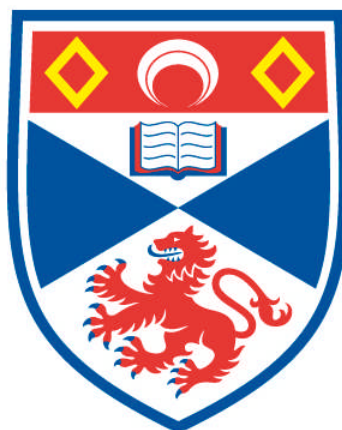


CHARACTERISATION OF INORGANIC MATERIALS USING SOLID-STATE NMR SPECTROSCOPY

Appendix C

Scott Sneddon

**A Thesis Submitted for the Degree of PhD
at the
University of St Andrews**



2016

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Appendix C

C.1 Cartesian coordinates for each model

Zn cluster

C.1.1 $[\text{Zn}(\text{bIm})_4]^{2+}$

C.1.1.1 Unoptimised

```
%nprocshared=4

%mem=20GB

%chk=zif7.chk

#p ginput b3lyp/gen opt=(modredundant)

zif7

2 1

C      -6.59412    15.74910   -22.12964
C     -11.26772    18.40860   -22.58379
C      -8.24391    15.42034   -20.78217
C     -10.57038    20.42344   -22.26795
C      -9.45843    15.31169   -20.14520
C     -10.39946    21.75623   -21.97291
C      -9.13873    22.27141   -22.12436
C      -9.45821    14.75291   -18.89398
C      -8.26606    14.28453   -18.28257
C      -8.04674    21.46870   -22.54584
C      -7.05870    14.95626   -20.17758
C      -9.48811    19.62408   -22.68668
C      -7.06127    14.37152   -18.92313
C      -8.21011    20.13885   -22.81827
C      -7.44000    17.88629   -25.79558
C     -10.90812    14.24936   -23.67474
```

C	-6.51009	16.24641	-26.75338
C	-11.47394	15.78881	-25.00938
C	-11.65559	16.98245	-25.77337
C	-5.75272	15.34122	-27.55870
C	-7.23618	15.77542	-25.69374
C	-12.32237	14.72971	-25.18367
C	-13.39798	14.75582	-26.14540
C	-7.29401	14.37169	-25.36400
C	-12.65345	17.02026	-26.69238
C	-5.80595	14.01583	-27.27196
C	-6.56736	13.50731	-26.18546
C	-13.53379	15.92414	-26.89809
H	-6.10829	16.01672	-22.87594
H	-11.83413	17.67381	-22.64598
H	-10.24362	15.60811	-20.54352
H	-11.10814	22.28501	-21.68797
H	-8.99337	23.17134	-21.94271
H	-10.26194	14.67508	-18.43358
H	-8.30511	13.91246	-17.43013
H	-7.20480	21.85473	-22.63931
H	-6.27874	14.05136	-18.53374
H	-7.49443	19.60400	-23.07944
H	-7.70213	18.75743	-25.60748
H	-10.44070	13.78647	-23.01883
H	-11.10297	17.71658	-25.64492
H	-5.23557	15.65216	-28.26347
H	-7.78779	14.05978	-24.64014
H	-13.97227	14.03258	-26.25589
H	-12.76346	17.79037	-27.20171
H	-5.32635	13.42340	-27.80450
H	-6.58336	12.59276	-26.02107
H	-14.20389	15.98428	-27.53921

H	-12.64415	19.86608	-21.90129
H	-12.35265	12.78740	-24.15798
H	-5.01388	14.97507	-20.92957
H	-6.22492	18.26062	-27.47529
N	-11.70072	19.60365	-22.18599
N	-7.91485	15.90295	-22.05309
N	-11.93805	13.71039	-24.29033
N	-7.85077	16.87460	-25.06217
N	-9.96250	18.32637	-22.88994
N	-6.00375	15.18317	-21.06415
N	-6.64342	17.61183	-26.80806
N	-10.56694	15.47136	-24.02870
Zn	-9.05525	16.66470	-23.48662

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N C H Zn 0
6-31g**

C.1.1.2 Optimised

```
%nprocshared=4  
%mem=20GB  
%chk=zif7.chk  
#p ginput b3lyp/gen nmr=all prop=efg
```

zif7

2 1

C	-0.86490200	2.74899700	-0.93351600
C	-1.69925100	-2.24238800	0.94042900
C	-1.85226100	2.37232000	0.94499500
C	-2.97292500	-3.00754400	-0.62095100
C	-2.33510300	1.87834800	2.13472100
C	-3.88594400	-3.67290800	-1.40598600
C	-4.02620900	-3.24291300	-2.69951500
C	-3.15171500	2.70101800	2.86557400
C	-3.47371000	4.01393100	2.43313800
C	-3.28259000	-2.14697300	-3.20978800
C	-2.17031100	3.67536900	0.51310400
C	-2.23319200	-1.91920500	-1.12486700
C	-2.97697100	4.51459400	1.26181800
C	-2.39083600	-1.47044400	-2.42461700
C	1.29587100	-0.54701200	-2.71945900
C	1.28435400	0.35787400	2.65958600
C	2.91974700	0.80422300	-2.81171800
C	1.70190700	-1.51608900	1.77344900
C	1.78558500	-2.70276900	0.98209600
C	4.05336300	1.61015800	-3.13867500
C	2.23846300	1.02338900	-1.64565900
C	2.38617500	-1.43273000	2.95528400
C	3.22841400	-2.50245100	3.43369300
C	2.63996500	2.03559200	-0.69867800
C	2.58363800	-3.71385700	1.40935000
C	4.45387500	2.55788700	-2.25373800
C	3.76812900	2.78849300	-1.03087500
C	3.31393300	-3.63821000	2.62579600
H	-0.25386000	2.61827100	-1.81646500

H	-1.21275800	-2.14155600	1.90120400
H	-2.09437600	0.87497500	2.47294300
H	-4.47095300	-4.50450000	-1.02531100
H	-4.73027100	-3.74379100	-3.35548500
H	-3.56803600	2.35030100	3.80450900
H	-4.12015400	4.62571400	3.05307600
H	-3.44743900	-1.84097100	-4.23772100
H	-3.21599800	5.52002900	0.92925100
H	-1.83925800	-0.61176700	-2.79574200
H	0.61667900	-1.34306900	-3.00264300
H	0.86875500	1.34661400	2.81868300
H	1.23534400	-2.77768400	0.05002400
H	4.58913000	1.45184800	-4.06970900
H	2.09369600	2.19214500	0.22338200
H	3.76914800	-2.42081200	4.36992700
H	2.66885300	-4.61658800	0.81219300
H	5.32122600	3.16746800	-2.48588400
H	4.12353000	3.55933400	-0.35559200
H	3.93789600	-4.46998200	2.93307400
H	-2.95930900	-3.86944600	1.37659600
H	2.44015100	0.21291500	4.40328500
H	-1.55651200	4.71354300	-1.29831500
H	2.55301800	-0.61933300	-4.38923500
N	-2.62485200	-3.17514000	0.72337000
N	-0.98631200	1.80889100	0.00206800
N	2.10115400	-0.18210000	3.53791500
N	1.15896000	0.11962600	-1.59385400
N	-1.41259700	-1.44287700	-0.10010000
N	-1.52539400	3.89615900	-0.70580800
N	2.30029600	-0.20852500	-3.50147100
N	0.98858400	-0.35681500	1.59341700
Zn	-0.09241200	0.03838800	-0.04315800

```

N C H O
6-311+g**
*****
Zn 0
6-311g**
*****

```

C.1.2 $[\text{Zn}(\text{mIm})_4]^{2+}$

C.1.2.1 Unoptimised

```

%nprocshared=4
%mem=20GB
%chk=zif8.chk
#p ginput b3lyp/gen opt=(modredundant)

zif8

2 1
C      -18.63665    14.87620    9.59020
C      -17.82322    10.82839    8.89569
C      -13.93484    14.02259    7.45267
C      -14.05852    13.29077    11.57308
C      -14.60159    14.94409    12.84215
C      -18.62745    16.18151    7.87702
C      -14.64935    12.03090    7.05075
C      -16.79747    10.68332    10.78399
C      -13.67633    12.31521    6.16545
C      -17.54787     9.57715    10.62701
C      -15.49479    14.87379    11.83786
C      -17.51162    15.42995    7.83904

```


C	-18.34666	11.36645	7.60641
C	-13.30071	12.15132	10.97885
C	-13.72472	15.34597	8.10861
C	-19.08114	14.15422	10.81775
H	-14.60534	15.57193	13.52752
H	-15.12272	11.23235	7.09759
H	-13.36637	11.74555	5.49961
H	-17.61253	8.87582	11.23354
H	-18.86899	16.82466	7.25097
H	-16.21760	15.44504	11.71474
H	-16.85488	15.46807	7.18240
H	-16.25804	10.87250	11.51690
H	-18.49674	10.52112	6.89335
H	-19.32485	11.87070	7.77676
H	-17.62873	12.08962	7.16911
H	-13.63157	11.96640	9.93644
H	-13.46931	11.23185	11.58922
H	-12.21163	12.38462	10.97927
H	-13.67515	16.14099	7.32941
H	-14.55812	15.56897	8.80954
H	-12.76287	15.33570	8.66992
H	-19.81531	13.36178	10.54161
H	-19.57366	14.87213	11.51215
H	-18.21034	13.69254	11.32862
H	-12.88606	13.73166	13.28551
H	-20.23993	16.23225	9.29177
H	-18.84327	8.97291	9.02623
H	-12.47892	14.08136	5.90915
N	-14.82577	13.11436	7.87148
N	-17.50508	14.59925	8.92923
N	-19.34806	15.84059	8.99197
N	-18.20069	9.65711	9.42449

N	-13.21865	13.58395	6.40927
N	-16.96128	11.48414	9.68377
N	-15.16111	13.82020	11.02716
N	-13.68583	13.93632	12.68591
Zn	-16.11331	13.25449	9.37791

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N C H Zn 0

6-31g**

C.1.2 [Zn(mIm)₄]²⁺

C.1.2.2 Optimised

%nprocshared=4

%mem=20GB

%chk=zif8.chk

#p gfinput b3lyp/gen nmr=all prop=efg

zif8

2 1

C	-2.15859100	-2.08525700	-0.18624100
C	-2.15900300	2.08504100	0.18442700
C	2.15782500	-0.18517100	2.08596600
C	2.15947300	0.18549500	-2.08431500
C	2.01493900	-1.63507300	-3.22605600
C	-2.01414600	-3.22693200	1.63436900
C	1.06085600	1.65860400	2.27582400
C	-1.06149800	2.27540900	-1.65897400
C	2.01214100	1.63536900	3.22759700
C	-2.01323900	3.22673300	-1.63606200
C	1.06289000	-1.65842900	-2.27505500
C	-1.06254200	-2.27548500	1.65804300
C	-2.65308800	1.55928400	1.49026000
C	2.65276900	1.49155600	-1.55839100
C	2.65171000	-1.49117600	1.56044800
C	-2.65168700	-1.55956300	-1.49246000

C10

H	2.25196700	-2.36492500	-3.98615900
H	0.33844100	2.43327700	2.07184700
H	2.24664900	2.36417200	3.98946500
H	-2.24848100	3.98812200	-2.36509600
H	-2.25040400	-3.98769300	2.36374800
H	0.34239500	-2.43449600	-2.06988400
H	-0.34101500	-2.07133400	2.43347900
H	-0.33550600	2.07347600	-2.43072300
H	-3.13248900	2.34637100	2.07873800
H	-3.39317200	0.76463000	1.34254100
H	-1.83708000	1.14787100	2.08665100
H	2.19097600	1.72329900	-0.59955300
H	2.43792900	2.31541000	-2.24875700
H	3.73789400	1.47203600	-1.41324300
H	3.12489600	-2.08292700	2.34877500
H	1.83613600	-2.08323900	1.14212000
H	3.39676500	-1.34222000	0.77084600
H	-3.38665700	-0.76018600	-1.34499400
H	-3.13649000	-2.34505400	-2.07856800
H	-1.83407500	-1.15432400	-2.09090900
H	3.50150700	-0.15895600	-3.67520400
H	-3.49323000	-3.68303200	0.15205900
H	-3.49396900	3.68223700	-0.15531900
H	3.49064500	0.15296100	3.68535000
N	1.14141400	0.50066900	1.54691900
N	-1.14231900	-1.54654900	0.50006700
N	-2.71404900	-3.11803600	0.46095600
N	-2.71407800	3.11773600	-0.46321700
N	2.71263700	0.46228900	3.11892100
N	-1.14211800	1.54645900	-0.50106100
N	1.14271800	-0.50047200	-1.54608900
N	2.71519800	-0.46190000	-3.11682200

Zn -0.00007600 0.00002400 -0.00004100

N C H O

6-311+g**

Zn 0

6-311g**

C.1.3 [Zn(pur)₄]²⁺

C.1.3.1 Unoptimised

%nprocshared=4

%mem=20GB

%chk=zif20.chk

#p gfinput b3lyp/gen opt=(modredundant)

zif20

2 1

C -5.92928 -8.58446 -51.71230

C -7.05075 -8.92128 -53.76176

C -10.72393 -16.28803 -51.73088

C -10.19183 -13.65529 -48.37285

C -11.18227 -15.23702 -49.36422

C -10.16108 -14.74640 -50.18233

C -10.05491 -8.67622 -48.11050

C -6.77553 -11.39964 -47.49360

C -8.47117 -10.27679 -48.10191

C -7.89824 -9.66199 -47.01807

C -8.39405 -8.52962 -46.48222

C12

C	-8.73440	-11.79134	-52.72318
C	-7.37854	-10.36651	-51.87509
C	-7.65283	-9.99669	-53.16722
C	-6.29214	-15.00100	-49.38609
C	-4.56137	-14.97530	-50.63262
C	-5.30403	-13.84449	-50.88147
C	-3.75122	-13.20149	-52.41056
C	-3.39291	-15.24144	-51.29782
C	-11.97488	-16.25326	-49.74864
H	-9.94574	-13.03885	-47.69601
H	-10.59386	-16.70422	-52.57055
H	-12.19167	-17.47186	-51.29049
H	-6.10822	-12.07496	-47.46328
H	-7.99932	-8.08147	-45.74822
H	-9.96738	-10.19333	-49.47127
H	-9.29225	-12.55275	-52.82267
H	-7.21402	-8.67074	-54.66170
H	-6.26886	-9.94505	-50.20920
H	-6.93784	-15.28476	-48.74858
H	-3.41294	-12.58223	-53.04825
H	-2.22898	-14.38496	-52.65150
H	-5.43396	-12.13686	-52.01389
H	-2.87855	-16.02783	-51.15761
H	-12.68113	-16.58914	-49.21356
H	-9.23644	-14.93418	-51.97320
H	-9.94540	-7.32287	-46.76674
H	-10.84583	-8.28910	-48.47013
H	-5.32063	-8.05315	-51.21393
H	-5.75913	-7.46194	-53.27965
H	-11.82116	-14.60883	-47.40675
H	-6.17675	-10.20150	-45.84178
H	-8.92734	-10.92363	-54.65517

H	-4.91092	-16.61511	-49.24824
N	-6.18865	-8.23477	-52.93416
N	-4.92303	-12.91162	-51.81055
N	-6.48468	-9.68447	-51.09511
N	-9.91464	-15.26342	-51.39915
N	-9.54596	-13.71469	-49.53564
N	-11.20017	-14.50943	-48.21040
N	-7.75146	-11.40029	-48.40898
N	-6.80618	-10.38595	-46.62076
N	-8.08521	-11.51767	-51.58452
N	-8.53658	-10.90912	-53.71081
N	-5.19992	-15.72473	-49.65304
N	-6.42692	-13.85644	-50.06419
N	-11.67793	-16.74636	-50.96662
N	-9.57184	-9.79347	-48.71030
N	-3.04433	-14.27785	-52.17369
N	-9.52301	-8.10544	-47.10427
Zn	-7.95096	-12.61273	-49.95890

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N C H Zn 0

6-31g**

C.1.3 $[\text{Zn}(\text{pur})_4]^{2+}$

C.1.3.2 Optimised

%nprocshared=4

%mem=20GB

%chk=zif20.chk

#p gfinput b3lyp/gen nmr=all prop=efg

zif20

2 1

C	4.09353000	1.46278000	1.02853500
C	3.33158500	1.83596800	3.23116900
C	-4.71720800	-0.50090100	1.94987400
C	-1.90384600	-2.62152900	-0.51563900
C	-3.75865800	-2.46291000	0.48444600
C	-3.00964800	-1.30564900	0.71372900
C	2.87390200	-3.82231700	0.26534600
C	1.34532700	-0.96727000	-2.57438700
C	1.85217700	-2.21117900	-0.93066400
C	2.66304600	-2.52590600	-1.99102900
C	3.60568800	-3.48602500	-1.92157900
C	0.12765300	0.58525100	2.66451200
C	1.94175300	0.83231100	1.55286600
C	2.14921700	1.27211300	2.83549400
C	-2.00359100	1.33546400	-2.05753200
C	-1.49232300	3.40390400	-1.95642900
C	-0.66336900	2.70041200	-1.11373300
C	0.36516400	4.64762600	-0.55403400
C	-1.40824700	4.76509100	-2.09325000
C	-4.98809000	-2.62859000	1.00387000
H	-1.10630300	-3.01847200	-1.12523700
H	-5.13893600	0.24037000	2.61621000

H	-6.31382200	-1.64632700	2.20386000
H	0.89135900	-0.17937800	-3.15662100
H	4.22896300	-3.86554100	-2.71267000
H	2.02835900	-2.22014300	1.07302700
H	-0.87034500	0.26754400	2.93217900
H	3.61042200	2.16118800	4.21852100
H	3.05385900	0.07517000	0.03896700
H	-2.52198600	0.42272000	-2.31403800
H	1.15985600	5.19989800	-0.06890800
H	-0.23302700	6.30765300	-1.45961900
H	0.25293100	3.07568700	0.64088500
H	-1.96177800	5.38999900	-2.77302200
H	-5.62244100	-3.49568800	0.92699300
H	-3.42619700	0.61721600	0.98382200
H	4.24601200	-4.90990700	-0.60447600
H	2.94268800	-4.43843300	1.15397900
H	4.87914200	1.61245500	0.29946100
H	5.18157500	2.31392100	2.44921300
H	-3.28196400	-4.20717900	-0.66857600
H	2.74590100	-1.70540700	-3.97525500
H	0.81448900	1.30331900	4.52979200
H	-3.10137600	2.71026700	-3.23187000
N	4.28969500	1.87867100	2.24140400
N	0.29965200	3.31568500	-0.35701200
N	2.90345800	0.92831500	0.58413500
N	-3.47695100	-0.29384200	1.46643700
N	-1.80949900	-1.43341800	0.07786600
N	-3.02280100	-3.30804800	-0.29354200
N	0.99826500	-1.20851000	-1.30485500
N	2.33610200	-1.72776800	-3.05435000
N	0.64125300	0.37829700	1.44538300
N	0.98263300	1.10201900	3.55603800

N	-2.35978200	2.51472500	-2.57759300
N	-0.99020900	1.35244200	-1.18531100
N	-5.41692800	-1.58200900	1.73569600
N	1.93877100	-2.83903600	0.25824700
N	-0.42387800	5.31723400	-1.35614900
N	3.62671000	-4.11451200	-0.71908700
Zn	-0.28323900	-0.19415100	-0.19090500

N C H O

6-311+g**

Zn 0

6-311g**

C.1.4 $[\text{Zn}(\text{nIm})_4]^{2+}$

C.1.4.1 Unoptimised

%nprocshared=4

%mem=20GB

%chk=zif65.chk

#p gfinput b3lyp/gen opt=(modredundant)

zif65

2 1

C	15.73502	15.48777	-18.48128
C	18.61188	12.63286	-21.85294
C	14.36498	12.93304	-22.88483
C	15.31515	11.15224	-18.01442
C	19.19049	10.65550	-21.47786

C18

C	13.35389	10.51078	-18.37141
C	18.07820	10.90353	-20.79935
C	14.48290	14.89415	-22.15986
C	17.74607	15.09425	-18.91286
C	13.79417	14.90605	-23.29327
C	17.68848	16.13358	-18.09092
C	13.71986	11.31398	-19.36139
H	13.18261	11.54322	-20.10867
H	19.66563	9.83464	-21.47079
H	12.51404	10.07587	-18.30009
H	17.63358	10.28778	-20.23123
H	14.66933	15.65385	-21.62348
H	18.54152	14.72107	-19.27009
H	13.41108	15.67559	-23.69409
H	18.43629	16.61981	-17.76850
H	20.34636	11.88240	-22.80380
H	14.39253	9.86894	-16.60878
H	13.26140	13.33252	-24.64405
H	16.02591	17.12623	-17.17223
N	16.39433	16.39418	-17.78196
N	14.98179	11.75767	-19.14031
N	19.54413	11.75739	-22.18424
N	14.36646	10.40718	-17.47577
N	17.67391	12.17444	-21.04339
N	14.88017	13.62716	-21.88579
N	16.49117	14.64665	-19.16397
N	13.72212	13.64717	-23.79150
N	16.54480	11.34693	-17.40191
N	14.35248	15.37832	-18.43977
N	18.57737	13.91640	-22.37871
N	14.55238	11.56426	-23.01307
O	17.67162	14.63540	-22.05658

O	13.74342	16.15927	-17.76134
O	16.75137	10.79037	-16.35851
O	13.83539	14.49979	-19.07372
O	19.44761	14.23936	-23.13995
O	14.08464	11.01691	-23.97366
O	17.33569	12.07282	-17.93919
O	15.18433	10.99791	-22.16397
Zn	16.00676	13.05148	-20.30836

1 F

2 F

3 F

4 F

5 F

6 F

7 F

8 F

9 F

10 F

11 F

12 F

25 F

26 F

27 F

28 F

29 F

30 F

31 F

32 F

33 F

34 F

35 F

C20

36 F
37 F
38 F
39 F
40 F
41 F
42 F
43 F
44 F
45 F

N C H Zn O O

6-31g**

C.1.4 [Zn(nIm)₄]²⁺

C.1.4.2 Optimised

%nprocshared=4

%mem=20GB

%chk=zif65.chk

#p ginput b3lyp/gen nmr=all prop=efg

zif65

2 1

C	2.13303800	-0.06489800	-2.18941300
C	-2.13303400	-2.18942500	0.06490400
C	-2.13305000	2.18941100	-0.06491400
C	2.13302700	0.06491100	2.18942500
C	-2.15029700	-2.91632200	2.02876500

C	2.15029500	2.02878000	2.91631900
C	-1.21246100	-1.98322700	1.93452300
C	-1.21246700	1.98321700	-1.93452600
C	1.21247000	-1.93451700	-1.98320900
C	-2.15032100	2.91630600	-2.02877300
C	2.15031400	-2.02876700	-2.91630800
C	1.21244900	1.93452300	1.98321500
H	0.56015400	2.71303300	1.62350700
H	-2.44208400	-3.51026400	2.88330500
H	2.44208100	2.88331700	3.51026500
H	-0.56017400	-1.62351900	2.71304000
H	-0.56021300	1.62347100	-2.71305400
H	0.56018100	-2.71303200	-1.62350100
H	-2.44215800	3.51019500	-2.88333300
H	2.44210200	-2.88330700	-3.51024900
H	-3.52563100	-3.67178900	0.54606500
H	3.52568300	0.54609200	3.67170900
H	-3.52508100	3.67237400	-0.54589500
H	3.52569500	-0.54612100	-3.67173900
N	2.77381200	-0.83259600	-3.05275700
N	1.19691100	0.67412900	1.48384600
N	-2.77379800	-3.05277300	0.83259500
N	2.77379300	0.83260300	3.05275600
N	-1.19691300	-1.48385200	0.67412600
N	-1.19692700	1.48384200	-0.67413500
N	1.19692000	-0.67413200	-1.48384400
N	-2.77382600	3.05275600	-0.83260200
N	2.47155400	-1.26478700	1.98347700
N	2.47155200	1.26480800	-1.98347000
N	-2.47154800	-1.98348800	-1.26479500
N	-2.47156600	1.98346500	1.26479100
O	-1.86532400	-1.14989300	-1.88020000

O	3.36276500	1.72972500	-2.63974400
O	3.36276800	-1.72970800	2.63975500
O	1.86532000	1.88019600	-1.14988200
O	-3.36276000	-2.63976500	-1.72971300
O	-3.36278400	2.63973600	1.72970500
O	1.86533100	-1.88018900	1.14989000
O	-1.86533500	1.14988400	1.88018600
Zn	0.00000200	-0.00000400	-0.00000100

N C H O 0

6-311+g**

Zn 0

6-311g**

C.1.5 [Zn(bIm)₂(nIm)₂]²⁺

C.1.5.1 Unoptimised

%nprocshared=4

%mem=20GB

%chk=zif68.chk

#p ginput b3lyp/gen opt=(modredundant)

zif68

2 1

C	13.58228	-7.30445	26.30539
C	13.64644	-8.16021	24.49559
C	13.96799	-9.08631	25.47816
C	13.67530	-8.53179	23.16122

C	14.31656	-10.37867	25.12071
C	14.29457	-10.69917	23.80456
C	13.98135	-9.83479	22.80952
C	15.64881	-5.33071	23.22368
C	16.72166	-4.41993	22.66035
C	14.89997	-3.46351	22.77683
C	11.51695	-5.36353	21.58511
C	10.44699	-6.56485	22.97819
C	9.76054	-6.56162	21.67609
C	9.92696	-7.28126	24.09137
C	8.56476	-7.30183	21.46384
C	8.17533	-7.95831	22.61064
C	8.75656	-8.01869	23.86025
C	10.31801	-3.01492	26.32493
C	10.54824	-3.77699	25.53131
C	12.55337	-3.44870	26.59388
H	13.45861	-6.63993	26.97219
H	13.48606	-7.88849	22.48598
H	14.56799	-11.00454	25.79202
H	13.96903	-10.09642	21.89708
H	15.78730	-6.22452	23.51196
H	17.63321	-4.65745	22.54272
H	12.19007	-4.79209	21.23167
H	10.34612	-7.26054	24.94465
H	8.13429	-7.33215	20.61649
H	8.40780	-8.55738	24.56179
H	9.47122	-2.61533	26.48380
H	9.92941	-4.13194	24.90439
H	14.55556	-11.73014	23.51482
H	14.11809	-8.91797	27.53485
H	10.33734	-5.53174	19.78999
H	7.25126	-8.54966	22.50280

H	16.69761	-2.51031	21.97396
H	11.60866	-2.09141	27.84310
N	13.92785	-8.52118	26.61292
N	13.41311	-7.03870	25.04005
N	16.23097	-3.32254	22.37816
N	14.56795	-4.73433	23.25137
N	14.06144	-2.57202	22.61764
N	10.50865	-5.74920	20.77257
N	11.61454	-5.75098	22.87584
N	11.95544	-4.12198	25.63187
N	11.54041	-2.74826	27.06247
N	13.73992	-3.47707	26.96535
O	12.86638	-2.87404	22.84638
O	14.43889	-1.53908	22.02070
O	14.00564	-2.75937	27.81452
O	14.42824	-4.15816	26.35781
Zn	12.91257	-5.29668	24.20880

1 F

2 F

3 F

4 F

5 F

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7 F

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9 F

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12 F

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47 F
48 F
49 F
50 F
51 F
52 F
53 F

N C H Zn O 0

6-31g**

C.1.6 [Zn(bIm)₂(nIm)₂]²⁺

C.1.6.1 Optimised

%nprocshared=4

%mem=20GB

C26

%chk=zif68.chk

#p ginput b3lyp/gen nmr=all prop=efg

zif68

2 1

C	0.63579600	2.07387200	1.87537600
C	1.76200000	2.01714900	0.22000100
C	2.22749100	2.99675600	1.08613600
C	2.37143800	1.83859900	-1.01132000
C	3.29974500	3.79218800	0.71596600
C	3.88138900	3.55229600	-0.48386600
C	3.46956700	2.60500900	-1.36045800
C	-1.28835300	2.01271900	-1.86053600
C	-2.41525300	2.32667300	-2.82458800
C	-2.52287200	0.38627200	-2.13893400
C	0.82776900	-1.89556800	-1.93520100
C	2.02675400	-1.83715200	-0.17802100
C	2.59755400	-2.78108000	-1.15263700
C	2.63023700	-1.62375100	1.09206200
C	3.79633200	-3.49658600	-0.88091500
C	4.28502200	-3.19231400	0.37063400
C	3.82011900	-2.32461900	1.33705400
C	-1.78570100	-2.66084000	2.75558300
C	-1.03533200	-2.33555200	1.98440000
C	-2.39649100	-0.50953100	2.24948100
H	-0.14610300	1.84059000	2.58639800
H	2.00457700	1.06896400	-1.68499700
H	3.67237900	4.57516800	1.36972400
H	3.96690800	2.45916000	-2.31228900
H	-0.52445400	2.72211700	-1.56898300
H	-2.57468500	3.27424000	-3.32447700

H	0.00414700	-1.70299200	-2.61333100
H	2.20364200	-0.92696100	1.80550600
H	4.26269800	-4.19997800	-1.55756800
H	4.35572600	-2.21222500	2.27175800
H	-1.95866200	-3.56912700	3.31741900
H	-0.19379200	-2.81336400	1.50761400
H	4.73250900	4.17269500	-0.75607000
H	1.54850300	3.60099300	2.94742200
H	1.82500800	-3.31738500	-3.17218500
H	5.20463200	-3.71440900	0.63717900
H	-3.94081500	1.11395300	-3.54852500
H	-3.47103200	-1.59499800	3.64997900
N	1.49614000	3.01904100	2.12213400
N	0.75099500	1.45090300	0.73565400
N	-3.11536100	1.32288400	-2.98869000
N	-1.36856200	0.83622100	-1.49432200
N	-2.92327000	-0.77793300	-2.05212200
N	1.76796700	-2.78915400	-2.31357000
N	0.84415200	-1.26849600	-0.73848100
N	-1.34129900	-0.96703300	1.60640300
N	-2.69392300	-1.55341200	2.99656100
N	-2.94903800	0.60253400	2.18092900
O	-2.20818200	-1.57330600	-1.39810500
O	-3.85991800	-1.11313100	-2.81113700
O	-3.87973400	0.72913200	2.83251800
O	-2.50242200	1.32620800	1.41698900
Zn	-0.39223400	-0.01745900	0.01935100

N C H O O

6-311+g**

Zn 0

6-311g**

C.1.7 [Zn(nbIm)₂(nIm)₂]²⁺

C.1.7.1 Unoptimised

%nprocshared=4

%mem=20GB

%chk=zif78.chk

#p opt=modredundant b3lyp/gen gfinput

zif78

2 1

C	2.89114100	0.54522900	2.29458400
C	-1.79582000	-1.33541100	0.50285800
C	-2.64121100	-1.73089300	1.53224700
C	-0.78676000	-1.06348300	2.37204300
C	0.55012500	0.80666800	-2.64760800
C	-0.59638500	1.93869000	-1.17642300
C	-0.93459500	2.39229700	-2.44332800
C	-1.18750400	2.47794000	0.00665400
C	-1.88169600	3.44177900	-2.64693100
C	-2.05091700	3.45906300	-0.19327100
C	-2.43356000	3.92243100	-1.54581100
C	2.41656800	2.15478700	1.04424800
C	3.45971400	2.54434200	2.05057900
C	-2.21672800	-1.37315800	-0.85150500
C	-3.95834900	-2.18791400	1.26920000
C	-3.46427900	-1.87637700	-1.07869000
C	-4.31284600	-2.27334500	-0.04542700

C	1.76232500	-3.02313900	-0.76690800
C	2.67982000	-3.68763700	-1.47978500
C	3.39379700	-1.38044900	-1.60765200
H	-0.11646000	-0.84706300	3.00919100
H	1.15477900	0.18215500	-3.03262800
H	-0.97467100	2.15616300	0.87573400
H	-2.10116800	3.77041600	-3.51178200
H	-3.09890400	4.59576600	-1.62552000
H	2.04277000	2.71471800	0.37773000
H	3.86624300	3.39569400	2.13684900
H	-1.66233900	-1.06580800	-1.55967700
H	-4.55921800	-2.42100200	1.96772500
H	2.68633700	-4.78026200	-1.64796800
H	0.89242400	-3.47812800	-0.26773500
H	4.37448300	1.37227100	3.57439300
H	4.44183600	-3.03350600	-2.54371000
H	-0.22952400	1.87217400	-4.39705800
H	-2.40232000	-1.76429200	3.64763100
H	-3.82955600	-1.96513600	-2.11674400
N	2.10772400	0.86751200	1.26382600
N	3.70901700	1.46551800	2.80860400
N	-0.62529800	-0.91016300	0.99995400
N	-2.03639500	-1.57028800	2.71819300
N	0.30263200	0.92342000	-1.26181400
N	-0.21401700	1.73476900	-3.38923300
N	2.97057200	-0.84598700	2.75078400
N	2.15708800	-1.61746100	-0.82257300
N	3.64524300	-2.74966400	-1.97284500
N	4.40012900	-0.43801800	-2.14870500
O	2.20850500	-1.66422700	2.22660100
O	3.72852300	-1.09658100	3.69297100
O	5.31950100	-0.85616900	-2.81723200

O	4.30781000	0.74729900	-1.93799100
Zn	1.00216100	-0.29104300	0.10822900
N	-2.68840300	4.10176400	0.96493700
N	-5.64126200	-2.80253000	-0.38627300
O	-3.48794800	4.99988100	0.74291400
O	-2.35727700	3.67918000	2.07336400
O	-6.36586600	-3.11150600	0.55373900
O	-5.91772400	-2.89706300	-1.57708100

51 F

41 F

39 F

37 F

44 F

N C H Zn O 0

6-31g**

C.1.7 $[\text{Zn}(\text{nbIm})_2(\text{nIm})_2]^{2+}$

C.1.7.2 Optimised

%nprocshared=4

%mem=20GB

%chk=zif78.chk

#p gfinput b3lyp/gen nmr=all prop=efg

zif78

2 1

C	3.02151800	0.65486600	2.07039800
---	------------	------------	------------

C	-1.71881700	-1.33851900	0.46931200
C	-2.61285500	-1.59067300	1.53070300
C	-0.68737800	-0.83975200	2.32512900
C	0.59555600	0.85861500	-2.69604900
C	-0.66583400	1.82554400	-1.21454500
C	-0.95740100	2.42453200	-2.45811400
C	-1.32193000	2.24830200	-0.05828300
C	-1.89899900	3.44798500	-2.60339600
C	-2.25429000	3.26153200	-0.21690100
C	-2.55309700	3.86442000	-1.45099100
C	2.41534400	2.29231300	0.82268400
C	3.35795100	2.78234100	1.70358100
C	-2.10631300	-1.58885800	-0.85449100
C	-3.90233900	-2.08129100	1.33696000
C	-3.38582400	-2.08015900	-1.07032900
C	-4.24847900	-2.31149900	0.01480300
C	1.94534200	-3.00106200	-0.72410100
C	2.96031800	-3.74138000	-1.29146500
C	3.37519800	-1.60220800	-1.50913700
H	0.05867000	-0.54068400	3.04501700
H	1.32414000	0.23029800	-3.18454000
H	-1.14899100	1.83156000	0.92379400
H	-2.11555800	3.90069900	-3.56470400
H	-3.29716000	4.65123300	-1.48034500
H	1.89278500	2.81715400	0.03916200
H	3.77686400	3.76975800	1.82665900
H	-1.43843700	-1.40727300	-1.68868400
H	-4.60710400	-2.28156600	2.13514900
H	3.10794800	-4.80740100	-1.37758900
H	1.05956500	-3.35527700	-0.21916700
H	4.40638000	1.70545300	3.24076400
H	4.73209500	-3.00444100	-2.26214300

H	-0.07268100	1.95447000	-4.36104900
H	-2.25792700	-1.31000100	3.63422100
H	-3.74973800	-2.29662700	-2.06718300
N	2.20941700	0.95393300	1.06199000
N	3.72923400	1.72224700	2.48324400
N	-0.51371700	-0.85723800	1.00397200
N	-1.91282400	-1.25674000	2.68368500
N	0.31811500	0.83940100	-1.39772500
N	-0.13327400	1.77456600	-3.36661500
N	3.14825700	-0.64135100	2.67286000
N	2.21109400	-1.65527700	-0.86741500
N	3.85455300	-2.83065600	-1.77973300
N	4.08715800	-0.41491300	-1.90415400
O	2.39402800	-1.51950600	2.23311200
O	3.97820800	-0.75969900	3.56193700
O	5.17675700	-0.58910100	-2.43419300
O	3.53114800	0.66248000	-1.67917000
Zn	1.07605500	-0.28239800	0.01944600
N	-2.97197700	3.71983000	0.99517200
N	-5.60834300	-2.83499300	-0.26683000
O	-3.77751000	4.62898300	0.86059800
O	-2.70090900	3.14516300	2.05011000
O	-6.33342200	-3.03652500	0.69998300
O	-5.89609400	-3.02271600	-1.44318700

N C H O 0

6-311+g**

Zn 0

6-311g**
