

23 O Isotropic = 279.8529 Anisotropy = 43.9501
 XX= 262.2717 YX= 0.2768 ZX= 14.6786
 XY= 0.3078 YY= 275.8979 ZY= 23.4525
 XZ= 11.7338 YZ= -0.4251 ZZ= 301.3891
 Eigenvalues: 257.6228 272.7830 309.1530

24 O Isotropic = -278.9563 Anisotropy = 1013.7645
 XX= -363.8334 YX= 56.0407 ZX= 34.9816
 XY= 3.2405 YY= -758.6302 ZY= -357.8892
 XZ= -10.7919 YZ= -359.2916 ZZ= 285.5947
 Eigenvalues: -871.9143 -361.8414 396.8867

25 O Isotropic = 305.7127 Anisotropy = 58.1985
 XX= 328.6976 YX= 34.8998 ZX= 9.1950
 XY= 3.9302 YY= 294.9928 ZY= -8.4456
 XZ= 26.0753 YZ= 21.9382 ZZ= 293.4475
 Eigenvalues: 285.1906 287.4357 344.5116

26 H Isotropic = 24.1651 Anisotropy = 13.3910
 XX= 31.8252 YX= -4.0042 ZX= 1.5403
 XY= -2.7167 YY= 20.7628 ZY= 0.0209
 XZ= 2.7236 YZ= -0.1709 ZZ= 19.9074
 Eigenvalues: 19.1907 20.2122 33.0925

27 H Isotropic = 27.7717 Anisotropy = 7.5164
 XX= 30.4666 YX= 0.1445 ZX= -0.0368
 XY= 1.8912 YY= 32.2179 ZY= 1.7050
 XZ= -0.6437 YZ= 0.9779 ZZ= 20.6305
 Eigenvalues: 20.4565 30.0759 32.7826

28 H Isotropic = 29.2395 Anisotropy = 7.8291
 XX= 29.1647 YX= -3.3652 ZX= -2.4333
 XY= -3.3750 YY= 25.7010 ZY= -0.6088
 XZ= -2.5473 YZ= 0.8292 ZZ= 32.8529
 Eigenvalues: 23.4784 29.7812 34.4589

29 H Isotropic = 28.2611 Anisotropy = 9.3401
 XX= 33.3178 YX= 3.4886 ZX= -3.3226
 XY= -2.2193 YY= 27.8900 ZY= -2.2094
 XZ= -2.6649 YZ= -3.5631 ZZ= 23.5756
 Eigenvalues: 21.6197 28.6759 34.4879

30 H Isotropic = 26.7242 Anisotropy = 4.0592
 XX= 25.9498 YX= -2.1414 ZX= -0.2074
 XY= -1.5630 YY= 25.5385 ZY= -0.0643
 XZ= -0.4289 YZ= -3.1611 ZZ= 28.6843
 Eigenvalues: 23.4832 27.2591 29.4303

31 H Isotropic = 24.4463 Anisotropy = 8.9503
 XX= 29.7596 YX= -0.7973 ZX= -2.3419
 XY= -0.2713 YY= 22.3168 ZY= 0.3229
 XZ= -2.2438 YZ= 1.7512 ZZ= 21.2626
 Eigenvalues: 20.2938 22.6320 30.4132

32 H Isotropic = 25.7093 Anisotropy = 8.9297
 XX= 29.4079 YX= 2.4647 ZX= -2.0986
 XY= 3.6051 YY= 23.4420 ZY= -2.5415
 XZ= -2.2024 YZ= -1.0609 ZZ= 24.2780
 Eigenvalues: 21.7662 23.6993 31.6624

33 H Isotropic = 29.4315 Anisotropy = 5.6614
 XX= 29.9322 YX= 0.4433 ZX= 0.7068
 XY= 1.7534 YY= 26.4303 ZY= -3.2688
 XZ= -0.2758 YZ= -2.5574 ZZ= 31.9319
 Eigenvalues: 24.9347 30.1540 33.2057

34 H Isotropic = 29.5508 Anisotropy = 5.7168
 XX= 31.9520 YX= -0.6185 ZX= -0.4327
 XY= -1.5625 YY= 31.7493 ZY= 2.4961
 XZ= -1.5562 YZ= 0.8366 ZZ= 24.9511
 Eigenvalues: 24.4926 30.7978 33.3620

35 H Isotropic = 30.1931 Anisotropy = 5.7230
 XX= 31.7092 YX= 0.2679 ZX= 0.0677
 XY= 0.2268 YY= 33.0768 ZY= 3.0583
 XZ= 0.6814 YZ= 2.2943 ZZ= 25.7934
 Eigenvalues: 24.9043 31.6666 34.0084

36 H Isotropic = 30.2979 Anisotropy = 4.9090
 XX= 32.1595 YX= 1.3098 ZX= -0.5287
 XY= 1.1231 YY= 26.6675 ZY= -3.0861
 XZ= 0.0628 YZ= -2.3704 ZZ= 32.0666
 Eigenvalues: 25.3704 31.9526 33.5705

37 H Isotropic = 30.3986 Anisotropy = 5.3229
 XX= 31.6425 YX= 1.1206 ZX= -0.2238
 XY= 1.4706 YY= 26.7526 ZY= -2.8141
 XZ= -0.2424 YZ= -2.3132 ZZ= 32.8008
 Eigenvalues: 25.5967 31.6519 33.9472

38 H Isotropic = 30.3218 Anisotropy = 5.4496
 XX= 31.9467 YX= -0.2004 ZX= 0.2708
 XY= -0.3056 YY= 32.9199 ZY= 3.1626
 XZ= 0.1363 YZ= 2.4956 ZZ= 26.0988
 Eigenvalues: 25.0669 31.9436 33.9548

39 H Isotropic = 30.2886 Anisotropy = 7.0954
 XX= 31.2852 YX= -1.0887 ZX= -0.1719
 XY= -0.9033 YY= 33.9337 ZY= 2.9794
 XZ= -0.3678 YZ= 2.4138 ZZ= 25.6470
 Eigenvalues: 24.8467 31.0003 35.0189

40 H Isotropic = 30.2562 Anisotropy = 6.7222
 XX= 30.6519 YX= 1.1119 ZX= 0.5664
 XY= 1.5172 YY= 26.6808 ZY= -3.4486
 XZ= 0.7012 YZ= -3.0216 ZZ= 33.4358
 Eigenvalues: 25.0059 31.0249 34.7376

41 H Isotropic = 30.8548 Anisotropy = 8.7506
XX= 31.0903 YX= 2.3062 ZX= -3.3974
XY= 1.8798 YY= 27.8247 ZY= -2.5478
XZ= -2.7343 YZ= -1.7905 ZZ= 33.6493
Eigenvalues: 26.7196 29.1563 36.6885

42 H Isotropic = 30.8327 Anisotropy = 8.8274
XX= 29.8499 YX= 2.5916 ZX= 0.5537
XY= 1.5330 YY= 34.2810 ZY= 3.9734
XZ= 0.5543 YZ= 3.4641 ZZ= 28.3672
Eigenvalues: 26.5181 29.2624 36.7176

43 H Isotropic = 30.6635 Anisotropy = 10.9759
XX= 37.0925 YX= -1.7450 ZX= 2.9989
XY= -0.5768 YY= 27.9085 ZY= -0.9176
XZ= 2.4912 YZ= -1.1704 ZZ= 26.9896
Eigenvalues: 25.9917 28.0181 37.9808

44 H Isotropic = 29.9140 Anisotropy = 9.1821
XX= 31.6317 YX= 0.5825 ZX= -3.7936
XY= 0.8584 YY= 26.4043 ZY= -0.5318
XZ= -4.8905 YZ= 0.5985 ZZ= 31.7060
Eigenvalues: 26.1394 27.5672 36.0354

45 H Isotropic = 30.0660 Anisotropy = 5.7127
XX= 33.2207 YX= -2.0790 ZX= 1.1053
XY= -0.3658 YY= 28.1337 ZY= 3.6750
XZ= 2.5215 YZ= 3.2273 ZZ= 28.8438
Eigenvalues: 24.5006 31.8230 33.8745

46 H Isotropic = 29.7926 Anisotropy = 9.2583
XX= 28.0488 YX= -2.3513 ZX= 1.5035
XY= -3.6998 YY= 34.6314 ZY= -0.5138
XZ= 1.2065 YZ= -0.9797 ZZ= 26.6976
Eigenvalues: 25.7103 27.7028 35.9648

47 H Isotropic = 27.0633 Anisotropy = 6.0990
XX= 26.2637 YX= -0.2889 ZX= -3.6080
XY= 0.7147 YY= 27.5225 ZY= -1.9439
XZ= -4.3975 YZ= -0.2011 ZZ= 27.4038
Eigenvalues: 22.7279 27.3328 31.1293

48 H Isotropic = 27.1547 Anisotropy = 10.1547
XX= 28.4646 YX= 2.9341 ZX= 0.3445
XY= 4.5039 YY= 30.9802 ZY= -1.2680
XZ= 0.4351 YZ= -3.6826 ZZ= 22.0193
Eigenvalues: 21.1055 26.4341 33.9245

49 H Isotropic = 25.8728 Anisotropy = 11.4259
XX= 26.8993 YX= 1.5158 ZX= 3.7653
XY= 3.8786 YY= 23.3939 ZY= 2.6935
XZ= 6.6326 YZ= 1.6669 ZZ= 27.3252
Eigenvalues: 21.6226 22.5058 33.4900

50 H Isotropic = 29.9004 Anisotropy = 14.7608
 XX= 23.3157 YX= -2.4902 ZX= 2.3204
 XY= -1.8580 YY= 27.1231 ZY= -0.4271
 XZ= 3.1629 YZ= 0.1391 ZZ= 39.2625
 Eigenvalues: 21.9806 27.9798 39.7410
 51 H Isotropic = 28.6737 Anisotropy = 16.9505
 XX= 32.6792 YX= 4.6668 ZX= 8.2578
 XY= 5.2309 YY= 31.0871 ZY= 1.5753
 XZ= 7.8787 YZ= 1.4254 ZZ= 22.2548
 Eigenvalues: 17.7698 28.2773 39.9740

Structure 1b conformation 4.

Level of theory & comments

B3PW91 D95** nmr

Ambuic acid, syn stereochemistry, C7 acceptor-C19 donor, s-cis at
 C8-C9-C11-C12, 90 degree dihedral at C3-C4-C5-C6.

Energy

-1190.7404830

Cartesian coordinates

C	6.24962	-1.61991	0.83269
C	5.37437	-1.17722	-0.29008
C	4.18477	-0.59559	-0.0272
C	3.21081	-0.10971	-1.07847
C	1.93787	0.51044	-0.50553
C	1.83742	1.95523	-0.20293
C	0.5129	2.68058	-0.21408
C	-0.71182	1.78199	-0.14709
C	-0.65625	0.43703	-0.37353
C	0.6272	-0.19917	-0.8178
C	-1.80105	-0.49449	-0.35897
C	-2.867	-0.46393	0.46729
C	-3.99266	-1.46436	0.44695
C	-5.37004	-0.80918	0.20495

C	-6.53021	-1.81502	0.26404
C	-7.90472	-1.17022	0.02432
C	-9.06188	-2.17937	0.0862
C	5.93514	-1.44125	-1.66696
C	-2.00479	2.53808	0.12959
O	7.33789	-2.15191	0.67912
O	5.74376	-1.38583	2.07764
O	1.99896	1.0074	0.85928
O	0.50086	3.64028	0.86568
O	0.64221	-1.25966	-1.43242
O	-1.99085	3.87643	-0.34758
H	3.89274	-0.45742	1.01019
H	2.90576	-0.94678	-1.71723
H	3.70531	0.61928	-1.73497
H	2.71303	2.58396	-0.37896
H	0.45165	3.29154	-1.12281
H	-1.71039	-1.32518	-1.05836
H	-2.93935	0.30974	1.23392
H	-4.02275	-1.98941	1.41513
H	-3.80004	-2.22458	-0.32167
H	-5.53335	-0.02026	0.95497
H	-5.36244	-0.30924	-0.7742
H	-6.52931	-2.31418	1.24543
H	-6.36521	-2.60628	-0.48328
H	-8.06928	-0.37921	0.77093
H	-7.90603	-0.67244	-0.95652
H	-9.10892	-2.66903	1.06824
H	-8.94229	-2.96578	-0.67111
H	-10.02858	-1.69023	-0.08983
H	6.9025	-0.93981	-1.7949
H	5.25631	-1.09981	-2.45361
H	6.12009	-2.51321	-1.80859
H	-2.22417	2.51453	1.21096
H	-2.83413	2.03126	-0.37557
H	6.41635	-1.72638	2.69517
H	0.67629	3.14513	1.68416
H	-1.34445	4.35647	0.19854

Computed NMR tensors

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 22.5884 Anisotropy = 84.4907

XX= 62.6768 YX= 7.8158 ZX= 12.6693
 XY= 8.6785 YY= 74.7053 ZY= -4.5522
 XZ= -13.9126 YZ= 8.7735 ZZ= -69.6170

Eigenvalues: -69.6521 58.5017 78.9155

2 C Isotropic = 60.6648 Anisotropy = 129.3983

XX= 79.3252 YX= 33.1021 ZX= -27.1057
 XY= 33.4404 YY= 130.4865 ZY= 18.3030
 XZ= -23.9040 YZ= 13.5869 ZZ= -27.8173

Eigenvalues: -36.8425 71.9065 146.9304

3 C Isotropic = 48.1398 Anisotropy = 163.4803

XX= 62.7431 YX= 44.4521 ZX= -22.3217
 XY= 46.7105 YY= 135.0780 ZY= 14.4389
 XZ= -11.5146 YZ= 7.3546 ZZ= -53.4016

Eigenvalues: -57.4916 44.7844 157.1267

4 C Isotropic = 164.1640 Anisotropy = 20.2657

XX= 174.6601 YX= -9.9253 ZX= -2.4892
 XY= -4.7875 YY= 158.9325 ZY= 0.1545
 XZ= 3.9628 YZ= -4.2216 ZZ= 158.8995

Eigenvalues: 155.2827 159.5349 177.6745

5 C Isotropic = 126.3850 Anisotropy = 70.0673

XX= 172.1572 YX= -9.5120 ZX= -3.6859
 XY= -6.2206 YY= 77.8320 ZY= -15.1898
 XZ= -3.9558 YZ= 8.9734 ZZ= 129.1659

Eigenvalues: 76.9568 129.1017 173.0965

6 C Isotropic = 123.6619 Anisotropy = 50.1860

XX= 156.3821 YX= -4.9478 ZX= -2.5634
 XY= -6.2473 YY= 88.4740 ZY= 4.0566
 XZ= -3.9496 YZ= -11.8397 ZZ= 126.1297

Eigenvalues: 87.5689 126.2977 157.1193

7 C Isotropic = 119.3414 Anisotropy = 43.1874

XX= 113.5115 YX= 0.1376 ZX= 3.1726
 XY= -1.0090 YY= 112.4815 ZY= 16.8422
 XZ= -5.4429 YZ= 30.9889 ZZ= 132.0311

Eigenvalues: 96.4159 113.4752 148.1329

8 C Isotropic = 33.5540 Anisotropy = 158.1156

XX= -40.5897 YX= -18.9980 ZX= 24.4322
 XY= -6.6502 YY= 8.6038 ZY= -12.1252
 XZ= 37.4633 YZ= -6.0081 ZZ= 132.6478

Eigenvalues: -48.1444 9.8419 138.9643

9 C Isotropic = 60.1658 Anisotropy = 130.8023

XX= -4.7804 YX= -0.5763 ZX= 34.7551
 XY= -5.8036 YY= 52.2582 ZY= -17.9407
 XZ= 35.4840 YZ= -29.2973 ZZ= 133.0197

Eigenvalues: -13.3088 46.4389 147.3674

10 C Isotropic = -5.9076 Anisotropy = 154.8762

XX= -87.7144 YX= 3.1986 ZX= 15.5032
 XY= -1.0598 YY= 4.5073 ZY= -49.5700
 XZ= 4.7785 YZ= -58.3595 ZZ= 65.4842
 Eigenvalues: -88.6688 -26.3973 97.3432
 11 C Isotropic = 65.3765 Anisotropy = 129.7837
 XX= 83.2191 YX= -45.2030 ZX= 10.8819
 XY= -53.3453 YY= 20.0454 ZY= -66.5643
 XZ= 14.4838 YZ= -63.1679 ZZ= 92.8649
 Eigenvalues: -30.2894 74.5199 151.8990
 12 C Isotropic = 46.1296 Anisotropy = 162.1412
 XX= 60.3346 YX= -62.1332 ZX= 26.0736
 XY= -50.4762 YY= 20.9602 ZY= -79.2221
 XZ= 22.2035 YZ= -82.0550 ZZ= 57.0940
 Eigenvalues: -52.3017 36.4668 154.2237
 13 C Isotropic = 150.4382 Anisotropy = 31.4310
 XX= 166.2830 YX= 12.8338 ZX= 3.9577
 XY= 5.7032 YY= 152.5317 ZY= 0.2595
 XZ= 5.8181 YZ= -1.2553 ZZ= 132.4999
 Eigenvalues: 131.6335 148.2890 171.3923
 14 C Isotropic = 155.7407 Anisotropy = 35.8327
 XX= 178.4637 YX= 5.2898 ZX= 1.7817
 XY= 6.0491 YY= 150.8243 ZY= -3.0179
 XZ= 2.2515 YZ= -2.9177 ZZ= 137.9341
 Eigenvalues: 137.0278 150.5650 179.6291
 15 C Isotropic = 154.4433 Anisotropy = 38.0836
 XX= 178.8060 YX= 5.2779 ZX= 2.8627
 XY= 4.8916 YY= 148.2595 ZY= -3.0429
 XZ= 4.1388 YZ= -3.2312 ZZ= 136.2644
 Eigenvalues: 134.9942 148.5034 179.8324
 16 C Isotropic = 164.0747 Anisotropy = 23.4045
 XX= 179.4209 YX= 3.1931 ZX= 1.9387
 XY= -3.6833 YY= 160.3999 ZY= -1.5947
 XZ= 3.2865 YZ= -0.7184 ZZ= 152.4035
 Eigenvalues: 152.0016 160.5449 179.6777
 17 C Isotropic = 174.3653 Anisotropy = 26.2635
 XX= 185.3798 YX= 7.5725 ZX= 0.7454
 XY= 13.9993 YY= 173.9588 ZY= -0.4223
 XZ= -0.0635 YZ= -1.2275 ZZ= 163.7573
 Eigenvalues: 163.5573 167.6643 191.8743
 18 C Isotropic = 173.4363 Anisotropy = 15.9574
 XX= 167.4048 YX= 2.4921 ZX= -9.0209
 XY= 3.6039 YY= 171.7348 ZY= 3.7585
 XZ= -4.1336 YZ= 2.4704 ZZ= 181.1692
 Eigenvalues: 162.9300 173.3043 184.0746
 19 C Isotropic = 121.3869 Anisotropy = 51.2495

XX= 111.2926 YX= -2.2974 ZX= 0.2367
 XY= -0.9936 YY= 149.9407 ZY= -12.5683
 XZ= -1.0616 YZ= -21.6458 ZZ= 102.9275
 Eigenvalues: 97.3034 111.3041 155.5533
 20 O Isotropic = -73.3014 Anisotropy = 541.3344
 XX= -179.7477 YX= 228.8928 ZX= 26.0070
 XY= 230.4987 YY= 174.6327 ZY= -7.7567
 XZ= 43.1597 YZ= -15.2941 ZZ= -214.7893
 Eigenvalues: -306.8356 -200.6569 287.5882
 21 O Isotropic = 137.0758 Anisotropy = 179.0262
 XX= 46.5414 YX= 59.4510 ZX= -116.4598
 XY= 58.1658 YY= 134.8021 ZY= 56.3342
 XZ= -27.1850 YZ= 12.6634 ZZ= 229.8839
 Eigenvalues: -9.3814 164.1822 256.4266
 22 O Isotropic = 244.3607 Anisotropy = 160.8897
 XX= 347.6302 YX= 13.9149 ZX= -21.8759
 XY= 20.8250 YY= 251.7430 ZY= 107.5111
 XZ= -31.6274 YZ= 64.2063 ZZ= 133.7090
 Eigenvalues: 84.7024 296.7593 351.6205
 23 O Isotropic = 280.1382 Anisotropy = 43.1635
 XX= 263.5187 YX= -2.9531 ZX= 12.2731
 XY= -2.1824 YY= 272.3082 ZY= 18.4575
 XZ= 11.6813 YZ= -4.0620 ZZ= 304.5878
 Eigenvalues: 258.7881 272.7127 308.9139
 24 O Isotropic = -279.0914 Anisotropy = 1004.4468
 XX= -367.1054 YX= 52.4269 ZX= 101.0384
 XY= 15.8476 YY= -533.4985 ZY= -540.9180
 XZ= 41.7211 YZ= -552.9842 ZZ= 63.3296
 Eigenvalues: -866.8344 -360.9796 390.5398
 25 O Isotropic = 305.2823 Anisotropy = 57.4828
 XX= 325.4583 YX= 36.1864 ZX= 15.3250
 XY= 2.0254 YY= 296.5206 ZY= -7.2122
 XZ= 23.1866 YZ= 22.8838 ZZ= 293.8681
 Eigenvalues: 284.4301 287.8128 343.6042
 26 H Isotropic = 24.0288 Anisotropy = 12.6176
 XX= 28.5990 YX= -5.5463 ZX= 1.7249
 XY= -5.3571 YY= 22.6486 ZY= -0.7174
 XZ= 3.2461 YZ= -1.2925 ZZ= 20.8390
 Eigenvalues: 19.2539 20.3921 32.4406
 27 H Isotropic = 27.5605 Anisotropy = 6.8837
 XX= 29.8978 YX= -1.0303 ZX= 1.2503
 XY= 1.6773 YY= 27.4352 ZY= 5.3046
 XZ= 0.5200 YZ= 5.4180 ZZ= 25.3485
 Eigenvalues: 20.9044 29.6274 32.1496
 28 H Isotropic = 29.4744 Anisotropy = 7.9660

XX= 30.9992 YX= -1.5975 ZX= -4.9597
 XY= -1.5206 YY= 29.3152 ZY= -3.8286
 XZ= -4.8058 YZ= -2.8975 ZZ= 28.1087
 Eigenvalues: 22.5135 31.1246 34.7850
 29 H Isotropic = 28.1619 Anisotropy = 9.3637
 XX= 32.5621 YX= 4.5966 ZX= -2.6500
 XY= -0.9114 YY= 29.1059 ZY= -1.5265
 XZ= -3.0259 YZ= -2.7829 ZZ= 22.8177
 Eigenvalues: 21.6833 28.3981 34.4044
 30 H Isotropic = 26.7504 Anisotropy = 4.0378
 XX= 26.1238 YX= -2.0005 ZX= -0.6191
 XY= -1.3477 YY= 26.0398 ZY= -0.6086
 XZ= -0.6003 YZ= -3.5723 ZZ= 28.0876
 Eigenvalues: 23.5464 27.2625 29.4423
 31 H Isotropic = 24.4707 Anisotropy = 8.6612
 XX= 29.3832 YX= 0.3874 ZX= -2.7064
 XY= 0.9198 YY= 21.9511 ZY= 0.1222
 XZ= -2.5479 YZ= 1.6548 ZZ= 22.0778
 Eigenvalues: 20.4805 22.6868 30.2448
 32 H Isotropic = 25.7162 Anisotropy = 8.9925
 XX= 28.8422 YX= 3.1047 ZX= -1.4911
 XY= 4.1513 YY= 24.7398 ZY= -2.9627
 XZ= -1.5486 YZ= -1.5587 ZZ= 23.5665
 Eigenvalues: 21.5780 23.8593 31.7112
 33 H Isotropic = 29.4283 Anisotropy = 5.7069
 XX= 30.0333 YX= 0.0731 ZX= 1.1866
 XY= 1.4515 YY= 28.3728 ZY= -4.3648
 XZ= 0.4628 YZ= -3.6957 ZZ= 29.8787
 Eigenvalues: 24.7893 30.2627 33.2329
 34 H Isotropic = 29.5036 Anisotropy = 5.6599
 XX= 31.7760 YX= -0.1526 ZX= -1.2619
 XY= -0.7263 YY= 30.2712 ZY= 3.9118
 XZ= -2.4309 YZ= 2.2366 ZZ= 26.4637
 Eigenvalues: 24.4750 30.7589 33.2769
 35 H Isotropic = 30.2162 Anisotropy = 5.7244
 XX= 31.7410 YX= 0.6475 ZX= -0.5390
 XY= 0.5543 YY= 31.4123 ZY= 4.4580
 XZ= 0.0711 YZ= 3.6747 ZZ= 27.4953
 Eigenvalues: 24.9011 31.7150 34.0325
 36 H Isotropic = 30.2803 Anisotropy = 4.9507
 XX= 31.9153 YX= 1.3460 ZX= 0.0235
 XY= 1.0244 YY= 28.5240 ZY= -4.1657
 XZ= 0.4462 YZ= -3.4501 ZZ= 30.4016
 Eigenvalues: 25.3626 31.8976 33.5807
 37 H Isotropic = 30.4029 Anisotropy = 5.3205

XX= 31.5555 YX= 1.0118 ZX= 0.3485
 XY= 1.2675 YY= 28.5998 ZY= -4.1423
 XZ= 0.4265 YZ= -3.6087 ZZ= 31.0535
 Eigenvalues: 25.5417 31.7171 33.9500
 38 H Isotropic = 30.2955 Anisotropy = 5.4713
 XX= 31.8654 YX= 0.1573 ZX= -0.4730
 XY= 0.1788 YY= 31.1144 ZY= 4.4474
 XZ= -0.5726 YZ= 3.7913 ZZ= 27.9068
 Eigenvalues: 25.0494 31.8941 33.9431
 39 H Isotropic = 30.3147 Anisotropy = 7.0677
 XX= 31.2274 YX= -0.6299 ZX= -1.1164
 XY= -0.3278 YY= 32.0321 ZY= 4.6470
 XZ= -1.2215 YZ= 4.1106 ZZ= 27.6846
 Eigenvalues: 24.8816 31.0360 35.0265
 40 H Isotropic = 30.2612 Anisotropy = 6.8009
 XX= 30.7211 YX= 0.6326 ZX= 1.2557
 XY= 0.9917 YY= 28.8127 ZY= -4.7605
 XZ= 1.4201 YZ= -4.2765 ZZ= 31.2500
 Eigenvalues: 24.9788 31.0097 34.7952
 41 H Isotropic = 30.8541 Anisotropy = 8.7656
 XX= 30.2705 YX= 2.8475 ZX= -2.2598
 XY= 2.1966 YY= 29.5854 ZY= -4.1150
 XZ= -1.7167 YZ= -3.4181 ZZ= 32.7064
 Eigenvalues: 26.6754 29.1890 36.6978
 42 H Isotropic = 30.8344 Anisotropy = 8.8204
 XX= 29.7658 YX= 2.6350 ZX= 0.9200
 XY= 1.6825 YY= 32.4382 ZY= 4.8171
 XZ= 0.6611 YZ= 4.2434 ZZ= 30.2993
 Eigenvalues: 26.5248 29.2638 36.7147
 43 H Isotropic = 30.6989 Anisotropy = 10.9353
 XX= 37.6805 YX= -1.8628 ZX= 1.4018
 XY= -0.5696 YY= 28.1305 ZY= -0.3549
 XZ= 1.2177 YZ= -0.4853 ZZ= 26.2858
 Eigenvalues: 26.0959 28.0118 37.9892
 44 H Isotropic = 29.9364 Anisotropy = 9.2311
 XX= 34.3085 YX= 2.0035 ZX= -2.1380
 XY= 3.1570 YY= 27.1167 ZY= -1.7640
 XZ= -2.7404 YZ= -0.7379 ZZ= 28.3839
 Eigenvalues: 26.1482 27.5706 36.0904
 45 H Isotropic = 30.1403 Anisotropy = 5.4113
 XX= 31.7537 YX= -3.5386 ZX= -0.2517
 XY= -3.1604 YY= 26.4236 ZY= 0.1522
 XZ= 1.6695 YZ= -0.6871 ZZ= 32.2435
 Eigenvalues: 24.8077 31.8654 33.7478
 46 H Isotropic = 29.8412 Anisotropy = 9.2691

XX= 27.1951 YX= -2.3465 ZX= 0.1023
 XY= -3.0774 YY= 33.9873 ZY= 2.9329
 XZ= -0.9586 YZ= 2.8668 ZZ= 28.3412
 Eigenvalues: 26.0236 27.4794 36.0206
 47 H Isotropic = 27.0672 Anisotropy = 6.1296
 XX= 25.9884 YX= 0.1244 ZX= -3.4073
 XY= 1.2921 YY= 28.0360 ZY= -2.2205
 XZ= -4.1178 YZ= -0.6112 ZZ= 27.1773
 Eigenvalues: 22.7445 27.3036 31.1536
 48 H Isotropic = 27.1534 Anisotropy = 10.1550
 XX= 27.8579 YX= 2.3814 ZX= 0.6772
 XY= 3.9254 YY= 32.2821 ZY= 0.5201
 XZ= 1.2261 YZ= -1.8091 ZZ= 21.3201
 Eigenvalues: 21.0657 26.4710 33.9233
 49 H Isotropic = 25.8851 Anisotropy = 11.3675
 XX= 23.9581 YX= -0.7478 ZX= 2.7236
 XY= -0.7849 YY= 23.0022 ZY= -1.4222
 XZ= 6.2350 YZ= -3.0857 ZZ= 30.6949
 Eigenvalues: 21.6078 22.5840 33.4634
 50 H Isotropic = 29.8924 Anisotropy = 14.8043
 XX= 23.7220 YX= -3.1009 ZX= 1.9787
 XY= -2.7192 YY= 27.1696 ZY= -2.5779
 XZ= 2.8401 YZ= -1.9933 ZZ= 38.7856
 Eigenvalues: 22.0031 27.9122 39.7620
 51 H Isotropic = 28.7166 Anisotropy = 16.8311
 XX= 32.2057 YX= 3.2974 ZX= 8.5007
 XY= 3.9252 YY= 31.0028 ZY= 3.8409
 XZ= 8.2191 YZ= 3.5377 ZZ= 22.9414
 Eigenvalues: 17.8633 28.3492 39.9373

Structure 1b conformation 5.

Level of theory & comments

B3PW91 D95** nmr

Ambuic acid, syn stereochemistry, C7 acceptor-C19 donor, s-cis at C8-C9-C11-C12, 120 degree dihedral at C3-C4-C5-C6.

Energy

-1190.7420386

Cartesian coordinates

C	5.62646	-2.32599	0.67365
C	5.1321	-1.30961	-0.29874
C	3.97051	-0.66456	-0.06531
C	3.36846	0.39685	-0.96307
C	2.05379	0.93101	-0.4244
C	1.86216	2.35865	-0.09011
C	0.48814	2.9869	-0.07447
C	-0.67233	2.00369	-0.04303
C	-0.52665	0.67234	-0.30779
C	0.80146	0.13677	-0.75279
C	-1.60416	-0.33557	-0.33317
C	-2.6875	-0.40238	0.46802
C	-3.73153	-1.48583	0.3962
C	-5.14842	-0.93714	0.11987
C	-6.22191	-2.03657	0.10672
C	-7.6354	-1.50196	-0.17375
C	-8.7051	-2.60508	-0.18244
C	6.0242	-1.09946	-1.49864
C	-2.01487	2.66038	0.25131
O	6.66863	-2.94761	0.53818
O	4.81847	-2.52184	1.7547
O	2.09712	1.40387	0.95126
O	0.41135	3.8987	1.04306
O	0.90315	-0.90905	-1.38426
O	-2.08882	4.01574	-0.16854
H	3.42352	-0.90553	0.84312
H	3.19807	-0.00861	-1.96735
H	4.07541	1.23128	-1.06568
H	2.68822	3.05265	-0.25901
H	0.38117	3.6271	-0.9584
H	-1.43964	-1.14251	-1.04678
H	-2.83571	0.34507	1.24949
H	-3.74991	-2.03015	1.35391
H	-3.45605	-2.21371	-0.37845
H	-5.40362	-0.18711	0.88396
H	-5.14662	-0.40949	-0.84467
H	-6.21748	-2.56141	1.07464
H	-5.96182	-2.78988	-0.65266
H	-7.89498	-0.74724	0.5834
H	-7.64044	-0.98056	-1.14222

H	-8.75	-3.12162	0.78586
H	-8.48991	-3.3595	-0.95107
H	-9.70172	-2.1937	-0.38808
H	7.03489	-0.81187	-1.18415
H	5.63145	-0.32717	-2.16647
H	6.12901	-2.03081	-2.06894
H	-2.23901	2.57546	1.32866
H	-2.80538	2.12149	-0.28242
H	5.26532	-3.20409	2.28808
H	0.62814	3.38435	1.83962
H	-1.47857	4.51431	0.40202

Computed NMR tensors

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 22.5797 Anisotropy = 84.9254

XX= 54.2237 YX= -14.6344 ZX= 45.7080

XY= 0.5490 YY= 46.4561 ZY= 46.4952

XZ= 24.7321 YZ= 61.0303 ZZ= -32.9408

Eigenvalues: -69.7862 58.3286 79.1966

2 C Isotropic = 61.1643 Anisotropy = 128.8128

XX= 90.1296 YX= 24.9786 ZX= 19.9418

XY= 23.1026 YY= 76.1721 ZY= 79.2731

XZ= 22.9220 YZ= 74.5886 ZZ= 17.1912

Eigenvalues: -35.8441 72.2975 147.0395

3 C Isotropic = 46.0536 Anisotropy = 160.4788

XX= 69.9225 YX= 33.5755 ZX= 31.5623

XY= 30.1157 YY= 73.5882 ZY= 87.5311

XZ= 41.5980 YZ= 80.0807 ZZ= -5.3500

Eigenvalues: -60.1300 45.2512 153.0395

4 C Isotropic = 158.4269 Anisotropy = 20.1568

XX= 168.1653 YX= -7.6910 ZX= -2.9077

XY= -6.2882 YY= 158.3990 ZY= 6.6827

XZ= 3.0095 YZ= -1.5836 ZZ= 148.7164

Eigenvalues: 147.9014 155.5146 171.8648

5 C Isotropic = 124.8025 Anisotropy = 67.7202

XX= 169.0084 YX= -4.7345 ZX= -4.2151

XY= -0.4008 YY= 78.3268 ZY= -17.3939

XZ= -8.2799 YZ= 5.0173 ZZ= 127.0722

Eigenvalues: 77.4320 127.0261 169.9493

6 C Isotropic = 122.8542 Anisotropy = 50.3136

XX= 156.0699 YX= -3.6553 ZX= -0.1870

XY= -2.7120 YY= 87.3548 ZY= 2.8025
 XZ= -4.9515 YZ= -11.9064 ZZ= 125.1378
 Eigenvalues: 86.6409 125.5251 156.3966
 7 C Isotropic = 118.9734 Anisotropy = 42.8361
 XX= 113.4244 YX= 0.0277 ZX= 1.9600
 XY= -0.6087 YY= 110.7833 ZY= 16.4399
 XZ= -7.4524 YZ= 29.8330 ZZ= 132.7124
 Eigenvalues: 96.0581 113.3312 147.5308
 8 C Isotropic = 33.1529 Anisotropy = 158.3380
 XX= -39.7214 YX= -23.0302 ZX= 23.7007
 XY= -10.6420 YY= 6.9099 ZY= -14.4188
 XZ= 35.5756 YZ= -8.1102 ZZ= 132.2702
 Eigenvalues: -48.6711 9.4182 138.7116
 9 C Isotropic = 60.5848 Anisotropy = 130.9012
 XX= -3.9214 YX= -5.2438 ZX= 34.5838
 XY= -11.1977 YY= 52.9542 ZY= -17.7989
 XZ= 36.7688 YZ= -28.8158 ZZ= 132.7216
 Eigenvalues: -12.7709 46.6730 147.8523
 10 C Isotropic = -6.6683 Anisotropy = 156.3657
 XX= -87.6000 YX= -3.7596 ZX= 18.2739
 XY= -6.4348 YY= 3.8952 ZY= -51.7022
 XZ= 8.2280 YZ= -58.5644 ZZ= 63.6999
 Eigenvalues: -88.7530 -28.8274 97.5755
 11 C Isotropic = 65.3843 Anisotropy = 130.2798
 XX= 89.2445 YX= -38.8527 ZX= 14.8610
 XY= -47.6998 YY= 16.1681 ZY= -68.1058
 XZ= 18.4149 YZ= -64.8826 ZZ= 90.7404
 Eigenvalues: -30.2989 74.2144 152.2376
 12 C Isotropic = 46.1309 Anisotropy = 162.4359
 XX= 66.3622 YX= -58.1339 ZX= 30.9895
 XY= -45.2252 YY= 16.7197 ZY= -79.4132
 XZ= 27.6044 YZ= -82.1100 ZZ= 55.3107
 Eigenvalues: -52.0107 35.9819 154.4215
 13 C Isotropic = 150.2899 Anisotropy = 31.7805
 XX= 164.3967 YX= 13.8746 ZX= 4.9993
 XY= 6.4607 YY= 154.0048 ZY= 1.4585
 XZ= 7.3601 YZ= 0.4397 ZZ= 132.4683
 Eigenvalues: 131.2697 148.1231 171.4769
 14 C Isotropic = 155.8386 Anisotropy = 35.6636
 XX= 177.1177 YX= 7.4399 ZX= 3.6270
 XY= 8.2699 YY= 152.1448 ZY= -2.4423
 XZ= 4.1714 YZ= -2.3683 ZZ= 138.2534
 Eigenvalues: 137.1270 150.7746 179.6144
 15 C Isotropic = 154.2303 Anisotropy = 38.5121
 XX= 177.5276 YX= 7.7466 ZX= 4.8289

XY= 7.1172 YY= 149.3322 ZY= -1.8896
 XZ= 6.0834 YZ= -1.7851 ZZ= 135.8312
 Eigenvalues: 134.5645 148.2214 179.9050
 16 C Isotropic = 164.1834 Anisotropy = 23.2675
 XX= 179.1057 YX= 4.6772 ZX= 3.2931
 XY= -2.2396 YY= 160.7207 ZY= -1.4053
 XZ= 4.2368 YZ= -0.2947 ZZ= 152.7239
 Eigenvalues: 152.0784 160.7768 179.6951
 17 C Isotropic = 174.1121 Anisotropy = 26.5350
 XX= 183.5520 YX= 8.3933 ZX= 1.7908
 XY= 14.5906 YY= 175.6483 ZY= 0.5786
 XZ= 0.8983 YZ= -0.2509 ZZ= 163.1358
 Eigenvalues: 162.9925 167.5417 191.8021
 18 C Isotropic = 173.7340 Anisotropy = 15.8368
 XX= 172.7575 YX= 6.7071 ZX= -8.9533
 XY= 5.5442 YY= 169.0720 ZY= 2.2137
 XZ= -5.0612 YZ= -0.4017 ZZ= 179.3725
 Eigenvalues: 162.8797 174.0305 184.2919
 19 C Isotropic = 121.3691 Anisotropy = 51.1959
 XX= 111.4206 YX= -5.0256 ZX= 0.9165
 XY= -3.4945 YY= 150.7714 ZY= -10.5029
 XZ= 0.0066 YZ= -19.8236 ZZ= 101.9153
 Eigenvalues: 97.5531 111.0545 155.4997
 20 O Isotropic = -73.7060 Anisotropy = 542.3144
 XX= -163.4469 YX= 210.6301 ZX= 142.6169
 XY= 202.4030 YY= 33.8310 ZY= 165.4814
 XZ= 157.1744 YZ= 155.8616 ZZ= -91.5021
 Eigenvalues: -308.0063 -200.9486 287.8370
 21 O Isotropic = 137.1774 Anisotropy = 178.8260
 XX= 106.3489 YX= 115.6692 ZX= -107.7685
 XY= 66.1840 YY= 90.8526 ZY= 40.5180
 XZ= -36.9155 YZ= -9.1817 ZZ= 214.3308
 Eigenvalues: -9.6748 164.8123 256.3947
 22 O Isotropic = 249.2599 Anisotropy = 158.9805
 XX= 350.5808 YX= 12.5413 ZX= -22.8547
 XY= 26.8541 YY= 249.1564 ZY= 105.2828
 XZ= -31.7768 YZ= 59.4667 ZZ= 148.0424
 Eigenvalues: 97.5228 295.0098 355.2469
 23 O Isotropic = 279.8970 Anisotropy = 43.6805
 XX= 263.6826 YX= -4.3704 ZX= 12.1830
 XY= -3.4631 YY= 271.1582 ZY= 18.7440
 XZ= 12.3530 YZ= -5.3478 ZZ= 304.8503
 Eigenvalues: 257.8747 272.7990 309.0174
 24 O Isotropic = -288.5023 Anisotropy = 1015.3279
 XX= -378.2133 YX= 71.1288 ZX= 138.6426

XY= 33.8929 YY= -530.8138 ZY= -551.5863
 XZ= 82.6543 YZ= -561.0849 ZZ= 43.5202
 Eigenvalues: -890.3466 -363.5432 388.3830
 25 O Isotropic = 305.7992 Anisotropy = 57.9279
 XX= 322.7468 YX= 36.9961 ZX= 17.5886
 XY= 3.3057 YY= 298.2658 ZY= -5.7300
 XZ= 22.3282 YZ= 25.6357 ZZ= 296.3850
 Eigenvalues: 285.3914 287.5884 344.4178
 26 H Isotropic = 24.1519 Anisotropy = 11.5908
 XX= 25.8615 YX= -5.1436 ZX= 0.9105
 XY= -6.1444 YY= 25.6270 ZY= -0.8760
 XZ= 2.8552 YZ= -1.8827 ZZ= 20.9671
 Eigenvalues: 19.9121 20.6644 31.8790
 27 H Isotropic = 28.1805 Anisotropy = 6.3239
 XX= 28.5946 YX= -3.2679 ZX= 0.0615
 XY= -0.3489 YY= 25.3581 ZY= 3.0500
 XZ= -0.8566 YZ= 3.1783 ZZ= 30.5886
 Eigenvalues: 23.4717 28.6733 32.3964
 28 H Isotropic = 29.8631 Anisotropy = 7.3340
 XX= 33.4898 YX= 0.0805 ZX= -3.6972
 XY= 0.4203 YY= 32.0772 ZY= -1.6082
 XZ= -3.2350 YZ= -0.5890 ZZ= 24.0223
 Eigenvalues: 22.7882 32.0488 34.7524
 29 H Isotropic = 28.1902 Anisotropy = 9.6909
 XX= 32.1757 YX= 4.9172 ZX= -2.6325
 XY= -0.2427 YY= 29.5871 ZY= -1.5225
 XZ= -3.0766 YZ= -2.9708 ZZ= 22.8078
 Eigenvalues: 21.6801 28.2397 34.6508
 30 H Isotropic = 26.7502 Anisotropy = 3.9846
 XX= 26.4208 YX= -1.8944 ZX= -0.6302
 XY= -1.2375 YY= 25.9793 ZY= -0.7737
 XZ= -0.4373 YZ= -3.6883 ZZ= 27.8505
 Eigenvalues: 23.5839 27.2601 29.4066
 31 H Isotropic = 24.4821 Anisotropy = 8.7752
 XX= 29.4698 YX= 0.9325 ZX= -2.5756
 XY= 1.4294 YY= 22.0074 ZY= -0.1231
 XZ= -2.4134 YZ= 1.4029 ZZ= 21.9692
 Eigenvalues: 20.5489 22.5652 30.3322
 32 H Isotropic = 25.7081 Anisotropy = 8.9301
 XX= 28.2956 YX= 3.4116 ZX= -1.1462
 XY= 4.4699 YY= 25.4513 ZY= -2.8840
 XZ= -1.1863 YZ= -1.4784 ZZ= 23.3774
 Eigenvalues: 21.6534 23.8095 31.6615
 33 H Isotropic = 29.4216 Anisotropy = 5.6825
 XX= 29.8396 YX= 0.2551 ZX= 1.4985

XY= 1.6361 YY= 28.6141 ZY= -4.2309
 XZ= 0.7858 YZ= -3.6330 ZZ= 29.8112
 Eigenvalues: 24.8101 30.2448 33.2100
 34 H Isotropic = 29.5156 Anisotropy = 5.6911
 XX= 32.0491 YX= -0.0623 ZX= -1.4243
 XY= -0.6761 YY= 30.0609 ZY= 3.8456
 XZ= -2.4008 YZ= 2.0973 ZZ= 26.4367
 Eigenvalues: 24.4681 30.7690 33.3097
 35 H Isotropic = 30.2044 Anisotropy = 5.6818
 XX= 31.6506 YX= 0.5173 ZX= -0.7677
 XY= 0.3554 YY= 31.2357 ZY= 4.5086
 XZ= -0.1232 YZ= 3.7901 ZZ= 27.7270
 Eigenvalues: 24.9206 31.7004 33.9923
 36 H Isotropic = 30.2978 Anisotropy = 4.9691
 XX= 31.7022 YX= 1.7098 ZX= 0.4324
 XY= 1.4158 YY= 28.9586 ZY= -4.1756
 XZ= 0.8398 YZ= -3.4010 ZZ= 30.2327
 Eigenvalues: 25.3472 31.9357 33.6106
 37 H Isotropic = 30.3847 Anisotropy = 5.2842
 XX= 31.3167 YX= 1.3635 ZX= 0.7175
 XY= 1.5978 YY= 28.9929 ZY= -4.0908
 XZ= 0.7429 YZ= -3.5626 ZZ= 30.8445
 Eigenvalues: 25.5297 31.7169 33.9075
 38 H Isotropic = 30.2960 Anisotropy = 5.4286
 XX= 31.9300 YX= 0.0946 ZX= -0.7006
 XY= 0.0733 YY= 30.8956 ZY= 4.4717
 XZ= -0.6763 YZ= 3.8160 ZZ= 28.0625
 Eigenvalues: 25.0458 31.9272 33.9151
 39 H Isotropic = 30.3033 Anisotropy = 7.0603
 XX= 31.4265 YX= -0.8091 ZX= -1.3880
 XY= -0.5416 YY= 31.7155 ZY= 4.6138
 XZ= -1.4676 YZ= 4.0431 ZZ= 27.7680
 Eigenvalues: 24.8748 31.0250 35.0102
 40 H Isotropic = 30.2595 Anisotropy = 6.8225
 XX= 30.4417 YX= 0.8853 ZX= 1.6354
 XY= 1.2886 YY= 29.1896 ZY= -4.6698
 XZ= 1.8037 YZ= -4.1749 ZZ= 31.1471
 Eigenvalues: 24.9583 31.0124 34.8078
 41 H Isotropic = 30.8354 Anisotropy = 8.7381
 XX= 29.9932 YX= 3.0574 ZX= -1.9427
 XY= 2.3958 YY= 30.2051 ZY= -4.2639
 XZ= -1.4524 YZ= -3.4995 ZZ= 32.3079
 Eigenvalues: 26.6697 29.1757 36.6608
 42 H Isotropic = 30.8241 Anisotropy = 8.7853
 XX= 29.4098 YX= 2.1925 ZX= 0.5373

XY= 1.2152 YY= 32.5509 ZY= 4.9571
 XZ= 0.3264 YZ= 4.4156 ZZ= 30.5115
 Eigenvalues: 26.5301 29.2612 36.6809
 43 H Isotropic = 30.7015 Anisotropy = 10.9438
 XX= 37.7039 YX= -1.0839 ZX= 1.8566
 XY= 0.2059 YY= 28.0297 ZY= -0.2161
 XZ= 1.6841 YZ= -0.4167 ZZ= 26.3709
 Eigenvalues: 26.0694 28.0377 37.9973
 44 H Isotropic = 29.9299 Anisotropy = 9.3239
 XX= 35.6631 YX= 1.2512 ZX= 0.4250
 XY= 2.8700 YY= 27.1537 ZY= -1.0528
 XZ= 0.5116 YZ= -0.3324 ZZ= 26.9728
 Eigenvalues: 26.0299 27.6139 36.1458
 45 H Isotropic = 30.1938 Anisotropy = 5.3217
 XX= 30.8177 YX= -2.8333 ZX= -2.2289
 XY= -3.4944 YY= 29.4567 ZY= -2.6258
 XZ= -0.6116 YZ= -3.5231 ZZ= 30.3070
 Eigenvalues: 24.8827 31.9571 33.7416
 46 H Isotropic = 29.8566 Anisotropy = 9.2451
 XX= 27.0279 YX= -2.0098 ZX= -1.0672
 XY= -2.0934 YY= 31.6053 ZY= 3.8234
 XZ= -2.3330 YZ= 4.0713 ZZ= 30.9365
 Eigenvalues: 26.2247 27.3250 36.0200
 47 H Isotropic = 27.0595 Anisotropy = 6.1351
 XX= 25.8963 YX= 0.1251 ZX= -3.2604
 XY= 1.2744 YY= 28.3052 ZY= -2.4205
 XZ= -4.0679 YZ= -0.8214 ZZ= 26.9771
 Eigenvalues: 22.6794 27.3496 31.1496
 48 H Isotropic = 27.1499 Anisotropy = 10.1449
 XX= 27.4106 YX= 2.0324 ZX= 0.7549
 XY= 3.5579 YY= 32.7006 ZY= 1.0196
 XZ= 1.5246 YZ= -1.2615 ZZ= 21.3384
 Eigenvalues: 21.0950 26.4415 33.9131
 49 H Isotropic = 25.8704 Anisotropy = 11.3105
 XX= 22.1780 YX= 0.1681 ZX= 0.2145
 XY= -1.7360 YY= 26.7931 ZY= -4.3464
 XZ= 3.1049 YZ= -6.3214 ZZ= 28.6402
 Eigenvalues: 21.5946 22.6059 33.4107
 50 H Isotropic = 29.8775 Anisotropy = 14.7486
 XX= 24.1132 YX= -3.4996 ZX= 2.0874
 XY= -3.1126 YY= 27.0392 ZY= -2.8960
 XZ= 2.9398 YZ= -2.3223 ZZ= 38.4800
 Eigenvalues: 21.9293 27.9932 39.7099
 51 H Isotropic = 28.7322 Anisotropy = 16.8600
 XX= 31.6612 YX= 2.9825 ZX= 8.3789

XY= 3.6383 YY= 31.1345 ZY= 4.7460
 XZ= 8.1611 YZ= 4.5057 ZZ= 23.4007
 Eigenvalues: 17.8792 28.3452 39.9721

Structure 1b conformation 6.

Level of theory & comments

B3PW91 D95** nmr

Ambuic acid, syn stereochemistry, C7 acceptor-C19 donor, s-cis at
 C8-C9-C11-C12, 150 degree dihedral at C3-C4-C5-C6.

Energy

-1190.7419250

Cartesian coordinates

C	5.29768	-2.71316	0.3639
C	5.02855	-1.38267	-0.25118
C	3.86536	-0.74647	-0.00211
C	3.49046	0.61313	-0.55542
C	2.1237	1.10322	-0.12148
C	1.85669	2.55	0.01899
C	0.46671	3.12208	-0.13242
C	-0.66096	2.10362	-0.06347
C	-0.44885	0.76066	-0.18022
C	0.92439	0.25153	-0.50019
C	-1.48182	-0.29257	-0.17303
C	-2.6155	-0.32524	0.55776
C	-3.61675	-1.4502	0.52595
C	-5.02114	-0.98679	0.08085
C	-6.06163	-2.11743	0.11229
C	-7.46034	-1.66712	-0.33829
C	-8.49778	-2.80021	-0.30035
C	6.13653	-0.86499	-1.13766
C	-2.04178	2.73044	0.07249
O	6.3175	-3.35764	0.1743
O	4.30689	-3.17596	1.17846

O	2.04276	1.72543	1.1834
O	0.28283	4.15459	0.86077
O	1.10274	-0.80977	-1.08715
O	-2.13589	4.02703	-0.50098
H	3.14656	-1.23281	0.65188
H	3.50976	0.5801	-1.65359
H	4.23118	1.36233	-0.24586
H	2.67062	3.25424	-0.16565
H	0.40443	3.65084	-1.09125
H	-1.23905	-1.15674	-0.79108
H	-2.84454	0.49024	1.24621
H	-3.69764	-1.88784	1.53375
H	-3.2585	-2.24663	-0.13969
H	-5.35615	-0.1647	0.73154
H	-4.95586	-0.57147	-0.93498
H	-6.12287	-2.52723	1.13239
H	-5.72145	-2.94334	-0.53103
H	-7.79912	-0.8396	0.3025
H	-7.3998	-1.26122	-1.35878
H	-8.60571	-3.20478	0.71507
H	-8.203	-3.629	-0.95798
H	-9.48516	-2.44942	-0.62708
H	7.07426	-0.7781	-0.57503
H	5.8935	0.11296	-1.56334
H	6.33082	-1.56427	-1.96014
H	-2.33465	2.75447	1.1365
H	-2.77461	2.10296	-0.44636
H	4.61934	-4.04317	1.49455
H	0.45954	3.74625	1.72566
H	-1.57765	4.60948	0.04282

Computed NMR tensors

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 22.2859 Anisotropy = 85.0822

XX= 37.7432 YX= -44.0917 ZX= 48.3977

XY= -20.2895 YY= 7.3446 ZY= 52.3715

XZ= 35.6232 YZ= 65.0761 ZZ= 21.7700

Eigenvalues: -69.8544 57.7047 79.0074

2 C Isotropic = 61.8864 Anisotropy = 126.5863

XX= 80.6926 YX= -3.1463 ZX= 36.1506

XY= -6.4130 YY= 19.8031 ZY= 75.5453

XZ= 37.4573 YZ= 72.6914 ZZ= 85.1636
 Eigenvalues: -33.8141 73.1961 146.2773
 3 C Isotropic = 45.1443 Anisotropy = 162.1109
 XX= 55.3214 YX= 2.2443 ZX= 52.1050
 XY= -8.1066 YY= 4.1515 ZY= 86.8809
 XZ= 58.3142 YZ= 82.2114 ZZ= 75.9600
 Eigenvalues: -61.9168 44.1315 153.2182
 4 C Isotropic = 155.0934 Anisotropy = 22.4918
 XX= 165.0257 YX= -7.1429 ZX= -1.2574
 XY= -8.1068 YY= 156.5244 ZY= 10.9328
 XZ= 2.6526 YZ= 5.9463 ZZ= 143.7301
 Eigenvalues: 138.8706 156.3217 170.0879
 5 C Isotropic = 125.4799 Anisotropy = 66.3392
 XX= 169.2404 YX= 0.4934 ZX= -2.4696
 XY= 4.9434 YY= 79.9877 ZY= -12.2945
 XZ= -5.4662 YZ= 7.9620 ZZ= 127.2117
 Eigenvalues: 79.8164 126.9173 169.7061
 6 C Isotropic = 126.8120 Anisotropy = 52.7751
 XX= 161.9545 YX= 0.0101 ZX= 2.1375
 XY= 2.5474 YY= 87.4023 ZY= 6.5683
 XZ= -0.5448 YZ= -10.3515 ZZ= 131.0791
 Eigenvalues: 87.2975 131.1431 161.9954
 7 C Isotropic = 118.9345 Anisotropy = 43.1545
 XX= 114.0576 YX= -1.7205 ZX= 0.7906
 XY= -2.7003 YY= 116.2852 ZY= 18.7357
 XZ= -9.5170 YZ= 31.5504 ZZ= 126.4608
 Eigenvalues: 95.6588 113.4405 147.7042
 8 C Isotropic = 33.9418 Anisotropy = 156.8726
 XX= -40.1421 YX= -22.1232 ZX= 14.8944
 XY= -10.1196 YY= 5.9382 ZY= -0.3543
 XZ= 27.2756 YZ= 5.9126 ZZ= 136.0293
 Eigenvalues: -47.6142 10.9160 138.5235
 9 C Isotropic = 60.0703 Anisotropy = 130.9410
 XX= -7.7812 YX= -3.2894 ZX= 26.9890
 XY= -9.2202 YY= 47.9468 ZY= -8.9133
 XZ= 29.2443 YZ= -18.5178 ZZ= 140.0453
 Eigenvalues: -13.1740 46.0206 147.3643
 10 C Isotropic = -7.9496 Anisotropy = 156.1506
 XX= -88.7048 YX= -2.9896 ZX= 7.0331
 XY= -6.4268 YY= -0.2644 ZY= -51.0834
 XZ= -2.9794 YZ= -58.1008 ZZ= 65.1205
 Eigenvalues: -88.9610 -31.0385 96.1509
 11 C Isotropic = 65.6449 Anisotropy = 129.3792
 XX= 89.8687 YX= -29.5037 ZX= 19.9970
 XY= -37.4917 YY= 0.8680 ZY= -61.0066

XZ= 24.1472 YZ= -57.0162 ZZ= 106.1979
 Eigenvalues: -29.6892 74.7261 151.8977
 12 C Isotropic = 46.2132 Anisotropy = 162.4740
 XX= 65.7679 YX= -46.2349 ZX= 39.4145
 XY= -34.7204 YY= -2.9540 ZY= -75.0889
 XZ= 35.5602 YZ= -77.7030 ZZ= 75.8257
 Eigenvalues: -51.7531 35.8635 154.5292
 13 C Isotropic = 150.2399 Anisotropy = 31.5353
 XX= 162.6646 YX= 14.6922 ZX= 5.6386
 XY= 7.1455 YY= 154.7278 ZY= -0.0613
 XZ= 9.2278 YZ= -0.4692 ZZ= 133.3272
 Eigenvalues: 131.1648 148.2914 171.2634
 14 C Isotropic = 155.6355 Anisotropy = 35.8868
 XX= 175.6383 YX= 9.0279 ZX= 5.8176
 XY= 10.2137 YY= 151.8670 ZY= -3.0644
 XZ= 5.9990 YZ= -3.3086 ZZ= 139.4011
 Eigenvalues: 136.7979 150.5485 179.5600
 15 C Isotropic = 154.0538 Anisotropy = 38.6927
 XX= 175.9909 YX= 9.4945 ZX= 7.0908
 XY= 8.5263 YY= 149.0695 ZY= -2.6023
 XZ= 8.7527 YZ= -2.2877 ZZ= 137.1008
 Eigenvalues: 134.2555 148.0569 179.8489
 16 C Isotropic = 164.0242 Anisotropy = 23.2257
 XX= 178.0319 YX= 5.6557 ZX= 4.8592
 XY= -0.4761 YY= 160.5800 ZY= -2.3287
 XZ= 6.3653 YZ= -0.9052 ZZ= 153.4607
 Eigenvalues: 151.7171 160.8476 179.5080
 17 C Isotropic = 174.1365 Anisotropy = 26.4358
 XX= 182.5891 YX= 8.9341 ZX= 2.3653
 XY= 14.7576 YY= 176.3620 ZY= 0.1688
 XZ= 0.9893 YZ= -1.1937 ZZ= 163.4583
 Eigenvalues: 162.9450 167.7042 191.7603
 18 C Isotropic = 174.0172 Anisotropy = 14.9251
 XX= 175.9325 YX= 9.4358 ZX= -6.1978
 XY= 6.1140 YY= 168.6084 ZY= 0.7230
 XZ= -3.5577 YZ= -1.7494 ZZ= 177.5107
 Eigenvalues: 163.3136 174.7708 183.9672
 19 C Isotropic = 121.6755 Anisotropy = 51.1919
 XX= 111.8698 YX= -4.7616 ZX= 2.4252
 XY= -3.9477 YY= 146.7705 ZY= -15.5560
 XZ= 1.9896 YZ= -25.1936 ZZ= 106.3861
 Eigenvalues: 97.8831 111.3399 155.8034
 20 O Isotropic = -72.7603 Anisotropy = 541.5719
 XX= -194.8525 YX= 134.0176 ZX= 188.9466
 XY= 118.8360 YY= -111.4650 ZY= 165.2331

XZ= 198.1828 YZ= 157.6853 ZZ= 88.0365
 Eigenvalues: -306.9822 -199.5864 288.2876
 21 O Isotropic = 137.1246 Anisotropy = 178.9335
 XX= 142.5475 YX= 149.1639 ZX= -72.3104
 XY= 69.6520 YY= 72.7422 ZY= 13.4884
 XZ= -27.3469 YZ= -27.7504 ZZ= 196.0842
 Eigenvalues: -10.0231 164.9833 256.4136
 22 O Isotropic = 243.6758 Anisotropy = 161.7995
 XX= 348.2057 YX= 10.3919 ZX= -24.6810
 XY= 20.6442 YY= 257.2269 ZY= 92.6273
 XZ= -20.5539 YZ= 37.5751 ZZ= 125.5947
 Eigenvalues: 95.9833 283.5019 351.5421
 23 O Isotropic = 280.2133 Anisotropy = 43.8176
 XX= 262.4707 YX= -3.7952 ZX= 8.2595
 XY= -4.9527 YY= 272.5313 ZY= 21.2097
 XZ= 9.5373 YZ= -2.0425 ZZ= 305.6380
 Eigenvalues: 257.8433 273.3716 309.4250
 24 O Isotropic = -292.4435 Anisotropy = 1016.4319
 XX= -399.0338 YX= 120.1512 ZX= 108.8556
 XY= 80.5088 YY= -577.1835 ZY= -525.7404
 XZ= 56.7706 YZ= -522.1662 ZZ= 98.8867
 Eigenvalues: -895.5685 -366.9398 385.1777
 25 O Isotropic = 306.0041 Anisotropy = 58.5120
 XX= 319.3392 YX= 37.9321 ZX= 15.4043
 XY= 6.9376 YY= 302.1892 ZY= -5.2754
 XZ= 22.7943 YZ= 28.3502 ZZ= 296.4838
 Eigenvalues: 285.2714 287.7287 345.0120
 26 H Isotropic = 24.0878 Anisotropy = 10.6847
 XX= 25.2926 YX= -4.1267 ZX= 0.3896
 XY= -6.0677 YY= 26.4057 ZY= 0.0241
 XZ= 2.5356 YZ= -1.6376 ZZ= 20.5650
 Eigenvalues: 19.9481 21.1044 31.2109
 27 H Isotropic = 28.4896 Anisotropy = 7.0685
 XX= 28.4165 YX= -4.4497 ZX= -2.2164
 XY= -1.7890 YY= 25.8050 ZY= 0.3768
 XZ= -2.8488 YZ= -0.0480 ZZ= 31.2471
 Eigenvalues: 23.5018 28.7650 33.2019
 28 H Isotropic = 29.9851 Anisotropy = 7.2280
 XX= 34.7423 YX= -0.1733 ZX= -0.9600
 XY= 0.7132 YY= 31.6637 ZY= 1.0478
 XZ= -0.5813 YZ= 2.1810 ZZ= 23.5493
 Eigenvalues: 23.1834 31.9681 34.8038
 29 H Isotropic = 28.4039 Anisotropy = 10.0836
 XX= 32.7764 YX= 5.2575 ZX= -2.4316
 XY= -0.0985 YY= 29.4037 ZY= -2.1301

XZ= -2.3619 YZ= -3.1723 ZZ= 23.0315
 Eigenvalues: 21.8766 28.2087 35.1263
 30 H Isotropic = 26.7835 Anisotropy = 4.0207
 XX= 26.5532 YX= -1.6789 ZX= -0.5478
 XY= -1.1610 YY= 25.4796 ZY= -0.5515
 XZ= -0.1981 YZ= -3.6154 ZZ= 28.3176
 Eigenvalues: 23.6654 27.2212 29.4639
 31 H Isotropic = 24.5135 Anisotropy = 8.8428
 XX= 29.7265 YX= 0.8754 ZX= -2.1460
 XY= 1.4971 YY= 22.1804 ZY= -0.1661
 XZ= -2.2472 YZ= 1.3279 ZZ= 21.6335
 Eigenvalues: 20.5853 22.5465 30.4087
 32 H Isotropic = 25.7374 Anisotropy = 8.8295
 XX= 28.1094 YX= 3.5029 ZX= -1.0573
 XY= 4.5969 YY= 25.3329 ZY= -2.7700
 XZ= -1.3321 YZ= -1.4314 ZZ= 23.7698
 Eigenvalues: 21.7521 23.8363 31.6237
 33 H Isotropic = 29.4265 Anisotropy = 5.6700
 XX= 29.5601 YX= 0.7534 ZX= 1.4893
 XY= 2.0431 YY= 27.8768 ZY= -3.8016
 XZ= 0.5924 YZ= -3.2919 ZZ= 30.8425
 Eigenvalues: 24.8693 30.2037 33.2065
 34 H Isotropic = 29.5415 Anisotropy = 5.7087
 XX= 32.3311 YX= -0.3269 ZX= -1.0721
 XY= -1.1527 YY= 30.6718 ZY= 3.2354
 XZ= -1.8695 YZ= 1.5401 ZZ= 25.6217
 Eigenvalues: 24.5144 30.7629 33.3473
 35 H Isotropic = 30.2115 Anisotropy = 5.6584
 XX= 31.7113 YX= 0.1960 ZX= -0.6105
 XY= -0.0086 YY= 32.1407 ZY= 3.9947
 XZ= 0.0380 YZ= 3.2892 ZZ= 26.7825
 Eigenvalues: 24.9273 31.7234 33.9838
 36 H Isotropic = 30.3199 Anisotropy = 4.9032
 XX= 31.5156 YX= 2.1077 ZX= 0.4025
 XY= 1.9066 YY= 28.2611 ZY= -3.7682
 XZ= 0.8543 YZ= -2.9249 ZZ= 31.1829
 Eigenvalues: 25.3968 31.9742 33.5887
 37 H Isotropic = 30.3633 Anisotropy = 5.2868
 XX= 31.1005 YX= 1.8081 ZX= 0.6266
 XY= 2.0537 YY= 28.2403 ZY= -3.6097
 XZ= 0.5612 YZ= -3.1029 ZZ= 31.7490
 Eigenvalues: 25.5164 31.6856 33.8878
 38 H Isotropic = 30.2961 Anisotropy = 5.4198
 XX= 32.0302 YX= -0.2416 ZX= -0.4732
 XY= -0.2984 YY= 31.8176 ZY= 3.9793

XZ= -0.3642 YZ= 3.3594 ZZ= 27.0404
 Eigenvalues: 25.0424 31.9365 33.9093
 39 H Isotropic = 30.2845 Anisotropy = 7.0432
 XX= 31.6998 YX= -1.2492 ZX= -1.0496
 XY= -1.0776 YY= 32.5663 ZY= 3.9359
 XZ= -1.1657 YZ= 3.2898 ZZ= 26.5873
 Eigenvalues: 24.8485 31.0249 34.9800
 40 H Isotropic = 30.2630 Anisotropy = 6.7898
 XX= 30.0969 YX= 1.4286 ZX= 1.5089
 XY= 1.8854 YY= 28.3250 ZY= -4.1451
 XZ= 1.6537 YZ= -3.6378 ZZ= 32.3672
 Eigenvalues: 24.9785 31.0210 34.7896
 41 H Isotropic = 30.8119 Anisotropy = 8.7497
 XX= 30.1337 YX= 3.0766 ZX= -2.3566
 XY= 2.5190 YY= 29.5213 ZY= -3.8575
 XZ= -1.8528 YZ= -3.0180 ZZ= 32.7806
 Eigenvalues: 26.6472 29.1434 36.6450
 42 H Isotropic = 30.8025 Anisotropy = 8.7851
 XX= 29.2717 YX= 1.7817 ZX= 0.1152
 XY= 0.7551 YY= 33.7006 ZY= 4.6650
 XZ= 0.0807 YZ= 4.2001 ZZ= 29.4353
 Eigenvalues: 26.5156 29.2327 36.6593
 43 H Isotropic = 30.6722 Anisotropy = 10.9892
 XX= 37.3644 YX= -0.4825 ZX= 2.8209
 XY= 0.7461 YY= 27.9346 ZY= -0.2895
 XZ= 2.5272 YZ= -0.5972 ZZ= 26.7175
 Eigenvalues: 25.9748 28.0434 37.9983
 44 H Isotropic = 29.9689 Anisotropy = 9.3789
 XX= 35.3273 YX= 0.4549 ZX= 2.2679
 XY= 2.0237 YY= 27.4107 ZY= -0.5331
 XZ= 2.9297 YZ= -0.1456 ZZ= 27.1687
 Eigenvalues: 26.0475 27.6377 36.2215
 45 H Isotropic = 30.2489 Anisotropy = 5.6008
 XX= 31.1791 YX= -1.4450 ZX= -2.7309
 XY= -2.6654 YY= 32.1296 ZY= -2.5072
 XZ= -1.6886 YZ= -3.3133 ZZ= 27.4380
 Eigenvalues: 24.7389 32.0250 33.9828
 46 H Isotropic = 29.8589 Anisotropy = 9.1910
 XX= 27.5965 YX= -1.9671 ZX= -2.4025
 XY= -1.4845 YY= 29.4995 ZY= 2.9538
 XZ= -3.7824 YZ= 3.3912 ZZ= 32.4806
 Eigenvalues: 26.0819 27.5085 35.9862
 47 H Isotropic = 27.0808 Anisotropy = 6.1161
 XX= 26.3364 YX= -0.2586 ZX= -3.2198
 XY= 0.8915 YY= 27.9624 ZY= -2.5651

XZ= -4.2187 YZ= -1.0809 ZZ= 26.9436
 Eigenvalues: 22.7049 27.3793 31.1582
 48 H Isotropic = 27.1770 Anisotropy = 10.1799
 XX= 27.0561 YX= 2.0427 ZX= 0.8759
 XY= 3.4565 YY= 32.8411 ZY= 0.1004
 XZ= 1.6081 YZ= -2.2529 ZZ= 21.6337
 Eigenvalues: 21.1135 26.4539 33.9636
 49 H Isotropic = 25.8602 Anisotropy = 11.2467
 XX= 21.9298 YX= 1.9394 ZX= -0.6165
 XY= -1.1249 YY= 30.5595 ZY= -3.8917
 XZ= 1.2750 YZ= -5.7208 ZZ= 25.0914
 Eigenvalues: 21.5883 22.6343 33.3580
 50 H Isotropic = 29.9015 Anisotropy = 14.7031
 XX= 24.0351 YX= -3.1320 ZX= 1.5358
 XY= -2.6333 YY= 26.3949 ZY= -1.5370
 XZ= 2.2790 YZ= -0.9331 ZZ= 39.2746
 Eigenvalues: 22.0517 27.9492 39.7036
 51 H Isotropic = 28.7102 Anisotropy = 16.9949
 XX= 30.4585 YX= 3.6645 ZX= 8.3542
 XY= 4.2880 YY= 32.3780 ZY= 4.3770
 XZ= 8.1027 YZ= 4.0509 ZZ= 23.2941
 Eigenvalues: 17.7612 28.3292 40.0402

Structure 1b conformation 7.

Level of theory & comments

B3PW91 D95** nmr

Ambuic acid, syn stereochemistry, C7 acceptor-C19 donor, s-cis at
 C8-C9-C11-C12, 180 degree dihedral at C3-C4-C5-C6.

Energy

-1190.7357772

Cartesian coordinates

C	5.29417	-2.82587	0.00931
C	5.09013	-1.35401	-0.10578

C	3.85645	-0.83065	0.05786
C	3.55325	0.65214	-0.01146
C	2.10714	1.10164	0.19361
C	1.81923	2.55472	0.12414
C	0.46549	3.1062	-0.26106
C	-0.6725	2.10304	-0.16616
C	-0.44378	0.76064	-0.12662
C	0.95499	0.24928	-0.31692
C	-1.46481	-0.30253	-0.08901
C	-2.63102	-0.28148	0.58886
C	-3.62748	-1.41071	0.612
C	-5.02561	-0.98511	0.11343
C	-6.06113	-2.11745	0.19941
C	-7.45756	-1.70136	-0.28951
C	-8.48969	-2.83603	-0.19574
C	6.34465	-0.57275	-0.41974
C	-2.05897	2.72909	-0.20914
O	6.37224	-3.37813	-0.14805
O	4.17144	-3.53586	0.31564
O	1.83658	1.86324	1.38925
O	0.19912	4.26812	0.55439
O	1.17207	-0.79022	-0.92749
O	-2.11067	3.93238	-0.96393
H	3.03888	-1.50813	0.27366
H	3.87601	1.02111	-0.99623
H	4.15363	1.19698	0.7288
H	2.65701	3.24011	-0.02285
H	0.51485	3.4972	-1.28472
H	-1.18717	-1.21057	-0.62425
H	-2.8898	0.59015	1.19353
H	-3.72502	-1.78145	1.64499
H	-3.25345	-2.24749	0.00726
H	-5.37546	-0.12569	0.70546
H	-4.94542	-0.63428	-0.92536
H	-6.13054	-2.4683	1.24076
H	-5.71085	-2.97719	-0.39209
H	-7.80645	-0.84033	0.29962
H	-7.38934	-1.35431	-1.33104
H	-8.60566	-3.18133	0.84044
H	-8.18426	-3.70009	-0.80105
H	-9.47551	-2.51039	-0.5519
H	7.10445	-0.73422	0.35497
H	6.14976	0.50093	-0.49573
H	6.78685	-0.91486	-1.36351
H	-2.4227	2.89938	0.81919

H	-2.75662	2.02998	-0.68254
H	4.45792	-4.46668	0.34866
H	0.2629	3.98184	1.48167
H	-1.58808	4.5886	-0.47115

Computed NMR tensors

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 22.2208 Anisotropy = 85.5137

XX= 22.9657 YX= -69.3592 ZX= 19.2106

XY= -40.2713 YY= -29.3027 ZY= 20.1102

XZ= 16.5817 YZ= 25.6556 ZZ= 72.9993

Eigenvalues: -69.7497 57.1821 79.2299

2 C Isotropic = 62.2968 Anisotropy = 125.9835

XX= 66.6165 YX= -26.0847 ZX= 17.0264

XY= -29.7891 YY= -20.6948 ZY= 22.5689

XZ= 17.1432 YZ= 21.6537 ZZ= 140.9688

Eigenvalues: -32.7866 73.3912 146.2858

3 C Isotropic = 46.4631 Anisotropy = 169.7511

XX= 33.4888 YX= -25.1763 ZX= 27.2306

XY= -36.4373 YY= -46.0230 ZY= 22.5294

XZ= 28.9988 YZ= 24.9949 ZZ= 151.9234

Eigenvalues: -61.3156 41.0744 159.6305

4 C Isotropic = 154.0437 Anisotropy = 30.9932

XX= 167.4823 YX= -12.1393 ZX= 0.7935

XY= -11.9567 YY= 152.7178 ZY= 10.6952

XZ= 2.3196 YZ= 10.1719 ZZ= 141.9310

Eigenvalues: 133.6738 153.7514 174.7058

5 C Isotropic = 127.4151 Anisotropy = 65.7166

XX= 170.7604 YX= 2.4995 ZX= 1.5627

XY= 9.5912 YY= 81.2882 ZY= -5.7536

XZ= 1.0983 YZ= 12.5461 ZZ= 130.1968

Eigenvalues: 80.6617 130.3575 171.2262

6 C Isotropic = 126.3780 Anisotropy = 55.3115

XX= 162.5821 YX= 3.9003 ZX= 2.4809

XY= 3.7255 YY= 87.1541 ZY= 13.5790

XZ= 5.0536 YZ= -3.9065 ZZ= 129.3979

Eigenvalues: 86.4579 129.4239 163.2524

7 C Isotropic = 119.1061 Anisotropy = 43.4454

XX= 114.8968 YX= -4.1253 ZX= 0.9771

XY= -5.6731 YY= 123.4933 ZY= 19.1514

XZ= -9.4210 YZ= 31.8429 ZZ= 118.9283

Eigenvalues: 95.6097 113.6390 148.0697
8 C Isotropic = 37.2872 Anisotropy = 152.4564
XX= -37.8790 YX= -21.4603 ZX= 3.7232
XY= -10.7331 YY= 13.4870 ZY= 13.0999
XZ= 18.5366 YZ= 20.1869 ZZ= 136.2535
Eigenvalues: -43.8252 16.7620 138.9247
9 C Isotropic = 58.1516 Anisotropy = 129.1919
XX= -13.5775 YX= -1.0961 ZX= 16.5435
XY= -6.0497 YY= 45.8163 ZY= 0.0982
XZ= 17.9485 YZ= -7.7178 ZZ= 142.2161
Eigenvalues: -15.6243 45.7996 144.2795
10 C Isotropic = -9.9582 Anisotropy = 154.2002
XX= -87.8979 YX= 2.7814 ZX= -9.7984
XY= -0.4763 YY= 2.6631 ZY= -54.9157
XZ= -22.0571 YZ= -58.9552 ZZ= 55.3601
Eigenvalues: -90.0106 -32.7061 92.8419
11 C Isotropic = 65.6826 Anisotropy = 126.9393
XX= 89.0086 YX= -24.7203 ZX= 20.6620
XY= -31.4581 YY= -8.4813 ZY= -52.5379
XZ= 25.6900 YZ= -47.0823 ZZ= 116.5206
Eigenvalues: -29.0750 75.8140 150.3088
12 C Isotropic = 46.6375 Anisotropy = 160.9918
XX= 65.1932 YX= -37.1744 ZX= 41.5630
XY= -28.7558 YY= -16.1919 ZY= -67.8452
XZ= 39.1353 YZ= -70.2487 ZZ= 90.9114
Eigenvalues: -51.3975 37.3447 153.9654
13 C Isotropic = 150.3972 Anisotropy = 31.4747
XX= 162.5774 YX= 14.9645 ZX= 5.7156
XY= 7.8922 YY= 154.4549 ZY= -1.3875
XZ= 9.1571 YZ= -1.8444 ZZ= 134.1592
Eigenvalues: 131.3881 148.4231 171.3803
14 C Isotropic = 155.7078 Anisotropy = 35.6947
XX= 175.2905 YX= 9.3773 ZX= 5.8113
XY= 10.7502 YY= 151.9064 ZY= -3.4153
XZ= 5.9579 YZ= -3.5551 ZZ= 139.9264
Eigenvalues: 136.9653 150.6538 179.5042
15 C Isotropic = 154.0195 Anisotropy = 38.7061
XX= 175.7071 YX= 10.0950 ZX= 7.0495
XY= 9.1365 YY= 148.7642 ZY= -3.2855
XZ= 8.6844 YZ= -2.8829 ZZ= 137.5871
Eigenvalues: 134.1551 148.0798 179.8236
16 C Isotropic = 163.9514 Anisotropy = 23.2647
XX= 177.7999 YX= 5.9790 ZX= 4.8163
XY= 0.1657 YY= 160.4728 ZY= -2.7090
XZ= 6.7404 YZ= -1.1204 ZZ= 153.5815

Eigenvalues: 151.5289 160.8641 179.4612
 17 C Isotropic = 174.1899 Anisotropy = 26.3951
 XX= 182.4188 YX= 9.0835 ZX= 2.0396
 XY= 14.8443 YY= 176.5030 ZY= -0.4436
 XZ= 0.3247 YZ= -1.8930 ZZ= 163.6478
 Eigenvalues: 162.9907 167.7923 191.7866
 18 C Isotropic = 174.7337 Anisotropy = 13.5861
 XX= 177.1374 YX= 11.7622 ZX= -1.3384
 XY= 6.6859 YY= 170.0368 ZY= -0.3951
 XZ= -1.0342 YZ= -1.3501 ZZ= 177.0270
 Eigenvalues: 163.7031 176.7068 183.7911
 19 C Isotropic = 122.2481 Anisotropy = 52.0437
 XX= 111.9521 YX= -2.6945 ZX= 3.2197
 XY= -2.9307 YY= 141.2081 ZY= -20.7486
 XZ= 2.8276 YZ= -30.7006 ZZ= 113.5842
 Eigenvalues: 98.1005 111.6999 156.9440
 20 O Isotropic = -71.8113 Anisotropy = 540.0220
 XX= -278.7192 YX= 41.7118 ZX= 110.3393
 XY= 21.3967 YY= -197.4079 ZY= 49.2160
 XZ= 110.1259 YZ= 46.9606 ZZ= 260.6930
 Eigenvalues: -304.9573 -198.6801 288.2033
 21 O Isotropic = 136.7891 Anisotropy = 179.2002
 XX= 153.6382 YX= 176.1842 ZX= -15.7441
 XY= 77.9655 YY= 88.3258 ZY= -8.6160
 XZ= -5.7970 YZ= -25.2597 ZZ= 168.4034
 Eigenvalues: -10.4811 164.5925 256.2559
 22 O Isotropic = 227.9359 Anisotropy = 174.8930
 XX= 344.2865 YX= 2.8513 ZX= -0.7710
 XY= 4.3096 YY= 248.5265 ZY= 88.2937
 XZ= 6.3410 YZ= 26.9546 ZZ= 90.9948
 Eigenvalues: 72.1579 267.1186 344.5312
 23 O Isotropic = 281.1459 Anisotropy = 42.3886
 XX= 261.8098 YX= -3.4480 ZX= 2.4617
 XY= -6.4313 YY= 276.1694 ZY= 20.6943
 XZ= 3.9197 YZ= 2.0715 ZZ= 305.4584
 Eigenvalues: 259.2642 274.7685 309.4049
 24 O Isotropic = -289.2718 Anisotropy = 1001.2298
 XX= -397.6451 YX= 160.4027 ZX= 56.5222
 XY= 115.8434 YY= -536.6015 ZY= -535.8060
 XZ= -5.4024 YZ= -525.5463 ZZ= 66.4313
 Eigenvalues: -881.6953 -364.3348 378.2148
 25 O Isotropic = 305.3894 Anisotropy = 56.6777
 XX= 316.5831 YX= 37.3633 ZX= 11.8155
 XY= 9.4439 YY= 305.6732 ZY= -6.5268
 XZ= 21.8049 YZ= 28.0477 ZZ= 293.9118

Eigenvalues: 284.5305 288.4631 343.1745
 26 H Isotropic = 23.2570 Anisotropy = 10.7457
 XX= 25.5330 YX= -3.9315 ZX= 0.2791
 XY= -6.0242 YY= 25.2477 ZY= 1.0116
 XZ= 2.2263 YZ= -0.6040 ZZ= 18.9901
 Eigenvalues: 18.4203 20.9298 30.4208
 27 H Isotropic = 28.4711 Anisotropy = 7.9716
 XX= 30.4491 YX= -4.0252 ZX= -4.4923
 XY= -2.0846 YY= 27.3813 ZY= -1.8754
 XZ= -4.1250 YZ= -2.9804 ZZ= 27.5828
 Eigenvalues: 21.8699 29.7578 33.7854
 28 H Isotropic = 29.5916 Anisotropy = 7.5380
 XX= 34.0229 YX= -2.0592 ZX= 2.1919
 XY= -0.9574 YY= 28.9578 ZY= 3.1712
 XZ= 1.9782 YZ= 4.0991 ZZ= 25.7940
 Eigenvalues: 22.8214 31.3364 34.6169
 29 H Isotropic = 28.5450 Anisotropy = 10.0016
 XX= 33.5407 YX= 5.2640 ZX= -1.6615
 XY= 0.0567 YY= 28.8927 ZY= -2.6461
 XZ= -0.9940 YZ= -2.6928 ZZ= 23.2017
 Eigenvalues: 22.1392 28.2831 35.2127
 30 H Isotropic = 26.8266 Anisotropy = 4.0906
 XX= 26.3645 YX= -1.3344 ZX= -0.6217
 XY= -1.0733 YY= 25.2619 ZY= -0.1395
 XZ= -0.3023 YZ= -3.3273 ZZ= 28.8533
 Eigenvalues: 23.8900 27.0361 29.5536
 31 H Isotropic = 24.6053 Anisotropy = 8.6281
 XX= 29.7902 YX= 0.6765 ZX= -1.7558
 XY= 1.5162 YY= 22.3575 ZY= -0.1455
 XZ= -2.1989 YZ= 1.2912 ZZ= 21.6683
 Eigenvalues: 20.7772 22.6814 30.3574
 32 H Isotropic = 25.7716 Anisotropy = 8.7656
 XX= 28.2953 YX= 3.4812 ZX= -1.0330
 XY= 4.5499 YY= 24.8108 ZY= -2.6451
 XZ= -1.6515 YZ= -1.4208 ZZ= 24.2086
 Eigenvalues: 21.7031 23.9963 31.6153
 33 H Isotropic = 29.4158 Anisotropy = 5.6663
 XX= 29.5606 YX= 0.9718 ZX= 1.4611
 XY= 2.1402 YY= 27.3675 ZY= -3.5256
 XZ= 0.4012 YZ= -3.0815 ZZ= 31.3192
 Eigenvalues: 24.8032 30.2509 33.1933
 34 H Isotropic = 29.5435 Anisotropy = 5.6311
 XX= 32.3931 YX= -0.3389 ZX= -0.8644
 XY= -1.3103 YY= 30.9288 ZY= 2.8418
 XZ= -1.6214 YZ= 1.2661 ZZ= 25.3087

Eigenvalues: 24.5265 30.8066 33.2976
 35 H Isotropic = 30.2200 Anisotropy = 5.6449
 XX= 31.7372 YX= 0.0897 ZX= -0.5255
 XY= -0.0705 YY= 32.5767 ZY= 3.6453
 XZ= 0.0592 YZ= 2.9012 ZZ= 26.3460
 Eigenvalues: 24.9355 31.7411 33.9832
 36 H Isotropic = 30.3138 Anisotropy = 4.9377
 XX= 31.4128 YX= 2.2009 ZX= 0.3149
 XY= 2.0556 YY= 27.9061 ZY= -3.5249
 XZ= 0.7543 YZ= -2.7023 ZZ= 31.6226
 Eigenvalues: 25.3904 31.9454 33.6056
 37 H Isotropic = 30.3597 Anisotropy = 5.2644
 XX= 31.1005 YX= 1.8875 ZX= 0.5643
 XY= 2.1231 YY= 27.8806 ZY= -3.3735
 XZ= 0.4316 YZ= -2.8718 ZZ= 32.0981
 Eigenvalues: 25.5000 31.7099 33.8694
 38 H Isotropic = 30.2928 Anisotropy = 5.4518
 XX= 32.0178 YX= -0.3086 ZX= -0.4045
 XY= -0.3597 YY= 32.2458 ZY= 3.6722
 XZ= -0.2744 YZ= 3.0707 ZZ= 26.6147
 Eigenvalues: 25.0338 31.9172 33.9273
 39 H Isotropic = 30.2790 Anisotropy = 7.0402
 XX= 31.7304 YX= -1.3386 ZX= -0.9260
 XY= -1.1887 YY= 32.9487 ZY= 3.5521
 XZ= -1.0828 YZ= 2.8820 ZZ= 26.1581
 Eigenvalues: 24.8434 31.0212 34.9725
 40 H Isotropic = 30.2587 Anisotropy = 6.7941
 XX= 30.0353 YX= 1.5500 ZX= 1.4436
 XY= 2.0251 YY= 27.9317 ZY= -3.8763
 XZ= 1.5520 YZ= -3.3560 ZZ= 32.8090
 Eigenvalues: 24.9752 31.0128 34.7881
 41 H Isotropic = 30.8030 Anisotropy = 8.7570
 XX= 30.1485 YX= 2.9676 ZX= -2.5246
 XY= 2.4424 YY= 29.1604 ZY= -3.6540
 XZ= -2.0258 YZ= -2.8003 ZZ= 33.1002
 Eigenvalues: 26.6397 29.1283 36.6410
 42 H Isotropic = 30.7984 Anisotropy = 8.7938
 XX= 29.2538 YX= 1.7159 ZX= 0.0041
 XY= 0.6893 YY= 34.2289 ZY= 4.3836
 XZ= 0.0365 YZ= 3.9360 ZZ= 28.9124
 Eigenvalues: 26.5147 29.2196 36.6609
 43 H Isotropic = 30.6585 Anisotropy = 11.0077
 XX= 37.3033 YX= -0.2569 ZX= 2.9634
 XY= 0.9457 YY= 27.8829 ZY= -0.3457
 XZ= 2.5937 YZ= -0.6592 ZZ= 26.7892

Eigenvalues: 25.9329 28.0456 37.9969
 44 H Isotropic = 29.9950 Anisotropy = 9.3548
 XX= 33.3497 YX= -0.6381 ZX= 3.9958
 XY= 0.6174 YY= 27.7334 ZY= -0.3089
 XZ= 5.1905 YZ= -0.2154 ZZ= 28.9018
 Eigenvalues: 25.9955 27.7579 36.2315
 45 H Isotropic = 30.3036 Anisotropy = 5.9713
 XX= 32.2914 YX= -0.1045 ZX= -1.4630
 XY= -1.8732 YY= 33.7939 ZY= -0.4684
 XZ= -1.1177 YZ= -0.8577 ZZ= 24.8256
 Eigenvalues: 24.5359 32.0904 34.2845
 46 H Isotropic = 29.9146 Anisotropy = 9.2384
 XX= 29.7193 YX= -1.3090 ZX= -4.1673
 XY= -0.2215 YY= 27.9128 ZY= 0.9923
 XZ= -5.4026 YZ= 1.2571 ZZ= 32.1117
 Eigenvalues: 25.9788 27.6915 36.0735
 47 H Isotropic = 27.1237 Anisotropy = 5.9560
 XX= 26.9657 YX= -0.6702 ZX= -3.0942
 XY= 0.4968 YY= 27.3749 ZY= -2.5154
 XZ= -4.1958 YZ= -1.1842 ZZ= 27.0304
 Eigenvalues: 22.9159 27.3608 31.0943
 48 H Isotropic = 27.2070 Anisotropy = 10.1115
 XX= 26.9343 YX= 2.2795 ZX= 0.9925
 XY= 3.5577 YY= 32.4813 ZY= -1.0158
 XZ= 1.5117 YZ= -3.4352 ZZ= 22.2053
 Eigenvalues: 21.1139 26.5590 33.9480
 49 H Isotropic = 25.8172 Anisotropy = 11.1732
 XX= 21.8516 YX= 2.8947 ZX= -0.0822
 XY= -0.8501 YY= 33.0266 ZY= -0.8242
 XZ= 0.4445 YZ= -1.7223 ZZ= 22.5733
 Eigenvalues: 21.6481 22.5374 33.2660
 50 H Isotropic = 29.9575 Anisotropy = 14.5827
 XX= 23.8045 YX= -2.7115 ZX= 0.0809
 XY= -2.1134 YY= 26.4007 ZY= 0.0036
 XZ= 0.6142 YZ= 0.5856 ZZ= 39.6671
 Eigenvalues: 22.3514 27.8417 39.6793
 51 H Isotropic = 28.7155 Anisotropy = 16.9893
 XX= 29.2279 YX= 4.6549 ZX= 8.3296
 XY= 5.1104 YY= 33.4916 ZY= 3.3707
 XZ= 7.9707 YZ= 2.7610 ZZ= 23.4268
 Eigenvalues: 17.6696 28.4351 40.0416

Structure 1b conformation 8.

Level of theory & comments

B3PW91 D95** nmr

Ambuic acid, syn stereochemistry, C7 acceptor-C19 donor, s-cis at
C8-C9-C11-C12, 210 degree dihedral at C3-C4-C5-C6.

Energy

-1190.6855334

Cartesian coordinates

C	5.26462	-2.8897	-0.41392
C	5.09142	-1.43329	0.02768
C	3.87507	-0.85084	0.03206
C	3.63497	0.60039	0.47747
C	2.14613	1.09757	0.41104
C	1.89887	2.57852	0.14787
C	0.59468	3.0495	-0.55784
C	-0.61831	2.11404	-0.27486
C	-0.43902	0.79045	-0.00035
C	0.96805	0.1465	-0.01119
C	-1.5154	-0.22984	0.20617
C	-2.74236	-0.05398	0.73593
C	-3.7535	-1.191	0.92845
C	-5.08058	-0.94021	0.13229
C	-6.12233	-2.07922	0.36068
C	-7.44924	-1.83138	-0.42316
C	-8.48977	-2.96558	-0.19614
C	6.39321	-0.73475	0.44932
C	-2.0098	2.81983	-0.40853
O	6.34706	-3.52895	-0.44657
O	4.02567	-3.48186	-0.80276
O	1.76757	2.03275	1.51066
O	0.28431	4.46259	-0.19615
O	1.11376	-1.069	-0.31382
O	-2.00069	3.99857	-1.26397
H	2.96357	-1.39753	-0.26622
H	4.2588	1.28329	-0.13151
H	3.97464	0.73075	1.52504

H	2.77575	3.22989	-0.03809
H	0.78114	3.09291	-1.65641
H	-1.18961	-1.2451	-0.07134
H	-3.07352	0.93428	1.0819
H	-4.00086	-1.28098	2.00358
H	-3.30455	-2.14616	0.60722
H	-5.51559	0.02448	0.44704
H	-4.84976	-0.86239	-0.94436
H	-6.34487	-2.15946	1.43916
H	-5.68566	-3.04238	0.04362
H	-7.88337	-0.86693	-0.10653
H	-7.22462	-1.75063	-1.5011
H	-8.7499	-3.04717	0.87039
H	-8.08668	-3.93497	-0.52718
H	-9.41201	-2.76336	-0.76227
H	7.22525	-1.45129	0.36532
H	6.33432	-0.37706	1.4908
H	6.6067	0.1343	-0.19535
H	-2.3625	3.05522	0.63174
H	-2.73764	2.09134	-0.82603
H	4.32711	-4.43191	-1.05896
H	0.15337	4.40224	0.82033
H	-1.16115	4.4837	-0.87765

Computed NMR tensors

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 7.7521 Anisotropy = 83.7356

XX= 3.5017 YX= -69.4061 ZX= -32.1002

XY= -43.9937 YY= -26.9708 ZY= -36.1496

XZ= -24.2818 YZ= -40.2261 ZZ= 46.7253

Eigenvalues: -87.2570 46.9373 63.5758

2 C Isotropic = 58.1302 Anisotropy = 122.2127

XX= 58.5051 YX= -25.8946 ZX= -20.4214

XY= -24.9559 YY= -4.5187 ZY= -50.4296

XZ= -19.8620 YZ= -50.1362 ZZ= 120.4042

Eigenvalues: -32.6412 67.4265 139.6054

3 C Isotropic = 43.2345 Anisotropy = 182.9047

XX= 23.0222 YX= -10.1636 ZX= -25.2854

XY= -25.7418 YY= -32.3097 ZY= -69.0547

XZ= -29.1167 YZ= -65.7937 ZZ= 138.9911

Eigenvalues: -63.5511 28.0837 165.1710

4 C Isotropic = 147.1821 Anisotropy = 39.9343
 XX= 162.1458 YX= -19.3210 ZX= 0.7696
 XY= -14.9630 YY= 148.0366 ZY= 7.3075
 XZ= 2.9067 YZ= 7.8581 ZZ= 131.3638
 Eigenvalues: 126.0877 141.6536 173.8049

5 C Isotropic = 120.0800 Anisotropy = 67.1579
 XX= 162.2417 YX= 5.3118 ZX= 8.4895
 XY= 12.1582 YY= 70.8539 ZY= -3.4638
 XZ= 6.3783 YZ= 19.1624 ZZ= 127.1443
 Eigenvalues: 69.1434 126.2446 164.8519

6 C Isotropic = 116.6440 Anisotropy = 54.3194
 XX= 152.3897 YX= 5.0372 ZX= 4.7517
 XY= -3.3250 YY= 76.6245 ZY= 19.9448
 XZ= 2.5010 YZ= 0.4085 ZZ= 120.9178
 Eigenvalues: 74.3982 122.6769 152.8569

7 C Isotropic = 105.1509 Anisotropy = 45.2028
 XX= 104.5735 YX= -6.3694 ZX= 3.3520
 XY= -10.1010 YY= 125.4493 ZY= 13.7365
 XZ= -4.7235 YZ= 24.8942 ZZ= 85.4299
 Eigenvalues: 77.3982 102.7683 135.2861

8 C Isotropic = 35.2705 Anisotropy = 146.2717
 XX= -35.7167 YX= -23.0098 ZX= 8.5454
 XY= -2.5271 YY= 19.1836 ZY= 31.6491
 XZ= 23.1345 YZ= 34.2568 ZZ= 122.3445
 Eigenvalues: -41.9113 14.9378 132.7849

9 C Isotropic = 53.7541 Anisotropy = 126.9751
 XX= -15.6590 YX= 6.4118 ZX= 12.4273
 XY= -0.5330 YY= 40.8369 ZY= 15.1042
 XZ= 15.8493 YZ= 4.3254 ZZ= 136.0843
 Eigenvalues: -17.0373 39.8954 138.4042

10 C Isotropic = -23.2217 Anisotropy = 156.1649
 XX= -102.6438 YX= 2.9761 ZX= -24.3201
 XY= -1.2615 YY= -33.5580 ZY= -29.0122
 XZ= -32.8913 YZ= -38.0160 ZZ= 66.5368
 Eigenvalues: -107.6603 -42.8929 80.8883

11 C Isotropic = 63.9561 Anisotropy = 124.7455
 XX= 81.1582 YX= -13.6437 ZX= 21.4464
 XY= -22.7752 YY= -24.3581 ZY= -18.6282
 XZ= 27.0490 YZ= -13.6931 ZZ= 135.0682
 Eigenvalues: -28.3177 73.0662 147.1198

12 C Isotropic = 45.6820 Anisotropy = 160.9784
 XX= 50.6757 YX= -22.6466 ZX= 45.4374
 XY= -9.0565 YY= -40.4206 ZY= -35.2520
 XZ= 37.6634 YZ= -36.3314 ZZ= 126.7908
 Eigenvalues: -48.3428 32.3879 153.0009

13 C Isotropic = 146.8794 Anisotropy = 33.5836
 XX= 157.2036 YX= 17.8305 ZX= 4.4599
 XY= 11.7253 YY= 150.6130 ZY= -5.1593
 XZ= 9.8839 YZ= -3.9616 ZZ= 132.8216
 Eigenvalues: 127.0974 144.2722 169.2684

14 C Isotropic = 152.6367 Anisotropy = 37.1944
 XX= 170.8991 YX= 12.4894 ZX= 7.9123
 XY= 13.6693 YY= 146.6914 ZY= -4.7812
 XZ= 8.1490 YZ= -5.0788 ZZ= 140.3197
 Eigenvalues: 132.5568 147.9204 177.4330

15 C Isotropic = 152.0069 Anisotropy = 38.6465
 XX= 170.5688 YX= 13.0011 ZX= 9.4790
 XY= 12.7160 YY= 145.9425 ZY= -3.6626
 XZ= 10.7727 YZ= -3.2924 ZZ= 139.5095
 Eigenvalues: 131.9923 146.2572 177.7712

16 C Isotropic = 160.8204 Anisotropy = 24.7474
 XX= 173.1945 YX= 8.3838 ZX= 6.8175
 XY= 3.3939 YY= 156.2200 ZY= -4.2042
 XZ= 10.2156 YZ= -1.6966 ZZ= 153.0466
 Eigenvalues: 147.1743 157.9682 177.3186

17 C Isotropic = 173.0596 Anisotropy = 26.1060
 XX= 180.3944 YX= 10.0600 ZX= 2.2043
 XY= 14.8004 YY= 175.0670 ZY= -0.9102
 XZ= -0.7646 YZ= -3.2156 ZZ= 163.7173
 Eigenvalues: 162.1980 166.5171 190.4636

18 C Isotropic = 174.4190 Anisotropy = 18.1326
 XX= 181.8180 YX= 7.5953 ZX= 3.5768
 XY= 10.3641 YY= 165.5351 ZY= -1.8260
 XZ= 4.1132 YZ= -2.2887 ZZ= 175.9040
 Eigenvalues: 160.7597 175.9900 186.5075

19 C Isotropic = 114.3932 Anisotropy = 54.7050
 XX= 100.6498 YX= -1.7283 ZX= -0.1842
 XY= -1.8918 YY= 132.3269 ZY= -22.7182
 XZ= 1.6662 YZ= -32.0311 ZZ= 110.2030
 Eigenvalues: 91.7218 100.5946 150.8632

20 O Isotropic = -107.5054 Anisotropy = 552.1160
 XX= -313.3557 YX= 55.1566 ZX= -74.0445
 XY= 41.1004 YY= -210.8090 ZY= -145.1594
 XZ= -79.9066 YZ= -143.3447 ZZ= 201.6486
 Eigenvalues: -333.3852 -249.7029 260.5720

21 O Isotropic = 87.7779 Anisotropy = 211.3325
 XX= 122.9325 YX= 194.5137 ZX= 62.6058
 XY= 85.6505 YY= 15.7454 ZY= -20.1511
 XZ= 27.7431 YZ= -3.3137 ZZ= 124.6558
 Eigenvalues: -86.6206 121.2881 228.6662

22 O Isotropic = 192.7700 Anisotropy = 197.5605
 XX= 318.1193 YX= -9.2190 ZX= 48.2223
 XY= -3.5166 YY= 214.0083 ZY= 90.1467
 XZ= 35.6647 YZ= 19.5296 ZZ= 46.1824
 Eigenvalues: 23.8500 229.9830 324.4770

23 O Isotropic = 252.3806 Anisotropy = 61.7018
 XX= 239.6999 YX= -5.2746 ZX= -0.9545
 XY= -6.9543 YY= 235.4118 ZY= 29.5374
 XZ= -10.1163 YZ= 19.2711 ZZ= 282.0300
 Eigenvalues: 224.1669 239.4597 293.5152

24 O Isotropic = -323.9171 Anisotropy = 1006.1770
 XX= -410.5515 YX= 141.5720 ZX= -54.7027
 XY= 81.4211 YY= -813.4858 ZY= -305.8587
 XZ= -109.1132 YZ= -296.3276 ZZ= 252.2858
 Eigenvalues: -908.1666 -410.4523 346.8675

25 O Isotropic = 279.8816 Anisotropy = 69.3474
 XX= 315.5913 YX= 34.6523 ZX= 6.7266
 XY= 10.9487 YY= 264.9149 ZY= -8.7843
 XZ= 10.4786 YZ= 24.6697 ZZ= 259.1384
 Eigenvalues: 252.4454 261.0861 326.1132

26 H Isotropic = 19.9382 Anisotropy = 11.8736
 XX= 25.0566 YX= -3.7694 ZX= 0.3484
 XY= -3.4693 YY= 22.6873 ZY= 2.5684
 XZ= -0.2344 YZ= 3.1053 ZZ= 12.0708
 Eigenvalues: 11.2919 20.6689 27.8539

27 H Isotropic = 28.6767 Anisotropy = 7.6224
 XX= 32.9731 YX= -1.5947 ZX= -3.1974
 XY= -1.0671 YY= 29.7445 ZY= -1.9579
 XZ= -1.9031 YZ= -2.7883 ZZ= 23.3124
 Eigenvalues: 21.8083 30.4634 33.7583

28 H Isotropic = 28.4682 Anisotropy = 7.2013
 XX= 30.6113 YX= -4.3351 ZX= 3.1448
 XY= -2.8237 YY= 25.9369 ZY= 1.6176
 XZ= 2.4637 YZ= 2.1143 ZZ= 28.8563
 Eigenvalues: 22.5397 29.5958 33.2690

29 H Isotropic = 27.7507 Anisotropy = 8.8965
 XX= 32.7675 YX= 4.6344 ZX= -1.2694
 XY= -0.4752 YY= 26.9490 ZY= -2.9174
 XZ= -0.0778 YZ= -2.8081 ZZ= 23.5355
 Eigenvalues: 21.8902 27.6801 33.6817

30 H Isotropic = 26.1539 Anisotropy = 3.1838
 XX= 25.1780 YX= -1.4131 ZX= -0.7815
 XY= -1.4404 YY= 25.2438 ZY= 1.4213
 XZ= -0.8719 YZ= -1.7936 ZZ= 28.0399
 Eigenvalues: 23.6630 26.5222 28.2764

31 H Isotropic = 24.2393 Anisotropy = 9.2061
XX= 30.0379 YX= 0.4640 ZX= -1.2855
XY= 0.8196 YY= 22.2896 ZY= 0.0525
XZ= -2.1866 YZ= 1.0503 ZZ= 20.3905
Eigenvalues: 19.9063 22.4350 30.3767

32 H Isotropic = 25.5362 Anisotropy = 8.9282
XX= 28.1983 YX= 3.4537 ZX= -1.4603
XY= 4.6501 YY= 24.3789 ZY= -2.0873
XZ= -2.0903 YZ= -0.9622 ZZ= 24.0315
Eigenvalues: 21.7423 23.3780 31.4883

33 H Isotropic = 29.2464 Anisotropy = 5.3346
XX= 29.1138 YX= 1.4831 ZX= 0.6974
XY= 2.5704 YY= 26.1991 ZY= -1.6287
XZ= -0.6208 YZ= -1.2867 ZZ= 32.4265
Eigenvalues: 24.9273 30.0092 32.8028

34 H Isotropic = 29.4084 Anisotropy = 5.5599
XX= 32.4599 YX= -0.4395 ZX= 0.2384
XY= -1.7490 YY= 31.2757 ZY= 1.0287
XZ= -0.3139 YZ= -0.5357 ZZ= 24.4895
Eigenvalues: 24.4806 30.6297 33.1150

35 H Isotropic = 29.9878 Anisotropy = 5.4215
XX= 31.5106 YX= -0.3076 ZX= 0.3677
XY= -0.3062 YY= 33.3775 ZY= 1.6672
XZ= 1.0488 YZ= 0.9809 ZZ= 25.0754
Eigenvalues: 24.7863 31.5751 33.6022

36 H Isotropic = 30.0585 Anisotropy = 4.6669
XX= 31.1769 YX= 2.5057 ZX= -0.3817
XY= 2.5220 YY= 26.5943 ZY= -1.8726
XZ= 0.0890 YZ= -0.9641 ZZ= 32.4042
Eigenvalues: 25.2672 31.7385 33.1697

37 H Isotropic = 30.2338 Anisotropy = 5.1007
XX= 30.8101 YX= 2.2359 ZX= -0.1875
XY= 2.5653 YY= 26.8031 ZY= -1.5242
XZ= -0.4320 YZ= -1.0817 ZZ= 33.0883
Eigenvalues: 25.5321 31.5351 33.6343

38 H Isotropic = 30.1554 Anisotropy = 5.3025
XX= 31.8786 YX= -0.5896 ZX= 0.4927
XY= -0.7791 YY= 33.1954 ZY= 1.9246
XZ= 0.5858 YZ= 1.2577 ZZ= 25.3923
Eigenvalues: 25.0163 31.7596 33.6904

39 H Isotropic = 30.0845 Anisotropy = 6.8328
XX= 31.7008 YX= -1.6638 ZX= 0.3427
XY= -1.6137 YY= 33.6534 ZY= 1.3210
XZ= 0.2408 YZ= 0.6831 ZZ= 24.8993
Eigenvalues: 24.7524 30.8614 34.6397

40 H Isotropic = 30.0553 Anisotropy = 6.5035
 XX= 29.5780 YX= 2.1693 ZX= 0.4684
 XY= 2.6298 YY= 26.5332 ZY= -1.8382
 XZ= 0.4216 YZ= -1.4099 ZZ= 34.0547
 Eigenvalues: 24.9195 30.8554 34.3910

41 H Isotropic = 30.7031 Anisotropy = 8.5820
 XX= 30.7365 YX= 2.4859 ZX= -3.5231
 XY= 2.2474 YY= 27.9873 ZY= -2.0004
 XZ= -3.0316 YZ= -1.1288 ZZ= 33.3855
 Eigenvalues: 26.6073 29.0776 36.4245

42 H Isotropic = 30.7071 Anisotropy = 8.6367
 XX= 29.2119 YX= 1.0217 ZX= -0.2797
 XY= 0.0005 YY= 35.7165 ZY= 2.7537
 XZ= -0.0120 YZ= 2.4061 ZZ= 27.1930
 Eigenvalues: 26.4448 29.2117 36.4649

43 H Isotropic = 30.5191 Anisotropy = 10.9017
 XX= 36.0824 YX= 0.8997 ZX= 4.2284
 XY= 1.8842 YY= 27.5754 ZY= -0.1443
 XZ= 3.6117 YZ= -0.6304 ZZ= 27.8996
 Eigenvalues: 25.8475 27.9229 37.7869

44 H Isotropic = 28.6706 Anisotropy = 8.6175
 XX= 31.9000 YX= -4.4447 ZX= 0.0252
 XY= -1.8449 YY= 30.3590 ZY= 1.9206
 XZ= 0.8838 YZ= 1.5164 ZZ= 23.7526
 Eigenvalues: 23.1468 28.4493 34.4156

45 H Isotropic = 30.2874 Anisotropy = 7.5481
 XX= 29.9810 YX= -0.2098 ZX= 2.0160
 XY= -0.6548 YY= 27.1962 ZY= 2.2723
 XZ= 1.8211 YZ= 3.5679 ZZ= 33.6849
 Eigenvalues: 25.7715 29.7712 35.3194

46 H Isotropic = 30.3266 Anisotropy = 7.8355
 XX= 31.1744 YX= 2.3793 ZX= -1.4916
 XY= 1.6559 YY= 31.8565 ZY= -3.1526
 XZ= -1.7671 YZ= -4.1381 ZZ= 27.9488
 Eigenvalues: 25.7385 29.6909 35.5503

47 H Isotropic = 26.7629 Anisotropy = 5.6951
 XX= 26.7231 YX= -0.7743 ZX= -3.0321
 XY= 0.0593 YY= 26.8447 ZY= -2.6469
 XZ= -4.0480 YZ= -0.9157 ZZ= 26.7210
 Eigenvalues: 22.6226 27.1066 30.5596

48 H Isotropic = 26.6736 Anisotropy = 9.4945
 XX= 26.6721 YX= 2.6002 ZX= 0.5871
 XY= 3.9625 YY= 30.6250 ZY= -1.6951
 XZ= 0.5710 YZ= -4.1700 ZZ= 22.7237
 Eigenvalues: 21.2150 25.8025 33.0033