Contents

Cartesian coordinate of reported complexes

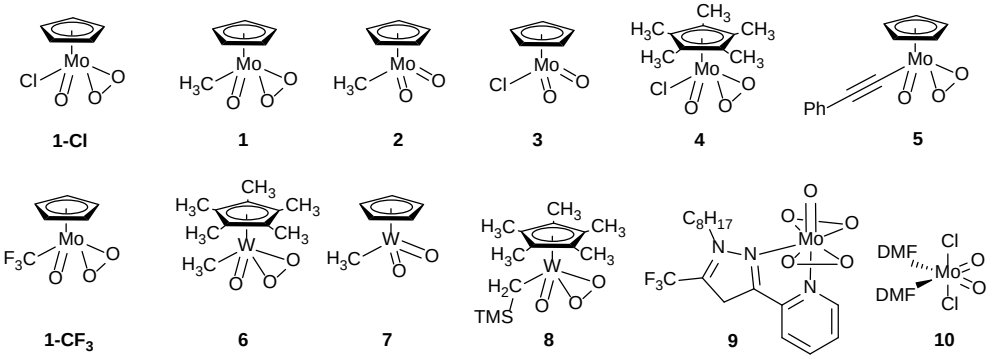

Table 1 and Figure 1

1-C1 at M06/def2-TZVP

Mo	-0.39394400	0.01079300	0.20693800
O	-1.87850900	-0.67009200	-0.79735600
O	-1.18024500	-1.69730400	-0.13516400
O	-0.84188400	0.50146600	1.73857800
C	-1.10753900	1.80111800	-0.79139100
C	1.55386100	-1.12503100	-0.78720600
C	1.76001800	-0.93215900	0.61234400
C	1.89384300	0.44970700	0.84709700
C	1.64834200	1.11230300	-0.36734200
C	1.47619900	0.12383400	-1.38843900
H	-2.18857000	1.78819100	-0.66043900
H	-0.86799800	1.78332300	-1.85395700
H	-0.68792500	2.69175300	-0.32313900
H	1.37476900	-2.07595900	-1.26512000
H	1.83526400	-1.71537000	1.35203900
H	2.03405000	0.91846700	1.80887400
H	1.64821100	2.17975500	-0.52285000
H	1.25459600	0.32534000	-2.42566000

1-C2 at M06/def2-TZVP

Mo	-0.39083700	0.00692200	0.20475100
O	-1.92047900	-0.60931000	-0.77444800
O	-1.21987300	-1.67235400	-0.17254300
O	-0.78820000	0.45084100	1.76467000
C	-1.09116400	1.83266100	-0.73219300
C	1.46759400	-0.82217000	-1.16627000
C	1.67040200	-1.20308500	0.18922800
C	1.92760200	-0.03752700	0.94308300
C	1.76380200	1.06216500	0.09297700
C	1.50164000	0.56882500	-1.22563200
H	-2.11720600	1.94327800	-0.38315800
H	-1.08981400	1.73476900	-1.81661700

H	-0.49854500	2.69516500	-0.42602100
H	1.20715200	-1.49208400	-1.97174800
H	1.64716600	-2.21482400	0.56669800
H	2.08730600	0.00357200	2.00954800
H	1.83543200	2.10223900	0.37274800
H	1.33283300	1.17853200	-2.09959300

Table 2

1-C2 at M06/SVP

Mo	-0.39532100	0.01733000	0.21017900
O	-1.84769300	-0.71497400	-0.81268200
O	-1.15742300	-1.71020000	-0.09210400
O	-0.87016100	0.55391600	1.71629200
C	-1.11768800	1.76550100	-0.83684200
C	1.57316800	-1.16412700	-0.71095300
C	1.76178800	-0.87409300	0.67975000
C	1.87518200	0.52805700	0.82385600
C	1.63145300	1.10703100	-0.44108600
C	1.48151400	0.04648900	-1.39806200
H	-2.20874200	1.73721600	-0.70419600
H	-0.87735500	1.72549900	-1.90929000
H	-0.71186200	2.68208600	-0.38301200
H	1.41292600	-2.15687800	-1.13130500
H	1.84878100	-1.61270400	1.47775200
H	2.01037000	1.06733700	1.76139400
H	1.62914700	2.17225200	-0.67059800
H	1.26991200	0.17425700	-2.46028900

1-C2 at M06/SVPD

Mo	-0.38642700	0.01082600	0.20653000
O	-1.92747600	-0.61449400	-0.76430300
O	-1.23499100	-1.67090900	-0.13914400
O	-0.76272500	0.48764900	1.76351700
C	-1.08240700	1.82072000	-0.74402000
C	1.42607400	-0.60339800	-1.31741000
C	1.61515200	-1.28370000	-0.08577200
C	1.90681300	-0.32158900	0.91973300
C	1.82044600	0.95326900	0.33101400
C	1.52310000	0.77845600	-1.05870800
H	-2.11771200	1.92383300	-0.39420600
H	-1.07577500	1.71773600	-1.83709200
H	-0.48801000	2.69052400	-0.42985700
H	1.13516300	-1.06445700	-2.26009300
H	1.52811700	-2.35903700	0.06232500
H	2.06508800	-0.52984500	1.97632100
H	1.92951300	1.90755700	0.84413700
H	1.40002800	1.57847100	-1.78537400

1-C2 at M06/TZVPD

Mo	-0.39102100	0.00647000	0.20496300
O	-1.92225500	-0.60782100	-0.77399200
O	-1.22487300	-1.67148500	-0.16967300
O	-0.78428200	0.45398500	1.76514500
C	-1.08988700	1.83343400	-0.73130100
C	1.46149600	-0.78224100	-1.19762000
C	1.66334000	-1.22120200	0.13878900
C	1.92734200	-0.09020700	0.94241700
C	1.77599100	1.04594800	0.13951300
C	1.50597600	0.61129800	-1.19705000
H	-2.11312700	1.94780700	-0.37577500
H	-1.09433700	1.73417000	-1.81534200
H	-0.49158600	2.69334700	-0.42898900
H	1.19495900	-1.41431700	-2.03105500
H	1.62961000	-2.24726400	0.47373700
H	2.08710300	-0.09630400	2.00951800
H	1.85222700	2.07265500	0.46373800
H	1.34374200	1.25856300	-2.04461400

Table 3

1-C2 at M06/Mo:LANL2TZ(f) and Non-Mo:6-311+G(d,p)

Mo	-0.38950500	0.01645600	0.21408800
O	-1.90615100	-0.64469500	-0.79475200
O	-1.23029900	-1.68732500	-0.13114200
O	-0.81242400	0.51563900	1.75042900
C	-1.09252500	1.80757800	-0.78925500
C	1.47665100	-0.85864500	-1.14376600
C	1.67393800	-1.19889000	0.22619800
C	1.92684500	-0.00928300	0.94742100
C	1.75819600	1.06634400	0.06274300
C	1.50838100	0.53110000	-1.24544300
H	-2.12504800	1.91484900	-0.45075400
H	-1.07755200	1.67443700	-1.87207800
H	-0.50724300	2.68320900	-0.49751600
H	1.22435700	-1.55515300	-1.93152700
H	1.65673000	-2.20149800	0.63292900
H	2.09004600	0.06378200	2.01370600
H	1.83630200	2.11628500	0.31010200
H	1.34368800	1.11473700	-2.14022100

1-C2 at M06/Mo:LANL2TZ(f) and Non-Mo:ACCT

Mo	-0.39118600	0.00670700	0.20712300
O	-1.93326500	-0.60182200	-0.77016300
O	-1.23974200	-1.67018400	-0.16854600
O	-0.77432100	0.45966500	1.76731800

C	-1.08768600	1.83855400	-0.73327200
C	1.45658700	-0.77160300	-1.21007700
C	1.66155700	-1.23008200	0.11802800
C	1.93437100	-0.11202300	0.93682200
C	1.78827500	1.03514900	0.15115200
C	1.50802800	0.62122100	-1.18937400
H	-2.10655300	1.95218100	-0.36922300
H	-1.09741400	1.73069400	-1.81512400
H	-0.48284300	2.69382900	-0.43538400
H	1.18455800	-1.38988600	-2.05034700
H	1.62459400	-2.25933100	0.43806800
H	2.09950400	-0.13467500	2.00149300
H	1.87141000	2.05571700	0.48882000
H	1.34838500	1.28119500	-2.02599300

1-C2 at M06/Mo:LANL2DZmod and Non-Mo:6-311+G(d,p)

Mo	-0.38430400	0.02824700	0.21981300
O	-1.91573800	-0.68091700	-0.78276600
O	-1.24458800	-1.70167800	-0.08340100
O	-0.80700500	0.59622800	1.75999200
C	-1.09534700	1.78291200	-0.85390000
C	1.46502500	-0.89340000	-1.12942400
C	1.67203200	-1.20216800	0.24638600
C	1.93483600	0.00369200	0.93848200
C	1.76415600	1.05957000	0.02887300
C	1.50064700	0.49394700	-1.26401400
H	-2.11946100	1.90729300	-0.49739700
H	-1.10245900	1.59456300	-1.92818600
H	-0.49795700	2.66522000	-0.61258200
H	1.20238800	-1.60683800	-1.89825600
H	1.65315600	-2.19470300	0.67667300
H	2.10932600	0.10086100	2.00095200
H	1.85295800	2.11457300	0.24940000
H	1.33337500	1.05625600	-2.17176800

1-C2 at M06/Mo:LANL2DZmod and Non-Mo:ACCT

Mo	-0.38665200	0.01215500	0.20780700
O	-1.93631700	-0.61560000	-0.76662800
O	-1.25099600	-1.67455600	-0.14402000
O	-0.77554400	0.49872900	1.77279700
C	-1.08437800	1.82684500	-0.76109400
C	1.44751900	-0.77589800	-1.21279300
C	1.65309400	-1.23951200	0.11271300
C	1.93311500	-0.12538200	0.93529400
C	1.79423500	1.02556800	0.15307000
C	1.50761300	0.61716300	-1.18755500
H	-2.10019600	1.94601100	-0.39118900

H	-1.10126200	1.70291600	-1.84078700
H	-0.47698500	2.68525900	-0.47856900
H	1.16779600	-1.38894200	-2.05423500
H	1.60895200	-2.26890700	0.43099800
H	2.10032300	-0.15263500	1.99951100
H	1.88405000	2.04441800	0.49388200
H	1.35237000	1.28010400	-2.02250400

Table 4

1-C2 at M06L/def2-TZVP

Mo	-0.39228800	0.00985600	0.20660100
O	-1.88847100	-0.66547700	-0.80417300
O	-1.17689900	-1.71124500	-0.13662400
O	-0.83698200	0.49856700	1.75653500
C	-1.10770900	1.81504400	-0.78595800
C	1.55769300	-1.16184800	-0.71746800
C	1.77457200	-0.87650400	0.66354800
C	1.88739300	0.52044900	0.80725700
C	1.63769500	1.09939000	-0.45118800
C	1.46754400	0.04654600	-1.40218300
H	-2.18778400	1.80537400	-0.66094100
H	-0.86636400	1.81305000	-1.84630500
H	-0.69201400	2.70198100	-0.31070600
H	1.38773500	-2.14227800	-1.13191400
H	1.86461400	-1.60776400	1.45143200
H	2.02581900	1.05281300	1.73414500
H	1.62239200	2.15315200	-0.67513900
H	1.23737100	0.17649200	-2.44776000

1-C2 at M06-2X/def2-TZVP

Mo	-0.39854100	0.00782600	0.20845100
O	-1.91908800	-0.57364200	-0.79463900
O	-1.22287600	-1.65808000	-0.21839200
O	-0.81113400	0.39181200	1.76787000
C	-1.07761600	1.83726800	-0.70709300
C	1.47061800	-0.78060200	-1.19511300
C	1.66383100	-1.22217800	0.14540500
C	1.93355400	-0.08999200	0.95006300
C	1.79181300	1.04747300	0.14544900
C	1.52457200	0.61287800	-1.19536300
H	-2.10464700	1.95005000	-0.36654800
H	-1.06646300	1.74343000	-1.79016100
H	-0.48152100	2.69128300	-0.38987000
H	1.20973600	-1.41152500	-2.02943900
H	1.62669200	-2.24689700	0.47992700
H	2.09258000	-0.09688100	2.01614400
H	1.87682100	2.07224500	0.46941100

H	1.36966800	1.25980300	-2.04321500

1-C2 at PBE0/def2-TZVP

Mo	-0.39273700	0.01018000	0.20300900
O	-1.88125500	-0.66053500	-0.79294200
O	-1.17109100	-1.69667900	-0.14460600
O	-0.84083500	0.47907300	1.74131400
C	-1.11750100	1.79498600	-0.77616800
C	1.56216600	-1.14950300	-0.73085100
C	1.77170300	-0.88418100	0.65688900
C	1.88312700	0.51004300	0.82235400
C	1.63584700	1.10891700	-0.42818200
C	1.47677400	0.06886700	-1.39779700
H	-2.19596100	1.78069600	-0.62068600
H	-0.90517900	1.77773900	-1.84461800
H	-0.69160700	2.68900800	-0.31943200
H	1.39765000	-2.12496300	-1.16201700
H	1.85548600	-1.62793000	1.43557200
H	2.02028700	1.02875800	1.75855700
H	1.62861900	2.16702100	-0.63611800
H	1.25841700	0.21248700	-2.44521800

1-C2 at B3LYP/def2-TZVP

Mo	-0.40730300	0.00872200	0.20234900
O	-1.89411700	-0.67661900	-0.81764700
O	-1.16671900	-1.72334800	-0.15460100
O	-0.88098000	0.47181600	1.74713000
C	-1.14475600	1.81118800	-0.78682900
C	1.60557600	-1.11558900	-0.77747400
C	1.79076600	-0.91832400	0.62937300
C	1.90206300	0.46878100	0.86545100
C	1.67330900	1.12999000	-0.35900800
C	1.52879200	0.13548600	-1.38439000
H	-2.22176600	1.79637800	-0.63313800
H	-0.92818800	1.79225700	-1.85291200
H	-0.71742800	2.70176600	-0.32800000
H	1.45575400	-2.06799800	-1.25874600
H	1.87048600	-1.69908300	1.36916500
H	2.03353000	0.93991300	1.82555800
H	1.67636400	2.19544800	-0.51528100
H	1.33799100	0.33102700	-2.42711400

1-C2 at B3PW91/def2-TZVP

Mo	-0.39667800	0.00941300	0.20099700
O	-1.88652100	-0.66840700	-0.79951600

O	-1.16977600	-1.70667800	-0.14399000
O	-0.85322900	0.47818900	1.74273800
C	-1.13071300	1.80050500	-0.77748900
C	1.57824100	-1.14302200	-0.73597100
C	1.77951300	-0.88713900	0.65621100
C	1.88741700	0.50720200	0.83241900
C	1.64643000	1.11517800	-0.41623900
C	1.49405900	0.08090500	-1.39503400
H	-2.20795400	1.78680800	-0.61617400
H	-0.92384000	1.78501100	-1.84665900
H	-0.70220500	2.69312600	-0.32114500
H	1.42321400	-2.11581200	-1.17592000
H	1.86405400	-1.63633000	1.42924900
H	2.02328800	1.01941200	1.77207500
H	1.64350000	2.17438600	-0.61706200
H	1.28696400	0.23146300	-2.44346500

1-C2 at MP2/def2-SVP

Mo	-0.39166400	0.00783000	0.20038100
O	-1.86827700	-0.66360600	-0.86784200
O	-1.18108800	-1.73321500	-0.15574600
O	-0.96220800	0.47339900	1.74138100
C	-1.11138200	1.82564900	-0.78308100
C	1.61028700	-1.19166300	-0.62274500
C	1.78131200	-0.81615900	0.75358100
C	1.86460200	0.60121900	0.81285300
C	1.65146000	1.10077900	-0.50082700
C	1.52955200	-0.01753200	-1.39198800
H	-2.20498100	1.81859100	-0.66765100
H	-0.86172300	1.82244400	-1.85435800
H	-0.69489900	2.72650500	-0.30564800
H	1.48073700	-2.20961500	-0.98890500
H	1.88142500	-1.50263300	1.59516900
H	2.00239000	1.20047800	1.71299200
H	1.64353700	2.14974100	-0.79260800
H	1.34099900	0.03924200	-2.46407800

1-C2 at MP2/def2-SVPD

Mo	-0.38856500	0.00523900	0.20192700
O	-1.90614900	-0.62825000	-0.84212900
O	-1.20249300	-1.72872700	-0.16915900
O	-0.90725100	0.46179400	1.77015700
C	-1.10342400	1.84250100	-0.76438700
C	1.58896800	-1.19622600	-0.65125000
C	1.79036900	-0.83624500	0.72899300
C	1.88373400	0.58260500	0.80369200
C	1.64975900	1.09901300	-0.50399200
C	1.50733000	-0.00991100	-1.40898800

H	-2.19693100	1.83421400	-0.65211800
H	-0.84538000	1.83833100	-1.83364400
H	-0.68508300	2.73806300	-0.27948000
H	1.43769400	-2.20695600	-1.02511400
H	1.88777400	-1.53190300	1.56154100
H	2.02368400	1.17032500	1.70919400
H	1.63670200	2.14998200	-0.78354100
H	1.28799100	0.05896300	-2.47313600

1-C2 at MP2/def2-TZVP

Mo	-0.38427700	0.00248800	0.20048400
O	-1.90410700	-0.62014200	-0.82249100
O	-1.19875600	-1.71902700	-0.17183200
O	-0.88549500	0.45989900	1.77139800
C	-1.10238800	1.83245900	-0.75861400
C	1.57344700	-1.16684400	-0.70130000
C	1.78049200	-0.86968500	0.68451500
C	1.88113100	0.53603300	0.81897200
C	1.64190800	1.10741800	-0.45400100
C	1.49010100	0.04374500	-1.40106800
H	-2.18795500	1.82407700	-0.64263800
H	-0.85258500	1.83001200	-1.82135600
H	-0.68752800	2.72340600	-0.28058000
H	1.41222600	-2.15262300	-1.11300300
H	1.86980900	-1.59585000	1.48094900
H	2.01551700	1.07870600	1.74384700
H	1.62429500	2.16219700	-0.68361500
H	1.26458100	0.16099400	-2.45155200

Table 5

1-CF_3 at M06L/def2-TZVP

Mo	0.28729000	0.45229800	-0.24543700
F	-2.05561100	-0.61205000	1.38001300
F	-1.91213000	-1.60345600	-0.54001200
F	-2.68130600	0.40710600	-0.41348300
O	-0.58970300	1.81429500	0.79286600
O	0.78141700	2.12602700	0.55007200
O	0.04980700	0.66414500	-1.89976900
C	2.21295100	-0.92778600	-0.73743800
C	1.11578100	-1.77439300	-0.53348600
C	0.71279200	-1.65095400	0.83098800
C	1.56516900	-0.72762100	1.45812100
C	2.46299600	-0.24338600	0.47943500
C	-1.74873500	-0.41012900	0.08305500
H	2.71446700	-0.75230300	-1.67578300
H	0.62993900	-2.38522600	-1.27741700
H	-0.10817400	-2.17584900	1.29117800

H	1.47725900	-0.36347900	2.46959700
H	3.20387200	0.52584300	0.63270500

1-CF_3 at M06-2X/def2-TZVP

Mo	-0.27395800	-0.45046900	-0.24641800
F	2.04530500	0.61151500	1.37544100
F	1.89301700	1.61544500	-0.52278200
F	2.67007200	-0.37847200	-0.42001000
O	0.60437500	-1.79282100	0.79304200
O	-0.73946700	-2.12032200	0.55067400
O	-0.02871500	-0.66431500	-1.88319000
C	-2.21880500	0.90120900	-0.75063500
C	-1.14108700	1.76492600	-0.52892700
C	-0.75413900	1.64240700	0.84136700
C	-1.59684600	0.70206900	1.45151900
C	-2.47098400	0.20438000	0.45875700
C	1.74487700	0.42598600	0.08629100
H	-2.70569000	0.72202400	-1.69730100
H	-0.66007300	2.39304800	-1.26316900
H	0.04319400	2.18919300	1.31949900
H	-1.51571800	0.33442900	2.46364600
H	-3.19866300	-0.58157300	0.59859000

1-CF3 at M06-2X/def2-TZVP

Mo	-0.26499500	-0.46260600	-0.24777500
F	2.01649200	0.65204000	1.36625900
F	1.85985800	1.62206900	-0.55423200
F	2.66603700	-0.36608000	-0.41253700
O	0.62713300	-1.76899700	0.81433400
O	-0.72443800	-2.10378700	0.60168700
O	-0.05120500	-0.74444200	-1.86540200
C	-2.19988900	0.92096900	-0.77039800
C	-1.12060500	1.77691800	-0.52705300
C	-0.75300800	1.64331600	0.85340900
C	-1.60576800	0.70073800	1.44299800
C	-2.46682900	0.20800700	0.43010300
C	1.71842000	0.43412500	0.07539400
H	-2.67497000	0.75289800	-1.72371600
H	-0.62562900	2.40829100	-1.24720500
H	0.04552600	2.17656200	1.34312000
H	-1.54205700	0.32595100	2.45219200
H	-3.20040100	-0.57314900	0.55505300

Table 6

1-Cl at M06L/def2-TZVP

Mo	-0.22796000	-0.27580100	0.19637100
O	-1.49779600	-1.39223400	-0.70451100
O	-0.23511900	-2.04237500	-0.54102000
O	-0.44302000	-0.45879700	1.85053100
C	1.93729100	0.62430600	0.90987300
C	1.29003600	1.59407000	0.14151100
C	1.19823300	1.11237000	-1.21083800
C	1.73074800	-0.16820300	-1.24193400
C	2.12640900	-0.51055800	0.09255000
H	2.10638100	0.66948800	1.97317500
H	0.91796500	2.54449400	0.48762100
H	0.72717800	1.63580100	-2.02675800
H	1.73749700	-0.84055600	-2.08449700
H	2.54378200	-1.45715200	0.39942800
Cl	-1.80866400	1.42746600	-0.23432400

1-Cl at M06/def2-TZVP

Mo	-0.23271400	-0.27335500	0.19731900
O	-1.49701700	-1.37104600	-0.71290700
O	-0.26340800	-2.02566700	-0.54693500
O	-0.45446800	-0.46779100	1.83306700
C	1.94797900	0.58106900	0.91567500
C	1.31209900	1.57553100	0.17187700
C	1.21422600	1.12500000	-1.19206300
C	1.72665000	-0.15920600	-1.25280400
C	2.11368100	-0.53904700	0.07455500
H	2.12098800	0.59994900	1.98048900
H	0.95727000	2.52614200	0.53920000
H	0.74990400	1.67434100	-1.99639400
H	1.72136700	-0.81402400	-2.11066200
H	2.51487000	-1.50061700	0.35945000
Cl	-1.79171200	1.43594400	-0.23227700

1-Cl at M06-2X/def2-TZVP

Mo	-0.23581000	-0.27947200	0.20368400
O	-1.49209600	-1.33336200	-0.74929400
O	-0.27175200	-2.01571500	-0.56862400
O	-0.47241500	-0.51350300	1.81833700
C	1.95632000	0.56518100	0.92142900
C	1.32183700	1.57432200	0.19236800
C	1.21661200	1.14081600	-1.18095000
C	1.72179800	-0.14580300	-1.26071500
C	2.11358900	-0.54587300	0.06308400
H	2.13737500	0.56972600	1.98382100
H	0.97072100	2.51965600	0.57295200
H	0.74985100	1.70085500	-1.97495700
H	1.70822000	-0.78929000	-2.12547400

H	2.50766900	-1.51302900	0.33348500
Cl	-1.78003800	1.44815800	-0.22112800

Table 7

2 at M06L/def2-TZVP

Mo	-0.53944000	-0.16624000	-0.00047000
O	-1.27470100	-0.81918200	-1.38988000
O	-1.30240100	-0.79416000	1.38515400
C	-1.31173500	1.84356000	-0.01977700
C	1.63217600	-0.38978000	-1.11009500
C	1.58038100	-1.12756500	0.10833300
C	1.60514700	-0.19863200	1.18565400
C	1.56147800	1.08235700	0.63664500
C	1.58297100	0.96370600	-0.78534300
H	-2.39500100	1.73220200	-0.06444600
H	-0.97373100	2.40466600	-0.88866700
H	-1.04644200	2.38547900	0.88582200
H	1.60409700	-0.81375800	-2.10078900
H	1.59482900	-2.20306100	0.19848400
H	1.55322600	-0.45164400	2.23203400
H	1.50073200	2.00852400	1.18592100
H	1.53309400	1.78455300	-1.48331200

2 at M06/def2-TZVP

Mo	-0.53308500	-0.17355900	-0.00059800
O	-1.24877100	-0.82984800	-1.38298700
O	-1.29506700	-0.79562200	1.37198400
C	-1.35066400	1.81291900	-0.02935100
C	1.64832400	-0.44138400	-1.07141400
C	1.60256800	-1.09660400	0.19359800
C	1.59891000	-0.09905200	1.20450300
C	1.52415700	1.14021700	0.57005400
C	1.56535100	0.92792800	-0.84060900
H	-2.42975300	1.67322900	-0.11453900
H	-0.99067600	2.39045900	-0.88064800
H	-1.12763500	2.34316400	0.89652500
H	1.63949800	-0.93170200	-2.03268500
H	1.63734500	-2.16419100	0.35576700
H	1.54080300	-0.28164800	2.26649200
H	1.43827400	2.10077700	1.05532600
H	1.50053800	1.69900300	-1.59376300

2 at M06-2X/def2-TZVP

Mo	0.54179800	-0.17421300	0.00001200
O	1.27557100	-0.80514700	1.37262600
O	1.27624800	-0.80510600	-1.37224800
C	1.35165100	1.80749900	0.00019300
C	-1.63772000	-0.27780900	1.15181400
C	-1.61926000	-1.11357900	-0.00238400
C	-1.63706800	-0.27366200	-1.15346900
C	-1.55165400	1.04633000	-0.71428300
C	-1.55218600	1.04375700	0.71754200
H	2.43341800	1.67537100	0.00089900
H	1.05405200	2.35702800	0.89102000
H	1.05518800	2.35670400	-0.89120500
H	-1.60738000	-0.62041500	2.17327000
H	-1.65637900	-2.19182800	-0.00437100
H	-1.60616500	-0.61251600	-2.17615100
H	-1.48228800	1.92215700	-1.33933000
H	-1.48309000	1.91726500	1.34586300

2 at PBE0/def2-TZVP

Mo	-0.52937900	-0.17363500	-0.00135600
O	-1.23132800	-0.83611200	-1.38760900
O	-1.29235400	-0.81042100	1.36333800
C	-1.38227300	1.78925900	-0.03042800
C	1.66140500	-0.57164600	-0.98446700
C	1.61530000	-1.04998500	0.35980300
C	1.58168000	0.07207700	1.22384100
C	1.50367300	1.21839300	0.42296800
C	1.57462000	0.81922300	-0.94415000
H	-2.45874700	1.62479000	-0.11602600
H	-1.03758200	2.37254800	-0.88476800
H	-1.17474900	2.32926000	0.89378600
H	1.67618800	-1.18760300	-1.87046900
H	1.65129300	-2.08561700	0.66541900
H	1.51158300	0.03520500	2.30022000
H	1.41148400	2.23436800	0.77529700
H	1.51746900	1.47805500	-1.79775300

2 at B3LYP/def2-TZVP

Mo	-0.54882000	-0.16928500	-0.00001000
O	-1.30639800	-0.80076300	-1.38466000
O	-1.30723900	-0.80023700	1.38440300
C	-1.35487200	1.83571200	-0.00049700
C	1.64783200	-0.29565600	-1.15372700
C	1.60617300	-1.13157600	0.00336700
C	1.64705600	-0.28972100	1.15604700

C	1.60311200	1.03398100	0.71426700
C	1.60377600	1.03027800	-0.71892100
H	-2.43757700	1.70335300	-0.00139900
H	-1.05765900	2.38703000	-0.89135000
H	-1.05913200	2.38674400	0.89102300
H	1.61965700	-0.63728800	-2.17537400
H	1.63016100	-2.21033300	0.00617100
H	1.61815300	-0.62601700	2.17944600
H	1.56322900	1.91168500	1.33898600
H	1.56424800	1.90471500	-1.34823500

2 at cam-B3LYP/def2-TZVP

Mo	-0.53713600	-0.17314400	-0.00000600
O	-1.28014600	-0.80767100	-1.37563100
O	-1.28094300	-0.80707400	1.37545000
C	-1.36468300	1.80673600	-0.00050900
C	1.63512100	-0.27768800	-1.14936600
C	1.60872300	-1.11161600	0.00284900
C	1.63431800	-0.27269400	1.15135100
C	1.55789900	1.04418400	0.71267000
C	1.55854900	1.04106400	-0.71656400
H	-2.44515900	1.66677600	-0.00147900
H	-1.07647700	2.36381400	-0.88934900
H	-1.07804800	2.36343800	0.88907300
H	1.61099900	-0.61929200	-2.17063800
H	1.65256600	-2.18912700	0.00522200
H	1.60948200	-0.60981100	2.17409800
H	1.49724800	1.92008500	1.33725300
H	1.49825900	1.91420100	-1.34504900

2 at B3PW91/def2-TZVP

Mo	-0.53342100	-0.17232500	-0.00138600
O	-1.24111300	-0.83471200	-1.39091000
O	-1.30326100	-0.80928200	1.36564500
C	-1.38808300	1.79632300	-0.03083100
C	1.66732300	-0.58072900	-0.98229100
C	1.61653800	-1.05396700	0.36534100
C	1.59015900	0.07295700	1.22527800
C	1.52270500	1.21760000	0.41892400
C	1.59185600	0.81219400	-0.94755300
H	-2.46450800	1.63086600	-0.11210400
H	-1.04694600	2.37777300	-0.88749700
H	-1.17733600	2.33783400	0.89150600
H	1.68377900	-1.20019600	-1.86552700
H	1.64972600	-2.08822900	0.67502700
H	1.52368800	0.04158400	2.30182700
H	1.44233300	2.23558800	0.76757200

H	1.54495900	1.46812700	-1.80369200

2 at wB97xD/def2-TZVP

Mo	-0.53303600	-0.17537700	-0.00124700
O	-1.23880000	-0.83444400	-1.38342300
O	-1.29774900	-0.80068800	1.36452500
C	-1.36419800	1.80602000	-0.03261400
C	1.66031100	-0.44542000	-1.06299300
C	1.60951000	-1.08969400	0.20903100
C	1.59512700	-0.08173500	1.21039100
C	1.51370600	1.15178500	0.56379000
C	1.56669100	0.92570700	-0.84657000
H	-2.44257500	1.66912700	-0.12386800
H	-1.00423300	2.38767500	-0.88030400
H	-1.15030100	2.33931500	0.89302600
H	1.66503400	-0.94421000	-2.01829100
H	1.65775100	-2.15364800	0.38169400
H	1.53763700	-0.25324500	2.27282600
H	1.42345700	2.11460200	1.03954600
H	1.50625200	1.68728400	-1.60725400

2 at MP2/def2-SVP

Mo	-0.53462100	-0.16981700	0.00001100
O	-1.35699100	-0.79512500	-1.38762100
O	-1.35400900	-0.80303200	1.38587300
C	-1.34277000	1.84622200	0.00470900
C	1.64868200	-0.27983600	-1.16654100
C	1.61324800	-1.14257100	-0.02223700
C	1.65271100	-0.32009500	1.15189700
C	1.59762300	1.02208800	0.73472200
C	1.59406900	1.04709200	-0.70219600
H	-2.43998800	1.75164700	0.01251600
H	-1.03879400	2.40124200	-0.89560200
H	-1.02595400	2.40428600	0.89864400
H	1.63935200	-0.60327800	-2.20734900
H	1.66322900	-2.23246700	-0.04133800
H	1.64806600	-0.67992500	2.18072900
H	1.56027800	1.89566300	1.38539700
H	1.55449100	1.94301200	-1.32158900

2 at MP2/def2-SVPD

Mo	-0.52306800	-0.17935300	-0.00000300
O	-1.31461600	-0.83686000	-1.40047000
O	-1.31457100	-0.83718500	1.40034300
C	-1.41431300	1.80769000	0.00017200
C	1.67445900	-0.86864300	-0.72162700

C	1.67450600	-0.86942000	0.72055300
C	1.59880300	0.47804700	1.15900200
C	1.50517400	1.30669000	0.00064900
C	1.59862400	0.47926400	-1.15864000
H	-2.50672200	1.67322300	0.00012400
H	-1.11871500	2.37019400	-0.89859300
H	-1.11877300	2.37017500	0.89896600
H	1.73038600	-1.74979200	-1.35944900
H	1.73053800	-1.75124200	1.35746600
H	1.53090300	0.80928300	2.19397000
H	1.40065200	2.38998900	0.00122000
H	1.53056300	0.81159800	-2.19324400

2 at MP2/def2-TZVP

Mo	0.51904300	-0.17736500	0.00036200
O	1.29642900	-0.85775800	1.39206300
O	1.31728700	-0.81165600	-1.40100100
C	1.40238600	1.80712100	0.02886500
C	-1.67032900	-0.66133100	0.92844800
C	-1.65066200	-1.01230300	-0.45993000
C	-1.60051500	0.18763100	-1.21513400
C	-1.50310300	1.26039400	-0.30506900
C	-1.57445400	0.73641000	1.02024600
H	2.48437300	1.66908800	0.10099600
H	1.05499700	2.38271600	0.88928500
H	1.17157100	2.35027700	-0.88998500
H	-1.69866500	-1.35746800	1.75451800
H	-1.70635600	-2.01503100	-0.86099800
H	-1.53687100	0.25344300	-2.29200200
H	-1.39750500	2.30396600	-0.56360600
H	-1.50102100	1.31011200	1.93354500

Table 8

MoO_4^{2-} at MP2/def2-SVP

Mo	0.00000000	0.00000000	0.00000000
O	1.04163200	1.04163200	1.04163200
O	-1.04163200	-1.04163200	1.04163200
O	-1.04163200	1.04163200	-1.04163200
O	1.04163200	-1.04163200	-1.04163200

MoO_4^{2-} at MP2/def2-SVPD

Mo	0.00000000	0.00000000	0.00000000
O	1.04889600	1.04889600	1.04889600

O	-1.04889600	-1.04889600	1.04889600
O	-1.04889600	1.04889600	-1.04889600
O	1.04889600	-1.04889600	-1.04889600

MoO_4^{2-} at MP2/def2-TZVP

Mo	0.00000000	0.00000000	0.00000000
O	1.04371700	1.04371700	1.04371700
O	-1.04371700	-1.04371700	1.04371700
O	-1.04371700	1.04371700	-1.04371700
O	1.04371700	-1.04371700	-1.04371700

MoO_4^{2-} at MP2/def2-TZVPD

Mo	0.00000000	0.00000000	0.00000000
O	1.04500000	1.04500000	1.04500000
O	-1.04500000	-1.04500000	1.04500000
O	-1.04500000	1.04500000	-1.04500000
O	1.04500000	-1.04500000	-1.04500000

MoO_4^{2-} at MP2/def2-QZVPD

Mo	0.00000000	0.00000000	0.00000000
O	1.04222100	1.04222100	1.04222100
O	-1.04222100	-1.04222100	1.04222100
O	-1.04222100	1.04222100	-1.04222100
O	1.04222100	-1.04222100	-1.04222100

MoO_4^{2-} at CCSD(T)/def2-SVP

Mo	-0.00000100	0.00000200	0.00000200
O	-0.44443100	1.69135700	-0.36121200
O	0.37592700	-0.85471800	-1.52210500
O	1.43254300	-0.02439100	1.06578800
O	-1.36403200	-0.81225700	0.81751800

MoO_4^{2-} at M06L/def2-SVP

Mo	0.00000000	0.00000000	0.00000000
O	1.02977800	1.02977800	1.02977800
O	-1.02977800	-1.02977800	1.02977800
O	-1.02977800	1.02977800	-1.02977800
O	1.02977800	-1.02977800	-1.02977800

MoO_4^{2-} at M06L/def2-SVPD

Mo	0.00000000	0.00000000	0.00000000
O	1.03190200	1.03190200	1.03190200
O	-1.03190200	-1.03190200	1.03190200
O	-1.03190200	1.03190200	-1.03190200
O	1.03190200	-1.03190200	-1.03190200

MoO_4^{2-} at M06L/def2-TZVP

Mo	0.00000000	0.00000000	0.00000000
O	1.03189400	1.03189400	1.03189400
O	-1.03189400	-1.03189400	1.03189400
O	-1.03189400	1.03189400	-1.03189400
O	1.03189400	-1.03189400	-1.03189400

MoO_4^{2-} at M06L/def2-TZVPD

Mo	0.00000000	0.00000000	0.00000000
O	1.03142500	1.03142500	1.03142500
O	-1.03142500	-1.03142500	1.03142500
O	-1.03142500	1.03142500	-1.03142500
O	1.03142500	-1.03142500	-1.03142500

Table 9

3 at M06L/def2-TZVP

Mo	0.28848700	-0.42967000	-0.00001200
O	0.59933100	-1.39928700	1.35649000
O	0.59952000	-1.39957000	-1.35629800
C	-1.74743400	0.27263700	1.15118300
C	-2.04369700	-0.51149500	-0.00014000
C	-1.74740800	0.27285800	-1.15131000
C	-1.19275800	1.47481100	-0.71349400
C	-1.19278400	1.47467400	0.71366800
H	-1.83786900	-0.05747700	2.17328700
H	-2.47205400	-1.50218200	-0.00023900
H	-1.83782100	-0.05694300	-2.17352900
H	-0.78047500	2.25174100	-1.33770900
H	-0.78052400	2.25142600	1.33811000
Cl	1.97329300	1.15585300	-0.00002400

4 at M06L/def2-TZVP

Mo	0.26005100	-0.55862800	-0.53665000
O	0.71416700	-2.42312900	-0.41604600
O	-0.70047100	-2.21086100	-0.32960100
O	0.08615400	-0.12538000	-2.15761100
C	-0.92383300	-0.01089000	1.48831300
C	-1.74484400	0.28999100	0.34050300
C	-1.19583300	1.42946300	-0.31372800
C	0.03113600	1.71962400	0.30560900
C	0.17489000	0.85479300	1.45896600
Cl	2.58961500	-0.21940800	-0.25423600
C	-1.21449600	-1.07158200	2.48437400
H	-2.06216400	-0.78788800	3.11174300
H	-1.46976700	-2.01210900	1.99589600
H	-0.36571500	-1.25349200	3.14001100
C	1.25734800	0.95073000	2.46790800
H	0.97762500	1.66872700	3.24289700
H	1.44691900	-0.00340300	2.95581300
H	2.19163800	1.28741200	2.02555500
C	0.97717800	2.79830100	-0.07500100
H	0.79141400	3.70168000	0.51089300
H	2.00847100	2.49680100	0.10152500
H	0.88488100	3.05858900	-1.12781800
C	-1.73666500	2.09124000	-1.52427400
H	-1.53490100	3.16100700	-1.50626800
H	-1.27694500	1.68380000	-2.42930900
H	-2.81290500	1.95490700	-1.60765600
C	-3.02677400	-0.38524600	0.01304600
H	-3.85022900	0.06228700	0.57459300
H	-3.26584800	-0.30703200	-1.04580400
H	-2.99550600	-1.44254700	0.27101400

5 at M06L/def2-TZVP

Mo	1.63806800	-0.45974200	0.06383300
O	1.24082200	-1.62785300	-1.41576500
O	2.64359800	-1.37925500	-1.29458600
O	1.80510200	-1.35497700	1.47944700
C	2.78616400	1.46129300	-0.93389800
C	3.49138100	1.03556500	0.23603600
C	2.68808900	1.31840800	1.35964800
C	1.45065900	1.77729700	0.89140000
C	1.53084100	1.90267900	-0.53843300
H	3.13333400	1.34153200	-1.94753300
H	4.48262700	0.60906300	0.25004500
H	2.92809300	1.07922700	2.38243700
H	0.58820600	2.02154900	1.48912100
H	0.72459700	2.21815000	-1.18032200
C	-0.43443700	-0.22255100	0.04346300
C	-1.64923100	-0.11424700	0.01670000
C	-3.06127600	-0.00834900	0.00580700

C	-3.69485700	1.07615800	-0.61526300
C	-3.85397300	-0.99017800	0.61525700
C	-5.07392800	1.17126600	-0.62600500
H	-3.08945700	1.83697300	-1.09082300
C	-5.23213900	-0.88462600	0.60200700
H	-3.37035800	-1.83082000	1.09468200
C	-5.84804600	0.19344900	-0.01802500
H	-5.54879600	2.01363400	-1.11276700
H	-5.83121900	-1.65105000	1.07717300
H	-6.92754100	0.27061400	-0.02792100

6 at M06L/def2-TZVP

O	-2.41091000	-0.50907400	0.06028000
O	-2.07003500	0.89278400	-0.15754500
O	-0.27326300	-0.42774900	-2.08873100
C	0.37829500	0.84829700	1.54722500
C	0.61531600	1.64533900	0.37894500
C	1.55305100	0.96067400	-0.44650600
C	1.80784900	-0.29427700	0.14792400
C	1.10648800	-0.34863300	1.40410900
C	-0.53279300	1.22912300	2.65868500
H	-0.11645800	2.05413900	3.24038400
H	-1.50228200	1.55543400	2.27927400
H	-0.70571900	0.40002700	3.34160400
C	1.23875200	-1.42657100	2.41657600
H	2.09693900	-1.22665500	3.06193900
H	0.36095100	-1.49735400	3.05611500
H	1.39748300	-2.40192600	1.96166400
C	2.73383500	-1.32632600	-0.39079100
H	3.77420800	-1.04449600	-0.21356200
H	2.57856200	-2.29611500	0.07741300
H	2.61156600	-1.45174600	-1.46639600
C	2.10830400	1.41803800	-1.74525900
H	3.17999000	1.60700800	-1.65972200
H	1.96415600	0.66620700	-2.52130200
H	1.63706500	2.33661000	-2.08734300
C	0.03278900	2.99391700	0.15078400
H	0.54150900	3.74065600	0.76394400
H	0.11873500	3.30536800	-0.88803700
H	-1.02318700	3.01630400	0.41961400
C	-0.56600400	-2.39049000	0.08193100
H	0.38558300	-2.88908000	-0.10496900
H	-0.86962200	-2.57433500	1.11134200
H	-1.31832900	-2.83176900	-0.57098200
W	-0.53963200	-0.26987200	-0.39911800

7 at M06L/def2-TZVP

O	-1.21251100	-0.73149500	-1.39448900
O	-1.21248600	-0.73141200	1.39454300
C	-1.11891700	1.92348100	-0.00003300
C	1.74578200	-0.32225200	-1.15199900
C	1.66875400	-1.15780200	-0.00007800
C	1.74579900	-0.32238300	1.15193900
C	1.76022400	1.00188700	0.71233800
C	1.76020700	1.00196800	-0.71223700
H	-2.20767200	1.87069800	-0.00006700
H	-0.80064700	2.47209100	-0.88508600
H	-0.80070100	2.47206400	0.88505700
H	1.69275000	-0.65911300	-2.17450000
H	1.64364600	-2.23693000	-0.00013600
H	1.69279500	-0.65937200	2.17439900
H	1.74450600	1.87959900	1.33864500
H	1.74447800	1.87976000	-1.33843400
W	-0.41459800	-0.10898600	0.00000100

8 at M06L/def2-TZVP

W	0.23105800	-0.39695500	-0.21972900
Si	-3.13826200	0.04680300	0.05963300
O	-0.38409500	0.04734400	-1.76572800
O	-0.41437500	-2.14218300	0.33882000
O	0.85515900	-2.22430500	-0.37405300
C	-1.49640800	0.18635000	0.96997300
C	1.14356600	1.77455500	0.27567300
C	1.94037800	1.24841000	-0.76696300
C	2.55482600	0.06152900	-0.28007800
C	2.22640400	-0.07607000	1.11060500
C	1.35636100	0.97482600	1.45446300
C	0.32362800	3.01224800	0.17687300
C	2.00865600	1.79699600	-2.14468700
C	3.46537200	-0.85427800	-1.01634800
C	2.70394200	-1.17349200	1.99199800
C	0.83814100	1.26638600	2.81595400
C	-4.51330400	0.14724900	1.33597300
C	-3.31552100	-1.54991600	-0.89129900
C	-3.29480900	1.51081000	-1.09719400
H	-1.51206600	-0.44641700	1.86051300
H	-1.43713600	1.22046900	1.31808800
H	-0.41256600	3.08104500	0.97542700
H	0.95379000	3.90205500	0.24223500
H	-0.21181000	3.06284200	-0.77117300
H	2.67197000	1.21403700	-2.77921800
H	1.02218700	1.79933200	-2.61248800
H	2.37654300	2.82384000	-2.13323600
H	3.35483900	-0.76417600	-2.09479000
H	4.50732100	-0.63997600	-0.76971000
H	3.27686000	-1.89350400	-0.74739500
H	2.56530500	-2.14695800	1.52007300

H	3.76849900	-1.06380900	2.20941200
H	2.17453100	-1.18515500	2.94254800
H	1.60759400	1.76599300	3.40872800
H	-0.02827600	1.92275800	2.79351400
H	0.55205600	0.36239100	3.35143300
H	-4.47284200	-0.68836900	2.03540000
H	-4.45297700	1.06523400	1.92184800
H	-5.49655400	0.12735300	0.86334800
H	-4.30504100	-1.61171400	-1.34709000
H	-2.57740500	-1.62781400	-1.68897800
H	-3.19229400	-2.42073900	-0.24795900
H	-4.24714000	1.49334100	-1.62860000
H	-3.24685000	2.45622500	-0.55397100
H	-2.50203500	1.51068400	-1.84485100

9 at M06L/def2-TZVP

Mo	-0.64368700	-1.71719200	0.55528500
O	-0.12870700	-1.97575100	-1.29500700
O	-0.40801400	-3.21538500	-0.62585400
O	-1.95767300	-1.38225200	1.94821500
O	-1.74113900	-2.78087500	1.72363700
O	0.81003800	-1.51391000	1.38173300
C	-3.55532500	-2.64221300	-0.86847000
C	-3.38919800	-0.37060500	-0.53872800
C	-4.90512400	-2.54516200	-1.17069900
H	-3.03054500	-3.59017600	-0.85906100
C	-4.73612500	-0.18730800	-0.82383500
C	-5.50057100	-1.29631700	-1.14138400
H	-5.17487000	0.80103400	-0.79875700
H	-6.55384200	-1.18385100	-1.36406200
N	-2.82238700	-1.58053100	-0.56388200
H	-5.47241500	-3.43213600	-1.41442600
C	-2.48822700	0.73440300	-0.24779200
C	-2.77631900	2.09620700	-0.16010000
N	-1.16601800	0.52251200	-0.09683900
C	-1.56168200	2.69775000	0.03192000
H	-3.73207900	2.58430300	-0.22308300
N	-0.60380000	1.74108500	0.06550200
C	-1.26842300	4.15541200	0.15716000
F	-0.48867500	4.60480000	-0.83856100
F	-0.64258100	4.44737300	1.30528600
F	-2.40602100	4.84864900	0.12376000
C	0.82619700	2.02927600	-0.16462500
H	0.90409300	2.38649900	-1.19535800
H	1.06770800	2.87379700	0.48113500
C	1.77536900	0.88939300	0.06108400
H	1.72779400	0.55682000	1.09642700
H	1.47965900	0.03251000	-0.54822000
C	3.20020700	1.28047700	-0.29206100

H	3.24770600	1.60415600	-1.33745900
H	3.50602000	2.14997800	0.29976400
C	4.17697100	0.14031100	-0.06635100
H	4.12749600	-0.17485900	0.98057900
H	3.85058900	-0.73169400	-0.64179900
C	5.60874300	0.48660200	-0.42936900
H	5.65414700	0.79431500	-1.47983800
H	5.92865100	1.36429000	0.14302000
C	6.58559600	-0.65065900	-0.19487200
H	6.26372100	-1.52949800	-0.76337800
H	6.54226000	-0.95652900	0.85582000
C	8.01925000	-0.30993600	-0.56179700
H	8.33636300	0.56954200	0.00677600
H	8.05850900	-0.00585000	-1.61213600
C	8.98531000	-1.45175700	-0.32157300
H	8.71141000	-2.33159000	-0.90510600
H	10.00678300	-1.18604500	-0.59058100
H	8.99070000	-1.75168300	0.72709700

10 at M06L/def2-TZVP

Mo	0.00001000	-1.27058900	-0.04712900
Cl	-0.00008700	-1.24609400	2.28774500
Cl	0.00009800	-0.15247600	-2.16350400
O	-1.34305500	-2.24883100	-0.34200100
O	1.34313300	-2.24878200	-0.34186300
O	-1.46452300	0.53923400	0.37638600
C	-2.52414600	0.61509300	-0.24498200
N	-3.45898700	1.54179100	-0.01522200
H	-2.78601900	-0.08564700	-1.04977700
C	-4.68160800	1.57560200	-0.77985800
H	-5.54879900	1.44733800	-0.12956900
H	-4.78413400	2.52853500	-1.30203500
H	-4.67467300	0.77468600	-1.51484200
C	-3.28165200	2.54216300	1.01323800
H	-4.08487200	2.47523800	1.74822600
H	-2.32847800	2.37485800	1.50458200
H	-3.29650700	3.54200300	0.57660000
O	1.46447300	0.53929800	0.37651300
C	2.52405100	0.61515400	-0.24494600
N	3.45895400	1.54178800	-0.01518800
H	2.78583300	-0.08552800	-1.04981900
C	4.68151300	1.57560200	-0.77992300
H	5.54875300	1.44724900	-0.12971600
H	4.67448000	0.77474100	-1.51496700
H	4.78403900	2.52856900	-1.30203700
C	3.28175800	2.54208500	1.01337000
H	3.29661200	3.54196000	0.57681200
H	2.32862400	2.37478000	1.50479200
H	4.08504500	2.47506700	1.74827500

Table 12

1-CF_3 PCM acetonitrile M06L/def2-TZVP

Mo	0.29848900	0.44683600	-0.25153700
F	-2.06447000	-0.59760200	1.39185900
F	-1.93101600	-1.59891300	-0.52171300
F	-2.66499200	0.42367300	-0.40755100
O	-0.57857900	1.82076700	0.78912600
O	0.78936400	2.14486100	0.52599000
O	-0.01313300	0.62006700	-1.90505200
C	2.21624300	-0.92278300	-0.73027400
C	1.11614200	-1.76731900	-0.53874500
C	0.70263900	-1.64572800	0.82383400
C	1.55516900	-0.72815600	1.46246100
C	2.46202200	-0.24569200	0.49432200
C	-1.73616300	-0.41220200	0.09774300
H	2.73223100	-0.74787900	-1.66073600
H	0.64028300	-2.38042500	-1.28716000
H	-0.11474200	-2.17879100	1.28075400
H	1.46496700	-0.37612500	2.47794500
H	3.20750000	0.51741400	0.65381600

1-CF_3 three acetonitrile M06L/def2-TZVP

Mo	-0.00913100	0.08243100	0.05609700
F	-2.37764900	-1.65411400	-0.77837200
F	-0.50325500	-2.68081600	-1.11198500
F	-1.12078800	-1.09238900	-2.43401400
O	-1.40394600	1.10632000	-0.81044500
O	-0.68512700	1.88595600	0.15249000
O	1.36835500	0.05280800	-0.92712700
C	1.39515100	-0.56075700	1.90197700
C	0.73082500	-1.70384400	1.44716700
C	-0.67000300	-1.52085900	1.69078000
C	-0.85538400	-0.26749200	2.29118400
C	0.41623300	0.35458000	2.36868600
C	-1.09014400	-1.46741400	-1.14296700
H	2.45084700	-0.36166200	1.81147000
H	1.19764200	-2.54929200	0.96621300
H	-1.44898000	-2.22694300	1.45100900
H	-1.81079600	0.18530700	2.51277000
H	0.61114100	1.35887500	2.71317300
H	0.75987900	4.07333900	-1.04681500
H	-4.04433800	2.04409300	-1.10574800
H	4.02086300	-0.11957300	-1.92304000
C	4.43035200	-0.24019000	-0.92209800
H	5.51744100	-0.24176500	-0.97890700
H	4.10542300	0.60763300	-0.31912000
C	3.95252400	-1.46786600	-0.33740400
N	3.57149500	-2.44416700	0.14584700

C	1.60629000	3.43084500	-1.27954800
H	1.24955300	2.61100300	-1.90253500
H	2.34726900	4.00391700	-1.83438500
C	2.17871800	2.90232000	-0.06726900
N	2.63636800	2.46130200	0.89685700
C	-4.46863800	1.06756600	-0.88181100
H	-5.54654800	1.10476300	-1.02997200
H	-4.03864500	0.34681000	-1.57466200
C	-4.15942000	0.69350100	0.47510700
N	-3.92290900	0.39204000	1.56324600

1-CF_3 PCM water M06L/def2-TZVP (Tight convergence criteria and ultrafine integration grid)

Mo	0.29650400	0.44800200	-0.25313700
F	-2.05393800	-0.61745100	1.39138100
F	-1.93151500	-1.59540100	-0.53529800
F	-2.66683600	0.42535800	-0.39100700
O	-0.58597500	1.81173500	0.79339500
O	0.77830500	2.14776000	0.52708100
O	-0.01926800	0.62179600	-1.90554200
C	2.23798600	-0.89650000	-0.71659300
C	1.14538100	-1.75737300	-0.55730800
C	0.70437200	-1.65798100	0.79732200
C	1.53544700	-0.74040700	1.46602000
C	2.45608600	-0.23608500	0.52314300
C	-1.73373200	-0.41647200	0.09735500
H	2.77020700	-0.70356300	-1.63399400
H	0.69150000	-2.36557900	-1.32280800
H	-0.11370800	-2.20784500	1.23211600
H	1.42175000	-0.40582800	2.48482100
H	3.18995000	0.53274500	0.70684500

1-CF_3 three water M06L/def2-TZVP (Tight convergence criteria and ultrafine integration grid)

Mo	0.03634400	0.09611800	-0.11005300
F	2.99867100	0.83497900	-0.31895800
F	2.59347800	-0.37476400	1.43013700
F	2.00980900	1.70034400	1.38555900
O	0.45128200	1.80494100	-0.89866100
O	-0.84992600	1.36348200	-1.28453200
O	-0.51577000	0.18685400	1.49307200
C	-0.64435100	-2.18662800	-0.42661200
C	0.67632000	-2.18992000	0.04171600
C	1.50034900	-1.60454100	-0.96686100
C	0.67952700	-1.24967300	-2.05176600
C	-0.64871200	-1.56833700	-1.70487300
C	2.08107500	0.59566900	0.63630100
H	-1.51551300	-2.50025300	0.12598900
H	1.01549400	-2.53642700	1.00473900

H	2.56591700	-1.46323900	-0.90188800
H	0.99497900	-0.71852000	-2.93581500
H	-1.53467200	-1.33458500	-2.27229100
H	-3.23409900	0.59546600	-0.19578500
H	-2.29988600	2.40536000	-0.51425400
O	-2.89775800	-0.31445900	-0.27627200
H	-3.06348000	-0.72207900	0.58905200
O	-3.17872800	2.46533800	-0.10610400
H	-3.67966200	3.05220100	-0.67715600
H	-1.81831500	-0.93050800	2.33745000
O	-2.53648100	-1.57628200	2.24177800
H	-3.02101100	-1.54778800	3.06988900

checkCIF results

$CpMo(\eta^2\text{-}O_2)OCH_3$

Reference: A. M. Al-Ajlouni, D. Veljanovski, A. Capapé, J. Zhao, E. Herdtweck, M. J. Calhorda and F. E. Kühn, *Organometallics*, 2009, **28**, 639.

Datablock: ZHAP-1041-173

Bond precision: C-C = 0.0114 A Wavelength=0.71073

Cell: a=6.5225(5) b=7.9532(5) c=13.9632(7)
alpha=90 beta=90 gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	724.34(8)	724.34(8)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C6 H8 Mo O3	C6 H8 Mo O3
Sum formula	C6 H8 Mo O3	C6 H8 Mo O3
Mr	224.06	224.06
Dx,g cm-3	2.055	2.055
Z	4	4
Mu (mm-1)	1.751	1.751
F000	440.0	440.0
F000'	433.28	
h,k,lmax	8,10,18	8,10,18
Nref	1716[1022]	1711
Tmin,Tmax	0.692,0.839	0.677,0.839
Tmin'	0.442	

Correction method= # Reported T Limits: Tmin=0.677 Tmax=0.839
AbsCorr = NUMERICAL

Data completeness= 1.67/1.00 Theta(max)= 27.810

R(reflections)= 0.0384(1662) wR2(reflections)= 0.0989(1711)

S = 1.094 Npar= 94

Alert level C

```
STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.510
          From the CIF: _refine_ls_abs_structure_Flack_su    0.150
PLAT234_ALERT_4_C Large Hirshfeld Difference O1     --  O2      ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13    --  C14     ..       0.16 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        O1 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        O2 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C14 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        Mo Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0114 Ang.
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT033_ALERT_4_G Flack x Value Deviates > 2*sigma from Zero .....     0.510 Note
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
2 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

$CpMo(\eta^2\text{-}O_2)OCl$

Reference: M. V. Galakhov, P. Gómez-Sal, T. Pedraz, M. A. Pellinghelli, P. Royo, A. Tiripicchio and A. Vázquez de Miguel, *Journal of Organometallic Chemistry*, 1999, **579**, 190.

Datablock: 6

```
Bond precision:  C-C = 0.0135 A          Wavelength=0.71073

Cell:            a=6.611(2)     b=9.472(3)          c=6.579(3)
                 alpha=90       beta=118.96(2)      gamma=90
Temperature:     293 K

                 Calculated                 Reported
Volume           360.5(2)                   360.5(2)
Space group      P 21/m                     P 21/m
Hall group       -P 2yb                     ?
Moiety formula   C9 H9 Cl Mo O6             ?
Sum formula      C9 H9 Cl Mo O6             C5 H5 Cl1 O3 Mo1
Mr               344.55                     244.49
Dx,g cm-3        1.587                      2.253
Z                1                          2
Mu (mm-1)        1.105                      2.128
F000             170.0                      236.0
F000'            168.51
h,k,lmax         8,12,8
Nref             837
Tmin,Tmax        0.591,0.682                0.587,1.000
Tmin'            0.569

Correction method= # Reported T Limits: Tmin=0.587 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.000          Theta(max)=

R(reflections)= 0.0460( 738)      wR2(reflections)= wR= 0.0569( 738)

S = 1.150                 Npar= 75
```

Alert level A

```
CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as
            calculated from the _atom_site* data lies outside
            the range 0.90 <> 1.10
           From the CIF: _cell_formula_units_Z                  2
           From the CIF: _chemical_formula_weight          244.49
           TEST: Calculate formula weight from _atom_site_*
           atom     mass     num      sum
           Mo       95.94     0.50   47.97
           Cl       35.45     0.50   17.73
           O        16.00     3.00   48.00
           C        12.01     4.50   54.05
           H         1.01     4.50    4.54
           Calculated formula weight             172.28
RADNT01_ALERT_1_A  The radiation type should contain one of the following
            * 'Cu K\a'
            * 'Mo K\a'
            * 'Ag K\a'
            * 'Ga K\a'
            * neutron
            * synchrotron
SHFSU01_ALERT_2_A  The absolute value of parameter shift to su ratio > 0.20
            Absolute value of the parameter shift to su ratio given   0.400
            Additional refinement cycles may be required.
WEIGH01_ALERT_1_A  The weighting scheme should be one of the following
            * sigma
            * calc
            Weighting scheme given as 0.6181(\s^2^(Fo)+0.0016Fo^2^)^-1^
PLAT026_ALERT_3_A Ratio Observed / Unique Reflections too Low ....          0 %
PLAT027_ALERT_3_A _diffrn_reflns_theta_full (too) Low .............       0.00 Degree
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low .......      0.000 Note
PLAT043_ALERT_1_A Calculated and Reported Mol. Weight Differ by ..     144.43 Check
PLAT051_ALERT_1_A Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .      48.10 %
PLAT080_ALERT_2_A Maximum Shift/Error ............................      0.40
```

Alert level B

```
CHEMS01_ALERT_1_B  The sum formula contains elements in the wrong order.
            O  precedes Mo
            Sequence must be C, H, then alphabetical.
```

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as empirical
HYDTR01_ALERT_1_C  The hydrogen treatment should only be one of the following
           keywords
           * refall
           * refxyz
           * refU
           * noref
           * undef
           * constr
           * none
           * mixed
           Hydrogen treatment given as refined isotropically
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT076_ALERT_1_C Occupancy      0.500 less than 1.0 for Sp.pos  .         MO
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:C5 H5 Cl1 Mo1 O3
            Atom count from the _atom_site data:  C4.5 H4.5 Cl0.5 Mo0.5 O3
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  C5 H5 Cl1 O3 Mo1
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           Mo          2.00       1.00    1.00
           Cl          2.00       1.00    1.00
           O           6.00       6.00    0.00
           C          10.00       9.00    1.00
           H          10.00       9.00    1.00
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by .............      0.50 Ratio
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.        2 Note
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)      293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)      293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *Mo     is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *Cl     is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O1     is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O2     is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O3     is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C1     is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H1     is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O1_a   is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O2_a   is Constrained at    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O3_a   is Constrained at    0.500 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =      53 Note
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found  Please Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....       ! Info
```

$CpMo(\eta^2\text{-}O_2)OCF3$

Reference: S. A. Hauser, R. M. Reich, J. Mink, A. Pothig, M. Cokoja and F. E. Kuhn, *Catalysis Science & Technology*, 2015. DOI: 10.1039/C4CY01604A

Datablock: Compound6

Bond precision: C-C = 0.0042 A Wavelength=0.71073

Cell: a=20.5911(3) b=6.9325(1) c=12.3919(2)
alpha=90 beta=117.372(1) gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	1570.87(4)	1570.87(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C6 H5 F3 Mo O3	C6 H5 F3 Mo O3
Sum formula	C6 H5 F3 Mo O3	C6 H5 F3 Mo O3
Mr	278.04	278.04
Dx,g cm-3	2.351	2.351
Z	8	8
Mu (mm-1)	1.693	1.693
F000	1072.0	1072.0
F000'	1058.95	
h,k,lmax	24,8,14	24,8,14
Nref	1446	1447
Tmin,Tmax	0.833,0.873	0.594,0.881
Tmin'	0.562	

Correction method= # Reported T Limits: Tmin=0.594 Tmax=0.881
AbsCorr = MULTI-SCAN

Data completeness= 1.001 Theta(max)= 25.400

R(reflections)= 0.0194(1266) wR2(reflections)= 0.0448(1447)

S = 1.043 Npar= 118

Datablock: Compound3

Bond precision: C-C = 0.0080 A Wavelength=0.71073

Cell: a=6.4530(2) b=6.5440(2) c=6.7851(2)
alpha=107.752(1) beta=97.132(1) gamma=107.192(1)
Temperature: 123 K

	Calculated	Reported
Volume	253.356(14)	253.356(14)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C9 H5 F3 Mo O3	C9 H5 F3 Mo O3
Sum formula	C9 H5 F3 Mo O3	C9 H5 F3 Mo O3
Mr	314.07	314.07
Dx,g cm-3	2.059	2.059
Z	1	1
Mu (mm-1)	1.326	1.326
F000	152.0	152.0
F000'	150.38	
h,k,lmax	7,7,8	7,7,8
Nref	1858[929]	910
Tmin,Tmax	0.839,0.911	0.529,0.913
Tmin'	0.482	

Correction method= # Reported T Limits: Tmin=0.529 Tmax=0.913
AbsCorr = MULTI-SCAN

Data completeness= 0.98/0.49 Theta(max)= 25.370

R(reflections)= 0.0147(905) wR2(reflections)= 0.0381(910)

S = 1.111 Npar= 145

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a Note
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo1 -- O1 .. 5.6 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo1 -- O2 .. 6.2 su