

Supplementary material to:

P.I. Arvidsson, T. Govender, H.G. Kruger, G.E.M. Maguire and T. Naicker,
S. Afr. J. Chem., 2009, **62**, 60–66.

Complex A (See Figure 1 in the Research Article)

HF = -2247.9843573 a.u.

C,-0.8756594364,4.1301826061,2.3090924325
C,-1.1340775472,4.0816214669,0.9396244623
C,-1.131728462,2.9339854417,0.1362875467
N,-1.591414696,3.0020501337,-1.2275178586
O,-0.8986441078,1.7124087323,0.6162318957
C,-1.5430258216,2.0210609763,-2.1454786634
O,-2.2410548344,2.3433786544,-3.2850503477
C,-2.4806636276,4.0687758713,-1.7056027036
C,-2.5895700208,3.7360580112,-3.1997126865
O,-0.9387896012,0.9058185189,-2.1083256434
H,-0.9253487471,5.0720528277,2.8464303404
H,-0.6663005895,3.2306537555,2.8799789037
H,-1.354103492,5.0308126999,0.4513070942
H,-2.040433659,5.0539759789,-1.5375728117
H,-3.437733325,4.0141694065,-1.1728512879
H,-1.8722415572,4.3093190875,-3.7993487669
H,-3.5933149068,3.8652506939,-3.6099528533
C,1.3959030419,-3.3891570099,0.0718219228
C,2.4645329659,-2.5429032244,-0.7232553636
C,3.3926997683,-3.6247891027,-1.3276418857
C,3.3861809481,-4.7390370186,-0.2601338401
C,1.8487990158,-4.8493167361,-0.1777773907
C,1.4311959192,-5.0503389605,-1.660513687
C,0.3433559501,-3.9918410244,-2.0091253808
C,1.3966343806,-3.1540585024,-2.7943350711
C,2.4952454895,-4.2061263387,-2.4524422915
C,1.6017491696,-1.9327024851,-1.8625172058
C,0.1060505951,-3.1219104796,-0.7477398546
H,1.3165931322,-3.1038794421,1.1243733503
H,2.9641327856,-1.7979409195,-0.1024529461
H,4.3748849596,-3.2656904345,-1.6496867476
H,3.8503074974,-4.4349121695,0.6858381354
H,3.8654556397,-5.6652092824,-0.6020135728
H,1.4498685718,-5.5860682096,0.525924843
H,1.2668732205,-6.0850800611,-1.9699341772
H,-0.564172227,-4.3006833184,-2.5331163953
H,1.1866365378,-2.9091921396,-3.8378767312
H,3.0222615495,-4.6925444436,-3.2764690883
O,0.2840099909,-1.7600293726,-1.2473145795
C,2.0767608877,-0.6585826375,-2.5423171187
C,-1.2434375513,-3.3240468669,-0.0725039598

C,2.3091751763,0.5018348038,-1.6213417751
N,1.7419934319,0.6902375571,-0.483964992
O,3.1851538324,1.4300288102,-2.0526355811
C,3.1655539793,2.5058705931,-1.0624382083
C,2.2362461096,1.9807191896,0.0713195503
C,-1.5765814294,-2.3693544003,1.032797006
N,-1.445433325,-1.0865794667,0.9928172121
O,-2.1746306939,-2.8933922446,2.1274697015
C,-2.2001924645,-0.5176865241,2.1550510338
C,-2.3587916363,-1.7725361212,3.0493411651
C,2.9229221876,1.8027660217,1.4130389255
C,-3.5155434322,0.1087520953,1.7170471614
C,2.5112603057,2.5698710081,2.5105316568
C,3.9881362978,0.9028257697,1.5704393645
C,3.1558800739,2.4342314215,3.7453293868
C,4.6306695527,0.7665882298,2.8026506884
C,4.2136620085,1.5347360804,3.8958749581
C,-4.5525709917,-0.6828681449,1.1889254682
C,-3.7225508401,1.4888596861,1.8582156617
C,-5.7646188583,-0.1070091099,0.8047268027
C,-5.9646753911,1.2701055426,0.9527335898
C,-4.9416298705,2.0613529261,1.4864785939
H,3.0116851232,-0.8708090593,-3.0748402003
H,1.3439332215,-0.3514899851,-3.3000519648
H,-2.0338684119,-3.2469223485,-0.8337427604
H,-1.2808574912,-4.345835197,0.319412826
H,2.7692292825,3.3961683955,-1.5572041198
H,4.1957172558,2.6787437524,-0.7457563291
H,1.3725577282,2.6424116635,0.1983163947
H,-1.5853134943,0.2504773228,2.6259518678
H,-1.575180638,-1.8486387677,3.8106424136
H,-3.3422678199,-1.878952685,3.5070416682
H,1.6720500869,3.2578342774,2.4045510823
H,4.3214978866,0.3027820785,0.7251002732
H,2.8235218682,3.0339896572,4.5891518653
H,5.4547798787,0.0649856125,2.9103314087
H,4.7128541369,1.431133431,4.8564104675
H,-4.4190824989,-1.7573902978,1.0757955397
H,-2.9235149096,2.1236588296,2.2323235959
H,-6.5534890321,-0.7331054657,0.3938214928
H,-6.9090779812,1.7197026522,0.6548759476
H,-5.0833888474,3.1320943942,1.6125418599
Mg,-0.3700771735,0.1516103329,-0.3450767155

Complex B (See Figure 1 in the Research Article)

HF = -2247.9763431 a.u.

C,-1.9513878222,4.2949257572,-1.3277690609
C,-1.4465462946,3.9974447165,-0.0618459512
C,-1.276024242,2.7280886183,0.492178156

N,-0.6875777494,2.5823370008,1.7935669022
O,-1.6385083479,1.5909717188,-0.133275965
C,-0.0872422071,1.4862150838,2.2849979823
O,0.1306436198,1.5754929859,3.6412736641
C,-0.9267642907,3.5329069449,2.8883564445
C,-0.0211474936,2.9645824393,3.990283666
O,0.2481335573,0.4196421354,1.6827202333
H,-2.1044468995,5.3263287032,-1.6310492859
H,-2.3429095398,3.5161742104,-1.9759623742
H,-1.1204995663,4.8428445394,0.546087738
H,-1.9928265879,3.529088267,3.1510782449
H,-0.6425456592,4.5471719816,2.6022032953
H,-0.4488746548,3.0217283235,4.9931500909
H,0.9694312903,3.4347145214,3.9823922812
C,1.4700183744,-2.4769773183,1.3234567459
C,2.4743238692,-1.7999575525,0.2988196076
C,3.7497517946,-2.6644255499,0.437109345
C,3.7418887398,-3.0810069735,1.9239060166
C,2.3033852673,-3.6405682197,1.909205882
C,2.3254465325,-4.6358196112,0.7192020913
C,1.1380790947,-4.288280117,-0.2285611478
C,2.118781708,-3.6251696811,-1.2300556607
C,3.3203903681,-3.9633182317,-0.2955849297
C,1.7939208018,-2.119783299,-1.0618075096
C,0.392965294,-3.0627592386,0.3670199077
H,1.0791303548,-1.7635315504,2.0506163461
H,2.6096671702,-0.7354935608,0.4964345031
H,4.6688620355,-2.1994719466,0.0673986009
H,3.86898493,-2.2356485397,2.6101864073
H,4.4968307924,-3.8415931338,2.1615424017
H,1.9331235902,-4.0484022825,2.8547907424
H,2.4910457522,-5.6843654,0.9778946101
H,0.4916275967,-5.0891704053,-0.5947275587
H,2.1225242822,-3.9835179865,-2.2623779589
H,4.1321552917,-4.5748454158,-0.6963620522
O,0.3649953814,-2.091889571,-0.7337827914
C,2.0860729137,-1.3095968702,-2.313446099
C,-0.9905958101,-3.4221874805,0.9075187072
C,1.7970579443,0.154977636,-2.27473766
N,1.0739938726,0.7890996828,-1.4177955055
O,2.3445601645,0.8684778473,-3.2809015512
C,1.7489845311,2.2019218114,-3.1761429917
C,1.2261652757,2.2509592796,-1.7220939872
C,-2.0625661319,-2.3786423639,0.9760551654
N,-2.1155773176,-1.253365383,0.3707943504
O,-3.1431641512,-2.7501323725,1.6983372186
C,-3.4856112537,-0.6849753448,0.5786311233
C,-4.0529509768,-1.6056230886,1.6828172639
C,2.1954591555,2.9543422911,-0.7831962063
C,-4.2574413636,-0.6671924834,-0.7331850988

C,1.9826959685,4.3138834839,-0.5041334488
C,3.3409554566,2.3338429526,-0.2651672712
C,2.8957690405,5.0329376642,0.2692592995
C,4.2533861116,3.0513189626,0.5158378784
C,4.0376506442,4.4045900261,0.7828438902
C,-4.8621645636,-1.824346211,-1.2483166325
C,-4.3439421872,0.5286870049,-1.4596151643
C,-5.5555650726,-1.7852299048,-2.4603646486
C,-5.6487908452,-0.5859286534,-3.1737930233
C,-5.0398352591,0.5672320835,-2.6715239004
H,3.1454559346,-1.4343542115,-2.5730850936
H,1.5244325755,-1.7467156163,-3.1527632022
H,-1.4192863501,-4.223977396,0.2896096403
H,-0.8683494547,-3.856493754,1.9068935645
H,0.9416420492,2.2578078596,-3.9131145326
H,2.52629632,2.9315358068,-3.4019963511
H,0.2497753718,2.7403607112,-1.6695049486
H,-3.3581589634,0.3421976006,0.9220686117
H,-4.0112759785,-1.1488220746,2.6758452005
H,-5.0577752489,-1.9820744384,1.4896658963
H,1.0872838087,4.7943154119,-0.8913082929
H,3.5257634261,1.281240133,-0.4619205154
H,2.7142292585,6.0855663627,0.4739439862
H,5.1338693198,2.5503220497,0.911886767
H,4.7494834454,4.964726291,1.3843691996
H,-4.7985138177,-2.7657585658,-0.7054404528
H,-3.8311955963,1.4123320082,-1.0861319665
H,-6.0232479196,-2.6885173637,-2.8449157639
H,-6.1916110998,-0.5530153828,-4.1154051716
H,-5.1013756804,1.5029030234,-3.2215225397
Mg,-0.4837761204,0.0570832323,-0.1423624541