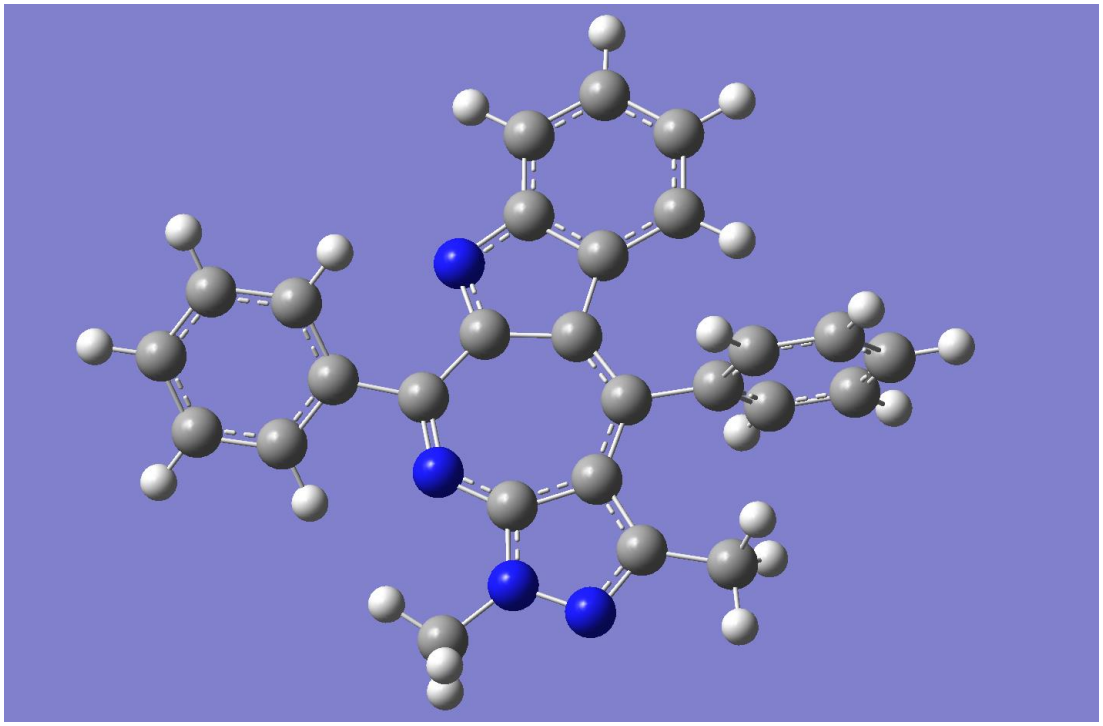
Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Computational details

All calculations were performed using Gaussian 16 package [1] based on density functional theory with the B3LYP functional [2-4] and a 6-31G(d,p) basis set. Nucleus-independent chemical shift (NICS) [5] calculations were performed using gauge-independent atomic orbitals (GIAO) [6,7] method.



Entering Gaussian System, Link 0=/public3/home/sc40234/g16/g16

Input=nics_nmr.gjf

Output=nics_nmr.log

Initial command:

/public3/home/sc40234/g16/l1.exe "/public3/home/sc40234/tmp/Gau-

44865.inp" -scrdir="/public3/home/sc40234/tmp/"

Entering Link 1 = /public3/home/sc40234/g16/l1.exe PID= 44867.

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Cite this work as:

Gaussian 16, Revision C.01,

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J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas,

J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2019.

****

Gaussian 16: ES64L-G16RevC.01 3-Jul-2019

19-May-2023

****

%mem=200GB

%nprocshared=64

Will use up to 64 processors via shared memory.

%chk=nics_opt.chk

---

nmr b3lyp/6-31g(d,p)

1/38=1,172=1/1;

2/12=2,17=6,18=5,40=1/2;

3/5=1,6=6,7=101,11=2,25=1,30=1,74=-5/1,2,3,8;

4//1;

5/5=2,38=5/2;

8/6=1,10=90,11=11/1;

10/13=100,45=16/2;

6/7=2,8=2,9=2,10=2,28=1/1;

99/9=1/99;

Title Card Required

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	0.90392	2.09855	-0.06891
C	2.13859	2.77458	-0.07738
H	3.07948	2.24559	-0.02068
C	2.14519	4.16335	-0.15733
H	3.09686	4.68683	-0.1622
C	0.95029	4.90495	-0.23175
H	0.99602	5.98835	-0.29449
C	-0.27896	4.2622	-0.22418
H	-1.2154	4.80741	-0.28042
C	-0.29353	2.8632	-0.14033
C	0.46683	0.707	-0.01159
C	-1.02185	0.81671	-0.03555
C	-2.02244	-0.23942	0.0089
C	-0.61168	-2.15712	-0.00963
C	0.7638	-1.76971	0.02378

C	1.25828	-0.43093	0.02448
C	-3.47506	0.11814	0.03809
C	-4.37283	-0.68428	-0.68666
H	-3.97945	-1.50147	-1.28108
C	-5.74189	-0.43388	-0.65626
H	-6.41677	-1.05497	-1.23821
C	-6.24403	0.61081	0.12198
H	-7.31238	0.80505	0.15279
C	-5.36429	1.4043	0.85936
H	-5.74692	2.21422	1.47361
C	-3.9911	1.17051	0.81232
H	-3.3162	1.80125	1.3742
C	1.47725	-3.02212	0.03825
C	-1.76414	-4.40438	-0.04424
H	-1.67621	-5.13691	0.76095
H	-2.65708	-3.79667	0.09059

H	-1.81159	-4.93153	-1.00166
C	2.94189	-3.34269	0.0807
H	3.42871	-2.9227	0.9647
H	3.04949	-4.4292	0.10234
H	3.47392	-2.95438	-0.79167
C	2.74771	-0.25765	0.04928
C	3.42586	-0.13512	1.2688
H	2.86483	-0.16631	2.19808
C	4.81073	0.0362	1.29146
H	5.32565	0.13266	2.24277
C	5.53089	0.08795	0.09644
H	6.60817	0.22305	0.11467
C	4.86007	-0.03192	-1.12225
H	5.41349	0.01189	-2.05566
C	3.47551	-0.20432	-1.14649
H	2.95279	-0.28889	-2.09459

N	-1.42423	2.0746	-0.11664
N	-1.80147	-1.53081	-0.00429
N	-0.61356	-3.52183	-0.01409
N	0.63248	-4.04523	0.01191
Bq	0.92758	3.51114	-0.14998
Bq	-0.27377	1.71201	-0.0746
Bq	-0.42408	-0.65775	-0.00056
Bq	0.32966	-2.9032	0.01004
Bq	4.14179	-0.08414	0.07287
Bq	-4.86487	0.36427	0.08147

Symmetry turned off:

Cannot cope with ghost atoms or with translation vectors.

Stoichiometry C27H20N4

Framework group C1[X(C27H20N4)]

NumDoF: NAt= 51 NAtoms= 57

Deg. of freedom 0

Full point group C1 NOp 1

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.903920	2.098552	-0.068909
2	6	0	2.138594	2.774577	-0.077382
3	1	0	3.079484	2.245589	-0.020679
4	6	0	2.145188	4.163347	-0.157333
5	1	0	3.096855	4.686826	-0.162197
6	6	0	0.950292	4.904954	-0.231745
7	1	0	0.996024	5.988352	-0.294490
8	6	0	-0.278963	4.262203	-0.224184
9	1	0	-1.215398	4.807411	-0.280423

10	6	0	-0.293532	2.863199	-0.140328
11	6	0	0.466825	0.707003	-0.011588
12	6	0	-1.021855	0.816710	-0.035553
13	6	0	-2.022444	-0.239424	0.008901
14	6	0	-0.611678	-2.157116	-0.009627
15	6	0	0.763803	-1.769709	0.023783
16	6	0	1.258280	-0.430934	0.024484
17	6	0	-3.475061	0.118142	0.038085
18	6	0	-4.372831	-0.684278	-0.686662
19	1	0	-3.979453	-1.501465	-1.281081
20	6	0	-5.741886	-0.433881	-0.656260
21	1	0	-6.416771	-1.054975	-1.238214
22	6	0	-6.244027	0.610814	0.121983
23	1	0	-7.312380	0.805053	0.152787
24	6	0	-5.364294	1.404300	0.859360
25	1	0	-5.746924	2.214218	1.473611

26	6	0	-3.991102	1.170511	0.812323
27	1	0	-3.316202	1.801247	1.374196
28	6	0	1.477249	-3.022117	0.038253
29	6	0	-1.764137	-4.404376	-0.044241
30	1	0	-1.676207	-5.136912	0.760949
31	1	0	-2.657075	-3.796670	0.090592
32	1	0	-1.811589	-4.931534	-1.001661
33	6	0	2.941890	-3.342691	0.080703
34	1	0	3.428707	-2.922695	0.964703
35	1	0	3.049494	-4.429198	0.102342
36	1	0	3.473922	-2.954376	-0.791667
37	6	0	2.747713	-0.257647	0.049284
38	6	0	3.425857	-0.135122	1.268799
39	1	0	2.864825	-0.166309	2.198080
40	6	0	4.810730	0.036204	1.291458
41	1	0	5.325647	0.132659	2.242766

42	6	0	5.530887	0.087949	0.096435
43	1	0	6.608171	0.223053	0.114671
44	6	0	4.860071	-0.031916	-1.122254
45	1	0	5.413488	0.011885	-2.055657
46	6	0	3.475510	-0.204318	-1.146491
47	1	0	2.952793	-0.288888	-2.094588
48	7	0	-1.424229	2.074601	-0.116643
49	7	0	-1.801468	-1.530808	-0.004286
50	7	0	-0.613558	-3.521832	-0.014093
51	7	0	0.632481	-4.045232	0.011906
52	0	0	0.927583	3.511139	-0.149980
53	0	0	-0.273774	1.712013	-0.074604
54	0	0	-0.424077	-0.657754	-0.000555
55	0	0	0.329659	-2.903201	0.010044
56	0	0	4.141795	-0.084142	0.072872
57	0	0	-4.864867	0.364268	0.081472

Rotational constants (GHZ): 0.2082431 0.1253609 0.0815285

Standard basis: 6-31G(d,p) (6D, 7F)

Warning: center 52 has no basis functions!

Warning: center 53 has no basis functions!

Warning: center 54 has no basis functions!

Warning: center 55 has no basis functions!

Warning: center 56 has no basis functions!

Warning: center 57 has no basis functions!

565 basis functions, 1008 primitive gaussians, 565 cartesian basis functions

105 alpha electrons 105 beta electrons

nuclear repulsion energy 2827.3863143055 Hartrees.

NAtoms= 57 NActive= 57 NUniq= 57 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned off.

One-electron integrals computed using PRISM.

NBasis= 565 RedAO= T EigKep= 2.75D-04 NBF= 565

NBsUse= 565 1.00D-06 EigRej= -1.00D+00 NBFU= 565

ExpMin= 1.61D-01 ExpMax= 4.17D+03 ExpMxC= 6.27D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Integral accuracy reduced to 1.0D-05 until final iterations.

Initial convergence to 1.0D-05 achieved. Increase integral accuracy.

SCF Done: E(RB3LYP) = -1259.94889794 A.U. after 17 cycles

NFock= 17 Conv=0.78D-08 -V/T= 2.0096

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 565

NBasis= 565 NAE= 105 NBE= 105 NFC= 0 NFV= 0

NROrb= 565 NOA= 105 NOB= 105 NVA= 460 NVB= 460

Differentiating once with respect to magnetic field using GIAOs.

Electric field/nuclear overlap derivatives assumed to be zero.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1=

0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 6100 IOpCl= 0 I1Cent= 7 NGrid= 57

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

FoFJK: IHMeth= 1 ICntrl= 6127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 1 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0 IntGTp=1.

There are 3 degrees of freedom in the 1st order CPHF. IDoFFX=0 NUNeed= 3.

3 vectors produced by pass 0 Test12= 1.61D-12 3.33D-08 XBig12= 1.33D+02 2.05D+00.

AX will form 3 AO Fock derivatives at one time.

3 vectors produced by pass 1 Test12= 1.61D-12 3.33D-08 XBig12= 3.88D-01 1.45D-01.

3 vectors produced by pass 2 Test12= 1.61D-12 3.33D-08 XBig12= 1.16D-03 1.43D-02.

3 vectors produced by pass 3 Test12= 1.61D-12 3.33D-08 XBig12= 1.04D-05 1.43D-03.

3 vectors produced by pass 4 Test12= 1.61D-12 3.33D-08 XBig12= 3.27D-08 6.27D-05.

3 vectors produced by pass 5 Test12= 1.61D-12 3.33D-08 XBig12= 1.03D-10 2.89D-06.

3 vectors produced by pass 6 Test12= 1.61D-12 3.33D-08 XBig12= 3.95D-13 3.09D-07.

InvSVY: IOpt=1 It= 1 EMax= 7.11D-15

Solved reduced A of dimension 21 with 3 vectors.

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 66.0425 Anisotropy = 153.4221

XX= 30.7247 YX= -2.3207 ZX= -2.9887

XY= 0.0060 YY= -0.1363 ZY= 9.1682

XZ= -5.1639 YZ= 11.9177 ZZ= 167.5390

Eigenvalues: -0.8223 30.6259 168.3239

2 C Isotropic = 72.2283 Anisotropy = 160.2094

XX= -5.2453 YX= 16.0344 ZX= -6.0400

XY= 22.1092 YY= 43.6283 ZY= 8.8014

XZ= -6.7571 YZ= 9.0286 ZZ= 178.3020

Eigenvalues: -12.2286 49.8790 179.0346

3 H Isotropic = 25.4304 Anisotropy = 17.7292

XX= 23.9150 YX= -0.7126 ZX= 0.1510

XY= -3.6184 YY= 36.8728 ZY= -0.7558

XZ= 0.1111 YZ= -0.6850 ZZ= 15.5032

Eigenvalues: 15.4785 23.5628 37.2498

4 C Isotropic = 72.7537 Anisotropy = 159.4516

XX= -7.8800 YX= -33.7116 ZX= -2.9785

XY= -35.8800 YY= 47.5378 ZY= 6.6823

XZ= -2.0953 YZ= 6.8169 ZZ= 178.6032

Eigenvalues: -24.6538 63.8601 179.0547

5 H Isotropic = 24.6010 Anisotropy = 8.0750

XX= 25.1116 YX= -1.4404 ZX= 0.1942

XY= -1.5086 YY= 29.5100 ZY= -0.4784

XZ= 0.1624 YZ= -0.5165 ZZ= 19.1814

Eigenvalues: 19.1555 24.6632 29.9844

6 C Isotropic = 69.1775 Anisotropy = 165.6929

XX= 55.2169 YX= 5.9039 ZX= -3.4736

XY= 1.7351 YY= -26.5026 ZY= 12.2240

XZ= -3.6727 YZ= 12.3288 ZZ= 178.8183

Eigenvalues: -27.4302 55.3233 179.6395

7 H Isotropic = 24.1404 Anisotropy = 5.1131

XX= 27.5482 YX= 0.2617 ZX= 0.1489

XY= -0.2885 YY= 25.4314 ZY= -0.2286

XZ= 0.0092 YZ= -0.4114 ZZ= 19.4415

Eigenvalues: 19.4237 25.4483 27.5491

8 C Isotropic = 73.7389 Anisotropy = 149.4439

XX= 17.6700 YX= 32.9325 ZX= -5.8814

XY= 36.5469 YY= 30.8908 ZY= 9.5366

XZ= -6.5852 YZ= 9.0359 ZZ= 172.6559

Eigenvalues: -11.7068 59.5553 173.3682

9 H Isotropic = 23.6596 Anisotropy = 6.8779

XX= 25.6295 YX= 1.6554 ZX= -0.0065

XY= 1.8272 YY= 27.0276 ZY= -0.2628

XZ= -0.4193 YZ= -0.9699 ZZ= 18.3218

Eigenvalues: 18.2772 24.4568 28.2449

10 C Isotropic = 42.5791 Anisotropy = 148.5046

XX= -16.6900 YX= -17.1536 ZX= -2.4449

XY= -8.3829 YY= 3.9620 ZY= 8.0840

XZ= -6.8905 YZ= 14.2919 ZZ= 140.4654

Eigenvalues: -22.7875 8.9427 141.5822

11 C Isotropic = 59.8482 Anisotropy = 126.4166

XX= 14.9697 YX= -20.1306 ZX= -0.7588

XY= -32.1700 YY= 21.2020 ZY= 4.0794

XZ= 1.3456 YZ= 14.8547 ZZ= 143.3729

Eigenvalues: -8.5297 43.9484 144.1260

12 C Isotropic = 42.2230 Anisotropy = 119.5002

XX= -18.3170 YX= -15.0067 ZX= 1.2879

XY= -31.0890 YY= 23.3392 ZY= 7.0422

XZ= -2.8459 YZ= 2.2123 ZZ= 121.6469

Eigenvalues: -28.5626 33.3419 121.8898

13 C Isotropic = 34.9890 Anisotropy = 141.1968

XX= -24.9556 YX= -4.2180 ZX= 4.1828

XY= 17.9226 YY= 1.4722 ZY= 1.8783

XZ= 3.3971 YZ= 14.9225 ZZ= 128.4504

Eigenvalues: -26.6454 2.4922 129.1202

14 C Isotropic = 49.5075 Anisotropy = 102.9327

XX= 23.7777 YX= 5.9983 ZX= -1.8429

XY= -2.6911 YY= 6.6736 ZY= 0.2897

XZ= -1.2511 YZ= 3.5793 ZZ= 118.0713

Eigenvalues: 6.4766 23.9167 118.1293

15 C Isotropic = 80.1168 Anisotropy = 108.1257

XX= 35.4229 YX= 5.0584 ZX= -2.7675

XY= 8.5884 YY= 52.8600 ZY= 0.9525

XZ= -1.1613 YZ= -7.0188 ZZ= 152.0674

Eigenvalues: 33.0639 55.0858 152.2006

16 C Isotropic = 45.7932 Anisotropy = 161.1323

XX= -16.2248 YX= -15.8055 ZX= -2.8829

XY= -1.3286 YY= 0.4813 ZY= 2.2322

XZ= -1.0548 YZ= 4.0394 ZZ= 153.1232

Eigenvalues: -19.8390 4.0039 153.2148

17 C Isotropic = 53.1906 Anisotropy = 162.0953

XX= -22.0858 YX= 24.6391 ZX= -8.4806

XY= 19.1488 YY= 81.9100 ZY= -59.6694

XZ= -11.2715 YZ= -74.7717 ZZ= 99.7474

Eigenvalues: -26.6606 24.9782 161.2541

18 C Isotropic = 65.3167 Anisotropy = 162.1715

XX= 47.5632 YX= 25.3668 ZX= 7.8711

XY= 27.2719 YY= 52.1497 ZY= -96.0728

XZ= -8.5686 YZ= -92.8552 ZZ= 96.2371

Eigenvalues: -28.3897 50.9087 173.4310

19 H Isotropic = 23.3649 Anisotropy = 9.2498

XX= 28.2280 YX= -0.0563 ZX= 2.1544

XY= -0.0451 YY= 22.1464 ZY= 0.7731

XZ= 4.9394 YZ= 1.6750 ZZ= 19.7205

Eigenvalues: 18.0977 22.4657 29.5315

20 C Isotropic = 69.8370 Anisotropy = 163.6457

XX= 27.6142 YX= -23.7451 ZX= -36.8347

XY= -22.5315 YY= 79.9396 ZY= -83.2210

XZ= -37.8515 YZ= -89.0503 ZZ= 101.9570

Eigenvalues: -28.0805 58.6573 178.9341

21 H Isotropic = 24.1694 Anisotropy = 5.3834

XX= 26.9683 YX= -1.5869 ZX= -0.2974

XY= -1.3939 YY= 24.0301 ZY= 2.0716

XZ= -0.1888 YZ= 1.7680 ZZ= 21.5097

Eigenvalues: 20.4333 24.3165 27.7583

22 C Isotropic = 67.3831 Anisotropy = 169.1909

XX= -27.3239 YX= 21.2942 ZX= -7.0293

XY= 19.6292 YY= 100.1843 ZY= -62.2838

XZ= -2.1888 YZ= -62.6647 ZZ= 129.2888

Eigenvalues: -30.7263 52.6985 180.1770

23 H Isotropic = 24.1956 Anisotropy = 4.2038

XX= 24.6743 YX= 0.0614 ZX= 0.4886

XY= -0.0039 YY= 24.9798 ZY= 2.8040

XZ= 0.7099 YZ= 2.7998 ZZ= 22.9326

Eigenvalues: 20.9129 24.6757 26.9981

24 C Isotropic = 70.8614 Anisotropy = 163.2764

XX= 48.1971 YX= 29.3111 ZX= 8.7261

XY= 28.7301 YY= 60.3125 ZY= -94.3370

XZ= 7.4314 YZ= -93.5183 ZZ= 104.0745

Eigenvalues: -24.8860 57.7578 179.7123

25 H Isotropic = 24.2367 Anisotropy = 5.1614

XX= 27.6046 YX= 0.3306 ZX= 0.8666

XY= 0.3453 YY= 23.3457 ZY= 1.6358

XZ= -0.1768 YZ= 2.0616 ZZ= 21.7596

Eigenvalues: 20.5396 24.4928 27.6776

26 C Isotropic = 61.7030 Anisotropy = 174.4968

XX= 16.0138 YX= -13.8282 ZX= -33.7410

XY= -9.4597 YY= 65.8225 ZY= -93.0461

XZ= -38.4497 YZ= -84.5478 ZZ= 103.2726

Eigenvalues: -29.4763 36.5511 178.0341

27 H Isotropic = 22.7638 Anisotropy = 11.1089

XX= 27.5356 YX= -1.5551 ZX= -2.5996

XY= -1.8192 YY= 22.6653 ZY= 2.0456

XZ= -6.5890 YZ= 2.2909 ZZ= 18.0905

Eigenvalues: 15.9257 22.1960 30.1697

28 C Isotropic = 48.1006 Anisotropy = 127.0471

XX= -14.5817 YX= 37.5435 ZX= -3.9145

XY= 8.2602 YY= 26.2409 ZY= 0.0850

XZ= -5.6788 YZ= 1.2994 ZZ= 132.6425

Eigenvalues: -24.9858 36.4888 132.7986

29 C Isotropic = 158.4260 Anisotropy = 47.4967

XX= 171.5058 YX= 21.4662 ZX= -0.0545

XY= 27.8774 YY= 157.2995 ZY= -0.3486

XZ= 3.0355 YZ= -1.0361 ZZ= 146.4726

Eigenvalues: 138.4659 146.7216 190.0904

30 H Isotropic = 28.0300 Anisotropy = 9.5374

XX= 27.4075 YX= 2.9231 ZX= -0.8115

XY= 1.6023 YY= 30.6256 ZY= -3.7016

XZ= -0.3506 YZ= -5.9399 ZZ= 26.0568

Eigenvalues: 22.8796 26.8221 34.3882

31 H Isotropic = 26.5321 Anisotropy = 7.9610

XX= 31.2578 YX= -1.9250 ZX= -0.5008

XY= -0.4372 YY= 29.4337 ZY= 0.4670

XZ= 0.1178 YZ= -0.6497 ZZ= 18.9046

Eigenvalues: 18.9005 28.8563 31.8394

32 H Isotropic = 28.0731 Anisotropy = 10.1139

XX= 27.4446 YX= 2.9500 ZX= 1.9431

XY= 2.2807 YY= 29.1290 ZY= 3.9592

XZ= 2.5227 YZ= 5.5740 ZZ= 27.6457

Eigenvalues: 23.5634 25.8402 34.8157

33 C Isotropic = 174.3808 Anisotropy = 21.3289

XX= 185.3854 YX= -9.5226 ZX= 0.9205

XY= -3.7973 YY= 174.6745 ZY= -0.2077

XZ= 0.4355 YZ= -0.5913 ZZ= 163.0826

Eigenvalues: 163.0580 171.4844 188.6001

34 H Isotropic = 30.1212 Anisotropy = 8.1225

XX= 28.9608 YX= 1.0392 ZX= 3.9985

XY= 2.6215 YY= 34.4318 ZY= -0.6731

XZ= 5.3018 YZ= 1.6277 ZZ= 26.9710

Eigenvalues: 23.1551 31.6724 35.5362

35 H Isotropic = 29.6941 Anisotropy = 10.5344

XX= 29.2797 YX= -2.7080 ZX= 0.1895

XY= 0.1003 YY= 36.4842 ZY= -0.1120

XZ= 0.2631 YZ= -0.2827 ZZ= 23.3182

Eigenvalues: 23.3080 29.0572 36.7170

36 H Isotropic = 30.0681 Anisotropy = 8.0613

XX= 29.3810 YX= 1.0236 ZX= -3.9481

XY= 2.5279 YY= 34.3156 ZY= 0.7908

XZ= -5.3400 YZ= -1.6808 ZZ= 26.5076

Eigenvalues: 23.0390 31.7230 35.4423

37 C Isotropic = 53.3967 Anisotropy = 173.1172

XX= -36.6459 YX= -24.6135 ZX= -0.5943

XY= -22.5931 YY= 165.9819 ZY= -4.1242

XZ= -0.9404 YZ= -4.0067 ZZ= 30.8542

Eigenvalues: -39.3805 30.7624 168.8082

38 C Isotropic = 68.1269 Anisotropy = 164.2977

XX= 37.6312 YX= -16.2191 ZX= 31.6714

XY= -15.6009 YY= 175.6459 ZY= -1.6677

XZ= 37.9739 YZ= -2.4990 ZZ= -8.8964

Eigenvalues: -27.6711 54.3931 177.6587

39 H Isotropic = 24.1079 Anisotropy = 9.0791

XX= 26.6873 YX= 0.6877 ZX= 2.8635

XY= 0.6536 YY= 21.8882 ZY= 0.7147

XZ= 6.4480 YZ= -0.1465 ZZ= 23.7482

Eigenvalues: 20.3172 21.8459 30.1607

40 C Isotropic = 67.6791 Anisotropy = 172.3768

XX= 36.3596 YX= -19.1116 ZX= -33.6636

XY= -19.2912 YY= 179.8539 ZY= -11.0009

XZ= -32.7155 YZ= -10.6380 ZZ= -13.1764

Eigenvalues: -31.4160 51.8562 182.5970

41 H Isotropic = 23.9388 Anisotropy = 4.6194

XX= 26.9098 YX= 0.7382 ZX= -0.8119

XY= 0.7662 YY= 21.3000 ZY= 0.0652

XZ= 0.4677 YZ= -0.2258 ZZ= 23.6068

Eigenvalues: 21.1995 23.5985 27.0185

42 C Isotropic = 68.7870 Anisotropy = 172.1541

XX= -24.6919 YX= -25.8401 ZX= -0.8278

XY= -26.3300 YY= 180.1675 ZY= -4.1165

XZ= -0.8386 YZ= -4.1191 ZZ= 50.8852

Eigenvalues: -27.9839 50.7884 183.5564

43 H Isotropic = 23.9584 Anisotropy = 2.6766

XX= 24.8123 YX= 0.4742 ZX= -0.0238

XY= 0.4220 YY= 21.3273 ZY= 0.1700

XZ= -0.0547 YZ= 0.1737 ZZ= 25.7355

Eigenvalues: 21.2637 24.8686 25.7428

44 C Isotropic = 67.5919 Anisotropy = 172.5933

XX= 33.5230 YX= -17.3990 ZX= 36.4174

XY= -17.5924 YY= 180.4713 ZY= -0.6212

XZ= 35.5857 YZ= -0.7552 ZZ= -11.2185

Eigenvalues: -31.5320 51.6537 182.6541

45 H Isotropic = 23.9458 Anisotropy = 4.6389

XX= 26.9043 YX= 0.7883 ZX= 0.9042

XY= 0.8020 YY= 21.3678 ZY= 0.1713

XZ= -0.4392 YZ= 0.4994 ZZ= 23.5654

Eigenvalues: 21.2175 23.5816 27.0384

46 C Isotropic = 68.0102 Anisotropy = 164.7320

XX= 39.9628 YX= -17.8393 ZX= -28.4383

XY= -17.5004 YY= 175.4397 ZY= -9.4314

XZ= -34.7933 YZ= -8.2947 ZZ= -11.3719

Eigenvalues: -27.6365 53.8355 177.8316

47 H Isotropic = 24.1408 Anisotropy = 9.0893

XX= 27.0266 YX= 0.5431 ZX= -2.7686

XY= 0.4739 YY= 22.0591 ZY= -0.4395

XZ= -6.5236 YZ= 0.5120 ZZ= 23.3366

Eigenvalues: 20.1305 22.0915 30.2003

48 N Isotropic = -54.9069 Anisotropy = 412.7336

XX= -102.6126 YX= -79.7303 ZX= 0.5578

XY= -108.9834 YY= -281.7797 ZY= 28.1638

XZ= -5.8392 YZ= 2.7620 ZZ= 219.6717

Eigenvalues: -322.6253 -62.3442 220.2488

49 N Isotropic = -16.8048 Anisotropy = 407.7722

XX= -125.7542 YX= 89.3603 ZX= 5.4869

XY= 93.2899 YY= -176.7003 ZY= -0.1761

XZ= -25.2964 YZ= 72.0177 ZZ= 252.0400

Eigenvalues: -248.4350 -57.0228 255.0433

50 N Isotropic = 59.0906 Anisotropy = 105.5851

XX= 11.4416 YX= -71.9105 ZX= -3.4164

XY= -47.0072 YY= 36.3577 ZY= -1.2690

XZ= 4.3460 YZ= 3.0129 ZZ= 129.4723

Eigenvalues: -36.8553 84.6463 129.4806

51 N Isotropic = -53.8191 Anisotropy = 309.7473

XX= -243.3653 YX= 23.1944 ZX= -9.9084

XY= 7.2891 YY= -70.4206 ZY= -2.2485

XZ= -13.5995 YZ= 1.8876 ZZ= 152.3284

Eigenvalues: -245.0424 -69.0941 152.6790

52 Bq Isotropic = 11.1328 Anisotropy = 5.3160

XX= 8.6083 YX= -0.9914 ZX= 0.0290

XY= -2.7390 YY= 10.1368 ZY= 0.0745

XZ= -0.3240 YZ= 0.3967 ZZ= 14.6533

Eigenvalues: 7.3569 11.3648 14.6768

53 Bq Isotropic = 9.0361 Anisotropy = 12.6490

XX= 16.8661 YX= -2.0447 ZX= 0.4488

XY= -2.4847 YY= 8.9474 ZY= -0.7022

XZ= -1.1675 YZ= -1.1335 ZZ= 1.2949

Eigenvalues: 1.1606 8.4790 17.4688

54 Bq Isotropic = 2.3580 Anisotropy = 8.0837

XX= 7.1770 YX= 0.6177 ZX= -0.0547

XY= 1.6543 YY= 5.2123 ZY= 1.1646

XZ= 0.9473 YZ= 0.7714 ZZ= -5.3152

Eigenvalues: -5.4128 4.7398 7.7472

55 Bq Isotropic = 12.4307 Anisotropy = 13.6459

XX= 14.8642 YX= 5.0136 ZX= 0.4033

XY= 6.4352 YY= 16.5611 ZY= 0.9933

XZ= -0.2190 YZ= 0.6074 ZZ= 5.8667

Eigenvalues: 5.7889 9.9752 21.5280

56 Bq Isotropic = 8.4023 Anisotropy = 10.8094

XX= 6.9908 YX= -0.8511 ZX= 0.1054

XY= -0.7526 YY= 15.5276 ZY= -0.2818

XZ= 0.0561 YZ= -0.2771 ZZ= 2.6886

Eigenvalues: 2.6816 6.9168 15.6086

57 Bq Isotropic = 8.6303 Anisotropy = 3.6668

XX= 8.3804 YX= -0.0588 ZX= -0.3037

XY= -0.0121 YY= 9.8373 ZY= -1.8905

XZ= -0.5726 YZ= -2.1805 ZZ= 7.6731

Eigenvalues: 6.3724 8.4436 11.0748

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

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Population analysis using the SCF Density.

****

Alpha occ. eigenvalues -- -14.41501 -14.35577 -14.34189 -14.31342 -10.26733

Alpha occ. eigenvalues -- -10.25349 -10.23651 -10.22807 -10.22594 -10.22560

Alpha occ. eigenvalues -- -10.21224 -10.21045 -10.20819 -10.20384 -10.20366

Alpha occ. eigenvalues -- -10.20300 -10.20286 -10.20272 -10.20269 -10.19415

Alpha occ. eigenvalues -- -10.18913 -10.18683 -10.18592 -10.18586 -10.18478

Alpha occ. eigenvalues -- -10.18404 -10.18340 -10.18298 -10.18298 -10.18242

Alpha occ. eigenvalues -- -10.18137 -1.05887 -0.95860 -0.93776 -0.87711

Alpha occ. eigenvalues -- -0.85755 -0.84831 -0.83397 -0.82414 -0.78868

Alpha occ. eigenvalues -- -0.76047 -0.75706 -0.75118 -0.73993 -0.73788

Alpha occ. eigenvalues -- -0.73070 -0.72660 -0.68813 -0.66904 -0.65214

Alpha occ. eigenvalues -- -0.61712 -0.61680 -0.61220 -0.59441 -0.59337

Alpha occ. eigenvalues -- -0.57354 -0.56722 -0.55740 -0.53928 -0.52469

Alpha occ. eigenvalues -- -0.50805 -0.49318 -0.49030 -0.48678 -0.48175

Alpha occ. eigenvalues -- -0.46598 -0.46358 -0.45978 -0.45147 -0.44195

Alpha occ. eigenvalues -- -0.43380 -0.43165 -0.42685 -0.42436 -0.42151

Alpha occ. eigenvalues -- -0.41879 -0.41702 -0.41293 -0.40984 -0.39651

Alpha occ. eigenvalues -- -0.39460 -0.39090 -0.39030 -0.37041 -0.36754

Alpha occ. eigenvalues -- -0.35922 -0.35811 -0.35196 -0.34910 -0.34138

Alpha occ. eigenvalues -- -0.33811 -0.33428 -0.32527 -0.31317 -0.30032

Alpha occ. eigenvalues -- -0.27020 -0.26965 -0.26470 -0.26017 -0.25930

Alpha occ. eigenvalues -- -0.25233 -0.24050 -0.23028 -0.21815 -

0.20409

Alpha virt. eigenvalues -- -0.07435 -0.07093 -0.01708 -0.01613 -0.00022

Alpha virt. eigenvalues -- 0.00814 0.02026 0.03778 0.04021 0.08443

Alpha virt. eigenvalues -- 0.10105 0.10938 0.11526 0.11974 0.12448

Alpha virt. eigenvalues -- 0.12946 0.13677 0.13973 0.14140 0.14681

Alpha virt. eigenvalues -- 0.15263 0.15761 0.16060 0.16464 0.16866

Alpha virt. eigenvalues -- 0.17243 0.17340 0.17544 0.17698 0.18194

Alpha virt. eigenvalues -- 0.18606 0.19213 0.19530 0.19742 0.20112

Alpha virt. eigenvalues -- 0.21101 0.21658 0.22843 0.23246 0.25314

Alpha virt. eigenvalues -- 0.25915 0.27482 0.27748 0.28381 0.29281

Alpha virt. eigenvalues -- 0.29461 0.29985 0.30681 0.31267 0.31576

Alpha virt. eigenvalues -- 0.32626 0.33242 0.34076 0.34274 0.34930

Alpha virt. eigenvalues -- 0.35467 0.37498 0.38466 0.40545 0.41454

Alpha virt. eigenvalues -- 0.44015 0.44119 0.44965 0.46263 0.47126

Alpha virt. eigenvalues -- 0.47524 0.49139 0.49529 0.50256 0.50883

Alpha virt. eigenvalues -- 0.51199 0.51897 0.52276 0.52852 0.53245

Alpha virt. eigenvalues -- 0.53869 0.54494 0.54603 0.54695 0.55411

Alpha virt. eigenvalues -- 0.55872 0.56295 0.56459 0.56697 0.56887

Alpha virt. eigenvalues -- 0.57054 0.58111 0.58135 0.59052 0.59228

Alpha virt. eigenvalues -- 0.59503 0.59920 0.60101 0.60326 0.60490

Alpha virt. eigenvalues -- 0.60918 0.61375 0.61539 0.61774 0.62039

Alpha virt. eigenvalues -- 0.62241 0.62328 0.63898 0.64401

0.64699

Alpha virt. eigenvalues -- 0.65088 0.65319 0.65620 0.66602 0.66836

Alpha virt. eigenvalues -- 0.67822 0.68148 0.68486 0.69997 0.70872

Alpha virt. eigenvalues -- 0.71815 0.72541 0.73634 0.74691 0.74767

Alpha virt. eigenvalues -- 0.75126 0.75964 0.77101 0.77766 0.78154

Alpha virt. eigenvalues -- 0.79182 0.80144 0.80265 0.80853 0.80915

Alpha virt. eigenvalues -- 0.81335 0.82472 0.82750 0.82804 0.83187

Alpha virt. eigenvalues -- 0.83347 0.83641 0.83759 0.84258 0.85120

Alpha virt. eigenvalues -- 0.85578 0.86403 0.87217 0.87749 0.88178

Alpha virt. eigenvalues -- 0.88510 0.88856 0.89705 0.90009 0.90177

Alpha virt. eigenvalues -- 0.90520 0.91477 0.91979 0.92608 0.92917

Alpha virt. eigenvalues -- 0.93365 0.95049 0.95665 0.96340 0.97136

Alpha virt. eigenvalues -- 0.97660 0.98282 0.98886 1.00807 1.01347

Alpha virt. eigenvalues -- 1.01718 1.03272 1.03690 1.04451 1.05094

Alpha virt. eigenvalues -- 1.08149 1.09399 1.09845 1.10650 1.12067

Alpha virt. eigenvalues -- 1.13075 1.13138 1.14224 1.15458 1.16118

Alpha virt. eigenvalues -- 1.16496 1.16971 1.18533 1.19369 1.20363

Alpha virt. eigenvalues -- 1.21217 1.22574 1.22689 1.24195 1.24734

Alpha virt. eigenvalues -- 1.25565 1.26685 1.27565 1.28005 1.28789

Alpha virt. eigenvalues -- 1.30040 1.30596 1.32109 1.33675 1.34165

Alpha virt. eigenvalues -- 1.34686 1.35783 1.35931 1.37139 1.38078

Alpha virt. eigenvalues -- 1.39061 1.39436 1.39620 1.40428

1.41079

Alpha virt. eigenvalues -- 1.41183 1.41433 1.41980 1.42286 1.43274

Alpha virt. eigenvalues -- 1.43604 1.44043 1.44485 1.45059 1.46151

Alpha virt. eigenvalues -- 1.47455 1.48213 1.48389 1.48648 1.50049

Alpha virt. eigenvalues -- 1.51792 1.55268 1.56386 1.59664 1.60736

Alpha virt. eigenvalues -- 1.65191 1.67245 1.68419 1.68651 1.71383

Alpha virt. eigenvalues -- 1.71981 1.73510 1.74026 1.74595 1.75403

Alpha virt. eigenvalues -- 1.76300 1.77534 1.77898 1.78869 1.79308

Alpha virt. eigenvalues -- 1.79500 1.80403 1.81449 1.83738 1.83976

Alpha virt. eigenvalues -- 1.84801 1.85331 1.86539 1.86942 1.87599

Alpha virt. eigenvalues -- 1.87967 1.88416 1.89225 1.89757 1.90475

Alpha virt. eigenvalues -- 1.91540 1.91913 1.91979 1.92882 1.93612

Alpha virt. eigenvalues -- 1.93890 1.94343 1.95544 1.96082 1.96601

Alpha virt. eigenvalues -- 1.97253 1.97436 1.97762 1.98542 1.99209

Alpha virt. eigenvalues -- 1.99506 1.99796 2.00076 2.00374 2.01254

Alpha virt. eigenvalues -- 2.01817 2.02083 2.02732 2.03472 2.04033

Alpha virt. eigenvalues -- 2.04474 2.06464 2.06864 2.07654 2.08256

Alpha virt. eigenvalues -- 2.09518 2.09605 2.10958 2.13608 2.13873

Alpha virt. eigenvalues -- 2.14920 2.15386 2.16303 2.18309 2.18652

Alpha virt. eigenvalues -- 2.20016 2.21001 2.22338 2.24274 2.24370

Alpha virt. eigenvalues -- 2.26026 2.26556 2.28607 2.29051 2.30002

Alpha virt. eigenvalues -- 2.30324 2.30521 2.31801 2.32134

2.34474

Alpha virt. eigenvalues -- 2.35553 2.36283 2.36809 2.37313 2.37865

Alpha virt. eigenvalues -- 2.37916 2.38570 2.38930 2.39171 2.39224

Alpha virt. eigenvalues -- 2.40273 2.40914 2.42003 2.43077 2.43241

Alpha virt. eigenvalues -- 2.43558 2.43919 2.44735 2.45280 2.45619

Alpha virt. eigenvalues -- 2.47185 2.47829 2.47917 2.49095 2.49773

Alpha virt. eigenvalues -- 2.50048 2.50262 2.50718 2.51993 2.52789

Alpha virt. eigenvalues -- 2.53278 2.54226 2.54837 2.55749 2.56148

Alpha virt. eigenvalues -- 2.56757 2.56892 2.57450 2.58614 2.60296

Alpha virt. eigenvalues -- 2.60627 2.61243 2.61527 2.62288 2.62975

Alpha virt. eigenvalues -- 2.64369 2.64448 2.65438 2.66178 2.66679

Alpha virt. eigenvalues -- 2.67577 2.68877 2.68968 2.71530 2.73699

Alpha virt. eigenvalues -- 2.74308 2.74986 2.75670 2.76347 2.77447

Alpha virt. eigenvalues -- 2.77900 2.78050 2.78418 2.80239 2.82880

Alpha virt. eigenvalues -- 2.83102 2.84257 2.86679 2.87194 2.88048

Alpha virt. eigenvalues -- 2.88391 2.89398 2.91758 2.92819 2.96705

Alpha virt. eigenvalues -- 2.98188 2.98627 3.03744 3.05749 3.06900

Alpha virt. eigenvalues -- 3.08792 3.09384 3.12635 3.14841 3.15973

Alpha virt. eigenvalues -- 3.19954 3.20532 3.21522 3.22765 3.23499

Alpha virt. eigenvalues -- 3.23606 3.24345 3.25376 3.26528 3.26735

Alpha virt. eigenvalues -- 3.31681 3.33360 3.34115 3.38411 3.39798

Alpha virt. eigenvalues -- 3.40276 3.40960 3.42640 3.43761

3.45193

Alpha virt. eigenvalues -- 3.46124 3.46235 3.47679 3.49661 3.51006

Alpha virt. eigenvalues -- 3.52578 3.86326 3.88386 3.90103 3.90544

Alpha virt. eigenvalues -- 4.04312 4.11140 4.12782 4.13837 4.15100

Alpha virt. eigenvalues -- 4.16270 4.16900 4.18456 4.18604 4.18951

Alpha virt. eigenvalues -- 4.21461 4.27372 4.29540 4.34696 4.37612

Alpha virt. eigenvalues -- 4.39800 4.41847 4.43309 4.43653 4.45871

Alpha virt. eigenvalues -- 4.47610 4.49404 4.50751 4.55098 4.62412

Alpha virt. eigenvalues -- 4.69231 4.78020 4.83080 4.84956 4.92275

Condensed to atoms (all electrons):

Mulliken charges:

1	C	0.064922
2	C	-0.129113
3	H	0.101651
4	C	-0.101891
5	H	0.081142
6	C	-0.092686
7	H	0.083457
8	C	-0.111158
9	H	0.093634
10	C	0.226589
11	C	0.040773
12	C	0.269720
13	C	0.152837
14	C	0.544199
15	C	-0.031527
16	C	-0.047162

17	C	0.086106
18	C	-0.084022
19	H	0.089551
20	C	-0.097420
21	H	0.083211
22	C	-0.076460
23	H	0.084349
24	C	-0.101874
25	H	0.085373
26	C	-0.063171
27	H	0.103477
28	C	0.285301
29	C	-0.174550
30	H	0.139114
31	H	0.158948
32	H	0.135333

33	C	-0.372953
34	H	0.127748
35	H	0.126951
36	H	0.127894
37	C	-0.021187
38	C	-0.086825
39	H	0.099639
40	C	-0.086352
41	H	0.095256
42	C	-0.081823
43	H	0.093015
44	C	-0.086136
45	H	0.095337
46	C	-0.086901
47	H	0.100355
48	N	-0.582234

49	N	-0.585833
50	N	-0.334836
51	N	-0.339767
52	Bq	0.000000
53	Bq	0.000000
54	Bq	0.000000
55	Bq	0.000000
56	Bq	0.000000
57	Bq	0.000000

Sum of Mulliken charges = -0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	0.064922
2	C	-0.027461
4	C	-0.020749
6	C	-0.009229

8	C	-0.017524
10	C	0.226589
11	C	0.040773
12	C	0.269720
13	C	0.152837
14	C	0.544199
15	C	-0.031527
16	C	-0.047162
17	C	0.086106
18	C	0.005529
20	C	-0.014209
22	C	0.007888
24	C	-0.016501
26	C	0.040306
28	C	0.285301
29	C	0.258845

33 C 0.009641

37 C -0.021187

38 C 0.012814

40 C 0.008904

42 C 0.011192

44 C 0.009201

46 C 0.013454

48 N -0.582234

49 N -0.585833

50 N -0.334836

51 N -0.339767

52 Bq 0.000000

53 Bq 0.000000

54 Bq 0.000000

55 Bq 0.000000

56 Bq 0.000000

57 Bq 0.000000

Electronic spatial extent (au): <R**2>= 12680.9359

Charge= -0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 2.1295 Y= -1.0382 Z= 0.2053 Tot= 2.3779

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -152.4610 YY= -173.7945 ZZ= -173.1522

XY= 7.3221 XZ= 0.1499 YZ= 3.4538

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 14.0082 YY= -7.3253 ZZ= -6.6829

XY= 7.3221 XZ= 0.1499 YZ= 3.4538

Octapole moment (field-independent basis, Debye-Ang**2):

XXX= 26.8609 YYY= 23.4441 ZZZ= 2.0871 XYY= -37.3153

XXY= -4.5105 XXZ= -1.9772 XZZ= 15.9191 YZZ= -16.4226

YYZ= -0.4525 XYZ= -16.7295

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX= -9517.9635 YYYY= -5991.9857 ZZZZ= -534.2262 XXXY= 13.0817

XXXZ= 30.6612 YYYX= 209.4953 YYYZ= -12.5522 ZZZX= 6.7003

ZZZY= 14.8898 XXYY= -2749.5575 XXZZ= -1812.4701 YYZZ= -1172.5756

XXYZ= 91.1113 YYXZ= -14.3262 ZZXY= -6.9494

N-N= 2.827386314305D+03 E-N=-8.575692147348D+03 KE= 1.247925640446D+03

Unable to Open any file for archive entry.

1\1\GINC-O2213\SP\RB3LYP\6-31G(d,p)\C27H20N4\SC40234\19-May-2023\0\\#

nmr b3lyp/6-31g(d,p)\\Title Card Required\\0,1\C,0,0.90392,2.098552,-0

.068909\C,0,2.138594,2.774577,-0.077382\H,0,3.079484,2.245589,-0.02067

9\C,0,2.145188,4.163347,-0.157333\H,0,3.096855,4.686826,-0.162197\C,0,

0.950292,4.904954,-0.231745\H,0,0.996024,5.988352,-0.29449\C,0,-0.2789

63,4.262203,-0.224184\H,0,-1.215398,4.807411,-0.280423\C,0,-0.293532,2

.863199,-0.140328\C,0,0.466825,0.707003,-0.011588\C,0,-1.021855,0.8167

1,-0.035553\C,0,-2.022444,-0.239424,0.008901\C,0,-0.611678,-2.157116,-

0.009627\C,0,0.763803,-1.769709,0.023783\C,0,1.25828,-0.430934,0.02448

4\C,0,-3.475061,0.118142,0.038085\C,0,-4.372831,-0.684278,-0.686662\H,

0,-3.979453,-1.501465,-1.281081\C,0,-5.741886,-0.433881,-0.65626\H,0,-

6.416771,-1.054975,-1.238214\C,0,-6.244027,0.610814,0.121983\H,0,-7.31

238,0.805053,0.152787\C,0,-5.364294,1.4043,0.85936\H,0,-5.746924,2.214

218,1.473611\C,0,-3.991102,1.170511,0.812323\H,0,-3.316202,1.801247,1.

374196\C,0,1.477249,-3.022117,0.038253\C,0,-1.764137,-4.404376,-0.0442

41\H,0,-1.676207,-5.136912,0.760949\H,0,-2.657075,-3.79667,0.090592\H,

0,-1.811589,-4.931534,-1.001661\C,0,2.94189,-3.342691,0.080703\H,0,3.428707,-2.922695,0.964703\H,0,3.049494,-4.429198,0.102342\H,0,3.473922,

-2.954376,-0.791667\C,0,2.747713,-0.257647,0.049284\C,0,3.425857,-0.135122,1.268799\H,0,2.864825,-0.166309,2.19808\C,0,4.81073,0.036204,1.291458\H,0,5.325647,0.132659,2.242766\C,0,5.530887,0.087949,0.096435\H,0

,6.608171,0.223053,0.114671\C,0,4.860071,-0.031916,-1.122254\H,0,5.413488,0.011885,-2.055657\C,0,3.47551,-0.204318,-1.146491\H,0,2.952793,-0.288888,-2.094588\N,0,-1.424229,2.074601,-0.116643\N,0,-1.801468,-1.530808,-0.004286\N,0,-0.613558,-3.521832,-0.014093\N,0,0.632481,-4.04523

2,0.011906\Bq,0,0.9275831667,3.5111386667,-0.1499801667\Bq,0,-0.273774

2,1.712013,-0.0746042\Bq,0,-0.4240767143,-0.657754,-

0.0005551429\Bq,0,

0.3296594,-2.9032012,0.0100444\Bq,0,4.1417946667,-0.0841416667,0.07287

18333\Bq,0,-4.8648668333,0.364268,0.0814715\\Version=ES64L-G16RevC.01\

HF=-1259.9488979\RMSD=7.844e-09\Dipole=0.8377937,-0.4084421,0.0807678\

Quadrupole=10.4147594,-5.4461581,-4.9686013,5.4438122,0.1114373,2.5678

194\PG=C01 [X(C27H20N4)]\\@

The archive entry for this job was punched.

IT IS A QUALITY OF REVOLUTIONS NOT TO GO BY OLD LINES OR OLD LAWS,

BUT TO BREAK UP BOTH, AND MAKE NEW ONES.

-- A. LINCOLN (1848)

Job cpu time: 0 days 0 hours 45 minutes 15.7 seconds.

Elapsed time: 0 days 0 hours 1 minutes 8.8 seconds.

File lengths (MBytes): RWF= 192 Int= 0 D2E= 0 Chk= 26 Scr= 1

Normal termination of Gaussian 16 at Fri May 19 08:50:04 2023.

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