

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

Supplementary Materials for

'Density-functional Theory Models of Xanthine Oxidoreductase Activity:
Comparison of Substrate Tautomerization and Protonation'

C.A. Bayse

Cartesian coordinates of optimized geometries (mPW1PW91)

1-MeXan

```
1\1\GINC-ORION-0-7\Freq\RmPW1PW91\Gen\C6H6N4O2\CBAYSE\11-Jun-2008\0\#\#
N GEOM=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RMPW1PW91/CHKBAS FREQ\test\
\0,1\H,-2.4902020936,1.9646511718,0.0000542787\C,-3.0168786483,-0.0
895054049,-0.0000011052\N,-2.3438115625,-1.2245748751,0.0000523626\C,-
1.0501293583,-0.8330438052,-0.000077264\C,-0.9252383747,0.5296497075,-
0.0001642711\N,-2.2165425796,0.9966683185,0.0000674127\H,-4.092301634,
-0.0151137677,0.0000454199\N,0.0588256769,-1.6258550344,-0.0000870819\
C,0.3334586724,1.2045514458,-0.0001003596\N,1.4107014364,0.3000560178,
-0.0000658898\C,1.3333270275,-1.0989325354,-0.0000426696\O,0.508023395
8,2.4076735428,0.0001161687\O,2.3111671344,-1.8127525961,0.0000923094\
H,-0.0129620772,-2.6299970308,0.0000570617\C,2.7394011884,0.8974959248
,0.0000691139\H,2.864131995,1.5219141878,-0.8830216497\H,2.8642167687,
1.5214202485,0.8835015805\H,3.4657389589,0.092404633,-0.0001728066\Ve
rsion=AM64L-G03RevC.02\State=1-A\HF=-601.8129734\RMSD=4.770e-09\RMSF=1
```

3-MeXan

```
1\1\GINC-ORION-0-8\Freq\RmPW1PW91\Gen\C6H6N4O2\CBAYSE\06-Jun-2008\0\#\#
N GEOM=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RMPW1PW91/CHKBAS FREQ\test\
\0,1\H,-3.193731144,0.5250291182,-0.0002673948\C,-2.3558362033,-1.4
215254549,0.0003081645\N,-1.129885376,-1.9075432018,0.0001444782\C,-0.
3366443059,-0.8108434038,0.0000398844\C,-1.0792884748,0.3459513527,-0.
0001909956\N,-2.3858669237,-0.0745507714,-0.0000836942\H,-3.2521905692
,-2.0203630596,0.0004450729\N,1.0333956183,-0.7965187097,-0.0000196015
\C,-0.5008226261,1.6520963747,0.0000058394\N,0.8920776664,1.5464843843
,-0.0000619391\C,1.7004726639,0.4131123663,0.0003603935\O,-1.073674294
1,2.7227976905,-0.0001886344\O,2.9085089293,0.4926534474,-0.0002619564
\H,1.4036011585,2.4166097442,-0.000227207\C,1.8168895848,-2.0199321569
,0.0000687009\H,2.4529965537,-2.05695772,-0.8828302001\H,2.4491182395,
-2.0595863263,0.8856752197\H,1.1248579526,-2.8565972387,-0.0025973906\
\Version=AM64L-G03RevC.02\State=1-A\HF=-601.8146788\RMSD=5.167e-09\RMS
```

7-MeXan

```
1\1\GINC-ORION-0-8\Freq\RmPW1PW91\Gen\C6H6N4O2\CBAYSE\07-Jun-2008\0\#\#
N GEOM=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RMPW1PW91/CHKBAS FREQ\test\
\0,1\C,2.0330693109,-1.4551428004,-0.0000579837\N,0.8772290048,-2.0
983170277,-0.0002615143\C,-0.0365381036,-1.1099055923,0.0001571603\C,0
.5514643176,0.1336864495,0.0004328364\N,1.9066408234,-0.1144911827,-0.
0000112172\H,2.9996182915,-1.934108238,-0.000242038\N,-1.3963617609,-1
.2534690449,0.0001188834\C,-0.204756075,1.3492996279,0.0004724369\N,-1
.5770848975,1.0651508331,0.0001989818\C,-2.234686727,-0.1604928563,0.0
004111889\O,0.2094007268,2.4909577392,-0.0002569944\O,-3.4401070285,-0
.2493214932,-0.0007681709\H,-2.1907674055,1.8664580629,-0.0003498756\H
,-1.8236268367,-2.1650615222,-0.000369243\C,2.9692238925,0.8694791376,
0.0000343297\H,2.8987804198,1.5007852121,-0.8835772284\H,2.8995798525,
1.4998284644,0.8843975266\H,3.9224442116,0.3453492129,-0.0006735668\Ve
rsion=AM64L-G03RevC.02\State=1-A\HF=-601.8160891\RMSD=2.732e-09\RMSF=
```

Xan

```
1\1\GINC-ORION-0-7\Freq\RmpW1PW91\Gen\C5H4N4O2\CBAYSE\27-May-2008\0\#\#  
N GEOM=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RMPW1PW91/CHKBAS FREQ\test\0,1\H,2.9171266996,0.0198049859,0.7744796772\C,2.3277676779,-0.997  
7860113,-0.9887883198\N,1.1805794665,-1.2040183472,-1.6073158442\C,0.2  
734189826,-0.5706824182,-0.8323300554\C,0.8575717598,0.022489535,0.258  
6149307\N,2.1940328433,-0.2675244922,0.136796614\H,3.2821521979,-1.365  
4495132,-1.3294643197\N,-1.0739935282,-0.4884790708,-1.0457586293\C,0.  
1203796533,0.7619255747,1.2374112053\N,-1.2406545987,0.7715119058,0.90  
5702251\C,-1.8983741299,0.1938353156,-0.176004667\O,0.5483434453,1.319  
5804753,2.225940416\O,-3.0925734096,0.2877329553,-0.3334192108\H,-1.84  
54556395,1.2714097342,1.540723585\H,-1.504316487,-0.9233945952,-1.8452  
978867\Version=AM64L-G03RevC.02\State=1-A\HF=-562.5034319\RMSD=3.421e
```

Xan_{1,7,9}

```
1\1\GINC-ORION-0-18\Freq\RmpW1PW91\Gen\C5H4N4O2\CBAYSE\27-May-2008\0\#\#  
N GEOM=ALLCHECK GUESS=READ SCRF=CHECK GENCHK RMPW1PW91/CHKBAS FREQ\test\0,1\H,1.4433107023,0.0004232408,2.5867532821\C,-0.6370565299,-0.0  
00738252,2.6305281422\N,-1.5426583345,-0.0006883312,1.6402798518\C,-0.  
8974931911,0.000217546,0.4003396297\C,0.4554601878,0.0010998372,0.7198  
048547\N,0.5677928365,0.0001313826,2.0863399617\H,-0.8527815375,-0.001  
1595616,3.6835133365\N,-1.4790710057,-0.0000182578,-0.7634984337\C,1.4  
409412949,0.0002481356,-0.3188889442\N,0.7935911649,0.0003591389,-1.53  
65536483\C,-0.6101110348,0.0010068046,-1.8254765015\O,2.6521088907,-0.  
0004761043,-0.1728648465\O,-0.9416690915,-0.0004015963,-2.9886416113\H  
,1.3810591165,-0.000282104,-2.3574484615\H,-2.5431336655,-0.0014519262  
,1.7554162986\Version=AM64L-G03RevC.02\State=1-A\HF=-562.4656124\RMSD
```

^{Mo}Xan_R

```
1\1\GINC-ORION-0-2\Freq\RmpW1PW91\Gen\C7H6Mo1N4O4S3(2-)\CBAYSE\05-Sep-  
2007\0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C  
HKBAS FREQ\test\0,-2,1\Mo,-2.3511044208,-0.7016809059,-0.3746041289\S,  
-4.329050402,0.3495265294,0.7017631627\C,-4.2704474103,2.0668191839,0.  
3611663021\C,-3.176853021,2.6514214831,-0.1690868614\S,-1.7632201959,1  
.7171397925,-0.6017458071\H,-5.1342797489,2.6538538777,0.6778552593\H,  
-3.1146665084,3.7318058074,-0.307231302\O,-3.0180290452,-1.1425809453,  
-1.8558290261\S,-2.7702555265,-2.3252014173,1.050746939\O,-0.521516859  
3,-0.8134261705,-0.6170648163\H,0.3631728674,-0.4005516506,-0.38046523  
68\C,1.8116485494,1.4124540606,0.8080383428\N,2.9982180207,1.914153481  
1,1.2512705743\C,3.8614620509,1.0359731267,0.752053676\C,3.215915457,0  
.0318756448,0.0310557339\N,1.8692061249,0.3070569059,0.0821125894\H,0.  
8693345432,1.894816733,1.0250870167\N,5.2362557841,1.0779560665,0.9041  
976416\C,3.9691393632,-0.9910517877,-0.6117959065\N,5.3715234735,-0.82  
31494065,-0.3670803262\C,6.0462876861,0.1391645238,0.3442620843\O,3.62  
76140887,-1.9364014208,-1.3013828025\O,7.2707969143,0.1457472306,0.458  
6536186\H,5.9550292251,-1.5240185283,-0.7934415573\H,5.6679526236,1.81  
24870439,1.4366611479\Version=AM64L-G03RevC.02\State=1-A\HF=-889.0211  
052\RMSD=9.147e-09\RMSF=4.950e-05\Dipole=0.3001734,1.5690686,0.1636236
```

^{Mo}XanH_R⁺

```
1\1\GINC-ORION-0-24\Freq\RmpW1PW91\Gen\C7H7Mo1N4O4S3(1-)\CBAYSE\18-Sep-  
2007\0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/  
CHKBAS FREQ\test\0,-1,1\Mo,2.5948972509,-0.2624270307,0.1875636997\S,1  
.270440252,0.5548035977,-1.7180330372\C,0.651394236,2.1419070818,-1.30
```

58424581\C,0.7261589705,2.6268537255,-0.0502038169\S,1.5329905741,1.72
14983376,1.2080635945\H,0.1398916318,2.6809894945,-2.1018291536\H,0.27
60533894,3.5765547673,0.2315528611\O,4.135876015,0.1104841154,-0.34405
62706\S,2.0526314733,-2.2495197354,-0.5421319477\O,2.8052953141,-0.571
9196153,2.0690103411\H,2.264745922,-0.1575571852,2.7440461779\C,-2.004
9729029,-2.6805061634,-0.1144965505\N,-1.350350753,-1.479549374,-0.259
0725807\C,-2.2924460719,-0.5241141578,-0.1233090048\C,-3.485483647,-1.
182817544,0.0971544037\N,-3.2790635795,-2.5417753536,0.0977171141\H,-1.
.4674772575,-3.6123482012,-0.1788821473\N,-2.1457599828,0.8286685585,-
0.180807563\C,-4.6924210967,-0.4241386266,0.2820197433\N,-4.4297467932
,0.9620150482,0.1990337783\C,-3.2447652472,1.6409703432,-0.0202121142\
O,-5.8239075491,-0.8105482661,0.4840004151\O,-3.1884745101,2.853019824
5,-0.0681570282\H,-5.2339307295,1.5581840504,0.3181893788\H,-1.2486218
001,1.2852612685,-0.3358346658\H,-0.3539943317,-1.3603926778,-0.436431
7084\\Version=AM64L-G03RevC.02\State=1-A\HF=-889.6424269\RMSD=1.455e-0

$2_{\text{H}}^{\text{Mo}}\cdot\text{Xan}_{\text{TS}}$

1\1\GINC-ORION-0-9\Freq\RmPW1PW91\Gen\C7H6Mo1N4O4S3(2-)\CBAYSE\29-Aug-
2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C
HKBAS FREQ\test\ -2,1\Mo,1.9714908512,-0.3820523809,0.2285562599\S,4.
1836404323,-0.3906120039,-0.8267307584\C,5.0008648287,1.0364373832,-0.
193617967\C,4.3448601544,2.0044653753,0.4802073452\S,2.6165263381,1.92
44331339,0.8010196393\H,6.0642217725,1.1341753851,-0.4215228238\H,4.86
47252317,2.9011973441,0.8225316886\O,2.1196843794,-1.3583796747,1.5908
336606\S,1.1544621513,-1.6205408231,-1.4612997858\O,0.1512468861,0.335
3204348,0.2817264389\C,-0.990099395,-0.1626037104,-0.2809879279\N,-1.8
392778823,-0.8847194871,0.6055496384\C,-3.1355890991,-0.4191768189,0.4
458937391\C,-3.0248715538,0.5032411614,-0.6025649902\N,-1.8123869836,0
.7016618959,-1.0439006538\C,-4.3630609992,-0.8029978252,0.9827660653\N
, -4.1601014136,1.1106438589,-1.1057652362\H,-1.4726947217,-1.262006819
6,1.4606018614\H,-0.4261112065,-0.9810624598,-1.0807809068\N,-5.444554
1217,-0.0648208617,0.3872269382\C,-5.4149774541,0.8516261637,-0.625144
5717\O,-4.6456658035,-1.619293634,1.8690206694\H,-4.0753814142,1.77681
27389,-1.8536262142\O,-6.4231836793,1.3977896322,-1.0698175993\H,-6.35
66085037,-0.2842033825,0.7504176387\\Version=AM64L-G03RevC.02\State=1-
A\HF=-888.9781111\RMSD=1.829e-09\RMSF=4.956e-06\Dipole=0.0023113,0.659

$2_{\text{H}}^{\text{Mo}}\cdot\text{XanH}^{\text{TS}}$

1\1\GINC-ORION-0-8\Freq\RmPW1PW91\Gen\C7H7Mo1N4O4S3(1-)\CBAYSE\27-Sep-
2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C
HKBAS FREQ\test\ -1,1\Mo,-2.106171509,-0.6520009828,-0.0578735149\S,-
3.6902341221,0.7237751966,1.1305435319\C,-4.2125750818,1.9255494046,-0
.0461962425\C,-3.5491697902,2.1331123014,-1.1995411673\S,-2.1298528683
,1.1827866961,-1.6318392488\H,-5.0712609752,2.5365842276,0.2315422757\
H,-3.851038489,2.9076420915,-1.9034037908\O,-2.962254285,-1.9800221351
, -0.6076964775\S,-1.0681809801,-1.0699517843,1.9315049968\O,-0.2255204
234,-0.9292746165,-0.7348516876\C,0.868200711,-0.8371422041,-0.0429050
89\N,2.0376646456,-1.4938212958,-0.4633234462\C,3.1322766704,-0.637670
47,-0.3418762958\C,2.6805566656,0.5131010659,0.2396816398\N,1.34624226
08,0.4511316519,0.3889751593\C,4.512602008,-0.8526036994,-0.5697088226
\N,3.5095993536,1.5266082639,0.6128526881\H,1.9699698861,-2.1958675452
, -1.1788459397\H,0.3037228617,-1.337678775,1.1869407262\N,5.2821962876
,0.277612324,-0.1818088803\C,4.8771029131,1.4534987407,0.3949778004\O,
5.0653729658,-1.8296567293,-1.0449877003\H,3.1664692014,2.3861411054,1
.0071151175\O,5.6275752717,2.3579209513,0.697852055\H,6.2745475553,0.1

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

962081598,-0.3396593915\H,0.7538102228,1.0357230719,0.9576610481\\Version=AM64L-G03RevC.02\State=1-A\HF=-889.5910578\RMSD=9.057e-09\RMSF=3.9

$2_{\text{H}}^{\text{Mo}}\cdot\text{Xan}_{\text{p}}$

1\1\GINC-ORION-0-29\Freq\RmpW1PW91\Gen\C7H6Mo1N4O4S3(2-)\CBAYSE\11-Sep-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CHKBAS FREQ\test\ -2,1\Mo,-1.8893478029,0.2686801923,0.2593598906\S,-4.2397145922,-0.1150580975,0.5031676307\C,-4.5468784758,-1.6425069254,-0.3412985228\C,-3.6132133079,-2.2265738989,-1.1182278312\S,-1.9991003057,-1.5224198541,-1.322223335\H,-5.5461782192,-2.0714807973,-0.2404277806\H,-3.8181292066,-3.1523092753,-1.6591067509\O,-1.1680421227,-0.2609094436,1.689927262\S,-2.4002786748,2.6382855309,0.2771753459\O,-0.1139926597,0.9193176469,-0.8094891893\C,1.0747989203,0.6058668222,-0.5833894484\N,1.4910730175,-0.1406852548,0.4890138904\C,2.8722262525,-0.2528396693,0.42189469\C,3.1925092626,0.4532232886,-0.731753757\N,2.1496811232,0.9769527695,-1.3539161041\H,0.8476197752,-0.4768730119,1.195718217\H,-1.2086738039,3.1198817814,-0.1752071974\C,3.8450570563,-0.8758481377,1.2159023904\O,3.7510301055,-1.5289513261,2.2521403046\N,4.5009016341,0.5658690604,-1.1499664455\H,4.7151483527,1.0744622783,-1.9899808163\C,5.53948692,0.0030592355,-0.4613143103\O,6.7095062408,0.0967728046,-0.8219969933\N,5.1548590367,-0.672056795,0.6662519966\H,5.9007820288,-1.0978505267,1.1907673609\\Version=AM64L-G03RevC.02\State=1-A\HF=-889.0311627\RMSD=1.420e-09\RMSF=2.361e-05\Dipole=1.8188131,-0.494118

$2_{\text{H}}^{\text{Mo}}\cdot\text{XanH}^{\text{p}}$

1\1\GINC-ORION-0-4\Freq\RmpW1PW91\Gen\C7H7Mo1N4O4S3(1-)\CBAYSE\05-Sep-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CHKBAS FREQ\test\ -1,1\Mo,-1.9015103749,0.2640373553,0.2485535263\S,-4.1352985551,-0.3159460793,0.6948045403\C,-4.4453043606,-1.7499447402,-0.3029140489\C,-3.5846856224,-2.1524901258,-1.2543758267\S,-2.0555889125,-1.2919057174,-1.5247863734\H,-5.3915871586,-2.2656428184,-0.1384138221\H,-3.782179358,-3.0168884395,-1.8873272045\O,-0.959623475,-0.3549447809,1.527746376\S,-2.5551779768,2.5700025507,0.4369492769\O,-0.1063598031,1.0753429572,-0.8541737215\C,1.0274533424,0.7127374743,-0.5644603719\N,1.4567647469,-0.038097493,0.472639448\C,2.8293709398,-0.2138859524,0.3878414622\C,3.252413676,0.4543060269,-0.7212513427\N,2.1715472309,1.0326278194,-1.3078129205\H,0.7517846395,-0.3953088955,1.143691971\H,-1.4009548438,3.1642586618,0.0227786032\C,3.7622688423,-0.8858504896,1.2363820032\O,3.5571162609,-1.4999114239,2.2583271458\N,4.555566251,0.5205228337,-1.1159185236\H,4.8534193286,1.0004382938,-1.9476140106\C,5.5488161445,-0.1126624272,-0.3853505266\O,6.7137392808,-0.0795224249,-0.7184114716\N,5.084015329,-0.7630518533,0.7310857219\H,5.7924953234,-1.2253373861,1.2805589722\H,2.1212741388,1.5495172341,-2.1674925158\\Version=AM64L-G03RevC.02\State=1-A\HF=-889.6184946\RMSD=3.525e-09\R

$2_{\text{H}}^{\text{Mo}}\cdot\text{Im}_{\text{R}}$

1\1\GINC-ORION-0-4\Freq\RmpW1PW91\Gen\C5H6Mo1N2O2S3(2-)\CBAYSE\17-Jul-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CHKBAS FREQ\test\ -2,1\Mo,0.8891142241,-0.6738273616,0.3567695433\S,3.0636955482,0.1643874452,-0.6812848024\C,3.074023934,1.9144090491,-0.5618526379\C,1.9892678356,2.6277455367,-0.1841895624\S,0.4752160966,1.8525875379,0.2293981086\H,3.9896379985,2.4217719746,-0.8765139048\H,2.0087110795,3.7201580131,-0.1762162156\O,1.3046829363,-0.8865619992,1.9884915801\S,1.4452835228,-2.5588159161,-0.7087103667\O,-0.8671436491,-0.6489235243,0.2658372852\H,-2.3037092532,-0.209804808,0.0487832109\C,-4

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

.4369204113, -0.6326650941, 0.0095837853\N, -5.5389576597, 0.056825886, -0.2294219968\C, -5.089103791, 1.3201258659, -0.5093643995\C, -3.719797379, 1.365273421, -0.432940565\N, -3.3200164983, 0.1083742114, -0.1004328168\H, -4.4029035228, -1.679758246, 0.2660215267\H, -5.7721411797, 2.1214114202, -0.7488146465\H, -3.0018315393, 2.1545765957, -0.5810947708\Version=AM64L-G03RevC.02\State=1-A\HF=-552.7334741\RMSD=4.982e-09\RMSF=1.067e-04\Dipo

$2_{\text{H}}^{\text{Mo}} \cdot \text{ImH}^+_{\text{R}}$

1\1\GINC-ORION-0-0\Freq\RmPW1PW91\Gen\C5H7Mo1N2O2S3(1-)\CBAYSE\07-Sep-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C HKBAS FREQ\test\ -1,1\Mo,1.2896211402, -0.8180969585, 0.2753489835\S, 0.7156415714, 0.6633909575, -1.5844214309\C, 1.1296986199, 2.3032878417, -1.1308281752\C, 1.4779670116, 2.6239115692, 0.1286894336\S, 1.6051731051, 1.3864608616, 1.3557441557\H, 1.0193089563, 3.0553652321, -1.910996876\H, 1.6752896352, 3.649297092, 0.4367080692\O, 2.7981519032, -1.378699549, -0.1831904642\S, -0.2198691202, -2.1581408883, -0.577711193\O, 1.1666048305, -1.2282285877, 2.1490662029\H, 0.920530897, -0.5691072589, 2.8007744715\C, -4.2049502046, -0.4681579351, -0.2566756011\N, -2.9392441998, -0.0070740134, -0.3662152169\C, -3.0004124023, 1.3560921849, -0.3339597293\C, -4.3292310825, 1.6540070796, -0.2060559365\N, -5.0780854356, 0.5072348039, -0.1587224087\H, -4.4346599414, -1.5214962138, -0.2531577057\H, -2.112869224, 1.9604795695, -0.4056767895\H, -4.788182537, 2.6277745213, -0.1449271738\H, -2.0938126501, -0.5701604613, -0.4446254775\Version=AM64L-G03RevC.02\State=1-A\HF=-553.3701311\RMSD=2.931e-09\RMSF=4.695e-06\Dipole=0.3284203, 1.0922426,

$2_{\text{H}}^{\text{Mo}} \cdot \text{ImTS}$

1\1\GINC-ORION-0-5\Freq\RmPW1PW91\Gen\C5H6Mo1N2O2S3(2-)\CBAYSE\19-Jun-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C HKBAS FREQ\test\ -2,1\Mo,0.4651106719, -0.2531190647, 0.2619468925\S, 2.7544201641, -1.0830152722, -0.217069136\C, 3.7833328236, 0.3467060053, -0.2007241171\C, 3.2830183464, 1.6016021408, -0.1849171257\S, 1.5539847858, 1.9322516189, -0.1706851452\H, 4.8614473258, 0.1776434413, -0.260456697\H, 3.9485105702, 2.467555697, -0.2205372834\O, 0.2528700638, -0.4627145086, 1.9295540942\S, -0.4118304304, -2.0304397042, -0.8044283706\O, -1.1055734528, 0.7121835829, -0.2843418433\C, -2.418583265, 0.0898163096, -0.4596289962\N, -3.0312509326, -0.1622346547, 0.7953880099\C, -4.276236565, 0.418440981, 0.8065343612\C, -4.4410464919, 0.9313529933, -0.4587912954\N, -3.3561812258, 0.7468411716, -1.2384270926\H, -4.9360529126, 0.3760732567, 1.6584149469\H, -5.3272265896, 1.4254930282, -0.839703546\H, -2.469259871, -0.4039520113, 1.5936506253\H, -2.0065159218, -0.9280677673, -0.9334764926\Version=AM64L-G03RevC.02\State=1-A\HF=-552.65431\RMSD=5.260e-09\RMSF=2.857e-06\Dipo

$2_{\text{H}}^{\text{Mo}} \cdot \text{ImH}^+_{\text{TS}}$

1\1\GINC-ORION-0-8\Freq\RmPW1PW91\Gen\C5H7Mo1N2O2S3(1-)\CBAYSE\14-Jan-2008\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C HKBAS FREQ\test\ -1,1\Mo,0.6507842306, -0.395433066, 0.4441566774\S, 2.4936763519, -0.8499522925, -1.0549239936\C, 3.4853286464, 0.6047255477, -1.0044038128\C, 3.0348855761, 1.7607074071, -0.4786715263\S, 1.4282950839, 1.8971913346, 0.2283013696\H, 4.4670686141, 0.5418516501, -1.4744112109\H, 3.6396412204, 2.6672220312, -0.4939205161\O, 1.0896797583, -1.0502236312, 1.9228183382\S, -0.6165975075, -1.8686795923, -0.7189642573\O, -1.1299379653, 0.4604105049, 0.7529869531\C, -2.2899809626, 0.176922077, 0.2008517971\N, -3.4559985558, 0.1529901608, 1.004787498\C, -4.5645438879, 0.4480362162, 0.2188638668\C, -4.123691878, 0.8776824952, -0.9745424951\N, -2.7372559481, 0.8698813703, -0.9585899027\H, -5.5679172598, 0.4102608681, 0.6062076234\H, -4

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

.6821610522,1.2662812206,-1.8086227538\H,-3.4876169397,-0.4915510506,1
.7740140412\H,-1.9798802801,-1.0621883727,-0.2364641071\H,-2.185192624
4,0.7693230628,-1.7944059014\\Version=AM64L-G03RevC.02\State=1-A\HF=-5
53.3169392\RMSD=5.346e-09\RMSF=7.562e-06\Dipole=-2.782113,0.6466103,-0

$2_{\text{H}}^{\text{Mo}} \cdot \text{Im}_p$

1\1\GINC-ORION-0-7\Freq\RmpW1PW91\Gen\C5H6Mo1N2O2S3(2-)\CBAYSE\19-Jun-
2007\0\#N GEOM=ALLCHECK GUESS=READ SCRf=CHECK TEST GENCHK RMPW1PW91/C
HKBAS FREQ\test\ -2,1\Mo,-0.5528296155,0.3933435035,0.2634046776\S,-2
.928732865,0.0074360501,0.1628639814\C,-3.1072980575,-1.7143051224,-0.
2158032548\C,-2.0535204483,-2.4787089496,-0.5697636995\S,-0.4090230567
, -1.8229955278,-0.6586297738\H,-4.1194479666,-2.1260345684,-0.19481287
74\H,-2.1777232464,-3.5315968879,-0.8333718655\O,-0.129018688,0.317423
5408,1.8955133782\S,-0.9975300417,2.6726413791,-0.4559101721\O,1.32934
01906,0.8081813406,-0.6649999126\C,2.4375027646,0.2334954836,-0.375412
5141\N,2.6015832692,-0.5295438921,0.7540854101\C,3.908291472,-0.968168
2736,0.7966348065\C,4.4843921328,-0.4336986162,-0.3196762825\N,3.59177
73828,0.3081519557,-1.0464875045\H,4.283794082,-1.6052664477,1.5801781
477\H,5.5084861673,-0.5520885416,-0.6477529215\H,1.8443853971,-0.70250
04322,1.3986165669\H,0.2716210631,2.9969666834,-0.8322054764\\Version=
AM64L-G03RevC.02\State=1-A\HF=-552.7210335\RMSD=4.197e-09\RMSF=1.135e-

$2_{\text{H}}^{\text{Mo}} \cdot \text{Im}_p^+$

1\1\GINC-ORION-0-2\Freq\RmpW1PW91\Gen\C5H7Mo1N2O2S3(1-)\CBAYSE\07-Sep-
2007\0\#N GEOM=ALLCHECK GUESS=READ SCRf=CHECK TEST GENCHK RMPW1PW91/C
HKBAS FREQ\test\ -1,1\Mo,-0.5602586275,0.3627565059,0.1914154517\S,-2
.8977593585,0.240524816,0.4705828075\C,-3.3210790138,-1.438803293,0.08
78889917\C,-2.4379772241,-2.282686269,-0.4758703588\S,-0.7742080824,-1
.768701847,-0.8205605071\H,-4.3491484469,-1.7433344681,0.2868604078\H,
-2.7026776521,-3.3059797978,-0.7412846434\O,0.1315791974,0.2196904556,
1.7424576763\S,-0.8581155765,2.6152066252,-0.5958101746\O,1.4030798933
,0.492183164,-0.8997293604\C,2.4345319606,0.049243982,-0.3813349093\N,
2.6187793515,-0.3774803895,0.8933499495\C,3.9194564634,-0.7931552807,1
.0766748459\C,4.5715388842,-0.627101281,-0.0909976939\N,3.6540866845,-
0.0993473024,-0.988439044\H,4.2713806624,-1.1736043176,2.0182528669\H,
5.5908580684,-0.8326261981,-0.3615631076\H,1.8181769545,-0.3310918399,
1.5410069304\H,0.3992062858,2.8512523029,-1.065229449\H,3.7982333602,0
.1049552995,-1.9592541082\\Version=AM64L-G03RevC.02\State=1-A\HF=-553.
3605506\RMSD=5.198e-09\RMSF=4.589e-06\Dipole=4.4291919,-1.2613571,-0.2

$2_{\text{CN}}^{\text{Mo}} \cdot \text{Im}_R$

1\1\GINC-ORION-0-29\Freq\RmpW1PW91\Gen\C7H4Mo1N4O2S3(2-)\CBAYSE\17-Jul-
2007\0\#N GEOM=ALLCHECK GUESS=READ SCRf=CHECK TEST GENCHK RMPW1PW91/
CHKBAS FREQ\test\ -2,1\Mo,0.0124358375,-1.1481557093,0.3705075426\S,2
.4194235579,-1.1719198055,-0.499989247\C,3.082731392,0.4326395049,-0.3
02516689\C,2.3010822233,1.5193531173,0.0326792709\S,0.5858303297,1.365
1592596,0.2924606439\O,0.1962903796,-1.4872766794,2.0192375386\S,-0.05
41850075,-3.0941146991,-0.6934950438\O,-1.5824125387,-0.4673051117,0.1
467903153\H,-2.9774115869,0.2715273568,-0.0355670908\C,-5.1276577617,0
.2001146963,-0.1567077431\N,-6.0942014963,1.0815316048,-0.3277102839\C
, -5.443281008,2.2808138803,-0.4431650173\C,-4.0881991381,2.0989868901,
-0.3396003589\N,-3.904109914,0.7624616144,-0.1566087266\H,-5.267221489
6,-0.8616794934,-0.0289905064\H,-5.9829977733,3.2032030318,-0.59384326
75\H,-3.2562363139,2.7814816182,-0.3784207971\C,2.8641779718,2.8284072
133,0.1224178077\N,3.2969918165,3.9132023035,0.2050859566\C,4.47617449

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

77,0.5939677348,-0.5705923835\N,5.6217864676,0.6932283773,-0.790971079
2\\Version=AM64L-G03RevC.02\State=1-A\HF=-737.2362212\RMSD=3.848e-09\R

2_{Me}^{MO}.Im_R

1\1\GINC-ORION-0-22\Freq\RmpW1PW91\Gen\C7H10Mo1N2O2S3(2-)\CBAYSE\17-Ju-
1-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91
/CHKBAS FREQ\test\ -2,1\Mo,-1.1331645426,0.3365544611,0.5270150684\S,
-0.2307268868,-0.7247325811,2.6322887097\C,1.5001633266,-0.3792893575,
2.7776627626\C,2.2022602488,0.1551727098,1.7475421412\S,1.3988843458,0
.5309489207,0.2227130157\O,-1.5241971335,1.9290853153,0.9649102025\S,-
2.919389931,-0.9185702263,1.0184623961\O,-1.0366634232,0.2691572256,-1
.2284903418\H,-0.3739753528,0.0202448952,-2.5843271492\C,-0.5186769903
, -0.2429291826,-4.7369473123\N,0.3341802355,-0.3947830427,-5.734843225
7\C,1.5640802523,-0.3697852869,-5.1304719866\C,1.4257288398,-0.2028926
802,-3.7753674759\N,0.0878711348,-0.1242870811,-3.5421890377\H,-1.5924
434828,-0.2153232662,-4.8372152727\H,2.4744419595,-0.4741364794,-5.701
8744431\H,2.13239903,-0.1321921156,-2.964784243\C,3.6846229841,0.43955
71835,1.7475007775\H,3.8734305229,1.5125406183,1.5995353464\H,4.179680
0054,0.1330171548,2.6763308353\H,4.1720923159,-0.0839050064,0.91220845
86\C,2.0804123643,-0.7893454717,4.1095673\H,1.6218329348,-0.2135871991
,4.9263452529\H,1.859536323,-1.8479070012,4.309009958\H,3.1666147945,-
0.651753724,4.1656621602\\Version=AM64L-G03RevC.02\State=1-A\HF=-631.3
55823\RMSD=8.136e-09\RMSF=7.639e-05\Dipole=2.6902402,0.2546197,0.75629

2_{Ph}^{MO}.Im_R

1\1\GINC-ORION-0-7\Freq\RmpW1PW91\Gen\C9H8Mo1N2O2S3(2-)\CBAYSE\09-Aug-
2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C
HKBAS FREQ\test\ -2,1\Mo,-0.035100982,-1.2824328164,0.2909276251\S,2.
2954139195,-1.0896286948,-0.6944458055\C,2.958862463,0.4959209973,-0.3
135708817\C,2.1287317433,1.5317874779,0.1895497674\S,0.4185440399,1.23
65388353,0.4420939951\O,0.225853447,-1.7751014608,1.8913599322\S,-0.07
81135458,-3.131019129,-0.9570509696\O,-1.6728791269,-0.6591972715,0.18
72850972\H,-2.9718774821,0.1555235003,0.0083122145\C,-5.1314920711,0.2
586597167,-0.1505505084\N,-6.0279085002,1.219374972,-0.2857088416\C,-5
.28471727,2.3694744813,-0.3247581016\C,-3.9493803949,2.0768811678,-0.2
121302532\N,-3.8697712712,0.7229113375,-0.1015068158\H,-5.3542582687,-
0.7946351002,-0.0856678994\H,-5.7501543503,3.3377006408,-0.4321808961\
H,-3.0645776057,2.6908239288,-0.2002407873\C,2.6948512411,2.7944827036
,0.442531419\H,2.0477439818,3.5813015755,0.8297885559\C,4.3184878964,0
.7727434107,-0.5454899627\H,4.9472440514,-0.0282573236,-0.9341861914\C
,4.8688331653,2.0307546492,-0.2863001378\H,5.9289226005,2.2089771712,-
0.4696508673\C,4.0490411847,3.0517825367,0.2127518398\H,4.458343792,4.
0399505551,0.4244603792\\Version=AM64L-G03RevC.02\State=1-A\HF=-706.38
00482\RMSD=6.399e-09\RMSF=3.538e-05\Dipole=1.3464773,2.1861673,0.27876

2_{CN}^{MO}.Im_{Ts}

1\1\GINC-ORION-0-4\Freq\RmpW1PW91\Gen\C7H4Mo1N4O2S3(2-)\CBAYSE\29-Jun-
2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C
HKBAS FREQ\test\ -2,1\Mo,-0.3005236304,-0.4571514031,0.3053395583\S,1
.8740370801,-1.5523632898,-0.188791144\C,3.0739453568,-0.2746083209,-0
.1302922925\C,2.7269729573,1.0588317792,-0.0812835489\S,1.0571410858,1
.5910481201,-0.0705636001\O,-0.5398172734,-0.678206817,1.9634849813\S,
-1.3404416999,-2.0997718219,-0.8095893777\O,-1.7035026989,0.7093589501
, -0.2221036679\C,-3.1159334414,0.2599304461,-0.4918879411\N,-3.8044897
027,0.0875974469,0.7292479304\C,-4.9274642005,0.8727598117,0.718171999

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

2\C, -4.9564359708, 1.4351455072, -0.5368918043\N, -3.8938462399, 1.0736586555, -1.2840097749\H, -5.6024847513, 0.94110568, 1.5555991635\H, -5.7247515026, 2.0874657691, -0.9320918696\H, -3.3438993206, -0.2960013859, 1.5363232147\H, -2.8072842023, -0.7705888698, -0.9675629396\C, 3.7315083736, 2.0728004402, -0.0810197368\N, 4.5306308661, 2.9287816228, -0.0762009504\C, 4.4445643318, -0.6688751314, -0.1909237532\N, 5.5580256676, -1.0285169615, -0.2375673636\\Version=AM64L-G03RevC.02\State=1-A\HF=-737.1583107\RMSD=1.299

2_{Me}^{MO}·Im_{TS}

1\1\GINC-ORION-0-29\Freq\RmpW1PW91\Gen\C7H10Mo1N2O2S3(2-)\CBAYSE\05-Jun-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CHKBAS FREQ\test\ -2,1\Mo, -0.0270779184, -0.3962116206, 0.2919787816\S, 2.1799166356, -1.394444436, -0.1717151424\C, 3.3701781982, -0.0759730056, -0.1275409798\C, 2.977918239, 1.2214174761, -0.1214629565\S, 1.2578780798, 1.6601104888, -0.147492497\O, -0.2800802576, -0.5767586881, 1.9576549072\S, -1.0376965425, -2.0970542681, -0.7822544925\O, -1.4964407137, 0.701832988, -0.2850395568\C, -2.857643888, 0.1975885362, -0.4852050172\N, -3.516422934, 0.0128017926, 0.7585993251\C, -4.7010711111, 0.7085242551, 0.7410505824\C, -4.7925570528, 1.223855356, -0.530582173\N, -3.715128382, 0.9317167975, -1.2872033679\H, -5.378149762, 0.7356513845, 1.5799214866\H, -5.6210575905, 1.7954534437, -0.9323652265\H, -2.9943326303, -0.2684383715, 1.5708710357\H, -2.5301292235, -0.8544805011, -0.9452174548\C, 3.9011629954, 2.4150118534, -0.1240964311\H, 3.765493435, 3.011451966, 0.7899318818\H, 4.9602910101, 2.1400662839, -0.1956974586\H, 3.6618362663, 3.0771176603, -0.9686985727\C, 4.8001617493, -0.5565925273, -0.1461987722\H, 5.0266716837, -1.1362492469, 0.7607196967\H, 4.9608706308, -1.2328776709, -0.9983380579\H, 5.5283401903, 0.2601883697, -0.2173220664\\Version=AM64L-G03RevC.02\State=1-A\HF=-631.2768465\RMSD=7.221e-09\RMSF=3.566e-06\Dipole=1.7274762, 0.6425337, 1.

2_{Ph}^{MO}·Im_{TS}

1\1\GINC-ORION-0-6\Freq\RmpW1PW91\Gen\C9H8Mo1N2O2S3(2-)\CBAYSE\30-Jun-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CHKBAS FREQ\test\ -2,1\Mo, 0.3845641367, 0.4557267698, 0.2920240186\S, -1.75336059, 1.6032681952, -0.185863246\C, -3.023978978, 0.3797549232, -0.1171285141\C, -2.6998837517, -1.001116745, -0.1007562587\S, -1.0188979495, -1.5340437073, -0.1397872262\O, 0.6415094932, 0.6318743539, 1.9549981379\S, 1.4917779267, 2.0866707022, -0.786579538\O, 1.7748481224, -0.7372967125, -0.2663894617\C, 3.1764664594, -0.3217764387, -0.4832809784\N, 3.84914349, -0.1782615258, 0.7564352802\C, 4.9722124401, -0.9677980646, 0.7448608726\C, 5.020869588, -1.4997614053, -0.522406606\N, 3.9706751306, -1.1247487058, -1.2805012896\H, 5.6417813052, -1.0472152207, 1.5861936589\H, 5.7985069728, -2.1410379822, -0.9196845795\H, 3.3578552144, 0.1585695587, 1.5666516117\H, 2.9139081443, 0.7378108924, -0.9479123539\C, -3.7445917278, -1.9423373457, -0.0854195236\H, -3.4828759973, -3.000512983, -0.0749321875\C, -4.3785918059, 0.7570606488, -0.1213062482\H, -4.6154544811, 1.8210594434, -0.138644656\C, -5.4070090845, -0.1889852671, -0.1011366396\H, -6.4473818634, 0.1380103258, -0.0981870346\C, -5.0867125979, -1.5530906475, -0.0829005533\H, -5.8726177515, -2.3087788665, -0.0663737266\\Version=AM64L-G03RevC.02\State=1-A\HF=-706.3015513\RMSD=4.182e-09\RMSF=3.361e-06\Dipole=-1.5762195, -0.4832

2_{CN}^{MO}·Im_P

1\1\GINC-ORION-0-9\Freq\RmpW1PW91\Gen\C7H4Mo1N4O2S3(2-)\CBAYSE\23-Jun-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CHKBAS FREQ\test\ -2,1\Mo, -0.2817825626, -0.8585469912, 0.2468655288\S, 2.0527526627, -1.389290421, 0.1678192827\C, 2.8863379719, 0.1645002108, 0.00

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

99303301\C,2.1955880799,1.3268845531,-0.2338385789\S,0.430575593,1.343
4614309,-0.3796406078\O,-0.6930825341,-0.8320896951,1.8775933325\S,-0.
6863533344,-3.0229799895,-0.7481753122\O,-2.120644811,-0.4520327781,-0.
.7070360771\C,-2.9389964561,0.485825282,-0.3758185255\N,-2.8805176212,
1.1214543855,0.8388372498\C,-3.9171231314,2.0288549835,0.899799411\C,-
4.5625541996,1.8914076908,-0.2940340129\N,-3.9689957103,0.9428275246,-
1.0845616241\H,-4.0749979306,2.6745861004,1.7471242694\H,-5.4296721171
,2.4385680165,-0.6364337809\H,-2.1819531858,0.9084038026,1.5339609095\
H,-1.9611653617,-2.7803255895,-1.1608113375\C,2.8746343541,2.568557794
1,-0.3982135887\N,3.3972336544,3.6074624356,-0.5387206708\C,4.30866268
8,0.157994793,0.1039677268\N,5.475362592,0.1064717858,0.194807804\Ver
sion=AM64L-G03RevC.02\State=1-A\HF=-737.2269684\RMSD=7.446e-09\RMSF=1.

$2_{Me}^{Mo} \cdot Im_p$

1\1\GINC-ORION-0-3\Freq\RmpW1PW91\Gen\C7H10Mo1N2O2S3(2-)\CBAYSE\07-Jul
-2007\0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/
CHKBAS FREQ\test\ -2,1\Mo,-0.025375073,0.7495813899,0.2453322184\S,-2
.4015569596,1.007325993,0.191508669\C,-3.1011400461,-0.6279281918,-0.0
056656738\C,-2.3079120273,-1.6831770269,-0.2966008911\S,-0.538749698,-
1.4717542957,-0.4644499442\O,0.4265859917,0.7002240922,1.8722758934\S,
0.146983508,2.9938465886,-0.6785614162\O,1.8642246564,0.5488506325,-0.
7428284175\C,2.7878915069,-0.2691928477,-0.395924013\N,2.7864987143,-0
.9135604417,0.8164328539\C,3.9292372201,-1.6804808503,0.9024324189\C,4
.5810738989,-1.4557283367,-0.2759367774\N,3.8911104624,-0.5887572944,-
1.0808158763\H,4.1508427784,-2.3026479834,1.7537262524\H,5.5211866334,
-1.8850884615,-0.5957252654\H,2.0414268516,-0.7911992668,1.4869078395\
H,1.4408091303,2.9167268938,-1.0993976478\C,-4.5994813939,-0.671165014
9,0.1475088057\H,-4.8916855103,-0.3878932168,1.1697312468\H,-5.0702712
656,0.0598709999,-0.5256698678\H,-5.0277727634,-1.6582548801,-0.067259
006\C,-2.7671689431,-3.1011229898,-0.5174190301\H,-3.8579868692,-3.210
9040882,-0.4759986161\H,-2.4237107005,-3.464643172,-1.4970217573\H,-2.
3286655396,-3.7726798722,0.2355290242\Version=AM64L-G03RevC.02\State=
1-A\HF=-631.3443196\RMSD=5.311e-09\RMSF=5.242e-06\Dipole=-1.3998754,-2

$2_{Ph}^{Mo} \cdot Im_p$

1\1\GINC-ORION-0-28\Freq\RmpW1PW91\Gen\C9H8Mo1N2O2S3(2-)\CBAYSE\24-Jun
-2007\0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/
CHKBAS FREQ\test\ -2,1\Mo,0.4115814234,0.8513295656,0.2564087653\S,-1
.8790311148,1.5515375357,0.2017198984\C,-2.8599205357,0.0809102192,0.0
279205993\C,-2.2416805965,-1.1557552622,-0.271119472\S,-0.4770407478,-
1.2563024138,-0.4530137051\O,0.8416786675,0.7271121788,1.8814625799\S,
0.9798235905,3.0241707823,-0.6630437899\O,2.2294201407,0.3254512263,-0
.7254424761\C,2.9847801686,-0.6592674357,-0.3974445618\N,2.8675380616,
-1.3118768639,0.804411953\C,3.8453631545,-2.2822783927,0.8678099602\C,
4.5218768453,-2.1631219979,-0.3115089905\N,4.0031089739,-1.1674438019,
-1.0959976959\H,3.9499022244,-2.9492686325,1.7072936732\H,5.3623487156
, -2.7558412393,-0.646341466\H,2.1621646869,-1.0677027825,1.4836284337\
H,2.2360004314,2.7132907098,-1.0888822835\C,-3.0428591748,-2.296937221
1,-0.4361845904\H,-2.5525208641,-3.2425495025,-0.6701921661\C,-4.25872
11785,0.1275956964,0.1478004208\H,-4.7247850971,1.0878106734,0.3727330
318\C,-4.4342766241,-2.2400155415,-0.3079532366\H,-5.030914986,-3.1434
519116,-0.4388073999\C,-5.0479613966,-1.0153412008,-0.0124962505\H,-6.
1315662243,-0.948619301,0.0927976782\Version=AM64L-G03RevC.02\State=1
-A\HF=-706.3694209\RMSD=3.935e-09\RMSF=1.781e-05\Dipole=-1.6498783,-1.

$2_{\text{H}}^{\text{Mo}}\cdot 1\text{-MeXan}_{\text{R}}$

1\1\GINC-ORION-0-0\Freq\RmpW1PW91\Gen\C8H8Mo1N4O4S3(2-)\CBAYSE\22-Jun-2008\0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C HKBAS FREQ\test\ -2,1\Mo,2.5266545271,-0.2905453441,-0.8466704605\S,4.6152894995,0.5381635923,0.2166194737\C,4.6576815094,-0.0767572896,1.8562728581\C,3.5840560712,-0.660798982,2.4265520847\S,2.0930790021,-0.8892775299,1.5416319967\O,3.0969580682,-1.7026640676,-1.564128223\S,2.9015751008,1.3635867521,-2.250239305\O,0.6865245574,-0.449260986,-0.8611640614\H,5.5719414678,0.1119706829,2.4216807568\H,3.5890002798,-0.9718475839,3.4722431804\H,-0.1615174904,-0.2605521921,-0.3521150946\C,-1.4347114241,0.6767992256,1.7145844881\N,-2.5717878431,1.0679486881,2.3547646205\C,-3.502915375,0.7199289822,1.4713572813\C,-2.9491857809,0.141948064,0.3358398536\N,-1.5854080303,0.12141995,0.5219628941\N,-4.8643797344,0.8847810159,1.6110530014\C,-3.7788729696,-0.3333329291,-0.7156728611\N,-5.1844735331,-0.1006558327,-0.4593397632\C,-5.7510352528,0.4851736121,0.6591329933\O,-3.4812866558,-0.8866696495,-1.7600538279\O,-6.9643529877,0.6420035364,0.8036747302\H,-0.4569447181,0.8003018199,2.1577816158\H,-5.2461864476,1.3116868356,2.4365334032\C,-6.0802256017,-0.555597447,-1.504961845\H,-7.098445633,-0.3036213044,-1.2098308687\H,-5.8248745953,-0.0735432062,-2.4536460669\H,-5.9807075685,-1.6369624653,-1.645025562\Version=AM64L-G03RevC.02\State=1-A\HF=-928.3170667\RMS

$2_{\text{H}}^{\text{Mo}}\cdot 3\text{-MeXan}_{\text{R}}$

1\1\GINC-ORION-0-6\Freq\RmpW1PW91\Gen\C8H8Mo1N4O4S3(2-)\CBAYSE\13-Jun-2008\0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C HKBAS FREQ\test\ -2,1\Mo,2.623279871,0.005289554,-0.69742349\S,4.3489968891,0.6409645688,0.978190413\C,4.3554222122,-0.590312609,2.2242585696\C,3.3810041909,-1.5194629722,2.3083273596\S,2.0762998751,-1.5824975507,1.1459639346\O,3.5690196238,-0.8579351741,-1.7899410875\S,2.7300651772,2.1358222825,-1.2363894708\O,0.8772331443,-0.4469818781,-1.1300832827\H,5.140955296,-0.5161216596,2.9782990786\H,3.3439488857,-2.2361209799,3.1301581784\H,-0.0495053627,-0.3186009448,-0.7661993475\C,-1.6487811538,1.3181354515,0.4330533586\N,-2.8682542246,1.7532562672,0.8519449874\C,-3.6662272003,0.7818391096,0.4139374308\C,-2.9414994407,-0.2095705151,-0.250075124\N,-1.621530261,0.1685702351,-0.2218522553\N,-5.0431560877,0.7470421199,0.5886647051\C,-3.6089380212,-1.333435249,-0.8098646491\N,-5.012485839,-1.2525264546,-0.5616304963\C,-5.7625199755,-0.3022673684,0.0906075484\O,-3.196357037,-2.2976227312,-1.4332680693\O,-6.9840580258,-0.4119391925,0.2016038267\C,-5.6979063368,1.8218615543,1.2965443718\H,-0.7483068934,1.8845262889,0.6235956032\H,-5.5464030906,-2.0228755278,-0.9289220574\H,-6.7662789255,1.6041942021,1.324453483\H,-5.5138789397,2.7736057231,0.7867836495\H,-5.296119019,1.9013150423,2.3122670848\Version=AM64L-G03RevC.02\State=1-A\HF=-928.3197554\RMSD=4

$2_{\text{H}}^{\text{Mo}}\cdot 7\text{-MeXan}_{\text{R}}$

1\1\GINC-ORION-0-7\Freq\RmpW1PW91\Gen\C8H8Mo1N4O4S3(2-)\CBAYSE\14-Jun-2008\0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C HKBAS FREQ\test\ -2,1\Mo,-0.2329103821,-0.6568829612,2.5882913895\S,0.9540389532,0.3238643642,4.5401243481\C,0.6622882292,2.0510487563,4.5271428125\C,0.1064429955,2.6721273724,3.4668141079\S,-0.4086251079,1.7791449148,2.0541477693\O,-1.7010836427,-1.0631191495,3.3048948175\S,1.1548706457,-2.332330353,2.9255440826\O,-0.5464216612,-0.7263306038,0.7695761677\H,1.0300859946,2.6116818628,5.3883017436\H,-0.002092933,3.7570949211,3.4304769914\H,-0.3356065516,-0.3067137686,-0.1213141634\C,0.8632162667,1.4823447319,-1.5809569231\N,1.2704368817,1.9841317893,-2.78

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

01727355\C,0.6874378451,1.1419496025,-3.6283550506\C,-0.0437257131,0.1
636249298,-2.9663267044\N,0.0847328317,0.4117822568,-1.6184280205\N,0.
7612760952,1.1858145275,-5.0041840975\C,-0.7739171463,-0.8147653502,-3
.6940187842\N,-0.6157169363,-0.6714126199,-5.1257323829\C,0.1188489717
,0.2881986006,-5.8001499269\O,-1.4851408623,-1.7201809147,-3.294147541
8\O,0.1980735259,0.3450371212,-7.0281862108\H,1.1482716314,1.937681302
9,-0.6433526095\H,1.3009482156,1.8968111166,-5.4653585848\C,-1.3303313
88,-1.6509589949,-5.9210459606\H,-1.1139665302,-1.4554070861,-6.970958
0737\H,-1.0133292137,-2.6614321254,-5.6452659267\H,-2.4067077655,-1.57
83758621,-5.7339255668\\Version=AM64L-G03RevC.02\State=1-A\HF=-928.317
068\RMSD=4.578e-09\RMSF=1.790e-05\Dipole=-0.1117009,1.1641401,-1.35715

2_{H}^{Mo} -1-MeXan_{TS}

1\1\GINC-ORION-0-23\Freq\RmpW1PW91\Gen\C8H8Mo1N4O4S3(2-)\CBAYSE\22-Jun
-2008\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/
CHKBAS FREQ\test - if no imag freq freeze 1, 7, 8, 28 and 9 for opt\\
-2,1\Mo,-2.2132187175,-0.42161385,-0.1396891981\S,-4.4145502262,-0.409
5696304,0.9451768598\C,-5.3568372607,0.7926337017,0.0681767419\C,-4.79
13072813,1.663400928,-0.7939687973\S,-3.0651144072,1.669826042,-1.1311
381488\O,-2.2871458565,-1.6493812194,-1.2865348619\S,-1.3040992645,-1.
2629118475,1.7300747908\O,-0.4774585424,0.4411162399,-0.360889758\C,0.
7147355151,0.1157451092,0.2232110442\N,1.5641354614,-0.7455203686,-0.5
465092887\C,2.8788089679,-0.3857946489,-0.2721656417\C,2.7519129991,0.
8038654584,0.4490303471\N,1.5280207648,1.1668250793,0.7196819302\C,4.1
004317069,-0.9070608343,-0.6826490173\N,3.8894077498,1.49575612,0.8009
772614\N,5.2277348701,-0.109401111,-0.2092110716\C,5.1531087183,1.0582
458382,0.5056989698\O,4.3308266872,-1.9234479112,-1.3507531621\O,6.150
2909734,1.6844942697,0.8660745973\H,-6.4231323639,0.8420943602,0.29761
82866\H,-5.3892249101,2.4297107117,-1.2906515447\H,0.2643160107,-0.530
8638013,1.1873382635\H,3.813161503,2.3421516076,1.3375710574\H,1.28773
01241,-1.6988350669,-0.7057584399\C,6.5600887809,-0.5767117684,-0.5223
632239\H,7.1312289607,-0.7671325183,0.3938123558\H,6.4428887523,-1.497
8682314,-1.0948579779\H,7.1055895318,0.1691998391,-1.1115105875\\Versi
on=AM64L-G03RevC.02\State=1-A\HF=-928.2755434\RMSD=7.300e-09\RMSF=1.17

2_{H}^{Mo} -3-MeXan_{TS}

1\1\GINC-ORION-0-9\Freq\RmpW1PW91\Gen\C8H8Mo1N4O4S3(2-)\CBAYSE\13-Jun-
2008\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C
HKBAS FREQ\test - if no imag freq freeze 1, 7, 8, 28 and 9 for opt\\-
2,1\Mo,-2.1432602245,-0.4810746382,-0.0300681914\S,-4.319300396,0.0474
749445,0.967508132\C,-5.1235818749,1.0868101875,-0.2063990113\C,-4.468
0337556,1.6431407314,-1.2467259495\S,-2.7534966942,1.3713306288,-1.534
9043607\O,-2.3588096657,-1.9455802615,-0.8302034143\S,-1.2993713648,-0
.8920353933,2.0138151654\O,-0.3119595398,0.0780179225,-0.427291168\C,0
.8391399576,-0.1716934689,0.2697252281\N,1.6357597859,-1.2364024304,-0
.2340281582\C,2.9468731093,-0.8007509087,-0.3239531057\C,2.9040349237,
0.492462926,0.2142501221\N,1.71047265,0.9056787746,0.5550943576\C,4.13
87885719,-1.4253261732,-0.6802566593\N,4.060099728,1.2422260337,0.3727
455879\N,5.2484836982,-0.53858056,-0.4959889158\C,5.2841324517,0.73074
03576,0.0112537655\O,4.3675291422,-2.5561930189,-1.1303563569\C,3.9517
460533,2.5747480208,0.9245551416\O,6.3389631202,1.3551207144,0.1292598
341\H,-6.1763875917,1.3108223839,-0.0227877343\H,-4.9784511874,2.31995
98605,-1.9344523621\H,1.2316488279,-1.955742976,-0.8055411558\H,6.1433
676433,-0.9203176351,-0.751492845\H,4.9539016664,3.0020174649,0.967837
1036\H,3.5068942334,2.529513758,1.9237979523\H,3.2974099027,3.18648176

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

09,0.2953851711\H,0.2851491025,-0.5380883052,1.3566864721\\Version=AM6
4L-G03RevC.02\State=1-A\HF=-928.2774143\RMSD=1.134e-09\RMSF=3.217e-06\

2_{H}^{Mo} -7-MeXan_{TS}

1\1\GINC-ORION-0-0\Freq\RmpW1PW91\Gen\C8H8Mo1N4O4S3(2-)\CBAYSE\12-Jun-
2008\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C
HKBAS FREQ\test - if no imag freq freeze 1, 7, 8, 23 and 9 for opt\\-
2,1\Mo,-2.0308431987,-0.3919078054,-0.0790235496\S,-4.1819430223,-0.08
80006228,1.0553122994\C,-5.0764370012,1.052993716,0.0548309956\C,-4.48
65379691,1.7660013672,-0.9276442018\S,-2.7765467266,1.6110757591,-1.30
82989751\O,-2.2350771253,-1.7444971183,-1.060366973\S,-1.1056839769,-1
.0411309926,1.858390528\O,-0.2496678613,0.3105017595,-0.4743160494\C,0
.9365893545,0.0855610545,0.1683446223\N,1.8187326362,-0.8455953482,-0.
4671347222\C,3.1171199407,-0.4119354467,-0.2273231857\C,2.9461023023,0
.8547552028,0.3514450377\N,1.7104035192,1.2090440054,0.5569130225\C,4.
3714745781,-0.8963009878,-0.6010875901\N,4.0505814954,1.6332159646,0.6
462406109\N,5.4205010379,-0.0035430838,-0.1876012601\C,5.3327765237,1.
225829817,0.4004905403\O,4.7087989877,-1.9345621644,-1.1870174669\O,6.
3151879064,1.909278211,0.6846191369\H,-6.1283016434,1.2050321554,0.304
9669439\H,-5.0508595986,2.5024280345,-1.5027689865\H,6.3513688965,-0.3
232846115,-0.3952822813\H,0.482700894,-0.4561761536,1.1956268743\H,3.9
20154935,2.5315597421,1.0778870544\C,1.433231646,-2.2206977858,-0.6413
340787\H,0.4595042682,-2.2590570489,-1.1365262269\H,2.1865034767,-2.72
82437242,-1.2487796749\H,1.3397403968,-2.7380947561,0.3287981644\\Vers
ion=AM64L-G03RevC.02\State=1-A\HF=-928.2801039\RMSD=1.225e-09\RMSF=7.5

2_{H}^{W} -Xan_R

1\1\GINC-ORION-0-29\Freq\RmpW1PW91\Gen\C7H6N4O4S3W1(2-)\CBAYSE\01-Sep-
2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C
HKBAS FREQ\test\\-2,1\W,-2.0304487269,-0.2325224327,-0.4978833185\S,-
3.8527910454,-0.1063553052,1.1892337786\C,-3.9202882372,1.5450459503,1
.7710199007\C,-2.9406294045,2.4322984505,1.5012365972\S,-1.5619890635,
2.001712848,0.5136621928\H,-4.7539173715,1.7983439678,2.4276906318\H,-
2.948562765,3.4378191047,1.9236188644\O,-2.9188219138,0.0550837797,-1.
9181389049\S,-2.0936128251,-2.4029360461,-0.0781948817\O,-0.2720813737
,0.0182010452,-1.0182307951\H,0.6641586989,-0.0298590541,-0.6465155205
\C,2.1893099004,-1.3111559063,0.9521437219\N,3.3974963402,-1.620247462
1,1.4986739562\C,4.2062863865,-0.7971168573,0.8397629213\C,3.507705356
4,-0.0128397843,-0.0772778328\N,2.1841675087,-0.3726955561,0.018176003
5\H,1.2805293448,-1.8084302173,1.2603729216\N,5.5756666163,-0.69926930
88,1.0121290817\C,4.1974841387,0.922349985,-0.8997802635\N,5.600689607
,0.9184605099,-0.6106942832\C,6.32693438,0.1724698862,0.286084729\O,3.
8027019067,1.6836189971,-1.7661981537\O,7.5445365759,0.2867151231,0.41
36826469\H,6.1407468704,1.5666906872,-1.1599096415\H,6.0469007693,-1.2
756475986,1.6868405859\\Version=AM64L-G03RevC.02\State=1-A\HF=-888.807
5968\RMSD=3.738e-09\RMSF=5.307e-06\Dipole=-0.8057289,0.5248314,0.57576

2_{H}^{W} -XanH_R⁺

1\1\GINC-ORION-0-0\Freq\RmpW1PW91\Gen\C7H7N4O4S3W1(1-)\CBAYSE\18-Sep-2
007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C
HKBAS FREQ\test\\-1,1\W,1.7515927387,-0.2613496962,-0.4793597435\S,3.1
352855159,1.6719628806,-0.0111842582\C,4.2033674488,1.2354861159,1.306
9471522\C,3.9947661423,0.1394336298,2.0584620356\S,2.6481858156,-0.926
4495409,1.7226039641\H,4.9987856156,1.9436437194,1.5318088226\H,4.6121
389853,-0.1018381588,2.9210742658\O,2.6669890291,-1.0250761767,-1.6757

438138\S,0.2833842425,1.0479319479,-1.4346798561\O,0.479000799,-1.6375
000283,0.1328128217\H,0.7507557077,-2.2502968103,0.820708244\C,-3.0621
246856,-2.4887928219,-0.0186937207\N,-2.2465795242,-1.3814818153,-0.02
25795586\C,-3.0722270627,-0.3251817592,0.1201186593\C,-4.3541870347,-0
.8306698648,0.2037577019\N,-4.3229991919,-2.2011626821,0.1122670486\H,
-2.6518714732,-3.4802008083,-0.1249923429\N,-2.7476562072,0.9972839813
,0.1906689318\C,-5.463613665,0.0677929242,0.3742681332\N,-5.0182301616
,1.4068570661,0.4338432337\C,-3.7448588069,1.9388463111,0.3225758234\O
, -6.6474569556,-0.1778412374,0.469378063\O,-3.53482747,3.1326576165,0.
3493740391\H,-5.7464645933,2.0959099939,0.5398904926\H,-1.8078870145,1
.3254826982,-0.0166312032\H,-1.2111307179,-1.3978321709,-0.0376560337\
\Version=AM64L-G03RevC.02\State=1-A\HF=-889.4294419\RMSD=2.536e-09\RMS

$2_{\text{H}}^{\text{W}}\text{-Xan}_{\text{p}}$

1\1\GINC-ORION-0-2\Freq\RmpW1PW91\Gen\C7H6N4O4S3W1(2-)\CBAYSE\16-Sep-2
007\0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CH
KBAS FREQ\test\ -2,1\W,-1.620947983,0.166906527,0.1770732008\S,-3.964
6601981,0.0058495997,0.5356378724\C,-4.4705113734,-1.5047649394,-0.259
4536442\C,-3.6331265713,-2.189416158,-1.0611042775\S,-1.9615410045,-1.
6420589962,-1.3334705435\H,-5.502158493,-1.8258245433,-0.1032543179\H,
-3.9410111184,-3.1018306745,-1.574137086\O,-0.8787118791,-0.3943178361
,1.6080241902\S,-1.8626908422,2.5613734841,0.1737937038\O,0.1371478154
,0.6150111164,-0.9766195096\C,1.3396937674,0.4133929005,-0.6911440274\
N,1.7735014242,-0.1371867004,0.4861108598\C,3.1606321236,-0.1737331947
,0.4516378781\C,3.4617545007,0.3510424524,-0.8003091907\N,2.4030291485
,0.7157110494,-1.5039328315\H,1.1310053419,-0.3985971177,1.2271420666\
H,-0.6684505934,2.9476764019,-0.3703284827\C,4.1491628857,-0.659520546
,1.3186299784\O,4.0722206533,-1.1792315283,2.429330387\N,4.7686639842,
0.4613495576,-1.2243868726\H,4.9696753626,0.847422705,-2.1303072222\C,
5.8231213105,0.0503365937,-0.4567397849\O,6.9918034711,0.1436769646,-0
.822085733\N,5.4556888775,-0.4737507208,0.7534125277\H,6.213138577,-0.
7905498514,1.3353696068\Version=AM64L-G03RevC.02\State=1-A\HF=-888.78
39644\RMSD=4.857e-09\RMSF=9.259e-06\Dipole=0.6952226,-0.3303786,-0.575

$2_{\text{H}}^{\text{W}}\text{-XanH}_{\text{p}}^{+}$

1\1\GINC-ORION-0-0\Freq\RmpW1PW91\Gen\C7H7N4O4S3W1(1-)\CBAYSE\07-Sep-2
007\0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CH
KBAS FREQ\test\ -1,1\W,-1.6345143733,0.1734263115,0.1863308992\S,-3.8
702956087,-0.2994254028,0.701879429\C,-4.3130374352,-1.6921398704,-0.3
17123861\C,-3.5118104947,-2.1177739395,-1.3073873524\S,-1.9351252006,-
1.338179243,-1.5961496856\H,-5.2836973344,-2.1496625856,-0.1275272962\
H,-3.7731948857,-2.952305256,-1.9563679616\O,-0.6799690983,-0.52231352
81,1.4395961544\S,-2.1067550656,2.5030628893,0.4580490058\O,0.13529415
22,0.9113124534,-0.9273345612\C,1.2847539265,0.6081678306,-0.617337187
2\N,1.7288918395,-0.1138564992,0.4328813445\C,3.1100688222,-0.22649158
34,0.3685360937\C,3.5169134413,0.4474976515,-0.7441097635\N,2.41934283
41,0.9677925036,-1.3527614462\H,1.0229702081,-0.4868716582,1.099017113
\H,-0.9691383808,3.0739646723,-0.0424600179\C,4.0614840431,-0.84704374
6,1.2345492001\O,3.8725337212,-1.4638777889,2.2584858675\N,4.821058859
8,0.5729948239,-1.1210754883\H,5.1075661677,1.0560259324,-1.9549253151
\C,5.8329899964,-0.0047753338,-0.3700748969\O,6.9995003659,0.080606995
2,-0.6886380616\N,5.3839199435,-0.665296117,0.7461097605\H,6.105374440
2,-1.0886527243,1.3098215393\H,2.3594561468,1.484708584,-2.211772376\
\Version=AM64L-G03RevC.02\State=1-A\HF=-889.3706068\RMSD=4.471e-09\RMSF

$2_{\text{H}}^{\text{W}} \cdot \text{Xan}_{\text{TS}}$

1\1\GINC-ORION-0-9\Freq\RmpW1PW91\Gen\C7H6N4O4S3W1(2-)\CBAYSE\24-Dec-2007\0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CHKBAS FREQ\test\ -2,1\W, -1.6952796662, -0.2075470186, -0.2363115267\S, -3.8745514601, -0.3268267812, 0.837211046\C, -4.7782062938, 1.06107971, 0.2223233053\C, -4.1821951488, 2.0548849481, -0.4676018704\S, -2.4565253523, 2.0468610269, -0.829877247\H, -5.8400991571, 1.1047458416, 0.4706751649\H, -4.7473786721, 2.9241668239, -0.8072623927\O, -1.7937184967, -1.2069496193, -1.6068456824\S, -0.7602347682, -1.4264514903, 1.4380347542\O, 0.0974243702, 0.5942922862, -0.2660326952\C, 1.2714350257, 0.1251173949, 0.1851316187\N, 2.0480727379, -0.6615139104, -0.7096259488\C, 3.378341952, -0.5278534301, -0.3167805955\C, 3.3411179155, 0.5153816768, 0.6131521192\N, 2.1440774601, 0.9637194256, 0.8947442625\C, 4.5720999779, -1.0803198194, -0.7774736811\N, 4.5159772116, 1.0014868832, 1.1543316448\H, 1.6688141851, -1.5265580096, -1.0561602626\H, 0.696581562, -0.7552842536, 1.0978389054\N, 5.704466319, -0.5079348428, -0.0976647418\C, 5.7446605087, 0.491860457, 0.8316037229\O, 4.7942368773, -1.9572982425, -1.6210745209\H, 4.4800371508, 1.731677653, 1.8439942699\O, 6.7880084268, 0.9037031952, 1.3357262126\H, 6.5944363766, -0.8987822371, -0.3567403031\Version=AM64L-G03RevC.02\State=1-A\HF=-888.7488818\RMSD=1.701e-09\RMSF=5.468e-06\Dipole=-1.0851503, 0.5388733, 0.116880

$2_{\text{H}}^{\text{W}} \cdot \text{XanH}^+_{\text{TS}}$

1\1\GINC-ORION-0-9\Freq\RmpW1PW91\Gen\C7H7N4O4S3W1(1-)\CBAYSE\15-Sep-2007\0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CHKBAS FREQ\test\ -1,1\W, -1.8314606503, -0.5147549873, -0.0307700862\S, -3.3827538862, 0.9152886662, 1.1137230574\C, -3.8672074099, 2.1153267352, -0.0865392286\C, -3.1970373268, 2.2785362049, -1.2422000612\S, -1.8092041316, 1.2685243885, -1.6543461413\H, -4.7096347625, 2.7537874302, 0.1773393314\H, -3.4748686596, 3.0429050729, -1.9661779989\O, -2.7286978134, -1.845295925, -0.565764593\S, -0.7958302951, -0.9386964342, 1.9835122825\O, 0.0300071748, -0.8794747711, -0.6838012042\C, 1.1619653433, -0.7757852565, -0.0753761505\N, 2.3062551182, -1.4347071648, -0.5323850064\C, 3.420083024, -0.6119985811, -0.3772264655\C, 2.9902407851, 0.5292670718, 0.2370920865\N, 1.6507263756, 0.4935069736, 0.3733574701\C, 4.7966897241, -0.8510156175, -0.604911884\N, 3.8389277706, 1.5126750218, 0.6452073959\H, 2.2385343552, -2.1676017667, -1.2146421382\H, 0.5172870877, -1.2882175705, 1.3147719216\N, 5.5884448076, 0.2480160258, -0.1765322659\C, 5.2057784702, 1.4155881601, 0.4324090168\O, 5.3286443933, -1.8273507197, -1.1053843129\H, 3.5118955392, 2.369062326, 1.0595596891\O, 5.9744937374, 2.2935921366, 0.76547159\H, 6.5798594518, 0.1491820241, -0.3304315463\H, 1.0804940154, 1.0431715577, 0.999151063\Version=AM64L-G03RevC.02\State=1-A\HF=-889.3575612\RMSD=3.287e-09\RMSF=3.8

$2_{\text{H}}^{\text{W}} \cdot \text{Im}_{\text{R}}$

1\1\GINC-ORION-0-4\Freq\RmpW1PW91\Gen\C5H6N2O2S3W1(2-)\CBAYSE\19-Jul-2007\0\#\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CHKBAS FREQ\test\ -2,1\W, 0.7368934182, -0.5242115167, 0.302829081\S, 2.9343078432, 0.2164269613, -0.7318371979\C, 3.0072625837, 1.9674002266, -0.6400546087\C, 1.9401816027, 2.7211648656, -0.2938186224\S, 0.3945929254, 1.9984615746, 0.1000086965\H, 3.9470622575, 2.4359531424, -0.941723876\H, 1.994255564, 3.8119272975, -0.2986821567\O, 1.1226549396, -0.7062462634, 1.9609682503\S, 1.2314242461, -2.4751896364, -0.6946519521\O, -1.0281930359, -0.4550982374, 0.1974405195\H, -2.4733874095, -0.0940077525, -0.019982411\C, -4.5921030222, -0.5958429127, -0.1536512799\N, -5.7149394893, 0.0679431494, -0.3695450355\C, -5.3092361988, 1.3656652794, -0.5349620335\C, -3.9452106177, 1.456006399, -0.4141596128\N, -3.5029730734, 0.1928363312, -0.1706882762\H,

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

-4.5236229962, -1.6584081955, 0.0191298268\H, -6.0173921829, 2.1570041419,
-0.7311147431\H, -3.2579017964, 2.2829377028, -0.4790514105\Version=AM64
L-G03RevC.02\State=1-A\HF=-552.5210425\RMSD=6.278e-09\RMSF=6.311e-06\D

$2_{\text{H}}^{\text{W}} \cdot \text{ImH}^{\text{R}}$

1\1\GINC-ORION-0-8\Freq\RmpW1PW91\Gen\C5H7N2O2S3W1(1-)\CBAYSE\04-Sep-2
007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CH
KBAS FREQ\test\ -1,1\W, -0.8885073882, -0.4907526789, -0.2843158945\S, -1
.7225206936, 0.9129773181, 1.5490663766\C, -1.7264832567, 2.5744086497, 0.9
917894524\C, -1.0872496901, 2.9414234655, -0.1355571722\S, -0.2687609055, 1
.7604163489, -1.1337202055\H, -2.2092434561, 3.3023362521, 1.6432595871\H,
-1.0292018955, 3.9821167012, -0.4524430837\O, -2.3200920202, -0.9494859999
, -1.0624130124\S, -0.4443411944, -1.965164847, 1.3017697\O, 0.4569952961, -
0.8973897246, -1.5543030878\H, 1.4043113858, -0.6909199199, -1.4279294363\
C, 2.9522813258, -0.5593183555, 0.6643108242\N, 3.9552057485, 0.0302225528,
1.3552733625\C, 4.8170710048, 0.5916774582, 0.4457202561\C, 4.2808790319, 0
.3033048799, -0.7745519314\N, 3.124487988, -0.413610947, -0.6264682653\H, 2
.1105151598, -1.0529440584, 1.1341289801\H, 5.6985166921, 1.1323643132, 0.7
424722774\H, 4.6542457817, 0.5752400962, -1.7478421301\H, 4.0182948997, 0.0
85591703, 2.3557006063\Version=AM64L-G03RevC.02\State=1-A\HF=-553.1423
217\RMSD=4.777e-09\RMSF=2.670e-05\Dipole=2.9690051, 1.1618613, 0.9129972

$2_{\text{CN}}^{\text{W}} \cdot \text{ImR}$

1\1\GINC-ORION-0-23\Freq\RmpW1PW91\Gen\C7H4N4O2S3W1(2-)\CBAYSE\18-Jul-
2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C
HKBAS FREQ\test\ -2,1\W, 0.0041998067, -0.9438292054, 0.2831737128\S, 2.4
037677979, -1.0282170955, -0.5815456611\C, 3.1212011693, 0.5461422006, -0.3
388427005\C, 2.3700819827, 1.6477763202, 0.0154362966\S, 0.6472377576, 1.53
54855492, 0.2536668468\O, 0.1788174467, -1.3506495149, 1.9335490258\S, -0.1
542115988, -2.8572244597, -0.8518481303\O, -1.5823881658, -0.2026953143, 0.
1052653617\H, -3.0063507774, 0.4582819425, -0.0561633347\C, -5.1629882869,
0.4098523145, 0.0476397204\N, -6.1384071184, 1.2711831741, -0.1712063566\C
, -5.4972012769, 2.4207778674, -0.54743795\C, -4.1396362925, 2.2295768553, -
0.5483823651\N, -3.9433721785, 0.9385101618, -0.1638783533\H, -5.294384500
9, -0.6133385618, 0.362125492\H, -6.0452506872, 3.3165882397, -0.7967100249
\H, -3.3129164299, 2.8786331343, -0.7823149685\C, 2.9687135645, 2.936766700
8, 0.1426954554\N, 3.4316147182, 4.0063987909, 0.2550584158\C, 4.5209216405
, 0.6690999104, -0.5923398209\N, 5.6703680275, 0.7366647535, -0.8041576652\
\Version=AM64L-G03RevC.02\State=1-A\HF=-737.0224024\RMSD=5.418e-09\RMS

$2_{\text{Me}}^{\text{W}} \cdot \text{ImR}$

1\1\GINC-ORION-0-28\Freq\RmpW1PW91\Gen\C7H10N2O2S3W1(2-)\CBAYSE\18-Jul-
2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/
CHKBAS FREQ\test\ -2,1\W, 0.2273646973, -0.9210259319, 0.2833341608\S, 2.
5576525955, -0.7785164899, -0.6855845881\C, 3.1680254825, 0.8721009825, -0.
4950243322\C, 2.3425954047, 1.8874324262, -0.1383760784\S, 0.6291471847, 1.
5806466118, 0.1564984422\O, 0.5022605477, -1.2708057576, 1.9364658741\S, 0.
1836429078, -2.8884759925, -0.8003090597\O, -1.4433340495, -0.3477993207, 0
.1575924192\H, -2.7255817193, 0.4253012899, 0.0265688713\C, -4.902165475, 0
.5517948231, -0.0559850414\N, -5.7950983723, 1.5195853582, -0.1748491647\C
, -5.0419260028, 2.6604362394, -0.2594207004\C, -3.7060801824, 2.3538651635
, -0.1891018614\N, -3.6348475176, 1.0016785392, -0.0593855145\H, -5.1341501
618, -0.4977777293, 0.0346799871\H, -5.5007217803, 3.6322002507, -0.3659398
205\H, -2.8143544293, 2.9574825824, -0.2192663079\C, 2.7391891055, 3.336046
6937, 0.0054095461\H, 2.5797377828, 3.6822350388, 1.0367549192\H, 3.7880497

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

568,3.5194327384,-0.2545967505\H,2.1121461617,3.9690331368,-0.63935226
54\C,4.635328089,1.0139269403,-0.8182529845\H,5.2476906369,0.447456009
1,-0.1019108138\H,4.8451444983,0.5933964493,-1.812139136\H,4.978379361
6,2.0550668576,-0.8095181717\Version=AM64L-G03RevC.02\State=1-A\HF=-6
31.1434293\RMSD=5.695e-09\RMSF=9.301e-06\Dipole=1.7148144,1.9234464,0.

$2_{Ph}^W \cdot Im_R$

1\1\GINC-ORION-0-29\Freq\RmpW1PW91\Gen\C9H8N2O2S3W1(2-)\CBAYSE\11-Aug-
2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C
HKBAS FREQ\test\ -2,1\W,-0.0667503652,-0.9673424868,0.2586367364\S,2.
3226452914,-1.0671340871,-0.5830429018\C,3.0999423141,0.4870871287,-0.
3046193106\C,2.3328882335,1.6281320402,0.0458944873\S,0.59114733,1.494
9587557,0.2113232051\O,0.0655517569,-1.3556616387,1.9186272057\S,-0.24
07708164,-2.9070700877,-0.8495528923\O,-1.6510442978,-0.2191391219,0.0
329501223\H,-3.0156382879,0.4502591277,-0.0911943377\C,-5.1796441491,0
.3545385316,-0.254924263\N,-6.1641483517,1.2290819819,-0.3652886137\C,
-5.5347669616,2.445045556,-0.3668343229\C,-4.1777338369,2.2771642105,-
0.2567939042\N,-3.9678891081,0.9343433687,-0.1866244313\H,-5.300644378
6,-0.7167124597,-0.2225103311\H,-6.0900618917,3.367523038,-0.447543528
7\H,-3.3583189623,2.9751926062,-0.2237130022\C,2.985186975,2.862106651
3,0.215622673\H,2.3848946816,3.7311371444,0.4841482081\C,4.4886691786,
0.6328872138,-0.4735319415\H,5.0693060827,-0.2482245491,-0.7457882368\
C,5.1254493196,1.8641398424,-0.2983845238\H,6.2052101766,1.9414744358,
-0.4294043081\C,4.3667078196,2.9898551663,0.0494024193\H,4.8444399098,
3.959311967,0.193033273\Version=AM64L-G03RevC.02\State=1-A\HF=-706.16
72512\RMSD=5.285e-09\RMSF=1.180e-04\Dipole=1.6073962,1.6546332,0.32797

$2_H^W \cdot Im_{TS}$

1\1\GINC-ORION-0-4\Freq\RmpW1PW91\Gen\C5H6N2O2S3W1(2-)\CBAYSE\23-Jun-2
007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CH
KBAS FREQ\test\ -2,1\W,0.4113399064,-0.1911158531,0.2349670536\S,2.62
53207773,-1.0717787386,-0.3575747769\C,3.7092835539,0.3231439296,-0.35
71940191\C,3.2497565714,1.5906445465,-0.2859278946\S,1.5297954458,1.96
7061277,-0.1779211907\H,4.7764922431,0.1181797586,-0.4685573093\H,3.93
56398755,2.4395326026,-0.3274829197\O,0.2502885082,-0.4262195183,1.918
8294705\S,-0.6183919101,-1.9150197342,-0.8155863008\O,-1.1740989422,0.
80871372,-0.2816388197\C,-2.4731185034,0.2513784246,-0.4354030821\N,-3
.1131082026,-0.0379215139,0.7926609332\C,-4.458441941,0.2281109253,0.6
634594326\C,-4.5815362607,0.8070259488,-0.576087838\N,-3.4071915666,0.
8684927294,-1.2412295252\H,-5.1654709072,0.0863533142,1.4652956695\H,-
5.4927778355,1.1986301575,-1.0130287398\H,-2.6665352391,-0.6120210275,
1.4858774045\H,-2.0571688846,-0.8480813189,-0.9229744352\Version=AM64
L-G03RevC.02\State=1-A\HF=-552.424465\RMSD=5.377e-09\RMSF=6.712e-06\Di

$2_H^W \cdot ImH^+_{TS}$

1\1\GINC-ORION-0-4\Freq\RmpW1PW91\Gen\C5H7N2O2S3W1(1-)\CBAYSE\10-Nov-2
007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CH
KBAS FREQ\test\ -1,1\W,0.4491577042,-0.1811721819,0.2312564348\S,2.57
07604454,-1.1203464523,-0.3915592842\C,3.7134846157,0.226244746,-0.342
2724802\C,3.3022366753,1.504661649,-0.2489605634\S,1.5937036298,1.9291
309024,-0.1300472743\H,4.7688278242,-0.0256715311,-0.4444611531\H,4.00
91907329,2.3335961146,-0.2553442697\O,0.2249644378,-0.4739481863,1.889
8843154\S,-0.6892790992,-1.825888671,-0.8641005417\O,-1.1708427693,0.8
690496949,-0.3225594049\C,-2.3875960048,0.388180102,-0.3256279453\N,-3
.0265278196,0.0256396415,0.8694839039\C,-4.3957794557,0.0579789008,0.6

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

855544302\C, -4.6426710924, 0.6414684334, -0.5004383097\N, -3.4196329198, 0.9811545553, -1.0703384797\H, -5.0849092764, -0.2718357829, 1.4431604887\H, -5.5804863568, 0.9129667784, -0.9521369358\H, -2.5322393926, -0.5714025604, 1.5142413844\H, -1.9801972594, -0.9314568304, -0.9326520593\H, -3.2887126, 1.114638373, -2.0566180733\\Version=AM64L-G03RevC.02\State=1-A\HF=-553.0843191\RMSD=4.085e-09\RMSF=7.098e-06\Dipole=-2.7469515, 0.56605, -0.2

$2_{CN}^W \cdot Im_{TS}$

1\1\GINC-ORION-0-14\Freq\RmpW1PW91\Gen\C7H4N4O2S3W1(2-)\CBAYSE\08-Jul-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C HKBAS FREQ\test\ -2,1\W, -0.2317812474, -0.3618911136, 0.2827661194\S, 1.8689793086, -1.4984837299, -0.262283667\C, 3.1173548147, -0.2544483949, -0.2230667793\C, 2.8055643036, 1.0838573588, -0.1438283331\S, 1.1414837724, 1.6510222713, -0.0719779238\O, -0.4632455389, -0.5935580785, 1.9563134966\S, -1.4013130652, -1.9375810908, -0.8357355615\O, -1.6532055235, 0.8286004456, -0.2440840006\C, -3.0287211574, 0.4219232287, -0.4859273464\N, -3.7468170735, 0.2298822301, 0.7102181718\C, -4.9812730153, 0.8142518105, 0.5925136723\C, -4.9833519884, 1.3786850378, -0.6608247175\N, -3.8207657436, 1.1756913686, -1.3173614154\H, -5.7178330742, 0.7950517282, 1.3789894245\H, -5.7945535746, 1.9329038321, -1.1155069629\H, -3.3596391999, -0.2561743079, 1.498939098\H, -2.7169302184, -0.6870724145, -0.9627367028\C, 3.8299388571, 2.0759748761, -0.1549395527\N, 4.6449189638, 2.9169273502, -0.1595802973\C, 4.4719600006, -0.6870703081, -0.3291758864\N, 5.570827529, -1.0829961247, -0.4148143973\\Version=AM64L-G03RevC.02\State=1-A\HF=-736.9282742\RMSD=6.028

$2_{Me}^W \cdot Im_{TS}$

1\1\GINC-ORION-0-5\Freq\RmpW1PW91\Gen\C7H10N2O2S3W1(2-)\CBAYSE\03-Jul-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C HKBAS FREQ\test\ -2,1\W, -0.001051106, -0.3009667465, 0.2837505052\S, 2.138053386, -1.3554751978, -0.2413786799\C, 3.3770961855, -0.0740250596, -0.2428096463\C, 3.0241609264, 1.2327939742, -0.2151344806\S, 1.312877479, 1.719215142, -0.1662956138\O, -0.2239105525, -0.4702318177, 1.9689573632\S, -1.1435460179, -1.9643032648, -0.75013893\O, -1.4793723444, 0.8139710802, -0.3071804112\C, -2.818294496, 0.3638211748, -0.4922916948\N, -3.5217763124, 0.1719952946, 0.7200849193\C, -4.8313645344, 0.5581844588, 0.5383615869\C, -4.8615732654, 1.1046744174, -0.7214328435\N, -3.6666321457, 1.0354767589, -1.3479191323\H, -5.5731394531, 0.5071680786, 1.3194610207\H, -5.7186045535, 1.5632713034, -1.2007887843\H, -3.1526203174, -0.4147451934, 1.4472632716\H, -2.4841933778, -0.778035431, -0.9330781543\C, 3.9775094594, 2.4006576648, -0.2468753108\H, 3.888869553, 2.9980235609, 0.6722718706\H, 5.0257774449, 2.0973203259, -0.3547569041\H, 3.7283083716, 3.0718095811, -1.0815385866\C, 4.7873201039, -0.6008098286, -0.3217059587\H, 5.0278018352, -1.2008943286, 0.5681845622\H, 4.8940343881, -1.2697295728, -1.188118441\H, 5.5393865033, 0.1923647618, -0.4094716975\\Version=AM64L-G03RevC.02\State=1-A\HF=-631.0471837\RMSD=7.968e-09\RMSF=4.069e-06\Dipole=1.9078022, 0.2513388, 1.2

$2_{Ph}^W \cdot Im_{TS}$

1\1\GINC-ORION-0-31\Freq\RmpW1PW91\Gen\C9H8N2O2S3W1(2-)\CBAYSE\09-Jul-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C HKBAS FREQ\test\ -2,1\W, 0.3060876367, 0.3576192147, 0.2763477218\S, -1.7681726376, 1.5415709771, -0.2540285529\C, -3.0794673435, 0.3525441161, -0.1960890566\C, -2.7914427111, -1.0330933488, -0.137397417\S, -1.1191699303, -1.6065018413, -0.1108399435\O, 0.5572834529, 0.5550462818, 1.9529032467\S, 1.5305422342, 1.9201869668, -0.8123731459\O, 1.7049137582, -0.8605296423, -0.2867251733\C, 3.0755662797, -0.4907807167, -0.4949207686\N, 3.7892257132

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

, -0.3152983441, 0.7100745382\C, 5.050373616, -0.8411721621, 0.5654391071\C, 5.0500024384, -1.4080147036, -0.686276445\N, 3.8744012231, -1.2399456248, -1.3304443695\H, 5.789379092, -0.8220524196, 1.3501336609\H, 5.8693877179, -1.9459820768, -1.1475596626\H, 3.4313430813, 0.2448036544, 1.4628508704\H, 2.8011079948, 0.6482460827, -0.9653210908\C, -3.8578493369, -1.9483737115, -0.1304583001\H, -3.6238456121, -3.0123572869, -0.0877569946\C, -4.4214873985, 0.7651097294, -0.2499155305\H, -4.6297457799, 1.8341660343, -0.3007772451\C, -5.4738635334, -0.1544614476, -0.2380109859\H, -6.5054322065, 0.1974590394, -0.2740636542\C, -5.1889218027, -1.5253013839, -0.1775639152\H, -5.9943015526, -2.26036612, -0.1670469195\\Version=AM64L-G03RevC.02\State=1-A\HF=-706.0717607\RMSD=7.907e-09\RMSF=4.360e-06\Dipole=-1.5203896, -0

$2_H^W \cdot \text{Im}_p$

1\1\GINC-ORION-0-0\Freq\RmpW1PW91\Gen\C5H6N2O2S3W1(2-)\CBAYSE\10-Jul-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CHKBAS FREQ\\test\\-2,1\W, 0.4573346404, -0.3273142053, 0.1929422936\S, 2.8191186079, 0.0075964017, 0.1444131324\C, 3.0639450397, 1.7387818547, -0.1921915546\C, 2.0341941195, 2.5354756787, -0.5392662293\S, 0.3724014742, 1.9074748132, -0.6452817197\H, 4.0888786581, 2.1139046754, -0.1501978423\H, 2.1752777798, 3.5912932438, -0.7782191465\O, 0.0012904394, -0.2986624979, 1.8395744397\S, 0.8158350321, -2.5815001268, -0.5871200999\O, -1.4122421566, -0.6593368502, -0.7594312769\C, -2.5250809501, -0.1098605821, -0.423863854\N, -2.6963370408, 0.5285781638, 0.7766879374\C, -4.0050899692, 0.9550768021, 0.8552757214\C, -4.5697536661, 0.5467563742, -0.3186983302\N, -3.6687967098, -0.112598026, -1.112374801\H, -4.3878796287, 1.5065165304, 1.6979219436\H, -5.5901563837, 0.7005366472, -0.6430046292\H, -1.9467869122, 0.6057931594, 1.451080583\H, -0.4455161839, -2.8791774216, -1.0263634171\\Version=AM64L-G03RevC.02\State=1-A\HF=-552.4743172\RMSD=4.166e-09\RMSF=1.987e-05\Di

$2_H^W \cdot \text{ImH}_p^+$

1\1\GINC-ORION-0-8\Freq\RmpW1PW91\Gen\C5H7N2O2S3W1(1-)\CBAYSE\06-Sep-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CHKBAS FREQ\\test\\-1,1\W, -0.4598297056, 0.2807362745, 0.137874966\S, -2.7823250417, 0.3183612933, 0.4587951837\C, -3.3453622089, -1.3363684861, 0.1100887535\C, -2.5325445476, -2.2469848657, -0.4513580848\S, -0.8318521821, -1.8478596012, -0.8080820565\H, -4.3908751422, -1.5561216006, 0.3265377658\H, -2.8634015919, -3.2549788143, -0.6985766849\O, 0.2514712698, 0.1397083542, 1.701330845\S, -0.5665138463, 2.5203909008, -0.6921605281\O, 1.4800439321, 0.2601066762, -0.9588236533\C, 2.5314598642, -0.0973268846, -0.4093161152\N, 2.7353278113, -0.3871384097, 0.8986838826\C, 4.0489551404, -0.7461363024, 1.1074805346\C, 4.6861418425, -0.6842862205, -0.0787298573\N, 3.746685937, -0.2765223515, -1.0153956656\H, 4.4202265915, -1.0173868532, 2.0789689477\H, 5.7085967173, -0.8878576418, -0.3387311153\H, 1.9279559877, -0.2986428654, 1.5418215048\H, 0.6792447685, 2.6617381069, -1.2391790659\H, 3.8785896073, -0.1617944907, -2.0024968611\\Version=AM64L-G03RevC.02\State=1-A\HF=-553.112589\RMSD=3.417e-09\RMSF=1.101e-05\Dipole=4.196202, -1.1361521,

$2_{CN}^W \cdot \text{Im}_p$

1\1\GINC-ORION-0-16\Freq\RmpW1PW91\Gen\C7H4N4O2S3W1(2-)\CBAYSE\04-Jul-2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CHKBAS FREQ\\test\\-2,1\W, -0.2323085998, -0.7145258689, 0.2045517155\S, 2.0707096463, -1.2576871682, 0.1748411812\C, 2.9491140408, 0.2901216926, -0.0149938112\C, 2.2708632673, 1.4488664927, -0.2843566414\S, 0.4878583693, 1.4594086445, -0.414736537\O, -0.6714845738, -0.669123355, 1.8493126048\S, -0.6809531571, -2.8664634365, -0.7786102319\O, -2.0612965743, -0.3119515801, -

Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

0.7561434055\C,-2.8962322108,0.6131175129,-0.4167165361\N,-2.864307129
,1.2163809177,0.8127455215\C,-3.9140646542,2.107593821,0.8789970138\C,
-4.5364831621,1.9946992599,-0.3296289198\N,-3.9172296484,1.0734657433,
-1.1332873101\H,-4.0943850389,2.7292076787,1.7397218993\H,-5.403774859
9,2.540318663,-0.6737291022\H,-2.1781112515,0.982155662,1.5151996066\H
, -1.9468845499,-2.6279648967,-1.2315991141\C,2.9472986885,2.6842925451
, -0.479050163\N,3.4633444583,3.7228332676,-0.6482149364\C,4.3677675825
,0.2595421331,0.080839665\N,5.5331669216,0.1796439699,0.1764384294\Version=AM64L-G03RevC.02\State=1-A\HF=-736.9821581\RMSD=7.192e-09\RMSF=1

$2_{Me}^W \cdot Imp$

1\1\GINC-ORION-0-6\Freq\RmPW1PW91\Gen\C7H10N2O2S3W1(2-)\CBAYSE\08-Jul-
2007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/C
HKBAS FREQ\test\ -2,1\W,-0.0260153598,0.6178619589,0.1998530686\S,-2.
3806641521,0.889441137,0.1870888666\C,-3.117842254,-0.7385165458,-0.03
7958395\C,-2.33792518,-1.7942995465,-0.3475430738\S,-0.5570583986,-1.5
850265963,-0.5020902403\O,0.455424632,0.5525258275,1.839366946\S,0.192
9656492,2.84928758,-0.7017389813\O,1.8467461199,0.4156806504,-0.797685
8178\C,2.7891863542,-0.3818816872,-0.4410714006\N,2.8179104531,-0.9789
757266,0.792318929\C,3.9754478866,-1.721999115,0.885349715\C,4.6003498
78,-1.5345530961,-0.3140697469\N,3.8810589903,-0.7090263978,-1.1372571
176\H,4.2232102919,-2.3074300138,1.7552211656\H,5.5403479266,-1.961832
9793,-0.6366294733\H,2.0875029451,-0.8242779025,1.4748900719\H,1.47574
54681,2.7814376073,-1.172573617\C,-4.614314957,-0.7588230071,0.1172740
414\H,-4.900468629,-0.4956145525,1.1468037648\H,-5.0737165723,-0.00276
70967,-0.5361004057\H,-5.0611973008,-1.7326325673,-0.121198808\C,-2.80
17005174,-3.2049893191,-0.5910410677\H,-3.8933351204,-3.3108833429,-0.
5510624511\H,-2.4599517843,-3.5555854761,-1.5762169092\H,-2.3662495549
, -3.890695615,0.151063129\Version=AM64L-G03RevC.02\State=1-A\HF=-631.
0980963\RMSD=8.452e-10\RMSF=4.363e-06\Dipole=-1.2996622,-1.6106854,1.1

$2_{Ph}^W \cdot Imp$

1\1\GINC-ORION-0-4\Freq\RmPW1PW91\Gen\C9H8N2O2S3W1(2-)\CBAYSE\30-Jun-2
007\0\#N GEOM=ALLCHECK GUESS=READ SCRF=CHECK TEST GENCHK RMPW1PW91/CH
KBAS FREQ\test\ -2,1\W,0.3446835029,0.710597837,0.2135090121\S,-1.922
1449745,1.4176988909,0.2059600724\C,-2.9349847709,-0.0405007786,0.0035
805874\C,-2.329523182,-1.2743829334,-0.3145163085\S,-0.5547482017,-1.3
791030435,-0.4805459753\O,0.8053321659,0.5676000893,1.8505742379\S,0.9
526427688,2.8641771322,-0.68661637\O,2.1389975952,0.1823762207,-0.7878
800893\C,2.9181663693,-0.7848421802,-0.4497944711\N,2.8501296674,-1.38
730566,0.7792279589\C,3.8456606127,-2.3387766887,0.8477121524\C,4.4770
971216,-2.261658678,-0.3598681276\N,3.9160804912,-1.3055882429,-1.1650
13954\H,3.9887629538,-2.9698005192,1.7089752763\H,5.3131843899,-2.8568
111662,-0.7009758464\H,2.1721504781,-1.1090476733,1.475549426\H,2.1985
488488,2.5656220655,-1.1646638635\C,-3.1370123363,-2.4052385755,-0.504
7556952\H,-2.6549621735,-3.351565618,-0.7549188575\C,-4.3317806475,0.0
22218623,0.118068633\H,-4.7890961402,0.9838530149,0.3572096027\C,-4.5
286500706,-2.3357266055,-0.38161784\H,-5.1348399624,-3.2298841693,-0.5
323519954\C,-5.1315146659,-1.1102471565,-0.0664046923\H,-6.2151808695,
-1.0356163001,0.035269078\Version=AM64L-G03RevC.02\State=1-A\HF=-706.
12327\RMSD=2.738e-09\RMSF=1.271e-05\Dipole=-1.2428317,-1.1867098,1.146