_4$H$_4$O}], (2*trans*)

W	0.952108000	-0.248919000	0.002661000
C	0.848422000	-1.758461000	1.386292000
O	0.778840000	-2.623272000	2.147484000
C	1.058644000	1.117023000	1.550154000
O	1.121873000	1.844745000	2.438019000
C	1.020400000	1.210987000	-1.460942000
O	1.051200000	1.995770000	-2.299996000
C	0.786914000	-1.724091000	-1.415409000
O	0.664341000	-2.575604000	-2.183617000
C	3.103831000	-0.234894000	-0.029221000
O	4.000218000	-1.234789000	-0.068028000
C	3.625980000	-2.625186000	-0.095721000
H	3.008269000	-2.808484000	-0.974728000
H	3.043693000	-2.854247000	0.796762000
C	4.908853000	-3.433100000	-0.141483000
H	4.670708000	-4.499658000	-0.162258000
H	5.525371000	-3.235596000	0.738124000
H	5.489641000	-3.193287000	-1.034869000
C	3.922751000	0.974507000	-0.018738000
C	5.286528000	1.166495000	-0.051339000
H	6.021487000	0.380742000	-0.093180000
C	5.512953000	2.567646000	-0.020431000
H	6.460079000	3.083088000	-0.033160000
C	4.277640000	3.143651000	0.029302000
H	3.939205000	4.165670000	0.066076000
O	3.309426000	2.202792000	0.031351000
P	-1.646106000	0.048497000	0.004146000
C	-2.471667000	-0.497410000	1.572338000

C	-2.396579000	-1.846936000	1.946884000
H	-1.897559000	-2.561865000	1.304338000
C	-2.954713000	-2.283090000	3.143846000
H	-2.888291000	-3.330686000	3.414624000
C	-3.582582000	-1.376017000	3.996288000
H	-4.009825000	-1.714915000	4.933302000
C	-3.650178000	-0.032752000	3.640409000
H	-4.131063000	0.681864000	4.299051000
C	-3.102253000	0.405569000	2.435309000
H	-3.168632000	1.453402000	2.172826000
C	-2.326440000	1.769220000	-0.221175000
C	-3.640114000	1.973110000	-0.668165000
H	-4.265361000	1.125174000	-0.918626000
C	-4.151874000	3.260005000	-0.803426000
H	-5.168788000	3.398472000	-1.153512000
C	-3.360947000	4.365854000	-0.495622000
H	-3.759530000	5.368318000	-0.604588000
C	-2.055249000	4.175632000	-0.054336000
H	-1.429188000	5.028485000	0.182446000
C	-1.540811000	2.886593000	0.078539000
H	-0.521841000	2.757110000	0.415237000
C	-2.580181000	-0.851538000	-1.327805000
C	-2.138292000	-0.696581000	-2.648816000
H	-1.265073000	-0.090786000	-2.861222000
C	-2.810876000	-1.311104000	-3.699550000
H	-2.453618000	-1.178984000	-4.714479000
C	-3.931889000	-2.100342000	-3.447828000
H	-4.451583000	-2.585879000	-4.266113000
C	-4.378209000	-2.262387000	-2.139972000
H	-5.250673000	-2.872536000	-1.933726000
C	-3.711538000	-1.638131000	-1.085563000
H	-4.080159000	-1.765631000	-0.076060000

5 *cis*-[W(PPh$_3$)(CO)$_4${C(CHA)C$_4$H$_4$S}], (3)

W	-0.516598000	-0.825431000	-1.188365000
C	0.798911000	-1.512514000	-2.564527000
O	1.512994000	-1.902928000	-3.386895000
C	-0.644359000	0.824229000	-2.381571000
O	-0.712108000	1.687491000	-3.150291000
C	-1.963693000	-1.605631000	-2.340244000
O	-2.761887000	-2.065636000	-3.037692000
C	-0.335198000	-2.635501000	-0.204894000
O	-0.199299000	-3.675271000	0.265911000
C	-2.123724000	-0.096735000	0.247562000
N	-2.510285000	1.145719000	0.529911000
H	-3.347849000	1.252291000	1.098953000
C	-2.965696000	-1.038063000	1.022154000
S	-3.596943000	-2.516550000	0.343822000
C	-3.380459000	-0.906030000	2.334964000

H	-3.072776000	-0.082018000	2.965983000
C	-4.187538000	-1.981488000	2.789841000
H	-4.586147000	-2.057794000	3.792905000
C	-4.401760000	-2.918276000	1.817553000
H	-4.987412000	-3.823030000	1.877215000
C	-1.947700000	2.427742000	0.096791000
H	-0.985746000	2.206585000	-0.364165000
C	-1.722562000	3.341412000	1.313139000
H	-1.039245000	2.858075000	2.014668000
H	-2.679206000	3.480771000	1.836397000
C	-1.177720000	4.711630000	0.883375000
H	-1.058424000	5.350726000	1.763582000
H	-0.175344000	4.580755000	0.457545000
C	-2.086601000	5.387674000	-0.152102000
H	-1.645474000	6.333960000	-0.480270000
H	-3.046447000	5.637796000	0.318177000
C	-2.336001000	4.472134000	-1.358449000
H	-3.038096000	4.940715000	-2.054455000
H	-1.401459000	4.329136000	-1.913238000
C	-2.876107000	3.100589000	-0.929663000
H	-2.999406000	2.448300000	-1.796234000
H	-3.868949000	3.223219000	-0.475713000
P	1.552742000	-0.049868000	0.282751000
C	2.659532000	-1.465852000	0.768877000
C	2.949856000	-1.790735000	2.097861000
H	2.538153000	-1.203064000	2.907475000
C	3.775687000	-2.874412000	2.398507000
H	3.984986000	-3.113816000	3.435226000
C	4.327399000	-3.641895000	1.378467000
H	4.966943000	-4.485139000	1.613660000
C	4.050187000	-3.320472000	0.050628000
H	4.473457000	-3.910868000	-0.754050000
C	3.221320000	-2.245661000	-0.252547000
H	3.018622000	-2.016802000	-1.290348000
C	2.786546000	1.130909000	-0.448806000
C	4.140101000	1.096908000	-0.084715000
H	4.495308000	0.348333000	0.612316000
C	5.040310000	2.014779000	-0.619840000
H	6.084821000	1.970299000	-0.332112000
C	4.604135000	2.980541000	-1.524705000
H	5.307508000	3.690497000	-1.945147000
C	3.262550000	3.021623000	-1.894068000
H	2.914339000	3.760414000	-2.606905000
C	2.361671000	2.100887000	-1.362306000
H	1.328824000	2.130797000	-1.677869000
C	1.177597000	0.727839000	1.929775000
C	1.801921000	1.894056000	2.386322000
H	2.531517000	2.398759000	1.766317000
C	1.496559000	2.416593000	3.643548000
H	1.989421000	3.322093000	3.979706000
C	0.573743000	1.776517000	4.465792000

H	0.345182000	2.178027000	5.446637000
C	-0.055910000	0.615336000	4.018474000
H	-0.773895000	0.106036000	4.651787000
C	0.234097000	0.102353000	2.757204000
H	-0.273175000	-0.792538000	2.416508000

6 *cis*-[W(PPh$_3$)(CO)$_4${C(CHA)C$_4$H$_4$O}], (4)

W	-0.348916000	-1.084661000	-1.124642000
C	1.081199000	-1.518919000	-2.486336000
O	1.860525000	-1.782368000	-3.300606000
C	-0.884269000	0.396456000	-2.428888000
O	-1.154155000	1.160766000	-3.254485000
C	-1.591042000	-2.298475000	-2.125169000
O	-2.287820000	-3.026620000	-2.691420000
C	0.285603000	-2.710814000	-0.036338000
O	0.658047000	-3.659591000	0.500718000
C	-2.091301000	-0.663090000	0.299150000
N	-2.703687000	0.489110000	0.560870000
H	-3.507016000	0.461337000	1.183886000
C	-2.742793000	-1.754949000	1.028471000
O	-3.680954000	-1.415632000	2.000308000
C	-2.704375000	-3.124356000	0.943177000
H	-2.096580000	-3.700325000	0.269451000
C	-3.638176000	-3.642608000	1.884175000
H	-3.861863000	-4.679391000	2.076950000
C	-4.196322000	-2.564598000	2.496970000
H	-4.930528000	-2.454593000	3.278076000
C	-2.436832000	1.829165000	0.036784000
H	-1.445904000	1.799791000	-0.416347000
C	-2.437989000	2.852811000	1.183809000
H	-1.672304000	2.587569000	1.915504000
H	-3.407470000	2.807359000	1.699875000
C	-2.213635000	4.277635000	0.655865000
H	-2.248367000	4.986921000	1.488453000
H	-1.204493000	4.347137000	0.231301000
C	-3.243858000	4.657519000	-0.416665000
H	-3.026134000	5.654404000	-0.812486000
H	-4.239244000	4.714980000	0.042851000
C	-3.269214000	3.628468000	-1.554532000
H	-4.054215000	3.875567000	-2.275483000
H	-2.322581000	3.664338000	-2.106144000
C	-3.486337000	2.203545000	-1.026780000
H	-3.454610000	1.481937000	-1.844997000
H	-4.482995000	2.128695000	-0.571112000
P	1.452297000	0.254611000	0.286292000
C	2.891691000	-0.817191000	0.783541000
C	3.241414000	-1.058298000	2.115744000

H	2.679597000	-0.602050000	2.919931000
C	4.319650000	-1.887643000	2.426325000
H	4.573069000	-2.066356000	3.465462000
C	5.064969000	-2.480171000	1.412807000
H	5.901281000	-3.125996000	1.655587000
C	4.727678000	-2.239586000	0.081568000
H	5.300155000	-2.696281000	-0.717805000
C	3.648973000	-1.419574000	-0.231627000
H	3.401763000	-1.251520000	-1.271674000
C	2.341498000	1.695321000	-0.480227000
C	3.637626000	2.050686000	-0.079456000
H	4.152029000	1.463971000	0.671583000
C	4.278206000	3.149048000	-0.646749000
H	5.282512000	3.406468000	-0.329072000
C	3.636342000	3.909041000	-1.622911000
H	4.139183000	4.759889000	-2.068732000
C	2.351432000	3.562543000	-2.030652000
H	1.848429000	4.137918000	-2.799517000
C	1.710315000	2.461589000	-1.464966000
H	0.722768000	2.191362000	-1.810593000
C	0.898049000	0.938240000	1.925096000
C	1.226221000	2.223217000	2.370916000
H	1.822506000	2.878182000	1.749017000
C	0.790841000	2.673455000	3.617598000
H	1.052945000	3.673089000	3.946243000
C	0.028969000	1.845685000	4.437489000
H	-0.304863000	2.196073000	5.407733000
C	-0.304942000	0.563993000	4.001562000
H	-0.900673000	-0.088642000	4.629805000
C	0.119179000	0.117699000	2.753284000
H	-0.153007000	-0.877358000	2.420990000

7 *mer*-[W(dppe)(CO)$_3${C(OEt)C$_4$H$_4$S}], (5)

W	0.046863000	-0.716738000	-0.448751000
C	0.132858000	0.517945000	-2.087403000
O	0.229831000	1.186127000	-3.022920000
C	0.992191000	-2.130356000	-1.504510000
O	1.583805000	-2.947357000	-2.082071000
C	0.072528000	-1.957981000	1.170102000
O	0.149469000	-2.643303000	2.101759000
C	-1.893991000	-1.360762000	-1.112464000
O	-2.463072000	-2.585892000	-1.035433000
C	-2.879733000	-0.547471000	-1.838666000
C	-2.971106000	0.821310000	-1.999543000
H	-2.262154000	1.509418000	-1.567713000
C	-4.085462000	1.241312000	-2.764463000
H	-4.304585000	2.277125000	-2.987134000
C	-4.854324000	0.192572000	-3.193396000

H	-5.748795000	0.229830000	-3.797488000
S	-4.241339000	-1.325895000	-2.656571000
C	-1.820066000	-3.737694000	-0.464035000
H	-1.781209000	-3.614777000	0.619015000
H	-0.800548000	-3.805732000	-0.844528000
C	-2.644872000	-4.951378000	-0.850526000
H	-2.198958000	-5.851136000	-0.418373000
H	-2.678104000	-5.069919000	-1.935639000
H	-3.668621000	-4.862362000	-0.480331000
P	2.292832000	0.301596000	0.268161000
P	-0.757422000	1.012247000	1.298515000
C	1.956226000	1.691429000	1.486227000
H	2.832068000	1.882695000	2.109514000
H	1.761101000	2.595070000	0.904076000
C	0.741796000	1.375088000	2.364527000
H	0.532674000	2.213605000	3.033906000
H	0.929627000	0.487673000	2.975353000
C	3.360232000	1.104086000	-1.020058000
C	3.878303000	2.399440000	-0.906932000
H	3.662020000	3.008662000	-0.038000000
C	4.686817000	2.931604000	-1.911243000
H	5.075824000	3.938700000	-1.808139000
C	4.993634000	2.175706000	-3.038190000
H	5.621254000	2.590388000	-3.818873000
C	4.486008000	0.883270000	-3.158668000
H	4.715740000	0.286943000	-4.034392000
C	3.673930000	0.353299000	-2.161529000
H	3.279991000	-0.649896000	-2.274400000
C	3.581162000	-0.707978000	1.162201000
C	4.712082000	-0.101482000	1.728462000
H	4.857572000	0.969841000	1.645570000
C	5.676057000	-0.863086000	2.380028000
H	6.543833000	-0.377650000	2.812938000
C	5.531985000	-2.247820000	2.466866000
H	6.284454000	-2.842215000	2.973008000
C	4.424090000	-2.861822000	1.892866000
H	4.307658000	-3.938314000	1.946756000
C	3.454611000	-2.096906000	1.243936000
H	2.600714000	-2.585535000	0.795689000
C	-2.039966000	0.470555000	2.513721000
C	-3.231394000	-0.076436000	2.017423000
H	-3.374278000	-0.176972000	0.948244000
C	-4.232176000	-0.498827000	2.887193000
H	-5.148199000	-0.917226000	2.485772000
C	-4.053676000	-0.395959000	4.265804000
H	-4.829916000	-0.734509000	4.942783000
C	-2.871154000	0.137868000	4.769260000
H	-2.721299000	0.216690000	5.840268000
C	-1.872035000	0.573879000	3.899810000
H	-0.964100000	0.991402000	4.316346000
C	-1.301986000	2.736641000	0.861225000

C	-2.263836000	3.431181000	1.606082000
H	-2.750037000	2.951880000	2.446576000
C	-2.612839000	4.737216000	1.268804000
H	-3.364342000	5.257483000	1.852362000
C	-2.005012000	5.371548000	0.188001000
H	-2.279600000	6.387373000	-0.073064000
C	-1.049489000	4.689567000	-0.561449000
H	-0.576790000	5.168970000	-1.411252000
C	-0.706038000	3.380060000	-0.231927000
H	0.017023000	2.853503000	-0.842162000

8 *mer*-[W(dppe)(CO)$_3${C(OEt)C$_4$H$_4$O}], (6)

W	0.008578000	-0.699368000	-0.564739000
C	0.175303000	0.664273000	-2.088487000
O	0.317243000	1.409738000	-2.958186000
C	1.080830000	-1.996223000	-1.646810000
O	1.747780000	-2.744699000	-2.235355000
C	-0.057674000	-2.070638000	0.943801000
O	-0.037300000	-2.831911000	1.817764000
C	-1.858742000	-1.334490000	-1.425040000
O	-2.413863000	-2.556901000	-1.494030000
C	-2.789592000	-0.460164000	-2.147254000
C	-2.941781000	0.906593000	-2.218474000
H	-2.331600000	1.637309000	-1.718858000
C	-4.059879000	1.168376000	-3.054129000
H	-4.461879000	2.130636000	-3.327926000
C	-4.524764000	-0.051969000	-3.445716000
H	-5.336435000	-0.361299000	-4.083963000
O	-3.786401000	-1.043697000	-2.909029000
C	-1.791351000	-3.742747000	-0.974692000
H	-1.842950000	-3.718257000	0.114751000
H	-0.742720000	-3.761058000	-1.273969000
C	-2.557357000	-4.926240000	-1.536415000
H	-2.133086000	-5.858131000	-1.153225000
H	-2.500284000	-4.941238000	-2.626812000
H	-3.609698000	-4.880001000	-1.247517000
P	2.170707000	0.312256000	0.389319000
P	-0.963077000	0.871211000	1.242551000
C	1.712000000	1.597808000	1.677730000
H	2.536058000	1.758549000	2.375900000
H	1.533072000	2.539809000	1.154405000
C	0.447382000	1.186675000	2.438334000
H	0.168872000	1.964840000	3.153654000
H	0.616408000	0.257563000	2.989632000
C	3.302735000	1.230436000	-0.759464000
C	3.752439000	2.536605000	-0.533744000
H	3.444099000	3.084485000	0.348201000

C	4.610968000	3.159462000	-1.439855000
H	4.945768000	4.173381000	-1.249879000
C	5.036678000	2.484805000	-2.579487000
H	5.702942000	2.970027000	-3.283780000
C	4.598191000	1.182269000	-2.811486000
H	4.920937000	0.648548000	-3.698218000
C	3.736469000	0.561814000	-1.913184000
H	3.397995000	-0.447787000	-2.115186000
C	3.421432000	-0.730151000	1.298383000
C	4.509686000	-0.142324000	1.960058000
H	4.643633000	0.933665000	1.942989000
C	5.446202000	-0.927772000	2.623206000
H	6.281688000	-0.457369000	3.129982000
C	5.317231000	-2.316811000	2.626757000
H	6.048946000	-2.929510000	3.141469000
C	4.251851000	-2.911068000	1.959117000
H	4.147772000	-3.990126000	1.948479000
C	3.309672000	-2.122563000	1.298230000
H	2.488440000	-2.594662000	0.777230000
C	-2.306565000	0.209072000	2.326982000
C	-3.450028000	-0.319374000	1.712402000
H	-3.520568000	-0.335169000	0.631869000
C	-4.493426000	-0.831940000	2.477097000
H	-5.370867000	-1.234889000	1.984052000
C	-4.405896000	-0.839073000	3.868186000
H	-5.214655000	-1.247816000	4.463410000
C	-3.271547000	-0.324903000	4.489070000
H	-3.191898000	-0.331377000	5.570437000
C	-2.230219000	0.200692000	3.724906000
H	-1.361473000	0.599171000	4.233115000
C	-1.528587000	2.612180000	0.905376000
C	-2.544977000	3.226242000	1.648857000
H	-3.062974000	2.671338000	2.421089000
C	-2.906735000	4.548130000	1.397793000
H	-3.699620000	5.005178000	1.979556000
C	-2.258609000	5.278801000	0.404714000
H	-2.543153000	6.306756000	0.210265000
C	-1.249297000	4.677725000	-0.343153000
H	-0.744152000	5.232773000	-1.125602000
C	-0.891211000	3.353282000	-0.099236000
H	-0.122495000	2.894941000	-0.708480000

9 *mer*-[W(dppe)(CO)$_3${C(CHA)C$_4$H$_4$S}], (7),

W	-0.001798000	-0.347054000	-0.412579000
C	0.639251000	0.698132000	-2.063742000
O	1.026200000	1.249895000	-3.000272000
C	0.202286000	-2.053001000	-1.424572000

O	0.334031000	-3.070388000	-1.975197000
C	-0.614295000	-1.397578000	1.216361000
O	-0.930714000	-2.001248000	2.157219000
C	-2.046295000	-0.093887000	-1.175235000
N	-3.089649000	-0.941706000	-1.096624000
H	-3.965903000	-0.647731000	-1.519967000
C	-3.160845000	-2.282099000	-0.515102000
H	-2.156268000	-2.534929000	-0.186734000
C	-3.591537000	-3.300011000	-1.586013000
H	-2.868190000	-3.287778000	-2.405696000
H	-4.561185000	-2.995396000	-2.004404000
C	-3.711956000	-4.711769000	-0.992961000
H	-4.055106000	-5.407922000	-1.764539000
H	-2.716492000	-5.055048000	-0.686013000
C	-4.657082000	-4.742445000	0.215864000
H	-4.684508000	-5.748008000	0.647538000
H	-5.678934000	-4.518049000	-0.117581000
C	-4.234621000	-3.720193000	1.279872000
H	-4.948558000	-3.714952000	2.109461000
H	-3.266909000	-4.011582000	1.704957000
C	-4.112124000	-2.306578000	0.692590000
H	-3.752097000	-1.606707000	1.450548000
H	-5.103184000	-1.955641000	0.372203000
C	-2.412485000	1.063643000	-2.023307000
C	-2.097380000	2.394550000	-1.887244000
H	-1.480323000	2.764847000	-1.083313000
C	-2.654147000	3.232342000	-2.890483000
H	-2.501273000	4.302793000	-2.929056000
C	-3.387465000	2.544057000	-3.813611000
H	-3.881063000	2.921041000	-4.696378000
S	-3.421911000	0.851068000	-3.464566000
P	2.430811000	-0.449756000	0.311064000
P	0.053850000	1.567369000	1.325328000
C	2.777801000	0.943267000	1.521627000
H	3.645951000	0.714125000	2.143052000
H	3.012484000	1.837983000	0.940244000
C	1.551247000	1.211475000	2.398357000
H	1.741373000	2.052457000	3.070362000
H	1.313972000	0.332046000	3.003318000
C	3.746883000	-0.236960000	-0.982831000
C	4.750871000	0.736485000	-0.929717000
H	4.809209000	1.429391000	-0.099637000
C	5.702346000	0.833867000	-1.945615000
H	6.470341000	1.597574000	-1.888200000
C	5.668153000	-0.042798000	-3.024797000
H	6.406931000	0.034343000	-3.814573000
C	4.675016000	-1.019289000	-3.085527000
H	4.636618000	-1.705866000	-3.923753000
C	3.721767000	-1.113380000	-2.077401000
H	2.949455000	-1.870824000	-2.145164000
C	3.123480000	-1.926898000	1.216721000

C	4.433317000	-1.916940000	1.718795000
H	5.067281000	-1.049099000	1.573725000
C	4.947677000	-3.023741000	2.385319000
H	5.962688000	-2.999313000	2.766648000
C	4.163711000	-4.165393000	2.553142000
H	4.565451000	-5.029856000	3.070024000
C	2.868915000	-4.191862000	2.046187000
H	2.255077000	-5.077763000	2.164138000
C	2.351756000	-3.079424000	1.381530000
H	1.346409000	-3.110782000	0.984558000
C	-1.332516000	1.673033000	2.547663000
C	-2.642611000	1.756956000	2.055844000
H	-2.818159000	1.749208000	0.986686000
C	-3.724359000	1.839814000	2.927376000
H	-4.730334000	1.908084000	2.528655000
C	-3.517796000	1.822938000	4.305900000
H	-4.361501000	1.877129000	4.984665000
C	-2.222734000	1.729056000	4.805888000
H	-2.052194000	1.708938000	5.876554000
C	-1.136649000	1.659879000	3.933854000
H	-0.139139000	1.593218000	4.348948000
C	0.354997000	3.358407000	0.908376000
C	-0.096825000	4.403259000	1.725987000
H	-0.683149000	4.185678000	2.610252000
C	0.191653000	5.728305000	1.406946000
H	-0.170921000	6.524397000	2.047980000
C	0.938048000	6.031429000	0.270251000
H	1.159821000	7.063560000	0.022949000
C	1.389370000	5.001535000	-0.551187000
H	1.962948000	5.225300000	-1.443608000
C	1.095475000	3.675624000	-0.238062000
H	1.432721000	2.888847000	-0.900731000

10 *mer*-[W(dppe)(CO)$_3${C(CHA)C$_4$H$_4$O}], (8))

W	-0.074386000	-0.394181000	-0.467768000
C	0.664018000	0.480334000	-2.176777000
O	1.076030000	0.924751000	-3.159474000
C	0.070715000	-2.174684000	-1.346564000
O	0.167403000	-3.236591000	-1.818055000
C	-0.845832000	-1.318254000	1.170472000
O	-1.276692000	-1.861983000	2.102226000
C	-2.069205000	-0.006213000	-1.277781000
N	-3.171466000	-0.777174000	-1.255317000
H	-4.019914000	-0.394935000	-1.662848000
C	-3.332532000	-2.140453000	-0.751473000
H	-2.357789000	-2.453899000	-0.384876000
C	-3.749896000	-3.083431000	-1.893949000
H	-2.982615000	-3.065397000	-2.672555000

H	-4.681018000	-2.711906000	-2.345150000
C	-3.966247000	-4.515190000	-1.381909000
H	-4.300641000	-5.155087000	-2.204400000
H	-3.004768000	-4.920548000	-1.044409000
C	-4.974122000	-4.558360000	-0.225028000
H	-5.071093000	-5.581329000	0.152285000
H	-5.965447000	-4.267727000	-0.597283000
C	-4.562316000	-3.611238000	0.910367000
H	-5.317640000	-3.613504000	1.702376000
H	-3.632270000	-3.969766000	1.367220000
C	-4.346570000	-2.177932000	0.403586000
H	-3.996170000	-1.532504000	1.212302000
H	-5.303653000	-1.766496000	0.052653000
C	-2.356270000	1.184196000	-2.094023000
C	-3.122963000	1.376077000	-3.218620000
H	-3.693335000	0.620444000	-3.735504000
C	-2.950422000	2.734898000	-3.618287000
H	-3.387806000	3.229485000	-4.471063000
C	-2.098886000	3.285062000	-2.713114000
H	-1.678091000	4.268191000	-2.587026000
O	-1.726306000	2.361821000	-1.788474000
P	2.306101000	-0.557130000	0.408745000
P	-0.002418000	1.651117000	1.117929000
C	2.642932000	0.894359000	1.552829000
H	3.461329000	0.670521000	2.240251000
H	2.948579000	1.740181000	0.931905000
C	1.373836000	1.260896000	2.329941000
H	1.552144000	2.116477000	2.986519000
H	1.053389000	0.415928000	2.944282000
C	3.710757000	-0.489675000	-0.802739000
C	4.773086000	0.417850000	-0.720290000
H	4.821439000	1.142990000	0.082601000
C	5.792997000	0.407282000	-1.672136000
H	6.605534000	1.121476000	-1.594101000
C	5.769934000	-0.513688000	-2.714431000
H	6.562578000	-0.520694000	-3.454165000
C	4.718686000	-1.424850000	-2.803452000
H	4.688601000	-2.144375000	-3.613949000
C	3.696898000	-1.410717000	-1.859993000
H	2.879228000	-2.116631000	-1.949779000
C	2.858396000	-2.001359000	1.455052000
C	4.126916000	-2.020221000	2.053580000
H	4.816133000	-1.197283000	1.898948000
C	4.529786000	-3.100381000	2.831505000
H	5.513811000	-3.098557000	3.287580000
C	3.674516000	-4.186995000	3.015988000
H	3.989331000	-5.030320000	3.620659000
C	2.421265000	-4.186535000	2.412926000
H	1.753092000	-5.030493000	2.542764000
C	2.016071000	-3.100717000	1.636149000
H	1.043403000	-3.110223000	1.163798000

C	-1.473595000	1.961816000	2.195847000
C	-2.605150000	2.554800000	1.615929000
H	-2.578915000	2.853359000	0.574855000
C	-3.758714000	2.763543000	2.363680000
H	-4.622083000	3.227690000	1.899690000
C	-3.808271000	2.375013000	3.702453000
H	-4.709408000	2.534000000	4.284004000
C	-2.695167000	1.778607000	4.285140000
H	-2.724093000	1.468343000	5.323742000
C	-1.534560000	1.573286000	3.538444000
H	-0.684502000	1.104785000	4.017283000
C	0.487194000	3.378886000	0.630259000
C	0.293640000	4.463944000	1.496737000
H	-0.208022000	4.316903000	2.446239000
C	0.726616000	5.739052000	1.142863000
H	0.565412000	6.568983000	1.822155000
C	1.363471000	5.949204000	-0.079456000
H	1.700597000	6.942673000	-0.353860000
C	1.561551000	4.877898000	-0.946371000
H	2.054023000	5.030891000	-1.900277000
C	1.122476000	3.601372000	-0.595302000
H	1.266525000	2.779326000	-1.283052000

11 *cis*-[W(PPh$_3$)(CO)$_4${C(OEt)C$_4$H$_4$S}], (9*cis*)

W	1.189184000	-1.074237000	-0.638662000
C	1.014898000	-0.233039000	-2.511270000
O	0.901148000	0.168339000	-3.581692000
C	2.848487000	-2.040079000	-1.301721000
O	3.772985000	-2.612048000	-1.682412000
C	1.326039000	-2.132930000	1.127166000
O	1.406982000	-2.809045000	2.054354000
C	0.067327000	-2.612822000	-1.359917000
O	-0.559218000	-3.474797000	-1.804474000
C	2.438936000	0.669017000	0.030210000
O	3.494052000	0.653636000	0.844800000
C	3.982269000	-0.528016000	1.519905000
H	4.124086000	-1.321315000	0.786696000
H	3.228580000	-0.841442000	2.242247000
C	5.284326000	-0.152713000	2.198644000
H	5.678680000	-1.020896000	2.732582000
H	5.132646000	0.654490000	2.918164000
H	6.028043000	0.167687000	1.466266000
C	2.299011000	2.048076000	-0.416185000
C	1.322138000	2.641578000	-1.197094000
H	0.474985000	2.106140000	-1.595245000
C	1.519301000	4.023386000	-1.409640000
H	0.853484000	4.642397000	-1.995251000
C	2.650425000	4.493246000	-0.792222000
H	3.036807000	5.501925000	-0.801649000

S	3.489945000	3.264867000	0.068289000
P	-0.897136000	0.062363000	0.139235000
O	-0.661086000	1.125358000	1.362442000
C	-1.487628000	2.144312000	1.839583000
C	-2.856872000	1.978731000	2.034993000
H	-3.337306000	1.045738000	1.774855000
C	-3.593449000	3.036262000	2.567989000
H	-4.659402000	2.912011000	2.721580000
C	-2.973654000	4.236414000	2.906690000
H	-3.554006000	5.050801000	3.324200000
C	-1.601585000	4.382617000	2.706931000
H	-1.109004000	5.312609000	2.967145000
C	-0.853847000	3.338680000	2.170900000
H	0.211401000	3.431391000	2.000769000
O	-1.708208000	1.046329000	-0.896111000
C	-2.768530000	0.774264000	-1.757435000
C	-2.808033000	-0.364041000	-2.556813000
H	-2.021453000	-1.104488000	-2.501391000
C	-3.874887000	-0.534373000	-3.436671000
H	-3.908904000	-1.420598000	-4.059848000
C	-4.883428000	0.422292000	-3.524187000
H	-5.708040000	0.283277000	-4.213297000
C	-4.823606000	1.560012000	-2.721667000
H	-5.602244000	2.311873000	-2.783048000
C	-3.767058000	1.740484000	-1.833306000
H	-3.701897000	2.614780000	-1.197947000
O	-2.206288000	-0.827145000	0.616262000
C	-2.181047000	-1.899667000	1.507059000
C	-1.839280000	-1.705847000	2.843145000
H	-1.537119000	-0.725641000	3.189059000
C	-1.892373000	-2.788168000	3.718551000
H	-1.620452000	-2.644952000	4.757896000
C	-2.291444000	-4.043380000	3.266268000
H	-2.330863000	-4.881433000	3.952075000
C	-2.637719000	-4.217961000	1.927464000
H	-2.947177000	-5.192324000	1.567451000
C	-2.584120000	-3.146656000	1.040134000
H	-2.843057000	-3.264882000	-0.003875000

12 *cis*-[W(PPh$_3$)(CO)$_4${C(OEt)C$_4$H$_4$O}], (10*cis*)

W	1.502365000	-0.054462000	0.627037000
C	0.917043000	-1.417884000	2.075840000
O	0.644614000	-2.138762000	2.924092000
C	3.427349000	-0.356624000	1.193529000
O	4.520657000	-0.498656000	1.529078000
C	2.197204000	1.393613000	-0.659246000
O	2.650453000	2.231032000	-1.305983000
C	1.365020000	1.395850000	2.056824000
O	1.294546000	2.209718000	2.872056000

C	1.603285000	-1.709046000	-0.855078000
O	2.474051000	-1.930904000	-1.840537000
C	3.555578000	-1.024420000	-2.151285000
H	4.099810000	-0.795845000	-1.235342000
H	3.126849000	-0.103582000	-2.547567000
C	4.438797000	-1.713092000	-3.172385000
H	5.266231000	-1.053195000	-3.444682000
H	3.877085000	-1.950976000	-4.078345000
H	4.855923000	-2.637421000	-2.767088000
C	0.701253000	-2.846051000	-0.891259000
C	0.649903000	-3.972070000	-1.686780000
H	1.343411000	-4.203897000	-2.477597000
C	-0.462792000	-4.736583000	-1.255587000
H	-0.806738000	-5.680944000	-1.646180000
C	-1.022336000	-4.031961000	-0.227334000
H	-1.872331000	-4.207468000	0.410606000
O	-0.337481000	-2.896543000	0.004707000
P	-0.871758000	0.409397000	-0.027077000
O	-1.278952000	-0.106304000	-1.523821000
C	-2.522919000	-0.228047000	-2.144523000
C	-3.616354000	0.581863000	-1.845520000
H	-3.546157000	1.332788000	-1.071727000
C	-4.800341000	0.402452000	-2.559326000
H	-5.653907000	1.029505000	-2.328020000
C	-4.893838000	-0.563329000	-3.558217000
H	-5.818873000	-0.691976000	-4.107824000
C	-3.788548000	-1.362319000	-3.846102000
H	-3.848452000	-2.117338000	-4.621847000
C	-2.600598000	-1.198637000	-3.140357000
H	-1.729985000	-1.809364000	-3.344409000
O	-2.155029000	-0.221255000	0.777451000
C	-2.408441000	-0.240498000	2.140672000
C	-2.037741000	0.792964000	2.996333000
H	-1.516680000	1.658766000	2.613959000
C	-2.360733000	0.700199000	4.349332000
H	-2.063412000	1.500009000	5.017668000
C	-3.060031000	-0.398741000	4.839832000
H	-3.309116000	-0.461370000	5.892472000
C	-3.440858000	-1.416690000	3.966333000
H	-3.990712000	-2.274479000	4.336562000
C	-3.115146000	-1.342882000	2.616515000
H	-3.403786000	-2.119690000	1.919668000
O	-1.407618000	1.983501000	0.008904000
C	-0.769043000	3.062159000	-0.601509000
C	-0.737888000	3.173088000	-1.989744000
H	-1.172277000	2.395167000	-2.603873000
C	-0.146053000	4.293748000	-2.567397000
H	-0.114935000	4.381366000	-3.647371000
C	0.400351000	5.295323000	-1.768535000
H	0.861237000	6.164013000	-2.223720000
C	0.353159000	5.174454000	-0.381216000

H	0.777855000	5.948304000	0.247765000
C	-0.231494000	4.057546000	0.209417000
H	-0.264303000	3.945946000	1.285358000

13 *cis*-[W(PPh$_3$)(CO)$_4${C(NHCy)C$_4$H$_4$S}], (11*cis*)

W	-0.675530000	0.193976000	-1.283870000
C	0.114979000	-1.374385000	-2.375410000
O	0.574494000	-2.198042000	-3.029104000
C	-2.298769000	0.202464000	-2.504161000
O	-3.229360000	0.223349000	-3.183432000
C	-1.392247000	1.863768000	-0.323424000
O	-1.793600000	2.836263000	0.147794000
C	0.274892000	1.426293000	-2.569646000
O	0.819535000	2.107125000	-3.331383000
C	-1.782804000	-1.338036000	0.016510000
C	-1.310893000	-2.727680000	0.138598000
C	-0.032265000	-3.221737000	0.259633000
H	0.845309000	-2.594028000	0.267050000
C	0.032468000	-4.632902000	0.392517000
H	0.958701000	-5.181682000	0.496992000
C	-1.194864000	-5.231038000	0.349484000
H	-1.429173000	-6.284398000	0.375565000
S	-2.463131000	-4.076182000	0.161653000
P	1.300067000	0.231596000	0.225295000
O	0.949498000	-0.092408000	1.796195000
C	1.784424000	-0.424746000	2.863165000
C	3.076598000	0.075083000	3.014192000
H	3.500155000	0.733383000	2.269086000
C	3.812359000	-0.290193000	4.141015000
H	4.818422000	0.095738000	4.260141000
C	3.269808000	-1.135042000	5.105748000
H	3.850180000	-1.410501000	5.978454000
C	1.974505000	-1.622998000	4.940787000
H	1.540835000	-2.281412000	5.684964000
C	1.229066000	-1.271426000	3.819872000
H	0.223080000	-1.642270000	3.668966000
O	2.510280000	-0.868944000	0.044327000
C	3.598305000	-0.902671000	-0.818960000
C	3.666058000	-0.176194000	-2.004398000
H	2.861170000	0.481370000	-2.300824000
C	4.792056000	-0.310197000	-2.815155000
H	4.843890000	0.254268000	-3.739065000
C	5.835937000	-1.156713000	-2.452586000
H	6.706196000	-1.254703000	-3.090624000
C	5.751561000	-1.877687000	-1.262640000
H	6.557668000	-2.540098000	-0.967986000
C	4.635411000	-1.753004000	-0.441742000
H	4.552408000	-2.300187000	0.489007000
O	2.283043000	1.560798000	0.304295000

C	1.863794000	2.875886000	0.507934000
C	1.377088000	3.274600000	1.750465000
H	1.274321000	2.551647000	2.549241000
C	1.031615000	4.609651000	1.946005000
H	0.648208000	4.923942000	2.909941000
C	1.177989000	5.535085000	0.915469000
H	0.906761000	6.572371000	1.072982000
C	1.672957000	5.120916000	-0.319582000
H	1.787570000	5.834143000	-1.127649000
C	2.018677000	3.788695000	-0.530336000
H	2.394909000	3.450824000	-1.486711000
N	-2.955689000	-1.177922000	0.621334000
H	-3.320948000	-1.961242000	1.161311000
C	-3.851150000	-0.016665000	0.641714000
H	-3.451353000	0.700128000	-0.070819000
C	-3.886114000	0.618869000	2.041038000
H	-2.879071000	0.941999000	2.316946000
H	-4.191412000	-0.143148000	2.771248000
C	-4.867376000	1.799466000	2.088843000
H	-4.904535000	2.203825000	3.104809000
H	-4.487477000	2.603560000	1.448083000
C	-6.271477000	1.390239000	1.623527000
H	-6.935330000	2.260052000	1.618604000
H	-6.697971000	0.675450000	2.339400000
C	-6.232269000	0.748177000	0.230137000
H	-7.230796000	0.413361000	-0.066027000
H	-5.924326000	1.497872000	-0.508623000
C	-5.256390000	-0.436686000	0.178532000
H	-5.198186000	-0.842953000	-0.835125000
H	-5.625786000	-1.241383000	0.829443000

14 *trans*-[W(PPh$_3$)(CO)$_4${C(NHCy)C$_4$H$_4$S}], (11*trans*)

W	0.496753000	-0.492744000	0.011135000
C	0.883951000	0.765767000	-1.580477000
O	1.179968000	1.440660000	-2.462839000
C	0.006207000	-2.012293000	-1.308355000
O	-0.323205000	-2.844293000	-2.026717000
C	0.289426000	-1.780487000	1.604335000
O	0.211963000	-2.515306000	2.486229000
C	0.771577000	1.031937000	1.343130000
O	0.865361000	1.906891000	2.093744000
C	2.660182000	-1.092154000	-0.135488000
C	3.039118000	-2.478321000	-0.465881000
C	2.516463000	-3.667903000	-0.014463000
H	1.695154000	-3.719293000	0.683218000
C	3.174763000	-4.817797000	-0.522828000
H	2.892604000	-5.830802000	-0.269127000
C	4.189961000	-4.514718000	-1.384880000
H	4.815438000	-5.189549000	-1.949073000

S	4.376075000	-2.809152000	-1.578673000
P	-1.879892000	0.041416000	0.013103000
O	-2.715925000	-0.612958000	-1.233928000
C	-4.083297000	-0.730909000	-1.473991000
C	-5.039260000	0.143918000	-0.961971000
H	-4.745143000	0.953967000	-0.310499000
C	-6.377481000	-0.049774000	-1.301823000
H	-7.124738000	0.626768000	-0.902494000
C	-6.758584000	-1.092967000	-2.141712000
H	-7.801944000	-1.232917000	-2.399216000
C	-5.787829000	-1.956008000	-2.648135000
H	-6.071400000	-2.772371000	-3.302814000
C	-4.448670000	-1.778980000	-2.316013000
H	-3.676140000	-2.437604000	-2.693355000
O	-2.894375000	-0.444238000	1.216894000
C	-2.744383000	-0.265339000	2.584375000
C	-2.474169000	0.980472000	3.146327000
H	-2.345505000	1.843034000	2.507572000
C	-2.392120000	1.094462000	4.533039000
H	-2.175294000	2.061655000	4.972128000
C	-2.592653000	-0.014991000	5.350136000
H	-2.530550000	0.082776000	6.427671000
C	-2.877102000	-1.251945000	4.773061000
H	-3.036339000	-2.121929000	5.399878000
C	-2.952192000	-1.382360000	3.390317000
H	-3.166335000	-2.334509000	2.921657000
O	-2.397227000	1.635280000	0.004721000
C	-1.913252000	2.617264000	-0.849983000
C	-2.242808000	2.604973000	-2.204254000
H	-2.845880000	1.800143000	-2.604385000
C	-1.791657000	3.636458000	-3.024159000
H	-2.042951000	3.625934000	-4.078555000
C	-1.026530000	4.675016000	-2.498311000
H	-0.679573000	5.475357000	-3.141378000
C	-0.711465000	4.680277000	-1.140812000
H	-0.119484000	5.486542000	-0.722416000
C	-1.150877000	3.651598000	-0.311486000
H	-0.904759000	3.637114000	0.742569000
N	3.734416000	-0.310653000	-0.056231000
H	4.647267000	-0.757238000	-0.125396000
C	3.828264000	1.135782000	0.168395000
H	2.814708000	1.527128000	0.124579000
C	4.660927000	1.787214000	-0.948662000
H	4.184140000	1.598758000	-1.914339000
H	5.653299000	1.316176000	-0.979696000
C	4.821346000	3.295925000	-0.709952000
H	5.450900000	3.725709000	-1.494744000
H	3.840612000	3.778572000	-0.800094000
C	5.412033000	3.592445000	0.675110000
H	5.468169000	4.673230000	0.836805000
H	6.442758000	3.216801000	0.717311000

C	4.585716000	2.933319000	1.787909000
H	5.050127000	3.107099000	2.763112000
H	3.592072000	3.394697000	1.830568000
C	4.424240000	1.424129000	1.556040000
H	3.783871000	0.982357000	2.323675000
H	5.403937000	0.932863000	1.632611000

15 *cis*-[W(PPh$_3$)(CO)$_4${C(NHCy)C$_4$H$_4$O}], (12*cis*)

W	0.805703000	-0.681400000	-1.039900000
C	0.041126000	0.050686000	-2.807057000
O	-0.398076000	0.400154000	-3.810412000
C	2.470920000	-1.232830000	-2.056673000
O	3.416714000	-1.562362000	-2.628805000
C	1.555316000	-1.563607000	0.664580000
O	1.996531000	-2.108834000	1.578012000
C	-0.033347000	-2.451576000	-1.524508000
O	-0.515398000	-3.457347000	-1.836210000
C	1.763969000	1.363401000	-0.596390000
C	1.109818000	2.628891000	-0.923641000
C	-0.112620000	2.972719000	-1.444185000
H	-0.900393000	2.296609000	-1.724812000
C	-0.161966000	4.392061000	-1.528761000
H	-0.977583000	4.994950000	-1.893599000
C	1.031793000	4.841372000	-1.055964000
H	1.455874000	5.824225000	-0.931008000
O	1.815701000	3.804843000	-0.682194000
P	-1.264008000	-0.050022000	0.185320000
O	-1.053205000	1.087204000	1.352488000
C	-1.980537000	1.848138000	2.060609000
C	-3.250918000	1.389761000	2.405929000
H	-3.581033000	0.406810000	2.100831000
C	-4.086209000	2.218304000	3.155035000
H	-5.074560000	1.863197000	3.424228000
C	-3.663537000	3.481397000	3.560523000
H	-4.320091000	4.115437000	4.144684000
C	-2.388075000	3.922415000	3.211037000
H	-2.046216000	4.903286000	3.521701000
C	-1.544767000	3.109844000	2.460248000
H	-0.551636000	3.433941000	2.175828000
O	-2.499533000	0.667180000	-0.631233000
C	-3.614845000	0.122724000	-1.259488000
C	-3.577909000	-1.080129000	-1.959258000
H	-2.670119000	-1.666000000	-2.006468000
C	-4.731675000	-1.520990000	-2.604527000
H	-4.704636000	-2.457470000	-3.149752000
C	-5.904421000	-0.771055000	-2.559367000
H	-6.795640000	-1.121476000	-3.066456000
C	-5.922177000	0.433594000	-1.859073000
H	-6.828582000	1.027040000	-1.817520000

C	-4.778976000	0.884541000	-1.205494000
H	-4.771638000	1.815586000	-0.652700000
O	-2.184422000	-1.208744000	0.928897000
C	-1.703894000	-2.196058000	1.787921000
C	-1.220037000	-1.859641000	3.049794000
H	-1.165975000	-0.820918000	3.349178000
C	-0.811391000	-2.875122000	3.911133000
H	-0.428400000	-2.618485000	4.892114000
C	-0.893703000	-4.209070000	3.519188000
H	-0.573857000	-4.994932000	4.193349000
C	-1.386954000	-4.528892000	2.255593000
H	-1.451173000	-5.564354000	1.941707000
C	-1.794723000	-3.523861000	1.382681000
H	-2.169133000	-3.754163000	0.394116000
N	2.967392000	1.580183000	-0.077438000
H	3.263667000	2.547932000	0.027476000
C	3.989211000	0.623761000	0.353557000
H	3.611167000	-0.369702000	0.127919000
C	4.228341000	0.741080000	1.868281000
H	3.295932000	0.532251000	2.399226000
H	4.510329000	1.776043000	2.106021000
C	5.339130000	-0.213861000	2.329653000
H	5.516957000	-0.079413000	3.400860000
H	4.996788000	-1.247251000	2.199288000
C	6.637474000	0.000757000	1.539624000
H	7.393401000	-0.725788000	1.852783000
H	7.043399000	0.993976000	1.771992000
C	6.395291000	-0.106610000	0.028105000
H	7.316915000	0.101821000	-0.523378000
H	6.108676000	-1.134564000	-0.224364000
C	5.288352000	0.849971000	-0.438859000
H	5.090215000	0.715955000	-1.505488000
H	5.618827000	1.888625000	-0.298691000

16 *trans*-[W(PPh$_3$)(CO)$_4${C(NHCy)C$_4$H$_4$O}], (12*trans*)

W	0.541464000	-0.560050000	-0.240463000
C	0.946458000	1.083914000	-1.411308000
O	1.208847000	1.968282000	-2.099943000
C	-0.096002000	-1.539388000	-1.934780000
O	-0.503470000	-2.085501000	-2.862125000
C	0.269272000	-2.291755000	0.849702000
O	0.158387000	-3.277517000	1.428822000
C	0.990114000	0.403077000	1.517058000
O	1.190631000	0.925988000	2.526140000
C	2.680970000	-1.213941000	-0.559379000
C	3.022721000	-2.564173000	-1.004177000
C	2.294788000	-3.682657000	-1.325840000
H	1.223584000	-3.769742000	-1.305766000

C	3.213511000	-4.704826000	-1.692996000
H	2.981354000	-5.710974000	-2.002274000
C	4.453604000	-4.157656000	-1.576578000
H	5.448396000	-4.536861000	-1.743447000
O	4.369656000	-2.872619000	-1.164296000
P	-1.769889000	0.147932000	0.011888000
O	-2.564005000	0.332091000	-1.411802000
C	-3.929247000	0.412194000	-1.685406000
C	-4.827189000	1.116042000	-0.886504000
H	-4.488917000	1.593264000	0.022464000
C	-6.163709000	1.183285000	-1.276138000
H	-6.867066000	1.727085000	-0.655589000
C	-6.598384000	0.564390000	-2.445796000
H	-7.639779000	0.624236000	-2.739902000
C	-5.684978000	-0.133165000	-3.234539000
H	-6.011555000	-0.619655000	-4.146772000
C	-4.347978000	-0.213067000	-2.856874000
H	-3.619960000	-0.752155000	-3.450453000
O	-2.921618000	-0.762095000	0.763788000
C	-2.832256000	-1.399957000	1.988122000
C	-2.216768000	-0.821706000	3.096244000
H	-1.771333000	0.160520000	3.018857000
C	-2.198823000	-1.519791000	4.302800000
H	-1.714833000	-1.073662000	5.164250000
C	-2.799028000	-2.771305000	4.408892000
H	-2.782216000	-3.306448000	5.351037000
C	-3.423972000	-3.330483000	3.294611000
H	-3.896420000	-4.303610000	3.366435000
C	-3.440750000	-2.650155000	2.082089000
H	-3.915354000	-3.067560000	1.202838000
O	-2.146982000	1.560532000	0.832491000
C	-1.570997000	2.801359000	0.602661000
C	-1.597105000	3.398116000	-0.657136000
H	-2.028082000	2.870156000	-1.497462000
C	-1.060742000	4.673937000	-0.817812000
H	-1.074024000	5.133705000	-1.799301000
C	-0.515686000	5.356366000	0.266959000
H	-0.105299000	6.350803000	0.135483000
C	-0.505045000	4.753000000	1.523817000
H	-0.086070000	5.276062000	2.376107000
C	-1.029195000	3.475349000	1.695784000
H	-1.020542000	2.990724000	2.663660000
N	3.779291000	-0.481690000	-0.393031000
H	4.671675000	-0.930468000	-0.584565000
C	3.919755000	0.909735000	0.042542000
H	2.915112000	1.301682000	0.183030000
C	4.631235000	1.736595000	-1.041838000
H	4.049496000	1.700585000	-1.966248000
H	5.608602000	1.282374000	-1.256069000
C	4.829454000	3.190155000	-0.587105000
H	5.370490000	3.745299000	-1.359229000

H	3.848123000	3.669872000	-0.490361000
C	5.573655000	3.271296000	0.752477000
H	5.652413000	4.313289000	1.077375000
H	6.600859000	2.907457000	0.619389000
C	4.874654000	2.433052000	1.831303000
H	5.448604000	2.452884000	2.762629000
H	3.896678000	2.872901000	2.060391000
C	4.674809000	0.978073000	1.381155000
H	4.123559000	0.414757000	2.138447000
H	5.653007000	0.491289000	1.265532000

[i] 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.

X-ray Crystallography

Table. Selected Bond Lengths (nm), Bond and Dihedral Angles (deg)

	2*cis*	**3**	**5**
W1-C6	0.21712(13)	0.2245(6)	0.2117(3)
W1-CO1[a]	0.20185(17)	0.1985(6)	
W1-CO*cis*[b]	0.20353(17)	0.2026(6)	0.2015(5)
W1-CO3	0.19870(15)	0.1988(6)	0.1982(4)
W1-P1	0.25488(3)	0.25578(15)	0.24930(9)
W1-P2			0.25145(9)
C6-C7	0.14475(19)	0.1493(8)	0.1459(5)
C7-C8	0.13725(19)	0.137(2)	0.1379(5)
C8-C9	0.1412(3)	0.152(3)	0.1421(5)
C9-C10	0.1351(3)	0.1340(14)	0.1332(5)
C10-S1/O6	0.13525(19)	0.1625(10)	0.1710(4)
C7-S1/O6	0.13671(19)	0.1705(8)	0.1741(3)
C6-N1/O7	0.13286(18)	0.1313(7)	0.1353(4)
C1-W1-C6	174.24(7)	175.5(2)	
P1-W1-P2			80.22(3)
W1-C6-O7/N1	130.76(10)	128.5(4)	130.5(2)
W1-C6-C7	124.70(10)	122.3(4)	125.5(2)
O7/N1-C6-C7	104.45(11)	109.3(5)	103.5(3)
O7/N1-C6-C7-S1/06	-175.64(12)	146.0(5)	-14.5(4)
W1-C6-O7/N1-C11	-0.3(2)	-2.0(8)	6.7(5)
W1-C6-C7-S1/O6	7.60(18)	-33.6(7)	158.36(18)
P1-C13-C14-P2			-55.4(3)

[a] *Trans* carbonyl bond length [b] Average *cis* carbonyl bond length