

Supplementary Data for “Structural Characterization of an Anhydrous Polymorph of Paclitaxel”

The following contains supplementary material for the paper, “Structural Characterization of an Anhydrous Polymorph of Paclitaxel”. Coordinates and calculated shielding eigenvalues are listed for partial structures (combination of Model ONE and Model THREE from Figure 3 in the paper) of paclitaxel **2a** and **2b** as given in Table 6 in the paper. Table 6 is included here for ease of reference.

Table 6 Dihedral values for model structures matching experimental CSPVs of paclitaxel **2a** and **2b** given in degrees. The symbols **a**, **b**, and **c** denote errors of $\pm 20.0^\circ \pm 30.0^\circ$ and $\pm 45.0^\circ$ respectively, in the predicted angle. All other dihedral angles have an error of $\pm 15.0^\circ$ or less.

Torsion angle	2a-i	2a-ii	2a-iii	2a-iv	2a-v	2b-i	2b-ii	2b-iii	2b-iv	2b-v	2b-vi	2b-vii	2b-viii
C30-O-C10-C9	-45.0	-45.0	-45.0	-45.0	-45.0	-60.0	-60.0	-60.0	-60.0	-60.0	-60.0	-60.0	-60.0
C1'-O-C13-C12	-165.0	-165.0	-165.0	-165.0	-165.0	-60.0	-60.0	-60.0	-60.0	-60.0	-60.0	-150.0	-150.0
C2'-C1'-O-C13	180.0	180.0	180.0	180.0	180.0	150.0	150.0	150.0	150.0	150.0	150.0	180.0	180.0
O-C2'-C1'=O	180.0 ^b	180.0 ^b	180.0 ^b	180.0 ^b	180.0 ^b	105.0	105.0	105.0	105.0	105.0	105.0	-15.0 ^c	-15.0 ^c
N-C3'-C2'-C1'	30.0	60.0	150.0	0.0	210.0	60.0	60.0	60.0	60.0	180.0	180.0	90.0	90.0
C4'-N-C3'-C2'	60.0	-15.0	-120.0	-120.0	-120.0	0.0	0.0	-105.0	-105.0	-105.0	-105.0	-135.0	-135.0
O=C4'-N-C3'	15.0	15.0	15.0	15.0	15.0	15.0 ^a	-170.0	15.0 ^a	-170.0	15.0 ^a	-170.0	15.0 ^a	-170.0
C-C3'ipso-C3'-C2'	-75.0	-75.0	-75.0	-75.0	-75.0	-60.0 ^b	-60.0 ^b	-60.0 ^b	-60.0 ^b	-60.0 ^b	-60.0 ^b	-60.0 ^b	-60.0 ^b
C-C4'ipso-C4'=O	± 45.0	± 45.0	± 45.0	± 45.0	± 45.0	± 45.0	± 45.0	± 45.0	± 45.0	± 45.0	± 45.0	± 45.0	± 45.0

Dihedral values measured for model structures matching experimental CSPVs of paclitaxel **2a** and **2b** given in degrees. The coordinates and computed shielding eigenvalues are given in the following supplementary data. These structures have the dihedral C-C4'ipso-C4'=O at -45.0°

Torsion angle	C30-O-C10-C9	C1'-O-C13-C12	C2'-C1'-O-C13	O-C2'-C1'=O	N-C3'-C2'-C1'	C4'-N-C3'-C2'	O=C4'-N-C3'	C-C3'ipso-C3'-C2'	C-C4'ipso-C4'=O	H-O-C2'-C1'
2a-i	-45.0	-165.0	-180.0	-180.0	30.0	60.0	15.0	-75.0	-47.1	44.5
2a-ii	-45.0	-165.0	180.0	180.0	60.0	15.0	15.0	-75.0	-46.6	-49.1
2a-iii	-45.0	-165.0	180.0	180.0	150.0	-120.0	15.0	-75.0	-46.8	43.7
2a-iv	-45.0	-165.0	-180.0	-180.0	0.0	-120.0	15.0	-75.0	-47.5	51.9
2a-v	-45.0	-165.0	-180.0	-180.0	-150.0	-120.0	15.0	-75.0	-46.8	51.8
2b-i	-60.0	-60.0	150.0	105.0	60.0	0.0	10.0	-60.0	-45.4	-63.0
2b-ii	-60.0	-60.0	150.0	105.0	60.0	0.0	-170.0	-60.0	-24.5	-82.2
2b-iii	-60.0	-60.0	150.0	105.0	60.0	-105.0	10.0	-60.0	-45.6	-68.7
2b-iv	-60.0	-60.0	150.0	60.0	60.0	-105.0	-170.0	-60.0	-52.1	-68.3
2b-v	-60.0	-60.0	150.0	105.0	-180.0	-105.0	10.0	-60.0	-45.6	-91.0
2b-vi	-60.0	-60.0	150.0	105.0	-180.0	-105.0	-170.0	-60.0	-48.4	-83.8
2b-vii	-60.0	-150.0	-180.0	105.0	90.0	-135.0	-10.0	-60.0	-42.5	-54.2
2b-viii	-60.0	-150.0	-180.0	105.0	90.0	-135.0	-170.0	-60.0	-45.0	-55.3

Dihedral values measured for model structures matching experimental CSPVs of paclitaxel **2a** given in degrees. The coordinates and computed shielding eigenvalues are included in the following supplementary data. These structures have the dihedral C-C4'ipso-C4'=O at +45.0°.

Torsion angle	C30-O-C10-C9	C1'-O-C13-C12	C2'-C1'-O-C13	O-C2'-C1'=O	N-C3'-C2'-C1'	C4'-N-C3'-C2'	O=C4'-N-C3'	C-C3'ipso-C3'-C2'	C-C4'ipso-C4'=O	H-O-C2'-C1'
2a-i	-45.0	-165.0	180.0	180.0	30.0	60.0	15.0	-75.0	45.0	-64.6
2a-i2	-45.0	-165.0	-180.0	-180.0	30.0	60.0	15.0	-75.0	-47.1	44.5
2a-ii	-45.0	-165.0	180.0	180.0	60.0	15.0	15.0	-75.0	45.0	-48.7
2a-iii	-45.0	-165.0	-180.0	180.0	150.0	-120.0	15.0	-75.0	45.0	-61.2
2a-iii2	-45.0	-165.0	-180.0	180.0	150.0	-120.0	15.0	-75.0	45.0	44.5
2a-iv	-45.0	-165.0	180.0	180.0	0.0	-120.0	15.0	-75.0	45.0	-59.2
2a-iv2	-45.0	-165.0	180.0	-180.0	0.0	-120.0	15.0	-75.0	45.0	51.8
2a-v	-45.0	-165.0	180.0	180.0	-150.0	-120.0	15.0	-75.0	45.0	-56.8
2a-v2	-45.0	-165.0	180.0	180.0	-150.0	-120.0	15.0	-75.0	45.0	51.8
2a-v3	-45.0	-165.0	180.0	-180.0	-150.0	-120.0	15.0	-75.0	45.0	51.8

Dihedral values measured for model structures matching experimental CSPVs of paclitaxel **2b** given in degrees. The coordinates and computed shielding eigenvalues are included in the following supplementary data. These structures have the dihedral C-C4'ipso-C4'=O at +45.0°.

Torsion angle	C30-O-C10-C9	C1'-O-C13-C12	C2'-C1'-O-C13	O-C2'-C1'=O	N-C3'-C2'-C1'	C4'-N-C3'-C2'	O=C4'-N-C3'	C-C3'ipso-C3'-C2'	C-C4'ipso-C4'=O	H-O-C2'-C1'
2b-i	-60.0	-60.0	150.0	105.0	60.0	0.0	10.0	-60.0	45.0	-62.3
2b-i2	-60.0	-60.0	150.0	105.0	60.0	0.0	10.0	-60.0	45.0	59.7
2b-ii	-60.0	-60.0	150.0	105.0	60.0	0.0	-170.0	-60.0	45.0	-47.6
2b-iii	-60.0	-60.0	150.0	105.0	60.0	-105.0	10.0	-60.0	45.0	72.6
2b-iii2	-60.0	-60.0	150.0	105.0	60.0	-105.0	10.0	-60.0	45.0	-68.3
2b-iv	-60.0	-60.0	150.0	105.0	60.0	-105.0	-170.0	-60.0	45.0	-72.0
2b-v	-60.0	-60.0	150.0	105.0	180.0	-105.0	10.0	-60.0	45.0	-90.7
2b-vi	-60.0	-60.0	150.0	105.0	180.0	-105.0	-170.0	-60.0	45.0	76.7
2b-vi2	-60.0	-60.0	150.0	105.0	180.0	-105.0	-170.0	-60.0	45.0	-56.6
2b-vii	-60.0	-150.0	180.0	105.0	90.0	-135.0	-10.0	-60.0	45.0	-52.5
2b-vii2	-60.0	-150.0	180.0	105.0	90.0	-135.0	-10.0	-60.0	44.5	61.7
2b-viii	-60.0	-150.0	-180.0	105.0	90.0	-135.0	-170.0	-60.0	45.0	-58.0
2b-viii2	-60.0	-150.0	180.0	105.0	90.0	-135.0	-170.0	-60.0	45.0	60.7

Structures with C-C4'ipso-C4'=O at -45.0°:

2a

2ai_neg45

C	2.654319	-1.113216	1.802027
C	3.50312	-2.257611	1.163139
C	3.125981	-2.635179	-0.279201
C	4.205056	-2.276059	-1.31669
C	4.549664	-0.77602	-1.407667
C	3.418477	0.239923	-1.445247
C	2.554039	0.26091	-0.217971
C	1.216961	0.086041	-0.38357
C	0.402653	-0.330446	0.810362
C	1.14308	-1.359502	1.668224
C	3.06754	0.268752	1.205261
C	4.561223	0.488044	1.385163
C	2.37965	1.393415	2.001645
C	0.493111	0.225206	-1.667604
C	5.459623	-3.095553	-1.11656
O	2.882114	-1.137943	2.10022
O	3.444611	-3.401553	2.001448
O	5.709786	-0.434272	-1.648885
O	3.758947	1.528528	-1.946665
O	-0.799641	-0.950587	0.290763
H	2.522701	-3.540332	2.251076
C	4.8778	2.24276	-1.610183
O	5.64564	1.847149	-0.739977
C	4.976787	3.488674	-2.428204
H	4.594138	-1.971025	1.205826
H	2.160805	-2.156194	-0.57945
H	2.776133	-0.136232	-2.316669
H	0.092173	0.559542	1.426664
H	0.681964	-1.346991	2.695168
H	0.96783	-2.379878	1.236906
H	5.187743	-0.106707	0.682026
H	4.813379	1.566344	1.226527
H	4.852772	0.224112	2.431987
H	3.133325	2.035911	2.519313
H	1.778811	2.050768	1.32958
H	1.715654	0.967018	2.793119
H	0.98536	0.977504	-2.332614
H	0.453105	-0.760725	-2.196802
H	-0.564556	0.554453	-1.490694
H	6.191199	-2.882615	-1.934107
H	5.948594	-2.847159	-0.144054
H	5.210756	-4.18379	-1.124236
H	4.025625	3.688837	-2.976815
H	5.210082	4.346593	-1.752237
H	5.808437	3.362354	-3.164396
H	3.814636	-1.340893	3.356943
C	-1.843753	-1.135979	1.145675
O	-1.735119	-0.798692	2.325184
H	3.7734	-2.52591	-2.330362
H	2.981852	-3.748457	-0.316584
C	-3.038091	-1.792332	0.480411
C	-4.312602	-0.902725	0.633281

O	-2.819577	-2.042391	-0.889985
H	-3.223024	-2.768467	1.016988
N	-4.080944	0.516957	0.707047
C	-5.395727	-1.357592	-0.311442
H	-4.67397-1.168235	1.685551	
H	-1.933426	-2.416766	-0.986504
C	-3.478282	1.346161	-0.228523
H	-4.123437	0.880737	1.634777
C	-5.35837-1.099555	-1.683677	
C	-6.405358	-1.522676	-2.504545
C	-7.492399	-2.205454	-1.963243
C	-7.531913	-2.469815	-0.593595
C	-6.492192	-2.044889	0.229681
H	-4.483732	-0.587234	-2.120641
O	-3.273894	1.023471	-1.412482
C	-3.118757	2.714579	0.261454
H	-6.366382	-1.313903	-3.583787
H	-8.316728	-2.536556	-2.611387
H	-8.385999	-3.011102	-0.161628
H	-6.539249	-2.252845	1.309306
C	-1.857494	3.226587	-0.062131
C	-1.497074	4.503408	0.365518
C	-2.395033	5.27216	1.106663
C	-3.656747	4.76536	1.418379
C	-4.021453	3.486049	0.998992
H	-1.163081	2.619302	-0.664825
H	-0.504578	4.905101	0.113268
H	-2.109429	6.280319	1.442148
H	-4.368138	5.375141	1.994731
H	-5.024104	3.099017	1.236262

2ai_neg45	E(RB+HF-PW91)	=	-2012.295236	
SCF GIAO	Magnetic shielding		tensor (ppm):	
1	C	Isotropic=	109.4472	Anisotropy = 28.2203
XX=	99.2759	YX=	2.7726	ZX= 14.3934
XY=	6.7608	YY=	106.4871	ZY= 3.9718
XZ=	7.9495	YZ=	3.1037	ZZ= 122.5786
Eigenvalues:	93.9657	106.1152	128.2607	
2	C	Isotropic=	112.3899	Anisotropy = 31.4138
XX=	94.0221	YX=	5.6601	ZX= -6.6662
XY=	-1.7555	YY=	126.8906	ZY= -4.9217
XZ=	-3.4981	YZ=	-14.9865	ZZ= 116.2569
Eigenvalues:	92.9141	110.9232	133.3324	
3	C	Isotropic=	142.1691	Anisotropy = 20.1208
XX=	121.2224	YX=	-4.8192	ZX= -0.7336
XY=	2.8591	YY=	154.0304	ZY= 2.018
XZ=	-1.4071	YZ=	3.0389	ZZ= 151.2546
Eigenvalues:	121.1601	149.7643	155.583	
4	C	Isotropic=	140.1891	Anisotropy = 24.9338
XX=	124.4913	YX=	1.3378	ZX= -0.4191
XY=	-10.827	YY=	156.0806	ZY= -1.5883
XZ=	7.3853	YZ=	1.1036	ZZ= 139.9955
Eigenvalues:	123.1047	140.6511	156.8116	
5	C	Isotropic=	-22.0021	Anisotropy = 179.0297
XX=	-58.2528	YX=	32.6886	ZX= 17.0765

XY=	14.6275	YY=	-102.5241	ZY=	16.164				
XZ=	13.8442	YZ=	7.7689	ZZ=	94.7706				
Eigenvalues:	-112.9025		-50.4548	97.351					
6	C	Isotropic=	102.0718	Anisotropy	=	41.3878			
XX=	86.2005	YX=	-6.7631	ZX=	2.0084				
XY=	6.8016	YY=	128.6368	ZY=	-7.3005				
XZ=	-6.37	YZ=	-5.2195	ZZ=	91.3781				
Eigenvalues:	85.2861	91.2656	129.6636						
7	C	Isotropic=	43.1597	Anisotropy	=	158.7611			
XX=	37.8527	YX=	-8.8565	ZX=	18.0884				
XY=	-30.6001	YY=	145.4938	ZY=	12.7625				
XZ=	32.4977	YZ=	-1.8094	ZZ=	-53.8673				
Eigenvalues:	-60.8936	41.3723	149.0005						
8	C	Isotropic=	41.4672	Anisotropy	=	155.6152			
XX=	41.4946	YX=	-20.7071	ZX=	10.0751				
XY=	-18.2307	YY=	136.0427	ZY=	25.0027				
XZ=	-4.0977	YZ=	42.243	ZZ=	-53.1356				
Eigenvalues:	-59.3284	38.5194	145.2107						
9	C	Isotropic=	110.3928	Anisotropy	=	48.9011			
XX=	126.679	YX=	17.6497	ZX=	17.303				
XY=	23.0745	YY=	108.3062	ZY=	-7.4909				
XZ=	19.1244	YZ=	-6.6411	ZZ=	96.1932				
Eigenvalues:	78.7697	109.4152	142.9936						
10	C	Isotropic=	147.8879	Anisotropy	=	41.5756			
XX=	168.263	YX=	4.8369	ZX=	12.1697				
XY=	4.0628	YY=	139.2182	ZY=	-1.0306				
XZ=	21.6424	YZ=	-11.3071	ZZ=	136.1824				
Eigenvalues:	125.0206	143.038	175.6049						
11	C	Isotropic=	147.9096	Anisotropy	=	14.1817			
XX=	142.8586	YX=	0.8907	ZX=	-2.2664				
XY=	-14.1051	YY=	153.5407	ZY=	-5.2547				
XZ=	1.8909	YZ=	-0.6314	ZZ=	147.3297				
Eigenvalues:	139.4287	146.9361	157.3641						
12	C	Isotropic=	155.6715	Anisotropy	=	24.4146			
XX=	165.23	YX=	-6.1695	ZX=	-13.3237				
XY=	0.3435	YY=	159.2548	ZY=	12.0552				
XZ=	-6.2074	YZ=	5.8569	ZZ=	142.5298				
Eigenvalues:	136.4056	158.6611	171.9479						
13	C	Isotropic=	148.2503	Anisotropy	=	54.7934			
XX=	145.6273	YX=	-22.1041	ZX=	-1.3557				
XY=	-25.6459	YY=	158.9859	ZY=	21.6234				
XZ=	4.0552	YZ=	24.7885	ZZ=	140.1377				
Eigenvalues:	115.7186	144.2531	184.7792						
14	C	Isotropic=	167.404	Anisotropy	=	10.5414			
XX=	164.1855	YX=	-8.5774	ZX=	2.5703				
XY=	3.1686	YY=	166.2295	ZY=	-0.1131				
XZ=	5.7176	YZ=	-3.0581	ZZ=	171.7969				
Eigenvalues:	161.5498	166.2306	174.4316						
15	C	Isotropic=	169.4453	Anisotropy	=	17.056			
XX=	174.2275	YX=	-4.831	ZX=	-5.2982				
XY=	-6.177	YY=	176.2155	ZY=	-2.3349				
XZ=	-0.9494	YZ=	-3.3487	ZZ=	157.8929				
Eigenvalues:	156.5323	170.9876	180.816						
16	O	Isotropic=	263.413	Anisotropy	=	83.3988			
XX=	313.9705	YX=	-8.684	ZX=	22.4058				
XY=	-2.3545	YY=	218.0866	ZY=	58.0346				

XZ= 11.2476 YZ= 20.909 ZZ= 258.1818
 Eigenvalues: 192.3453 278.8814 319.0122
 17 O Isotropic= 265.4467 Anisotropy = 45.761
 XX= 253.4332 YX= 18.3743 ZX= -15.4707
 XY= -5.5442 YY= 251.6851 ZY= 7.6878
 XZ= -12.3192 YZ= 2.2666 ZZ= 291.2218
 Eigenvalues: 242.447 257.9391 295.954
 18 O Isotropic= -371.0033 Anisotropy = 1096.9297
 XX= -964.2542 YX= -137.5683 ZX= 243.0799
 XY= -119.8988 YY= -467.6227 ZY= 117.8501
 XZ= 169.2326 YZ= 96.6598 ZZ= 318.8668
 Eigenvalues: -1033.4509 -439.8422 360.2831
 19 O Isotropic= 95.5206 Anisotropy = 126.5988
 XX= 154.7838 YX= 100.5907 ZX= -80.9643
 XY= -7.758 YY= 61.2018 ZY= 41.456
 XZ= -22.5367 YZ= 130.4481 ZZ= 70.5761
 Eigenvalues: -44.3212 150.9631 179.9198
 20 O Isotropic= 72.5564 Anisotropy = 191.1219
 XX= 73.4358 YX= -58.9422 ZX= -17.9355
 XY= -75.3003 YY= 143.6038 ZY= -75.4271
 XZ= -145.7311 YZ= -121.6629 ZZ= 0.6298
 Eigenvalues: -108.8292 126.5275 199.971
 21 H Isotropic= 31.1773 Anisotropy = 13.4296
 XX= 35.9224 YX= 2.1847 ZX= -5.2473
 XY= 1.624 YY= 31.9848 ZY= -5.8822
 XZ= -4.9773 YZ= -5.0359 ZZ= 25.6245
 Eigenvalues: 21.5581 31.8434 40.1303
 22 C Isotropic= 21.4223 Anisotropy = 77.8233
 XX= 10.4585 YX= -88.5588 ZX= 15.7849
 XY= -57.4382 YY= -18.2093 ZY= 18.7372
 XZ= -2.2315 YZ= -6.8613 ZZ= 72.0177
 Eigenvalues: -78.7921 69.7545 73.3045
 23 O Isotropic= -141.4296 Anisotropy = 605.9282
 XX= -238.4687 YX= -131.8076 ZX= -288.2985
 XY= -159.7844 YY= -129.3831 ZY= 160.9203
 XZ= -249.9241 YZ= 176.211 ZZ= -56.4369
 Eigenvalues: -433.4138 -253.3975 262.5226
 24 C Isotropic= 165.9973 Anisotropy = 37.4452
 XX= 155.3383 YX= 5.3732 ZX= 2.7865
 XY= 4.5484 YY= 181.0844 ZY= -15.3798
 XZ= 4.6385 YZ= -18.2992 ZZ= 161.5692
 Eigenvalues: 147.5995 159.4317 190.9608
 25 H Isotropic= 27.4185 Anisotropy = 2.8772
 XX= 27.9174 YX= -0.0592 ZX= -1.4207
 XY= 0.7326 YY= 28.3282 ZY= -0.3056
 XZ= -1.9328 YZ= -1.1347 ZZ= 26.01
 Eigenvalues: 24.9715 27.9474 29.3367
 26 H Isotropic= 28.2215 Anisotropy = 8.6116
 XX= 29.5249 YX= -4.6844 ZX= -0.449
 XY= -4.3353 YY= 29.2074 ZY= 0.8917
 XZ= 0.0777 YZ= 1.0803 ZZ= 25.9322
 Eigenvalues: 24.5885 26.1134 33.9626
 27 H Isotropic= 25.2281 Anisotropy = 4.0148
 XX= 25.8543 YX= 2.4218 ZX= -1.8311
 XY= 1.5799 YY= 25.66 ZY= 0.0742
 XZ= 1.5037 YZ= -1.8398 ZZ= 24.17

Eigenvalues:	23.3552	24.4245	27.9046		
28	H	Isotropic=	25.1557	Anisotropy	= 6.572
XX=	29.2288	YX=	-0.2341	ZX=	1.5734
XY=	-0.6179	YY=	25.2543	ZY=	3.1386
XZ=	1.6524	YZ=	0.0257	ZZ=	20.9842
Eigenvalues:	20.1562	25.774	29.537		
29	H	Isotropic=	27.6586	Anisotropy	= 7.3172
XX=	31.9981	YX=	-0.5414	ZX=	-1.597
XY=	-1.5824	YY=	21.9824	ZY=	-3.1235
XZ=	-1.156	YZ=	-1.418	ZZ=	28.9952
Eigenvalues:	21.1268	29.3123	32.5367		
30	H	Isotropic=	29.7798	Anisotropy	= 5.5686
XX=	33.1329	YX=	-0.4684	ZX=	1.0343
XY=	-1.1013	YY=	31.3199	ZY=	0.1885
XZ=	0.8558	YZ=	0.5906	ZZ=	24.8866
Eigenvalues:	24.745	31.1022	33.4922		
31	H	Isotropic=	29.4099	Anisotropy	= 8.314
XX=	31.2289	YX=	-0.7537	ZX=	-3.3681
XY=	-1.1994	YY=	26.6978	ZY=	3.473
XZ=	-3.3345	YZ=	1.9984	ZZ=	30.3031
Eigenvalues:	25.1027	28.1744	34.9526		
32	H	Isotropic=	29.2137	Anisotropy	= 8.9089
XX=	28.7226	YX=	4.8828	ZX=	-2.2094
XY=	4.4346	YY=	30.7419	ZY=	-1.0506
XZ=	-1.3184	YZ=	-1.5804	ZZ=	28.1766
Eigenvalues:	24.8602	27.6279	35.153		
33	H	Isotropic=	30.3686	Anisotropy	= 6.8424
XX=	32.1343	YX=	2.1877	ZX=	2.6382
XY=	1.8932	YY=	27.3229	ZY=	-0.3321
XZ=	3.1242	YZ=	-1.1086	ZZ=	31.6486
Eigenvalues:	25.9916	30.1841	34.9302		
34	H	Isotropic=	30.1569	Anisotropy	= 8.872
XX=	29.7457	YX=	0.3884	ZX=	0.3279
XY=	1.3492	YY=	31.7207	ZY=	4.9603
XZ=	2.1965	YZ=	5.4336	ZZ=	29.0041
Eigenvalues:	24.9433	29.4557	36.0715		
35	H	Isotropic=	30.2709	Anisotropy	= 7.3812
XX=	30.6348	YX=	-2.5611	ZX=	2.3217
XY=	-3.4252	YY=	33.1907	ZY=	0.6973
XZ=	1.2725	YZ=	0.6406	ZZ=	26.9871
Eigenvalues:	25.7621	29.8589	35.1917		
36	H	Isotropic=	28.5414	Anisotropy	= 5.6108
XX=	28.7966	YX=	0.1095	ZX=	-2.0191
XY=	-1.4323	YY=	27.9574	ZY=	3.8046
XZ=	-2.2035	YZ=	1.3792	ZZ=	28.8704
Eigenvalues:	25.4979	27.8444	32.282		
37	H	Isotropic=	28.7855	Anisotropy	= 7.1169
XX=	29.9879	YX=	1.5048	ZX=	0.506
XY=	1.8396	YY=	27.7198	ZY=	-5.2474
XZ=	-0.9488	YZ=	-4.4307	ZZ=	28.649
Eigenvalues:	23.1455	29.681	33.5302		
38	H	Isotropic=	29.0288	Anisotropy	= 6.6662
XX=	28.3672	YX=	0.8955	ZX=	0.7339
XY=	1.2854	YY=	28.7312	ZY=	3.8449
XZ=	1.2667	YZ=	3.4296	ZZ=	29.9881
Eigenvalues:	25.6536	27.9598	33.4729		

39	H	Isotropic=	27.7601	Anisotropy	=	10.5469
XX=	34.2927	YX=	-1.7528	ZX=	-2.0616	
XY=	-2.5829	YY=	23.7195	ZY=	-2.2025	
XZ=	-0.3643	YZ=	-1.7649	ZZ=	25.268	
Eigenvalues:	21.8711	26.6178	34.7913			
40	H	Isotropic=	29.1406	Anisotropy	=	10.8516
XX=	31.9939	YX=	-0.1911	ZX=	-5.8051	
XY=	-2.0508	YY=	27.036	ZY=	-0.2751	
XZ=	-5.8104	YZ=	0.511	ZZ=	28.3919	
Eigenvalues:	24.0024	27.0444	36.375			
41	H	Isotropic=	29.6267	Anisotropy	=	5.8603
XX=	31.8971	YX=	-1.7635	ZX=	1.8426	
XY=	-2.4454	YY=	26.2431	ZY=	1.2892	
XZ=	2.0654	YZ=	0.8308	ZZ=	30.74	
Eigenvalues:	25.0571	30.2895	33.5335			
42	H	Isotropic=	30.4735	Anisotropy	=	9.7477
XX=	28.9302	YX=	-1.707	ZX=	-1.1033	
XY=	-1.8482	YY=	36.3367	ZY=	1.1802	
XZ=	-1.3703	YZ=	1.4822	ZZ=	26.1534	
Eigenvalues:	25.643	28.8054	36.9719			
43	H	Isotropic=	28.9742	Anisotropy	=	5.2797
XX=	30.3923	YX=	1.1894	ZX=	1.6915	
XY=	-0.4379	YY=	29.1554	ZY=	-3.8843	
XZ=	2.9279	YZ=	-2.7529	ZZ=	27.3749	
Eigenvalues:	24.1324	30.2962	32.494			
44	H	Isotropic=	29.1467	Anisotropy	=	7.6625
XX=	26.5242	YX=	1.1187	ZX=	0.901	
XY=	2.9722	YY=	33.2872	ZY=	2.3815	
XZ=	0.3835	YZ=	0.6279	ZZ=	27.6287	
Eigenvalues:	25.9203	27.2647	34.255			
45	H	Isotropic=	28.8295	Anisotropy	=	8.37
XX=	29.8241	YX=	0.3748	ZX=	-3.6258	
XY=	1.5503	YY=	26.9479	ZY=	-1.7023	
XZ=	-4.7338	YZ=	-1.6064	ZZ=	29.7165	
Eigenvalues:	25.3762	26.7028	34.4095			
46	H	Isotropic=	30.7859	Anisotropy	=	18.2838
XX=	38.1828	YX=	-3.5651	ZX=	7.6686	
XY=	-2.3438	YY=	23.0844	ZY=	-3.2574	
XZ=	5.7853	YZ=	-1.7339	ZZ=	31.0905	
Eigenvalues:	22.2755	27.1071	42.9751			
47	C	Isotropic=	11.5135	Anisotropy	=	93.9043
XX=	-54.3583	YX=	-52.3361	ZX=	9.2495	
XY=	-40.639	YY=	56.897	ZY=	4.4354	
XZ=	52.8103	YZ=	10.5943	ZZ=	32.0019	
Eigenvalues:	-80.206	40.6302	74.1164			
48	O	Isotropic=	-95.4827	Anisotropy	=	621.907
XX=	-168.3538	YX=	-183.5899	ZX=	23.1361	
XY=	-185.6966	YY=	218.4062	ZY=	-103.3795	
XZ=	72.7686	YZ=	-143.3727	ZZ=	-336.5005	
Eigenvalues:	-363.2371	-242.3329	319.122			
49	H	Isotropic=	28.6661	Anisotropy	=	6.5098
XX=	28.1489	YX=	-2.3321	ZX=	0.4485	
XY=	-1.8104	YY=	25.5122	ZY=	1.8851	
XZ=	1.7832	YZ=	2.369	ZZ=	32.3372	
Eigenvalues:	23.707	29.2853	33.006			
50	H	Isotropic=	29.444	Anisotropy	=	6.6604

XX=	27.6552	YX=	0.5645	ZX=	-1.5583					
XY=	0.4241	YY=	33.5195	ZY=	1.0518					
XZ=	-1.5473	YZ=	2.0683	ZZ=	27.1574					
Eigenvalues:	25.5444	28.9034	33.8843							
51	C	Isotropic=	108.7305	Anisotropy	=	19.2214				
XX=	105.8908	YX=	-0.519	ZX=	1.7766					
XY=	-3.0388	YY=	102.5806	ZY=	8.594					
XZ=	-4.1863	YZ=	7.8675	ZZ=	117.7201					
Eigenvalues:	98.7798	105.867	121.5447							
52	C	Isotropic=	123.1704	Anisotropy	=	30.3375				
XX=	132.9263	YX=	14.2981	ZX=	10.5604					
XY=	11.9035	YY=	121.2284	ZY=	-2.526					
XZ=	7.564	YZ=	1.4404	ZZ=	115.3567					
Eigenvalues:	107.8365	118.2794	143.3954							
53	O	Isotropic=	279.7447	Anisotropy	=	87.8121				
XX=	335.599	YX=	-22.4195	ZX=	-16.9569					
XY=	-3.4369	YY=	261.0134	ZY=	-11.3762					
XZ=	2.0021	YZ=	6.6003	ZZ=	242.6216					
Eigenvalues:	241.3758	259.5722	338.2861							
54	H	Isotropic=	26.3941	Anisotropy	=	6.0706				
XX=	25.119	YX=	0.4519	ZX=	-0.1361					
XY=	-0.4376	YY=	27.189	ZY=	-3.691					
XZ=	-1.6404	YZ=	-2.9753	ZZ=	26.8742					
Eigenvalues:	23.4436	25.2974	30.4411							
55	N	Isotropic=	131.076	Anisotropy	=	101.5179				
XX=	175.8905	YX=	29.8215	ZX=	-10.4981					
XY=	7.5282	YY=	139.4575	ZY=	-33.1722					
XZ=	-4.9271	YZ=	-98.5786	ZZ=	77.8802					
Eigenvalues:	35.8633	158.6102	198.7546							
56	C	Isotropic=	58.0586	Anisotropy	=	177.5847				
XX=	28.5353	YX=	-71.661	ZX=	-42.9126					
XY=	-69.0973	YY=	139.4055	ZY=	3.5137					
XZ=	-39.227	YZ=	4.9272	ZZ=	6.2349					
Eigenvalues:	-36.2502	33.9776	176.4483							
57	H	Isotropic=	26.3978	Anisotropy	=	7.591				
XX=	26.9822	YX=	2.8595	ZX=	-2.2685					
XY=	3.5146	YY=	25.0479	ZY=	-1.6156					
XZ=	-2.7588	YZ=	-1.7164	ZZ=	27.1632					
Eigenvalues:	22.6764	25.0586	31.4584							
58	H	Isotropic=	29.9246	Anisotropy	=	18.6763				
XX=	40.0148	YX=	-4.9187	ZX=	-2.1898					
XY=	-5.7798	YY=	24.1816	ZY=	5.3763					
XZ=	-2.3815	YZ=	3.0872	ZZ=	25.5774					
Eigenvalues:	20.1885	27.2098	42.3755							
59	C	Isotropic=	15.0606	Anisotropy	=	122.0279				
XX=	73.4554	YX=	-57.1394	ZX=	6.98					
XY=	-55.6974	YY=	-49.1803	ZY=	8.4365					
XZ=	21.957	YZ=	19.7436	ZZ=	20.9067					
Eigenvalues:	-74.7357	23.5049	96.4125							
60	H	Isotropic=	25.7361	Anisotropy	=	7.2625				
XX=	21.0204	YX=	-0.2432	ZX=	-1.7209					
XY=	2.0081	YY=	30.2899	ZY=	3.2849					
XZ=	-3.5687	YZ=	-0.9913	ZZ=	25.8979					
Eigenvalues:	19.7085	26.9219	30.5777							
61	C	Isotropic=	51.557	Anisotropy	=	187.8908				
XX=	19.0661	YX=	-84.506	ZX=	11.6612					

XY= -85.9582 YY= 125.7618 ZY= 35.5703
 XZ= 10.9592 YZ= 34.3301 ZZ= 9.8431
 Eigenvalues: -42.6538 20.5072 176.8175
 62 C Isotropic= 62.2191 Anisotropy = 174.1436
 XX= 78.9064 YX= -52.4658 ZX= -4.9096
 XY= -52.9775 YY= 144.3989 ZY= 31.8892
 XZ= -2.9088 YZ= 35.4946 ZZ= -36.648
 Eigenvalues: -42.9952 51.3377 178.3148
 63 C Isotropic= 63.9147 Anisotropy = 175.2725
 XX= 30.6074 YX= -72.9008 ZX= -47.9332
 XY= -76.095 YY= 139.4473 ZY= 0.1543
 XZ= -48.8354 YZ= 1.8265 ZZ= 21.6893
 Eigenvalues: -38.6749 49.6559 180.763
 64 C Isotropic= 64.7002 Anisotropy = 168.2356
 XX= 27.3423 YX= -84.4306 ZX= 18.4825
 XY= -85.7258 YY= 124.1132 ZY= 34.513
 XZ= 19.3873 YZ= 34.8291 ZZ= 42.6453
 Eigenvalues: -36.8808 54.1243 176.8573
 65 C Isotropic= 61.677 Anisotropy = 141.666
 XX= 80.2441 YX= -41.8131 ZX= -0.8011
 XY= -32.5131 YY= 132.3832 ZY= 30.9765
 XZ= -1.0771 YZ= 31.8841 ZZ= -27.5964
 Eigenvalues: -33.8876 62.7976 156.121
 66 H Isotropic= 20.8272 Anisotropy = 10.3077
 XX= 21.8048 YX= 4.0146 ZX= 5.0861
 XY= 2.7103 YY= 17.3562 ZY= -0.1735
 XZ= 3.7948 YZ= 1.0079 ZZ= 23.3207
 Eigenvalues: 15.0693 19.7133 27.699
 67 O Isotropic= -109.1324 Anisotropy = 659.5703
 XX= 239.3037 YX= -157.3292 ZX= 122.9557
 XY= -157.9097 YY= -151.6493 ZY= -36.7574
 XZ= 186.3242 YZ= -66.6367 ZZ= -415.0515
 Eigenvalues: -450.7263 -207.2519 330.5811
 68 C Isotropic= 53.7774 Anisotropy = 172.5732
 XX= 28.1081 YX= -33.8355 ZX= 41.6168
 XY= -19.5681 YY= 1.7013 ZY= -66.4984
 XZ= 15.9469 YZ= -65.2856 ZZ= 131.5227
 Eigenvalues: -29.5063 22.0122 168.8262
 69 H Isotropic= 23.6704 Anisotropy = 5.8733
 XX= 25.8887 YX= 2.857 ZX= 1.4505
 XY= 2.6965 YY= 21.3465 ZY= -0.0911
 XZ= 1.1764 YZ= 0.147 ZZ= 23.776
 Eigenvalues: 19.9508 23.4746 27.586
 70 H Isotropic= 23.8063 Anisotropy = 3.479
 XX= 24.4872 YX= 2.1681 ZX= -0.0898
 XY= 1.8527 YY= 21.572 ZY= -1.0764
 XZ= -0.318 YZ= -0.9096 ZZ= 25.3598
 Eigenvalues: 20.4175 24.8758 26.1257
 71 H Isotropic= 23.9314 Anisotropy = 4.3369
 XX= 24.769 YX= 2.1073 ZX= 1.3053
 XY= 2.1715 YY= 21.4492 ZY= -0.0309
 XZ= 1.2054 YZ= -0.1289 ZZ= 25.5759
 Eigenvalues: 20.324 24.6475 26.8227
 72 H Isotropic= 24.2093 Anisotropy = 8.1702
 XX= 27.9466 YX= 3.6054 ZX= 0.0109
 XY= 3.551 YY= 22.161 ZY= 0.0442

XZ=	0.1817	YZ=	-0.0587	ZZ=	22.5202				
Eigenvalues:	20.4514	22.5204	29.6561						
73	C	Isotropic=	62.5959	Anisotropy	=	174.6955			
XX=	27.4295	YX=	4.5065	ZX=	70.4541				
XY=	6.2986	YY=	46.1803	ZY=	-64.776				
XZ=	73.7099	YZ=	-67.8319	ZZ=	114.1779				
Eigenvalues:	-34.7742	43.5024	179.0595						
74	C	Isotropic=	61.7369	Anisotropy	=	176.0548			
XX=	-7.5674	YX=	-49.1189	ZX=	59.7476				
XY=	-45.954	YY=	57.6458	ZY=	-36.8766				
XZ=	60.7977	YZ=	-35.9783	ZZ=	135.1323				
Eigenvalues:	-41.5692	47.6732	179.1068						
75	C	Isotropic=	62.0567	Anisotropy	=	177.9536			
XX=	58.6994	YX=	-40.0425	ZX=	34.7172				
XY=	-40.2801	YY=	-6.6623	ZY=	-68.249				
XZ=	35.2665	YZ=	-68.2082	ZZ=	134.1331				
Eigenvalues:	-40.8612	46.3389	180.6924						
76	C	Isotropic=	62.8395	Anisotropy	=	174.9391			
XX=	30.4475	YX=	14.1311	ZX=	70.3215				
XY=	9.6174	YY=	40.5021	ZY=	-67.034				
XZ=	72.8104	YZ=	-67.6467	ZZ=	117.569				
Eigenvalues:	-38.6931	47.746	179.4656						
77	C	Isotropic=	66.8771	Anisotropy	=	162.9543			
XX=	1.6978	YX=	-38.0341	ZX=	55.5822				
XY=	-45.2222	YY=	60.2421	ZY=	-32.8799				
XZ=	52.7782	YZ=	-32.7979	ZZ=	138.6915				
Eigenvalues:	-27.6934	52.8115	175.5133						
78	H	Isotropic=	23.3849	Anisotropy	=	5.5603			
XX=	24.2982	YX=	1.3049	ZX=	-0.4489				
XY=	0.7673	YY=	26.7006	ZY=	0.2276				
XZ=	-0.8512	YZ=	0.7185	ZZ=	19.1559				
Eigenvalues:	19.0274	24.0355	27.0918						
79	H	Isotropic=	23.8069	Anisotropy	=	6.1052			
XX=	23.287	YX=	-0.7514	ZX=	-1.3927				
XY=	-0.4432	YY=	27.0593	ZY=	1.961				
XZ=	-1.4363	YZ=	2.0122	ZZ=	21.0745				
Eigenvalues:	20.0292	23.5145	27.8771						
80	H	Isotropic=	23.7362	Anisotropy	=	4.247			
XX=	25.3856	YX=	-0.1678	ZX=	-2.2094				
XY=	-0.1642	YY=	24.3946	ZY=	1.4105				
XZ=	-2.0011	YZ=	1.4546	ZZ=	21.4283				
Eigenvalues:	20.1434	24.4976	26.5675						
81	H	Isotropic=	23.9022	Anisotropy	=	4.3631			
XX=	24.6236	YX=	1.1362	ZX=	-1.294				
XY=	1.1333	YY=	26.0091	ZY=	1.751				
XZ=	-0.9469	YZ=	1.5099	ZZ=	21.074				
Eigenvalues:	20.1381	24.7576	26.811						
82	H	Isotropic=	23.9616	Anisotropy	=	8.3821			
XX=	22.89	YX=	-1.1391	ZX=	-1.671				
XY=	-1.0763	YY=	28.1135	ZY=	3.5029				
XZ=	-1.0243	YZ=	2.5328	ZZ=	20.8813				
Eigenvalues:	19.5341	22.801	29.5497						
2a11_neg45									
	C	2.785647	-1.395202	1.615519					
	C	3.647288	-2.388374	0.773221					
	C	3.313866	-2.445888	-0.726998					

C	4.427549	-1.88824	-1.631704
C	4.784068	-0.407662	-1.391015
C	3.6609	0.607396	-1.245118
C	2.758041	0.378058	-0.067769
C	1.425917	0.25832	-0.306743
C	0.571522	-0.391882	0.746536
C	1.278392	-1.588921	1.387093
C	3.226227	0.076844	1.338818
C	4.714818	0.232786	1.605877
C	2.520738	1.015418	2.335565
C	0.744721	0.667064	-1.555738
C	5.669928	-2.747616	-1.573965
O	2.970061	-1.718019	2.993043
O	3.55443	-3.682527	1.348847
O	5.953424	-0.037134	-1.520034
O	4.025918	1.969028	-1.44963
O	-0.618479	-0.872006	0.073701
H	2.620837	-3.871043	1.505108
C	5.137386	2.580245	-0.935112
O	5.876283	1.999383	-0.147581
C	5.26951	3.971393	-1.463538
H	4.738119	-2.132027	0.909164
H	2.361134	-1.902405	-0.947003
H	3.04477	0.434195	-2.195671
H	0.249443	0.351307	1.528936
H	0.784557	-1.789682	2.378499
H	1.109801	-2.491141	0.742238
H	5.359339	-0.206419	0.810682
H	4.979397	1.316462	1.68929
H	4.970415	-0.253281	2.580046
H	3.26158	1.52285	3.000703
H	1.946343	1.808602	1.801015
H	1.82867	0.439208	2.997481
H	1.260946	1.534413	-2.036625
H	0.716955	-0.189734	-2.276223
H	-0.316861	0.963745	-1.344951
H	6.42958	-2.373362	-2.303155
H	6.127612	-2.720843	-0.555959
H	5.414822	-3.805358	-1.823751
H	4.339114	4.294388	-1.988593
H	5.481005	4.662242	-0.611895
H	6.126519	3.996676	-2.180686
H	3.89064	-1.981958	3.116163
C	-1.685923	-1.219624	0.84287
O	-1.61473	-1.126979	2.069683
H	4.026254	-1.911179	-2.687537
H	3.163889	-3.523748	-1.005078
C	-2.866394	-1.704983	0.025349
C	-4.160274	-0.992986	0.50501
O	-2.642718	-1.695617	-1.35451
H	-3.007203	-2.804234	0.272487
N	-4.244603	0.445821	0.431227
C	-5.339518	-1.659962	-0.170161
H	-4.209264	-1.237964	1.618821
H	-2.279742	-0.8365	-1.619487
C	-3.471138	1.359284	-0.248787

H	-4.903537	0.825891	1.076409
C	-5.618796	-1.421791	-1.519318
C	-6.718597	-2.031362	-2.122165
C	-7.54196-2.879161	-1.381493	
C	-7.263242	-3.119912	-0.035943
C	-6.166784	-2.509729	0.571533
H	-4.947583	-0.773188	-2.105166
O	-2.681395	1.045031	-1.164197
C	-3.648718	2.792359	0.139686
H	-6.932443	-1.844926	-3.184882
H	-8.408868	-3.359961	-1.858009
H	-7.909183	-3.791226	0.548637
H	-5.954418	-2.701628	1.634129
C	-2.502436	3.574612	0.319725
C	-2.628817	4.91701	0.673701
C	-3.894327	5.480966	0.837692
C	-5.036334	4.703276	0.644325
C	-4.917529	3.357763	0.29701
H	-1.508549	3.124765	0.168054
H	-1.727882	5.531375	0.819387
H	-3.992149	6.541118	1.115702
H	-6.034156	5.150861	0.763743
H	-5.824432.756706	0.131019	

2aii_neg45	E(RB+HF-PW91)	=	-2012.310485	
SCF GIAO	Magnetic shielding	tensor (ppm):		
1 C	Isotropic=	109.2929	Anisotropy	= 28.9353
XX=	98.4129	YX= 0.1504	ZX= 13.8448	
XY=	5.3743	YY= 105.165	ZY= -0.1353	
XZ=	8.8623	YZ= -0.9923	ZZ= 124.3008	
Eigenvalues:	93.4758	105.8197	128.5831	
2 C	Isotropic=	112.1051	Anisotropy	= 30.1066
XX=	94.5958	YX= 7.637	ZX= -5.6914	
XY=	-0.5	YY= 129.5211	ZY= -1.239	
XZ=	-4.8609	YZ= -11.109	ZZ= 112.1983	
Eigenvalues:	93.0415	111.0976	132.1761	
3 C	Isotropic=	142.0073	Anisotropy	= 20.2056
XX=	121.2284	YX= -4.4239	ZX= -2.3324	
XY=	3.1318	YY= 152.5663	ZY= 2.6062	
XZ=	-1.2225	YZ= 3.3788	ZZ= 152.2271	
Eigenvalues:	121.1196	149.4245	155.4777	
4 C	Isotropic=	140.033	Anisotropy	= 24.9577
XX=	124.3681	YX= 1.7856	ZX= -0.7701	
XY=	-11.8464	YY= 155.4825	ZY= 1.6148	
XZ=	5.1039	YZ= 4.1992	ZZ= 140.2484	
Eigenvalues:	123.1766	140.2509	156.6715	
5 C	Isotropic=	-22.3042	Anisotropy	= 179.6482
XX=	-59.7602	YX= 28.4299	ZX= 19.0171	
XY=	11.4005	YY= -99.0995	ZY= -25.9622	
XZ=	11.8287	YZ= -33.6721	ZZ= 91.9472	
Eigenvalues:	-112.8894	-51.4843	97.4613	
6 C	Isotropic=	101.8469	Anisotropy	= 41.212
XX=	86.2138	YX= -6.2204	ZX= 0.3969	
XY=	9.4874	YY= 129.1457	ZY= 1.2896	
XZ=	-4.7261	YZ= 3.0934	ZZ= 90.1812	

Eigenvalues:	85.1321	91.087	129.3216			
7	C	Isotropic=	44.0249	Anisotropy	=	156.8144
XX=	37.7281	YX=	-12.357	ZX=	18.5442	
XY=	-37.112	YY=	134.5033	ZY=	51.3368	
XZ=	27.1827	YZ=	38.1725	ZZ=	-40.1568	
Eigenvalues:	-59.2061	142.7129	148.5678			
8	C	Isotropic=	40.4927	Anisotropy	=	157.6004
XX=	38.7285	YX=	-24.5081	ZX=	8.3868	
XY=	-18.6573	YY=	114.3702	ZY=	60.9216	
XZ=	-4.4817	YZ=	77.7461	ZZ=	-31.6204	
Eigenvalues:	-60.2918	136.2104	145.5597			
9	C	Isotropic=	110.5778	Anisotropy	=	48.699
XX=	126.0067	YX=	13.2845	ZX=	21.6155	
XY=	18.3731	YY=	110.1038	ZY=	-4.114	
XZ=	23.8261	YZ=	-2.7683	ZZ=	95.6231	
Eigenvalues:	79.5442	109.1455	143.0438			
10	C	Isotropic=	148.0868	Anisotropy	=	41.8436
XX=	167.743	YX=	2.4893	ZX=	13.8979	
XY=	-0.5862	YY=	141.1091	ZY=	-0.5872	
XZ=	22.4953	YZ=	-10.9628	ZZ=	135.4083	
Eigenvalues:	125.2147	143.0631	175.9825			
11	C	Isotropic=	147.9351	Anisotropy	=	13.8042
XX=	143.0024	YX=	1.315	ZX=	-2.1868	
XY=	-13.2568	YY=	154.5853	ZY=	-3.6501	
XZ=	-0.7113	YZ=	1.2798	ZZ=	146.2176	
Eigenvalues:	139.9587	146.7087	157.138			
12	C	Isotropic=	155.6844	Anisotropy	=	24.1397
XX=	165.8415	YX=	-3.522	ZX=	-13.3814	
XY=	1.6151	YY=	155.0447	ZY=	14.74	
XZ=	-5.5832	YZ=	8.5564	ZZ=	146.167	
Eigenvalues:	136.2651	159.0105	171.7775			
13	C	Isotropic=	147.997	Anisotropy	=	54.568
XX=	144.6929	YX=	-21.6636	ZX=	-5.7625	
XY=	-26.2512	YY=	148.6013	ZY=	23.1737	
XZ=	-1.1434	YZ=	25.9981	ZZ=	150.697	
Eigenvalues:	115.4175	144.1979	184.3757			
14	C	Isotropic=	168.342	Anisotropy	=	11.651
XX=	164.6915	YX=	-8.7172	ZX=	1.4619	
XY=	1.9921	YY=	168.0675	ZY=	-1.7517	
XZ=	6.2551	YZ=	-4.4375	ZZ=	172.2669	
Eigenvalues:	162.239	166.6775	176.1093			
15	C	Isotropic=	169.3229	Anisotropy	=	17.1314
XX=	174.3027	YX=	-3.6086	ZX=	-5.6255	
XY=	-6.1347	YY=	176.375	ZY=	1.6409	
XZ=	-1.3493	YZ=	0.7672	ZZ=	157.2911	
Eigenvalues:	156.6008	170.6241	180.7439			
16	O	Isotropic=	262.7719	Anisotropy	=	84.1078
XX=	312.5139	YX=	-16.0936	ZX=	22.0333	
XY=	-7.3426	YY=	202.9357	ZY=	45.0357	
XZ=	11.9955	YZ=	8.365	ZZ=	272.8662	
Eigenvalues:	191.609	277.8629	318.8438			
17	O	Isotropic=	265.7118	Anisotropy	=	45.3124
XX=	255.114	YX=	22.3293	ZX=	-11.5042	
XY=	-2.8299	YY=	250.5202	ZY=	-1.2277	
XZ=	-12.2919	YZ=	-5.8775	ZZ=	291.5013	
Eigenvalues:	242.305	258.9104	295.9201			

18	O	Isotropic=	-369.2569	Anisotropy	=	1094.5255
XX=	-975.004	YX=	-177.0899	ZX=	168.7202	
XY=	-143.656	YY=	-470.2009	ZY=	-62.1284	
XZ=	97.744	YZ=	-83.303	ZZ=	337.4344	
Eigenvalues:	-1030.2322		-437.9651		360.4268	
19	O	Isotropic=	94.7726	Anisotropy	=	127.3827
XX=	157.5043	YX=	110.7945	ZX=	-56.6023	
XY=	-5.3752	YY=	23.7629	ZY=	33.0753	
XZ=	-22.0673	YZ=	124.6357	ZZ=	103.0505	
Eigenvalues:	-45.9635	150.5869		179.6944		
20	O	Isotropic=	72.2524	Anisotropy	=	189.0704
XX=	73.6767	YX=	-48.2181	ZX=	-26.4074	
XY=	-48.5291	YY=	176.7342	ZY=	-35.5644	
XZ=	-158.2377	YZ=	-78.82	ZZ=	-33.6536	
Eigenvalues:	-106.0351		124.493		198.2994	
21	H	Isotropic=	31.1395	Anisotropy	=	13.5464
XX=	36.4779	YX=	3.5599	ZX=	-3.878	
XY=	3.0035	YY=	33.8402	ZY=	-3.8259	
XZ=	-3.6878	YZ=	-2.8728	ZZ=	23.1005	
Eigenvalues:	21.5903	31.6578		40.1705		
22	C	Isotropic=	21.3445	Anisotropy	=	78.0062
XX=	9.7765	YX=	-89.0253	ZX=	-4.707	
XY=	-55.5487	YY=	-15.5176	ZY=	-2.6344	
XZ=	-16.4449	YZ=	-28.3751	ZZ=	69.7745	
Eigenvalues:	-78.6061	169.2909		73.3486		
23	O	Isotropic=	-141.0557	Anisotropy	=	606.4197
XX=	-223.4832	YX=	-71.3515	ZX=	-315.5263	
XY=	-105.7863	YY=	-193.6681	ZY=	131.8488	
XZ=	-283.3479	YZ=	146.3315	ZZ=	-6.0157	
Eigenvalues:	-433.5867		-252.8044		263.2241	
24	C	Isotropic=	165.7211	Anisotropy	=	37.7788
XX=	155.013	YX=	5.428	ZX=	3.7656	
XY=	4.278	YY=	187.0028	ZY=	-9.9669	
XZ=	5.9925	YZ=	-12.7061	ZZ=	155.1475	
Eigenvalues:	146.8184		159.438		190.907	
25	H	Isotropic=	27.455	Anisotropy	=	3.0369
XX=	28.1034	YX=	0.322	ZX=	-1.2912	
XY=	1.2317	YY=	28.5541	ZY=	0.2539	
XZ=	-1.7847	YZ=	-0.5179	ZZ=	25.7076	
Eigenvalues:	24.9418	27.9437		29.4797		
26	H	Isotropic=	28.1039	Anisotropy	=	8.5026
XX=	29.431	YX=	-4.5374	ZX=	-1.2989	
XY=	-4.2158	YY=	28.5765	ZY=	1.2412	
XZ=	-0.6658	YZ=	1.5439	ZZ=	26.3042	
Eigenvalues:	24.5131	26.0263		33.7723		
27	H	Isotropic=	25.1971	Anisotropy	=	4.0936
XX=	25.917	YX=	2.7301	ZX=	-1.1291	
XY=	1.2877	YY=	25.9135	ZY=	0.3939	
XZ=	1.8575	YZ=	-1.3815	ZZ=	23.7608	
Eigenvalues:	23.2215	24.4436		27.9262		
28	H	Isotropic=	25.0274	Anisotropy	=	6.9361
XX=	29.1235	YX=	0.1163	ZX=	2.0928	
XY=	-0.3225	YY=	23.5176	ZY=	3.6371	
XZ=	1.6059	YZ=	1.3167	ZZ=	22.4411	
Eigenvalues:	20.185	25.2458		29.6515		
29	H	Isotropic=	27.621	Anisotropy	=	7.4942

XX=	32.1626	YX=	0.0125	ZX=	-1.5611		
XY=	-1.1125	YY=	22.9411	ZY=	-4.3577		
XZ=	-1.307	YZ=	-2.5779	ZZ=	27.7591		
Eigenvalues:	21.0074	29.2383	32.6171				
30	H	Isotropic=	29.6059	Anisotropy	=	5.6064	
XX=	33.0032	YX=	-0.6049	ZX=	1.2246		
XY=	-1.2399	YY=	30.563	ZY=	1.444		
XZ=	0.8772	YZ=	1.925	ZZ=	25.2514		
Eigenvalues:	24.5708	30.9033	33.3434				
31	H	Isotropic=	29.3771	Anisotropy	=	8.2664	
XX=	31.3625	YX=	-0.0724	ZX=	-3.3137		
XY=	-0.4804	YY=	25.7516	ZY=	2.4431		
XZ=	-3.6343	YZ=	1.0522	ZZ=	31.0171		
Eigenvalues:	25.102	28.1413	34.888				
32	H	Isotropic=	29.2003	Anisotropy	=	9.0603	
XX=	28.7839	YX=	5.3011	ZX=	-0.9758		
XY=	4.7798	YY=	31.1387	ZY=	-0.3255		
XZ=	-0.5008	YZ=	-0.756	ZZ=	27.6782		
Eigenvalues:	24.7646	27.5958	35.2405				
33	H	Isotropic=	30.2652	Anisotropy	=	6.7705	
XX=	31.8456	YX=	1.6052	ZX=	3.1228		
XY=	1.3269	YY=	27.7743	ZY=	-1.2557		
XZ=	3.3786	YZ=	-1.855	ZZ=	31.1757		
Eigenvalues:	25.8588	30.158	34.7789				
34	H	Isotropic=	30.1035	Anisotropy	=	9.1183	
XX=	29.4072	YX=	0.2734	ZX=	0.3593		
XY=	1.0608	YY=	29.4303	ZY=	5.136		
XZ=	2.1781	YZ=	5.5505	ZZ=	31.4729		
Eigenvalues:	24.9912	29.1369	36.1824				
35	H	Isotropic=	30.1885	Anisotropy	=	6.512	
XX=	29.9581	YX=	-2.6287	ZX=	1.8791		
XY=	-2.8974	YY=	32.6291	ZY=	1.6712		
XZ=	0.1115	YZ=	1.9502	ZZ=	27.9783		
Eigenvalues:	26.2246	29.8111	34.5298				
36	H	Isotropic=	28.3834	Anisotropy	=	5.8749	
XX=	28.6964	YX=	0.8184	ZX=	-2.0107		
XY=	-0.5521	YY=	26.6491	ZY=	3.4748		
XZ=	-2.7588	YZ=	1.2525	ZZ=	29.8047		
Eigenvalues:	24.8922	27.958	32.3				
37	H	Isotropic=	28.9393	Anisotropy	=	7.3177	
XX=	30.2493	YX=	1.3301	ZX=	1.0755		
XY=	2.2544	YY=	29.9838	ZY=	-5.2896		
XZ=	-0.4847	YZ=	-4.2047	ZZ=	26.5847		
Eigenvalues:	23.0128	29.9872	33.8177				
38	H	Isotropic=	28.9555	Anisotropy	=	6.4834	
XX=	28.3295	YX=	0.485	ZX=	0.87		
XY=	0.9818	YY=	27.277	ZY=	3.129		
XZ=	1.4473	YZ=	2.9432	ZZ=	31.26		
Eigenvalues:	25.6338	27.9549	33.2777				
39	H	Isotropic=	27.4234	Anisotropy	=	12.0928	
XX=	35.1428	YX=	-1.4121	ZX=	-2.2032		
XY=	-2.234	YY=	23.9458	ZY=	-3.2291		
XZ=	-0.2274	YZ=	-2.0488	ZZ=	23.1816		
Eigenvalues:	20.5895	26.1955	35.4853				
40	H	Isotropic=	29.1539	Anisotropy	=	10.8191	
XX=	32.3623	YX=	0.9937	ZX=	-5.5632		

XY=	-0.7864	YY=	27.0811	ZY=	-0.5653				
XZ=	-5.9957	YZ=	0.3567	ZZ=	28.0184				
Eigenvalues:	24.016	27.0791	36.3667						
41	H	Isotropic=	29.6254	Anisotropy	=	5.824			
XX=	31.7449	YX=	-2.1922	ZX=	1.4639				
XY=	-2.8516	YY=	26.0868	ZY=	0.1058				
XZ=	1.4661	YZ=	-0.2759	ZZ=	31.0446				
Eigenvalues:	25.0916	30.2766	33.5081						
42	H	Isotropic=	30.4662	Anisotropy	=	9.7136			
XX=	28.9924	YX=	-1.4481	ZX=	-1.2998				
XY=	-1.4546	YY=	35.3163	ZY=	3.1799				
XZ=	-1.6639	YZ=	3.4982	ZZ=	27.09				
Eigenvalues:	25.6322	28.8246	36.942						
43	H	Isotropic=	29.0289	Anisotropy	=	5.4254			
XX=	30.2579	YX=	0.8072	ZX=	2.0909				
XY=	-0.9862	YY=	30.5935	ZY=	-3.2849				
XZ=	2.898	YZ=	-2.1124	ZZ=	26.2354				
Eigenvalues:	24.1249	30.316	32.6459						
44	H	Isotropic=	29.1798	Anisotropy	=	7.6371			
XX=	26.4717	YX=	0.8394	ZX=	1.1678				
XY=	2.7424	YY=	32.4457	ZY=	3.462				
XZ=	0.9933	YZ=	1.6195	ZZ=	28.6221				
Eigenvalues:	25.8965	27.3718	34.2712						
45	H	Isotropic=	28.8678	Anisotropy	=	8.259			
XX=	30.1438	YX=	1.1222	ZX=	-3.36				
XY=	2.5653	YY=	27.832	ZY=	-2.0312				
XZ=	-4.2516	YZ=	-1.9519	ZZ=	28.6276				
Eigenvalues:	25.4137	26.8159	34.3738						
46	H	Isotropic=	30.7049	Anisotropy	=	18.1789			
XX=	37.3459	YX=	-5.5324	ZX=	6.7964				
XY=	-3.7487	YY=	24.7508	ZY=	-4.9417				
XZ=	5.3891	YZ=	-3.2056	ZZ=	30.0179				
Eigenvalues:	22.3856	26.9049	42.8242						
47	C	Isotropic=	10.2845	Anisotropy	=	92.5759			
XX=	-57.0833	YX=	-50.3728	ZX=	-4.4702				
XY=	-45.4754	YY=	54.1424	ZY=	3.4068				
XZ=	38.8907	YZ=	12.476	ZZ=	33.7944				
Eigenvalues:	-78.0767	36.9284	72.0017						
48	O	Isotropic=	-88.3282	Anisotropy	=	610.4001			
XX=	-174.1478	YX=	-171.7025	ZX=	-5.4906				
XY=	-181.151	YY=	254.4023	ZY=	-13.3528				
XZ=	39.1529	YZ=	-26.9859	ZZ=	-345.2391				
Eigenvalues:	-346.9	-236.6898	318.6052						
49	H	Isotropic=	28.6288	Anisotropy	=	6.4196			
XX=	28.0474	YX=	-2.4739	ZX=	-0.1677				
XY=	-2.1391	YY=	24.9891	ZY=	0.188				
XZ=	1.1961	YZ=	0.6401	ZZ=	32.8499				
Eigenvalues:	23.7105	29.2675	32.9086						
50	H	Isotropic=	29.4483	Anisotropy	=	6.628			
XX=	27.7635	YX=	0.903	ZX=	-1.3399				
XY=	0.8357	YY=	32.5001	ZY=	2.2673				
XZ=	-1.3803	YZ=	3.3412	ZZ=	28.0812				
Eigenvalues:	25.5547	28.9231	33.8669						
51	C	Isotropic=	110.7433	Anisotropy	=	24.8596			
XX=	113.8031	YX=	-5.1799	ZX=	5.3646				
XY=	-6.6544	YY=	91.8786	ZY=	-5.3275				

XZ= -5.4016 YZ= -4.7354 ZZ= 126.5481
 Eigenvalues: 89.735 115.1785 127.3163
 52 C Isotropic= 123.306 Anisotropy = 20.0497
 XX= 125.4655 YX= 13.55 ZX= 7.5008
 XY= 7.5499 YY= 126.2783 ZY= -5.478
 XZ= 9.0857 YZ= -5.3527 ZZ= 118.1743
 Eigenvalues: 106.8593 126.3863 136.6725
 53 O Isotropic= 284.9082 Anisotropy = 66.3805
 XX= 284.9159 YX= 17.9763 ZX= -19.3852
 XY= 19.746 YY= 316.1253 ZY= -27.4965
 XZ= -6.4342 YZ= 0.6451 ZZ= 253.6834
 Eigenvalues: 248.3379 277.2248 329.1619
 54 H Isotropic= 26.4056 Anisotropy = 4.4
 XX= 26.9066 YX= 0.4098 ZX= 0.0288
 XY= -1.0823 YY= 27.5952 ZY= -2.6383
 XZ= -1.0863 YZ= -3.0406 ZZ= 24.7151
 Eigenvalues: 22.874 27.0039 29.339
 55 N Isotropic= 121.9757 Anisotropy = 96.4491
 XX= 132.2563 YX= 70.1127 ZX= 29.8466
 XY= 40.3143 YY= 129.802 ZY= -26.8928
 XZ= 54.1266 YZ= -61.7036 ZZ= 103.8688
 Eigenvalues: 27.2135 152.4385 186.2751
 56 C Isotropic= 50.5841 Anisotropy = 186.7033
 XX= 34.1536 YX= -91.9822 ZX= -31.6138
 XY= -84.1059 YY= 111.1278 ZY= 11.1926
 XZ= -38.5156 YZ= 20.461 ZZ= 6.4709
 Eigenvalues: -35.1693 11.8686 175.0529
 57 H Isotropic= 26.0392 Anisotropy = 6.5874
 XX= 25.3127 YX= 2.374 ZX= -0.693
 XY= 1.9906 YY= 24.8339 ZY= -2.7293
 XZ= -0.9309 YZ= -3.1745 ZZ= 27.9711
 Eigenvalues: 22.2538 25.433 30.4309
 58 H Isotropic= 26.8101 Anisotropy = 18.1151
 XX= 24.116 YX= 7.3768 ZX= -1.9848
 XY= 6.7242 YY= 33.409 ZY= -5.1042
 XZ= -2.9043 YZ= -4.0349 ZZ= 22.9052
 Eigenvalues: 20.3184 21.225 38.8868
 59 C Isotropic= 16.133 Anisotropy = 121.3456
 XX= 66.4344 YX= -28.9192 ZX= 35.4342
 XY= -20.0412 YY= -59.9941 ZY= 1.1128
 XZ= 43.0526 YZ= 10.6607 ZZ= 41.9588
 Eigenvalues: -66.2917 17.6607 97.0301
 60 H Isotropic= 26.2275 Anisotropy = 8.8873
 XX= 23.9879 YX= -1.1688 ZX= -4.6311
 XY= -0.1966 YY= 32.0944 ZY= 2.038
 XZ= -4.5146 YZ= -2.962 ZZ= 22.6002
 Eigenvalues: 18.6218 27.9082 32.1524
 61 C Isotropic= 58.6991 Anisotropy = 180.7536
 XX= 60.7979 YX= -90.7778 ZX= 1.4919
 XY= -87.7252 YY= 93.8127 ZY= 59.0776
 XZ= 7.4682 YZ= 54.5118 ZZ= 21.4867
 Eigenvalues: -41.9499 38.8456 179.2015
 62 C Isotropic= 62.1228 Anisotropy = 175.1113
 XX= 89.4097 YX= -55.5063 ZX= -32.1675
 XY= -55.3588 YY= 124.8728 ZY= 40.5106
 XZ= -34.5496 YZ= 41.7086 ZZ= -27.9142

Eigenvalues: -41.509549.0142 178.8637
 63 C Isotropic= 64.2495 Anisotropy = 174.6759
 XX= 40.3923 YX= -87.3201 ZX= -47.6669
 XY= -91.6147 YY= 110.3644 ZY= 9.0417
 XZ= -49.3962 YZ= 9.5628 ZZ= 41.9918
 Eigenvalues: -37.234149.2825 180.7
 64 C Isotropic= 63.1585 Anisotropy = 171.3141
 XX= 61.9354 YX= -87.3435 ZX= 7.4325
 XY= -88.5678 YY= 93.9656 ZY= 54.7006
 XZ= 9.8257 YZ= 55.3046 ZZ= 33.5747
 Eigenvalues: -38.285750.3933 177.368
 65 C Isotropic= 64.1612 Anisotropy = 148.0398
 XX= 87.2244 YX= -46.1362 ZX= -28.919
 XY= -35.2913 YY= 124.2897 ZY= 36.6829
 XZ= -29.3598 YZ= 38.5463 ZZ= -19.0304
 Eigenvalues: -31.557961.1871 162.8544
 66 H Isotropic= 22.76 Anisotropy = 10.7381
 XX= 25.3585 YX= 2.1067 ZX= 5.3624
 XY= 1.09 YY= 19.0697 ZY= -0.2425
 XZ= 4.6705 YZ= 1.4775 ZZ= 23.8517
 Eigenvalues: 18.5123 19.8489 29.9187
 67 O Isotropic= -56.6802 Anisotropy = 572.9196
 XX= 30.7972 YX= -31.9 ZX= 301.5302
 XY= -36.4469 YY= -148.0406 ZY= -23.1391
 XZ= 356.0438 YZ= -43.9841 ZZ= -52.7971
 Eigenvalues: -342.4683 -152.8385 325.2662
 68 C Isotropic= 55.2981 Anisotropy = 169.7751
 XX= 26.2765 YX= 4.1368 ZX= -0.0948
 XY= 14.3609 YY= -12.4532 ZY= -47.4674
 XZ= -25.2506 YZ= -55.8741 ZZ= 152.0708
 Eigenvalues: -27.880725.2934 168.4815
 69 H Isotropic= 23.6564 Anisotropy = 5.6148
 XX= 25.1774 YX= 3.1689 ZX= 1.2925
 XY= 3.0599 YY= 22.3257 ZY= -0.2509
 XZ= 1.1354 YZ= -0.1062 ZZ= 23.4661
 Eigenvalues: 20.1245 23.4451 27.3996
 70 H Isotropic= 23.7523 Anisotropy = 3.2784
 XX= 23.7541 YX= 2.2863 ZX= 0.431
 XY= 1.9762 YY= 22.2533 ZY= -1.3841
 XZ= 0.2748 YZ= -1.3179 ZZ= 25.2494
 Eigenvalues: 20.3893 24.9296 25.9379
 71 H Isotropic= 23.847 Anisotropy = 4.4188
 XX= 24.4674 YX= 2.4635 ZX= 1.4922
 XY= 2.6147 YY= 22.2533 ZY= -0.2402
 XZ= 1.5144 YZ= -0.383 ZZ= 24.8203
 Eigenvalues: 20.3169 24.4312 26.7929
 72 H Isotropic= 24.1037 Anisotropy = 8.1852
 XX= 26.6336 YX= 4.1963 ZX= -0.6397
 XY= 4.0305 YY= 23.2804 ZY= -0.822
 XZ= -0.5821 YZ= -1.2087 ZZ= 22.397
 Eigenvalues: 20.3816 22.3689 29.5605
 73 C Isotropic= 61.7661 Anisotropy = 173.3326
 XX= -24.669 YX= 23.5606 ZX= 11.1636
 XY= 23.6661 YY= 43.4504 ZY= -35.8108
 XZ= 15.7847 YZ= -39.4147 ZZ= 166.5169
 Eigenvalues: -35.110643.0877 177.3212

74	C	Isotropic=	61.6523	Anisotropy	=	177.2527
XX=	-14.0276	YX=	-41.8766	ZX=	-7.5969	
XY=	-38.6335	YY=	29.4837	ZY=	-39.0009	
XZ=	-6.9145	YZ=	-39.5546	ZZ=	169.5008	
Eigenvalues:	-41.4751	46.6112	179.8208			
75	C	Isotropic=	61.5403	Anisotropy	=	178.7092
XX=	44.2469	YX=	6.834	ZX=	3.1657	
XY=	6.8617	YY=	-26.3211	ZY=	-54.3018	
XZ=	3.8589	YZ=	-53.2208	ZZ=	166.6951	
Eigenvalues:	-40.9474	44.8885	180.6798			
76	C	Isotropic=	62.9893	Anisotropy	=	175.4244
XX=	-23.473	YX=	33.0373	ZX=	9.6705	
XY=	29.1978	YY=	41.2972	ZY=	-36.0428	
XZ=	10.9891	YZ=	-33.6696	ZZ=	171.1437	
Eigenvalues:	-38.5421	47.5712	179.9389			
77	C	Isotropic=	67.7594	Anisotropy	=	161.5897
XX=	-2.1792	YX=	-32.5065	ZX=	-9.1415	
XY=	-39.5072	YY=	38.5008	ZY=	-35.5829	
XZ=	-10.485	YZ=	-32.7636	ZZ=	166.9567	
Eigenvalues:	-26.732	54.5244	175.4859			
78	H	Isotropic=	23.4545	Anisotropy	=	7.1484
XX=	23.656	YX=	0.6008	ZX=	0.1022	
XY=	0.3928	YY=	27.819	ZY=	1.6094	
XZ=	-0.1667	YZ=	1.9963	ZZ=	18.8885	
Eigenvalues:	18.5352	23.6083	28.2201			
79	H	Isotropic=	23.7256	Anisotropy	=	6.0255
XX=	24.5481	YX=	-1.7088	ZX=	-0.582	
XY=	-1.4559	YY=	26.5719	ZY=	1.4657	
XZ=	-0.4705	YZ=	1.4422	ZZ=	20.0568	
Eigenvalues:	19.7394	23.6949	27.7426			
80	H	Isotropic=	23.7145	Anisotropy	=	3.9249
XX=	26.3239	YX=	-0.1519	ZX=	-0.152	
XY=	-0.0543	YY=	24.4175	ZY=	0.9003	
XZ=	0.073	YZ=	1.1078	ZZ=	20.4022	
Eigenvalues:	20.1651	24.6474	26.3311			
81	H	Isotropic=	23.8929	Anisotropy	=	4.8449
XX=	24.5048	YX=	0.1494	ZX=	-0.0112	
XY=	0.248	YY=	26.7676	ZY=	1.4333	
XZ=	0.2858	YZ=	1.5674	ZZ=	20.4064	
Eigenvalues:	20.0684	24.4875	27.1229			
82	H	Isotropic=	24.0825	Anisotropy	=	8.7022
XX=	24.3218	YX=	-2.9906	ZX=	-0.6624	
XY=	-2.7122	YY=	28.2063	ZY=	1.2968	
XZ=	0.0856	YZ=	1.3681	ZZ=	19.7194	
Eigenvalues:	19.5096	22.854	29.884			

2aiii_neg45

C	3.311112	1.818486	-0.070032
C	4.102714	1.729001	1.272965
C	3.697596	0.574195	2.204328
C	4.78339	-0.505606	2.361917
C	5.194087	-1.213961	1.055507
C	4.109265	-1.687730	1.00604
C	3.256413	-0.59279	-0.471807
C	1.911332	-0.68507	-0.304437
C	1.088576	0.563634	-0.46334

C	1.789441	1.78229	0.142996
C	3.781532	0.701522	-1.053709
C	5.285104	0.787798	-1.261912
C	3.151761	0.944071	-2.438268
C	1.183813	-1.917818	0.072059
C	6.001553	0.034792	3.075771
O	3.548271	3.110457	-0.62614
O	3.998971	2.968372	1.957549
O	6.366428	-1.563409	0.899495
O	4.50178	-2.678586	-0.843706
O	-0.148125	0.34282	0.258815
H	3.078509	3.255687	1.915029
C	5.652995	-2.659575	-1.58496
O	6.416667	-1.701027	-1.546901
C	5.790297	-3.9153	-2.382155
H	5.205764	1.659893	1.04362
H	2.752681	0.089378	1.853322
H	3.444488	-2.328018	0.779682
H	0.826779	0.745649	-1.543782
H	1.337573	2.704107	-0.319387
H	1.565141	1.816809	1.241293
H	5.878189	0.410273	-0.397975
H	5.583473	0.189161	-2.158683
H	5.574529	1.850544	-1.454755
H	3.93808	1.150643	-3.204979
H	2.574047	0.051941	-2.777876
H	2.477354	1.834982	-2.413885
H	1.717229	-2.832971	-0.286397
H	1.066167	-1.972687	1.184036
H	0.158584	-1.914026	-0.378609
H	6.73441	-0.788437	3.260448
H	6.510115	0.816845	2.462301
H	5.703946	0.484343	4.053295
H	4.846797	-4.511369	-2.363524
H	6.045146	-3.646885	-3.435996
H	6.620603	-4.522534	-1.944892
H	4.477883	3.328925	-0.483685
C	-1.188726	1.193569	0.013159
O	-1.026398	2.125496	-0.772744
H	4.333094	-1.325637	2.995141
H	3.503176	1.006179	3.222684
C	-2.417101	0.847322	0.834934
C	-3.636962	0.641966	-0.130218
O	-2.223495	-0.304674	1.627601
H	-2.616343	1.731853	1.509468
N	-4.616475	-0.295634	0.349686
C	-4.236842	2.007674	-0.392898
H	-3.219398	0.224025	-1.100058
H	-1.347367	-0.238692	2.031482
C	-4.944938	-1.444087	-0.351303
H	-5.180489	-0.016746	1.115696
C	-5.008456	2.6569	0.57712
C	-5.575836	3.90042	0.30393
C	-5.374326	4.503963	-0.937579
C	-4.6006	3.862718	-1.904166
C	-4.034671	2.616521	-1.635622

H	-5.164519	2.197143	1.564374
O	-4.228878	-1.866697	-1.27961
C	-6.173786	-2.165650	0.089965
H	-6.182287	4.40586	1.069683
H	-5.822704	5.485184	-1.151855
H	-4.432616	4.33905	-2.881471
H	-3.411162	1.20807	-2.396021
C	-7.071446	-2.61015	-0.887173
C	-8.224696	-3.295301	-0.507619
C	-8.478179	-3.545052	0.841358
C	-7.576144	-3.112231	1.813537
C	-6.423634	-2.420402	1.4417
H	-6.852425	-2.424992	-1.950478
H	-8.931913	-3.642868	-1.275165
H	-9.387798	-4.087902	1.138563
H	-7.771065	-3.318512	2.876233
H	-5.70795	-2.096311	2.212546

2a	ii	_neg45	E(RB+HF-PW91)	=	-2012.300821	
SCF	GIAO	Magnetic	shielding	tensor (ppm):		
1	C	Isotropic=	109.3639	Anisotropy	=	28.0246
XX=	99.8252	YX=	11.8025	ZX=	-9.249	
XY=	4.4987	YY=	117.0662	ZY=	-8.2078	
XZ=	-9.3738	YZ=	-8.2156	ZZ=	111.2002	
Eigenvalues:	94.0543	105.9903	128.0469			
2	C	Isotropic=	112.2144	Anisotropy	=	30.5256
XX=	94.4575	YX=	-8.9487	ZX=	-3.7036	
XY=	-3.3619	YY=	124.9385	ZY=	14.715	
XZ=	1.5823	YZ=	5.081	ZZ=	117.2473	
Eigenvalues:	93.2273	110.8511	132.5648			
3	C	Isotropic=	142.1527	Anisotropy	=	20.658
XX=	120.836	YX=	1.289	ZX=	2.8907	
XY=	-2.6648	YY=	149.9021	ZY=	-1.5806	
XZ=	-3.8656	YZ=	-0.6198	ZZ=	155.72	
Eigenvalues:	120.8122	149.7212	155.9247			
4	C	Isotropic=	140.028	Anisotropy	=	25.1278
XX=	124.4756	YX=	-1.7842	ZX=	-2.4908	
XY=	11.4497	YY=	142.3692	ZY=	5.5429	
XZ=	5.0062	YZ=	7.9072	ZZ=	153.2392	
Eigenvalues:	123.2471	140.057	156.7798			
5	C	Isotropic=	-21.931	Anisotropy	=	178.6717
XX=	-55.6794	YX=	4.3464	ZX=	-35.9529	
XY=	8.7132	YY=	50.8947	ZY=	-78.7695	
XZ=	-18.2501	YZ=	-86.9307	ZZ=	-61.0084	
Eigenvalues:	-112.8708	-50.1057	97.1834			
6	C	Isotropic=	102.0164	Anisotropy	=	41.1153
XX=	86.2805	YX=	3.7968	ZX=	3.3453	
XY=	-9.5551	YY=	102.755	ZY=	16.6699	
XZ=	-5.8364	YZ=	19.3706	ZZ=	117.0138	
Eigenvalues:	85.5499	91.0728	129.4266			
7	C	Isotropic=	43.4045	Anisotropy	=	157.9153
XX=	36.7055	YX=	17.6268	ZX=	-4.2996	
XY=	38.8402	YY=	-21.3235	ZY=	80.8495	
XZ=	9.9902	YZ=	66.0651	ZZ=	114.8316	
Eigenvalues:	-59.8006	41.3329	148.6814			

8	C	Isotropic=	41.6659	Anisotropy	=	154.6931
XX=	40.215	YX=	15.6198	ZX=	9.5691	
XY=	2.5556	YY=	-44.8023	ZY=	41.012	
XZ=	13.3945	YZ=	59.6311	ZZ=	129.585	
Eigenvalues:			-58.6256		38.8288	144.7946
9	C	Isotropic=	110.4544	Anisotropy	=	48.815
XX=	128.516	YX=	7.8105	ZX=	-22.8763	
XY=	6.6936	YY=	104.2266	ZY=	7.4803	
XZ=	-27.5324	YZ=	9.2892	ZZ=	98.6206	
Eigenvalues:			79.4729		108.8925	142.9977
10	C	Isotropic=	148.0427	Anisotropy	=	41.4686
XX=	169.351	YX=	8.4489	ZX=	-8.3026	
XY=	17.3945	YY=	141.5599	ZY=	10.5519	
XZ=	-11.3787	YZ=	0.4839	ZZ=	133.2171	
Eigenvalues:			125.3332		143.1064	175.6884
11	C	Isotropic=	147.9573	Anisotropy	=	13.8226
XX=	142.1637	YX=	-2.692	ZX=	-0.3674	
XY=	6.9154	YY=	150.1952	ZY=	2.3736	
XZ=	10.4037	YZ=	6.5287	ZZ=	151.5131	
Eigenvalues:			139.9772		146.7224	157.1724
12	C	Isotropic=	155.5537	Anisotropy	=	24.9164
XX=	164.8923	YX=	-8.9456	ZX=	11.0918	
XY=	-6.5762	YY=	137.9693	ZY=	3.2401	
XZ=	2.5629	YZ=	-2.9049	ZZ=	163.7996	
Eigenvalues:			135.7531		158.7434	172.1647
13	C	Isotropic=	148.1698	Anisotropy	=	55.1843
XX=	143.4935	YX=	8.1982	ZX=	18.7634	
XY=	14.3641	YY=	125.3755	ZY=	-9.0093	
XZ=	20.3456	YZ=	-6.3229	ZZ=	175.6404	
Eigenvalues:			115.5853		143.9648	184.9593
14	C	Isotropic=	167.8606	Anisotropy	=	12.2319
XX=	164.2336	YX=	6.4845	ZX=	5.3968	
XY=	3.8367	YY=	173.5982	ZY=	0.1929	
XZ=	-5.6539	YZ=	-2.6159	ZZ=	165.7501	
Eigenvalues:			161.9105		165.6562	176.0153
15	C	Isotropic=	169.377	Anisotropy	=	17.0134
XX=	173.6216	YX=	-3.1044	ZX=	6.609	
XY=	1.3653	YY=	163.2714	ZY=	9.3716	
XZ=	6.0319	YZ=	8.5252	ZZ=	171.2379	
Eigenvalues:			156.3798		171.0319	180.7193
16	O	Isotropic=	263.4401	Anisotropy	=	85.9605
XX=	315.618	YX=	28.1252	ZX=	0.2752	
XY=	12.1065	YY=	220.2905	ZY=	-21.8613	
XZ=	0.8763	YZ=	-58.2621	ZZ=	254.4119	
Eigenvalues:			191.4298		278.1435	320.7471
17	O	Isotropic=	265.3273	Anisotropy	=	46.0998
XX=	252.8189	YX=	-20.5018	ZX=	-9.4759	
XY=	-9.6321	YY=	279.2861	ZY=	-16.0718	
XZ=	12.4666	YZ=	-21.3727	ZZ=	263.8768	
Eigenvalues:			243.0267		256.8947	296.0605
18	O	Isotropic=	-372.455	Anisotropy	=	1098.4022
XX=	-974.7061	YX=	283.722	ZX=	-6.7879	
XY=	206.4865	YY=	103.0499	ZY=	-349.6772	
XZ=	10.057	YZ=	-367.07	ZZ=	-245.7087	
Eigenvalues:			-1036.5586		-440.6194	359.8132
19	O	Isotropic=	95.0833	Anisotropy	=	127.6604

XX=	157.2978	YX=	-114.6071	ZX=	-57.1875		
XY=	-11.7394	YY=	3.4008	ZY=	-105.0102		
XZ=	18.3197	YZ=	-21.8677	ZZ=	124.5512		
Eigenvalues:	-45.1071	150.1668		180.1902			
20	O	Isotropic=	78.6207	Anisotropy	=	177.2258	
XX=	72.982	YX=	2.9483	ZX=	56.4515		
XY=	-106.2073	YY=	104.5526	ZY=	127.9508		
XZ=	123.3428	YZ=	90.8604	ZZ=	58.3275		
Eigenvalues:	-93.614	132.7049		196.7713			
21	H	Isotropic=	31.1612	Anisotropy	=	13.4827	
XX=	35.9876	YX=	-6.1649	ZX=	0.9436		
XY=	-5.5508	YY=	30.7731	ZY=	4.9735		
XZ=	1.2468	YZ=	5.8236	ZZ=	26.7231		
Eigenvalues:	21.604	31.73		40.1497			
22	C	Isotropic=	21.396	Anisotropy	=	78.8584	
XX=	4.3405	YX=	53.0707	ZX=	74.1469		
XY=	22.0921	YY=	53.5049	ZY=	-23.8436		
XZ=	53.2105	YZ=	-47.4891	ZZ=	6.3426		
Eigenvalues:	-78.6518	68.8715		73.9682			
23	O	Isotropic=	-140.8478	Anisotropy	=	606.5144	
XX=	-257.3379	YX=	-203.7919	ZX=	227.8779		
XY=	-155.628	YY=	-195.6168	ZY=	-152.2123		
XZ=	236.3849	YZ=	-141.3566	ZZ=	30.4114		
Eigenvalues:	-432.7749		-253.2636		263.4952		
24	C	Isotropic=	165.6191	Anisotropy	=	38.0036	
XX=	155.781	YX=	-0.4452	ZX=	-6.543		
XY=	1.7303	YY=	177.4218	ZY=	20.2204		
XZ=	-6.7171	YZ=	17.5578	ZZ=	163.6543		
Eigenvalues:	146.6487		159.2537		190.9548		
25	H	Isotropic=	27.4796	Anisotropy	=	3.0232	
XX=	28.0239	YX=	-1.3552	ZX=	0.538		
XY=	-2.2605	YY=	26.9227	ZY=	1.5068		
XZ=	0.0409	YZ=	0.8574	ZZ=	27.4923		
Eigenvalues:	25.0555	27.8882		29.4951			
26	H	Isotropic=	28.2543	Anisotropy	=	8.163	
XX=	29.1661	YX=	1.424	ZX=	4.2623		
XY=	1.7586	YY=	25.8453	ZY=	0.4236		
XZ=	3.6218	YZ=	0.6809	ZZ=	29.7517		
Eigenvalues:	24.7563	26.3103		33.6964			
27	H	Isotropic=	25.3207	Anisotropy	=	4.1849	
XX=	26.0301	YX=	-2.5621	ZX=	-1.6152		
XY=	0.5538	YY=	25.3408	ZY=	2.1257		
XZ=	-2.1765	YZ=	0.0914	ZZ=	24.5911		
Eigenvalues:	23.2104	24.6409		28.1106			
28	H	Isotropic=	25.0037	Anisotropy	=	6.6258	
XX=	29.1033	YX=	0.5065	ZX=	-1.5926		
XY=	0.2426	YY=	20.0434	ZY=	0.3711		
XZ=	-0.4227	YZ=	-1.5763	ZZ=	25.8643		
Eigenvalues:	19.9736	25.6166		29.4209			
29	H	Isotropic=	27.6612	Anisotropy	=	8.49	
XX=	32.5792	YX=	-1.6823	ZX=	1.3696		
XY=	-0.4524	YY=	28.8529	ZY=	-2.6748		
XZ=	2.4529	YZ=	-0.7886	ZZ=	21.5514		
Eigenvalues:	20.9283	28.734		33.3212			
30	H	Isotropic=	29.8318	Anisotropy	=	5.7651	
XX=	33.4658	YX=	0.7495	ZX=	0.0144		

XY=	1.1075	YY=	25.4638	ZY=	1.6765				
XZ=	0.6154	YZ=	2.1014	ZZ=	30.5658				
Eigenvalues:	24.7696	31.0506	33.6752						
31	H	Isotropic=	29.4514	Anisotropy	=	8.3401			
XX=	31.0294	YX=	-2.5369	ZX=	2.0462				
XY=	-2.6103	YY=	27.5576	ZY=	-2.5971				
XZ=	2.5515	YZ=	-3.9567	ZZ=	29.7671				
Eigenvalues:	25.075	28.2677	35.0115						
32	H	Isotropic=	29.2199	Anisotropy	=	9.1206			
XX=	28.9068	YX=	-4.1697	ZX=	-3.6657				
XY=	-3.5565	YY=	29.6608	ZY=	1.8377				
XZ=	-3.4112	YZ=	1.3822	ZZ=	29.0921				
Eigenvalues:	24.6106	27.7488	35.3003						
33	H	Isotropic=	30.3573	Anisotropy	=	6.7694			
XX=	32.3237	YX=	1.5421	ZX=	-3.0163				
XY=	1.7998	YY=	31.347	ZY=	-0.9154				
XZ=	-2.8761	YZ=	-1.4964	ZZ=	27.4013				
Eigenvalues:	25.9928	30.2089	34.8703						
34	H	Isotropic=	30.1095	Anisotropy	=	9.319			
XX=	29.5569	YX=	-0.0557	ZX=	-0.9471				
XY=	0.7663	YY=	25.4545	ZY=	-2.7149				
XZ=	-2.3199	YZ=	-2.2617	ZZ=	35.317				
Eigenvalues:	24.862	29.1443	36.3221						
35	H	Isotropic=	30.1766	Anisotropy	=	6.2371			
XX=	29.5259	YX=	2.614	ZX=	0.6016				
XY=	1.0523	YY=	27.9689	ZY=	1.4538				
XZ=	2.3085	YZ=	1.8507	ZZ=	33.0349				
Eigenvalues:	26.6926	29.5025	34.3346						
36	H	Isotropic=	28.4378	Anisotropy	=	6.4309			
XX=	28.6058	YX=	-2.3576	ZX=	0.2269				
XY=	-2.354	YY=	26.3017	ZY=	-1.4467				
XZ=	2.1642	YZ=	-3.5138	ZZ=	30.4058				
Eigenvalues:	24.4027	28.1856	32.725						
37	H	Isotropic=	28.9211	Anisotropy	=	7.7688			
XX=	30.1089	YX=	0.028	ZX=	-1.8675				
XY=	-1.7672	YY=	32.7947	ZY=	2.4797				
XZ=	-1.496	YZ=	3.311	ZZ=	23.8596				
Eigenvalues:	22.7444	29.9185	34.1003						
38	H	Isotropic=	29.1988	Anisotropy	=	6.8503			
XX=	28.6208	YX=	0.565	ZX=	-1.8447				
XY=	0.4955	YY=	27.5442	ZY=	-2.6039				
XZ=	-2.4634	YZ=	-2.896	ZZ=	31.4316				
Eigenvalues:	25.9827	27.8481	33.7657						
39	H	Isotropic=	28.387	Anisotropy	=	8.1586			
XX=	33.4707	YX=	-0.3741	ZX=	1.7273				
XY=	0.7176	YY=	28.8481	ZY=	0.7331				
XZ=	2.0859	YZ=	1.2698	ZZ=	22.8422				
Eigenvalues:	22.3689	28.966	33.8261						
40	H	Isotropic=	29.1681	Anisotropy	=	10.839			
XX=	31.8161	YX=	-5.1543	ZX=	2.7544				
XY=	-4.3555	YY=	27.9676	ZY=	-1.2363				
XZ=	4.4302	YZ=	-0.3392	ZZ=	27.7207				
Eigenvalues:	24.0561	27.0542	36.3941						
41	H	Isotropic=	29.6434	Anisotropy	=	5.8164			
XX=	31.7844	YX=	2.5187	ZX=	0.9528				
XY=	2.9649	YY=	29.1584	ZY=	-2.0645				

XZ=	1.4287	YZ=	-2.4926	ZZ=	27.9873				
Eigenvalues:	25.1294	30.2796	33.521						
42	H	Isotropic=	30.5168	Anisotropy	=	9.6478			
XX=	28.8531	YX=	-0.4399	ZX=	1.6366				
XY=	-0.6165	YY=	26.9444	ZY=	2.8074				
XZ=	1.7815	YZ=	3.1857	ZZ=	35.753				
Eigenvalues:	25.6802	28.9216	36.9487						
43	H	Isotropic=	29.0422	Anisotropy	=	5.5363			
XX=	30.3361	YX=	1.1187	ZX=	-1.816				
XY=	2.9382	YY=	30.4196	ZY=	2.4437				
XZ=	-0.7882	YZ=	3.4345	ZZ=	26.3709				
Eigenvalues:	24.1008	30.2928	32.733						
44	H	Isotropic=	29.1769	Anisotropy	=	7.6924			
XX=	26.5056	YX=	0.434	ZX=	-1.6633				
XY=	-0.8879	YY=	27.6253	ZY=	1.9682				
XZ=	-3.0337	YZ=	0.1957	ZZ=	33.3997				
Eigenvalues:	25.7755	27.45	34.3052						
45	H	Isotropic=	28.8973	Anisotropy	=	8.2361			
XX=	29.8866	YX=	-3.3482	ZX=	1.1984				
XY=	-4.9306	YY=	30.4964	ZY=	-0.0498				
XZ=	0.5937	YZ=	0.0574	ZZ=	26.3089				
Eigenvalues:	25.4854	26.8185	34.3881						
46	H	Isotropic=	30.8009	Anisotropy	=	18.1979			
XX=	38.2968	YX=	8.2833	ZX=	0.2614				
XY=	6.2165	YY=	31.5337	ZY=	-2.2772				
XZ=	-0.0121	YZ=	-0.3564	ZZ=	22.5723				
Eigenvalues:	22.257	27.2129	42.9329						
47	C	Isotropic=	11.1512	Anisotropy	=	92.011			
XX=	-56.823	YX=	30.5273	ZX=	34.8902				
XY=	67.2679	YY=	27.8342	ZY=	2.5041				
XZ=	5.6889	YZ=	8.96	ZZ=	62.4424				
Eigenvalues:	-80.9869	41.9487	72.4918						
48	O	Isotropic=	-100.4972	Anisotropy	=	609.9723			
XX=	-182.462	YX=	81.4585	ZX=	141.9639				
XY=	108.1301	YY=	-161.9937	ZY=	320.5226				
XZ=	130.0961	YZ=	263.3647	ZZ=	42.9642				
Eigenvalues:	-368.9346	-238.7079	306.1511						
49	H	Isotropic=	28.7083	Anisotropy	=	6.5553			
XX=	28.0086	YX=	1.5538	ZX=	1.8857				
XY=	2.4026	YY=	29.659	ZY=	-4.087				
XZ=	0.851	YZ=	-3.6913	ZZ=	28.4571				
Eigenvalues:	23.8185	29.2278	33.0785						
50	H	Isotropic=	29.4879	Anisotropy	=	6.5465			
XX=	27.8367	YX=	-1.8156	ZX=	-0.1526				
XY=	-1.6434	YY=	27.0344	ZY=	0.6634				
XZ=	-0.2365	YZ=	1.7553	ZZ=	33.5927				
Eigenvalues:	25.5726	29.0389	33.8523						
51	C	Isotropic=	110.2547	Anisotropy	=	35.1689			
XX=	102.6217	YX=	-16.3126	ZX=	17.2586				
XY=	-5.1993	YY=	118.0888	ZY=	-9.625				
XZ=	4.8334	YZ=	-13.3542	ZZ=	110.0537				
Eigenvalues:	94.3761	102.6875	133.7007						
52	C	Isotropic=	129.0503	Anisotropy	=	31.39			
XX=	130.6437	YX=	-2.0448	ZX=	6.3185				
XY=	3.5497	YY=	131.7816	ZY=	-20.0278				
XZ=	5.8135	YZ=	-21.6339	ZZ=	124.7257				

Eigenvalues:	106.0493	131.1247	149.977		
53	O	Isotropic=	288.1793	Anisotropy	= 92.4415
XX=	340.3372	YX=	-9.1645	ZX=	33.4212
XY=	-0.2251	YY=	253.1858	ZY=	-0.425
XZ=	20.8432	YZ=	7.3847	ZZ=	271.0149
Eigenvalues:	250.9129	263.8179	349.807		
54	H	Isotropic=	26.4806	Anisotropy	= 5.5332
XX=	25.9808	YX=	-4.0329	ZX=	1.6676
XY=	-2.4145	YY=	27.6831	ZY=	1.4067
XZ=	0.2639	YZ=	-0.2148	ZZ=	25.7779
Eigenvalues:	23.0333	26.2392	30.1694		
55	N	Isotropic=	129.0928	Anisotropy	= 94.5171
XX=	105.368	YX=	0.1341	ZX=	55.8639
XY=	21.7746	YY=	185.9712	ZY=	-10.1215
XZ=	71.8748	YZ=	24.5411	ZZ=	95.9391
Eigenvalues:	36.5785	158.5956	192.1042		
56	C	Isotropic=	49.7011	Anisotropy	= 190.4584
XX=	118.5323	YX=	79.5914	ZX=	40.7038
XY=	74.4068	YY=	6.1567	ZY=	31.9598
XZ=	46.783	YZ=	33.0691	ZZ=	24.4143
Eigenvalues:	-34.8729	7.3029	176.6734		
57	H	Isotropic=	25.1928	Anisotropy	= 2.3298
XX=	24.8883	YX=	1.1996	ZX=	-1.3512
XY=	1.7458	YY=	24.4238	ZY=	0.4917
XZ=	-0.5303	YZ=	0.8776	ZZ=	26.2664
Eigenvalues:	22.794	26.0385	26.746		
58	H	Isotropic=	29.9771	Anisotropy	= 19.2123
XX=	40.096	YX=	-0.3955	ZX=	6.05
XY=	-0.6007	YY=	21.9395	ZY=	-3.0586
XZ=	6.0794	YZ=	-4.729	ZZ=	27.8959
Eigenvalues:	19.7238	27.4223	42.7853		
59	C	Isotropic=	17.7779	Anisotropy	= 118.3449
XX=	8.6814	YX=	-53.8119	ZX=	23.392
XY=	-68.102	YY=	-21.0375	ZY=	-34.3561
XZ=	10.396	YZ=	-33.7581	ZZ=	65.69
Eigenvalues:	-71.0162	227.6756	96.6745		
60	H	Isotropic=	26.0998	Anisotropy	= 8.2082
XX=	24.8616	YX=	1.9786	ZX=	-4.9695
XY=	4.8527	YY=	29.5679	ZY=	0.8994
XZ=	-3.562	YZ=	1.1414	ZZ=	23.8699
Eigenvalues:	19.1551	27.5724	31.5719		
61	C	Isotropic=	67.2576	Anisotropy	= 165.8039
XX=	138.0956	YX=	36.7213	ZX=	45.5467
XY=	42.335	YY=	63.4807	ZY=	49.344
XZ=	46.3895	YZ=	52.2125	ZZ=	0.1965
Eigenvalues:	-31.0809	55.0602	177.7935		
62	C	Isotropic=	63.1852	Anisotropy	= 176.8851
XX=	111.9674	YX=	70.0525	ZX=	70.3514
XY=	71.0584	YY=	59.3156	ZY=	-6.6513
XZ=	74.2498	YZ=	-9.0948	ZZ=	18.2727
Eigenvalues:	-40.9859	49.433	181.1086		
63	C	Isotropic=	64.5904	Anisotropy	= 174.1269
XX=	123.7129	YX=	78.3272	ZX=	31.7582
XY=	79.0659	YY=	7.4964	ZY=	38.4004
XZ=	31.3456	YZ=	35.495	ZZ=	62.5619
Eigenvalues:	-36.1922	49.2884	180.675		

64	C	Isotropic=	62.1589	Anisotropy	=	175.6622
XX=	133.7647	YX=	41.4723	ZX=	52.1416	
XY=	43.5487	YY=	57.6382	ZY=	54.3643	
XZ=	49.7622	YZ=	54.5343	ZZ=	-4.9262	
Eigenvalues:	-40.0569	47.2666	179.2671			
65	C	Isotropic=	55.5629	Anisotropy	=	158.1969
XX=	98.4597	YX=	62.6115	ZX=	65.153	
XY=	62.4089	YY=	53.0452	ZY=	-11.2327	
XZ=	69.0397	YZ=	-6.8322	ZZ=	15.1839	
Eigenvalues:	-40.6137	46.275	161.0275			
66	H	Isotropic=	24.0715	Anisotropy	=	9.1537
XX=	23.2746	YX=	-3.6232	ZX=	-2.1934	
XY=	-3.5241	YY=	27.29	ZY=	2.3188	
XZ=	-1.8434	YZ=	1.3157	ZZ=	21.65	
Eigenvalues:	20.2166	21.824	30.174			
67	O	Isotropic=	-89.2499	Anisotropy	=	656.7691
XX=	-92.6301	YX=	-95.0372	ZX=	297.3093	
XY=	-77.3561	YY=	-110.9272	ZY=	-319.8053	
XZ=	244.7648	YZ=	-234.6941	ZZ=	-64.1924	
Eigenvalues:	-428.7178	-187.6281	348.5962			
68	C	Isotropic=	54.1137	Anisotropy	=	172.5714
XX=	16.0365	YX=	-84.2939	ZX=	-4.9382	
XY=	-70.3394	YY=	124.0007	ZY=	42.1806	
XZ=	7.3086	YZ=	18.9811	ZZ=	22.3041	
Eigenvalues:	-29.1091	22.289	169.1614			
69	H	Isotropic=	23.8054	Anisotropy	=	5.0445
XX=	22.0508	YX=	-2.5586	ZX=	-1.0065	
XY=	-2.1036	YY=	25.691	ZY=	-1.541	
XZ=	-0.8174	YZ=	-1.643	ZZ=	23.6745	
Eigenvalues:	20.2151	24.0328	27.1684			
70	H	Isotropic=	23.8254	Anisotropy	=	3.1562
XX=	22.3507	YX=	-2.0251	ZX=	-1.6315	
XY=	-1.572	YY=	23.9594	ZY=	-0.8122	
XZ=	-1.6741	YZ=	-0.8206	ZZ=	25.166	
Eigenvalues:	20.4695	25.0771	25.9295			
71	H	Isotropic=	23.7832	Anisotropy	=	4.7234
XX=	22.6237	YX=	-2.9284	ZX=	-0.8891	
XY=	-2.5577	YY=	25.1802	ZY=	-0.753	
XZ=	-0.9498	YZ=	-0.683	ZZ=	23.5457	
Eigenvalues:	20.441	23.9764	26.9321			
72	H	Isotropic=	23.6196	Anisotropy	=	7.9228
XX=	22.2749	YX=	-2.2504	ZX=	1.0257	
XY=	-0.9057	YY=	24.3127	ZY=	-3.99	
XZ=	1.2703	YZ=	-4.1049	ZZ=	24.2711	
Eigenvalues:	20.1895	21.7678	28.9015			
73	C	Isotropic=	61.4537	Anisotropy	=	175.5964
XX=	73.6259	YX=	-60.2461	ZX=	8.4642	
XY=	-57.6256	YY=	144.5722	ZY=	16.066	
XZ=	6.509	YZ=	18.8894	ZZ=	-33.8369	
Eigenvalues:	-37.3958	843.239	178.518			
74	C	Isotropic=	62.0615	Anisotropy	=	176.617
XX=	44.5992	YX=	-73.5526	ZX=	-42.439	
XY=	-73.2726	YY=	139.034	ZY=	-10.7934	
XZ=	-44.5945	YZ=	-12.062	ZZ=	2.5514	
Eigenvalues:	-40.4162	46.7946	179.8062			
75	C	Isotropic=	62.4439	Anisotropy	=	177.5456

XX=	20.5038	YX=	-92.3874	ZX=	15.3507				
XY=	-93.2557	YY=	126.2173	ZY=	19.0987				
XZ=	15.1404	YZ=	20.1924	ZZ=	40.6106				
Eigenvalues:	-40.0748	46.5988	180.8076						
76	C	Isotropic=	63.5723	Anisotropy	=	174.5935			
XX=	80.0822	YX=	-57.7893	ZX=	9.5355				
XY=	-60.8156	YY=	143.3801	ZY=	21.2047				
XZ=	11.2063	YZ=	25.2861	ZZ=	-32.7455				
Eigenvalues:	-38.9337	49.6826	179.9679						
77	C	Isotropic=	67.3823	Anisotropy	=	163.5623			
XX=	52.1461	YX=	-66.3146	ZX=	-46.2581				
XY=	-69.0518	YY=	137.7803	ZY=	-7.9729				
XZ=	-38.9299	YZ=	-5.7608	ZZ=	12.2206				
Eigenvalues:	-27.6388	53.3619	176.4239						
78	H	Isotropic=	23.4615	Anisotropy	=	8.0818			
XX=	25.9992	YX=	4.4327	ZX=	1.126				
XY=	3.3779	YY=	21.9196	ZY=	1.1131				
XZ=	1.4799	YZ=	1.3624	ZZ=	22.4658				
Eigenvalues:	19.4974	22.0378	28.8494						
79	H	Isotropic=	23.8002	Anisotropy	=	4.4466			
XX=	24.4662	YX=	2.7641	ZX=	-0.7392				
XY=	2.6781	YY=	22.1007	ZY=	-0.6569				
XZ=	-0.8622	YZ=	-0.5343	ZZ=	24.8338				
Eigenvalues:	20.3156	24.3205	26.7646						
80	H	Isotropic=	23.7492	Anisotropy	=	3.6613			
XX=	23.728	YX=	2.0981	ZX=	0.6915				
XY=	1.8522	YY=	21.6198	ZY=	-0.1461				
XZ=	0.6846	YZ=	0.1237	ZZ=	25.8999				
Eigenvalues:	20.4106	24.647	26.1901						
81	H	Isotropic=	23.8465	Anisotropy	=	5.098			
XX=	25.3391	YX=	3.189	ZX=	0.0752				
XY=	2.9718	YY=	22.2577	ZY=	-0.5992				
XZ=	0.1546	YZ=	-0.1199	ZZ=	23.9428				
Eigenvalues:	20.3172	23.9773	27.2452						
82	H	Isotropic=	23.6821	Anisotropy	=	8.5369			
XX=	24.1907	YX=	3.6848	ZX=	-2.445				
XY=	3.5924	YY=	22.5802	ZY=	-2.9892				
XZ=	-2.3901	YZ=	-1.8206	ZZ=	24.2754				
Eigenvalues:	19.6169	22.056	29.3733						

2aiv_neg45

C	-2.772688	0.929612	-1.757447
C	-3.84426	-0.090273	-2.257299
C	-3.75869	-1.496146	-1.639776
C	-4.945161	-1.844024	-0.722706
C	-5.121374	-0.917156	0.496725
C	-3.900654	-0.548021	3.2541
C	-2.848174	0.222326	0.581937
C	-1.586263	-0.280901	0.567386
C	-0.639341	0.204678	-0.495369
C	-1.344566	0.368234	-1.844467
C	-3.115139	1.412932	-0.312932
C	-4.522763	1.986365	-0.275176
C	-2.179526	2.574561	0.070948
C	-1.077566	-1.320769	1.48988
C	-6.236694	-1.942875	-1.502299

O	-2.764895	2.030595	-2.664076
O	-3.782101	-0.172525	-3.672989
O	-6.257047	-0.655020.899598	
O	-4.164231	-0.064243	2.638523
O	0.388907	-0.804261	-0.633593
H	-2.853394	-0.242007	-3.926773
C	-5.119563	0.860125	2.968322
O	-5.777723	1.428323	2.10402
C	-5.199688	1.033955	4.449696
H	-4.871940.339984	-2.075797	
H	-2.807196	-1.624516	-1.065982
H	-3.461929	-1.573569	1.587765
H	-0.138451.165358	-0.18699	
H	-0.721441.061437	-2.47626	
H	-1.364399	-0.626215	-2.36246
H	-5.322053	1.211284	-0.306193
H	-4.670707	2.581286	0.660587
H	-4.665501	2.679317	-1.141192
H	-2.758053	3.516032	0.237693
H	-1.623928	2.347771	1.011533
H	-1.450165	2.780783	-0.750488
H	-1.589025	-1.270954	2.483128
H	-1.231511	-2.337898	1.047856
H	0.021352	-1.186719	1.656198
H	-7.063198	-2.286529	-0.833209
H	-6.525826	-0.950473	-1.924358
H	-6.121603	-2.669068	-2.342333
H	-4.341879	0.537032	4.962387
H	-5.198042	2.1258 4.685122	
H	-6.157118	0.581058	4.807091
H	-3.677586	2.208284	-2.924492
C	1.532724	-0.46267-1.306102	
O	1.617212	0.66147 -1.794497	
H	-4.720394	-2.856364	-0.274546
H	-3.754598	-2.240963	-2.480491
C	2.510264	-1.622353	-1.366462
C	3.936095	-1.296281	-0.80191
O	2.012699	-2.741087	-0.661306
H	2.619839	-1.877556	-2.461495
N	4.057102	0.058963	-0.324589
C	4.372028	-2.313558	0.226913
H	4.625246	-1.392585	-1.703434
H	1.119925	-2.9182 -0.987869	
C	4.98498 0.939797	-0.871789	
H	3.728949	0.239276	0.595691
C	3.838921	-2.316141	1.520003
C	4.293581	-3.236318	2.463805
C	5.281227	-4.159614	2.121788
C	5.811623	-4.163398	0.831892
C	5.362516	-3.241994	-0.113123
H	3.035395	-1.613575	1.786216
O	5.54658 0.696581	-1.956238	
C	5.221886	2.205177	-0.120459
H	3.868838	-3.234897	3.478219
H	5.639532	-4.884714	2.866965
H	6.588099	-4.892704	0.557964

H	5.790872	-3.246605	-1.127033
C	6.539621	2.635207	0.069951
C	6.786932	3.822451	0.757532
C	5.723787	4.584068	1.243547
C	4.410062	4.161425	1.039252
C	4.154797	2.97131	0.358408
H	7.371036	2.038009	-0.335795
H	7.822514	4.160422	0.910271
H	5.921441	5.52231	1.783092
H	3.571899	4.769268	1.410627
H	3.116468	2.651603	0.178887

2aiv_neg45	E(RB+HF-PW91)	=	-2012.29318
SCF GIAO	Magnetic shielding tensor (ppm):		
1 C	Isotropic=	109.1214	Anisotropy = 28.5312
XX=	95.0286	YX= -7.8075	ZX= 4.7464
XY=	-6.1019	YY= 123.1251	ZY= -8.8595
XZ=	-2.5987	YZ= -7.0851	ZZ= 109.2106
Eigenvalues:	93.3583	105.8637	128.1422
2 C	Isotropic=	112.3591	Anisotropy = 30.8717
XX=	96.1775	YX= 4.1691	ZX= -9.1793
XY=	6.7531	YY= 109.0957	ZY= 0.2841
XZ=	0.1794	YZ= 8.3971	ZZ= 131.8039
Eigenvalues:	93.3207	110.8163	132.9402
3 C	Isotropic=	141.8702	Anisotropy = 20.5067
XX=	122.8692	YX= 10.2406	ZX= 3.2007
XY=	6.4979	YY= 152.5263	ZY= 2.2627
XZ=	-3.0735	YZ= 2.0127	ZZ= 150.215
Eigenvalues:	120.6625	149.4067	155.5413
4 C	Isotropic=	140.0614	Anisotropy = 25.0743
XX=	125.2139	YX= 3.523	ZX= 0.1511
XY=	5.1783	YY= 145.0379	ZY= 9.5797
XZ=	13.9333	YZ= 3.8091	ZZ= 149.9323
Eigenvalues:	123.0381	140.3685	156.7776
5 C	Isotropic=	-21.8054	Anisotropy = 178.9904
XX=	-64.5863	YX= -13.9072	ZX= -35.056
XY=	0.1103	YY= 35.4125	ZY= -93.2105
XZ=	-21.5457	YZ= -87.6725	ZZ= -36.2426
Eigenvalues:	-113.1747	-49.7631	97.5215
6 C	Isotropic=	102.0435	Anisotropy = 41.2352
XX=	87.3634	YX= 4.6661	ZX= 9.5475
XY=	2.8106	YY= 98.8379	ZY= 16.3342
XZ=	-6.5004	YZ= 17.4522	ZZ= 119.9292
Eigenvalues:	85.5172	91.0796	129.5336
7 C	Isotropic=	42.7754	Anisotropy = 159.3381
XX=	32.306	YX= -10.5021	ZX= 36.1306
XY=	-7.295	YY= 33.5458	ZY= 86.4317
XZ=	63.8716	YZ= 94.0775	ZZ= 62.4746
Eigenvalues:	-60.8717	40.1972	149.0009
8 C	Isotropic=	42.522	Anisotropy = 153.4474
XX=	46.7261	YX= 5.7574	ZX= 42.6278
XY=	15.5031	YY= 50.6795	ZY= 101.2625
XZ=	28.5154	YZ= 85.5796	ZZ= 30.1604
Eigenvalues:	-57.3677	40.1135	144.8203
9 C	Isotropic=	110.7055	Anisotropy = 47.6275

XX=	114.6849	YX=	-28.5827	ZX=	-1.8657				
XY=	-32.0887	YY=	106.9281	ZY=	5.0595				
XZ=	-5.5493	YZ=	4.195	ZZ=	110.5035				
Eigenvalues:	80.1887	109.4707		142.4571					
10	C	Isotropic=	147.8145	Anisotropy	=	41.144			
XX=	160.5365	YX=	-18.3757	ZX=	2.8082				
XY=	-24.9284	YY=	138.9717	ZY=	-5.3243				
XZ=	10.924	YZ=	3.311	ZZ=	143.9352				
Eigenvalues:	125.1422		143.0574		175.2438				
11	C	Isotropic=	147.8619	Anisotropy	=	14.3229			
XX=	143.9193	YX=	2.0886	ZX=	-1.2525				
XY=	7.7262	YY=	145.6863	ZY=	5.4073				
XZ=	11.8614	YZ=	-1.9543	ZZ=	153.9801				
Eigenvalues:	139.1286		147.0465		157.4105				
12	C	Isotropic=	155.7462	Anisotropy	=	24.1403			
XX=	168.624	YX=	11.6909	ZX=	-1.6649				
XY=	2.4188	YY=	154.3584	ZY=	7.962				
XZ=	-1.6211	YZ=	13.8887	ZZ=	144.2561				
Eigenvalues:	136.4089		158.9899		171.8397				
13	C	Isotropic=	148.3898	Anisotropy	=	54.5814			
XX=	151.4061	YX=	18.4876	ZX=	18.9333				
XY=	16.8906	YY=	164.2656	ZY=	12.3097				
XZ=	24.1592	YZ=	7.7739	ZZ=	129.4979				
Eigenvalues:	116.269	144.1231		184.7774					
14	C	Isotropic=	167.605	Anisotropy	=	12.0446			
XX=	163.8856	YX=	3.0051	ZX=	6.6922				
XY=	-5.6464	YY=	168.587	ZY=	-6.9522				
XZ=	0.1308	YZ=	-3.1764	ZZ=	170.3425				
Eigenvalues:	162.2415		164.9388		175.6347				
15	C	Isotropic=	169.3394	Anisotropy	=	17.0802			
XX=	175.8243	YX=	4.1437	ZX=	2.1633				
XY=	1.7846	YY=	160.4397	ZY=	7.665				
XZ=	5.9982	YZ=	7.7077	ZZ=	171.7542				
Eigenvalues:	156.5172		170.7747		180.7262				
16	O	Isotropic=	263.3099	Anisotropy	=	84.0384			
XX=	308.9725	YX=	-18.4963	ZX=	16.313				
XY=	-12.1682	YY=	285.578	ZY=	-33.3425				
XZ=	10.9619	YZ=	5.1737	ZZ=	195.3791				
Eigenvalues:	192.134	278.4601		319.3355					
17	O	Isotropic=	265.3699	Anisotropy	=	45.77			
XX=	257.573	YX=	5.8853	ZX=	-26.9192				
XY=	20.2811	YY=	276.5268	ZY=	-14.2916				
XZ=	-6.3568	YZ=	-14.1811	ZZ=	262.01				
Eigenvalues:	242.9965		257.23		295.8833				
18	O	Isotropic=	-372.3457	Anisotropy	=	1098.6952			
XX=	-958.3452	YX=	122.266	ZX=	170.7702				
XY=	170.9728	YY=	98.2391	ZY=	-416.4226				
XZ=	114.3222	YZ=	-384.037	ZZ=	-256.931				
Eigenvalues:	-1036.4138		-440.7411		360.1178				
19	O	Isotropic=	95.4966	Anisotropy	=	126.9337			
XX=	160.0302	YX=	-2.6546	ZX=	-113.8481				
XY=	19.6167	YY=	146.5468	ZY=	80.9981				
XZ=	-12.9846	YZ=	-28.7717	ZZ=	-20.0871				
Eigenvalues:	-44.128	150.4987		180.1191					
20	O	Isotropic=	73.1067	Anisotropy	=	182.2427			
XX=	108.8668	YX=	24.3479	ZX=	34.1489				

XY=	134.9513	YY=	-70.3918	ZY=	20.2354		
XZ=	-30.7053	YZ=	78.9552	ZZ=	180.8449		
Eigenvalues:	-107.9529		132.6711		194.6018		
21	H	Isotropic=	31.0595	Anisotropy	=	13.4792	
XX=	36.5671	YX=	0.0187	ZX=	-4.3665		
XY=	0.1817	YY=	22.1452	ZY=	3.3695		
XZ=	-4.1068	YZ=	2.3546	ZZ=	34.4662		
Eigenvalues:	21.4391		31.6938		40.0456		
22	C	Isotropic=	21.5826	Anisotropy	=	79.1551	
XX=	26.4432	YX=	46.7402	ZX=	66.1719		
XY=	41.3829	YY=	24.1493	ZY=	-70.3977		
XZ=	35.806	YZ=	-38.5444	ZZ=	14.1553		
Eigenvalues:	-78.7116		69.1067		74.3527		
23	O	Isotropic=	-141.4119	Anisotropy	=	606.2308	
XX=	-106.2535	YX=	345.6438	ZX=	-76.9581		
XY=	331.8455	YY=	-51.1882	ZY=	22.9876		
XZ=	-33.9876	YZ=	0.3553	ZZ=	-266.794		
Eigenvalues:	-432.9577		-254.02		262.742		
24	C	Isotropic=	165.8166	Anisotropy	=	37.6929	
XX=	152.819	YX=	-5.8022	ZX=	-1.7358		
XY=	-6.0929	YY=	154.8019	ZY=	5.0006		
XZ=	0.5597	YZ=	7.304	ZZ=	189.829		
Eigenvalues:	147.4718		159.0329		190.9452		
25	H	Isotropic=	27.4094	Anisotropy	=	3.0446	
XX=	28.3386	YX=	0.5982	ZX=	-0.7137		
XY=	0.6573	YY=	25.8391	ZY=	0.8303		
XZ=	-1.6586	YZ=	1.7176	ZZ=	28.0506		
Eigenvalues:	24.9098		27.8793		29.4391		
26	H	Isotropic=	28.2652	Anisotropy	=	8.4309	
XX=	30.5869	YX=	2.6566	ZX=	3.7326		
XY=	2.2886	YY=	27.2153	ZY=	1.2549		
XZ=	3.5103	YZ=	0.8133	ZZ=	26.9935		
Eigenvalues:	24.6427		26.2672		33.8858		
27	H	Isotropic=	25.3383	Anisotropy	=	4.1082	
XX=	25.3953	YX=	-0.6482	ZX=	-3.0507		
XY=	-2.4287	YY=	24.4771	ZY=	0.133		
XZ=	-0.0982	YZ=	1.3743	ZZ=	26.1425		
Eigenvalues:	23.2732		24.6646		28.0771		
28	H	Isotropic=	24.9648	Anisotropy	=	6.6293	
XX=	28.6929	YX=	-2.0948	ZX=	0.4167		
XY=	-1.0689	YY=	25.6606	ZY=	1.1737		
XZ=	0.5872	YZ=	3.0072	ZZ=	20.5409		
Eigenvalues:	19.6806		25.8295		29.3843		
29	H	Isotropic=	27.4151	Anisotropy	=	7.9519	
XX=	32.5379	YX=	-0.049	ZX=	-1.2319		
XY=	0.3063	YY=	23.5198	ZY=	-2.6238		
XZ=	-0.5507	YZ=	-4.7882	ZZ=	26.1875		
Eigenvalues:	20.9005		28.6283		32.7164		
30	H	Isotropic=	29.7195	Anisotropy	=	5.6048	
XX=	32.8475	YX=	-1.5745	ZX=	1.7783		
XY=	-0.8871	YY=	28.2329	ZY=	3.2928		
XZ=	1.7854	YZ=	2.591	ZZ=	28.0782		
Eigenvalues:	24.6547		31.0478		33.456		
31	H	Isotropic=	29.3773	Anisotropy	=	8.3777	
XX=	32.4861	YX=	2.7963	ZX=	-1.7995		
XY=	3.3327	YY=	30.2534	ZY=	-1.4762		

XZ=	-1.3777	YZ=	-0.1911	ZZ=	25.3923				
Eigenvalues:	25.045	28.1244	34.9624						
32	H	Isotropic=	29.1604	Anisotropy	=	9.1497			
XX=	28.0108	YX=	-1.4757	ZX=	-4.9728				
XY=	-1.6192	YY=	28.5268	ZY=	1.7705				
XZ=	-4.3369	YZ=	2.0737	ZZ=	30.9436				
Eigenvalues:	24.5931	27.6279	35.2602						
33	H	Isotropic=	30.2533	Anisotropy	=	6.7346			
XX=	30.498	YX=	-3.7582	ZX=	-0.526				
XY=	-3.7811	YY=	30.6315	ZY=	-2.4959				
XZ=	-0.1134	YZ=	-2.0154	ZZ=	29.6304				
Eigenvalues:	25.8689	30.148	34.743						
34	H	Isotropic=	30.0278	Anisotropy	=	9.1906			
XX=	29.1604	YX=	0.7877	ZX=	0.2272				
XY=	-1.0299	YY=	35.5851	ZY=	2.709				
XZ=	0.096	YZ=	2.2514	ZZ=	25.3378				
Eigenvalues:	24.7613	29.1672	36.1548						
35	H	Isotropic=	30.1636	Anisotropy	=	6.354			
XX=	30.1468	YX=	-0.2075	ZX=	3.4128				
XY=	1.8542	YY=	30.3209	ZY=	2.5666				
XZ=	2.461	YZ=	2.3638	ZZ=	30.0231				
Eigenvalues:	26.6509	29.4403	34.3996						
36	H	Isotropic=	28.2931	Anisotropy	=	6.4535			
XX=	29.6809	YX=	1.9215	ZX=	-1.9358				
XY=	3.3137	YY=	30.1777	ZY=	-0.426				
XZ=	-0.7826	YZ=	1.5053	ZZ=	25.0207				
Eigenvalues:	24.3528	27.9311	32.5955						
37	H	Isotropic=	28.8962	Anisotropy	=	7.7841			
XX=	29.2754	YX=	-3.2175	ZX=	-1.07				
XY=	-1.8649	YY=	24.0585	ZY=	-1.1977				
XZ=	-2.5904	YZ=	-1.8317	ZZ=	33.3547				
Eigenvalues:	22.6114	29.9916	34.0856						
38	H	Isotropic=	29.1434	Anisotropy	=	6.3865			
XX=	28.1539	YX=	-0.681	ZX=	-0.22				
XY=	-0.6717	YY=	33.3136	ZY=	-0.1256				
XZ=	-0.2936	YZ=	-0.0384	ZZ=	25.9627				
Eigenvalues:	25.9295	28.0996	33.4011						
39	H	Isotropic=	28.5267	Anisotropy	=	8.678			
XX=	34.1678	YX=	-1.2125	ZX=	-0.272				
XY=	-0.932	YY=	22.9564	ZY=	-1.8294				
XZ=	0.7607	YZ=	-3.113	ZZ=	28.4558				
Eigenvalues:	21.9405	29.3275	34.312						
40	H	Isotropic=	29.1631	Anisotropy	=	10.8568			
XX=	33.9846	YX=	3.3669	ZX=	-3.3582				
XY=	4.6129	YY=	26.0812	ZY=	0.5398				
XZ=	-2.2154	YZ=	-0.6116	ZZ=	27.4234				
Eigenvalues:	24.0334	27.0549	36.401						
41	H	Isotropic=	29.6076	Anisotropy	=	5.823			
XX=	31.6681	YX=	-0.7034	ZX=	2.1161				
XY=	-0.356	YY=	30.112	ZY=	-2.6242				
XZ=	2.7394	YZ=	-2.3985	ZZ=	27.0426				
Eigenvalues:	25.0746	30.2586	33.4896						
42	H	Isotropic=	30.4631	Anisotropy	=	9.7285			
XX=	29.8186	YX=	2.1568	ZX=	1.741				
XY=	2.564	YY=	30.5339	ZY=	5.2069				
XZ=	1.4664	YZ=	4.9157	ZZ=	31.0368				

Eigenvalues:	25.6118	28.8287	36.9488			
43	H	Isotropic=	29.0631	Anisotropy	=	5.5608
XX=	29.1703	YX=	-3.1528	ZX=	0.3703	
XY=	-3.0009	YY=	26.0521	ZY=	0.5937	
XZ=	2.1245	YZ=	-0.9257	ZZ=	31.9667	
Eigenvalues:	24.1277	30.2912	32.7702			
44	H	Isotropic=	29.1689	Anisotropy	=	7.638
XX=	25.8784	YX=	-0.3001	ZX=	0.2137	
XY=	-0.9434	YY=	31.9464	ZY=	2.1291	
XZ=	-1.2037	YZ=	4.2227	ZZ=	29.6819	
Eigenvalues:	25.802	27.4437	34.2609			
45	H	Isotropic=	28.873	Anisotropy	=	8.2995
XX=	30.8571	YX=	1.6684	ZX=	-2.767	
XY=	1.8762	YY=	26.0289	ZY=	-1.0832	
XZ=	-4.4473	YZ=	-0.8063	ZZ=	29.733	
Eigenvalues:	25.4229	26.7901	34.406			
46	H	Isotropic=	30.6757	Anisotropy	=	18.1733
XX=	36.0591	YX=	-5.9018	ZX=	6.7651	
XY=	-5.2677	YY=	27.2875	ZY=	-4.9997	
XZ=	4.2602	YZ=	-6.2819	ZZ=	28.6807	
Eigenvalues:	22.2667	26.9692	42.7913			
47	C	Isotropic=	13.1351	Anisotropy	=	88.8704
XX=	-51.6144	YX=	42.5952	ZX=	46.7134	
XY=	-1.4719	YY=	50.4368	ZY=	9.8693	
XZ=	63.1599	YZ=	-4.5717	ZZ=	40.5828	
Eigenvalues:	-79.6059	46.6292	72.382			
48	O	Isotropic=	-120.1099	Anisotropy	=	649.4702
XX=	-155.9367	YX=	77.0155	ZX=	197.2634	
XY=	53.5786	YY=	-304.5816	ZY=	207.2082	
XZ=	227.7704	YZ=	265.6782	ZZ=	100.1886	
Eigenvalues:	-418.1544	-255.0455	312.8702			
49	H	Isotropic=	28.7203	Anisotropy	=	6.461
XX=	28.507	YX=	1.7463	ZX=	1.5569	
XY=	0.479	YY=	31.3894	ZY=	-2.9847	
XZ=	1.7661	YZ=	-3.6277	ZZ=	26.2646	
Eigenvalues:	23.8072	29.3262	33.0277			
50	H	Isotropic=	29.4475	Anisotropy	=	6.6559
XX=	28.2058	YX=	1.3996	ZX=	-0.5877	
XY=	1.5678	YY=	30.7277	ZY=	4.2774	
XZ=	-0.8661	YZ=	3.0702	ZZ=	29.409	
Eigenvalues:	25.4822	28.9755	33.8847			
51	C	Isotropic=	114.4655	Anisotropy	=	29.4706
XX=	113.1337	YX=	7.5039	ZX=	-4.313	
XY=	5.1207	YY=	130.4002	ZY=	-6.4987	
XZ=	-2.4635	YZ=	-7.0964	ZZ=	99.8627	
Eigenvalues:	98.1234	111.1606	134.1126			
52	C	Isotropic=	130.7509	Anisotropy	=	33.7759
XX=	132.3349	YX=	-6.0076	ZX=	13.6954	
XY=	-5.4173	YY=	141.4686	ZY=	-10.3465	
XZ=	12.5281	YZ=	-15.5107	ZZ=	118.4493	
Eigenvalues:	108.2771	130.7075	153.2682			
53	O	Isotropic=	276.1049	Anisotropy	=	111.3802
XX=	341.0128	YX=	-0.2868	ZX=	27.9391	
XY=	-18.7994	YY=	239.9059	ZY=	14.9743	
XZ=	33.0711	YZ=	10.3755	ZZ=	247.3959	
Eigenvalues:	224.1151	253.8411	350.3583			

54	H	Isotropic=	26.1148	Anisotropy	=	5.9768
XX=	25.3954	YX=	0.069	ZX=	-0.0911	
XY=	0.609	YY=	23.2331	ZY=	1.6827	
XZ=	-1.6693	YZ=	0.8902	ZZ=	29.716	
Eigenvalues:	22.8845	25.3606	30.0994			
55	N	Isotropic=	121.8883	Anisotropy	=	88.7289
XX=	151.6671	YX=	41.7651	ZX=	33.808	
XY=	12.9362	YY=	145.4515	ZY=	-39.5788	
XZ=	20.11	YZ=	-70.2337	ZZ=	68.5464	
Eigenvalues:	28.9958	155.6283	181.041			
56	C	Isotropic=	53.6677	Anisotropy	=	188.1702
XX=	84.5969	YX=	89.469	ZX=	25.5756	
XY=	74.8471	YY=	66.0712	ZY=	64.8218	
XZ=	18.1369	YZ=	62.2961	ZZ=	10.3352	
Eigenvalues:	-40.02	21.9086	179.1146			
57	H	Isotropic=	24.5378	Anisotropy	=	6.4294
XX=	26.3095	YX=	-0.9582	ZX=	-3.4527	
XY=	-0.6447	YY=	23.5272	ZY=	-0.0573	
XZ=	-3.5289	YZ=	-0.1522	ZZ=	23.7768	
Eigenvalues:	21.1992	23.5902	28.8241			
58	H	Isotropic=	30.2435	Anisotropy	=	19.3633
XX=	41.2136	YX=	3.0803	ZX=	4.7578	
XY=	4.0695	YY=	27.2882	ZY=	-0.3882	
XZ=	4.8742	YZ=	0.8585	ZZ=	22.2288	
Eigenvalues:	21.0131	26.5651	43.1523			
59	C	Isotropic=	17.1902	Anisotropy	=	118.2925
XX=	51.7748	YX=	-68.4701	ZX=	10.5661	
XY=	-64.6856	YY=	-35.2426	ZY=	-17.3885	
XZ=	27.3578	YZ=	-6.8121	ZZ=	35.0383	
Eigenvalues:	-71.293	26.8117	96.0518			
60	H	Isotropic=	26.5073	Anisotropy	=	7.863
XX=	23.385	YX=	2.551	ZX=	-0.6664	
XY=	2.1934	YY=	31.0564	ZY=	1.4595	
XZ=	-3.344	YZ=	-1.0272	ZZ=	25.0805	
Eigenvalues:	21.5786	26.1941	31.7493			
61	C	Isotropic=	61.7461	Anisotropy	=	169.9746
XX=	68.6449	YX=	99.6187	ZX=	43.1456	
XY=	94.9501	YY=	61.9523	ZY=	11.0475	
XZ=	44.9327	YZ=	7.8443	ZZ=	54.6412	
Eigenvalues:	-38.6331	148.8089	175.0625			
62	C	Isotropic=	63.9181	Anisotropy	=	173.5783
XX=	99.0865	YX=	58.6684	ZX=	63.281	
XY=	57.7542	YY=	105.5806	ZY=	25.0468	
XZ=	58.821	YZ=	23.5242	ZZ=	-12.9129	
Eigenvalues:	-39.7694	151.8867	179.637			
63	C	Isotropic=	65.0092	Anisotropy	=	173.544
XX=	107.3044	YX=	76.7384	ZX=	8.4942	
XY=	79.9094	YY=	65.1429	ZY=	62.7762	
XZ=	7.5887	YZ=	61.8996	ZZ=	22.5803	
Eigenvalues:	-35.7421	150.0645	180.7052			
64	C	Isotropic=	62.4506	Anisotropy	=	172.9968
XX=	70.5879	YX=	99.513	ZX=	40.6066	
XY=	101.0619	YY=	63.1139	ZY=	8.6164	
XZ=	42.7567	YZ=	8.246	ZZ=	53.6501	
Eigenvalues:	-39.5107	149.0807	177.7818			
65	C	Isotropic=	58.9333	Anisotropy	=	151.4028

XX=	90.1173	YX=	51.5252	ZX=	54.196				
XY=	46.156	YY=	103.5928	ZY=	15.2898				
XZ=	53.0576	YZ=	19.0172	ZZ=	-16.9102				
Eigenvalues:	-39.2221	56.1536	159.8685						
66	H	Isotropic=	23.9385	Anisotropy	=	8.0176			
XX=	22.2568	YX=	-1.2026	ZX=	0.4727				
XY=	-0.2809	YY=	21.7659	ZY=	-2.9099				
XZ=	-0.0246	YZ=	-3.6872	ZZ=	27.7928				
Eigenvalues:	20.1454	22.3865	29.2835						
67	O	Isotropic=	-94.8331	Anisotropy	=	667.189			
XX=	72.5767	YX=	-168.464	ZX=	268.0149				
XY=	-200.0795	YY=	-91.2837	ZY=	-82.658				
XZ=	327.0891	YZ=	-136.9898	ZZ=	-265.7923				
Eigenvalues:	-438.9134	-195.5455	349.9596						
68	C	Isotropic=	54.7871	Anisotropy	=	172.2931			
XX=	23.6846	YX=	-7.9289	ZX=	-3.3808				
XY=	7.7705	YY=	23.0281	ZY=	-85.0166				
XZ=	-26.7141	YZ=	-87.0105	ZZ=	117.6486				
Eigenvalues:	-28.9799	23.692	169.6492						
69	H	Isotropic=	23.8707	Anisotropy	=	5.8798			
XX=	23.2091	YX=	-3.1446	ZX=	0.4935				
XY=	-3.0625	YY=	24.022	ZY=	-1.8256				
XZ=	0.2002	YZ=	-2.4529	ZZ=	24.381				
Eigenvalues:	20.1316	23.6899	27.7905						
70	H	Isotropic=	23.8419	Anisotropy	=	3.522			
XX=	23.5015	YX=	-2.7282	ZX=	-1.2225				
XY=	-2.4823	YY=	23.2596	ZY=	-0.3872				
XZ=	-1.297	YZ=	-0.8904	ZZ=	24.7648				
Eigenvalues:	20.3656	24.9704	26.1899						
71	H	Isotropic=	23.8372	Anisotropy	=	4.1323			
XX=	22.7896	YX=	-2.2939	ZX=	-0.6681				
XY=	-2.172	YY=	23.5365	ZY=	-1.7801				
XZ=	-0.5875	YZ=	-1.9725	ZZ=	25.1854				
Eigenvalues:	20.2892	24.6303	26.592						
72	H	Isotropic=	23.852	Anisotropy	=	8.2708			
XX=	24.4487	YX=	-4.4612	ZX=	-0.1974				
XY=	-4.2288	YY=	25.3102	ZY=	-0.9952				
XZ=	-0.002	YZ=	-1.7397	ZZ=	21.7971				
Eigenvalues:	19.9509	22.2393	29.3659						
73	C	Isotropic=	61.3591	Anisotropy	=	174.7431			
XX=	-7.1686	YX=	29.8051	ZX=	25.8066				
XY=	29.2543	YY=	59.7088	ZY=	-71.5524				
XZ=	27.9547	YZ=	-75.7495	ZZ=	131.5372				
Eigenvalues:	-37.5397	43.7626	177.8546						
74	C	Isotropic=	62.4475	Anisotropy	=	176.0126			
XX=	-30.8887	YX=	-26.8243	ZX=	-7.4831				
XY=	-25.1109	YY=	74.2935	ZY=	-61.2399				
XZ=	-5.0785	YZ=	-61.1104	ZZ=	143.9377				
Eigenvalues:	-39.5323	47.0856	179.7893						
75	C	Isotropic=	62.3638	Anisotropy	=	177.2434			
XX=	44.5834	YX=	-14.315	ZX=	-4.0242				
XY=	-15.1918	YY=	16.7871	ZY=	-95.33				
XZ=	-3.1535	YZ=	-93.8169	ZZ=	125.721				
Eigenvalues:	-40.383	46.9485	180.5261						
76	C	Isotropic=	63.6787	Anisotropy	=	174.5299			
XX=	-1.6788	YX=	37.6171	ZX=	26.5933				

XY=	33.3172	YY=	54.956	ZY=	-73.5272				
XZ=	27.0999	YZ=	-71.505	ZZ=	137.7588				
Eigenvalues:	-39.2356	50.2396	180.0319						
77	C	Isotropic=	66.3208	Anisotropy	=	165.6195			
XX=	-20.6701	YX=	-16.8335	ZX=	-7.5572				
XY=	-22.4516	YY=	74.8925	ZY=	-58.6059				
XZ=	-12.8647	YZ=	-55.551	ZZ=	144.7401				
Eigenvalues:	-27.6156	49.8442	176.7338						
78	H	Isotropic=	23.5395	Anisotropy	=	7.8499			
XX=	25.3492	YX=	3.6654	ZX=	0.587				
XY=	2.9138	YY=	24.3794	ZY=	1.8931				
XZ=	0.9452	YZ=	2.8005	ZZ=	20.8899				
Eigenvalues:	19.5532	22.2925	28.7728						
79	H	Isotropic=	23.8475	Anisotropy	=	4.1352			
XX=	24.6247	YX=	0.235	ZX=	-0.5804				
XY=	0.1969	YY=	25.2329	ZY=	2.5532				
XZ=	-0.3109	YZ=	2.6412	ZZ=	21.685				
Eigenvalues:	20.2577	24.6806	26.6043						
80	H	Isotropic=	23.7963	Anisotropy	=	4.1564			
XX=	26.5369	YX=	0.458	ZX=	-0.3089				
XY=	0.1407	YY=	23.6092	ZY=	1.6152				
XZ=	-0.0391	YZ=	1.8296	ZZ=	21.2427				
Eigenvalues:	20.3224	24.4992	26.5672						
81	H	Isotropic=	23.8856	Anisotropy	=	6.046			
XX=	25.154	YX=	2.0054	ZX=	0.6252				
XY=	1.5149	YY=	25.2769	ZY=	2.5635				
XZ=	0.8856	YZ=	2.7479	ZZ=	21.226				
Eigenvalues:	19.9092	23.8314	27.9163						
82	H	Isotropic=	23.713	Anisotropy	=	7.3662			
XX=	23.9566	YX=	0.668	ZX=	-0.3531				
XY=	-0.3898	YY=	27.1311	ZY=	3.5553				
XZ=	0.4456	YZ=	3.5862	ZZ=	20.0511				
Eigenvalues:	18.563	23.9521	28.6238						

2av_neg45

C	-3.142151	-0.049893	-1.892929
C	-3.85833-1.436606	-1.941899	
C	-3.552196	-2.381438	-0.767713
C	-4.757584	-2.633648	0.155966
C	-5.332695	-1.375605	0.836938
C	-4.376439	-0.378431	1.472827
C	-3.424053	0.275432	0.514012
C	-2.094632	0.178782	0.777096
C	-1.127527	0.425172	-0.347982
C	-1.62822-0.179883	-1.662447	
C	-3.810690.869474	-0.822904	
C	-5.300013	0.996839	-1.100789
C	-3.238229	2.294042	-0.946095
C	-1.513611	-0.203481	2.083675
C	-5.851424	-3.395417	-0.557305
O	-3.242428	0.534439	-3.190344
O	-3.554434	-2.073301	-3.173881
O	-6.547544	-1.295338	1.03336
O	-4.949065	0.509499	2.427583
O	0.112143	-0.229707	0.014325
H	-2.607671	-1.975076	-3.333701

C	-6.130012	1.186008	2.27662
O	-6.757971	1.140309	1.224505
C	-6.478284	1.92879	3.524934
H	-4.972584	-1.270877	-2.01281
H	-2.700211	-1.995206	-0.154464
H	-3.76182-1.040822		2.177491
H	-0.912434	1.52449	-0.468289
H	-1.088843	0.336168	-2.505329
H	-1.336989	-1.262397	-1.693892
H	-5.885103	0.089847	-0.825734
H	-5.725971	1.856246	-0.525019
H	-5.459846	1.207125	-2.187366
H	-4.035153	3.021943	-1.23571
H	-2.802999	2.636316	0.022579
H	-2.453153	2.336086	-1.740505
H	-2.1768	0.10157	2.930825
H	-1.350277	-1.310354	2.124825
H	-0.519183	0.291331	2.223995
H	-6.672752	-3.646563	0.157707
H	-6.289338	-2.785884	-1.383909
H	-5.441193	-4.340122	-0.987972
H	-5.621122	1.942976	4.239642
H	-6.760664	2.975114	3.254771
H	-7.351982	1.423052	4.004826
H	-4.124904	0.345673	-3.533564
C	1.237676	0.105527	-0.688627
O	1.138873	0.900166	-1.621315
H	-4.380855	-3.267572	1.011798
H	-3.244038	-3.373002	-1.195884
C	2.451369	-0.658122	-0.197971
C	3.61906	0.247617	0.321223
O	2.131906	-1.474406	0.912761
H	2.782635	-1.294781	-1.069067
N	4.88991	-0.406503	0.101727
C	3.581733	1.63968	-0.256094
H	3.463153	0.316199	1.448741
H	1.363595	-2.010389	0.676127
C	5.743146	-0.715822	1.155787
H	5.293888	-0.29346-0.799426	
C	3.969161	1.9002	-1.575081
C	3.985481	3.208761	-2.056327
C	3.617964	4.265631	-1.223969
C	3.232367	4.011295	0.092004
C	3.219243	2.704766	0.577689
H	4.233771	1.073156	-2.250423
O	5.355523	-0.702803	2.338233
C	7.135893	-1.103844	0.78649
H	4.282946	3.404845	-3.096926
H	3.62961	5.297153	-1.605453
H	2.940651	4.84231	0.750975
H	2.925011	2.512176	1.621048
C	8.196141	-0.547069	1.510401
C	9.508632	-0.894235	1.193549
C	9.763648	-1.800268	0.163776
C	8.705187	-2.362694	-0.550096
C	7.390039	-2.01465-0.243091	

H	7.98363	0.151891	2.334548
H	10.342587	-0.455517	1.761186
H	10.800109	-2.074897	-0.082875
H	8.906231	-3.084221	-1.355636
H	6.558774	-2.471322	-0.80105

2av_neg45	E(RB+HF-PW91)	=	-2012.296904
SCF GIAO	Magnetic shielding	tensor (ppm):	
1 C	Isotropic=	109.3025	Anisotropy = 28.351
XX=	99.2578	YX= -8.6528	ZX= 9.9256
XY=	-9.4508	YY= 110.4342	ZY= -9.771
XZ=	2.0635	YZ= -9.3405	ZZ= 118.2155
Eigenvalues:	94.1895	105.5148	128.2032
2 C	Isotropic=	111.7927	Anisotropy = 29.7538
XX=	96.8056	YX= -6.2268	ZX= -12.5854
XY=	-0.3132	YY= 116.2997	ZY= 4.2261
XZ=	-7.6533	YZ= 13.5068	ZZ= 122.2728
Eigenvalues:	93.2729	110.4765	131.6286
3 C	Isotropic=	141.6918	Anisotropy = 20.1467
XX=	121.5482	YX= 1.7872	ZX= -2.603
XY=	-5.0979	YY= 154.9793	ZY= -0.4575
XZ=	-6.3931	YZ= -1.2032	ZZ= 148.5479
Eigenvalues:	120.7274	149.2251	155.1229
4 C	Isotropic=	140.0614	Anisotropy = 25.0097
XX=	123.6156	YX= -4.6344	ZX= -4.7966
XY=	2.2023	YY= 152.5708	ZY= 8.5176
XZ=	7.8078	YZ= 6.0403	ZZ= 143.9979
Eigenvalues:	123.3908	140.059	156.7345
5 C	Isotropic=	-21.7523	Anisotropy = 179.0167
XX=	-53.6602	YX= -24.9066	ZX= -5.0758
XY=	-6.6994	YY= -58.1903	ZY= -92.1336
XZ=	-0.4013	YZ= -85.671	ZZ= 46.5937
Eigenvalues:	-112.8416	-50.0074	97.5922
6 C	Isotropic=	101.8794	Anisotropy = 41.262
XX=	87.8213	YX= -0.3171	ZX= 0.3336
XY=	-9.942	YY= 115.2404	ZY= 19.0573
XZ=	-12.8492	YZ= 16.7928	ZZ= 102.5764
Eigenvalues:	85.3723	90.8784	129.3873
7 C	Isotropic=	43.4109	Anisotropy = 157.885
XX=	29.78	YX= -19.9817	ZX= 19.6525
XY=	-4.4046	YY= 109.6279	ZY= 71.5428
XZ=	40.7659	YZ= 85.3146	ZZ= -9.1752
Eigenvalues:	-59.9224	44.14875	148.6676
8 C	Isotropic=	41.889	Anisotropy = 154.6468
XX=	36.4548	YX= -1.3688	ZX= 21.7397
XY=	-0.249	YY= 126.8838	ZY= 67.1551
XZ=	10.3322	YZ= 47.3239	ZZ= -37.6716
Eigenvalues:	-58.1786	38.8588	144.9869
9 C	Isotropic=	110.4988	Anisotropy = 49.101
XX=	130.3016	YX= -20.7274	ZX= 9.1942
XY=	-26.8467	YY= 95.4162	ZY= 5.2365
XZ=	8.505	YZ= 4.7405	ZZ= 105.7785
Eigenvalues:	80.4808	107.7827	143.2328
10 C	Isotropic=	148.3298	Anisotropy = 40.9233
XX=	166.7388	YX= -7.0219	ZX= 11.6447

XY=	-9.7832	YY=	132.6716	ZY=	-1.2558				
XZ=	19.365	YZ=	10.3379	ZZ=	145.579				
Eigenvalues:	126.3697		143.0077		175.612				
11	C	Isotropic=	147.9425	Anisotropy	=	13.9163			
XX=	141.6911	YX=	-0.8733	ZX=	-4.568				
XY=	9.4332	YY=	151.1062	ZY=	7.8624				
XZ=	6.0645	YZ=	2.7459	ZZ=	151.0303				
Eigenvalues:	139.8732		146.7344		157.2201				
12	C	Isotropic=	155.6672	Anisotropy	=	24.6175			
XX=	165.8283	YX=	10.9457	ZX=	-4.9554				
XY=	2.6914	YY=	164.4653	ZY=	-1.8361				
XZ=	-2.6939	YZ=	5.3668	ZZ=	136.7079				
Eigenvalues:	135.9598		158.9628		172.0789				
13	C	Isotropic=	148.5852	Anisotropy	=	54.3862			
XX=	138.601	YX=	17.4431	ZX=	10.6219				
XY=	18.1926	YY=	177.8525	ZY=	-1.529				
XZ=	17.2494	YZ=	-4.1524	ZZ=	129.302				
Eigenvalues:	116.3908		144.5221		184.8427				
14	C	Isotropic=	167.7989	Anisotropy	=	12.2191			
XX=	163.0305	YX=	5.3664	ZX=	4.9004				
XY=	-5.6684	YY=	165.6198	ZY=	-3.3006				
XZ=	2.3671	YZ=	0.6886	ZZ=	174.7464				
Eigenvalues:	161.9821		165.4696		175.945				
15	C	Isotropic=	169.3063	Anisotropy	=	17.1533			
XX=	172.9606	YX=	5.5728	ZX=	-2.1114				
XY=	4.9705	YY=	171.3971	ZY=	9.0566				
XZ=	2.56	YZ=	10.5544	ZZ=	163.5612				
Eigenvalues:	156.4278		170.7493		180.7418				
16	O	Isotropic=	264.051	Anisotropy	=	84.7297			
XX=	307.5327	YX=	5.5722	ZX=	42.678				
XY=	10.1813	YY=	258.6308	ZY=	-54.451				
XZ=	25.7478	YZ=	-19.207	ZZ=	225.9895				
Eigenvalues:	192.4458		279.1697		320.5375				
17	O	Isotropic=	265.365	Anisotropy	=	46.1581			
XX=	257.0425	YX=	-6.9178	ZX=	-22.4671				
XY=	13.9906	YY=	264.9954	ZY=	-21.2202				
XZ=	-11.0019	YZ=	-18.6363	ZZ=	274.0569				
Eigenvalues:	242.7698		257.1881		296.137				
18	O	Isotropic=	-371.7967	Anisotropy	=	1098.6529			
XX=	-1021.8562	YX=	-10.5401	ZX=	157.5747				
XY=	10.7835	YY=	-224.5282	ZY=	-363.7829				
XZ=	80.545	YZ=	-352.8417	ZZ=	130.9944				
Eigenvalues:	-1035.9221		-440.1065		360.6386				
19	O	Isotropic=	95.2029	Anisotropy	=	127.445			
XX=	172.2235	YX=	-37.315	ZX=	-92.1958				
XY=	23.0406	YY=	127.1723	ZY=	-20.2303				
XZ=	17.68	YZ=	-106.5118	ZZ=	-13.7872				
Eigenvalues:	-44.5281		149.9706		180.1662				
20	O	Isotropic=	72.132	Anisotropy	=	185.7548			
XX=	66.2423	YX=	45.6184	ZX=	-9.5987				
XY=	116.3124	YY=	60.6388	ZY=	107.0893				
XZ=	-125.2994	YZ=	132.7088	ZZ=	89.5148				
Eigenvalues:	-109.0063		129.4337		195.9685				
21	H	Isotropic=	31.2122	Anisotropy	=	13.5353			
XX=	37.3846	YX=	1.178	ZX=	-5.5059				
XY=	1.0805	YY=	26.5843	ZY=	5.5976				

XZ= -5.0958 YZ= 4.7376 ZZ= 29.6677
 Eigenvalues: 21.6053 31.7955 40.2357
 22 C Isotropic= 21.4907 Anisotropy = 78.4607
 XX= -12.3312 YX= 74.2633 ZX= 49.5617
 XY= 57.6094 YY= 16.0896 ZY= -38.8806
 XZ= 17.1654 YZ= -14.3543 ZZ= 60.7138
 Eigenvalues: -78.6424 69.3167 73.7978
 23 O Isotropic= -141.2136 Anisotropy = 606.2417
 XX= -238.5267 YX= 235.5547 ZX= -192.4612
 XY= 240.6394 YY= 65.6093 ZY= -112.0177
 XZ= -143.5611 YZ= -121.1403 ZZ= -250.7233
 Eigenvalues: -433.3936 -253.1947 262.9475
 24 C Isotropic= 166.0225 Anisotropy = 37.5764
 XX= 157.1263 YX= -9.3741 ZX= -4.5831
 XY= -9.4237 YY= 162.4469 ZY= 15.4174
 XZ= -2.4684 YZ= 18.2858 ZZ= 178.4944
 Eigenvalues: 147.3469 159.6472 191.0734
 25 H Isotropic= 27.5106 Anisotropy = 3.1913
 XX= 28.5377 YX= 0.5295 ZX= -1.2122
 XY= 0.0454 YY= 27.387 ZY= 0.84
 XZ= -2.2623 YZ= 1.6519 ZZ= 26.6072
 Eigenvalues: 24.9631 27.9306 29.6382
 26 H Isotropic= 28.3236 Anisotropy = 8.281
 XX= 28.2775 YX= 4.2515 ZX= 1.7547
 XY= 3.3374 YY= 30.1954 ZY= 1.44
 XZ= 2.0856 YZ= 1.2726 ZZ= 26.4981
 Eigenvalues: 24.8671 26.2595 33.8443
 27 H Isotropic= 25.3685 Anisotropy = 4.1433
 XX= 26.5047 YX= -1.542 ZX= -2.6268
 XY= -2.0811 YY= 24.3241 ZY= -0.3377
 XZ= 0.5359 YZ= 1.9589 ZZ= 25.2767
 Eigenvalues: 23.2772 24.6976 28.1307
 28 H Isotropic= 25.5671 Anisotropy = 7.5677
 XX= 30.3619 YX= -0.3113 ZX= 1.5741
 XY= 0.1093 YY= 25.9966 ZY= -1.2687
 XZ= 1.6045 YZ= 0.7382 ZZ= 20.3428
 Eigenvalues: 20.0865 26.0026 30.6122
 29 H Isotropic= 27.8146 Anisotropy = 8.8013
 XX= 32.7191 YX= 3.1965 ZX= -0.705
 XY= 3.1468 YY= 21.9975 ZY= -0.529
 XZ= 0.1245 YZ= -2.469 ZZ= 28.7271
 Eigenvalues: 20.8892 28.8724 33.6821
 30 H Isotropic= 29.9231 Anisotropy = 5.7489
 XX= 33.0785 YX= 0.3753 ZX= 1.6924
 XY= 0.2635 YY= 30.5626 ZY= 2.5245
 XZ= 1.8022 YZ= 1.988 ZZ= 26.1282
 Eigenvalues: 24.9064 31.1072 33.7557
 31 H Isotropic= 29.4939 Anisotropy = 8.3743
 XX= 31.4085 YX= 2.6141 ZX= -1.7644
 XY= 3.1528 YY= 30.1967 ZY= -3.5903
 XZ= -1.9045 YZ= -2.2513 ZZ= 26.8765
 Eigenvalues: 25.1729 28.232 35.0767
 32 H Isotropic= 29.2946 Anisotropy = 9.2021
 XX= 30.5369 YX= -3.6094 ZX= -4.3406
 XY= -3.4249 YY= 28.5866 ZY= 0.723
 XZ= -3.6401 YZ= 1.2159 ZZ= 28.7602

Eigenvalues:	24.7535	27.7009	35.4293		
33	H	Isotropic=	30.4389	Anisotropy	= 6.7459
XX=	32.3344	YX=	-2.5029	ZX=	1.6145
XY=	-2.4971	YY=	27.1533	ZY=	-1.8372
XZ=	1.9054	YZ=	-1.2033	ZZ=	31.8291
Eigenvalues:	26.0339	30.3467	34.9362		
34	H	Isotropic=	30.2547	Anisotropy	= 9.0204
XX=	29.9607	YX=	-0.8451	ZX=	0.5886
XY=	-2.436	YY=	35.2134	ZY=	-2.186
XZ=	1.4895	YZ=	-2.412	ZZ=	25.59
Eigenvalues:	24.9784	29.5174	36.2683		
35	H	Isotropic=	30.42	Anisotropy	= 6.1848
XX=	29.5891	YX=	0.3427	ZX=	2.4315
XY=	1.8202	YY=	33.081	ZY=	2.4482
XZ=	1.3501	YZ=	1.7916	ZZ=	28.5898
Eigenvalues:	26.9271	29.7897	34.5432		
36	H	Isotropic=	28.6558	Anisotropy	= 6.3776
XX=	29.6976	YX=	0.7112	ZX=	-1.5864
XY=	2.561	YY=	30.6576	ZY=	-3.1163
XZ=	-1.7262	YZ=	-1.2352	ZZ=	25.6122
Eigenvalues:	24.5873	28.4726	32.9075		
37	H	Isotropic=	28.9595	Anisotropy	= 7.9802
XX=	30.5042	YX=	-1.4957	ZX=	-0.869
XY=	-1.4479	YY=	23.5571	ZY=	2.8979
XZ=	-2.0823	YZ=	1.9478	ZZ=	32.8172
Eigenvalues:	22.8047	29.7942	34.2797		
38	H	Isotropic=	29.1554	Anisotropy	= 6.5528
XX=	28.4312	YX=	-1.3345	ZX=	0.4676
XY=	-2.1493	YY=	31.3837	ZY=	-3.0086
XZ=	0.8137	YZ=	-2.535	ZZ=	27.6512
Eigenvalues:	26.1401	27.802	33.5239		
39	H	Isotropic=	28.5128	Anisotropy	= 7.848
XX=	33.0306	YX=	2.8285	ZX=	-0.7861
XY=	2.3731	YY=	23.1123	ZY=	1.3508
XZ=	1.3898	YZ=	0.88	ZZ=	29.3955
Eigenvalues:	22.3266	29.467	33.7448		
40	H	Isotropic=	29.1803	Anisotropy	= 10.8726
XX=	32.5214	YX=	3.3661	ZX=	-4.4452
XY=	4.8042	YY=	28.1674	ZY=	-0.0141
XZ=	-3.568	YZ=	-0.9498	ZZ=	26.852
Eigenvalues:	24.0151	27.097	36.4286		
41	H	Isotropic=	29.6497	Anisotropy	= 5.7876
XX=	30.8609	YX=	1.4168	ZX=	2.9088
XY=	1.8406	YY=	28.2278	ZY=	-2.1573
XZ=	3.3057	YZ=	-1.7547	ZZ=	29.8604
Eigenvalues:	25.1254	30.3156	33.5081		
42	H	Isotropic=	30.4985	Anisotropy	= 9.6497
XX=	28.7852	YX=	0.9367	ZX=	-0.3549
XY=	1.0157	YY=	35.676	ZY=	3.5761
XZ=	-0.6247	YZ=	3.2453	ZZ=	27.0342
Eigenvalues:	25.6515	28.9124	36.9316		
43	H	Isotropic=	29.0597	Anisotropy	= 5.5859
XX=	30.0251	YX=	-1.8463	ZX=	0.654
XY=	-1.0903	YY=	26.0071	ZY=	3.2697
XZ=	2.7783	YZ=	2.2514	ZZ=	31.1469
Eigenvalues:	24.0955	30.3	32.7837		

44	H	Isotropic=	29.2171	Anisotropy	=	7.6634
XX=	26.9741	YX=	-2.2554	ZX=	0.1507	
XY=	-3.384	YY=	33.0544	ZY=	0.0195	
XZ=	-1.1705	YZ=	1.8418	ZZ=	27.6229	
Eigenvalues:	25.8567	27.4687	34.326			
45	H	Isotropic=	28.9111	Anisotropy	=	8.2535
XX=	30.8496	YX=	1.6148	ZX=	-3.3215	
XY=	0.9866	YY=	26.43	ZY=	-0.1413	
XZ=	-4.7634	YZ=	-0.2613	ZZ=	29.4538	
Eigenvalues:	25.4737	26.8462	34.4134			
46	H	Isotropic=	30.8718	Anisotropy	=	18.2609
XX=	36.3294	YX=	1.3221	ZX=	9.0081	
XY=	0.6908	YY=	22.738	ZY=	-0.101	
XZ=	6.9643	YZ=	-1.941	ZZ=	33.548	
Eigenvalues:	22.2879	27.2818	43.0458			
47	C	Isotropic=	13.5952	Anisotropy	=	89.7221
XX=	-68.7328	YX=	28.3643	ZX=	14.4979	
XY=	-5.0243	YY=	65.1904	ZY=	10.3373	
XZ=	50.8111	YZ=	9.3369	ZZ=	44.3278	
Eigenvalues:	-78.0224	44.3981	73.4099			
48	O	Isotropic=	-124.2759	Anisotropy	=	651.4567
XX=	-231.29	YX=	107.9989	ZX=	51.4808	
XY=	81.7464	YY=	18.42	ZY=	310.9796	
XZ=	74.7911	YZ=	380.2266	ZZ=	-159.9577	
Eigenvalues:	-428.0702	-254.7863	10.0285			
49	H	Isotropic=	28.7072	Anisotropy	=	6.4927
XX=	27.3113	YX=	2.3802	ZX=	1.4396	
XY=	1.1138	YY=	28.8308	ZY=	-3.4378	
XZ=	2.4042	YZ=	-3.6858	ZZ=	29.9794	
Eigenvalues:	23.8649	29.221	33.0356			
50	H	Isotropic=	29.5105	Anisotropy	=	6.5502
XX=	28.2568	YX=	-0.3903	ZX=	-1.8199	
XY=	-0.6982	YY=	33.4983	ZY=	1.8508	
XZ=	-1.6635	YZ=	0.7385	ZZ=	26.7766	
Eigenvalues:	25.5443	29.11	33.8773			
51	C	Isotropic=	107.9054	Anisotropy	=	22.6756
XX=	111.3156	YX=	5.4853	ZX=	-8.3641	
XY=	6.6661	YY=	109.8844	ZY=	-8.3239	
XZ=	-7.0653	YZ=	-8.4871	ZZ=	102.5161	
Eigenvalues:	96.1061	104.5875	123.0225			
52	C	Isotropic=	121.7808	Anisotropy	=	27.3452
XX=	117.3438	YX=	17.7131	ZX=	-0.5533	
XY=	9.3925	YY=	131.8301	ZY=	-1.3384	
XZ=	-0.8909	YZ=	-0.5141	ZZ=	116.1684	
Eigenvalues:	109.2171	116.1144	140.0109			
53	O	Isotropic=	276.9404	Anisotropy	=	85.2033
XX=	306.2274	YX=	40.6592	ZX=	6.4643	
XY=	35.3919	YY=	272.2907	ZY=	8.5673	
XZ=	19.6398	YZ=	7.1178	ZZ=	252.303	
Eigenvalues:	247.4844	249.5941	333.7426			
54	H	Isotropic=	26.6285	Anisotropy	=	4.0302
XX=	26.4014	YX=	0.9164	ZX=	-1.3383	
XY=	-0.9268	YY=	25.5284	ZY=	1.31	
XZ=	-1.8034	YZ=	1.4718	ZZ=	27.9555	
Eigenvalues:	24.5785	25.9916	29.3153			
55	N	Isotropic=	118.623	Anisotropy	=	92.7657

XX=	132.1314	YX=	-5.7448	ZX=	49.7876		
XY=	-1.6695	YY=	152.5018	ZY=	-0.6808		
XZ=	87.1987	YZ=	-25.5263	ZZ=	71.2357		
Eigenvalues:	26.088	149.3142		180.4668			
56	C	Isotropic=	50.8244	Anisotropy	=	195.0521	
XX=	171.548	YX=	8.2342	ZX=	28.0893		
XY=	18.4321	YY=	-32.7983	ZY=	22.1487		
XZ=	44.0121	YZ=	21.0455	ZZ=	13.7236		
Eigenvalues:	-41.2817	12.8958		180.8592			
57	H	Isotropic=	24.7741	Anisotropy	=	2.504	
XX=	24.4594	YX=	-0.8447	ZX=	0.674		
XY=	-0.4395	YY=	23.867	ZY=	1.2325		
XZ=	0.6307	YZ=	0.6758	ZZ=	25.9958		
Eigenvalues:	23.0091	24.8697		26.4434			
58	H	Isotropic=	30.0955	Anisotropy	=	18.49	
XX=	36.4142	YX=	8.1881	ZX=	1.9832		
XY=	8.5118	YY=	30.7304	ZY=	-2.6835		
XZ=	2.1281	YZ=	-0.4888	ZZ=	23.142		
Eigenvalues:	21.3161	26.5482		42.4222			
59	C	Isotropic=	17.4394	Anisotropy	=	116.0319	
XX=	-46.4696	YX=	42.3166	ZX=	-16.4018		
XY=	45.9729	YY=	76.568	ZY=	28.2137		
XZ=	-35.4609	YZ=	22.6616	ZZ=	22.2197		
Eigenvalues:	-72.0529	29.577		94.794			
60	H	Isotropic=	26.0763	Anisotropy	=	9.9642	
XX=	28.8536	YX=	-5.4485	ZX=	-2.0693		
XY=	-6.2008	YY=	23.218	ZY=	-2.4299		
XZ=	1.9094	YZ=	-2.1708	ZZ=	26.1573		
Eigenvalues:	19.0033	26.5065		32.7191			
61	C	Isotropic=	61.9502	Anisotropy	=	173.8249	
XX=	159.2125	YX=	29.85	ZX=	50.1471		
XY=	32.0251	YY=	0.906	ZY=	-33.8138		
XZ=	49.9635	YZ=	-38.65	ZZ=	25.732		
Eigenvalues:	-40.1816	48.1987		177.8335			
62	C	Isotropic=	62.5992	Anisotropy	=	177.5595	
XX=	163.261	YX=	8.5577	ZX=	54.9625		
XY=	8.5913	YY=	46.8815	ZY=	14.9786		
XZ=	60.4851	YZ=	17.973	ZZ=	-22.3447		
Eigenvalues:	-40.9217	47.7472		180.9722			
63	C	Isotropic=	64.5043	Anisotropy	=	175.9571	
XX=	168.5827	YX=	15.1366	ZX=	36.9966		
XY=	12.0984	YY=	-25.4134	ZY=	30.2247		
XZ=	37.971	YZ=	32.2402	ZZ=	50.3436		
Eigenvalues:	-36.6293	48.3332		181.809			
64	C	Isotropic=	62.5876	Anisotropy	=	175.8719	
XX=	160.0928	YX=	31.7888	ZX=	52.812		
XY=	29.7394	YY=	-0.7068	ZY=	-35.9515		
XZ=	51.0295	YZ=	-36.9174	ZZ=	28.3768		
Eigenvalues:	-40.7719	48.6991		179.8355			
65	C	Isotropic=	61.536	Anisotropy	=	151.5919	
XX=	147.0358	YX=	-1.3515	ZX=	50.4616		
XY=	6.1557	YY=	54.6199	ZY=	14.9177		
XZ=	53.8561	YZ=	14.5259	ZZ=	-17.0476		
Eigenvalues:	-34.2685	56.2793		162.5973			
66	H	Isotropic=	23.9145	Anisotropy	=	8.1097	
XX=	22.1822	YX=	0.3036	ZX=	-1.5337		

XY=	-0.2859	YY=	24.1303	ZY=	-4.7488				
XZ=	-1.1218	YZ=	-3.945	ZZ=	25.431				
Eigenvalues:	20.024	22.3985	29.321						
67	O	Isotropic=	-99.2879	Anisotropy	=	670.2212			
XX=	-157.147	YX=	153.0215	ZX=	49.6325				
XY=	140.293	YY=	290.7757	ZY=	128.4846				
XZ=	57.0662	YZ=	49.5982	ZZ=	-431.4922				
Eigenvalues:	-447.1104	-198.2795	347.5263						
68	C	Isotropic=	54.4882	Anisotropy	=	173.0609			
XX=	-21.9069	YX=	16.4691	ZX=	9.1354				
XY=	4.3255	YY=	87.1693	ZY=	-89.4547				
XZ=	18.4138	YZ=	-64.4083	ZZ=	98.2023				
Eigenvalues:	-28.5076	22.11	169.8622						
69	H	Isotropic=	23.8407	Anisotropy	=	4.5787			
XX=	21.3598	YX=	-0.198	ZX=	-1.5079				
XY=	-0.4875	YY=	26.7355	ZY=	-0.8384				
XZ=	-0.897	YZ=	-0.6329	ZZ=	23.4267				
Eigenvalues:	20.743	23.8859	26.8931						
70	H	Isotropic=	23.8629	Anisotropy	=	2.7851			
XX=	21.4609	YX=	0.2141	ZX=	-1.7547				
XY=	-0.2215	YY=	25.0912	ZY=	0.1645				
XZ=	-1.4687	YZ=	0.2612	ZZ=	25.0366				
Eigenvalues:	20.8404	25.0287	25.7196						
71	H	Isotropic=	23.8863	Anisotropy	=	4.1882			
XX=	21.1817	YX=	0.5026	ZX=	-0.9398				
XY=	0.3752	YY=	26.1749	ZY=	-0.9307				
XZ=	-0.835	YZ=	-0.9733	ZZ=	24.3024				
Eigenvalues:	20.9404	24.0401	26.6785						
72	H	Isotropic=	23.9883	Anisotropy	=	6.959			
XX=	21.6036	YX=	-0.118	ZX=	0.0706				
XY=	-0.6191	YY=	28.1796	ZY=	1.9391				
XZ=	0.2257	YZ=	1.4001	ZZ=	22.1816				
Eigenvalues:	21.4198	21.9174	28.6276						
73	C	Isotropic=	61.2407	Anisotropy	=	176.1522			
XX=	41.7777	YX=	10.9207	ZX=	4.4505				
XY=	8.372	YY=	89.0118	ZY=	-104.2121				
XZ=	5.7482	YZ=	-107.9039	ZZ=	52.9327				
Eigenvalues:	-37.8954	442.9421	178.6755						
74	C	Isotropic=	62.0213	Anisotropy	=	176.7269			
XX=	-0.9318	YX=	-22.0568	ZX=	-36.741				
XY=	-23.5865	YY=	108.1128	ZY=	-84.7077				
XZ=	-38.5417	YZ=	-84.9309	ZZ=	78.8828				
Eigenvalues:	-40.5584	446.783	179.8392						
75	C	Isotropic=	62.0741	Anisotropy	=	177.4023			
XX=	-30.1581	YX=	24.6381	ZX=	15.065				
XY=	25.5984	YY=	117.3692	ZY=	-70.6239				
XZ=	14.6712	YZ=	-71.7036	ZZ=	99.011				
Eigenvalues:	-40.535	46.4149	180.3423						
76	C	Isotropic=	63.5818	Anisotropy	=	174.542			
XX=	47.2394	YX=	13.2651	ZX=	6.691				
XY=	17.9216	YY=	85.9161	ZY=	-105.8914				
XZ=	7.3924	YZ=	-107.8567	ZZ=	57.5899				
Eigenvalues:	-38.8789	49.6811	179.9431						
77	C	Isotropic=	67.2488	Anisotropy	=	163.5896			
XX=	9.6842	YX=	-24.7217	ZX=	-37.5891				
XY=	-17.5835	YY=	105.3179	ZY=	-80.4072				

XZ=	-33.263	YZ=	-78.297	ZZ=	86.7443				
Eigenvalues:	-27.9034	53.3413	176.3086						
78	H	Isotropic=	23.4731	Anisotropy	=	8.0114			
XX=	28.4308	YX=	-0.5336	ZX=	1.793				
XY=	0.6641	YY=	20.1316	ZY=	1.1899				
XZ=	1.4195	YZ=	1.0524	ZZ=	21.8567				
Eigenvalues:	19.5277	22.0775	28.814						
79	H	Isotropic=	23.7943	Anisotropy	=	4.45			
XX=	25.9987	YX=	-1.2659	ZX=	-0.3477				
XY=	-1.2234	YY=	22.237	ZY=	2.3254				
XZ=	-0.4722	YZ=	2.1513	ZZ=	23.1472				
Eigenvalues:	20.3165	24.3056	26.761						
80	H	Isotropic=	23.7561	Anisotropy	=	3.6731			
XX=	24.8944	YX=	-0.0197	ZX=	0.8039				
XY=	0.2776	YY=	22.8006	ZY=	2.772				
XZ=	0.7497	YZ=	2.5022	ZZ=	23.5732				
Eigenvalues:	20.4828	24.5807	26.2048						
81	H	Isotropic=	23.8236	Anisotropy	=	5.0608			
XX=	27.1174	YX=	-0.8325	ZX=	0.2083				
XY=	-0.4438	YY=	22.1099	ZY=	2.0084				
XZ=	0.249	YZ=	1.6435	ZZ=	22.2434				
Eigenvalues:	20.2933	23.9799	27.1974						
82	H	Isotropic=	23.7602	Anisotropy	=	8.2964			
XX=	26.1627	YX=	-3.497	ZX=	-1.7128				
XY=	-3.0919	YY=	23.107	ZY=	3.0514				
XZ=	-1.3924	YZ=	2.0864	ZZ=	22.011				
Eigenvalues:	19.7501	22.2394	29.2911						

2b

2bi_neg45

C	3.460459	-1.365445	1.595714
C	4.202478	-2.164579	0.478094
C	3.510705	-2.179315	-0.895358
C	4.276966	-1.406494	-1.984093
C	4.487192	0.093224	-1.694616
C	3.315394	0.917448	-1.184047
C	2.777557	0.483494	0.148738
C	1.445706	0.214081	0.248212
C	0.995115	-0.636366	1.40399
C	1.98278	-1.767457	1.709782
C	3.63087	0.166465	1.359589
C	5.111882	0.505942	1.270668
C	3.103944	0.936464	2.585775
C	0.425824	0.665993	-0.718605
C	5.594749	-2.071141	-2.311442
O	4.018805	-1.742929	2.853568
O	4.423907	-3.491044	0.933626
O	5.531808	0.6415	-2.055697
O	3.41116	2.316548	-1.412602
O	-0.248564	-1.343384	1.22767
H	3.583531	-3.835057	1.260572
C	4.401363	3.134973	-0.942566
O	5.385973	2.675204	-0.374058
C	4.108798	4.564624	-1.261736

H	5.250641	-1.760133	0.370516
H	2.47276	-1.767632	-0.823997
H	2.515743	0.667036	-1.97006
H	0.849673	0.031227	2.304868
H	1.785766	-2.122669	2.75782
H	1.766637	-2.628851	0.024442
H	5.569863	0.261965	0.286092
H	5.272561	1.597959	1.451952
H	5.667436	-0.047811	2.068154
H	3.927067	1.49744	3.092366
H	2.322941	1.6764	2.289889
H	2.680701	0.230758	3.341883
H	0.832609	1.362465	-1.49198
H	-0.042871	-0.213192	-1.230642
H	-0.379684	1.234479	-0.180726
H	6.086909	-1.546109	-3.166417
H	6.28964	-2.032684	-1.438416
H	5.426092	-3.139487	-2.587849
H	3.161316	4.663471	-1.84348
H	4.018734	5.133085	-0.304189
H	4.95843	4.978301	-1.857942
H	4.960734	-1.911134	2.723813
C	-1.419811	-0.674055	0.989268
O	-1.609447	0.395607	1.562247
H	3.628323	-1.426204	-2.908866
H	3.43362	-3.247826	-1.232014
C	-2.372505	-1.517094	0.147378
C	-3.848296	-1.226556	0.518431
O	-2.068178	-1.397673	-1.2178
H	-2.178423	-2.609011	0.376898
N	-4.365490	0.112591	0.366434
C	-4.750497	-2.236724	-0.159495
H	-3.887075	-1.439226	1.640316
H	-2.197738	-0.476683	-1.492852
C	-3.746068	1.259142	-0.078443
H	-5.281940	0.219284	0.74367
C	-4.794121	-2.362317	-1.550614
C	-5.638745	-3.301694	-2.142322
C	-6.445157	-4.117165	-1.349346
C	-6.405601	-3.993251	0.039707
C	-5.563505	-3.054999	0.633875
H	-4.147807	-1.72916	-2.178989
O	-2.613961	1.257249	-0.608011
C	-4.507365	2.532705	0.095834
H	-5.664447	-3.398793	-3.237793
H	-7.110136	-4.857987	-1.817211
H	-7.039095	-4.636204	0.668304
H	-5.538054	-2.963909	1.730464
C	-3.822087	3.646388	0.59438
C	-4.495707	4.856197	0.757604
C	-5.844543	4.957792	0.41657
C	-6.523017	3.849012	-0.090483
C	-5.858068	2.633714	-0.250338
H	-2.753552	3.555235	0.848133
H	-3.959136	5.731359	1.153137
H	-6.373665	5.914023	0.544209

H	-7.584403	3.932087	-0.367068
H	-6.397414	1.768406	-0.664233

```

2bi_neg45      E(RB+HF-PW91)      =      -2012.289735
SCF GIAO      Magnetic      shielding      tensor (ppm):
1      C      Isotropic=      110.8104      Anisotropy      30.2473
XX= 105.3667      YX= -2.6698      ZX= 20.3176
XY= 3.8172      YY= 107.7222      ZY= 1.3804
XZ= 14.0894      YZ= 0.505      ZZ= 119.3422
Eigenvalues: 93.7858 107.6702      130.9753
2      C      Isotropic=      112.3854      Anisotropy      31.5501
XX= 92.9188      YX= -0.4225      ZX= -0.7063
XY= -5.3283      YY= 131.862      ZY= -0.0691
XZ= 1.0375      YZ= -10.5777      ZZ= 112.3754
Eigenvalues: 92.705 111.0324      133.4188
3      C      Isotropic=      141.3093      Anisotropy      20.1082
XX= 122.5023      YX= -8.3551      ZX= 4.8824
XY= 0.0095      YY= 150.8159      ZY= 2.4386
XZ= 5.4541      YZ= 5.534      ZZ= 150.6097
Eigenvalues: 120.8036      148.4095      154.7147
4      C      Isotropic=      141.2256      Anisotropy      23.1406
XX= 129.144      YX= -1.4213      ZX= 2.2783
XY= -14.9339      YY= 153.0314      ZY= 5.489
XZ= 6.8342      YZ= 5.499      ZZ= 141.5014
Eigenvalues: 124.455 142.5691      156.6527
5      C      Isotropic=      -23.7235      Anisotropy      182.1764
XX= -46.5498      YX= 17.8494      ZX= 59.3165
XY= 3.7415      YY= -92.3514      ZY= -37.4187
XZ= 54.394      YZ= -46.903      ZZ= 67.7307
Eigenvalues: -113.7951      -55.1028      97.7275
6      C      Isotropic=      101.2128      Anisotropy      41.2333
XX= 88.1819      YX= -14.7565      ZX= 0.7795
XY= 3.5546      YY= 127.103      ZY= 3.3894
XZ= -5.3364      YZ= 7.4969      ZZ= 88.3534
Eigenvalues: 85.9852 88.9515 128.7016
7      C      Isotropic=      47.7282      Anisotropy      150.2205
XX= 49.735      YX= -12.755      ZX= -6.6378
XY= -29.3968      YY= 117.4592      ZY= 76.613
XZ= -0.8482      YZ= 55.142      ZZ= -24.0096
Eigenvalues: -50.1192      45.4286 147.8752
8      C      Isotropic=      38.3888      Anisotropy      161.5635
XX= 32.4344      YX= -9.3259      ZX= -13.7034
XY= -11.0943      YY= 89.4378      ZY= 80.0824
XZ= -26.0959      YZ= 98.809      ZZ= -6.7058
Eigenvalues: -61.6971      30.7657 146.0978
9      C      Isotropic=      110.9531      Anisotropy      55.3628
XX= 131.7536      YX= 25.7573      ZX= 11.2859
XY= 24.8743      YY= 104.0627      ZY= -8.658
XZ= 18.4343      YZ= -13.6471      ZZ= 97.043
Eigenvalues: 75.143 109.8546      147.8616
10     C      Isotropic=      146.8402      Anisotropy      44.1848
XX= 175.2076      YX= 5.7656      ZX= 3.0693
XY= 0.0355      YY= 133.5466      ZY= -4.7102
XZ= 10.4651      YZ= -12.683      ZZ= 131.7663
Eigenvalues: 122.9796      141.2441      176.2967

```

11	C	Isotropic=	147.6409	Anisotropy	11.718
XX=	143.4375	YX=	0.4197	ZX=	-0.4325
XY=	-13.9886	YY=	151.5566	ZY=	-0.8321
XZ=	-2.1037	YZ=	0.7907	ZZ=	147.9284
Eigenvalues:	139.4443		148.0254		155.4529
12	C	Isotropic=	155.0014	Anisotropy	22.5276
XX=	159.0954	YX=	1.6683	ZX=	-17.7406
XY=	6.3976	YY=	154.2496	ZY=	13.14
XZ=	-8.8143	YZ=	7.9326	ZZ=	151.6593
Eigenvalues:	135.2999		159.6846		170.0198
13	C	Isotropic=	148.2986	Anisotropy	54.3517
XX=	147.9542	YX=	-13.1251	ZX=	-8.5307
XY=	-19.6678	YY=	140.4223	ZY=	26.7084
XZ=	-5.7879	YZ=	29.4291	ZZ=	156.5193
Eigenvalues:	116.4658		143.8969		184.5331
14	C	Isotropic=	166.3249	Anisotropy	14.4665
XX=	170.8405	YX=	-9.4873	ZX=	5.1426
XY=	1.6168	YY=	161.6643	ZY=	4.6664
XZ=	8.6257	YZ=	2.4797	ZZ=	166.4699
Eigenvalues:	156.3113		166.6942		175.9692
15	C	Isotropic=	169.2414	Anisotropy	17.2103
XX=	172.597	YX=	-2.7704	ZX=	-9.9264
XY=	-5.2128	YY=	175.0078	ZY=	3.5122
XZ=	-6.0124	YZ=	2.4816	ZZ=	160.1194
Eigenvalues:	156.1865		170.8228		180.715
16	O	Isotropic=	263.1645	Anisotropy	82.4088
XX=	316.329	YX=	-0.305	ZX=	5.2909
XY=	18.9307	YY=	199.6345	ZY=	38.9468
XZ=	4.3608	YZ=	3.9808	ZZ=	273.5301
Eigenvalues:	193.3633		278.0265		318.1038
17	O	Isotropic=	265.5808	Anisotropy	44.6953
XX=	250.112	YX=	22.419	ZX=	1.4404
XY=	-0.6538	YY=	254.607	ZY=	-6.3822
XZ=	2.611	YZ=	-16.9098	ZZ=	292.0233
Eigenvalues:	239.6491		261.7156		295.3777
18	O	Isotropic=	-353.6597	Anisotropy	1076.0025
XX=	-736.3592	YX=	-268.6312	ZX=	432.8534
XY=	-233.7787	YY=	-514.418	ZY=	-46.8894
XZ=	376.2778	YZ=	-55.323	ZZ=	189.7982
Eigenvalues:	-990.3313		-434.323		363.6753
19	O	Isotropic=	87.531	Anisotropy	124.0561
XX=	100.9909	YX=	160.6628	ZX=	-58.0194
XY=	21.969	YY=	36.2835	ZY=	19.4856
XZ=	-36.4455	YZ=	78.8765	ZZ=	125.3187
Eigenvalues:	-53.701		146.0589		170.2351
20	O	Isotropic=	98.8197	Anisotropy	153.9063
XX=	135.1718	YX=	-28.5511	ZX=	5.1722
XY=	-152.1678	YY=	55.5671	ZY=	-76.4105
XZ=	-84.7816	YZ=	-112.7572	ZZ=	105.7202
Eigenvalues:	-63.9255		158.9607		201.4239
21	H	Isotropic=	31.1503	Anisotropy	13.6279
XX=	33.1925	YX=	3.5257	ZX=	-5.1418
XY=	2.9558	YY=	35.5546	ZY=	-4.314
XZ=	-5.0779	YZ=	-3.2667	ZZ=	24.7039
Eigenvalues:	21.9564		31.2591		40.2356
22	C	Isotropic=	20.1202	Anisotropy	74.469

XX=	39.2284	YX=	-78.2685	ZX=	-8.2363		
XY=	-39.1181	YY=	-45.5247	ZY=	-9.4339		
XZ=	-11.0081	YZ=	-26.6765	ZZ=	66.657		
Eigenvalues:	-78.4249	69.0194	69.7663				
23	O	Isotropic=	-130.6818	Anisotropy		599.4029	
XX=	-267.6521	YX=	-19.0684	ZX=	-293.6992		
XY=	-40.3789	YY=	-252.7962	ZY=	25.8401		
XZ=	-248.3172	YZ=	31.1333	ZZ=	128.4028		
Eigenvalues:	-406.4957	-254.4699	268.9201				
24	C	Isotropic=	166.1151	Anisotropy		36.8895	
XX=	158.3361	YX=	-3.9665	ZX=	6.117		
XY=	-4.6204	YY=	187.8881	ZY=	-9.1049		
XZ=	5.5385	YZ=	-7.7322	ZZ=	152.1212		
Eigenvalues:	147.9145	159.7228	190.7082				
25	H	Isotropic=	27.3884	Anisotropy		2.9316	
XX=	26.7796	YX=	0.1667	ZX=	-1.466		
XY=	1.3326	YY=	28.8078	ZY=	0.0328		
XZ=	-1.8494	YZ=	-0.5256	ZZ=	26.578		
Eigenvalues:	24.9875	27.8349	29.3429				
26	H	Isotropic=	27.9567	Anisotropy		8.2842	
XX=	29.7357	YX=	-3.7345	ZX=	-1.9487		
XY=	-3.3615	YY=	27.1857	ZY=	1.8159		
XZ=	-1.7109	YZ=	2.8455	ZZ=	26.9486		
Eigenvalues:	24.257	26.1335	33.4795				
27	H	Isotropic=	25.2236	Anisotropy		3.4858	
XX=	25.7728	YX=	2.1097	ZX=	-1.2938		
XY=	0.4616	YY=	26.6015	ZY=	0.6489		
XZ=	1.618	YZ=	-1.3803	ZZ=	23.2965		
Eigenvalues:	23.2133	24.91	27.5475				
28	H	Isotropic=	24.4501	Anisotropy		7.387	
XX=	28.9773	YX=	1.4446	ZX=	1.286		
XY=	-0.1888	YY=	21.0984	ZY=	3.6842		
XZ=	0.8809	YZ=	2.4684	ZZ=	23.2746		
Eigenvalues:	18.9221	25.0534	29.3748				
29	H	Isotropic=	28.5448	Anisotropy		6.4766	
XX=	29.7109	YX=	0.7011	ZX=	-1.5047		
XY=	0.0476	YY=	25.8749	ZY=	-4.2646		
XZ=	-0.7478	YZ=	-3.6514	ZZ=	30.0486		
Eigenvalues:	23.476	29.2958	32.8625				
30	H	Isotropic=	29.0358	Anisotropy		4.5591	
XX=	32.0007	YX=	0.557	ZX=	0.2309		
XY=	0.238	YY=	29.641	ZY=	1.6392		
XZ=	-0.4572	YZ=	2.4071	ZZ=	25.4657		
Eigenvalues:	24.6375	30.3948	32.0752				
31	H	Isotropic=	29.2348	Anisotropy		8.1781	
XX=	29.017	YX=	1.1365	ZX=	-2.8927		
XY=	1.0909	YY=	25.4721	ZY=	1.477		
XZ=	-2.8819	YZ=	-0.1215	ZZ=	33.2152		
Eigenvalues:	24.8455	28.172	34.6869				
32	H	Isotropic=	29.1245	Anisotropy		9.087	
XX=	27.0288	YX=	4.5832	ZX=	-0.2419		
XY=	3.8244	YY=	32.8671	ZY=	-0.8947		
XZ=	0.5791	YZ=	-1.4142	ZZ=	27.4775		
Eigenvalues:	24.6586	27.5324	35.1825				
33	H	Isotropic=	30.3382	Anisotropy		6.5482	
XX=	33.1067	YX=	1.311	ZX=	2.8231		

XY=	1.2862	YY=	28.7918	ZY=	-1.3488		
XZ=	3.0916	YZ=	-1.993	ZZ=	29.1162		
Eigenvalues:	25.9862	30.3249	34.7037				
34	H	Isotropic=	30.0902	Anisotropy		9.0822	
XX=	29.5562	YX=	1.6325	ZX=	0.514		
XY=	2.0131	YY=	29.0302	ZY=	4.451		
XZ=	2.0448	YZ=	5.3949	ZZ=	31.6842		
Eigenvalues:	25.1459	28.9797	36.145				
35	H	Isotropic=	30.0388	Anisotropy		6.4931	
XX=	30.5672	YX=	-2.304	ZX=	1.407		
XY=	-2.7247	YY=	31.4102	ZY=	2.956		
XZ=	-1.0564	YZ=	2.9496	ZZ=	28.1389		
Eigenvalues:	25.8987	29.8501	34.3675				
36	H	Isotropic=	28.3705	Anisotropy		6.2407	
XX=	27.0266	YX=	1.0831	ZX=	-1.3969		
XY=	0.3703	YY=	26.5892	ZY=	3.0662		
XZ=	-2.1007	YZ=	0.7443	ZZ=	31.4959		
Eigenvalues:	25.0224	27.5582	32.531				
37	H	Isotropic=	28.7359	Anisotropy		6.7154	
XX=	31.7381	YX=	1.1315	ZX=	-0.1351		
XY=	1.2609	YY=	27.7071	ZY=	-4.5469		
XZ=	-1.7457	YZ=	-4.2301	ZZ=	26.7624		
Eigenvalues:	22.8197	30.175	33.2128				
38	H	Isotropic=	28.2564	Anisotropy		11.2546	
XX=	32.0244	YX=	4.6129	ZX=	1.3769		
XY=	5.5848	YY=	26.5365	ZY=	0.8269		
XZ=	2.9201	YZ=	1.9812	ZZ=	26.2082		
Eigenvalues:	23.4852	25.5246	35.7594				
39	H	Isotropic=	27.4599	Anisotropy		11.2656	
XX=	33.5775	YX=	-2.0541	ZX=	-3.6942		
XY=	-3.1179	YY=	25.843	ZY=	-0.8501		
XZ=	-2.4427	YZ=	-1.0129	ZZ=	22.9592		
Eigenvalues:	21.5106	25.8988	34.9703				
40	H	Isotropic=	29.1656	Anisotropy		10.7659	
XX=	29.2639	YX=	1.7648	ZX=	-5.5462		
XY=	-0.0318	YY=	27.2557	ZY=	-1.4921		
XZ=	-6.2254	YZ=	-1.1844	ZZ=	30.9771		
Eigenvalues:	24.1559	26.998	36.3428				
41	H	Isotropic=	29.6106	Anisotropy		5.8867	
XX=	32.9325	YX=	-1.3876	ZX=	0.9938		
XY=	-1.8688	YY=	25.3861	ZY=	0.5028		
XZ=	0.9265	YZ=	-0.0445	ZZ=	30.5132		
Eigenvalues:	25.0174	30.2794	33.5351				
42	H	Isotropic=	30.47	Anisotropy		9.6103	
XX=	28.469	YX=	-1.2839	ZX=	-2.0448		
XY=	-1.3232	YY=	34.3267	ZY=	3.7197		
XZ=	-2.4889	YZ=	4.0547	ZZ=	28.6144		
Eigenvalues:	25.7425	28.7907	36.8769				
43	H	Isotropic=	28.9696	Anisotropy		5.455	
XX=	30.2858	YX=	0.7741	ZX=	2.9875		
XY=	-1.1776	YY=	30.4761	ZY=	-2.5661		
XZ=	3.1885	YZ=	-1.3534	ZZ=	26.147		
Eigenvalues:	24.072	30.2306	32.6063				
44	H	Isotropic=	29.1603	Anisotropy		6.918	
XX=	26.2841	YX=	-0.9302	ZX=	-0.5878		
XY=	0.389	YY=	31.8744	ZY=	3.4306		

XZ= -0.1973 YZ= 2.3248 ZZ= 29.3223
 Eigenvalues: 26.2312 27.4773 33.7723
 45 H Isotropic= 28.9481 Anisotropy 8.815
 XX= 29.5096 YX= 1.6773 ZX= -2.273
 XY= 3.8293 YY= 29.9053 ZY= -3.0793
 XZ= -3.1593 YZ= -3.2686 ZZ= 27.4294
 Eigenvalues: 25.0613 26.9583 34.8248
 46 H Isotropic= 30.5945 Anisotropy 17.9354
 XX= 40.491 YX= -5.1274 ZX= 4.2369
 XY= -3.3843 YY= 24.1857 ZY= -3.507
 XZ= 2.6164 YZ= -1.658 ZZ= 27.1067
 Eigenvalues: 22.4057 26.8263 42.5514
 47 C Isotropic= 8.1295 Anisotropy 92.436
 XX= -69.5596 YX= -3.0722 ZX= -59.6878
 XY= 29.8844 YY= 46.124 ZY= 0.806
 XZ= -39.7157 YZ= -10.6076 ZZ= 47.8242
 Eigenvalues: -88.662 43.2971 69.7535
 48 O Isotropic= -151.1358 Anisotropy 690.1624
 XX= -254.7757 YX= 112.7375 ZX= -170.0099
 XY= 113.5061 YY= -305.7852 ZY= -275.9542
 XZ= -181.4666 YZ= -243.6162 ZZ= 107.1534
 Eigenvalues: -436.684-325.6959 308.9724
 49 H Isotropic= 28.6562 Anisotropy 6.4772
 XX= 29.3105 YX= -1.808 ZX= 0.8747
 XY= -1.8434 YY= 24.2891 ZY= 0.0589
 XZ= 2.0909 YZ= 1.0176 ZZ= 32.369
 Eigenvalues: 23.5852 29.4091 32.9743
 50 H Isotropic= 29.4361 Anisotropy 6.5805
 XX= 26.8172 YX= 1.0457 ZX= -0.9134
 XY= 0.7593 YY= 32.3646 ZY= 2.0202
 XZ= -1.2627 YZ= 3.1905 ZZ= 29.1264
 Eigenvalues: 25.7875 28.6977 33.8231
 51 C Isotropic= 112.4579 Anisotropy 15.4782
 XX= 122.6796 YX= 2.9883 ZX= 0.1796
 XY= 0.1203 YY= 97.8877 ZY= -5.835
 XZ= 0.4621 YZ= -4.9183 ZZ= 116.8065
 Eigenvalues: 96.371 118.2261 122.7767
 52 C Isotropic= 125.0033 Anisotropy 15.909
 XX= 117.9538 YX= 8.7552 ZX= 6.548
 XY= 8.135 YY= 131.5676 ZY= -4.4273
 XZ= 7.1227 YZ= -2.3671 ZZ= 125.4885
 Eigenvalues: 110.1228 129.2777 135.6093
 53 O Isotropic= 262.7151 Anisotropy 42.4517
 XX= 262.2264 YX= -3.6665 ZX= -4.3318
 XY= 7.5949 YY= 286.3612 ZY= -31.8844
 XZ= -10.0699 YZ= 2.9001 ZZ= 239.5577
 Eigenvalues: 233.9756 263.1535 291.0163
 54 H Isotropic= 26.4173 Anisotropy 5.8292
 XX= 29.6858 YX= 1.9056 ZX= 1.7853
 XY= -2.4247 YY= 25.8918 ZY= -2.7547
 XZ= 1.2188 YZ= -3.1392 ZZ= 23.6742
 Eigenvalues: 21.487 27.4615 30.3034
 55 N Isotropic= 120.7895 Anisotropy 101.4516
 XX= 60.7636 YX= 67.1073 ZX= 25.9718
 XY= 38.4737 YY= 166.2327 ZY= -4.6946
 XZ= 46.1662 YZ= -17.2665 ZZ= 135.3724

Eigenvalues: 25.9969 147.9477 188.424
 56 C Isotropic= 52.5618 Anisotropy 187.3371
 XX= 80.3824 YX= -101.9553 ZX= -3.425
 XY= -96.948 YY= 74.114 ZY= -24.0657
 XZ= -8.4042 YZ= -19.7942 ZZ= 3.189
 Eigenvalues: -33.2552 13.4874 177.4532
 57 H Isotropic= 26.6042 Anisotropy 6.9982
 XX= 25.0679 YX= 1.8751 ZX= -0.3396
 XY= 1.6074 YY= 26.233 ZY= -2.9267
 XZ= -2.0785 YZ= -3.168 ZZ= 28.5118
 Eigenvalues: 23.5479 24.9951 31.2697
 58 H Isotropic= 27.574 Anisotropy 13.6552
 XX= 22.3512 YX= -0.4613 ZX= -0.4349
 XY= -1.5343 YY= 35.816 ZY= -4.1037
 XZ= -0.5564 YZ= -2.158 ZZ= 24.5549
 Eigenvalues: 21.9973 24.0473 36.6775
 59 C Isotropic= 16.4394 Anisotropy 117.2289
 XX= 42.8986 YX= 2.102 ZX= 29.4603
 XY= 16.644 YY= -62.6393 ZY= 18.3591
 XZ= 35.9917 YZ= 24.5049 ZZ= 69.0588
 Eigenvalues: -66.2083 20.9344 94.592
 60 H Isotropic= 26.3423 Anisotropy 9.2735
 XX= 26.9574 YX= -1.8883 ZX= -3.4888
 XY= -1.3973 YY= 31.8622 ZY= 0.3843
 XZ= -2.262 YZ= -4.8557 ZZ= 20.2072
 Eigenvalues: 18.6097 27.8925 32.5246
 61 C Isotropic= 59.2547 Anisotropy 180.0028
 XX= 91.5744 YX= -96.4568 ZX= 26.0909
 XY= -90.5694 YY= 79.3432 ZY= 29.9428
 XZ= 31.6854 YZ= 20.8033 ZZ= 6.8464
 Eigenvalues: -39.7342 38.2417 179.2565
 62 C Isotropic= 61.9379 Anisotropy 176.7923
 XX= 119.3812 YX= -65.3224 ZX= 2.604
 XY= -65.8052 YY= 107.9469 ZY= -8.0339
 XZ= 3.4605 YZ= -10.3596 ZZ= -41.5142
 Eigenvalues: -42.0853 48.0996 179.7995
 63 C Isotropic= 63.3533 Anisotropy 176.3112
 XX= 87.8549 YX= -100.4691 ZX= -16.6757
 XY= -102.8973 YY= 69.1023 ZY= -29.5024
 XZ= -18.0653 YZ= -28.0215 ZZ= 33.1025
 Eigenvalues: -38.7856 47.9513 180.8941
 64 C Isotropic= 62.8756 Anisotropy 173.0979
 XX= 89.2347 YX= -93.6557 ZX= 31.7558
 XY= -93.5874 YY= 79.4216 ZY= 26.2845
 XZ= 33.9286 YZ= 27.2384 ZZ= 19.9704
 Eigenvalues: -39.2857 49.6383 178.2742
 65 C Isotropic= 62.0682 Anisotropy 146.0113
 XX= 113.0071 YX= -50.5536 ZX= 3.7945
 XY= -46.5676 YY= 107.673 ZY= -8.6232
 XZ= 3.7891 YZ= -10.0761 ZZ= -34.4756
 Eigenvalues: -35.0907 61.8862 159.409
 66 H Isotropic= 22.4879 Anisotropy 11.8347
 XX= 23.7552 YX= 4.0203 ZX= 4.6426
 XY= 3.326 YY= 19.528 ZY= 2.484
 XZ= 3.891 YZ= 3.8076 ZZ= 24.1806
 Eigenvalues: 17.3089 19.7771 30.3777

67	O	Isotropic=	-72.8961	Anisotropy	579.4056
XX=	-212.9094	YX=	-10.1277	ZX=	256.6269
XY=	-46.9622	YY=	-167.9902	ZY=	74.9643
XZ=	291.5654	YZ=	81.8142	ZZ=	162.2113
Eigenvalues:	-376.2394		-155.8231		313.3743
68	C	Isotropic=	55.0221	Anisotropy	170.3961
XX=	28.0723	YX=	36.209	ZX=	-30.8763
XY=	40.5896	YY=	1.5733	ZY=	-37.2145
XZ=	-51.2796	YZ=	-55.5412	ZZ=	135.4206
Eigenvalues:	-27.4287	23.8754	168.6195		
69	H	Isotropic=	23.6467	Anisotropy	5.5433
XX=	23.617	YX=	3.4862	ZX=	0.4378
XY=	3.4393	YY=	23.7149	ZY=	0.8612
XZ=	0.4468	YZ=	0.7694	ZZ=	23.6081
Eigenvalues:	20.1828	23.415	27.3422		
70	H	Isotropic=	23.6942	Anisotropy	3.2477
XX=	22.803	YX=	2.4347	ZX=	-0.4186
XY=	2.2418	YY=	22.7536	ZY=	-0.2669
XZ=	-0.5138	YZ=	-0.1953	ZZ=	25.5259
Eigenvalues:	20.4346	24.7886	25.8593		
71	H	Isotropic=	23.7656	Anisotropy	4.4843
XX=	23.0309	YX=	2.8923	ZX=	0.6273
XY=	2.9163	YY=	23.3709	ZY=	1.0378
XZ=	0.5413	YZ=	0.8648	ZZ=	24.8949
Eigenvalues:	20.2799	24.2617	26.7551		
72	H	Isotropic=	24.1223	Anisotropy	8.0602
XX=	25.0442	YX=	4.2456	ZX=	-0.6959
XY=	4.2728	YY=	24.9999	ZY=	-0.7185
XZ=	-0.9846	YZ=	-1.1092	ZZ=	22.3227
Eigenvalues:	20.7606	22.1105	29.4957		
73	C	Isotropic=	60.5306	Anisotropy	177.2969
XX=	-24.4081	YX=	8.9415	ZX=	-52.3257
XY=	9.274	YY=	49.804	ZY=	-33.9756
XZ=	-46.7872	YZ=	-34.8501	ZZ=	156.1958
Eigenvalues:	-37.1134	39.9766	178.7285		
74	C	Isotropic=	61.7587	Anisotropy	177.6294
XX=	32.2579	YX=	-27.1215	ZX=	-48.0952
XY=	-24.4978	YY=	2.6219	ZY=	-57.4612
XZ=	-47.2756	YZ=	-59.0515	ZZ=	150.3964
Eigenvalues:	-41.3656	46.4635	180.1784		
75	C	Isotropic=	61.8787	Anisotropy	178.2636
XX=	34.3413	YX=	45.4595	ZX=	-27.6235
XY=	45.5175	YY=	-9.9532	ZY=	-42.1183
XZ=	-26.9879	YZ=	-41.6784	ZZ=	161.248
Eigenvalues:	-40.8304	45.7454	180.7211		
76	C	Isotropic=	63.6933	Anisotropy	174.864
XX=	-23.8359	YX=	15.9925	ZX=	-53.0081
XY=	13.36	YY=	57.3613	ZY=	-31.4101
XZ=	-52.1771	YZ=	-27.8557	ZZ=	157.5546
Eigenvalues:	-38.4434	49.254	180.2693		
77	C	Isotropic=	67.7184	Anisotropy	161.0099
XX=	42.7444	YX=	-21.6272	ZX=	-44.9869
XY=	-26.9138	YY=	14.0288	ZY=	-54.3711
XZ=	-48.2386	YZ=	-50.3394	ZZ=	146.3821
Eigenvalues:	-27.2868	55.3837	175.0584		
78	H	Isotropic=	23.1222	Anisotropy	8.1828

XX=	22.4732	YX=	-1.0351	ZX=	0.1512				
XY=	-1.1296	YY=	27.8481	ZY=	2.334				
XZ=	0.1781	YZ=	2.25	ZZ=	19.0454				
Eigenvalues:	18.4401	22.3492	28.5774						
79	H	Isotropic=	23.6648	Anisotropy	5.3189				
XX=	25.3701	YX=	-2.0161	ZX=	0.661				
XY=	-1.7489	YY=	25.2826	ZY=	1.0131				
XZ=	0.8746	YZ=	0.8352	ZZ=	20.3417				
Eigenvalues:	19.932	23.8517	27.2107						
80	H	Isotropic=	23.7075	Anisotropy	3.7308				
XX=	25.4726	YX=	0.1417	ZX=	1.3851				
XY=	0.3386	YY=	24.6379	ZY=	1.2349				
XZ=	1.5703	YZ=	1.3536	ZZ=	21.012				
Eigenvalues:	20.2503	24.6775	26.1947						
81	H	Isotropic=	23.9111	Anisotropy	5.1378				
XX=	24.2317	YX=	-1.2189	ZX=	0.8104				
XY=	-1.0136	YY=	26.7479	ZY=	1.3497				
XZ=	1.0729	YZ=	1.4979	ZZ=	20.7537				
Eigenvalues:	20.096	24.3011	27.3363						
82	H	Isotropic=	24.1138	Anisotropy	8.8201				
XX=	26.0341	YX=	-3.95	ZX=	1.0645				
XY=	-3.4287	YY=	26.3713	ZY=	-0.0611				
XZ=	1.8	YZ=	0.0717	ZZ=	19.9361				
Eigenvalues:	19.4856	22.862	29.9939						

2bii_neg45

C	-3.169448	-1.913519	-1.25179
C	-3.689192	-2.522658	0.088769
C	-2.924244	-2.092552	1.351702
C	-3.748378	-1.208415	2.305042
C	-4.238358	0.122821	1.700992
C	-3.264294	0.971875	0.898843
C	-2.739362	0.316407	-0.345629
C	-1.390660.247776	-0.514898	
C	-0.848759	-0.785253	-1.460415
C	-1.654031	-2.091795	-1.423368
C	-3.590506	-0.418009	-1.360697
C	-5.100071	-0.299237	-1.2124
C	-3.267328	0.100398	-2.7756
C	-0.417498	1.134614	0.149927
C	-4.90585-1.972309	2.907026	
O	-3.728433	-2.667115	-2.32681
O	-3.702537	-3.937251	-0.025254
O	-5.340151	0.571325	2.026704
O	-3.590779	2.351382	0.808693
O	0.485765	-1.252659	-1.187549
H	-2.832406	-4.217468	-0.334908
C	-4.739189	2.862479	0.264923
O	-5.653647	2.123366	-0.081986
C	-4.690445	4.35415	0.217273
H	-4.783713	-2.271496	0.204616
H	-1.981332	-1.554171.0823	
H	-2.384477	1.047473	1.634065
H	-0.828619	-0.347526	-2.502253
H	-1.463579	-2.638045	-2.387272
H	-1.252678	-2.735133	-0.596059

H	-5.452184	-0.359362	-0.158122
H	-5.456835	0.675511	-1.629401
H	-5.594547	-1.112635	-1.799943
H	-4.201962	0.361921	-3.329508
H	-2.630172	1.015228	-2.732387
H	-2.745782	-0.685879	-3.374316
H	-0.896031	1.898736	0.810509
H	0.318163	0.545348	0.756548
H	0.128969	1.698918	-0.652859
H	-5.431218	-1.338993	3.663212
H	-5.647522	-2.258109	2.122937
H	-4.534392	-2.900563	3.40363
H	-3.762825	4.74474	0.699593
H	-4.718471	4.678381	-0.851701
H	-5.586821	4.757833	0.748624
H	-4.607508	-2.964509	-2.059233
C	1.589335	-0.43873	-1.162485
O	1.703203	0.405939	-2.046132
H	-3.052407	-0.899662	3.139668
H	-2.639537	-3.020752	1.916152
C	2.608198	-1.015164	-0.175521
C	4.057608	-0.954851	-0.691858
O	2.375464	-0.467615	1.101359
H	2.359047	-2.115779	-0.045577
N	4.80459	0.220246	-1.058001
C	4.913244	-1.813501	0.231653
H	3.959659	-1.536863	-1.677504
H	2.801259	0.401479	1.139538
C	4.791679	1.597983	-1.173924
H	5.629395	-0.121931	-1.53919
C	5.031345	-1.549414	1.597794
C	5.828475	-2.364678	2.402064
C	6.515821	-3.442354	1.845597
C	6.406659	-3.704444	0.479585
C	5.611237	-2.891863	-0.325989
H	4.494699	-0.701203	2.048563
O	5.798695	2.042259	-1.782273
C	4.014717	2.579092	-0.363372
H	5.914076	-2.152483	4.78099
H	7.144616	-4.083422	4.80956
H	6.950723	-4.551191	0.035615
H	5.534527	-3.102309	-1.403781
C	4.760131	3.699998	0.061562
C	4.1665	4.698617	0.826219
C	2.816716	4.610074	1.172585
C	2.070964	3.517041	0.741875
C	2.670262	2.512144	-0.021129
H	5.821845	3.782503	-0.228209
H	4.762949	5.564135	1.151681
H	2.346497	5.401429	1.774617
H	1.001565	3.437034	0.990965
H	2.052582	1.679659	-0.373811

2bii_neg45 E(RB+HF-PW91) = -2012.243685
 SCF GIAO Magnetic shielding tensor (ppm):

1	C	Isotropic=	110.779	Anisotropy	31.4935
XX=	108.2912	YX=	7.4289	ZX=	20.0193
XY=	-1.976	YY=	107.7858	ZY=	3.5845
XZ=	16.0013	YZ=	4.9286	ZZ=	116.2599
Eigenvalues:	93.808	106.7543		131.7747	
2	C	Isotropic=	111.9499	Anisotropy	30.1978
XX=	92.9646	YX=	-4.8883	ZX=	2.1204
XY=	-0.856	YY=	131.8706	ZY=	-5.4158
XZ=	0.7383	YZ=	5.4866	ZZ=	111.0144
Eigenvalues:	92.6427	111.1252		132.0817	
3	C	Isotropic=	141.4587	Anisotropy	19.9586
XX=	123.258	YX=	4.5225	ZX=	6.6115
XY=	-2.4055	YY=	149.8841	ZY=	-1.3693
XZ=	9.1029	YZ=	-4.6763	ZZ=	151.234
Eigenvalues:	121.0903	148.5214		154.7645	
4	C	Isotropic=	140.4362	Anisotropy	24.2513
XX=	127.0401	YX=	-2.7704	ZX=	4.6945
XY=	11.7882	YY=	151.4558	ZY=	-9.1916
XZ=	5.3223	YZ=	-7.5318	ZZ=	142.8129
Eigenvalues:	123.8343	140.8706		156.6037	
5	C	Isotropic=	-22.9271	Anisotropy	180.4945
XX=	-36.8262	YX=	6.0754	ZX=	58.2871
XY=	18.093	YY=	-59.194	ZY=	77.8701
XZ=	47.6533	YZ=	87.6395	ZZ=	27.239
Eigenvalues:	-113.9686	-52.2151		197.4026	
6	C	Isotropic=	101.4255	Anisotropy	40.5992
XX=	88.0176	YX=	7.4047	ZX=	0.0191
XY=	-11.3301	YY=	122.9023	ZY=	-11.2446
XZ=	-1.2174	YZ=	-16.5974	ZZ=	93.3566
Eigenvalues:	86.611	89.1739		128.4916	
7	C	Isotropic=	45.0635	Anisotropy	154.9534
XX=	38.9595	YX=	-2.4379	ZX=	5.7094
XY=	13.4115	YY=	80.5746	ZY=	-107.7879
XZ=	4.0297	YZ=	-81.8605	ZZ=	15.6563
Eigenvalues:	-52.6688	39.4934		148.3657	
8	C	Isotropic=	42.1054	Anisotropy	156.8731
XX=	35.9766	YX=	-11.3192	ZX=	1.0714
XY=	-9.0079	YY=	39.4038	ZY=	-89.3065
XZ=	-12.5608	YZ=	-113.258	ZZ=	50.9359
Eigenvalues:	-57.6488	37.2776		146.6875	
9	C	Isotropic=	110.7428	Anisotropy	55.7829
XX=	138.7293	YX=	-17.3271	ZX=	13.9578
XY=	-15.535	YY=	104.4558	ZY=	9.7877
XZ=	21.214	YZ=	15.2046	ZZ=	89.0433
Eigenvalues:	73.5751	110.7218		147.9314	
10	C	Isotropic=	145.9312	Anisotropy	44.6128
XX=	174.248	YX=	3.8116	ZX=	0.2602
XY=	8.6895	YY=	137.9238	ZY=	2.1072
XZ=	6.1759	YZ=	11.7098	ZZ=	125.6216
Eigenvalues:	122.5197	139.6007		175.673	
11	C	Isotropic=	147.1637	Anisotropy	12.4135
XX=	140.1842	YX=	-2.4201	ZX=	1.2884
XY=	12.7465	YY=	152.6498	ZY=	-1.5894
XZ=	-3.7981	YZ=	-2.8375	ZZ=	148.6571
Eigenvalues:	138.3048	147.7469		155.4394	
12	C	Isotropic=	155.344	Anisotropy	22.0043

XX=	159.3646	YX=	-4.8916	ZX=	-14.4134		
XY=	-8.3816	YY=	147.5068	ZY=	-13.6864		
XZ=	-6.1587	YZ=	-7.3454	ZZ=	159.1607		
Eigenvalues:	135.963	160.0554		170.0136			
13	C	Isotropic=	148.2243	Anisotropy		54.6338	
XX=	141.7611	YX=	10.3031	ZX=	-5.6168		
XY=	19.2831	YY=	131.9028	ZY=	-22.9455		
XZ=	-3.8595	YZ=	-23.7771	ZZ=	171.0091		
Eigenvalues:	115.6695		144.3567		184.6469		
14	C	Isotropic=	164.0951	Anisotropy		13.2268	
XX=	167.141	YX=	12.5087	ZX=	2.0413		
XY=	2.8531	YY=	161.3372	ZY=	-5.2298		
XZ=	7.7891	YZ=	-2.6885	ZZ=	163.807		
Eigenvalues:	152.6863		166.6859		172.9129		
15	C	Isotropic=	169.2734	Anisotropy		17.1835	
XX=	170.5233	YX=	-0.5444	ZX=	-9.9428		
XY=	2.7764	YY=	173.2415	ZY=	-8.4344		
XZ=	-6.9408	YZ=	-6.6165	ZZ=	164.0554		
Eigenvalues:	156.2665		170.8247		180.729		
16	O	Isotropic=	262.774	Anisotropy		82.8581	
XX=	316.7222	YX=	23.9171	ZX=	2.8733		
XY=	0.1487	YY=	193.6409	ZY=	-16.8586		
XZ=	1.7088	YZ=	16.0056	ZZ=	277.959		
Eigenvalues:	192.4706		277.8387		318.0128		
17	O	Isotropic=	265.8469	Anisotropy		45.2686	
XX=	254.4378	YX=	-20.1867	ZX=	8.3036		
XY=	2.2367	YY=	258.4459	ZY=	14.6556		
XZ=	1.7144	YZ=	26.6842	ZZ=	284.657		
Eigenvalues:	239.8403		261.6744		296.026		
18	O	Isotropic=	-358.1164	Anisotropy		1080.6087	
XX=	-774.0548	YX=	331.8748	ZX=	408.0761		
XY=	283.8235	YY=	-351.3519	ZY=	236.2952		
XZ=	358.9018	YZ=	232.9337	ZZ=	51.0575		
Eigenvalues:	-997.3843		-439.2543		362.2894		
19	O	Isotropic=	89.0508	Anisotropy		125.2786	
XX=	130.5978	YX=	-156.8524	ZX=	-13.4944		
XY=	-12.1223	YY=	-8.944	ZY=	7.6598		
XZ=	-17.2132	YZ=	-38.1317	ZZ=	145.4987		
Eigenvalues:	-50.8523	145.4349		172.5699			
20	O	Isotropic=	89.1233	Anisotropy		163.1124	
XX=	93.1494	YX=	31.9468	ZX=	-5.3394		
XY=	126.901	YY=	126.8586	ZY=	73.3216		
XZ=	-131.5019	YZ=	97.9656	ZZ=	47.362		
Eigenvalues:	-70.3565	139.8615		197.8649			
21	H	Isotropic=	31.1779	Anisotropy		13.7097	
XX=	33.8997	YX=	-5.1345	ZX=	-5.093		
XY=	-4.3567	YY=	35.2071	ZY=	1.1077		
XZ=	-5.0746	YZ=	0.0922	ZZ=	24.4268		
Eigenvalues:	22.06	31.1559	40.3177				
22	C	Isotropic=	20.161	Anisotropy		75.2825	
XX=	13.5986	YX=	87.3554	ZX=	-28.8751		
XY=	47.0446	YY=	-9.465	ZY=	25.1595		
XZ=	-24.7343	YZ=	39.4573	ZZ=	56.3494		
Eigenvalues:	-79.1235	69.2571	70.3493				
23	O	Isotropic=	-132.743	Anisotropy		601.0282	
XX=	-309.7545	YX=	-55.8641	ZX=	-254.1892		

XY=	-20.3654	YY=	-258.7819	ZY=	23.7253		
XZ=	-212.705	YZ=	28.6429	ZZ=	170.3075		
Eigenvalues:	-408.9376		-257.2338		267.9425		
24	C	Isotropic=	166.2052	Anisotropy		37.0062	
XX=	158.359	YX=	-0.0311	ZX=	4.0528		
XY=	-0.1746	YY=	190.8756	ZY=	1.0219		
XZ=	3.5034	YZ=	-0.8562	ZZ=	149.3812		
Eigenvalues:	148.0025		159.7371		190.8761		
25	H	Isotropic=	27.3634	Anisotropy		2.9955	
XX=	27.0025	YX=	-0.8352	ZX=	-1.2719		
XY=	-2.0159	YY=	28.3172	ZY=	-0.5676		
XZ=	-1.5227	YZ=	0.0086	ZZ=	26.7705		
Eigenvalues:	25.0354	27.6943	29.3604				
26	H	Isotropic=	27.9622	Anisotropy		8.1683	
XX=	28.4271	YX=	3.1476	ZX=	-2.4334		
XY=	3.1668	YY=	27.0504	ZY=	-2.0916		
XZ=	-2.2166	YZ=	-3.2181	ZZ=	28.409		
Eigenvalues:	24.342	26.1368	33.4077				
27	H	Isotropic=	25.3441	Anisotropy		3.3851	
XX=	26.188	YX=	-2.2993	ZX=	-0.6897		
XY=	-0.1312	YY=	26.5414	ZY=	-1.4025		
XZ=	1.1949	YZ=	1.344	ZZ=	23.303		
Eigenvalues:	23.279	25.1526	27.6009				
28	H	Isotropic=	24.5647	Anisotropy		6.6675	
XX=	28.7981	YX=	0.1256	ZX=	1.5405		
XY=	1.2425	YY=	19.9947	ZY=	-2.1773		
XZ=	0.2647	YZ=	-1.0119	ZZ=	24.9013		
Eigenvalues:	19.4324	25.252	29.0097				
29	H	Isotropic=	28.4317	Anisotropy		6.5881	
XX=	29.3405	YX=	-0.3698	ZX=	-2.0607		
XY=	0.5698	YY=	27.5739	ZY=	4.6646		
XZ=	-1.5435	YZ=	4.0227	ZZ=	28.3809		
Eigenvalues:	23.3306	29.1408	32.8238				
30	H	Isotropic=	29.1081	Anisotropy		4.9968	
XX=	32.4293	YX=	-0.3715	ZX=	0.1831		
XY=	-0.0293	YY=	28.3715	ZY=	-2.0254		
XZ=	-0.4628	YZ=	-2.9343	ZZ=	26.5235		
Eigenvalues:	24.7942	30.0909	32.4393				
31	H	Isotropic=	29.1799	Anisotropy		8.0949	
XX=	29.0751	YX=	-1.0787	ZX=	-2.0834		
XY=	-1.1579	YY=	25.091	ZY=	0.3325		
XZ=	-2.4567	YZ=	1.8851	ZZ=	33.3734		
Eigenvalues:	24.7645	28.1987	34.5764				
32	H	Isotropic=	29.1391	Anisotropy		9.1194	
XX=	28.743	YX=	-5.1625	ZX=	0.9079		
XY=	-4.3802	YY=	31.6761	ZY=	0.0707		
XZ=	1.4381	YZ=	0.7267	ZZ=	26.9984		
Eigenvalues:	24.627	27.5717	35.2187				
33	H	Isotropic=	30.2049	Anisotropy		6.6918	
XX=	33.6231	YX=	0.2626	ZX=	2.4001		
XY=	0.2541	YY=	29.4711	ZY=	1.7508		
XZ=	2.5047	YZ=	2.3549	ZZ=	27.5206		
Eigenvalues:	25.7199	30.2288	34.6661				
34	H	Isotropic=	30.0438	Anisotropy		9.3085	
XX=	30.3205	YX=	-1.2851	ZX=	1.8594		
XY=	-1.3505	YY=	26.1967	ZY=	-2.7454		

XZ=	3.6594	YZ=	-3.2907	ZZ=	33.6141		
Eigenvalues:	25.1002	28.7817	36.2494				
35	H	Isotropic=	30.1542	Anisotropy	5.9142		
XX=	29.6398	YX=	2.0925	ZX=	1.4519		
XY=	1.7242	YY=	30.7337	ZY=	-3.1376		
XZ=	-0.9135	YZ=	-3.4691	ZZ=	30.0891		
Eigenvalues:	26.3748	29.9909	34.097				
36	H	Isotropic=	28.4332	Anisotropy	6.3376		
XX=	27.1835	YX=	-1.2974	ZX=	-0.3541		
XY=	-0.9115	YY=	25.6454	ZY=	-1.685		
XZ=	-1.5775	YZ=	0.6109	ZZ=	32.4706		
Eigenvalues:	24.9532	27.6881	32.6582				
37	H	Isotropic=	28.328	Anisotropy	6.7623		
XX=	31.9426	YX=	0.1239	ZX=	-1.2895		
XY=	-0.0741	YY=	29.0854	ZY=	4.4384		
XZ=	-2.5946	YZ=	4.03	ZZ=	23.9559		
Eigenvalues:	21.2952	30.8525	32.8361				
38	H	Isotropic=	27.7594	Anisotropy	11.2421		
XX=	33.3601	YX=	-3.2989	ZX=	2.4758		
XY=	-3.3882	YY=	25.5373	ZY=	1.4318		
XZ=	3.6225	YZ=	-0.2064	ZZ=	24.3807		
Eigenvalues:	22.4046	25.6194	35.2541				
39	H	Isotropic=	28.2867	Anisotropy	8.3299		
XX=	31.3529	YX=	2.891	ZX=	-2.9164		
XY=	3.0179	YY=	28.7856	ZY=	-0.2804		
XZ=	-2.6407	YZ=	0.7861	ZZ=	24.7216		
Eigenvalues:	23.3736	27.6465	33.8399				
40	H	Isotropic=	29.1426	Anisotropy	10.8184		
XX=	28.8303	YX=	-2.75	ZX=	-5.108		
XY=	-1.007	YY=	27.3982	ZY=	1.5676		
XZ=	-6.1907	YZ=	1.1826	ZZ=	31.1994		
Eigenvalues:	24.1197	26.9533	36.3549				
41	H	Isotropic=	29.5993	Anisotropy	6.018		
XX=	32.3307	YX=	2.7212	ZX=	0.2978		
XY=	3.2059	YY=	26.3524	ZY=	0.5271		
XZ=	0.0161	YZ=	1.107	ZZ=	30.1147		
Eigenvalues:	25.0366	30.15	33.6113				
42	H	Isotropic=	30.4604	Anisotropy	9.5559		
XX=	28.0667	YX=	-0.4488	ZX=	-1.2682		
XY=	-0.3926	YY=	32.263	ZY=	-4.8778		
XZ=	-1.6922	YZ=	-5.2935	ZZ=	31.0516		
Eigenvalues:	25.7072	28.8431	36.831				
43	H	Isotropic=	28.9763	Anisotropy	5.714		
XX=	30.4625	YX=	-0.2165	ZX=	2.4703		
XY=	1.7973	YY=	31.4731	ZY=	1.892		
XZ=	2.7782	YZ=	0.8117	ZZ=	24.9933		
Eigenvalues:	23.8145	30.3288	32.7856				
44	H	Isotropic=	29.1287	Anisotropy	6.8303		
XX=	26.339	YX=	-0.1658	ZX=	0.0851		
XY=	-1.3902	YY=	30.2467	ZY=	-3.5514		
XZ=	0.8478	YZ=	-2.5349	ZZ=	30.8004		
Eigenvalues:	26.1842	27.5196	33.6823				
45	H	Isotropic=	28.8974	Anisotropy	8.922		
XX=	30.3195	YX=	-2.1417	ZX=	-2.4074		
XY=	-4.5381	YY=	30.1357	ZY=	2.2229		
XZ=	-2.5807	YZ=	2.1561	ZZ=	26.237		

Eigenvalues: 24.9479 26.899 34.8454
 46 H Isotropic= 30.4866 Anisotropy 17.9828
 XX= 38.4098 YX= 8.581 ZX= 0.8142
 XY= 6.6744 YY= 27.5669 ZY= 3.5216
 XZ= 0.0808 YZ= 1.1581 ZZ= 25.4832
 Eigenvalues: 22.4354 26.5493 42.4752
 47 C Isotropic= 5.8197 Anisotropy 98.8753
 XX= -69.6143 YX= -20.1292 ZX= -57.2117
 XY= -50.3962 YY= 40.4383 ZY= 0.3292
 XZ= -28.7244 YZ= 11.1514 ZZ= 46.6352
 Eigenvalues: -91.4909 37.2135 71.7366
 48 O Isotropic= -148.5247 Anisotropy 690.4455
 XX= -244.0667 YX= -169.3047 ZX= -142.5729
 XY= -160.3301 YY= -134.1921 ZY= 320.3475
 XZ= -155.7996 YZ= 325.026 ZZ= -67.3153
 Eigenvalues: -429.7356 -327.6108 311.7723
 49 H Isotropic= 28.6584 Anisotropy 6.3289
 XX= 28.7359 YX= 2.6981 ZX= 0.4377
 XY= 3.1583 YY= 25.4399 ZY= 1.7323
 XZ= 1.5295 YZ= 1.1354 ZZ= 31.7993
 Eigenvalues: 23.6571 29.4404 32.8776
 50 H Isotropic= 29.4766 Anisotropy 6.2717
 XX= 27.4487 YX= -2.2612 ZX= 0.0784
 XY= -1.8142 YY= 30.4583 ZY= -2.1855
 XZ= -0.1673 YZ= -3.4766 ZZ= 30.5228
 Eigenvalues: 25.922 28.8501 33.6577
 51 C Isotropic= 108.6593 Anisotropy 12.6283
 XX= 116.7296 YX= -6.0491 ZX= 2.3356
 XY= 1.6052 YY= 102.5054 ZY= 6.6212
 XZ= 0.3055 YZ= 7.2611 ZZ= 106.7429
 Eigenvalues: 97.031 111.8686 117.0782
 52 C Isotropic= 122.6821 Anisotropy 19.8725
 XX= 114.408 YX= -6.2771 ZX= 8.9934
 XY= -5.4588 YY= 134.2563 ZY= 3.0041
 XZ= 7.4806 YZ= -0.507 ZZ= 119.382
 Eigenvalues: 107.1777 124.9382 135.9304
 53 O Isotropic= 267.6905 Anisotropy 41.1946
 XX= 290.0247 YX= 16.1071 ZX= -0.4848
 XY= -3.6019 YY= 287.4623 ZY= 15.5761
 XZ= 3.7519 YZ= -15.2041 ZZ= 225.5844
 Eigenvalues: 225.543 282.3748 295.1535
 54 H Isotropic= 26.0677 Anisotropy 6.8718
 XX= 30.2357 YX= -2.0233 ZX= 2.5485
 XY= 2.9401 YY= 26.551 ZY= 1.9723
 XZ= 0.4994 YZ= 1.8475 ZZ= 21.4163
 Eigenvalues: 20.6053 26.9489 30.6489
 55 N Isotropic= 119.4647 Anisotropy 107.3194
 XX= 81.466 YX= -31.0879 ZX= 27.5927
 XY= -46.4644 YY= 176.497 ZY= 0.1221
 XZ= 51.775 YZ= 12.4718 ZZ= 100.4312
 Eigenvalues: 41.1671 126.2161 191.011
 56 C Isotropic= 51.1472 Anisotropy 185.675
 XX= 94.6718 YX= 91.4068 ZX= -36.0034
 XY= 88.9879 YY= 61.1774 ZY= 2.1281
 XZ= -40.9103 YZ= -4.4224 ZZ= -2.4075
 Eigenvalues: -34.316 12.8272 174.9306

57	H	Isotropic=	26.219	Anisotropy	6.3677
XX=	25.2794	YX=	-0.3248	ZX=	0.423
XY=	-0.8143	YY=	27.7842	ZY=	4.2093
XZ=	-1.864	YZ=	2.6997	ZZ=	25.5933
Eigenvalues:	23.0366	25.1562	30.4641		
58	H	Isotropic=	29.4927	Anisotropy	16.1934
XX=	25.1435	YX=	3.9754	ZX=	0.2945
XY=	6.1488	YY=	38.4945	ZY=	3.4761
XZ=	-0.8088	YZ=	-0.7954	ZZ=	24.8402
Eigenvalues:	23.1595	25.0304	40.2883		
59	C	Isotropic=	19.9414	Anisotropy	114.381
XX=	59.1072	YX=	26.556	ZX=	33.256
XY=	16.6683	YY=	-63.5393	ZY=	-13.9007
XZ=	35.1604	YZ=	-10.8678	ZZ=	64.2563
Eigenvalues:	-69.7903	33.4191	96.1954		
60	H	Isotropic=	25.7893	Anisotropy	7.6498
XX=	27.3368	YX=	0.4334	ZX=	-7.4114
XY=	-1.4969	YY=	28.7871	ZY=	-0.6312
XZ=	-4.2936	YZ=	-1.2806	ZZ=	21.244
Eigenvalues:	17.5858	28.8929	30.8891		
61	C	Isotropic=	61.4343	Anisotropy	175.0356
XX=	112.6797	YX=	89.6599	ZX=	-7.2652
XY=	87.839	YY=	41.6028	ZY=	-46.7596
XZ=	-1.7216	YZ=	-38.8235	ZZ=	30.0203
Eigenvalues:	-35.8776	42.0557	178.1247		
62	C	Isotropic=	61.973	Anisotropy	176.1986
XX=	129.9568	YX=	59.1576	ZX=	-25.7932
XY=	59.3816	YY=	88.7126	ZY=	-34.5614
XZ=	-24.0798	YZ=	-31.2256	ZZ=	-32.7503
Eigenvalues:	-41.7343	48.2146	179.4387		
63	C	Isotropic=	63.5125	Anisotropy	176.473
XX=	101.7583	YX=	91.1692	ZX=	-46.1192
XY=	91.2428	YY=	65.194	ZY=	15.6319
XZ=	-46.8849	YZ=	14.7702	ZZ=	23.5851
Eigenvalues:	-38.4515	47.8278	181.1611		
64	C	Isotropic=	61.985	Anisotropy	173.9503
XX=	106.8029	YX=	94.1009	ZX=	-1.6252
XY=	93.0356	YY=	42.3275	ZY=	-40.6461
XZ=	1.1644	YZ=	-42.9931	ZZ=	36.8246
Eigenvalues:	-39.9503	47.9534	177.9519		
65	C	Isotropic=	63.1612	Anisotropy	145.9582
XX=	122.3137	YX=	46.9291	ZX=	-17.6605
XY=	44.3379	YY=	92.1483	ZY=	-29.3108
XZ=	-16.0467	YZ=	-29.2735	ZZ=	-24.9782
Eigenvalues:	-32.1513	61.1684	160.4667		
66	H	Isotropic=	23.2195	Anisotropy	11.5029
XX=	24.0638	YX=	-3.5397	ZX=	5.3911
XY=	-2.8613	YY=	20.5951	ZY=	-1.0249
XZ=	4.7553	YZ=	-2.8451	ZZ=	24.9997
Eigenvalues:	18.3832	20.3873	30.8881		
67	O	Isotropic=	-135.741	Anisotropy	579.1153
XX=	-165.5335	YX=	-48.9988	ZX=	282.5916
XY=	-126.5658	YY=	-262.686	ZY=	54.061
XZ=	334.3829	YZ=	44.5006	ZZ=	20.9963
Eigenvalues:	-448.3278	-209.2312	250.3359		
68	C	Isotropic=	59.1201	Anisotropy	163.8028

XX=	29.5776	YX=	3.5484	ZX=	41.4619		
XY=	18.4602	YY=	46.0147	ZY=	-77.3381		
XZ=	29.0486	YZ=	-95.5157	ZZ=	101.768		
Eigenvalues:	-31.8336	40.8718	168.322				
69	H	Isotropic=	23.8189	Anisotropy	5.9446		
XX=	23.2732	YX=	-3.4039	ZX=	1.4605		
XY=	-3.3047	YY=	24.2037	ZY=	-0.6602		
XZ=	1.6061	YZ=	-0.8283	ZZ=	23.9799		
Eigenvalues:	20.2211	23.4537	27.782				
70	H	Isotropic=	23.7398	Anisotropy	3.3371		
XX=	22.4452	YX=	-2.3841	ZX=	0.3401		
XY=	-2.3955	YY=	23.6255	ZY=	1.1339		
XZ=	0.44	YZ=	0.8836	ZZ=	25.1488		
Eigenvalues:	20.3901	24.8648	25.9646				
71	H	Isotropic=	23.7397	Anisotropy	4.4808		
XX=	22.7589	YX=	-2.6118	ZX=	1.3392		
XY=	-2.7058	YY=	23.3257	ZY=	-0.3106		
XZ=	1.4149	YZ=	-0.5311	ZZ=	25.1344		
Eigenvalues:	20.2487	24.2434	26.7268				
72	H	Isotropic=	24.0841	Anisotropy	7.9665		
XX=	24.3088	YX=	-3.9977	ZX=	0.2162		
XY=	-4.4862	YY=	25.8559	ZY=	0.3879		
XZ=	0.1205	YZ=	0.0999	ZZ=	22.0875		
Eigenvalues:	20.7112	22.1459	29.3951				
73	C	Isotropic=	51.8744	Anisotropy	178.7839		
XX=	-29.7846	YX=	-31.1966	ZX=	40.0975		
XY=	-28.0217	YY=	65.6514	ZY=	-51.6063		
XZ=	53.3059	YZ=	-62.4861	ZZ=	119.7563		
Eigenvalues:	-45.0089	29.5683	171.0636				
74	C	Isotropic=	60.974	Anisotropy	174.461		
XX=	26.8397	YX=	-53.8008	ZX=	13.2053		
XY=	-54.1128	YY=	25.6912	ZY=	-72.5263		
XZ=	10.0203	YZ=	-75.12	ZZ=	130.391		
Eigenvalues:	-41.5066	47.1472	177.2813				
75	C	Isotropic=	60.4441	Anisotropy	179.1291		
XX=	34.8964	YX=	13.8355	ZX=	50.4239		
XY=	11.9418	YY=	32.0312	ZY=	-90.8318		
XZ=	48.5221	YZ=	-86.7885	ZZ=	114.4046		
Eigenvalues:	-43.8867	45.3555	179.8635				
76	C	Isotropic=	63.812	Anisotropy	171.573		
XX=	-23.7042	YX=	-15.2818	ZX=	47.4153		
XY=	-18.794	YY=	79.6448	ZY=	-52.1868		
XZ=	51.3785	YZ=	-48.5241	ZZ=	135.4955		
Eigenvalues:	-37.8507	51.0927	178.194				
77	C	Isotropic=	65.3608	Anisotropy	176.1831		
XX=	22.9724	YX=	-33.3589	ZX=	21.5476		
XY=	-40.4135	YY=	43.2889	ZY=	-72.9986		
XZ=	14.331	YZ=	-82.1772	ZZ=	129.821		
Eigenvalues:	-17.3458	30.6119	182.8162				
78	H	Isotropic=	22.7293	Anisotropy	7.7056		
XX=	21.4053	YX=	1.7064	ZX=	-1.0268		
XY=	1.088	YY=	25.7603	ZY=	3.293		
XZ=	-1.0806	YZ=	4.1014	ZZ=	21.0223		
Eigenvalues:	18.1945	22.1271	27.8664				
79	H	Isotropic=	23.6894	Anisotropy	3.701		
XX=	25.2218	YX=	0.1531	ZX=	-1.7134		

XY=	0.1276	YY=	24.2993	ZY=	2.0632
XZ=	-1.6302	YZ=	1.8888	ZZ=	21.5471
Eigenvalues:	20.0457	24.8657	26.1567		
80	H	Isotropic=	23.7374	Anisotropy	5.4009
XX=	25.4236	YX=	2.208	ZX=	-0.2351
XY=	2.0047	YY=	24.6189	ZY=	1.7579
XZ=	-0.3317	YZ=	2.0034	ZZ=	21.1699
Eigenvalues:	20.0833	23.7909	27.338		
81	H	Isotropic=	23.9485	Anisotropy	9.0508
XX=	24.2386	YX=	2.1476	ZX=	0.0058
XY=	1.9518	YY=	27.4581	ZY=	4.0708
XZ=	0.3432	YZ=	4.2	ZZ=	20.1489
Eigenvalues:	18.2027	23.6605	29.9824		
82	H	Isotropic=	22.6109	Anisotropy	5.4021
XX=	25.1598	YX=	0.3545	ZX=	-1.9123
XY=	1.3182	YY=	24.6509	ZY=	3.7849
XZ=	-0.8231	YZ=	3.1851	ZZ=	18.0219
Eigenvalues:	16.2444	25.3759	26.2123		

2biii_neg45

C	3.53907	-1.19598	1.673404
C	4.330556	-2.035424	0.621185
C	3.68201	-2.134551	-0.769749
C	4.466556	-1.402446	-1.873499
C	4.638806	0.11413	-1.655613
C	3.436119	0.938732	-1.223511
C	2.86577	0.562177	0.113205
C	1.536862	0.272294	0.188333
C	1.065949	-0.529624	1.370646
C	2.066548	-1.621687	1.764115
C	3.68726	0.324983	1.363844
C	5.16312	0.691258	1.301348
C	3.107183	1.145171	2.532172
C	0.541902	0.660935	-0.832491
C	5.806699	-2.055012	-2.126054
O	4.065699	-1.496942	9.64709
O	4.563428	-3.332154	1.150123
O	5.682532	0.665659	-2.0136
O	3.509587	2.32636	-1.519312
O	-0.156203	-1.272003	1.191306
H	3.721916	-3.673696	1.477041
C	4.469737	3.187341	-1.059757
O	5.450275	2.771784	-0.452277
C	4.151566	4.59578	-1.441106
H	5.373518	-1.615107	0.524058
H	2.634458	-1.742124	-0.750521
H	2.667672	0.630083	-2.019616
H	0.878299	0.179298	2.231721
H	1.84377	-1.925276	2.823416
H	1.888328	-2.522362	1.119603
H	5.656888	0.404597	0.345987
H	5.296164	1.794629	1.428266
H	5.70397	0.193109	2.144341
H	3.903202	1.74811	3.033861
H	2.321362	1.852588	2.175781
H	2.674293	0.469898	3.310401

H	0.963774	1.3395	-1.614404
H	0.122699	-0.251873	-1.328369
H	-0.291503	1.228275	-0.342821
H	6.315209	-1.564055	-2.991639
H	6.472961	-1.95763	-1.235453
H	5.667469	-3.13937	-2.35192
H	3.263372	4.641372	-2.115443
H	3.941185	5.178094	-0.510882
H	5.038537	5.035506	-1.959099
H	5.014716	-1.649731	2.872508
C	-1.329863	-0.633684	0.882407
O	-1.544480.467434	1.379083	
H	3.847877	-1.482953	-2.815286
H	3.636262	-3.22028	-1.052928
C	-2.239481	-1.530728	0.054838
C	-3.750017	-1.241089	0.278291
O	-1.834748	-1.462322	-1.297145
H	-2.044611	-2.605969	0.346266
N	-4.140577	0.105924	-0.057464
C	-4.593689	-2.281016	-0.416749
H	-3.890689	-1.358578	1.404113
H	-2.041964	-0.574466	-1.619275
C	-4.405753	1.057791	0.925436
H	-4.532190.243877	-0.959641	
C	-4.52693-2.478593	-1.798974	
C	-5.326776	-3.444531	-2.408995
C	-6.199807	-4.216325	-1.643064
C	-6.271039	-4.021213	-0.263654
C	-5.473175	-3.056188	0.348894
H	-3.827329	-1.884677	-2.406995
O	-4.143677	0.84864	2.122292
C	-5.007112	2.339202	0.454876
H	-5.264813	-3.598025	-3.496461
H	-6.830046	-4.978175	-2.12509
H	-6.958276	-4.628586	0.34383
H	-5.537241	-2.905261	1.437699
C	-6.084109	2.871509	1.172794
C	-6.664464	4.070971	0.763137
C	-6.167684	4.743161	-0.353928
C	-5.086776	4.217441	-1.061968
C	-4.505723	3.014463	-0.661534
H	-6.455065	2.344637	2.06593
H	-7.511682	4.489131	1.326639
H	-6.625357	5.691156	-0.673779
H	-4.688512	4.753096	-1.936185
H	-3.643776	2.612643	-1.214526

2biii_neg45 E(RB+HF-PW91) = -2012.286874
SCF GIAO Magnetic shielding tensor (ppm):
1 C Isotropic= 110.8585 Anisotropy 30.2133
XX= 104.2733 YX= -1.7285 ZX= 19.8953
XY= 4.6774 YY= 107.9469 ZY= 2.6404
XZ= 13.2621 YZ= 1.2964 ZZ= 120.3553
Eigenvalues: 93.8855 107.6894 131.0007
2 C Isotropic= 112.2945 Anisotropy 30.8444

XX=	93.2627	YX=	-1.1725	ZX=	-1.1899				
XY=	-6.0477	YY=	130.599	ZY=	-1.1175				
XZ=	1.1217	YZ=	-11.2609	ZZ=	113.0217				
Eigenvalues:	92.8965	111.1296		132.8574					
3	C	Isotropic=	141.1819	Anisotropy		20.1423			
XX=	122.4817	YX=	-8.9171	ZX=	4.4185				
XY=	-0.6683	YY=	150.6678	ZY=	2.5505				
XZ=	4.466	YZ=	5.5916	ZZ=	150.3962				
Eigenvalues:	120.8174	148.1182		154.6101					
4	C	Isotropic=	141.0258	Anisotropy		23.2282			
XX=	129.155	YX=	-1.9505	ZX=	1.8611				
XY=	-15.3516	YY=	153.0356	ZY=	4.5176				
XZ=	7.239	YZ=	4.9935	ZZ=	140.8867				
Eigenvalues:	124.289	142.2771		156.5113					
5	C	Isotropic=	-23.2969	Anisotropy		181.343			
XX=	-49.9275	YX=	24.2314	ZX=	55.2274				
XY=	9.199	YY=	-94.5957	ZY=	-27.7678				
XZ=	51.4797	YZ=	-37.1798	ZZ=	74.6324				
Eigenvalues:	-113.9144	-53.5748		97.5984					
6	C	Isotropic=	101.3819	Anisotropy		41.359			
XX=	88.97	YX=	-15.7468	ZX=	1.6468				
XY=	2.1165	YY=	127.5095	ZY=	1.4999				
XZ=	-5.467	YZ=	4.683	ZZ=	87.666				
Eigenvalues:	86.225	88.966		128.9546					
7	C	Isotropic=	45.7908	Anisotropy		153.3822			
XX=	47.5184	YX=	-16.6734	ZX=	-3.9532				
XY=	-34.1702	YY=	122.387	ZY=	69.635				
XZ=	3.0399	YZ=	47.989	ZZ=	-32.533				
Eigenvalues:	-52.9348	42.2616		148.0456					
8	C	Isotropic=	40.497	Anisotropy		156.0242			
XX=	37.616	YX=	-11.2244	ZX=	-16.4503				
XY=	-12.6275	YY=	97.419	ZY=	71.7228				
XZ=	-29.3832	YZ=	90.5965	ZZ=	-13.5441				
Eigenvalues:	-58.6726	35.6504		144.5131					
9	C	Isotropic=	111.3408	Anisotropy		54.1634			
XX=	130.0363	YX=	26.6597	ZX=	10.6227				
XY=	25.7806	YY=	104.2965	ZY=	-7.4587				
XZ=	17.8126	YZ=	-12.3132	ZZ=	99.6895				
Eigenvalues:	76.6452	109.9274		147.4497					
10	C	Isotropic=	146.8605	Anisotropy		44.1002			
XX=	174.5922	YX=	7.0133	ZX=	4.073				
XY=	1.6576	YY=	132.7216	ZY=	-4.3271				
XZ=	11.9079	YZ=	-12.4995	ZZ=	133.2678				
Eigenvalues:	123.1045	141.2164		176.2607					
11	C	Isotropic=	147.4823	Anisotropy		12.15			
XX=	143.4991	YX=	0.1074	ZX=	-0.2942				
XY=	-14.8035	YY=	151.1054	ZY=	-1.1622				
XZ=	-1.5284	YZ=	0.5598	ZZ=	147.8423				
Eigenvalues:	138.9302	147.9343		155.5823					
12	C	Isotropic=	155.1399	Anisotropy		22.4204			
XX=	159.9708	YX=	0.4807	ZX=	-17.698				
XY=	5.6613	YY=	155.633	ZY=	12.6024				
XZ=	-9.0115	YZ=	7.4567	ZZ=	149.816				
Eigenvalues:	135.5514	159.7816		170.0869					
13	C	Isotropic=	148.2492	Anisotropy		54.6658			
XX=	149.3504	YX=	-14.3736	ZX=	-8.557				

XY=	-20.9851	YY=	142.1887	ZY=	26.8111		
XZ=	-5.7144	YZ=	29.6518	ZZ=	153.2084		
Eigenvalues:	116.04	144.0145		184.693			
14	C	Isotropic=	167.8239	Anisotropy		13.198	
XX=	171.0872	YX=	-7.9434	ZX=	3.665		
XY=	2.8093	YY=	162.445	ZY=	3.1805		
XZ=	8.452	YZ=	0.7956	ZZ=	169.9396		
Eigenvalues:	160.0758	166.7733		176.6225			
15	C	Isotropic=	169.1989	Anisotropy		17.2795	
XX=	173.268	YX=	-3.4343	ZX=	-9.4193		
XY=	-5.7158	YY=	174.9556	ZY=	2.3682		
XZ=	-5.2951	YZ=	1.4945	ZZ=	159.3732		
Eigenvalues:	156.2015	170.6767		180.7186			
16	O	Isotropic=	263.1281	Anisotropy		82.3399	
XX=	315.6376	YX=	1.9671	ZX=	5.8779		
XY=	20.1361	YY=	202.1572	ZY=	43.7083		
XZ=	3.9436	YZ=	7.6462	ZZ=	271.5894		
Eigenvalues:	193.0345	278.3285		318.0213			
17	O	Isotropic=	265.5695	Anisotropy		44.718	
XX=	249.2323	YX=	22.398	ZX=	-0.9346		
XY=	-1.0044	YY=	254.0754	ZY=	-3.9388		
XZ=	0.8667	YZ=	-13.5839	ZZ=	293.4009		
Eigenvalues:	240.1079	261.2192		295.3815			
18	O	Isotropic=	-356.8384	Anisotropy		1079.1815	
XX=	-755.1087	YX=	-251.4305	ZX=	420.5097		
XY=	-220.104	YY=	-531.1859	ZY=	-6.888		
XZ=	359.5634	YZ=	-18.9117	ZZ=	215.7793		
Eigenvalues:	-996.0721	-437.0591		362.6159			
19	O	Isotropic=	89.3458	Anisotropy		125.8045	
XX=	102.0699	YX=	159.3466	ZX=	-65.6843		
XY=	21.6938	YY=	46.3873	ZY=	22.5683		
XZ=	-37.7102	YZ=	81.6091	ZZ=	119.5802		
Eigenvalues:	-51.4064	146.2283		173.2154			
20	O	Isotropic=	96.0726	Anisotropy		158.8401	
XX=	141.3739	YX=	-28.6642	ZX=	9.9364		
XY=	-155.7162	YY=	34.2465	ZY=	-74.2687		
XZ=	-69.5525	YZ=	-107.0095	ZZ=	112.5973		
Eigenvalues:	-67.6298	153.8816		201.966			
21	H	Isotropic=	31.1021	Anisotropy		13.622	
XX=	33.2911	YX=	3.2112	ZX=	-5.0408		
XY=	2.772	YY=	35.1098	ZY=	-4.9639		
XZ=	-5.04	YZ=	-3.8909	ZZ=	24.9053		
Eigenvalues:	21.8997	31.2231		40.1834			
22	C	Isotropic=	20.3752	Anisotropy		74.8678	
XX=	42.3644	YX=	-76.889	ZX=	-5.3239		
XY=	-38.1738	YY=	-48.9862	ZY=	-6.4444		
XZ=	-9.1407	YZ=	-24.7593	ZZ=	67.7474		
Eigenvalues:	-78.7867	69.6251		70.287			
23	O	Isotropic=	-133.2259	Anisotropy		602.2066	
XX=	-259.0799	YX=	-29.5694	ZX=	-305.6228		
XY=	-52.0224	YY=	-254.702	ZY=	32.8975		
XZ=	-252.8019	YZ=	38.3637	ZZ=	114.104		
Eigenvalues:	-410.7273	-257.1956		268.2451			
24	C	Isotropic=	166.146	Anisotropy		36.9487	
XX=	158.1433	YX=	-3.9654	ZX=	6.7308		
XY=	-3.5649	YY=	186.8595	ZY=	-11.592		

XZ=	5.4415	YZ=	-9.4688	ZZ=	153.4352		
Eigenvalues:	147.9674			159.6921		190.7784	
25	H	Isotropic=		27.3951	Anisotropy		2.941
XX=	26.899	YX=	0.0334	ZX=	-1.4647		
XY=	1.2018	YY=	28.7622	ZY=	-0.1366		
XZ=	-1.8745	YZ=	-0.7489	ZZ=	26.5242		
Eigenvalues:	25.0296	27.7999	29.3557				
26	H	Isotropic=		28.0313	Anisotropy		8.2257
XX=	30.0722	YX=	-3.9302	ZX=	-1.6961		
XY=	-3.3921	YY=	27.2104	ZY=	1.5624		
XZ=	-1.5231	YZ=	2.5908	ZZ=	26.8112		
Eigenvalues:	24.3318	26.247	33.515				
27	H	Isotropic=		25.3868	Anisotropy		3.4694
XX=	25.8211	YX=	2.0255	ZX=	-1.4228		
XY=	0.5445	YY=	26.7539	ZY=	0.3515		
XZ=	1.7428	YZ=	-1.6177	ZZ=	23.5854		
Eigenvalues:	23.3837	25.0769	27.6997				
28	H	Isotropic=		24.4244	Anisotropy		7.4288
XX=	29.0442	YX=	1.2839	ZX=	1.2019		
XY=	0.0459	YY=	21.1554	ZY=	3.7702		
XZ=	0.6529	YZ=	2.6508	ZZ=	23.0738		
Eigenvalues:	18.7638	25.1326	29.377				
29	H	Isotropic=		28.4575	Anisotropy		6.6002
XX=	29.7455	YX=	0.6524	ZX=	-1.4741		
XY=	0.2597	YY=	25.2377	ZY=	-4.0693		
XZ=	-0.8518	YZ=	-3.4287	ZZ=	30.3892		
Eigenvalues:	23.2619	29.2529	32.8576				
30	H	Isotropic=		29.0247	Anisotropy		4.5789
XX=	32.0291	YX=	0.3917	ZX=	0.3637		
XY=	0.2321	YY=	29.7221	ZY=	1.3545		
XZ=	-0.4464	YZ=	2.1857	ZZ=	25.3229		
Eigenvalues:	24.6964	30.3005	32.0773				
31	H	Isotropic=		29.2744	Anisotropy		8.186
XX=	29.2436	YX=	1.0159	ZX=	-3.0973		
XY=	0.9665	YY=	25.5954	ZY=	1.8135		
XZ=	-3.0593	YZ=	0.1643	ZZ=	32.9842		
Eigenvalues:	24.8878	28.2036	34.7317				
32	H	Isotropic=		29.1887	Anisotropy		9.0441
XX=	26.9497	YX=	4.4419	ZX=	-0.4948		
XY=	3.8195	YY=	32.9053	ZY=	-1.0667		
XZ=	0.4	YZ=	-1.6211	ZZ=	27.7111		
Eigenvalues:	24.7211	27.6269	35.2181				
33	H	Isotropic=		30.3161	Anisotropy		6.6309
XX=	32.8797	YX=	1.5593	ZX=	2.9321		
XY=	1.5902	YY=	28.5849	ZY=	-1.2805		
XZ=	3.191	YZ=	-1.9216	ZZ=	29.4839		
Eigenvalues:	25.8943	30.3174	34.7367				
34	H	Isotropic=		30.106	Anisotropy		9.0484
XX=	29.4855	YX=	1.4623	ZX=	0.3017		
XY=	2.113	YY=	29.5077	ZY=	4.6501		
XZ=	1.7539	YZ=	5.4985	ZZ=	31.3248		
Eigenvalues:	25.1345	29.0453	36.1383				
35	H	Isotropic=		30.1158	Anisotropy		6.3317
XX=	30.8432	YX=	-2.4261	ZX=	1.5041		
XY=	-2.731	YY=	31.4834	ZY=	2.7374		
XZ=	-1.0036	YZ=	2.5251	ZZ=	28.0207		

Eigenvalues:	26.0905	29.9199	34.3369		
36	H	Isotropic=	28.3587	Anisotropy	6.3187
XX=	27.1825	YX=	0.8969	ZX=	-1.6418
XY=	0.259	YY=	26.6697	ZY=	3.3091
XZ=	-2.3686	YZ=	0.8679	ZZ=	31.224
Eigenvalues:	24.9754	27.5296	32.5712		
37	H	Isotropic=	28.9259	Anisotropy	7.2461
XX=	31.7419	YX=	1.4586	ZX=	-0.2107
XY=	1.6555	YY=	27.5491	ZY=	-4.8298
XZ=	-1.4771	YZ=	-4.7482	ZZ=	27.4867
Eigenvalues:	22.7003	30.3207	33.7566		
38	H	Isotropic=	28.324	Anisotropy	11.3029
XX=	31.5129	YX=	4.925	ZX=	1.2216
XY=	6.194	YY=	26.8598	ZY=	0.8281
XZ=	2.7561	YZ=	2.0252	ZZ=	26.5993
Eigenvalues:	23.1572	25.9556	35.8592		
39	H	Isotropic=	28.5357	Anisotropy	9.4707
XX=	33.1897	YX=	-1.7052	ZX=	-4.16
XY=	-2.2057	YY=	26.8276	ZY=	-1.659
XZ=	-3.1948	YZ=	-1.9618	ZZ=	25.5897
Eigenvalues:	22.6669	28.0907	34.8495		
40	H	Isotropic=	29.1648	Anisotropy	10.7807
XX=	29.6159	YX=	1.5333	ZX=	-5.6573
XY=	-0.2678	YY=	27.1335	ZY=	-1.4616
XZ=	-6.2174	YZ=	-1.1225	ZZ=	30.7449
Eigenvalues:	24.1591	26.9833	36.3519		
41	H	Isotropic=	29.5907	Anisotropy	5.9484
XX=	32.9442	YX=	-1.221	ZX=	1.1164
XY=	-1.6826	YY=	25.3024	ZY=	0.6864
XZ=	1.103	YZ=	0.1508	ZZ=	30.5254
Eigenvalues:	24.9669	30.2488	33.5563		
42	H	Isotropic=	30.4495	Anisotropy	9.5632
XX=	28.6562	YX=	-1.6645	ZX=	-2.0462
XY=	-1.684	YY=	34.6104	ZY=	3.2692
XZ=	-2.4987	YZ=	3.5911	ZZ=	28.0818
Eigenvalues:	25.7399	28.7836	36.8249		
43	H	Isotropic=	29.0511	Anisotropy	5.6336
XX=	29.738	YX=	0.9855	ZX=	3.1818
XY=	-0.7881	YY=	30.2859	ZY=	-2.8745
XZ=	3.7553	YZ=	-1.5555	ZZ=	27.1293
Eigenvalues:	24.138	30.2084	32.8068		
44	H	Isotropic=	29.1787	Anisotropy	6.6537
XX=	26.5022	YX=	-1.2759	ZX=	-1.1455
XY=	-0.1097	YY=	31.9111	ZY=	3.0988
XZ=	-0.5527	YZ=	2.0958	ZZ=	29.1229
Eigenvalues:	26.2496	27.672	33.6146		
45	H	Isotropic=	28.9719	Anisotropy	8.9105
XX=	29.8559	YX=	1.7859	ZX=	-1.9974
XY=	4.1362	YY=	29.9465	ZY=	-3.0347
XZ=	-2.8433	YZ=	-3.3956	ZZ=	27.1134
Eigenvalues:	24.9578	27.0457	34.9123		
46	H	Isotropic=	30.5849	Anisotropy	17.9917
XX=	40.4499	YX=	-4.5276	ZX=	4.9925
XY=	-2.7453	YY=	23.7038	ZY=	-3.3899
XZ=	3.1896	YZ=	-1.6286	ZZ=	27.6009
Eigenvalues:	22.3201	26.8552	42.5794		

47 C Isotropic= 9.7573 Anisotropy 92.2443
 XX= -63.5045 YX= -12.0353 ZX= -64.2771
 XY= 26.7549 YY= 47.3293 ZY= 3.3183
 XZ= -51.0427 YZ= -7.3541 ZZ= 45.4472
 Eigenvalues: -88.6141 46.6326 71.2535

48 O Isotropic= -160.5397 Anisotropy 717.1929
 XX= -237.2735 YX= 142.9747 ZX= -197.0211
 XY= 119.2954 YY= -353.6446 ZY= -245.4631
 XZ= -215.9825 YZ= -237.1048 ZZ= 109.299
 Eigenvalues: -467.408 -331.8 317.5889

49 H Isotropic= 28.6934 Anisotropy 6.5022
 XX= 29.3263 YX= -1.7124 ZX= 0.8521
 XY= -1.6336 YY= 24.3093 ZY= 0.3687
 XZ= 2.0756 YZ= 1.3448 ZZ= 32.4445
 Eigenvalues: 23.6227 29.4293 33.0281

50 H Isotropic= 29.4283 Anisotropy 6.4445
 XX= 26.8492 YX= 0.7455 ZX= -1.0862
 XY= 0.493 YY= 32.5949 ZY= 1.7297
 XZ= -1.4321 YZ= 2.9682 ZZ= 28.8409
 Eigenvalues: 25.8123 28.748 33.7247

51 C Isotropic= 111.9503 Anisotropy 14.7587
 XX= 121.6357 YX= -0.0707 ZX= -0.7214
 XY= -3.1584 YY= 97.6213 ZY= -2.4437
 XZ= -0.4932 YZ= -1.3205 ZZ= 116.594
 Eigenvalues: 97.3222 116.7393 121.7895

52 C Isotropic= 130.5395 Anisotropy 24.6531
 XX= 137.6598 YX= 7.7876 ZX= 0.5781
 XY= 9.929 YY= 137.5946 ZY= -4.5381
 XZ= -3.6575 YZ= -3.3103 ZZ= 116.3642
 Eigenvalues: 115.662 128.9817 146.9749

53 O Isotropic= 274.7452 Anisotropy 39.8753
 XX= 284.8697 YX= -2.3104 ZX= 32.3463
 XY= 11.0633 YY= 278.997 ZY= -16.9021
 XZ= 19.1654 YZ= -4.2469 ZZ= 260.3689
 Eigenvalues: 240.7664 282.1405 301.3287

54 H Isotropic= 26.7163 Anisotropy 5.5455
 XX= 29.4811 YX= 1.6359 ZX= 2.0077
 XY= -2.2171 YY= 25.8497 ZY= -3.2754
 XZ= 1.3298 YZ= -2.5146 ZZ= 24.818
 Eigenvalues: 22.2222 27.5133 30.4132

55 N Isotropic= 137.0455 Anisotropy 119.6671
 XX= 136.7517 YX= 19.7208 ZX= -13.798
 XY= 19.0748 YY= 178.4419 ZY= 49.3426
 XZ= -39.8322 YZ= 86.4353 ZZ= 95.9429
 Eigenvalues: 45.8494 148.4635 216.8235

56 C Isotropic= 53.0931 Anisotropy 188.936
 XX= 81.7919 YX= -101.8742 ZX= 5.0905
 XY= -95.4204 YY= 71.1672 ZY= -35.6085
 XZ= 2.735 YZ= -29.9602 ZZ= 6.3202
 Eigenvalues: -34.2059 14.4348 179.0504

57 H Isotropic= 25.2579 Anisotropy 5.6248
 XX= 24.4823 YX= 2.3356 ZX= -1.5536
 XY= 1.7237 YY= 24.638 ZY= -0.8579
 XZ= -3.5963 YZ= -0.3403 ZZ= 26.6534
 Eigenvalues: 21.9585 24.8075 29.0078

58 H Isotropic= 30.2638 Anisotropy 11.2522

XX= 27.4442 YX= -1.4077 ZX= -2.0801
 XY= -1.8351 YY= 33.6708 ZY= -6.3118
 XZ= -0.2108 YZ= -5.1063 ZZ= 29.6763
 Eigenvalues: 24.4438 28.5823 37.7653
 59 C Isotropic= 19.1488 Anisotropy 117.869
 XX= 71.5895 YX= 49.2116 ZX= -18.7596
 XY= 53.72 YY= -46.3996 ZY= -27.1252
 XZ= 0.5148 YZ= -40.209 ZZ= 32.2566
 Eigenvalues: -73.4664 33.1847 97.7281
 60 H Isotropic= 26.9069 Anisotropy 8.1571
 XX= 22.4915 YX= -3.1415 ZX= 3.5604
 XY= -1.7356 YY= 31.4126 ZY= 1.4823
 XZ= 0.4133 YZ= 2.0983 ZZ= 26.8165
 Eigenvalues: 20.8981 27.4775 32.345
 61 C Isotropic= 62.5474 Anisotropy 169.9965
 XX= 85.3304 YX= -91.0273 ZX= 42.255
 XY= -87.6436 YY= 82.8737 ZY= 20.5121
 XZ= 43.3836 YZ= 12.4959 ZZ= 19.438
 Eigenvalues: -37.1191 48.8828 175.8784
 62 C Isotropic= 62.4463 Anisotropy 175.9525
 XX= 117.2233 YX= -62.8129 ZX= 17.8471
 XY= -63.6641 YY= 107.7519 ZY= -21.2606
 XZ= 18.9034 YZ= -24.1137 ZZ= -37.6363
 Eigenvalues: -41.6637 49.2547 179.748
 63 C Isotropic= 63.4848 Anisotropy 176.3947
 XX= 88.6115 YX= -99.0988 ZX= -8.3918
 XY= -100.0891 YY= 67.9885 ZY= -38.9582
 XZ= -8.9363 YZ= -38.116 ZZ= 33.8544
 Eigenvalues: -38.5828 47.956 181.0813
 64 C Isotropic= 61.7333 Anisotropy 174.9407
 XX= 81.3865 YX= -93.8625 ZX= 42.4985
 XY= -93.9266 YY= 82.3263 ZY= 14.8603
 XZ= 44.3324 YZ= 16.1527 ZZ= 21.4873
 Eigenvalues: -40.7973 47.6369 178.3605
 65 C Isotropic= 60.1585 Anisotropy 149.2947
 XX= 109.4624 YX= -49.7337 ZX= 18.5039
 XY= -50.1764 YY= 102.0536 ZY= -21.1191
 XZ= 17.0792 YZ= -20.0668 ZZ= -31.0405
 Eigenvalues: -34.9732 55.7604 159.6882
 66 H Isotropic= 23.0095 Anisotropy 10.962
 XX= 23.2229 YX= 3.9903 ZX= 3.7402
 XY= 2.8281 YY= 20.5987 ZY= 3.3188
 XZ= 3.2158 YZ= 3.8304 ZZ= 25.2068
 Eigenvalues: 18.0197 20.6912 30.3175
 67 O Isotropic= -122.3426 Anisotropy 708.13
 XX= 238.8996 YX= 188.2595 ZX= -209.2642
 XY= 184.8583 YY= -148.4747 ZY= -83.3229
 XZ= -115.4314 YZ= -17.9631 ZZ= -457.4526
 Eigenvalues: -493.7193 -223.0525 349.7441
 68 C Isotropic= 54.3388 Anisotropy 171.6228
 XX= 57.4521 YX= 65.0285 ZX= 57.5165
 XY= 51.0154 YY= 23.426 ZY= 68.5107
 XZ= 34.3411 YZ= 60.0889 ZZ= 82.1384
 Eigenvalues: -28.5861 22.8486 168.7541
 69 H Isotropic= 23.8174 Anisotropy 5.5831
 XX= 23.595 YX= 3.6775 ZX= 0.2683

XY=	3.3214	YY=	24.0068	ZY=	1.1188		
XZ=	0.1102	YZ=	1.0557	ZZ=	23.8504		
Eigenvalues:	20.1909	23.7218	27.5395				
70	H	Isotropic=	23.7581	Anisotropy		3.4261	
XX=	22.8468	YX=	2.5783	ZX=	-0.8725		
XY=	2.2939	YY=	22.9062	ZY=	-0.0078		
XZ=	-0.9262	YZ=	0.209	ZZ=	25.5214		
Eigenvalues:	20.3415	24.8906	26.0422				
71	H	Isotropic=	23.7676	Anisotropy		4.6029	
XX=	22.8699	YX=	3.0148	ZX=	0.2402		
XY=	2.7441	YY=	23.5113	ZY=	1.2532		
XZ=	0.2185	YZ=	1.4778	ZZ=	24.9215		
Eigenvalues:	20.1722	24.2943	26.8361				
72	H	Isotropic=	23.7907	Anisotropy		8.5911	
XX=	24.4388	YX=	4.9683	ZX=	-1.0255		
XY=	4.4041	YY=	24.926	ZY=	-0.6867		
XZ=	-1.0651	YZ=	-0.1838	ZZ=	22.0074		
Eigenvalues:	19.8852	21.9688	29.5181				
73	C	Isotropic=	60.399	Anisotropy		175.2316	
XX=	84.893	YX=	32.2432	ZX=	73.5848		
XY=	28.8188	YY=	63.8175	ZY=	67.9643		
XZ=	74.9738	YZ=	70.296	ZZ=	32.4867		
Eigenvalues:	-39.1031	143.0801	177.2201				
74	C	Isotropic=	61.8527	Anisotropy		176.9533	
XX=	48.8668	YX=	67.5593	ZX=	83.617		
XY=	66.6494	YY=	69.5669	ZY=	23.4393		
XZ=	85.8908	YZ=	22.1937	ZZ=	67.1243		
Eigenvalues:	-40.6896	146.4261	179.8215				
75	C	Isotropic=	62.194	Anisotropy		177.8043	
XX=	86.1499	YX=	73.0122	ZX=	38.935		
XY=	74.3612	YY=	15.5679	ZY=	61.8255		
XZ=	39.9915	YZ=	61.677	ZZ=	84.8642		
Eigenvalues:	-40.5837	146.4355	180.7302				
76	C	Isotropic=	63.8181	Anisotropy		174.3598	
XX=	91.8707	YX=	23.1079	ZX=	74.2247		
XY=	27.9813	YY=	61.1574	ZY=	71.0654		
XZ=	74.9853	YZ=	72.8476	ZZ=	38.4261		
Eigenvalues:	-38.8191	150.2154	180.0579				
77	C	Isotropic=	66.8679	Anisotropy		162.4266	
XX=	50.8848	YX=	55.4663	ZX=	82.978		
XY=	61.6302	YY=	73.0667	ZY=	21.1526		
XZ=	76.0907	YZ=	22.9984	ZZ=	76.6523		
Eigenvalues:	-27.7911	153.2426	175.1523				
78	H	Isotropic=	23.345	Anisotropy		7.8983	
XX=	23.9796	YX=	-4.6781	ZX=	-1.8188		
XY=	-3.5592	YY=	24.4494	ZY=	0.4734		
XZ=	-1.5969	YZ=	0.0526	ZZ=	21.6061		
Eigenvalues:	19.4965	21.9281	28.6106				
79	H	Isotropic=	23.7541	Anisotropy		4.2229	
XX=	22.7281	YX=	-1.8298	ZX=	-1.4927		
XY=	-1.8214	YY=	25.0702	ZY=	-1.8386		
XZ=	-1.1883	YZ=	-2.0168	ZZ=	23.464		
Eigenvalues:	20.2642	24.4287	26.5693				
80	H	Isotropic=	23.7473	Anisotropy		3.8835	
XX=	23.852	YX=	-1.6326	ZX=	-2.5841		
XY=	-1.3332	YY=	23.5423	ZY=	-1.0444		

XZ= -2.3096 YZ= -1.1012 ZZ= 23.8476
 Eigenvalues: 20.3692 24.5363 26.3363
 81 H Isotropic= 23.8876 Anisotropy 5.5526
 XX= 23.812 YX= -3.036 ZX= -1.41
 XY= -2.6681 YY= 25.4166 ZY= -1.3352
 XZ= -1.1641 YZ= -1.2119 ZZ= 22.4343
 Eigenvalues: 20.2028 23.8707 27.5893
 82 H Isotropic= 23.8925 Anisotropy 8.0812
 XX= 22.0389 YX= -1.8771 ZX= -1.0434
 XY= -1.5196 YY= 27.3252 ZY= -3.8382
 XZ= -0.3101 YZ= -3.0351 ZZ= 22.3135
 Eigenvalues: 19.702 22.6956 29.28

2biv_neg45

C	3.05435	-0.093067	2.139806
C	3.849277	-1.423679	1.950479
C	3.372827	-2.320693	0.795708
C	4.38222	-2.430665	-0.36135
C	4.731476	-1.097152	-1.051938
C	3.608205	-0.138961	-1.416998
C	2.828685	0.387615	-0.246968
C	1.473635	0.247775	-0.25952
C	0.75511	0.341759	1.058405
C	1.537639	-0.328035	2.192801
C	3.447372	0.926077	1.02694
C	4.955907	1.128347	1.032875
C	2.844853	2.305193	1.357107
C	0.677491	-0.030478	-1.472679
C	5.64174	-3.147773	0.068785
O	3.368162	0.431753	3.428777
O	3.834298	-2.142982	3.174251
O	5.877466	-0.908713	-1.467528
O	3.906338	0.783234	-2.4552
O	-0.528952	-0.311612	1.133
H	2.91719	-2.207397	3.468017
C	4.910045	1.714126	-2.429174
O	5.732527	1.727902	-1.520027
C	4.846147	2.601984	-3.628202
H	4.943931	-1.183057	1.817009
H	2.394798	-1.961320	3.88235
H	2.910357	-0.840511	-2.000914
H	0.563127	1.432735	1.285554
H	1.144533	0.074394	3.166069
H	1.319816	-1.428361	2.179921
H	5.52098	0.307792	0.536882
H	5.223607	2.080788	0.510919
H	5.312417	1.217661	2.089451
H	3.647635	3.06065	1.540907
H	2.214331	2.680175	0.516384
H	2.230527	2.253365	2.289224
H	1.28226	0.027644	-2.411372
H	0.210414	-1.04615	-1.401879
H	-0.130465	0.739225	-1.575873
H	6.314571	-3.301159	-0.810239
H	6.200896	-2.552182	0.829825
H	5.385091	-4.140889	0.509317

H	4.051013	2.26838	-4.336982
H	4.6281	3.644175	-3.28932
H	5.838329	2.580965	-4.141759
H	4.285873	0.206754	3.628514
C	-1.554490	0.05275	0.303297
O	-1.670067	1.237989	0.00208
H	3.881357	-3.042919	-1.167916
H	3.21496	-3.354882	1.203945
C	-2.475196	-1.123712	0.01286
C	-3.947379	-0.700333	-0.277193
O	-1.896022	-1.901331	-1.014658
H	-2.478594	-1.810223	0.910979
N	-4.093463	0.170672	-1.407817
C	-4.830758	-1.921486	-0.370509
H	-4.23983	-0.122078	0.656041
H	-1.923846	-1.380069	-1.829272
C	-4.343043	1.534609	-1.418532
H	-4.165356	-0.28386	-2.293771
C	-4.607688	-2.919785	-1.322846
C	-5.448108	-4.031356	-1.383155
C	-6.517138	-4.1504	-0.495952
C	-6.745177	-3.154596	0.454153
C	-5.907508	-2.042470	0.516283
H	-3.758215	-2.839081	-2.018499
O	-4.619884	2.039205	-2.527093
C	-4.436664	2.34826	-0.176088
H	-5.264195	-4.814804	-2.133254
H	-7.179826	-5.027065	-0.545009
H	-7.588539	-3.244533	1.154736
H	-6.097348	-1.258575	1.265466
C	-3.770842	3.580043	-0.143843
C	-3.925147	4.427206	0.952669
C	-4.764718	4.06394	2.005254
C	-5.461103	2.856332	1.954897
C	-5.307393	2.003033	0.862977
H	-3.117495	3.86369	-0.983605
H	-3.388245	0.386879	0.980928
H	-4.886143	4.733196	2.8698
H	-6.141808	2.579109	2.77306
H	-5.900645	1.076827	0.812292

2biv_neg45	E(RB+HF-PW91)	=	-2012.278777
SCF	GIAO	Magnetic shielding tensor (ppm):	
1	C	Isotropic=	111.0947
		Anisotropy	30.1198
XX=	101.1868	YX=	9.4201
		ZX=	14.3276
XY=	10.5622	YY=	113.5876
		ZY=	8.5781
XZ=	5.7661	YZ=	7.7562
		ZZ=	118.5098
Eigenvalues:	94.3656	107.7441	131.1746
2	C	Isotropic=	112.6409
		Anisotropy	31.3456
XX=	93.746	YX=	2.2126
		ZX=	-6.7762
XY=	-2.9671	YY=	118.6087
		ZY=	-5.5994
XZ=	-1.989	YZ=	-15.6263
		ZZ=	125.568
Eigenvalues:	93.0088	111.3759	133.538
3	C	Isotropic=	142.0351
		Anisotropy	20.462
XX=	121.29	YX=	-3.0141
		ZX=	3.7918

XY=	3.4622	YY=	155.5995	ZY=	0.1547		
XZ=	-0.6825	YZ=	1.2149	ZZ=	149.2159		
Eigenvalues:	121.2027		149.2261		155.6765		
4	C	Isotropic=	140.7787	Anisotropy		24.1225	
XX=	126.2598	YX=	1.2511	ZX=	-0.3905		
XY=	-6.266	YY=	153.7365	ZY=	-6.6338		
XZ=	12.5951	YZ=	-4.8282	ZZ=	142.3397		
Eigenvalues:	124.1953		141.2803		156.8603		
5	C	Isotropic=	-23.1356	Anisotropy		180.7802	
XX=	-55.9122	YX=	39.1217	ZX=	12.941		
XY=	23.0251	YY=	-67.0689	ZY=	81.8631		
XZ=	18.6522	YZ=	75.0896	ZZ=	53.5743		
Eigenvalues:	-113.7968		-52.9945		97.3845		
6	C	Isotropic=	101.8044	Anisotropy		40.9186	
XX=	88.58	YX=	-7.2356	ZX=	8.1758		
XY=	3.2425	YY=	117.0548	ZY=	-19.5051		
XZ=	-8.1489	YZ=	-17.8897	ZZ=	99.7784		
Eigenvalues:	87.0469		89.2828		129.0835		
7	C	Isotropic=	45.6159	Anisotropy		154.5824	
XX=	38.5724	YX=	-0.443	ZX=	18.523		
XY=	-14.5323	YY=	124.0888	ZY=	-51.8203		
XZ=	34.167	YZ=	-71.8534	ZZ=	-25.8134		
Eigenvalues:	-53.4883		41.6652		148.6709		
8	C	Isotropic=	41.376	Anisotropy		155.2117	
XX=	39.3578	YX=	-11.2522	ZX=	9.0133		
XY=	-16.6906	YY=	136.7151	ZY=	-44.6513		
XZ=	0.761	YZ=	-24.3515	ZZ=	-51.945		
Eigenvalues:	-58.115		37.3925		144.8505		
9	C	Isotropic=	111.1868	Anisotropy		54.9816	
XX=	133.6092	YX=	27.2341	ZX=	-4.1133		
XY=	29.8863	YY=	90.5034	ZY=	3.6127		
XZ=	2.6707	YZ=	-2.6456	ZZ=	109.4478		
Eigenvalues:	76.2591		109.4602		147.8412		
10	C	Isotropic=	147.3168	Anisotropy		43.9979	
XX=	173.3008	YX=	7.1966	ZX=	4.6175		
XY=	5.687	YY=	124.6996	ZY=	2.7112		
XZ=	13.9263	YZ=	-5.0644	ZZ=	143.95		
Eigenvalues:	123.5623		141.7393		176.6487		
11	C	Isotropic=	147.3647	Anisotropy		12.0949	
XX=	141.589	YX=	0.4716	ZX=	-1.9621		
XY=	-11.2872	YY=	149.9877	ZY=	-4.9916		
XZ=	6.5423	YZ=	-0.9844	ZZ=	150.5176		
Eigenvalues:	138.8896		147.7766		155.428		
12	C	Isotropic=	154.7984	Anisotropy		22.9116	
XX=	163.5949	YX=	-9.4338	ZX=	-10.2416		
XY=	-1.4725	YY=	163.3206	ZY=	3.1293		
XZ=	-6.8413	YZ=	-3.9288	ZZ=	137.4797		
Eigenvalues:	134.7982		159.5242		170.0728		
13	C	Isotropic=	147.93	Anisotropy		55.874	
XX=	145.4226	YX=	-18.1402	ZX=	6.5675		
XY=	-21.8465	YY=	174.7599	ZY=	8.2129		
XZ=	13.7729	YZ=	11.2953	ZZ=	123.6075		
Eigenvalues:	114.5904		144.0202		185.1794		
14	C	Isotropic=	168.2	Anisotropy		12.6617	
XX=	168.6679	YX=	-4.6047	ZX=	8.1989		
XY=	5.7254	YY=	168.008	ZY=	6.647		

XZ=	5.6159	YZ=	2.0747	ZZ=	167.9241				
Eigenvalues:	160.2687			167.6902		176.6411			
15	C	Isotropic=		169.3189	Anisotropy		17.2312		
XX=	173.7448	YX=	-6.9724	ZX=	-3.8052				
XY=	-6.6204	YY=	171.6742	ZY=	-7.8174				
XZ=	0.7175	YZ=	-8.7868	ZZ=	162.5378				
Eigenvalues:	156.2208			170.9296		180.8064			
16	O	Isotropic=		262.992	Anisotropy		83.0449		
XX=	314.1699	YX=	-1.4597	ZX=	23.6577				
XY=	4.64	YY=	250.5949	ZY=	59.5395				
XZ=	8.2956	YZ=	22.6954	ZZ=	224.2111				
Eigenvalues:	193.0253			277.5953		318.3552			
17	O	Isotropic=		265.3043	Anisotropy		44.7402		
XX=	253.2974	YX=	15.7741	ZX=	-19.8477				
XY=	-3.3797	YY=	258.3725	ZY=	21.824				
XZ=	-3.0078	YZ=	14.9294	ZZ=	284.2431				
Eigenvalues:	239.6709			261.111		295.1311			
18	O	Isotropic=		-356.6249	Anisotropy		1080.2506		
XX=	-894.8543	YX=	7.0342	ZX=	340.9515				
XY=	-6.6025	YY=	-275.4338	ZY=	350.888				
XZ=	271.8169	YZ=	343.1766	ZZ=	100.4135				
Eigenvalues:	-995.8245			-437.5923		363.5422			
19	O	Isotropic=		89.3589	Anisotropy		125.25		
XX=	137.5437	YX=	70.4483	ZX=	-129.1508				
XY=	-10.1674	YY=	122.062	ZY=	21.0556				
XZ=	-22.4991	YZ=	95.7662	ZZ=	8.4709				
Eigenvalues:	-51.4244		146.6422			172.8589			
20	O	Isotropic=		92.5563	Anisotropy		157.2284		
XX=	118.4671	YX=	-23.3051	ZX=	14.7935				
XY=	-175.0707	YY=	-20.7598	ZY=	-0.8813				
XZ=	30.3236	YZ=	-6.4278	ZZ=	179.9617				
Eigenvalues:	-72.5298		152.8235			197.3753			
21	H	Isotropic=		31.2279	Anisotropy		13.5004		
XX=	35.6617	YX=	0.4643	ZX=	-5.5811				
XY=	0.3177	YY=	27.4488	ZY=	-6.617				
XZ=	-5.1528	YZ=	-5.5272	ZZ=	30.5734				
Eigenvalues:	22.0099		31.4457			40.2282			
22	C	Isotropic=		20.1955	Anisotropy		74.709		
XX=	27.1352	YX=	-73.0077	ZX=	42.3344				
XY=	-48.7816	YY=	-17.2307	ZY=	52.1974				
XZ=	15.1918	YZ=	29.284	ZZ=	50.682				
Eigenvalues:	-79.0308		69.6158			70.0015			
23	O	Isotropic=		-131.5479	Anisotropy		599.9472		
XX=	-190.102	YX=	-237.0738	ZX=	-240.803				
XY=	-223.0667	YY=	-67.8796	ZY=	151.1541				
XZ=	-187.4029	YZ=	153.1534	ZZ=	-136.6621				
Eigenvalues:	-407.0185			-256.0422		268.4169			
24	C	Isotropic=		166.3823	Anisotropy		36.6918		
XX=	156.3514	YX=	4.4402	ZX=	3.2879				
XY=	4.4244	YY=	164.7805	ZY=	-19.2245				
XZ=	2.692	YZ=	-17.3452	ZZ=	178.0151				
Eigenvalues:	148.3714			159.9321		190.8435			
25	H	Isotropic=		27.4414	Anisotropy		2.7947		
XX=	27.6565	YX=	-0.5882	ZX=	-1.3113				
XY=	-0.1689	YY=	27.6803	ZY=	-0.8683				
XZ=	-2.2462	YZ=	-1.5117	ZZ=	26.9875				

Eigenvalues:	25.0017	28.018	29.3045		
26	H	Isotropic=	28.1315	Anisotropy	8.5027
XX=	29.4843	YX=	-4.4201	ZX=	1.6684
XY=	-3.7317	YY=	29.4625	ZY=	-0.7239
XZ=	1.7626	YZ=	0.0946	ZZ=	25.4477
Eigenvalues:	24.3183	26.2762	33.8		
27	H	Isotropic=	25.4381	Anisotropy	3.4991
XX=	26.1615	YX=	1.2278	ZX=	-2.4389
XY=	1.4783	YY=	25.0892	ZY=	-0.1934
XZ=	1.0407	YZ=	-2.4839	ZZ=	25.0636
Eigenvalues:	23.6214	24.9221	27.7708		
28	H	Isotropic=	24.7236	Anisotropy	7.989
XX=	29.5826	YX=	1.0827	ZX=	1.5944
XY=	-0.913	YY=	25.203	ZY=	2.2689
XZ=	2.65	YZ=	1.403	ZZ=	19.3852
Eigenvalues:	18.4863	25.6349	30.0496		
29	H	Isotropic=	28.7076	Anisotropy	6.2832
XX=	30.6366	YX=	-1.1126	ZX=	-1.9061
XY=	-1.0412	YY=	23.8476	ZY=	0.9512
XZ=	-0.8553	YZ=	1.4936	ZZ=	31.6386
Eigenvalues:	23.5527	29.6737	32.8964		
30	H	Isotropic=	29.1846	Anisotropy	4.6609
XX=	32.1643	YX=	0.4609	ZX=	1.0894
XY=	-0.0188	YY=	30.1202	ZY=	-1.9478
XZ=	0.803	YZ=	-1.1899	ZZ=	25.2693
Eigenvalues:	24.6804	30.5816	32.2919		
31	H	Isotropic=	29.2969	Anisotropy	8.2725
XX=	30.3207	YX=	-1.5689	ZX=	-2.8498
XY=	-2.077	YY=	29.3904	ZY=	4.469
XZ=	-2.6888	YZ=	2.8862	ZZ=	28.1796
Eigenvalues:	24.8488	28.23	34.8119		
32	H	Isotropic=	29.1739	Anisotropy	9.001
XX=	28.34	YX=	3.8809	ZX=	-3.7511
XY=	3.6396	YY=	29.5677	ZY=	-1.8278
XZ=	-2.5024	YZ=	-2.3769	ZZ=	29.6141
Eigenvalues:	24.8127	27.5345	35.1746		
33	H	Isotropic=	30.3034	Anisotropy	6.6552
XX=	32.6167	YX=	2.8446	ZX=	1.7409
XY=	2.7456	YY=	27.1743	ZY=	0.675
XZ=	1.9187	YZ=	0.1455	ZZ=	31.1193
Eigenvalues:	25.971	30.1991	34.7402		
34	H	Isotropic=	30.133	Anisotropy	8.9571
XX=	29.8482	YX=	1.0497	ZX=	-0.0615
XY=	2.2789	YY=	34.9141	ZY=	2.3733
XZ=	0.9769	YZ=	2.969	ZZ=	25.6368
Eigenvalues:	24.9227	29.372	36.1044		
35	H	Isotropic=	30.2255	Anisotropy	6.5196
XX=	30.3851	YX=	-0.7005	ZX=	2.8398
XY=	-2.9105	YY=	32.9769	ZY=	-1.4709
XZ=	1.4095	YZ=	-1.1886	ZZ=	27.3145
Eigenvalues:	26.206	29.8986	34.5719		
36	H	Isotropic=	28.5676	Anisotropy	6.3596
XX=	28.3119	YX=	-0.5052	ZX=	-1.8278
XY=	-2.2444	YY=	30.5331	ZY=	3.6246
XZ=	-1.6458	YZ=	1.5692	ZZ=	26.8577
Eigenvalues:	25.1846	27.7109	32.8073		

37	H	Isotropic=	28.9347	Anisotropy	7.4326
XX=	32.2232	YX=	1.0815	ZX=	-1.4068
XY=	0.2833	YY=	23.1128	ZY=	-1.0045
XZ=	-2.3701	YZ=	-0.8894	ZZ=	31.4681
Eigenvalues:	22.9819	29.9324	33.8898		
38	H	Isotropic=	28.4761	Anisotropy	11.2757
XX=	32.4089	YX=	4.1967	ZX=	-1.0789
XY=	6.3105	YY=	28.2536	ZY=	1.3766
XZ=	-0.251	YZ=	1.8988	ZZ=	24.766
Eigenvalues:	22.99	26.4452	35.9933		
39	H	Isotropic=	28.6567	Anisotropy	9.6831
XX=	33.4086	YX=	-3.7095	ZX=	-2.1738
XY=	-4.1266	YY=	25.5909	ZY=	-0.984
XZ=	-0.5695	YZ=	-1.5348	ZZ=	26.9708
Eigenvalues:	23.1986	27.6595	35.1121		
40	H	Isotropic=	29.1861	Anisotropy	10.8563
XX=	31.2909	YX=	-2.5446	ZX=	-5.3687
XY=	-4.2861	YY=	27.5343	ZY=	0.659
XZ=	-4.6086	YZ=	1.3748	ZZ=	28.7332
Eigenvalues:	24.1599	26.9748	36.4237		
41	H	Isotropic=	29.6497	Anisotropy	5.9429
XX=	32.2068	YX=	-0.8331	ZX=	2.3499
XY=	-1.3503	YY=	27.7945	ZY=	2.6004
XZ=	2.7554	YZ=	2.0804	ZZ=	28.9478
Eigenvalues:	25.0902	30.2473	33.6117		
42	H	Isotropic=	30.5098	Anisotropy	9.6322
XX=	28.8402	YX=	-1.9124	ZX=	-0.4917
XY=	-2.1265	YY=	35.8133	ZY=	-2.7947
XZ=	-0.6953	YZ=	-2.4602	ZZ=	26.8759
Eigenvalues:	25.7284	28.8698	36.9313		
43	H	Isotropic=	29.0133	Anisotropy	5.4718
XX=	28.874	YX=	2.9176	ZX=	1.4726
XY=	1.9166	YY=	26.884	ZY=	-2.4239
XZ=	3.0662	YZ=	-1.0454	ZZ=	31.2819
Eigenvalues:	24.2109	30.1678	32.6612		
44	H	Isotropic=	29.1593	Anisotropy	6.8715
XX=	26.3903	YX=	-1.0821	ZX=	-0.4035
XY=	-0.1452	YY=	33.6032	ZY=	-0.1361
XZ=	-0.6871	YZ=	-1.4158	ZZ=	27.4843
Eigenvalues:	26.0641	27.6734	33.7403		
45	H	Isotropic=	28.9308	Anisotropy	8.9405
XX=	31.174	YX=	0.426	ZX=	-2.9079
XY=	1.4951	YY=	25.7403	ZY=	-1.5017
XZ=	-4.9455	YZ=	-2.0186	ZZ=	29.8782
Eigenvalues:	25.0287	26.8727	34.8911		
46	H	Isotropic=	30.5617	Anisotropy	18.1251
XX=	37.8628	YX=	-1.8739	ZX=	8.6314
XY=	-1.1121	YY=	22.9863	ZY=	-0.2774
XZ=	6.3107	YZ=	1.693	ZZ=	30.8359
Eigenvalues:	22.4165	26.6234	42.6451		
47	C	Isotropic=	8.5684	Anisotropy	96.4747
XX=	-43.5975	YX=	-42.785	ZX=	-62.3064
XY=	-5.4081	YY=	41.1145	ZY=	7.0555
XZ=	-72.4421	YZ=	-10.1598	ZZ=	28.1882
Eigenvalues:	-87.6415	40.4618	72.8849		
48	O	Isotropic=	-149.9024	Anisotropy	699.1779

XX=	-134.3947	YX=	-50.3363	ZX=	-289.6526		
XY=	-71.9164	YY=	-387.4681	ZY=	155.2897		
XZ=	-284.4088	YZ=	179.5219	ZZ=	72.1556		
Eigenvalues:	-447.705	-318.2183		316.2162			
49	H	Isotropic=	28.707	Anisotropy		6.5011	
XX=	28.4615	YX=	-1.7577	ZX=	1.724		
XY=	-0.8395	YY=	28.1534	ZY=	3.6906		
XZ=	2.6853	YZ=	4.2467	ZZ=	29.5061		
Eigenvalues:	23.5884	29.4916	33.041				
50	H	Isotropic=	29.539	Anisotropy		6.5175	
XX=	27.6127	YX=	0.2071	ZX=	-1.5112		
XY=	0.1618	YY=	33.6777	ZY=	-1.6403		
XZ=	-1.5028	YZ=	-0.502	ZZ=	27.3265		
Eigenvalues:	25.8966	28.8363	33.884				
51	C	Isotropic=	112.7237	Anisotropy		14.2109	
XX=	121.2271	YX=	-3.2032	ZX=	-0.714		
XY=	-5.1811	YY=	103.6119	ZY=	8.0317		
XZ=	3.8431	YZ=	8.9647	ZZ=	113.332		
Eigenvalues:	97.8489	118.1246		122.1976			
52	C	Isotropic=	128.7163	Anisotropy		14.4793	
XX=	131.7242	YX=	1.1192	ZX=	-1.3313		
XY=	7.9705	YY=	127.4349	ZY=	-6.324		
XZ=	-4.6443	YZ=	-7.3135	ZZ=	126.9897		
Eigenvalues:	120.2802		127.4995		138.3692		
53	O	Isotropic=	276.065	Anisotropy		46.2391	
XX=	281.0905	YX=	22.8246	ZX=	30.5098		
XY=	23.184	YY=	265.6655	ZY=	-11.9768		
XZ=	13.1747	YZ=	-2.9576	ZZ=	281.439		
Eigenvalues:	239.9034		281.4005		306.8911		
54	H	Isotropic=	27.0337	Anisotropy		4.8106	
XX=	29.3256	YX=	1.9165	ZX=	0.2657		
XY=	-0.834	YY=	23.5638	ZY=	-1.4409		
XZ=	2.4498	YZ=	-0.7749	ZZ=	28.2118		
Eigenvalues:	23.1963	27.6641	30.2408				
55	N	Isotropic=	140.2624	Anisotropy		136.9533	
XX=	135.0311	YX=	15.6304	ZX=	-22.4486		
XY=	8.8524	YY=	227.0991	ZY=	33.5031		
XZ=	-13.9277	YZ=	15.5501	ZZ=	58.6571		
Eigenvalues:	50.5222	138.7004		231.5646			
56	C	Isotropic=	53.8746	Anisotropy		186.0317	
XX=	53.436	YX=	-70.8711	ZX=	61.4421		
XY=	-65.5417	YY=	20.4813	ZY=	-58.0199		
XZ=	55.3949	YZ=	-51.5545	ZZ=	87.7065		
Eigenvalues:	-33.836	17.5641	177.8957				
57	H	Isotropic=	25.2968	Anisotropy		9.3911	
XX=	24.8776	YX=	-3.2021	ZX=	-4.6924		
XY=	-0.9081	YY=	27.9116	ZY=	2.9892		
XZ=	-5.0687	YZ=	1.6858	ZZ=	23.1012		
Eigenvalues:	19	25.3329	31.5576				
58	H	Isotropic=	30.2419	Anisotropy		10.5636	
XX=	27.8042	YX=	-1.7672	ZX=	-3.1903		
XY=	-0.1522	YY=	26.9872	ZY=	-3.4366		
XZ=	-1.0911	YZ=	-2.9433	ZZ=	35.9342		
Eigenvalues:	25.0026	28.4387	37.2843				
59	C	Isotropic=	14.5562	Anisotropy		117.6742	
XX=	84.3531	YX=	33.8335	ZX=	-2.6085		

XY= 29.4463 YY= -54.321 ZY= -42.7532
 XZ= -3.5529 YZ= -34.2272 ZZ= 13.6364
 Eigenvalues: -76.4816 27.1445 93.0056
 60 H Isotropic= 26.8858 Anisotropy 6.3032
 XX= 22.4571 YX= -0.8583 ZX= 1.7528
 XY= 1.7645 YY= 28.859 ZY= 4.2091
 XZ= 0.0653 YZ= -0.4885 ZZ= 29.3413
 Eigenvalues: 22.3318 27.2377 31.088
 61 C Isotropic= 62.4009 Anisotropy 171.0443
 XX= 47.8966 YX= -40.934 ZX= 92.6966
 XY= -37.5218 YY= 77.2968 ZY= -33.3471
 XZ= 90.2644 YZ= -41.9345 ZZ= 62.0093
 Eigenvalues: -36.9044 47.6768 176.4304
 62 C Isotropic= 61.5178 Anisotropy 176.4415
 XX= 91.4793 YX= -26.2965 ZX= 61.2549
 XY= -26.3774 YY= 34.0222 ZY= -82.0125
 XZ= 62.265 YZ= -85.8984 ZZ= 59.0519
 Eigenvalues: -42.1194 47.5273 179.1454
 63 C Isotropic= 62.9965 Anisotropy 175.8302
 XX= 62.308 YX= -79.193 ZX= 48.5047
 XY= -79.197 YY= 23.4779 ZY= -44.4956
 XZ= 48.4409 YZ= -44.1557 ZZ= 103.2038
 Eigenvalues: -38.8594 47.6324 180.2167
 64 C Isotropic= 61.5085 Anisotropy 174.0537
 XX= 41.7581 YX= -43.0206 ZX= 92.1127
 XY= -40.5748 YY= 77.8712 ZY= -36.8039
 XZ= 93.9199 YZ= -36.2768 ZZ= 64.8962
 Eigenvalues: -40.9018 47.8831 177.5443
 65 C Isotropic= 62.1724 Anisotropy 147.5917
 XX= 90.4345 YX= -15.9774 ZX= 52.3134
 XY= -15.2426 YY= 37.0294 ZY= -75.2672
 XZ= 52.171 YZ= -74.863 ZZ= 59.0533
 Eigenvalues: -32.488 58.4384 160.5669
 66 H Isotropic= 22.953 Anisotropy 11.3537
 XX= 23.2295 YX= 4.5112 ZX= 1.1089
 XY= 4.2167 YY= 25.1588 ZY= 4.4519
 XZ= 1.4086 YZ= 4.4461 ZZ= 20.4706
 Eigenvalues: 17.4349 20.9019 30.5221
 67 O Isotropic= -138.676 Anisotropy 630.0335
 XX= 221.6112 YX= 151.9638 ZX= -171.7094
 XY= 141.3893 YY= -269.8269 ZY= 102.1529
 XZ= -103.2442 YZ= 68.7458 ZZ= -367.8124
 Eigenvalues: -471.8003 -225.5741 281.3463
 68 C Isotropic= 55.9066 Anisotropy 170.6133
 XX= 104.7233 YX= -58.1492 ZX= 52.4517
 XY= -36.0876 YY= 47.7102 ZY= -61.9936
 XZ= 50.1141 YZ= -63.4719 ZZ= 15.2863
 Eigenvalues: -34.6193 32.6903 169.6488
 69 H Isotropic= 23.7007 Anisotropy 5.4676
 XX= 24.4247 YX= 2.8616 ZX= -1.6932
 XY= 2.8181 YY= 24.5022 ZY= 1.1626
 XZ= -1.6384 YZ= 0.8939 ZZ= 22.1753
 Eigenvalues: 19.9602 23.7962 27.3458
 70 H Isotropic= 23.6649 Anisotropy 3.5477
 XX= 23.6721 YX= 1.1128 ZX= -2.2853
 XY= 1.1473 YY= 23.7749 ZY= 1.7991

XZ=	-2.2572	YZ=	1.7989	ZZ=	23.5476		
Eigenvalues:	20.1393	24.8253	26.03				
71	H	Isotropic=	23.6901	Anisotropy	4.9865		
XX=	23.4286	YX=	2.3561	ZX=	-1.3957		
XY=	2.3865	YY=	25.2679	ZY=	1.7809		
XZ=	-1.383	YZ=	1.7675	ZZ=	22.3738		
Eigenvalues:	19.893	24.1629	27.0144				
72	H	Isotropic=	23.6751	Anisotropy	8.4347		
XX=	24.9484	YX=	3.2021	ZX=	-3.2643		
XY=	3.9537	YY=	24.5419	ZY=	-0.2692		
XZ=	-3.4665	YZ=	-0.3119	ZZ=	21.5349		
Eigenvalues:	18.8701	22.8569	29.2982				
73	C	Isotropic=	56.6112	Anisotropy	183.9766		
XX=	96.4727	YX=	-65.1884	ZX=	78.5505		
XY=	-65.322	YY=	56.0788	ZY=	-7.8876		
XZ=	86.8828	YZ=	-12.6117	ZZ=	17.2822		
Eigenvalues:	-43.3262	33.8976	179.2623				
74	C	Isotropic=	61.6564	Anisotropy	177.9239		
XX=	101.7148	YX=	-87.0147	ZX=	47.9829		
XY=	-83.9885	YY=	8.9413	ZY=	-28.091		
XZ=	45.4098	YZ=	-26.7345	ZZ=	74.3132		
Eigenvalues:	-41.9471	146.644	180.2723				
75	C	Isotropic=	63.3155	Anisotropy	176.948		
XX=	123.4154	YX=	-39.2982	ZX=	57.8918		
XY=	-40.247	YY=	42.945	ZY=	-70.6571		
XZ=	53.2792	YZ=	-68.1258	ZZ=	23.586		
Eigenvalues:	-38.7092	247.3747	181.2808				
76	C	Isotropic=	65.5486	Anisotropy	170.8142		
XX=	93.1675	YX=	-55.4677	ZX=	86.705		
XY=	-58.2574	YY=	73.8472	ZY=	-10.8803		
XZ=	83.4602	YZ=	-10.8872	ZZ=	29.6312		
Eigenvalues:	-35.2744	52.4955	179.4248				
77	C	Isotropic=	67.2452	Anisotropy	164.7085		
XX=	99.8196	YX=	-80.7713	ZX=	38.7983		
XY=	-81.0882	YY=	30.4979	ZY=	-24.446		
XZ=	42.5951	YZ=	-34.4626	ZZ=	71.418		
Eigenvalues:	-22.9403	347.6251	177.0509				
78	H	Isotropic=	23.1631	Anisotropy	6.5834		
XX=	21.2824	YX=	1.0612	ZX=	0.3088		
XY=	0.873	YY=	26.6858	ZY=	2.1764		
XZ=	0.0475	YZ=	1.926	ZZ=	21.5212		
Eigenvalues:	20.7481	21.1893	27.552				
79	H	Isotropic=	23.6982	Anisotropy	4.1359		
XX=	22.2191	YX=	-0.1926	ZX=	-2.1058		
XY=	0.3353	YY=	24.336	ZY=	1.4311		
XZ=	-2.1283	YZ=	1.3366	ZZ=	24.5394		
Eigenvalues:	20.7862	23.8529	26.4554				
80	H	Isotropic=	23.7745	Anisotropy	3.3782		
XX=	23.142	YX=	1.766	ZX=	-1.937		
XY=	1.6009	YY=	24.7353	ZY=	0.4823		
XZ=	-2.0873	YZ=	0.6607	ZZ=	23.4461		
Eigenvalues:	20.6183	24.6784	26.0266				
81	H	Isotropic=	23.8474	Anisotropy	4.7729		
XX=	22.7119	YX=	1.078	ZX=	-2.139		
XY=	1.0199	YY=	25.3262	ZY=	2.5501		
XZ=	-1.564	YZ=	2.3273	ZZ=	23.5042		

Eigenvalues: 20.0933 24.4196 27.0294
 82 H Isotropic= 23.6446 Anisotropy 7.5861
 XX= 22.7118 YX= -0.8577 ZX= -4.5766
 XY= -0.787 YY= 24.9255 ZY= 3.0145
 XZ= -3.9888 YZ= 1.6698 ZZ= 23.2967
 Eigenvalues: 18.5398 23.6921 28.702

2bv_neg45

C	-3.569884	1.446422	-1.337586
C	-4.042579	0.346639	-2.340242
C	-3.279507	-0.986657	-2.268261
C	-4.128491	-2.159764	-1.745959
C	-4.68605-1.97804-0.320038		
C	-3.7625	-1.463376	0.773265
C	-3.226786	-0.080221	0.541328
C	-1.878227	0.104795	0.591143
C	-1.317737	1.327688	-0.082561
C	-2.050472	1.661459	-1.386745
C	-4.061545	1.104763	0.101191
C	-5.572346	0.922167	0.09438
C	-3.793132	2.303418	1.031659
C	-0.93148-0.820021.247748		
C	-5.241418	-2.509242	-2.707601
O	-4.109032	2.696175	-1.766429
O	-3.991453	0.874889	-3.657055
O	-5.801794	-2.424501	-0.041396
O	-4.151761	-1.786379	2.100773
O	0.055751	1.233233	-0.514968
H	-3.117001	1.262428	-3.785957
C	-5.327988	-1.420332	2.697001
O	-6.217174	-0.871796	2.055048
C	-5.343084	-1.817158	4.136794
H	-5.145585	0.161032	-2.188948
H	-2.366156	-0.889366	-1.629369
H	-2.878724	-2.190012	0.668298
H	-1.362163	2.192239	0.644022
H	-1.847084	2.740303	-1.628321
H	-1.605393	1.049463	-2.215139
H	-5.902734	-0.066546	-0.295594
H	-5.981761.026429	1.130116	
H	-6.039509	1.724674	-0.529327
H	-4.749622.738291	1.412203	
H	-3.184805	1.997443	1.915538
H	-3.263639	3.118876	0.480771
H	-1.437556	-1.675296	1.759056
H	-0.196742	-1.225934	0.505161
H	-0.372548	-0.263241	2.045157
H	-5.784229	-3.418862	-2.351448
H	-5.980328	-1.675763	-2.784051
H	-4.821263	-2.709247	-3.722338
H	-4.417548	-2.377114	4.41197
H	-5.418347	-0.893511	4.76094
H	-6.237995	-2.460546	4.320473
H	-4.9777 2.529816	-2.154	
C	1.057959	0.99407 0.383371	
O	0.972037	1.473543	1.512441

H	-3.434725	-3.047812	-1.665728
H	-2.944818	-1.249936	-3.30733
C	2.216378	0.233365	-0.2501
C	3.545452	0.522432	0.505991
O	1.903585	-1.140691	-0.304244
H	2.289103	0.555012	-1.330612
N	4.644908	-0.200575	-0.096541
C	3.82119	2.007801	0.507451
H	3.409618	0.160473	1.573021
H	2.227641	-1.556345	0.509962
C	5.178349	-1.326301	0.507921
H	5.15072	0.254485	-0.818704
C	3.974017	2.707888	-0.694694
C	4.245529	4.074825	-0.678481
C	4.368579	4.748854	0.536918
C	4.217507	4.053658	1.736223
C	3.946538	2.685422	1.724281
H	3.873605	2.184012	-1.657231
O	4.605857	-1.849351	1.486248
C	6.436298	-1.875772	-0.068591
H	4.359967	4.621979	-1.625779
H	4.581367	5.828048	0.548344
H	4.308409	4.583721	2.695963
H	3.812564	2.142698	2.67289
C	7.464606	-2.245562	0.805654
C	8.652626	-2.766598	0.295095
C	8.812059	-2.926405	-1.081657
C	7.781919	-2.566785	-1.951177
C	6.59339	-2.038246	-1.448413
H	7.321313	-2.133471	1.89189
H	9.462329	-3.055874	0.981408
H	9.749598	-3.340353	-1.4822
H	7.904637	-2.701681	-3.036016
H	5.779596	-1.768603	-2.138482

2bv_neg45 E(RB+HF-PW91) = -2012.301265

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic= 111.2262 Anisotropy 30.3275

XX= 108.5077 YX= -20.4755 ZX= 1.5182

XY= -14.5122 YY= 118.0806 ZY= -1.8584

XZ= -5.294 YZ= -2.4615 ZZ= 107.0903

Eigenvalues: 94.5278 107.7063 131.4445

2 C Isotropic= 112.4652 Anisotropy 31.5035

XX= 93.7497 YX= -0.3599 ZX= -7.6973

XY= 0.4767 YY= 113.0604 ZY= -12.4627

XZ= -3.2424 YZ= -0.7034 ZZ= 130.5855

Eigenvalues: 92.9131 111.0149 133.4675

3 C Isotropic= 141.7062 Anisotropy 20.4177

XX= 123.0791 YX= -7.4077 ZX= 0.557

XY= -8.1787 YY= 149.5147 ZY= 3.7714

XZ= -6.7022 YZ= 1.0042 ZZ= 152.5248

Eigenvalues: 120.7792 149.0214 155.318

4 C Isotropic= 140.4225 Anisotropy 24.4501

XX= 127.0409 YX= -3.5514 ZX= -5.1782

XY= -8.3392 YY= 138.4931 ZY= 3.5327

XZ=	8.135	YZ=	4.9584	ZZ=	155.7334				
Eigenvalues:	124.2166			140.3282		156.7225			
5	C	Isotropic=		-23.3397	Anisotropy		181.5252		
XX=	-37.0611	YX=	-55.6121	ZX=	-6.9113				
XY=	-49.5244	YY=	66.5337	ZY=	-50.3947				
XZ=	7.2254	YZ=	-41.0616	ZZ=	-99.4917				
Eigenvalues:	-113.8984			-53.7979	97.6771				
6	C	Isotropic=		102.0013	Anisotropy		41.9336		
XX=	87.889	YX=	-2.0703	ZX=	5.6454				
XY=	4.0605	YY=	88.6959	ZY=	6.607				
XZ=	-12.3863	YZ=	0.2024	ZZ=	129.4189				
Eigenvalues:	86.6981	89.3487	129.957						
7	C	Isotropic=		46.7208	Anisotropy		152.622		
XX=	42.6837	YX=	-7.0068	ZX=	-8.0909				
XY=	-8.3143	YY=	-31.539	ZY=	45.7194				
XZ=	6.7255	YZ=	72.3304	ZZ=	129.0176				
Eigenvalues:	-51.4335	43.127	148.4687						
8	C	Isotropic=		39.4517	Anisotropy		157.6881		
XX=	33.911	YX=	-0.8582	ZX=	-12.2121				
XY=	7.4723	YY=	-12.2759	ZY=	97.3036				
XZ=	-8.3714	YZ=	74.7964	ZZ=	96.7199				
Eigenvalues:	-60.2915	34.0695	144.5771						
9	C	Isotropic=		110.9809	Anisotropy		55.938		
XX=	142.8663	YX=	-5.0933	ZX=	-16.7319				
XY=	-11.7137	YY=	97.2014	ZY=	-17.2797				
XZ=	-16.6561	YZ=	-10.4165	ZZ=	92.875				
Eigenvalues:	76.0484	108.6213	148.2729						
10	C	Isotropic=		147.2039	Anisotropy		44.4236		
XX=	175.3389	YX=	0.4697	ZX=	4.9267				
XY=	-5.4332	YY=	132.355	ZY=	-14.4934				
XZ=	8.8013	YZ=	-4.7698	ZZ=	133.9177				
Eigenvalues:	123.3121	141.4799	176.8196						
11	C	Isotropic=		147.3287	Anisotropy		11.4689		
XX=	140.3297	YX=	0.161	ZX=	-3.3316				
XY=	0.0456	YY=	147.9673	ZY=	0.7395				
XZ=	12.0091	YZ=	-0.7363	ZZ=	153.6891				
Eigenvalues:	139.0432	147.9682	154.9746						
12	C	Isotropic=		154.7342	Anisotropy		22.5563		
XX=	159.5526	YX=	14.9313	ZX=	-0.1194				
XY=	7.4945	YY=	151.1691	ZY=	9.7491				
XZ=	-5.9379	YZ=	16.5916	ZZ=	153.4808				
Eigenvalues:	134.665	159.7659	169.7717						
13	C	Isotropic=		147.8445	Anisotropy		55.8202		
XX=	140.4376	YX=	0.9278	ZX=	11.3175				
XY=	-3.0967	YY=	153.3743	ZY=	31.7881				
XZ=	19.1231	YZ=	30.7351	ZZ=	149.7216				
Eigenvalues:	114.5418	143.9338	185.058						
14	C	Isotropic=		166.9521	Anisotropy		11.0127		
XX=	168.9642	YX=	-3.9826	ZX=	9.2773				
XY=	-7.534	YY=	166.8754	ZY=	0.5375				
XZ=	-0.8651	YZ=	3.2098	ZZ=	165.0168				
Eigenvalues:	159.0583	167.5042	174.2939						
15	C	Isotropic=		169.2898	Anisotropy		17.1672		
XX=	170.0391	YX=	9.4979	ZX=	2.1625				
XY=	5.8856	YY=	160.76	ZY=	2.9157				
XZ=	4.3673	YZ=	4.8025	ZZ=	177.0703				

Eigenvalues:	156.2595	170.8754	180.7346		
16	O	Isotropic=	263.5909	Anisotropy	83.2104
XX=	316.6435	YX=	-11.9219	ZX=	26.4294
XY=	-1.6372	YY=	270.4997	ZY=	8.1986
XZ=	5.0235	YZ=	40.2488	ZZ=	203.6294
Eigenvalues:	193.4167	278.2914	319.0645		
17	O	Isotropic=	265.2263	Anisotropy	44.8363
XX=	254.6989	YX=	-1.4316	ZX=	-20.724
XY=	-1.7139	YY=	292.8809	ZY=	-16.1707
XZ=	1.9263	YZ=	-4.3104	ZZ=	248.099
Eigenvalues:	239.7901	260.7716	295.1172		
18	O	Isotropic=	-354.9641	Anisotropy	1078.2072
XX=	-784.5375	YX=	-483.788	ZX=	179.2222
XY=	-423.0062	YY=	149.4337	ZY=	-97.3817
XZ=	148.5364	YZ=	-103.4613	ZZ=	-429.7884
Eigenvalues:	-992.3488	-436.3841	363.8407		
19	O	Isotropic=	87.9817	Anisotropy	125.225
XX=	134.877	YX=	59.0607	ZX=	-140.475
XY=	18.4326	YY=	123.5465	ZY=	81.3253
XZ=	0.3756	YZ=	37.4308	ZZ=	5.5216
Eigenvalues:	-52.9505	145.4306	171.465		
20	O	Isotropic=	94.0586	Anisotropy	152.4066
XX=	85.2256	YX=	11.2038	ZX=	46.9232
XY=	98.5531	YY=	120.3882	ZY=	-90.0537
XZ=	172.6533	YZ=	-62.786	ZZ=	76.562
Eigenvalues:	-73.7958	160.3086	195.663		
21	H	Isotropic=	31.1324	Anisotropy	13.7017
XX=	34.1149	YX=	6.8268	ZX=	-3.0158
XY=	6.4356	YY=	25.6626	ZY=	-2.6508
XZ=	-2.8104	YZ=	-3.6038	ZZ=	33.6197
Eigenvalues:	21.8577	31.2726	40.2669		
22	C	Isotropic=	20.2466	Anisotropy	74.1959
XX=	7.4382	YX=	1.6788	ZX=	92.7201
XY=	10.309	YY=	69.0249	ZY=	-13.646
XZ=	53.029	YZ=	-0.1259	ZZ=	-15.7234
Eigenvalues:	-78.4965	69.5257	69.7105		
23	O	Isotropic=	-130.9746	Anisotropy	599.8743
XX=	-311.2065	YX=	252.6724	ZX=	19.6082
XY=	204.0369	YY=	149.1811	ZY=	106.6953
XZ=	39.1016	YZ=	114.2386	ZZ=	-230.8985
Eigenvalues:	-406.686	-255.1796	268.9416		
24	C	Isotropic=	166.2552	Anisotropy	37.0239
XX=	158.4917	YX=	-3.3045	ZX=	-2.5814
XY=	-3.2966	YY=	153.0248	ZY=	-10.9066
XZ=	-2.155	YZ=	-12.5639	ZZ=	187.2489
Eigenvalues:	147.9707	159.857	190.9377		
25	H	Isotropic=	27.441	Anisotropy	3.0149
XX=	27.1054	YX=	1.5966	ZX=	-0.4057
XY=	2.055	YY=	26.7781	ZY=	-0.1872
XZ=	-1.6573	YZ=	0.1219	ZZ=	28.4395
Eigenvalues:	24.972	27.9	29.451		
26	H	Isotropic=	27.9438	Anisotropy	8.3959
XX=	27.9619	YX=	1.5573	ZX=	3.9093
XY=	1.014	YY=	26.798	ZY=	3.3499
XZ=	3.3952	YZ=	2.2884	ZZ=	29.0714
Eigenvalues:	24.288	26.0023	33.541		

27	H	Isotropic=	25.3591	Anisotropy	3.6238
XX=	26.3449	YX=	1.4823	ZX=	-2.1094
XY=	-1.074	YY=	23.5778	ZY=	-2.1352
XZ=	-0.7474	YZ=	0.7462	ZZ=	26.1546
Eigenvalues:	23.3923	24.91	27.775		
28	H	Isotropic=	24.7694	Anisotropy	7.9411
XX=	29.9341	YX=	-0.9328	ZX=	0.0712
XY=	-0.8349	YY=	22.7894	ZY=	2.6073
XZ=	1.4742	YZ=	3.5729	ZZ=	21.5849
Eigenvalues:	18.917	25.3278	30.0635		
29	H	Isotropic=	28.6509	Anisotropy	6.3698
XX=	30.027	YX=	2.6672	ZX=	0.9176
XY=	1.4768	YY=	30.5319	ZY=	-3.0686
XZ=	1.022	YZ=	-3.3285	ZZ=	25.3939
Eigenvalues:	23.3718	29.6836	32.8975		
30	H	Isotropic=	29.054	Anisotropy	5.036
XX=	32.3787	YX=	0.2607	ZX=	0.2045
XY=	0.4249	YY=	25.0896	ZY=	2.2825
XZ=	0.0037	YZ=	1.4764	ZZ=	29.6936
Eigenvalues:	24.4094	30.3413	32.4113		
31	H	Isotropic=	29.3237	Anisotropy	8.1941
XX=	29.1027	YX=	2.3375	ZX=	-0.2234
XY=	2.612	YY=	33.4533	ZY=	0.8713
XZ=	-0.2673	YZ=	2.4354	ZZ=	25.4149
Eigenvalues:	24.9407	28.2439	34.7864		
32	H	Isotropic=	29.2177	Anisotropy	9.1502
XX=	29.2486	YX=	0.9203	ZX=	-5.3348
XY=	0.1395	YY=	27.7322	ZY=	-1.94
XZ=	-4.6832	YZ=	-1.1132	ZZ=	30.6724
Eigenvalues:	24.7697	27.5655	35.3179		
33	H	Isotropic=	30.3502	Anisotropy	6.5743
XX=	33.8634	YX=	-2.0642	ZX=	-0.1854
XY=	-2.2333	YY=	28.9811	ZY=	-2.5753
XZ=	-0.3002	YZ=	-2.0053	ZZ=	28.2061
Eigenvalues:	25.9402	30.3773	34.733		
34	H	Isotropic=	30.1568	Anisotropy	9.105
XX=	30.86	YX=	-1.3422	ZX=	-1.7791
XY=	-3.0581	YY=	31.0568	ZY=	4.8764
XZ=	-2.1891	YZ=	4.3815	ZZ=	28.5534
Eigenvalues:	24.9985	29.245	36.2268		
35	H	Isotropic=	30.2305	Anisotropy	6.2774
XX=	29.9105	YX=	-1.7432	ZX=	1.2984
XY=	0.5915	YY=	27.8908	ZY=	2.9615
XZ=	1.9101	YZ=	2.4101	ZZ=	32.8901
Eigenvalues:	26.319	29.957	34.4154		
36	H	Isotropic=	28.5804	Anisotropy	6.1016
XX=	27.7224	YX=	0.7021	ZX=	-1.0506
XY=	1.7183	YY=	31.4006	ZY=	1.4352
XZ=	-0.3316	YZ=	3.6533	ZZ=	26.6183
Eigenvalues:	25.0382	28.0548	32.6482		
37	H	Isotropic=	28.9611	Anisotropy	7.2293
XX=	31.6657	YX=	1.7363	ZX=	-0.2466
XY=	2.9961	YY=	28.1432	ZY=	-4.0854
XZ=	-0.1394	YZ=	-4.4271	ZZ=	27.0743
Eigenvalues:	23.0724	30.0301	33.7806		
38	H	Isotropic=	27.9453	Anisotropy	12.8169

XX=	34.3963	YX=	-0.6885	ZX=	-4.2001		
XY=	-2.6108	YY=	25.4584	ZY=	0.5523		
XZ=	-5.3794	YZ=	-0.3303	ZZ=	23.9813		
Eigenvalues:	22.0377	25.3083	36.49				
39	H	Isotropic=	28.6488	Anisotropy	8.0435		
XX=	30.3476	YX=	4.6368	ZX=	1.9186		
XY=	4.0743	YY=	26.2127	ZY=	-0.5841		
XZ=	3.1294	YZ=	0.0822	ZZ=	29.3862		
Eigenvalues:	23.0486	28.8867	34.0112				
40	H	Isotropic=	29.1738	Anisotropy	10.7881		
XX=	28.8276	YX=	5.7286	ZX=	-1.0355		
XY=	6.1678	YY=	31.6699	ZY=	0.4601		
XZ=	0.814	YZ=	0.0161	ZZ=	27.0238		
Eigenvalues:	24.1142	27.0412	36.3658				
41	H	Isotropic=	29.648	Anisotropy	5.8696		
XX=	32.0424	YX=	-1.033	ZX=	2.7878		
XY=	-1.0071	YY=	30.287	ZY=	0.1166		
XZ=	3.2059	YZ=	0.6391	ZZ=	26.6147		
Eigenvalues:	25.1713	30.2118	33.5611				
42	H	Isotropic=	30.4953	Anisotropy	9.6075		
XX=	28.076	YX=	1.1623	ZX=	-0.3424		
XY=	1.5171	YY=	28.3533	ZY=	4.1544		
XZ=	-0.3917	YZ=	3.7686	ZZ=	35.0568		
Eigenvalues:	25.7184	28.8673	36.9003				
43	H	Isotropic=	29.0161	Anisotropy	5.5544		
XX=	30.2944	YX=	-2.0772	ZX=	-0.9595		
XY=	-2.8696	YY=	26.3919	ZY=	-2.4587		
XZ=	1.0974	YZ=	-3.3867	ZZ=	30.3621		
Eigenvalues:	24.0749	30.2545	32.719				
44	H	Isotropic=	29.1891	Anisotropy	6.9823		
XX=	26.3598	YX=	-0.1766	ZX=	-0.5313		
XY=	-0.3937	YY=	29.1166	ZY=	2.1279		
XZ=	-1.7891	YZ=	3.2316	ZZ=	32.0909		
Eigenvalues:	26.1046	27.6187	33.844				
45	H	Isotropic=	28.9623	Anisotropy	8.8548		
XX=	30.3671	YX=	3.1253	ZX=	-1.2737		
XY=	4.053	YY=	28.0379	ZY=	-2.6426		
XZ=	-3.359	YZ=	-2.7334	ZZ=	28.4819		
Eigenvalues:	25.08	26.9414	34.8655				
46	H	Isotropic=	30.6022	Anisotropy	18.063		
XX=	38.2428	YX=	-2.9857	ZX=	8.3574		
XY=	-1.8797	YY=	26.9848	ZY=	-1.5991		
XZ=	6.6183	YZ=	-3.9248	ZZ=	26.579		
Eigenvalues:	22.4173	26.7451	42.6442				
47	C	Isotropic=	7.6935	Anisotropy	96.4878		
XX=	-59.2086	YX=	58.7809	ZX=	-15.4748		
XY=	41.5226	YY=	50.7416	ZY=	0.1308		
XZ=	-52.6448	YZ=	9.5625	ZZ=	31.5475		
Eigenvalues:	-88.0654	39.1271	72.0187				
48	O	Isotropic=	-143.6085	Anisotropy	696.6184		
XX=	-204.8795	YX=	228.1398	ZX=	-89.0271		
XY=	239.0531	YY=	146.8214	ZY=	-180.3975		
XZ=	-76.5224	YZ=	-183.1187	ZZ=	-372.7673		
Eigenvalues:	-430.629	-321.0002	320.8038				
49	H	Isotropic=	28.669	Anisotropy	6.3488		
XX=	28.4972	YX=	-1.1556	ZX=	2.6863		

XY= -2.5461 YY= 32.0749 ZY= 0.8096
 XZ= 2.4747 YZ= 0.2814 ZZ= 25.4348
 Eigenvalues: 23.7258 29.3797 32.9015
 50 H Isotropic= 29.482 Anisotropy 6.5569
 XX= 27.5969 YX= 0.5457 ZX= -2.2571
 XY= 0.5314 YY= 28.9168 ZY= 3.1436
 XZ= -2.2792 YZ= 1.8828 ZZ= 31.9321
 Eigenvalues: 25.7608 28.8319 33.8532
 51 C Isotropic= 108.5634 Anisotropy 21.5041
 XX= 114.0671 YX= 10.4697 ZX= 3.6849
 XY= 5.1644 YY= 115.8159 ZY= -3.5451
 XZ= 5.1089 YZ= -0.1795 ZZ= 95.8074
 Eigenvalues: 94.1451 108.6457 122.8995
 52 C Isotropic= 127.1059 Anisotropy 22.7944
 XX= 127.3911 YX= 8.9643 ZX= 2.5031
 XY= -0.5106 YY= 133.2888 ZY= 9.4732
 XZ= 6.1293 YZ= 13.3421 ZZ= 120.6377
 Eigenvalues: 113.7191 125.2965 142.3021
 53 O Isotropic= 272.3438 Anisotropy 47.8247
 XX= 288.1065 YX= 11.7856 ZX= 35.5707
 XY= 2.5282 YY= 266.1281 ZY= -13.1955
 XZ= 13.7247 YZ= -31.5603 ZZ= 262.7968
 Eigenvalues: 232.1902 280.6143 304.227
 54 H Isotropic= 26.6023 Anisotropy 3.9522
 XX= 27.2338 YX= 1.8402 ZX= 0.4452
 XY= 0.6972 YY= 25.7937 ZY= -3.1906
 XZ= 0.8899 YZ= -2.5134 ZZ= 26.7793
 Eigenvalues: 22.9345 27.6353 29.2371
 55 N Isotropic= 121.3263 Anisotropy 113.096
 XX= 99.6925 YX= -28.1173 ZX= 48.2854
 XY= -43.0049 YY= 180.428 ZY= 18.0426
 XZ= 69.796 YZ= -6.4547 ZZ= 83.8583
 Eigenvalues: 27.0339 140.2213 196.7236
 56 C Isotropic= 52.4019 Anisotropy 190.0101
 XX= 170.5953 YX= -43.5 ZX= -5.7367
 XY= -40.0945 YY= -28.0518 ZY= 2.4151
 XZ= 0.6235 YZ= -0.6561 ZZ= 14.6621
 Eigenvalues: -36.4905 14.6209 179.0753
 57 H Isotropic= 25.0761 Anisotropy 3.2255
 XX= 23.568 YX= -0.6396 ZX= 0.2141
 XY= -1.9773 YY= 24.4806 ZY= 0.3331
 XZ= 0.2985 YZ= 0.3615 ZZ= 27.1798
 Eigenvalues: 22.6018 25.4002 27.2264
 58 H Isotropic= 29.4217 Anisotropy 14.388
 XX= 28.1822 YX= -1.8011 ZX= 4.9026
 XY= -0.8832 YY= 29.9789 ZY= -6.8193
 XZ= 5.6165 YZ= -6.8927 ZZ= 30.104
 Eigenvalues: 21.6896 27.5618 39.0137
 59 C Isotropic= 15.7996 Anisotropy 123.7924
 XX= -3.9481 YX= 56.3103 ZX= 32.219
 XY= 66.9655 YY= -8.8759 ZY= 32.4461
 XZ= 20.9049 YZ= 29.0527 ZZ= 60.2228
 Eigenvalues: -68.2225 17.2934 98.3278
 60 H Isotropic= 26.4924 Anisotropy 9.41
 XX= 25.8933 YX= -4.543 ZX= -4.6531
 XY= -5.1338 YY= 29.2838 ZY= -1.9828

XZ= -2.491 YZ= -1.6333 ZZ= 24.3
 Eigenvalues: 19.3059 27.4055 32.7657
 61 C Isotropic= 67.4255 Anisotropy 166.239
 XX= 173.8378 YX= -23.4492 ZX= -7.889
 XY= -25.847 YY= 40.5706 ZY= -35.5663
 XZ= -6.2708 YZ= -38.606 ZZ= -12.132
 Eigenvalues: -32.8017 56.8267 178.2514
 62 C Isotropic= 62.7122 Anisotropy 176.5406
 XX= 174.7842 YX= -28.8269 ZX= 8.2659
 XY= -28.7327 YY= 32.9007 ZY= 35.942
 XZ= 8.5842 YZ= 39.0262 ZZ= -19.5482
 Eigenvalues: -41.1154 48.8462 180.406
 63 C Isotropic= 63.7223 Anisotropy 176.5161
 XX= 173.3521 YX= -40.7489 ZX= 1.7944
 XY= -41.5575 YY= -29.6504 ZY= -1.9977
 XZ= 1.2059 YZ= -0.6199 ZZ= 47.4652
 Eigenvalues: -37.6875 47.4547 181.3996
 64 C Isotropic= 61.0687 Anisotropy 177.2698
 XX= 173.908 YX= -27.6076 ZX= -2.4085
 XY= -28.191 YY= 31.9185 ZY= -35.6932
 XZ= -4.7475 YZ= -37.2376 ZZ= -22.6204
 Eigenvalues: -42.0575 46.015 179.2486
 65 C Isotropic= 56.735 Anisotropy 160.0923
 XX= 158.7286 YX= -24.7781 ZX= 10.2629
 XY= -24.9414 YY= 31.1454 ZY= 34.6688
 XZ= 9.6267 YZ= 35.7202 ZZ= -19.6691
 Eigenvalues: -39.7561 46.4979 163.4632
 66 H Isotropic= 24.0402 Anisotropy 8.5536
 XX= 21.6789 YX= 1.5803 ZX= -1.0498
 XY= 1.5649 YY= 27.1444 ZY= -4.1312
 XZ= -0.8972 YZ= -3.1048 ZZ= 23.2973
 Eigenvalues: 21.1191 21.2589 29.7426
 67 O Isotropic= -75.362 Anisotropy 625.3786
 XX= -69.7283 YX= 92.062 ZX= 259.462
 XY= 91.8706 YY= -104.0299 ZY= 330.7414
 XZ= 213.4311 YZ= 225.7421 ZZ= -52.3279
 Eigenvalues: -393.8633 -173.7799 341.5571
 68 C Isotropic= 55.8759 Anisotropy 169.9783
 XX= 2.6261 YX= 66.5001 ZX= 6.6392
 XY= 51.3956 YY= 143.7065 ZY= -40.8737
 XZ= 14.1459 YZ= -18.6866 ZZ= 21.2953
 Eigenvalues: -27.4598 25.8928 169.1948
 69 H Isotropic= 23.8456 Anisotropy 4.9467
 XX= 20.9675 YX= 1.7889 ZX= -0.1332
 XY= 1.4063 YY= 26.6577 ZY= 0.4288
 XZ= 0.0226 YZ= 0.5675 ZZ= 23.9116
 Eigenvalues: 20.54 23.8534 27.1434
 70 H Isotropic= 23.8141 Anisotropy 3.0989
 XX= 20.9166 YX= 1.2888 ZX= 0.014
 XY= 0.9941 YY= 24.6808 ZY= 0.2137
 XZ= 0.0221 YZ= 0.1401 ZZ= 25.8449
 Eigenvalues: 20.5973 24.965 25.88
 71 H Isotropic= 23.7867 Anisotropy 4.4576
 XX= 20.9473 YX= 1.6593 ZX= 0.2554
 XY= 1.3683 YY= 26.3258 ZY= -0.1938
 XZ= 0.0348 YZ= -0.5207 ZZ= 24.0868

Eigenvalues: 20.5355 24.0661 26.7584
 72 H Isotropic= 23.5356 Anisotropy 8.0414
 XX= 21.0101 YX= 1.6883 ZX= 1.0581
 XY= 1.4046 YY= 25.8817 ZY= 3.9494
 XZ= 0.7609 YZ= 3.1143 ZZ= 23.7149
 Eigenvalues: 20.5462 21.1641 28.8965
 73 C Isotropic= 61.495 Anisotropy 176.1739
 XX= 61.3747 YX= 48.1067 ZX= 3.8092
 XY= 46.0437 YY= 159.4764 ZY= -11.5277
 XZ= 2.0182 YZ= -13.8853 ZZ= -36.3662
 Eigenvalues: -37.589 43.1297 178.9442
 74 C Isotropic= 61.8012 Anisotropy 177.0479
 XX= 19.9991 YX= 62.5359 ZX= -41.8584
 XY= 62.619 YY= 154.6987 ZY= 6.6971
 XZ= -44.6334 YZ= 7.1791 ZZ= 10.7057
 Eigenvalues: -40.5702 46.1406 179.8331
 75 C Isotropic= 61.6484 Anisotropy 179.1026
 XX= 2.3716 YX= 74.8204 ZX= 24.106
 XY= 75.496 YY= 148.7771 ZY= -19.2983
 XZ= 23.8032 YZ= -20.3395 ZZ= 33.7965
 Eigenvalues: -41.2175 45.1126 181.0502
 76 C Isotropic= 63.1989 Anisotropy 174.8525
 XX= 67.7498 YX= 46.2758 ZX= 4.9423
 XY= 49.7514 YY= 158.095 ZY= -16.4044
 XZ= 7.3354 YZ= -19.5576 ZZ= -36.248
 Eigenvalues: -39.0511 48.8807 179.7673
 77 C Isotropic= 66.9864 Anisotropy 164.3024
 XX= 29.4321 YX= 55.8042 ZX= -46.9032
 XY= 59.3739 YY= 152.5204 ZY= 2.0472
 XZ= -39.0164 YZ= 2.5622 ZZ= 19.0066
 Eigenvalues: -28.8074 53.2452 176.5213
 78 H Isotropic= 23.3807 Anisotropy 8.0086
 XX= 27.0083 YX= -3.8743 ZX= 0.8874
 XY= -2.8675 YY= 20.8401 ZY= -0.7923
 XZ= 1.112 YZ= -0.6534 ZZ= 22.2938
 Eigenvalues: 19.3315 22.091 28.7198
 79 H Isotropic= 23.7474 Anisotropy 4.4334
 XX= 24.8688 YX= -2.3341 ZX= -0.8244
 XY= -2.1727 YY= 21.2997 ZY= 0.5988
 XZ= -1.0487 YZ= 0.5831 ZZ= 25.0739
 Eigenvalues: 20.2064 24.3328 26.7031
 80 H Isotropic= 23.7012 Anisotropy 3.8302
 XX= 24.2238 YX= -1.8605 ZX= 0.8385
 XY= -1.5491 YY= 21.0649 ZY= 0.1574
 XZ= 0.8095 YZ= -0.0331 ZZ= 25.8149
 Eigenvalues: 20.2927 24.5563 26.2547
 81 H Isotropic= 23.8263 Anisotropy 5.2164
 XX= 26.0287 YX= -2.859 ZX= -0.2585
 XY= -2.5168 YY= 21.4238 ZY= 0.6324
 XZ= -0.0916 YZ= 0.3026 ZZ= 24.0266
 Eigenvalues: 20.1549 24.0201 27.304
 82 H Isotropic= 23.7456 Anisotropy 8.5039
 XX= 24.4973 YX= -3.3769 ZX= -2.7729
 XY= -3.0196 YY= 21.4866 ZY= 2.7353
 XZ= -2.6119 YZ= 1.692 ZZ= 25.253
 Eigenvalues: 19.4134 22.4086 29.4149

2bvi_neg45

C	-3.34721	-2.040909	0.26176
C	-4.019212	-1.568146	1.589611
C	-3.323153	-0.397084	2.303232
C	-4.144070	0.905163	2.303587
C	-4.473661	1.469471	0.907137
C	-3.372882	1.536447	-0.14021
C	-2.807478	0.20471	-0.541081
C	-1.458939	0.028326	-0.466926
C	-0.943811	-1.383755	-0.408192
C	-1.842806	-2.296624	0.432711
C	-3.636892	-1.017551	-0.877528
C	-5.139558	-0.818789	-1.013727
C	-3.173045	-1.605522	-2.224224
C	-0.473621	1.128311	-0.420513
C	-5.404233	0.76522	3.127018
O	-3.879418	-3.321881	-0.072603
O	-4.137611	-2.680386	2.463654
O	-5.556605	2.028297	0.715914
O	-3.576122	2.485706	-1.177323
O	0.345957	-1.557249	0.216459
H	-3.271273	-3.101319	2.525525
C	-4.631121	2.49718	-2.049663
O	-5.574563	1.727077	-1.908108
C	-4.455101	3.556815	-3.087244
H	-5.095616	-1.299621	1.381433
H	-2.321168	-0.192293	1.849571
H	-2.553231	2.08919	0.445109
H	-0.838271	-1.774035	-1.463678
H	-1.622664	-3.359499	0.140095
H	-1.557098	-2.186924	1.512128
H	-5.574104	-0.142539	-0.243908
H	-5.386344	-0.386733	-2.015547
H	-5.651366	-1.811134	-0.945266
H	-4.03906	-1.764444	-2.912411
H	-2.455295	-0.921311	-2.735673
H	-2.692436	-2.603134	-2.073677
H	-0.940713	2.138556	-0.522712
H	0.108731	1.093421	0.5362
H	0.234622	1.020564	-1.283325
H	-5.932683	1.747965	3.189074
H	-6.103601	0.02731	2.665585
H	-5.150854	0.421641	4.15852
H	-3.526571	4.149425	-2.907364
H	-4.396379	3.068218	-4.090346
H	-5.342799	4.234987	-3.0588
H	-4.799241	-3.349899	0.220363
C	1.455516	-0.936501	-0.282506
O	1.565385	-0.7963	-1.499683
H	-3.492782	1.695707	2.780208
H	-3.160592	-0.692512	3.374416
C	2.472433	-0.623180	0.807936
C	3.91595	-0.573304	0.216437
O	2.10022	0.556521	1.481972
H	2.395071	-1.430697	1.595699

N	4.887208	-0.277992	1.236568
C	4.231864	-1.892851	-0.451834
H	3.903692	0.243716	-0.564205
H	2.42822	1.308939	0.969576
C	5.553521	0.913178	1.456763
H	5.194872	-1.056241	1.78087
C	4.216634	-3.086301	0.278439
C	4.528545	-4.292297	-0.347225
C	4.860482	-4.312284	-1.702113
C	4.879177	-3.123735	-2.431438
C	4.568793	-1.915088	-1.808822
H	3.956468	-3.079392	1.347859
O	6.494824	0.895828	2.277318
C	5.231301	2.15955	0.707307
H	4.512299	-5.228627	0.22999
H	5.106012	-5.264878	-2.194531
H	5.137385	-3.137084	-3.500721
H	4.572218	-0.980774	-2.390739
C	5.12459	3.346083	1.446214
C	4.927403	4.560993	0.79269
C	4.871893	4.604571	-0.600556
C	5.032738	3.432777	-1.339544
C	5.226858	2.2138	-0.689905
H	5.200794	3.307702	2.544699
H	4.830094	5.487388	1.378253
H	4.717353	5.564074	-1.116404
H	5.020121	3.468671	-2.439117
H	5.413802	1.308616	-1.289047

2bvi_neg45	E(RB+HF-PW91)	=	-2012.286626
SCF GIAO	Magnetic shielding	tensor (ppm):	
1 C	Isotropic=	111.2007	Anisotropy 30.6153
XX=	106.2764	YX= 18.3818	ZX= 8.8328
XY=	9.4194	YY= 116.5401	ZY= 5.0284
XZ=	12.0881	YZ= 5.6618	ZZ= 110.7857
Eigenvalues:	94.2687	107.7227	131.6109
2 C	Isotropic=	112.2642	Anisotropy 30.853
XX=	92.7956	YX= -1.4261	ZX= 1.4794
XY=	1.7631	YY= 122.7054	ZY= -16.3169
XZ=	-2.0035	YZ= -5.3012	ZZ= 121.2917
Eigenvalues:	92.793	111.1667	132.8329
3 C	Isotropic=	141.6225	Anisotropy 20.0254
XX=	122.4339	YX= 7.5095	ZX= -2.1794
XY=	3.578	YY= 147.6992	ZY= 2.3719
XZ=	4.8707	YZ= -0.6798	ZZ= 154.7344
Eigenvalues:	121.232	148.6628	154.9728
4 C	Isotropic=	140.8101	Anisotropy 24.0598
XX=	127.8063	YX= 1.9424	ZX= 1.8783
XY=	12.9005	YY= 139.4359	ZY= -4.0597
XZ=	-7.2574	YZ= -3.9304	ZZ= 155.188
Eigenvalues:	124.1779	141.4024	156.8499
5 C	Isotropic=	-23.0113	Anisotropy 181.522
XX=	-43.7514	YX= 39.1674	ZX= 43.6732
XY=	42.4222	YY= 62.7369	ZY= 49.2956
XZ=	28.3937	YZ= 58.9756	ZZ= -88.0193

Eigenvalues:	-113.7568	-53.280498	0.0034		
6	C	Isotropic=	102.0519	Anisotropy	41.557
XX=	88.3786	YX=	7.6608	ZX=	-9.3409
XY=	-7.4233	YY=	95.7113	ZY=	-13.6825
XZ=	2.7649	YZ=	-18.1067	ZZ=	122.0657
Eigenvalues:	86.9113	89.4877	129.7565		
7	C	Isotropic=	46.1167	Anisotropy	153.6056
XX=	43.5105	YX=	4.1505	ZX=	-6.1424
XY=	16.737	YY=	-44.1611	ZY=	-50.5542
XZ=	-18.0742	YZ=	-25.9511	ZZ=	139.0006
Eigenvalues:	-52.4792	42.3088	148.5204		
8	C	Isotropic=	40.4718	Anisotropy	155.8421
XX=	35.5694	YX=	-6.3345	ZX=	-6.128
XY=	-15.4874	YY=	-57.498	ZY=	5.4454
XZ=	-14.1142	YZ=	-15.5387	ZZ=	143.3441
Eigenvalues:	-58.9495	35.9984	144.3666		
9	C	Isotropic=	110.8976	Anisotropy	56.3267
XX=	135.9454	YX=	-3.9795	ZX=	25.2171
XY=	2.4367	YY=	108.061	ZY=	-9.0003
XZ=	28.7698	YZ=	-3.155	ZZ=	88.6865
Eigenvalues:	75.5994	108.6447	148.4488		
10	C	Isotropic=	147.2134	Anisotropy	44.429
XX=	175.9629	YX=	1.0995	ZX=	2.8083
XY=	9.4419	YY=	141.0597	ZY=	-8.7211
XZ=	2.8771	YZ=	-0.0786	ZZ=	124.6175
Eigenvalues:	123.1988	141.6086	176.8327		
11	C	Isotropic=	147.3806	Anisotropy	11.8747
XX=	142.0665	YX=	-0.7419	ZX=	1.2601
XY=	6.1529	YY=	149.0151	ZY=	-1.2314
XZ=	-12.4925	YZ=	-2.9878	ZZ=	151.0601
Eigenvalues:	139.1172	147.7274	155.297		
12	C	Isotropic=	154.9467	Anisotropy	22.4734
XX=	160.0468	YX=	-14.5163	ZX=	-7.8055
XY=	-10.4176	YY=	141.5869	ZY=	0.9171
XZ=	0.727	YZ=	6.7435	ZZ=	163.2063
Eigenvalues:	135.1824	159.7286	169.9289		
13	C	Isotropic=	148.3175	Anisotropy	55.0937
XX=	145.7689	YX=	1.8825	ZX=	-14.7009
XY=	8.4191	YY=	125.9576	ZY=	19.6033
XZ=	-19.2017	YZ=	17.2862	ZZ=	173.226
Eigenvalues:	115.6086	144.2973	185.0467		
14	C	Isotropic=	167.3856	Anisotropy	12.3644
XX=	170.6474	YX=	7.8675	ZX=	-5.6795
XY=	6.0643	YY=	165.1024	ZY=	1.9454
XZ=	5.2014	YZ=	4.099	ZZ=	166.4068
Eigenvalues:	159.3705	167.1577	175.6285		
15	C	Isotropic=	169.3838	Anisotropy	17.1421
XX=	172.0746	YX=	-6.6105	ZX=	-7.5669
XY=	-2.3582	YY=	161.8677	ZY=	-6.2653
XZ=	-7.4128	YZ=	-4.9055	ZZ=	174.2092
Eigenvalues:	156.3923	170.9473	180.8118		
16	O	Isotropic=	263.1733	Anisotropy	83.0118
XX=	317.6184	YX=	12.8445	ZX=	-4.3667
XY=	-2.2621	YY=	232.3394	ZY=	25.2684
XZ=	10.6851	YZ=	59.4972	ZZ=	239.5623
Eigenvalues:	193.3895	277.616	318.5145		

17	O	Isotropic=	265.6254	Anisotropy	45.1729
XX=	252.089	YX=	-11.2132	ZX=	19.6259
XY=	2.0977	YY=	291.2857	ZY=	8.4766
XZ=	0.187	YZ=	18.8211	ZZ=	253.5014
Eigenvalues:	239.6432		261.4922		295.7407
18	O	Isotropic=	-355.6368	Anisotropy	1079.4212
XX=	-774.5421	YX=	499.1571	ZX=	26.8277
XY=	430.0314	YY=	64.7094	ZY=	268.6353
XZ=	23.0871	YZ=	273.2289	ZZ=	-357.0776
Eigenvalues:	-993.9736		-436.9141		363.9774
19	O	Isotropic=	88.703	Anisotropy	124.4942
XX=	117.2672	YX=	-130.4899	ZX=	100.0728
XY=	-33.0123	YY=	47.6011	ZY=	96.0148
XZ=	-2.2178	YZ=	39.1458	ZZ=	101.2406
Eigenvalues:	-51.8365	146.2463			171.6991
20	O	Isotropic=	93.5367	Anisotropy	151.9661
XX=	120.1579	YX=	15.478	ZX=	-31.5759
XY=	5.9199	YY=	176.3167	ZY=	-31.5899
XZ=	-184.5758	YZ=	1.7764	ZZ=	-15.8646
Eigenvalues:	-75.7951	161.5578			194.8474
21	H	Isotropic=	31.2093	Anisotropy	13.6202
XX=	33.9496	YX=	-6.469	ZX=	-0.1187
XY=	-6.233	YY=	30.8028	ZY=	-5.5998
XZ=	-0.1152	YZ=	-6.5771	ZZ=	28.8756
Eigenvalues:	21.9638	31.3747	40.2895		
22	C	Isotropic=	20.4126	Anisotropy	74.5722
XX=	29.1224	YX=	39.1749	ZX=	-76.0294
XY=	14.2541	YY=	52.5774	ZY=	30.8287
XZ=	-45.5092	YZ=	47.7975	ZZ=	-20.4619
Eigenvalues:	-78.5325	69.643	70.1274		
23	O	Isotropic=	-131.4574	Anisotropy	600.6546
XX=	-274.4021	YX=	-234.2318	ZX=	-172.2981
XY=	-182.4277	YY=	-30.363	ZY=	194.8554
XZ=	-166.3621	YZ=	193.4464	ZZ=	-89.607
Eigenvalues:	-407.2327		-256.1184		268.9791
24	C	Isotropic=	166.3991	Anisotropy	36.7905
XX=	158.0144	YX=	5.2327	ZX=	1.6319
XY=	5.1693	YY=	171.5941	ZY=	-19.2971
XZ=	1.0286	YZ=	-20.8202	ZZ=	169.5888
Eigenvalues:	148.3285		159.9426		190.9261
25	H	Isotropic=	27.4573	Anisotropy	2.9392
XX=	27.1188	YX=	-1.3672	ZX=	-0.6568
XY=	-2.4398	YY=	27.3386	ZY=	-1.3607
XZ=	0.2032	YZ=	-0.7377	ZZ=	27.9144
Eigenvalues:	25.0406	27.9145	29.4167		
26	H	Isotropic=	28.1338	Anisotropy	8.4792
XX=	29.477	YX=	0.742	ZX=	-4.5899
XY=	0.5835	YY=	25.1478	ZY=	1.1973
XZ=	-3.7239	YZ=	0.1841	ZZ=	29.7767
Eigenvalues:	24.3376	26.2772	33.7866		
27	H	Isotropic=	25.5648	Anisotropy	3.4242
XX=	26.4172	YX=	-2.1694	ZX=	1.0438
XY=	1.0923	YY=	24.99	ZY=	-2.7409
XZ=	1.3639	YZ=	-0.4059	ZZ=	25.2872
Eigenvalues:	23.4887	25.3581	27.8476		
28	H	Isotropic=	24.88	Anisotropy	8.0917

XX=	30.0987	YX=	0.4685	ZX=	1.3126		
XY=	0.9172	YY=	19.9711	ZY=	1.8124		
XZ=	0.0195	YZ=	2.7507	ZZ=	24.5703		
Eigenvalues:	19.0176	25.348	30.2745				
29	H	Isotropic=	28.7122	Anisotropy		6.373	
XX=	30.423	YX=	-1.6724	ZX=	-1.1832		
XY=	-0.844	YY=	32.2462	ZY=	0.678		
XZ=	-0.6417	YZ=	0.2424	ZZ=	23.4674		
Eigenvalues:	23.3396	29.8362	32.9609				
30	H	Isotropic=	29.1684	Anisotropy		4.9806	
XX=	32.4818	YX=	0.09	ZX=	-0.1612		
XY=	-0.525	YY=	24.8625	ZY=	-0.6571		
XZ=	0.0173	YZ=	-1.3808	ZZ=	30.1611		
Eigenvalues:	24.6667	30.3498	32.4888				
31	H	Isotropic=	29.3409	Anisotropy		8.1532	
XX=	29.3634	YX=	-2.7658	ZX=	-0.7974		
XY=	-2.9057	YY=	30.1863	ZY=	3.1078		
XZ=	-0.894	YZ=	4.7603	ZZ=	28.4731		
Eigenvalues:	24.9472	28.2992	34.7764				
32	H	Isotropic=	29.2478	Anisotropy		9.1146	
XX=	27.9868	YX=	-2.9725	ZX=	4.0451		
XY=	-1.9289	YY=	29.9707	ZY=	-2.8822		
XZ=	3.8581	YZ=	-2.3432	ZZ=	29.786		
Eigenvalues:	24.8109	27.6083	35.3242				
33	H	Isotropic=	30.3455	Anisotropy		6.7148	
XX=	33.4592	YX=	1.8166	ZX=	2.2237		
XY=	1.9022	YY=	30.6215	ZY=	-0.914		
XZ=	2.4331	YZ=	-0.3527	ZZ=	26.9558		
Eigenvalues:	25.8979	30.3166	34.822				
34	H	Isotropic=	30.2064	Anisotropy		9.1153	
XX=	30.1417	YX=	-0.1658	ZX=	1.88		
XY=	0.912	YY=	26.4786	ZY=	3.7675		
XZ=	3.1088	YZ=	2.9822	ZZ=	33.9989		
Eigenvalues:	25.1194	29.2165	36.2833				
35	H	Isotropic=	30.3342	Anisotropy		6.1566	
XX=	30.6141	YX=	2.3687	ZX=	-0.771		
XY=	0.4731	YY=	26.8262	ZY=	-0.3694		
XZ=	-2.5327	YZ=	-0.5511	ZZ=	33.5624		
Eigenvalues:	26.3513	30.2128	34.4387				
36	H	Isotropic=	28.6333	Anisotropy		6.1074	
XX=	27.7271	YX=	-1.6284	ZX=	0.2695		
XY=	-1.9895	YY=	28.2348	ZY=	2.0022		
XZ=	-0.7106	YZ=	4.322	ZZ=	29.9378		
Eigenvalues:	25.105	28.0899	32.7048				
37	H	Isotropic=	29.2836	Anisotropy		7.0679	
XX=	32.615	YX=	-0.99	ZX=	0.5505		
XY=	-2.1476	YY=	31.7691	ZY=	-1.7997		
XZ=	-0.1368	YZ=	-2.0472	ZZ=	23.4668		
Eigenvalues:	23.0409	30.8145	33.9956				
38	H	Isotropic=	28.5309	Anisotropy		12.454	
XX=	33.5792	YX=	-0.7887	ZX=	4.6533		
XY=	-0.3458	YY=	25.6454	ZY=	1.1118		
XZ=	7.0064	YZ=	-0.0631	ZZ=	26.3682		
Eigenvalues:	22.9209	25.8383	36.8336				
39	H	Isotropic=	29.0835	Anisotropy		8.302	
XX=	32.5792	YX=	-2.2097	ZX=	-3.3194		

XY=	-1.4993	YY=	27.7374	ZY=	-1.7069		
XZ=	-4.2248	YZ=	-1.3254	ZZ=	26.9337		
Eigenvalues:	23.8024	28.8299	34.6181				
40	H	Isotropic=	29.215	Anisotropy	10.8175		
XX=	29.4621	YX=	-5.6068	ZX=	-1.84		
XY=	-5.1687	YY=	30.6966	ZY=	1.6133		
XZ=	-3.5783	YZ=	1.2151	ZZ=	27.4863		
Eigenvalues:	24.2008	27.0175	36.4267				
41	H	Isotropic=	29.6669	Anisotropy	6.0191		
XX=	32.7892	YX=	1.9214	ZX=	-1.1822		
XY=	2.1114	YY=	28.9517	ZY=	1.9027		
XZ=	-1.5001	YZ=	2.4818	ZZ=	27.26		
Eigenvalues:	25.0875	30.2337	33.6797				
42	H	Isotropic=	30.4931	Anisotropy	9.5894		
XX=	28.3513	YX=	-1.0171	ZX=	-1.7714		
XY=	-1.3913	YY=	26.6951	ZY=	-0.9301		
XZ=	-1.8418	YZ=	-1.2626	ZZ=	36.433		
Eigenvalues:	25.7439	28.8494	36.8861				
43	H	Isotropic=	29.1368	Anisotropy	5.5725		
XX=	30.3477	YX=	1.8345	ZX=	2.3586		
XY=	3.4633	YY=	29.7703	ZY=	-2.2307		
XZ=	0.8582	YZ=	-3.4211	ZZ=	27.2922		
Eigenvalues:	24.1371	30.4214	32.8518				
44	H	Isotropic=	29.2552	Anisotropy	6.8954		
XX=	26.3437	YX=	-0.1145	ZX=	-0.5177		
XY=	-0.3786	YY=	27.5706	ZY=	-0.5095		
XZ=	0.6581	YZ=	0.5788	ZZ=	33.8513		
Eigenvalues:	26.2953	27.6182	33.8522				
45	H	Isotropic=	29.0036	Anisotropy	8.8627		
XX=	30.1162	YX=	-3.0614	ZX=	0.142		
XY=	-4.8498	YY=	30.7351	ZY=	-2.2115		
XZ=	1.4449	YZ=	-2.0947	ZZ=	26.1594		
Eigenvalues:	25.1045	26.9942	34.912				
46	H	Isotropic=	30.5833	Anisotropy	18.1464		
XX=	39.6876	YX=	6.9564	ZX=	-3.6339		
XY=	4.7004	YY=	28.9129	ZY=	0.8144		
XZ=	-2.5971	YZ=	-1.2381	ZZ=	23.1495		
Eigenvalues:	22.4306	26.6385	42.681				
47	C	Isotropic=	7.5325	Anisotropy	98.0104		
XX=	-61.8981	YX=	-56.9366	ZX=	-31.4924		
XY=	-59.2857	YY=	46.5859	ZY=	-2.7592		
XZ=	9.4738	YZ=	6.2119	ZZ=	37.9097		
Eigenvalues:	-87.8541	37.5788	72.8727				
48	O	Isotropic=	-143.4609	Anisotropy	699.5459		
XX=	-211.9926	YX=	-248.1332	ZX=	1.138		
XY=	-252.4242	YY=	192.9636	ZY=	93.3082		
XZ=	-15.1879	YZ=	94.251	ZZ=	-411.3536		
Eigenvalues:	-433.0716	-320.2141	322.9031				
49	H	Isotropic=	28.7781	Anisotropy	6.4185		
XX=	29.206	YX=	1.9764	ZX=	-1.5442		
XY=	3.0055	YY=	29.8531	ZY=	4.0449		
XZ=	-0.6085	YZ=	3.2569	ZZ=	27.2752		
Eigenvalues:	23.6791	29.5982	33.0571				
50	H	Isotropic=	29.5115	Anisotropy	6.3914		
XX=	27.1312	YX=	-1.4017	ZX=	0.5382		
XY=	-1.5911	YY=	27.7145	ZY=	0.2873		

XZ= 0.5843 YZ= -0.9447 ZZ= 33.6888
 Eigenvalues: 25.8918 28.8704 33.7724
 51 C Isotropic= 108.9032 Anisotropy 18.3834
 XX= 115.9364 YX= -4.7788 ZX= -5.8557
 XY= -1.7851 YY= 113.7454 ZY= 5.8928
 XZ= -4.5976 YZ= 7.6506 ZZ= 97.0278
 Eigenvalues: 93.9286 111.6222 121.1588
 52 C Isotropic= 125.1258 Anisotropy 8.9464
 XX= 127.4265 YX= -1.9751 ZX= -0.8299
 XY= -1.3874 YY= 121.9369 ZY= 6.0779
 XZ= -1.7069 YZ= 5.2264 ZZ= 126.0139
 Eigenvalues: 117.9213 126.366 131.0901
 53 O Isotropic= 266.1947 Anisotropy 50.3691
 XX= 285.9095 YX= 10.8617 ZX= -27.8261
 XY= 7.9456 YY= 273.9966 ZY= -10.8429
 XZ= -0.3491 YZ= -30.2983 ZZ= 238.6779
 Eigenvalues: 227.7782 271.0317 299.7741
 54 H Isotropic= 26.7663 Anisotropy 4.948
 XX= 27.0535 YX= -0.7422 ZX= -1.593
 XY= -0.2127 YY= 29.4112 ZY= -2.3144
 XZ= -1.0066 YZ= -1.7185 ZZ= 23.834
 Eigenvalues: 22.7377 27.4961 30.0649
 55 N Isotropic= 125.9572 Anisotropy 126.4013
 XX= 90.0599 YX= 53.4587 ZX= -52.1302
 XY= 24.7022 YY= 196.0182 ZY= 16.4008
 XZ= -31.1499 YZ= 35.6364 ZZ= 91.7935
 Eigenvalues: 35.9221 131.7248 210.2247
 56 C Isotropic= 52.89 Anisotropy 188.112
 XX= 162.8455 YX= 28.0872 ZX= 48.9713
 XY= 28.3043 YY= -21.4303 ZY= -14.0453
 XZ= 41.0277 YZ= -16.7802 ZZ= 17.2549
 Eigenvalues: -36.3454 16.7175 178.298
 57 H Isotropic= 25.2805 Anisotropy 7.9351
 XX= 22.0951 YX= 5.3648 ZX= -1.0308
 XY= 2.5477 YY= 27.4284 ZY= -1.3129
 XZ= -1.1247 YZ= -2.2988 ZZ= 26.318
 Eigenvalues: 19.9889 25.2821 30.5706
 58 H Isotropic= 31.2849 Anisotropy 16.9128
 XX= 30.1362 YX= 6.6961 ZX= -4.4744
 XY= 4.109 YY= 38.6017 ZY= -3.1152
 XZ= -3.1949 YZ= -3.7802 ZZ= 25.117
 Eigenvalues: 23.0244 28.2702 42.5601
 59 C Isotropic= 17.6791 Anisotropy 116.207
 XX= 49.7215 YX= -32.3426 ZX= -24.112
 XY= -25.0381 YY= -61.972 ZY= 33.989
 XZ= -24.9605 YZ= 31.1219 ZZ= 65.2879
 Eigenvalues: -73.9949 31.8818 95.1504
 60 H Isotropic= 26.6346 Anisotropy 7.0088
 XX= 23.1633 YX= 2.5896 ZX= 4.312
 XY= -2.0946 YY= 30.6201 ZY= -2.8215
 XZ= 3.3431 YZ= -0.4456 ZZ= 26.1205
 Eigenvalues: 20.4119 28.1849 31.3072
 61 C Isotropic= 66.6574 Anisotropy 166.7214
 XX= 165.3585 YX= 11.883 ZX= 47.7432
 XY= 12.6907 YY= 56.7988 ZY= 4.4063
 XZ= 46.2835 YZ= 1.5628 ZZ= -22.1852

Eigenvalues: -33.310655.4777 177.805
 62 C Isotropic= 61.9326 Anisotropy 177.2882
 XX= 170.9766 YX= 14.0031 ZX= 30.9429
 XY= 13.5729 YY= -13.2071 ZY= 41.8403
 XZ= 30.9488 YZ= 45.779 ZZ= 28.0282
 Eigenvalues: -41.129846.8028 180.1247
 63 C Isotropic= 63.3557 Anisotropy 176.1261
 XX= 167.1471 YX= 33.6345 ZX= 38.5068
 XY= 32.225 YY= -14.0902 ZY= -29.445
 XZ= 38.2844 YZ= -28.0618 ZZ= 37.0101
 Eigenvalues: -37.513746.8076 180.7731
 64 C Isotropic= 61.3314 Anisotropy 177.1509
 XX= 165.8839 YX= 16.8739 ZX= 47.8685
 XY= 15.242 YY= 48.3162 ZY= 5.5574
 XZ= 49.5585 YZ= 3.3053 ZZ= -30.2059
 Eigenvalues: -41.645446.2076 179.432
 65 C Isotropic= 58.3758 Anisotropy 157.447
 XX= 156.4024 YX= 10.8676 ZX= 24.9854
 XY= 9.8564 YY= -9.5668 ZY= 42.9689
 XZ= 25.8268 YZ= 43.8017 ZZ= 28.2917
 Eigenvalues: -38.119949.9068 163.3404
 66 H Isotropic= 23.9982 Anisotropy 8.9643
 XX= 21.2511 YX= -1.3718 ZX= 0.022
 XY= -2.185 YY= 29.5284 ZY= -1.4218
 XZ= -0.2758 YZ= -0.3388 ZZ= 21.215
 Eigenvalues: 20.6848 21.3354 29.9744
 67 O Isotropic= -132.5541 Anisotropy 618.6464
 XX= -192.531 YX= -83.8825 ZX= -378.7534
 XY= -106.4779 YY= -194.5417 ZY= 63.9604
 XZ= -304.2932 YZ= 80.0765 ZZ= -10.5895
 Eigenvalues: -459.0491 -218.49 279.8769
 68 C Isotropic= 58.11 Anisotropy 171.1219
 XX= 162.9472 YX= 52.6609 ZX= 2.935
 XY= 27.7674 YY= -5.6247 ZY= 33.2034
 XZ= -6.4803 YZ= 24.4106 ZZ= 17.0076
 Eigenvalues: -31.495133.6338 172.1913
 69 H Isotropic= 23.7436 Anisotropy 4.8639
 XX= 20.9788 YX= -1.5306 ZX= -1.2606
 XY= -1.584 YY= 25.6459 ZY= 0.9974
 XZ= -1.3644 YZ= 1.1226 ZZ= 24.6061
 Eigenvalues: 20.2814 23.9632 26.9862
 70 H Isotropic= 23.7471 Anisotropy 3.2
 XX= 20.9704 YX= -0.7311 ZX= -1.2812
 XY= -0.8548 YY= 24.9424 ZY= -0.6162
 XZ= -1.3461 YZ= -0.6138 ZZ= 25.3286
 Eigenvalues: 20.4134 24.9475 25.8804
 71 H Isotropic= 23.7276 Anisotropy 4.8308
 XX= 20.924 YX= -1.1464 ZX= -1.3686
 XY= -1.3263 YY= 26.4274 ZY= 0.7018
 XZ= -1.3256 YZ= 0.4795 ZZ= 23.8315
 Eigenvalues: 20.2484 23.9863 26.9482
 72 H Isotropic= 23.5472 Anisotropy 7.9349
 XX= 20.7639 YX= -0.7307 ZX= -1.9662
 XY= -1.6606 YY= 23.6319 ZY= 3.2027
 XZ= -2.3896 YZ= 2.5004 ZZ= 26.246
 Eigenvalues: 19.9883 21.8163 28.8372

73 C Isotropic= 58.261 Anisotropy 179.912
 XX= 173.8939 YX= 21.6942 ZX= -23.3555
 XY= 17.5969 YY= 41.7157 ZY= -3.1222
 XZ= -11.9502 YZ= -1.8003 ZZ= -40.8266
 Eigenvalues: -42.277 38.8578 178.2024

74 C Isotropic= 61.3575 Anisotropy 179.2164
 XX= 177.4098 YX= 24.7239 ZX= 1.4582
 XY= 25.3404 YY= -11.749 ZY= -40.1912
 XZ= -1.0859 YZ= -41.7006 ZZ= 18.4117
 Eigenvalues: -42.262545.4999 180.8351

75 C Isotropic= 61.9867 Anisotropy 178.9788
 XX= 177.3551 YX= 24.8808 ZX= -3.6582
 XY= 30.9953 YY= -17.1613 ZY= 34.5151
 XZ= -9.3582 YZ= 34.6395 ZZ= 25.7664
 Eigenvalues: -39.907644.5619 181.3059

76 C Isotropic= 64.3927 Anisotropy 174.8405
 XX= 178.1057 YX= 17.5539 ZX= -0.9555
 XY= 20.7106 YY= 51.7832 ZY= 3.2373
 XZ= -3.7224 YZ= 5.1573 ZZ= -36.7107
 Eigenvalues: -36.959149.1842 180.9531

77 C Isotropic= 63.9014 Anisotropy 169.4496
 XX= 168.1165 YX= 43.4722 ZX= -0.2985
 XY= 33.6094 YY= 4.3959 ZY= -34.5877
 XZ= 4.8611 YZ= -26.9929 ZZ= 19.1919
 Eigenvalues: -25.260540.0968 176.8678

78 H Isotropic= 23.2188 Anisotropy 6.6889
 XX= 20.3005 YX= -0.0438 ZX= 0.9254
 XY= -0.0688 YY= 27.5133 ZY= 0.771
 XZ= 0.7686 YZ= 1.1845 ZZ= 21.8427
 Eigenvalues: 19.8988 22.0796 27.6781

79 H Isotropic= 23.6385 Anisotropy 3.7321
 XX= 20.583 YX= 0.4176 ZX= 0.7656
 XY= 0.077 YY= 25.3019 ZY= -0.9071
 XZ= 0.5673 YZ= -0.9706 ZZ= 25.0305
 Eigenvalues: 20.4543 24.3346 26.1265

80 H Isotropic= 23.7195 Anisotropy 3.4543
 XX= 20.7911 YX= -0.3548 ZX= 0.0613
 XY= 0.1753 YY= 25.0346 ZY= 0.8029
 XZ= -0.1207 YZ= 0.8452 ZZ= 25.3328
 Eigenvalues: 20.7892 24.347 26.0224

81 H Isotropic= 23.6933 Anisotropy 4.8466
 XX= 20.4566 YX= 0.1232 ZX= -0.8969
 XY= -0.056 YY= 26.8043 ZY= -0.6565
 XZ= -0.3953 YZ= -0.5448 ZZ= 23.8191
 Eigenvalues: 20.3358 23.8197 26.9244

82 H Isotropic= 23.4254 Anisotropy 7.4904
 XX= 19.6425 YX= 2.5029 ZX= -1.4754
 XY= 1.52 YY= 25.5274 ZY= -3.0014
 XZ= -0.6513 YZ= -2.0749 ZZ= 25.1064
 Eigenvalues: 19.0066 22.8506 28.419

2bvii_neg45

C	-2.882157	0.407911	1.829944
C	-3.757154	1.670379	1.549163
C	-3.707146	2.202963	0.107293
C	-5.031301	2.039434	-0.660577

C	-5.516598	0.58501	-0.822701
C	-4.520383	-0.481938	-1.249683
C	-3.391014	-0.70622	-0.286289
C	-2.123108	-0.591682	-0.760927
C	-1.012551	-0.367499	0.227011
C	-1.432148	0.584401	1.349525
C	-3.544634	-0.862315	1.212133
C	-4.960566	-1.009924	1.748138
C	-2.782449	-2.114718	1.684653
C	-1.747297	-0.610924	-2.192279
C	-6.124993	2.898063	-0.06712
O	-2.758751	0.266095	3.244341
O	-3.400371	2.692809	2.466397
O	-6.724290.337356		-0.786501
O	-5.091264	-1.63832	-1.847025
O	0.078093	0.262911	-0.487752
H	-2.438473	2.772214	2.46271
C	-5.990104	-2.482114	-1.252198
O	-6.485171	-2.211132	-0.163788
C	-6.266618		-3.66574-2.120079
H	-4.826517	1.442663	1.830762
H	-2.887405	1.710797	-0.473327
H	-4.066058	-0.010304	-2.194211
H	-0.649512	-1.349142	0.646158
H	-0.740586	0.414776	2.220508
H	-1.278729	1.639872	1.002083
H	-5.696675	-0.336667	1.253831
H	-5.321325	-2.059804	1.610857
H	-4.966325	-0.798981	2.84653
H	-3.436042	-2.768861	2.312056
H	-2.429401	-2.720585	0.816868
H	-1.906636	-1.828591	2.317377
H	-2.462377		-1.22386-2.795185
H	-1.723042	0.432212	-2.598642
H	-0.723933	-1.046782	-2.315947
H	-7.047718	2.830978	-0.693991
H	-6.384511	2.558719	0.964406
H	-5.792424	3.962704	-0.020385
H	-5.709412	-3.599545	-3.084895
H	-5.957018		-4.58971-1.573533
H	-7.36432-3.709011		-2.324951
H	-3.587814	0.552952	3.64798
C	1.349216	0.019288	-0.055197
O	1.529331	-0.705531	0.921474
H	-4.836376	2.390152	-1.716633
H	-3.480273.302015		0.154145
C	2.377952	0.74911	-0.904277
C	3.699251	0.953235	-0.099288
O	2.546817	0.097539	-2.14469
H	1.961851	1.763008	-1.182836
N	4.630372	-0.132867	-0.256486
C	4.282559	2.287465	-0.510585
H	3.420867	1.001457	1.001354
H	2.758721	-0.829537	-1.972469
C	5.30614 -0.690938		0.820992
H	4.909953	-0.366676	-1.178676

C	4.630433	2.526116	-1.844428
C	5.188047	3.748843	-2.212827
C	5.402974	4.736474	-1.250589
C	5.060683	4.498663	0.080122
C	4.505336	3.274488	0.45348
H	4.442046	1.748121	-2.601358
O	5.281014	-0.163943	1.94805
C	6.104931	-1.917341	0.535866
H	5.458709	3.934236	-3.262558
H	5.843808	5.701203	-1.541743
H	5.233446	5.274534	0.840542
H	4.253816	3.083023	1.508283
C	7.397805	-2.008777	1.063844
C	8.164864	-3.147774	0.823332
C	7.642131	-4.196387	0.066006
C	6.349261	-4.108484	-0.450927
C	5.579024	-2.969113	-0.22004
H	7.792984	-1.183552	1.67721
H	9.181682	-3.219686	1.236987
H	8.248078	-5.095734	-0.119932
H	5.933876	-4.939912	-1.039161
H	4.554901	-2.910639	-0.617813

2bvii_neg45 E(RB+HF-PW91) = -2012.306279

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic= 109.7766 Anisotropy 27.943

XX= 96.3356 YX= 4.079 ZX= -7.1092

XY= 7.2699 YY= 107.6631 ZY= -7.0824

XZ= -0.4884 YZ= -5.967 ZZ= 125.3312

Eigenvalues: 93.9456 106.9791 128.4053

2 C Isotropic= 112.0943 Anisotropy 30.3377

XX= 99.23 YX= 9.9304 ZX= 12.6983

XY= 0.9001 YY= 123.4417 ZY= 5.2185

XZ= 9.5491 YZ= 13.0149 ZZ= 113.6112

Eigenvalues: 93.1691 110.7944 132.3194

3 C Isotropic= 141.9233 Anisotropy 19.6542

XX= 123.5485 YX= -3.2553 ZX= 6.8734

XY= 4.1047 YY= 154.2749 ZY= -2.6531

XZ= 8.8442 YZ= -1.4654 ZZ= 147.9465

Eigenvalues: 121.2066 149.5372 155.0261

4 C Isotropic= 140.2115 Anisotropy 24.9475

XX= 123.8181 YX= 3.1666 ZX= 5.7958

XY= -7.0862 YY= 156.1535 ZY= 5.3951

XZ= -4.0037 YZ= 0.7985 ZZ= 140.663

Eigenvalues: 123.63 140.1614 156.8432

5 C Isotropic= -23.1792 Anisotropy 181.0775

XX= -55.964 YX= 20.6612 ZX= 22.7622

XY= 3.2282 YY= -100.1789 ZY= -41.0879

XZ= 23.0539 YZ= -39.39 ZZ= 86.6053

Eigenvalues: -113.29 -53.7868 97.5391

6 C Isotropic= 101.822 Anisotropy 42.3106

XX= 88.703 YX= -2.228 ZX= -3.6728

XY= 11.1597 YY= 126.4481 ZY= 9.8839

XZ= 9.2034 YZ= 11.6518 ZZ= 90.3148

Eigenvalues: 86.2032 89.2337 130.029

7	C	Isotropic=	43.5341	Anisotropy	158.3657
XX=	18.0295	YX=	5.6142	ZX=	-36.3448
XY=	-16.9585	YY=	145.5448	ZY=	17.0115
XZ=	-51.0375	YZ=	26.3803	ZZ=	-32.9721
Eigenvalues:	-59.3229	40.8139	149.1112		
8	C	Isotropic=	40.5829	Anisotropy	157.1034
XX=	29.9855	YX=	-17.6275	ZX=	-33.9174
XY=	-13.2686	YY=	143.1916	ZY=	1.8856
XZ=	-19.8295	YZ=	-15.7207	ZZ=	-51.4282
Eigenvalues:	-60.1063	36.5366	145.3185		
9	C	Isotropic=	112.6208	Anisotropy	48.2188
XX=	121.9363	YX=	22.7429	ZX=	-18.7543
XY=	27.5034	YY=	103.3516	ZY=	5.9232
XZ=	-19.2585	YZ=	5.8814	ZZ=	112.5745
Eigenvalues:	78.1472	114.9486	144.7667		
10	C	Isotropic=	148.2393	Anisotropy	44.3216
XX=	161.5966	YX=	9.6216	ZX=	-16.7221
XY=	5.4903	YY=	133.0788	ZY=	2.0406
XZ=	-25.4468	YZ=	10.7683	ZZ=	150.0425
Eigenvalues:	123.7898	143.1412	177.787		
11	C	Isotropic=	147.7499	Anisotropy	12.4088
XX=	142.4734	YX=	1.9801	ZX=	4.454
XY=	-10.5019	YY=	152.4667	ZY=	8.2889
XZ=	-1.4932	YZ=	0.8231	ZZ=	148.3096
Eigenvalues:	139.7434	147.4839	156.0225		
12	C	Isotropic=	155.2665	Anisotropy	22.1271
XX=	167.1401	YX=	-6.7061	ZX=	3.5125
XY=	-1.9777	YY=	162.2885	ZY=	-8.9097
XZ=	-1.6022	YZ=	-0.7424	ZZ=	136.3708
Eigenvalues:	135.5004	160.2812	170.0179		
13	C	Isotropic=	147.9738	Anisotropy	55.3804
XX=	139.5792	YX=	-25.0616	ZX=	-3.3349
XY=	-27.1993	YY=	167.3305	ZY=	-12.6378
XZ=	-9.4496	YZ=	-16.3904	ZZ=	137.0117
Eigenvalues:	115.5619	143.4653	184.8941		
14	C	Isotropic=	167.8309	Anisotropy	12.7738
XX=	162.3195	YX=	-6.6297	ZX=	-1.4193
XY=	3.7575	YY=	165.3707	ZY=	-1.0611
XZ=	-2.1267	YZ=	4.4221	ZZ=	175.8025
Eigenvalues:	161.6684	165.4775	176.3468		
15	C	Isotropic=	169.2874	Anisotropy	17.1552
XX=	173.959	YX=	-3.6769	ZX=	1.0687
XY=	-4.9737	YY=	175.6991	ZY=	5.8142
XZ=	-3.7463	YZ=	6.6573	ZZ=	158.2042
Eigenvalues:	156.209	170.9291	180.7242		
16	O	Isotropic=	262.5879	Anisotropy	82.4239
XX=	297.7563	YX=	-17.012	ZX=	-38.8001
XY=	-20.4471	YY=	227.2998	ZY=	-57.3921
XZ=	-26.6542	YZ=	-18.6582	ZZ=	262.7076
Eigenvalues:	192.1685	278.0579	317.5372		
17	O	Isotropic=	265.7868	Anisotropy	44.6975
XX=	263.7418	YX=	15.4341	ZX=	23.2862
XY=	-8.5025	YY=	252.0207	ZY=	-11.4728
XZ=	15.7399	YZ=	-11.5007	ZZ=	281.5979
Eigenvalues:	241.9098	259.8655	295.5851		
18	O	Isotropic=	-358.6864	Anisotropy	1082.484

XX=	-972.4243	YX=	-123.5141	ZX=	72.0067
XY=	-115.5657	YY=	-422.0021	ZY=	-161.7071
XZ=	143.2789	YZ=	-152.5847	ZZ=	318.3671
Eigenvalues:	-1001.5133		-437.5155		362.9695
19	O	Isotropic=	91.5283	Anisotropy	118.2647
XX=	167.263	YX=	54.0331	ZX=	63.8089
XY=	-22.9364	YY=	86.0105	ZY=	-45.4146
XZ=	-22.3271	YZ=	-145.309	ZZ=	21.3114
Eigenvalues:	-50.128		154.3414		170.3715
20	O	Isotropic=	71.1796	Anisotropy	162.9203
XX=	110.7134	YX=	-20.3442	ZX=	0.9627
XY=	-80.0005	YY=	84.2833	ZY=	118.0808
XZ=	120.0784	YZ=	129.7445	ZZ=	18.5422
Eigenvalues:	-105.3537		139.0994		179.7932
21	H	Isotropic=	31.1519	Anisotropy	14.0017
XX=	38.5642	YX=	3.0151	ZX=	2.3511
XY=	2.8852	YY=	30.3053	ZY=	5.6518
XZ=	2.2011	YZ=	4.6417	ZZ=	24.5863
Eigenvalues:	21.5444		31.425		40.4864
22	C	Isotropic=	20.1098	Anisotropy	74.9086
XX=	18.9933	YX=	-81.3055	ZX=	-5.7576
XY=	-59.1805	YY=	-28.2005	ZY=	-9.6456
XZ=	14.6673	YZ=	21.0122	ZZ=	69.5365
Eigenvalues:	-79.0545		69.335		70.0488
23	O	Isotropic=	-132.2505	Anisotropy	602.4868
XX=	-31.6745	YX=	-203.4407	ZX=	282.4975
XY=	-204.2808	YY=	-139.2823	ZY=	-99.566
XZ=	230.5723	YZ=	-100.2848	ZZ=	-225.7946
Eigenvalues:	-409.3383		-256.8206		269.4074
24	C	Isotropic=	166.382	Anisotropy	37.0059
XX=	155.1915	YX=	9.5704	ZX=	0.258
XY=	9.5451	YY=	175.676	ZY=	17.7424
XZ=	0.5858	YZ=	16.2152	ZZ=	168.2785
Eigenvalues:	148.4851		159.6083		191.0526
25	H	Isotropic=	27.477	Anisotropy	3.1435
XX=	28.8165	YX=	0.2304	ZX=	0.7899
XY=	0.7237	YY=	28.178	ZY=	0.3128
XZ=	1.7075	YZ=	1.1242	ZZ=	25.4365
Eigenvalues:	24.9346		27.9237		29.5727
26	H	Isotropic=	28.2502	Anisotropy	7.9355
XX=	28.6919	YX=	-4.3987	ZX=	-0.8338
XY=	-3.7962	YY=	29.8123	ZY=	0.7087
XZ=	-1.0753	YZ=	0.4258	ZZ=	26.2465
Eigenvalues:	25.0081		26.2021		33.5405
27	H	Isotropic=	25.3655	Anisotropy	4.3329
XX=	26.1363	YX=	2.8289	ZX=	1.6808
XY=	1.7908	YY=	25.5545	ZY=	-0.2584
XZ=	-1.5262	YZ=	1.7555	ZZ=	24.4058
Eigenvalues:	23.2739		24.5686		28.2541
28	H	Isotropic=	24.6443	Anisotropy	7.0815
XX=	28.7268	YX=	0.6034	ZX=	-2.5674
XY=	-0.6785	YY=	23.9798	ZY=	-2.8045
XZ=	-1.8161	YZ=	-1.0934	ZZ=	21.2262
Eigenvalues:	19.7771		24.7905		29.3653
29	H	Isotropic=	28.1488	Anisotropy	6.891
XX=	32.4942	YX=	-0.7836	ZX=	1.2

XY=	-1.019	YY=	22.6007	ZY=	2.1667		
XZ=	0.5143	YZ=	0.5858	ZZ=	29.3515		
Eigenvalues:	22.2231	29.4806	32.7428				
30	H	Isotropic=	29.5694	Anisotropy	5.4683		
XX=	32.2837	YX=	0.2578	ZX=	-2.9143		
XY=	-0.4263	YY=	30.9741	ZY=	0.7316		
XZ=	-2.4006	YZ=	0.0586	ZZ=	25.4503		
Eigenvalues:	24.5199	30.9733	33.2149				
31	H	Isotropic=	29.283	Anisotropy	8.304		
XX=	32.1321	YX=	-1.5229	ZX=	2.5333		
XY=	-2.4792	YY=	27.3981	ZY=	-3.5928		
XZ=	2.6278	YZ=	-2.3311	ZZ=	28.3189		
Eigenvalues:	24.8564	28.1737	34.819				
32	H	Isotropic=	29.2182	Anisotropy	9.2628		
XX=	29.9015	YX=	5.2499	ZX=	2.3308		
XY=	4.6624	YY=	30.4421	ZY=	0.0109		
XZ=	1.3561	YZ=	0.4423	ZZ=	27.3111		
Eigenvalues:	24.6426	27.6187	35.3935				
33	H	Isotropic=	30.2626	Anisotropy	6.4208		
XX=	31.0997	YX=	2.4456	ZX=	-2.251		
XY=	2.1658	YY=	27.0455	ZY=	-0.1046		
XZ=	-2.3847	YZ=	0.3615	ZZ=	32.6425		
Eigenvalues:	25.8157	30.4288	34.5431				
34	H	Isotropic=	30.0679	Anisotropy	9.1338		
XX=	28.9622	YX=	-0.4509	ZX=	-0.5525		
XY=	0.9577	YY=	32.8606	ZY=	-4.8944		
XZ=	-1.876	YZ=	-4.9983	ZZ=	28.381		
Eigenvalues:	24.9912	29.0555	36.1571				
35	H	Isotropic=	30.2492	Anisotropy	6.3082		
XX=	28.8804	YX=	-1.4075	ZX=	-2.4675		
XY=	-2.1722	YY=	33.7283	ZY=	0.7722		
XZ=	-0.4072	YZ=	0.2037	ZZ=	28.1388		
Eigenvalues:	26.9386	29.3543	34.4546				
36	H	Isotropic=	28.367	Anisotropy	6.3187		
XX=	29.8359	YX=	-0.2426	ZX=	1.7667		
XY=	-2.2722	YY=	28.5875	ZY=	-3.7639		
XZ=	2.2768	YZ=	-2.1471	ZZ=	26.6776		
Eigenvalues:	24.3569	28.1646	32.5795				
37	H	Isotropic=	28.984	Anisotropy	8.0107		
XX=	30.3117	YX=	2.7901	ZX=	-0.3372		
XY=	3.2256	YY=	26.4375	ZY=	4.8094		
XZ=	1.3001	YZ=	4.0374	ZZ=	30.2028		
Eigenvalues:	22.8036	29.824	34.3245				
38	H	Isotropic=	29.0673	Anisotropy	6.7945		
XX=	27.5801	YX=	0.6651	ZX=	-0.5768		
XY=	1.09	YY=	29.6112	ZY=	-3.7407		
XZ=	-0.7649	YZ=	-3.4248	ZZ=	30.0106		
Eigenvalues:	26.197	27.408	33.597				
39	H	Isotropic=	28.8941	Anisotropy	7.5931		
XX=	33.5541	YX=	-1.1195	ZX=	0.0637		
XY=	-1.4199	YY=	24.3791	ZY=	3.5397		
XZ=	-1.2053	YZ=	2.7496	ZZ=	28.7491		
Eigenvalues:	22.6658	30.0603	33.9562				
40	H	Isotropic=	29.1872	Anisotropy	10.8871		
XX=	34.3594	YX=	-1.3565	ZX=	4.1761		
XY=	-2.9011	YY=	27.2797	ZY=	0.5632		

XZ=	3.9709	YZ=	-0.7232	ZZ=	25.9224				
Eigenvalues:	24.0931	27.0232	36.4452						
41	H	Isotropic=	29.619	Anisotropy	5.7726				
XX=	30.5515	YX=	-1.9839	ZX=	-2.1852				
XY=	-2.6835	YY=	26.7351	ZY=	-1.0365				
XZ=	-2.3077	YZ=	-0.7608	ZZ=	31.5705				
Eigenvalues:	25.1083	30.2814	33.4674						
42	H	Isotropic=	30.5003	Anisotropy	9.5557				
XX=	29.1793	YX=	-1.3501	ZX=	0.0612				
XY=	-1.3783	YY=	36.6245	ZY=	0.4595				
XZ=	0.4448	YZ=	0.0647	ZZ=	25.697				
Eigenvalues:	25.6663	28.9638	36.8707						
43	H	Isotropic=	29.0509	Anisotropy	5.7189				
XX=	27.4799	YX=	2.746	ZX=	-1.4417				
XY=	1.8255	YY=	28.1907	ZY=	3.2409				
XZ=	-2.7029	YZ=	1.4591	ZZ=	31.482				
Eigenvalues:	24.1952	30.0939	32.8635						
44	H	Isotropic=	29.2017	Anisotropy	7.0434				
XX=	26.5501	YX=	-0.5941	ZX=	0.7413				
XY=	0.1281	YY=	33.7577	ZY=	-1.7002				
XZ=	0.9213	YZ=	-0.1015	ZZ=	27.2972				
Eigenvalues:	26.0006	27.7072	33.8973						
45	H	Isotropic=	28.9245	Anisotropy	8.7824				
XX=	33.0254	YX=	1.5594	ZX=	1.5608				
XY=	2.9156	YY=	26.8072	ZY=	1.3989				
XZ=	3.2178	YZ=	2.1917	ZZ=	26.9408				
Eigenvalues:	25.077	26.917	34.7794						
46	H	Isotropic=	30.577	Anisotropy	18.0713				
XX=	33.4022	YX=	-3.7865	ZX=	-8.4885				
XY=	-2.0438	YY=	23.2198	ZY=	3.5154				
XZ=	-6.513	YZ=	1.9709	ZZ=	35.1091				
Eigenvalues:	22.3735	26.733	42.6246						
47	C	Isotropic=	11.381	Anisotropy	89.5339				
XX=	-79.9001	YX=	-24.7623	ZX=	17.2872				
XY=	1.3421	YY=	59.4347	ZY=	13.2472				
XZ=	-9.8254	YZ=	13.8345	ZZ=	54.6083				
Eigenvalues:	-81.0519	44.1246	71.0702						
48	O	Isotropic=	-100.7396	Anisotropy	632.3839				
XX=	-257.3757	YX=	-18.8769	ZX=	-40.7053				
XY=	-23.1917	YY=	100.3125	ZY=	280.5752				
XZ=	-55.5221	YZ=	353.2154	ZZ=	-145.1555				
Eigenvalues:	-369.3418	-253.7265	320.8497						
49	H	Isotropic=	28.6998	Anisotropy	6.5345				
XX=	27.4329	YX=	-2.9715	ZX=	0.2169				
XY=	-2.1341	YY=	26.3615	ZY=	-2.042				
XZ=	-0.9417	YZ=	-2.3012	ZZ=	32.3051				
Eigenvalues:	23.8447	29.1986	33.0562						
50	H	Isotropic=	29.5154	Anisotropy	6.4508				
XX=	28.6707	YX=	0.5507	ZX=	1.2065				
XY=	0.7166	YY=	33.6339	ZY=	-0.5003				
XZ=	1.3212	YZ=	-1.5494	ZZ=	26.2418				
Eigenvalues:	25.5282	29.2022	33.816						
51	C	Isotropic=	108.8653	Anisotropy	23.0406				
XX=	119.8435	YX=	1.2955	ZX=	9.5058				
XY=	2.3986	YY=	98.9775	ZY=	5.7082				
XZ=	5.7003	YZ=	5.7447	ZZ=	107.775				

Eigenvalues:	96.0089	106.3613	124.2257		
52	C	Isotropic=	131.5447	Anisotropy	19.9783
XX=	136.0592	YX=	5.9317	ZX=	-2.3198
XY=	6.6931	YY=	139.7805	ZY=	6.2488
XZ=	-3.1334	YZ=	5.16	ZZ=	118.7944
Eigenvalues:	116.3902		133.3803	144.8636	
53	O	Isotropic=	294.7481	Anisotropy	21.7465
XX=	289.5435	YX=	-1.2204	ZX=	-15.7253
XY=	-3.9174	YY=	304.4087	ZY=	-16.4377
XZ=	-10.9095	YZ=	-0.4224	ZZ=	290.2921
Eigenvalues:	274.5564		300.4421	309.2458	
54	H	Isotropic=	26.367	Anisotropy	6.4234
XX=	30.3577	YX=	2.928	ZX=	-0.0554
XY=	-0.7513	YY=	26.3783	ZY=	-0.2454
XZ=	0.4631	YZ=	1.334	ZZ=	22.365
Eigenvalues:	22.292	26.1597	30.6493		
55	N	Isotropic=	138.5931	Anisotropy	104.496
XX=	156.5199	YX=	-4.2159	ZX=	10.219
XY=	20.3289	YY=	149.8009	ZY=	-58.9796
XZ=	60.5131	YZ=	-82.7036	ZZ=	109.4586
Eigenvalues:	45.9486	161.5736	208.2571		
56	C	Isotropic=	46.7499	Anisotropy	196.3016
XX=	144.2898	YX=	-72.3058	ZX=	27.607
XY=	-71.2828	YY=	-6.3745	ZY=	-0.8512
XZ=	32.5599	YZ=	-1.375	ZZ=	2.3345
Eigenvalues:	-37.9293	0.5614	177.6176		
57	H	Isotropic=	25.1507	Anisotropy	2.7496
XX=	25.0567	YX=	0.3328	ZX=	-0.8029
XY=	2.108	YY=	24.0604	ZY=	1.4161
XZ=	0.4082	YZ=	1.159	ZZ=	26.335
Eigenvalues:	22.832	25.6364	26.9838		
58	H	Isotropic=	29.972	Anisotropy	15.3294
XX=	25.3043	YX=	-2.7039	ZX=	2.097
XY=	-4.6271	YY=	39.0971	ZY=	3.1469
XZ=	0.9198	YZ=	0.9361	ZZ=	25.5146
Eigenvalues:	22.8598	26.8646	40.1916		
59	C	Isotropic=	17.8433	Anisotropy	113.3996
XX=	36.1796	YX=	72.6221	ZX=	-17.5174
XY=	71.7469	YY=	1.293	ZY=	21.8504
XZ=	-37.7666	YZ=	30.625	ZZ=	16.0575
Eigenvalues:	-71.7568	31.8437	93.4431		
60	H	Isotropic=	26.5223	Anisotropy	6.106
XX=	25.5015	YX=	-4.9008	ZX=	-1.7702
XY=	-3.3445	YY=	26.3917	ZY=	-0.8617
XZ=	2.3153	YZ=	-1.8635	ZZ=	27.6738
Eigenvalues:	21.7135	27.2605	30.593		
61	C	Isotropic=	65.6839	Anisotropy	169.1723
XX=	155.7966	YX=	-50.826	ZX=	15.4139
XY=	-49.8668	YY=	27.6801	ZY=	-50.5658
XZ=	10.2584	YZ=	-49.1627	ZZ=	13.575
Eigenvalues:	-32.97	51.5564	178.4654		
62	C	Isotropic=	61.897	Anisotropy	177.2835
XX=	153.6608	YX=	-46.9405	ZX=	40.7355
XY=	-46.5681	YY=	64.9695	ZY=	2.2903
XZ=	41.6694	YZ=	4.6629	ZZ=	-32.9394
Eigenvalues:	-43.3625	48.9674	180.0859		

63 C Isotropic= 64.8009 Anisotropy 174.5678
 XX= 145.9089 YX= -74.5099 ZX= 28.6355
 XY= -74.4525 YY= 0.3455 ZY= 11.0783
 XZ= 30.0312 YZ= 11.6459 ZZ= 48.1483
 Eigenvalues: -36.7955 50.0187 181.1794

64 C Isotropic= 61.9894 Anisotropy 174.6139
 XX= 154.9392 YX= -53.8743 ZX= 10.3102
 XY= -53.2182 YY= 22.5574 ZY= -49.4339
 XZ= 10.335 YZ= -52.5821 ZZ= 8.4717
 Eigenvalues: -40.2786 47.8482 178.3987

65 C Isotropic= 61.5522 Anisotropy 152.9742
 XX= 142.482 YX= -39.1429 ZX= 31.3465
 XY= -39.8532 YY= 66.7756 ZY= 7.5551
 XZ= 34.6104 YZ= 4.9764 ZZ= -24.6011
 Eigenvalues: -32.8698 53.9914 163.5349

66 H Isotropic= 23.1902 Anisotropy 10.5087
 XX= 21.5284 YX= 4.1611 ZX= -3.1271
 XY= 3.4477 YY= 24.1442 ZY= -3.7847
 XZ= -2.2086 YZ= -3.6712 ZZ= 23.898
 Eigenvalues: 18.8134 20.5613 30.196

67 O Isotropic= -111.8273 Anisotropy 677.8911
 XX= 157.1079 YX= 242.353 ZX= -90.4747
 XY= 246.0659 YY= -62.2123 ZY= -113.6907
 XZ= -85.1689 YZ= -123.7076 ZZ= -430.3776
 Eigenvalues: -465.8249 -209.7571 340.1001

68 C Isotropic= 55.8295 Anisotropy 171.6634
 XX= 20.8962 YX= 41.611 ZX= -39.7807
 XY= 32.4386 YY= 9.8831 ZY= -64.4497
 XZ= -16.1345 YZ= -52.5927 ZZ= 136.7091
 Eigenvalues: -27.6763 24.893 170.2717

69 H Isotropic= 23.7793 Anisotropy 5.2638
 XX= 21.5436 YX= 2.5608 ZX= -0.8411
 XY= 2.4221 YY= 26.1506 ZY= -0.1581
 XZ= -0.5582 YZ= -0.1393 ZZ= 23.6438
 Eigenvalues: 20.3505 23.699 27.2885

70 H Isotropic= 23.8131 Anisotropy 3.1061
 XX= 21.4007 YX= 1.7345 ZX= -0.7859
 XY= 1.5381 YY= 24.4158 ZY= 0.7151
 XZ= -0.6924 YZ= 0.5207 ZZ= 25.6227
 Eigenvalues: 20.5153 25.0401 25.8838

71 H Isotropic= 23.7791 Anisotropy 4.6495
 XX= 21.5783 YX= 2.3661 ZX= -0.9969
 XY= 2.2619 YY= 25.3347 ZY= -0.5393
 XZ= -0.9393 YZ= -0.8209 ZZ= 24.4243
 Eigenvalues: 20.3886 24.07 26.8788

72 H Isotropic= 23.6377 Anisotropy 8.1199
 XX= 21.3441 YX= 2.8466 ZX= 0.7106
 XY= 2.6207 YY= 27.4383 ZY= 2.1435
 XZ= 0.7426 YZ= 1.539 ZZ= 22.1308
 Eigenvalues: 20.2973 21.565 29.051

73 C Isotropic= 59.2789 Anisotropy 177.3653
 XX= 44.2565 YX= -1.3798 ZX= -59.5177
 XY= -5.4231 YY= 25.1486 ZY= -80.419
 XZ= -58.6123 YZ= -84.275 ZZ= 108.4316
 Eigenvalues: -41.0545 41.3688 177.5224

74 C Isotropic= 61.8402 Anisotropy 176.5011

XX=	-9.7829	YX=	24.6399	ZX=	-70.5322		
XY=	22.5656	YY=	70.135	ZY=	-45.6705		
XZ=	-71.3638	YZ=	-45.3214	ZZ=	125.1685		
Eigenvalues:	-40.3634	46.3764	179.5076				
75	C	Isotropic=	61.463	Anisotropy		178.6739	
XX=	38.0413	YX=	58.8532	ZX=	-32.4082		
XY=	60.4195	YY=	10.1256	ZY=	-59.1776		
XZ=	-34.3534	YZ=	-58.7194	ZZ=	136.2222		
Eigenvalues:	-41.5779	45.388	180.579				
76	C	Isotropic=	63.6695	Anisotropy		173.4845	
XX=	55.5594	YX=	-7.8384	ZX=	-57.4105		
XY=	-3.5061	YY=	21.615	ZY=	-79.6247		
XZ=	-58.8884	YZ=	-80.755	ZZ=	113.8341		
Eigenvalues:	-38.7353	50.4179	179.3258				
77	C	Isotropic=	65.7382	Anisotropy		162.9724	
XX=	-2.2701	YX=	14.5383	ZX=	-67.0738		
XY=	23.1733	YY=	71.4668	ZY=	-40.7323		
XZ=	-62.6123	YZ=	-40.8657	ZZ=	128.0179		
Eigenvalues:	-29.0797	51.9079	174.3865				
78	H	Isotropic=	23.3675	Anisotropy		8.058	
XX=	26.3858	YX=	-4.0195	ZX=	2.1296		
XY=	-2.8673	YY=	22.9321	ZY=	0.275		
XZ=	1.5268	YZ=	0.588	ZZ=	20.7847		
Eigenvalues:	19.3674	21.9956	28.7395				
79	H	Isotropic=	23.7755	Anisotropy		4.2996	
XX=	23.972	YX=	-1.4446	ZX=	1.2938		
XY=	-1.4961	YY=	25.4814	ZY=	1.9002		
XZ=	1.1161	YZ=	1.8618	ZZ=	21.8733		
Eigenvalues:	20.275	24.4096	26.6419				
80	H	Isotropic=	23.694	Anisotropy		3.9066	
XX=	25.2214	YX=	-0.4094	ZX=	2.1763		
XY=	-0.1745	YY=	23.8405	ZY=	1.6143		
XZ=	1.8814	YZ=	1.5694	ZZ=	22.0202		
Eigenvalues:	20.336	24.4476	26.2984				
81	H	Isotropic=	23.8374	Anisotropy		5.5891	
XX=	25.4324	YX=	-2.4637	ZX=	1.3216		
XY=	-2.2566	YY=	24.9471	ZY=	1.2817		
XZ=	1.0127	YZ=	1.0683	ZZ=	21.1325		
Eigenvalues:	20.1179	23.8308	27.5634				
82	H	Isotropic=	23.816	Anisotropy		8.4225	
XX=	22.8333	YX=	-2.5173	ZX=	0.7938		
XY=	-2.4036	YY=	28.1563	ZY=	2.4812		
XZ=	0.402	YZ=	1.5334	ZZ=	20.4582		
Eigenvalues:	19.4806	22.5363	29.4309				

2bviii_neg45

C	-2.444753	-0.836698	1.581257
C	-3.165126	0.300257	2.372887
C	-3.199448	1.671588	1.67761
C	-4.608771	2.1102	1.240367
C	-5.302018	1.170387	0.233734
C	-4.512254	0.655886	-0.959873
C	-3.326341	-0.194452	-0.60712
C	-2.113516	0.180002	-1.091745
C	-0.882714	-0.359785	-0.418568
C	-1.044811	-0.417881	1.02198

C	-3.336833	-1.326538	0.398819
C	-4.693529	-1.762881	0.930745
C	-2.705896	-2.584173	-0.227994
C	-1.900525	1.131638	-2.204969
C	-5.504826	2.361567	2.431788
O	-2.188208	-1.906892	2.489581
O	-2.574911	0.412912	3.658711
O	-6.521028	0.995995	0.302276
O	-5.296182	0.233042	-2.067226
O	0.200927	0.558896	-0.700889
H	-1.617423	0.447692	3.543123
C	-6.23185-0.765932	-2.04732	
O	-6.564892	-1.297106	-0.993652
C	-6.758658	-1.031654	-3.419301
H	-4.218601	-0.030422.608439	
H	-2.522078	1.686482	0.7875
H	-4.102615	1.632879	-1.405694
H	-0.614489	-1.372731	-0.834716
H	-0.292686	-1.153567	1.500089
H	-0.788125	0.586833	1.529863
H	-5.380184	-0.914445	1.150155
H	-5.206463	-2.426593	0.190665
H	-4.552578	-2.358346	1.866937
H	-3.370807	-3.473014	-0.09918
H	-2.534827	-2.444501	-1.32164
H	-1.735944	-2.829473	0.270169
H	-2.753164	1.112838	-2.928313
H	-1.778991	2.17085 -1.806131	
H	-0.965243	0.870392	-2.761483
H	-6.490322	2.76436 2.091959	
H	-5.695339	1.416783	2.99537
H	-5.027413.099006	3.12062	
H	-6.29868-0.345366	-4.169782	
H	-6.528101	-2.090376	-3.691814
H	-7.866631	-0.88627-3.410113	
H	-2.928315	-1.958857	3.107651
C	1.465424	0.051003	-0.76941
O	1.64725 -1.150528	-0.580826	
H	-4.483275	3.081715	0.677619
H	-2.821494	2.437028	2.407536
C	2.487817	1.135312	-1.071702
C	3.906856	0.685476	-0.579625
O	2.432971	1.504808	-2.43046
H	2.191689	2.075607	-0.518839
N	4.626056	-0.022724	-1.603083
C	4.625712	1.933025	-0.11078
H	3.742464	-0.011022	0.297763
H	2.550837	0.7096 -2.968495	
C	5.353206	-1.196863	-1.478342
H	4.834422	0.519275	-2.417256
C	4.85205 2.98567	-1.005203	
C	5.507739	4.13867 -0.578113	
C	5.930182	4.252197	0.746967
C	5.686435	3.214184	1.645486
C	5.032456	2.057543	1.220273
H	4.496097	2.901178	-2.045021

O	6.053605	-1.527856	-2.458189
C	5.317241	-2.034678	-0.251032
H	5.689151	4.960232	-1.286917
H	6.450813	5.161046	1.083165
H	6.009178	3.305577	2.693187
H	4.828785	1.253063	1.94335
C	5.185854	-3.42057-0.412897	
C	5.230146	-4.258821	0.699642
C	5.435099	-3.723651	1.971511
C	5.609348	-2.348763	2.128244
C	5.559194	-1.504988	1.019103
H	5.046539	-3.836917	-1.423069
H	5.110685	-5.344783	0.570811
H	5.469053	-4.386292.849032	
H	5.795085	-1.927663	3.127126
H	5.742991	-0.426588	1.143477

2bviii_neg45	E(RB+HF-PW91)	=	-2012.298902	
SCF GIAO	Magnetic shielding tensor (ppm):			
1	C	Isotropic=	109.7958	Anisotropy = 27.2212
XX=	97.7477	YX=	6.873	ZX= -0.6796
XY=	4.3539	YY=	121.9224	ZY= -10.0933
XZ=	6.314	YZ=	-9.8652	ZZ= 109.7174
Eigenvalues:	94.5459	106.8983	127.9433	
2	C	Isotropic=	112.4529	Anisotropy = 30.7635
XX=	104.1012	YX=	0.2422	ZX= 20.6644
XY=	-5.2082	YY=	110.461	ZY= 2.218
XZ=	12.1424	YZ=	9.2704	ZZ= 122.7964
Eigenvalues:	93.0813	111.3154	132.9619	
3	C	Isotropic=	141.9994	Anisotropy = 19.4872
XX=	126.3826	YX=	-5.8216	ZX= 7.0499
XY=	-1.9426	YY=	153.482	ZY= 2.7684
XZ=	13.3268	YZ=	4.5289	ZZ= 146.1337
Eigenvalues:	121.2905	149.7169	154.9909	
4	C	Isotropic=	140.5271	Anisotropy = 24.3282
XX=	124.5818	YX=	-0.1643	ZX= 11.1254
XY=	-0.2925	YY=	146.379	ZY= 9.7981
XZ=	-2.5771	YZ=	5.4421	ZZ= 150.6204
Eigenvalues:	123.7987	141.0367	156.7458	
5	C	Isotropic=	-22.9379	Anisotropy = 181.2464
XX=	-47.8985	YX=	-14.8514	ZX= 29.4625
XY=	-27.3705	YY=	27.5573	ZY= -94.4078
XZ=	17.5486	YZ=	-94.6658	ZZ= -48.4725
Eigenvalues:	-113.3152	-53.3916	97.8931	
6	C	Isotropic=	101.7246	Anisotropy = 42.5428
XX=	91.5414	YX=	4.3803	ZX= 1.2008
XY=	5.4319	YY=	98.5357	ZY= 17.4614
XZ=	19.2475	YZ=	18.908	ZZ= 115.0966
Eigenvalues:	86.0171	89.0702	130.0864	
7	C	Isotropic=	43.8654	Anisotropy = 157.6426
XX=	10.4483	YX=	45.6213	ZX= -9.5176
XY=	37.3023	YY=	39.6164	ZY= 80.9661
XZ=	-35.7942	YZ=	89.7837	ZZ= 81.5315
Eigenvalues:	-58.8245	41.4603	148.9604	
8	C	Isotropic=	40.7016	Anisotropy = 157.077

XX=	20.9503	YX=	26.0554	ZX=	-31.8869		
XY=	23.1578	YY=	59.4999	ZY=	103.5106		
XZ=	-19.3475	YZ=	85.3172	ZZ=	41.6545		
Eigenvalues:	-59.8602	36.5454	145.4196				
9	C	Isotropic=	112.8143	Anisotropy	=	48.0058	
XX=	124.8367	YX=	27.3031	ZX=	0.1		
XY=	31.1581	YY=	100.2385	ZY=	-9.9532		
XZ=	2.8828	YZ=	-9.5081	ZZ=	113.3675		
Eigenvalues:	78.5189	115.1058	144.8181				
10	C	Isotropic=	148.4244	Anisotropy	=	44.2078	
XX=	159.0515	YX=	16.5938	ZX=	-7.559		
XY=	18.2884	YY=	133.8557	ZY=	-15.5139		
XZ=	-16.7896	YZ=	-6.3512	ZZ=	152.366		
Eigenvalues:	124.1575	143.2195	177.8963				
11	C	Isotropic=	147.6885	Anisotropy	=	11.7899	
XX=	142.5634	YX=	-1.4469	ZX=	7.0462		
XY=	-5.8143	YY=	145.8305	ZY=	7.0752		
XZ=	-6.2522	YZ=	-1.3667	ZZ=	154.6716		
Eigenvalues:	139.9648	147.5523	155.5485				
12	C	Isotropic=	155.2	Anisotropy	=	22.0796	
XX=	165.7654	YX=	-4.6092	ZX=	-5.5284		
XY=	1.0259	YY=	155.0753	ZY=	8.4878		
XZ=	-5.933	YZ=	17.734	ZZ=	144.7594		
Eigenvalues:	135.3594	160.3209	169.9198				
13	C	Isotropic=	148.2234	Anisotropy	=	55.0577	
XX=	131.7876	YX=	-12.7273	ZX=	-17.9627		
XY=	-9.7762	YY=	168.4617	ZY=	18.4052		
XZ=	-24.5697	YZ=	15.0469	ZZ=	144.4207		
Eigenvalues:	115.8974	143.8442	184.9285				
14	C	Isotropic=	168.0749	Anisotropy	=	12.8246	
XX=	161.9167	YX=	-4.0962	ZX=	-3.6666		
XY=	3.2771	YY=	168.8813	ZY=	-8.3994		
XZ=	3.3129	YZ=	-1.5521	ZZ=	173.4268		
Eigenvalues:	161.8656	165.7346	176.6246				
15	C	Isotropic=	169.3713	Anisotropy	=	16.8646	
XX=	172.5632	YX=	-1.9627	ZX=	-1.6518		
XY=	-0.1873	YY=	161.7733	ZY=	8.6184		
XZ=	-5.6481	YZ=	10.0938	ZZ=	173.7774		
Eigenvalues:	156.617	170.8826	180.6144				
16	O	Isotropic=	263.5306	Anisotropy	=	82.1103	
XX=	283.9823	YX=	13.4622	ZX=	-53.9148		
XY=	-4.5836	YY=	282.7233	ZY=	-37.5321		
XZ=	-47.1971	YZ=	-2.0643	ZZ=	223.8864		
Eigenvalues:	192.5789	279.7422	318.2708				
17	O	Isotropic=	265.6125	Anisotropy	=	45.1143	
XX=	268.2871	YX=	-7.2453	ZX=	24.8687		
XY=	-18.9575	YY=	277.7344	ZY=	-13.7527		
XZ=	3.1189	YZ=	-14.8668	ZZ=	250.816		
Eigenvalues:	241.6119	259.5369	295.6887				
18	O	Isotropic=	-358.4965	Anisotropy	=	1084.1339	
XX=	-961.4513	YX=	-174.8546	ZX=	94.5991		
XY=	-217.3011	YY=	88.1275	ZY=	-352.1219		
XZ=	151.5905	YZ=	-352.1593	ZZ=	-202.1655		
Eigenvalues:	-1001.9261	-437.8227	364.2595				
19	O	Isotropic=	91.8044	Anisotropy	=	118.2144	
XX=	170.012	YX=	-8.1214	ZX=	48.0806		

XY=	12.2302	YY=	151.6908	ZY=	72.6443				
XZ=	-70.1325	YZ=	-24.0989	ZZ=	-46.2897				
Eigenvalues:	-49.7921	154.5912		170.614					
20	O	Isotropic=	70.9086	Anisotropy	=	163.2302			
XX=	111.783	YX=	-12.5288	ZX=	-0.79				
XY=	-136.5657	YY=	-66.3745	ZY=	60.0599				
XZ=	44.2328	YZ=	47.5491	ZZ=	167.3173				
Eigenvalues:	-105.7662	138.7633		179.7287					
21	H	Isotropic=	31.3101	Anisotropy	=	14.074			
XX=	39.9718	YX=	0.3839	ZX=	2.5032				
XY=	0.7244	YY=	22.6766	ZY=	3.5563				
XZ=	2.3134	YZ=	2.5467	ZZ=	31.2818				
Eigenvalues:	21.7021	31.5354		40.6928					
22	C	Isotropic=	20.3697	Anisotropy	=	75.4439			
XX=	1.2454	YX=	-60.6323	ZX=	-56.1742				
XY=	-63.8634	YY=	14.8491	ZY=	-51.9088				
XZ=	-25.8562	YZ=	-21.6759	ZZ=	45.0147				
Eigenvalues:	-79.043	69.4865		70.6657					
23	O	Isotropic=	-132.2239	Anisotropy	=	601.4125			
XX=	-38.5393	YX=	-330.6471	ZX=	25.2753				
XY=	-296.3396	YY=	-63.4528	ZY=	87.2149				
XZ=	-12.3066	YZ=	92.585	ZZ=	-294.6796				
Eigenvalues:	-408.7573	-256.6323		268.7178					
24	C	Isotropic=	166.1732	Anisotropy	=	37.3352			
XX=	158.8547	YX=	7.4874	ZX=	12.1649				
XY=	7.3802	YY=	154.3991	ZY=	4.2413				
XZ=	12.3074	YZ=	2.7836	ZZ=	185.266				
Eigenvalues:	148.1564	159.2999		191.0634					
25	H	Isotropic=	27.5665	Anisotropy	=	3.2145			
XX=	29.3537	YX=	-0.2161	ZX=	0.4517				
XY=	-0.5567	YY=	26.3537	ZY=	1.069				
XZ=	1.4984	YZ=	1.778	ZZ=	26.9922				
Eigenvalues:	25.0187	27.9714		29.7095					
26	H	Isotropic=	28.3572	Anisotropy	=	7.8583			
XX=	27.6144	YX=	-2.4788	ZX=	-3.3011				
XY=	-1.729	YY=	27.8529	ZY=	2.3286				
XZ=	-3.1302	YZ=	2.139	ZZ=	29.6043				
Eigenvalues:	25.1433	26.3323		33.5961					
27	H	Isotropic=	25.4526	Anisotropy	=	4.3085			
XX=	26.8407	YX=	1.0898	ZX=	3.0591				
XY=	2.0959	YY=	24.3253	ZY=	-0.929				
XZ=	0.0243	YZ=	1.3657	ZZ=	25.1917				
Eigenvalues:	23.3785	24.6543		28.3249					
28	H	Isotropic=	24.8773	Anisotropy	=	7.0789			
XX=	28.6025	YX=	2.2435	ZX=	-2.224				
XY=	0.4403	YY=	24.8148	ZY=	0.2217				
XZ=	-2.7958	YZ=	1.6254	ZZ=	21.2146				
Eigenvalues:	20.0891	24.9462		29.5966					
29	H	Isotropic=	28.4964	Anisotropy	=	8.0738			
XX=	33.2785	YX=	-2.6699	ZX=	-0.4942				
XY=	-2.0309	YY=	24.6449	ZY=	-2.1764				
XZ=	-1.2313	YZ=	-3.7467	ZZ=	27.5658				
Eigenvalues:	22.2562	29.354		33.879					
30	H	Isotropic=	29.7673	Anisotropy	=	5.5615			
XX=	32.0601	YX=	2.103	ZX=	-2.3617				
XY=	1.6364	YY=	28.1585	ZY=	2.8459				

XZ=	-2.5089	YZ=	2.0817	ZZ=	29.0834		
Eigenvalues:	24.8568	30.9701	33.475				
31	H	Isotropic=	29.3994	Anisotropy	=	8.3908	
XX=	32.1018	YX=	-2.8956	ZX=	-0.3807		
XY=	-3.7635	YY=	31.111	ZY=	-0.7002		
XZ=	-1.0475	YZ=	0.4346	ZZ=	24.9856		
Eigenvalues:	24.8698	28.3352	34.9933				
32	H	Isotropic=	29.3083	Anisotropy	=	9.3189	
XX=	31.8149	YX=	2.4406	ZX=	4.9601		
XY=	2.5875	YY=	28.744	ZY=	0.7948		
XZ=	3.699	YZ=	1.2569	ZZ=	27.3658		
Eigenvalues:	24.6663	27.7376	35.5209				
33	H	Isotropic=	30.413	Anisotropy	=	6.3669	
XX=	31.4681	YX=	2.7624	ZX=	-0.2089		
XY=	2.4877	YY=	29.5341	ZY=	-3.5251		
XZ=	-0.5437	YZ=	-3.0573	ZZ=	30.2368		
Eigenvalues:	25.9862	30.5952	34.6576				
34	H	Isotropic=	30.1595	Anisotropy	=	9.0357	
XX=	29.0128	YX=	0.5944	ZX=	-1.0747		
XY=	2.3375	YY=	35.6855	ZY=	1.5818		
XZ=	-1.1882	YZ=	1.7276	ZZ=	25.7803		
Eigenvalues:	25.0341	29.2611	36.1833				
35	H	Isotropic=	30.3568	Anisotropy	=	6.0576	
XX=	28.4551	YX=	1.1613	ZX=	-1.8972		
XY=	-0.8022	YY=	30.7143	ZY=	3.3111		
XZ=	-1.0703	YZ=	2.3661	ZZ=	31.9011		
Eigenvalues:	27.2772	29.398	34.3952				
36	H	Isotropic=	28.5649	Anisotropy	=	6.5375	
XX=	30.3841	YX=	-1.0282	ZX=	0.4394		
XY=	-3.3661	YY=	30.8448	ZY=	0.5348		
XZ=	-0.6805	YZ=	1.7041	ZZ=	24.4658		
Eigenvalues:	24.2634	28.5081	32.9232				
37	H	Isotropic=	29.068	Anisotropy	=	8.2162	
XX=	31.3226	YX=	1.6962	ZX=	2.0834		
XY=	1.0927	YY=	23.8073	ZY=	-1.5388		
XZ=	3.4902	YZ=	-2.4538	ZZ=	32.074		
Eigenvalues:	22.8521	29.8064	34.5454				
38	H	Isotropic=	29.1809	Anisotropy	=	6.8508	
XX=	27.7805	YX=	0.855	ZX=	-0.0446		
XY=	1.3556	YY=	33.4642	ZY=	-0.9908		
XZ=	-0.0072	YZ=	-0.5355	ZZ=	26.298		
Eigenvalues:	26.2118	27.5828	33.7481				
39	H	Isotropic=	28.9763	Anisotropy	=	7.3132	
XX=	33.0092	YX=	-1.5911	ZX=	-1.011		
XY=	-0.6697	YY=	23.4567	ZY=	-1.6186		
XZ=	-2.3614	YZ=	-2.1994	ZZ=	30.4629		
Eigenvalues:	22.7428	30.3344	33.8517				
40	H	Isotropic=	29.2224	Anisotropy	=	10.9852	
XX=	34.4819	YX=	-4.0269	ZX=	0.7912		
XY=	-4.8003	YY=	27.0175	ZY=	2.0351		
XZ=	-0.4251	YZ=	0.6833	ZZ=	26.1679		
Eigenvalues:	24.1244	26.997	36.5459				
41	H	Isotropic=	29.7008	Anisotropy	=	5.7132	
XX=	29.474	YX=	-0.4122	ZX=	-3.1672		
XY=	-0.884	YY=	30.0265	ZY=	-2.4494		
XZ=	-3.74	YZ=	-2.2475	ZZ=	29.6018		

Eigenvalues:	25.1382	30.4545	33.5096			
42	H	Isotropic=	30.5547	Anisotropy	=	9.4968
XX=	29.0559	YX=	-0.1242	ZX=	-0.3618	
XY=	-0.3044	YY=	31.4136	ZY=	5.7782	
XZ=	-0.1124	YZ=	5.3573	ZZ=	31.1946	
Eigenvalues:	25.7351	29.043	36.8859			
43	H	Isotropic=	29.0396	Anisotropy	=	5.6942
XX=	27.8123	YX=	2.538	ZX=	1.6476	
XY=	3.032	YY=	27.1674	ZY=	-1.1425	
XZ=	0.0245	YZ=	-2.8171	ZZ=	32.1392	
Eigenvalues:	24.1623	30.1208	32.8358			
44	H	Isotropic=	29.2057	Anisotropy	=	7.0148
XX=	26.8038	YX=	-0.0771	ZX=	0.7538	
XY=	-0.0012	YY=	31.7034	ZY=	2.3511	
XZ=	1.3989	YZ=	3.9981	ZZ=	29.1098	
Eigenvalues:	25.9485	27.7862	33.8822			
45	H	Isotropic=	28.9359	Anisotropy	=	8.8613
XX=	34.0191	YX=	-0.1484	ZX=	1.363	
XY=	-0.392	YY=	25.1275	ZY=	-0.3501	
XZ=	3.4809	YZ=	0.3394	ZZ=	27.6611	
Eigenvalues:	25.1168	26.8474	34.8435			
46	H	Isotropic=	30.7292	Anisotropy	=	17.9746
XX=	31.5803	YX=	1.7987	ZX=	-8.7119	
XY=	1.768	YY=	25.9227	ZY=	-5.1761	
XZ=	-6.0558	YZ=	-6.8325	ZZ=	34.6845	
Eigenvalues:	22.3305	27.1448	42.7122			
47	C	Isotropic=	11.4012	Anisotropy	=	88.9083
XX=	-76.9063	YX=	-26.1507	ZX=	22.5389	
XY=	11.4163	YY=	43.9199	ZY=	0.7355	
XZ=	19.6339	YZ=	8.4165	ZZ=	67.1901	
Eigenvalues:	-80.4361	143.9664	70.6734			
48	O	Isotropic=	-100.2155	Anisotropy	=	629.2166
XX=	-253.6001	YX=	44.8767	ZX=	55.589	
XY=	35.9967	YY=	-331.5379	ZY=	103.6344	
XZ=	43.6929	YZ=	170.3718	ZZ=	284.4917	
Eigenvalues:	-368.4034	-251.5052	319.2623			
49	H	Isotropic=	28.7771	Anisotropy	=	6.6591
XX=	26.7561	YX=	-2.8139	ZX=	-1.7679	
XY=	-1.2777	YY=	31.4967	ZY=	-2.8278	
XZ=	-2.1064	YZ=	-2.8196	ZZ=	28.0787	
Eigenvalues:	23.8902	29.2247	33.2165			
50	H	Isotropic=	29.5927	Anisotropy	=	6.3682
XX=	29.3023	YX=	0.0458	ZX=	1.2777	
XY=	0.3409	YY=	31.3456	ZY=	4.0732	
XZ=	1.4883	YZ=	3.0567	ZZ=	28.1303	
Eigenvalues:	25.5235	29.4165	33.8382			
51	C	Isotropic=	108.9751	Anisotropy	=	22.8908
XX=	122.1194	YX=	-6.0567	ZX=	4.6648	
XY=	-3.0699	YY=	97.1379	ZY=	-4.7194	
XZ=	3.3112	YZ=	-3.0794	ZZ=	107.6679	
Eigenvalues:	95.4652	107.2245	124.2356			
52	C	Isotropic=	129.9161	Anisotropy	=	9.4202
XX=	132.3612	YX=	0.5701	ZX=	-0.9898	
XY=	4.3406	YY=	124.1736	ZY=	4.9117	
XZ=	0.8302	YZ=	6.3533	ZZ=	133.2137	
Eigenvalues:	121.0232	132.5289	136.1963			

53 O Isotropic= 296.6955 Anisotropy = 22.9984
 XX= 290.9654 YX= 12.7168 ZX= -15.7183
 XY= 4.7308 YY= 308.4143 ZY= -1.5099
 XZ= -9.9939 YZ= 12.0885 ZZ= 290.7066
 Eigenvalues: 275.0269 303.0317 312.0277

54 H Isotropic= 26.7045 Anisotropy = 6.4448
 XX= 30.9075 YX= 2.0795 ZX= 1.3893
 XY= -0.7138 YY= 24.4194 ZY= 0.9298
 XZ= -0.9978 YZ= 2.2952 ZZ= 24.7866
 Eigenvalues: 22.9618 26.1507 31.001

55 N Isotropic= 134.6878 Anisotropy = 120.4533
 XX= 121.7305 YX= -9.9684 ZX= 53.1001
 XY= -13.0623 YY= 211.4522 ZY= -15.1983
 XZ= 41.0645 YZ= -5.0887 ZZ= 70.8807
 Eigenvalues: 42.7495 146.3239 214.99

56 C Isotropic= 46.2692 Anisotropy = 195.4072
 XX= 128.6781 YX= -79.2691 ZX= -46.7785
 XY= -76.2538 YY= 3.7854 ZY= 8.6186
 XZ= -39.4691 YZ= 7.4187 ZZ= 6.3442
 Eigenvalues: -37.2474 -0.4856 176.5407

57 H Isotropic= 25.5009 Anisotropy = 6.9948
 XX= 24.9264 YX= -3.3147 ZX= 2.7315
 XY= 0.184 YY= 26.0823 ZY= -2.4904
 XZ= 3.0685 YZ= -2.4321 ZZ= 25.4939
 Eigenvalues: 22.1984 24.1402 30.1641

58 H Isotropic= 29.8081 Anisotropy = 14.5629
 XX= 24.5522 YX= -2.4629 ZX= 2.0416
 XY= -1.6397 YY= 30.7358 ZY= 7.8527
 XZ= -0.8516 YZ= 5.8057 ZZ= 34.1363
 Eigenvalues: 22.9249 26.9827 39.5167

59 C Isotropic= 14.9527 Anisotropy = 114.2621
 XX= 47.7958 YX= 56.4735 ZX= 1.5414
 XY= 50.682 YY= -21.0997 ZY= 56.5459
 XZ= 5.4601 YZ= 50.4169 ZZ= 18.1621
 Eigenvalues: -73.9826 27.7134 91.1275

60 H Isotropic= 26.3438 Anisotropy = 6.7206
 XX= 23.2528 YX= -2.3549 ZX= -2.367
 XY= 0.8027 YY= 27.8091 ZY= -4.2152
 XZ= -2.144 YZ= -1.3099 ZZ= 27.9695
 Eigenvalues: 21.7717 26.4355 30.8242

61 C Isotropic= 64.7801 Anisotropy = 171.5973
 XX= 141.3909 YX= -52.6944 ZX= -51.4214
 XY= -44.7352 YY= 71.5481 ZY= 7.7025
 XZ= -51.4771 YZ= 10.9798 ZZ= -18.5988
 Eigenvalues: -33.9609 49.1229 179.1783

62 C Isotropic= 60.2374 Anisotropy = 178.9238
 XX= 147.7818 YX= -56.0701 ZX= -21.3339
 XY= -57.5186 YY= 19.9964 ZY= 55.9508
 XZ= -20.0308 YZ= 58.3232 ZZ= 12.934
 Eigenvalues: -44.2061 45.3983 179.5199

63 C Isotropic= 63.9677 Anisotropy = 174.8165
 XX= 132.4082 YX= -79.0266 ZX= -40.145
 XY= -81.8922 YY= 11.8992 ZY= -9.8909
 XZ= -40.9028 YZ= -9.7078 ZZ= 47.5957
 Eigenvalues: -37.3932 48.7842 180.512

64 C Isotropic= 61.5399 Anisotropy = 173.6828

XX= 141.0253 YX= -50.0641 ZX= -48.7784
 XY= -48.6973 YY= 69.6945 ZY= 6.1915
 XZ= -51.6784 YZ= 4.3996 ZZ= -26.1
 Eigenvalues: -40.7023 47.9936 177.3284
 65 C Isotropic= 65.1025 Anisotropy = 149.2791
 XX= 136.659 YX= -49.2815 ZX= -16.2994
 XY= -47.7297 YY= 33.4002 ZY= 54.645
 XZ= -13.7433 YZ= 50.494 ZZ= 25.2484
 Eigenvalues: -26.7375 57.4232 164.6219
 66 H Isotropic= 22.8967 Anisotropy = 10.5627
 XX= 21.5341 YX= 5.0794 ZX= 0.1733
 XY= 4.7636 YY= 26.875 ZY= -1.7439
 XZ= 0.3101 YZ= -1.187 ZZ= 20.2811
 Eigenvalues: 18.1515 20.6002 29.9386
 67 O Isotropic= -134.8045 Anisotropy = 631.5079
 XX= -52.9319 YX= 257.7077 ZX= 312.4235
 XY= 247.7491 YY= -108.3812 ZY= 48.8385
 XZ= 224.983 YZ= 61.5793 ZZ= -243.1004
 Eigenvalues: -470.8129 -219.8014 286.2007
 68 C Isotropic= 58.8759 Anisotropy = 168.6434
 XX= 163.5431 YX= -35.9396 ZX= -22.0446
 XY= -12.6995 YY= 19.7266 ZY= 36.1467
 XZ= -17.7682 YZ= 34.7121 ZZ= -6.6419
 Eigenvalues: -31.2942 36.6171 171.3049
 69 H Isotropic= 23.6147 Anisotropy = 5.1242
 XX= 21.7616 YX= 2.6461 ZX= 1.4249
 XY= 2.6396 YY= 24.836 ZY= 0.5133
 XZ= 1.5545 YZ= 0.8589 ZZ= 24.2464
 Eigenvalues: 20.0134 23.7998 27.0308
 70 H Isotropic= 23.7238 Anisotropy = 3.4448
 XX= 21.541 YX= 1.9923 ZX= 1.1553
 XY= 1.6965 YY= 24.1647 ZY= -1.0246
 XZ= 1.0202 YZ= -0.9999 ZZ= 25.4656
 Eigenvalues: 20.1985 24.9526 26.0203
 71 H Isotropic= 23.7337 Anisotropy = 5.0915
 XX= 21.5422 YX= 2.5127 ZX= 1.0948
 XY= 2.6461 YY= 25.8869 ZY= -0.0698
 XZ= 1.0874 YZ= -0.1448 ZZ= 23.772
 Eigenvalues: 20.053 24.0201 27.128
 72 H Isotropic= 23.6532 Anisotropy = 7.2552
 XX= 20.9324 YX= 0.8705 ZX= 2.5371
 XY= 1.8064 YY= 25.1194 ZY= 2.5804
 XZ= 2.9334 YZ= 2.1509 ZZ= 24.908
 Eigenvalues: 19.5358 22.9339 28.49
 73 C Isotropic= 57.7521 Anisotropy = 179.5291
 XX= 174.0541 YX= -17.8222 ZX= -15.4699
 XY= -16.1634 YY= 24.835 ZY= -29.6168
 XZ= -25.4573 YZ= -29.7833 ZZ= -25.6326
 Eigenvalues: -42.4319 38.2501 177.4382
 74 C Isotropic= 61.597 Anisotropy = 177.9185
 XX= 175.483 YX= -25.7854 ZX= -18.7503
 XY= -22.9107 YY= -36.7774 ZY= -10.4611
 XZ= -16.3873 YZ= -11.8054 ZZ= 46.0852
 Eigenvalues: -41.5025 46.0841 180.2093
 75 C Isotropic= 61.7319 Anisotropy = 179.2046
 XX= 177.1775 YX= -11.6406 ZX= -22.6957

XY= -12.8085 YY= 15.967 ZY= 43.331
 XZ= -17.9642 YZ= 43.613 ZZ= -7.9488
 Eigenvalues: -41.4375 45.4315 181.2016
 76 C Isotropic= 65.3323 Anisotropy = 172.6094
 XX= 174.6049 YX= -17.2336 ZX= -29.7244
 XY= -20.0478 YY= 41.61 ZY= -29.3577
 XZ= -28.6105 YZ= -27.6327 ZZ= -20.2179
 Eigenvalues: -36.8124 52.4042 180.4053
 77 C Isotropic= 63.9738 Anisotropy = 172.3858
 XX= 171.8075 YX= -34.5256 ZX= -12.2925
 XY= -31.7608 YY= -20.1436 ZY= -11.7861
 XZ= -19.656 YZ= -2.9727 ZZ= 40.2575
 Eigenvalues: -27.1872 40.2109 178.8977
 78 H Isotropic= 23.2181 Anisotropy = 6.7403
 XX= 20.0924 YX= -0.379 ZX= -0.3527
 XY= -0.3304 YY= 27.3016 ZY= -1.7563
 XZ= -0.2999 YZ= -1.1997 ZZ= 22.2604
 Eigenvalues: 19.9946 21.9481 27.7117
 79 H Isotropic= 23.6325 Anisotropy = 3.6768
 XX= 20.6873 YX= -0.7972 ZX= 0.6329
 XY= -0.2694 YY= 24.5008 ZY= -0.6256
 XZ= 0.5907 YZ= -0.6198 ZZ= 25.7093
 Eigenvalues: 20.56 24.2537 26.0837
 80 H Isotropic= 23.6346 Anisotropy = 3.6167
 XX= 20.85 YX= 0.2761 ZX= 0.7495
 XY= 0.1544 YY= 25.7208 ZY= 0.6658
 XZ= 0.9669 YZ= 0.6724 ZZ= 24.3331
 Eigenvalues: 20.6494 24.2087 26.0458
 81 H Isotropic= 23.7405 Anisotropy = 5.3281
 XX= 20.6839 YX= -0.2144 ZX= 1.8405
 XY= 0.0921 YY= 26.2502 ZY= -1.7191
 XZ= 1.1494 YZ= -1.5869 ZZ= 24.2875
 Eigenvalues: 20.0993 23.8296 27.2926
 82 H Isotropic= 23.1623 Anisotropy = 7.353
 XX= 18.8456 YX= -3.5598 ZX= 3.7486
 XY= -1.1928 YY= 25.4865 ZY= -1.7641
 XZ= 2.357 YZ= -0.5252 ZZ= 25.1549
 Eigenvalues: 17.2102 24.2124 28.0643

Structures with C-C4'ipso-C4'=O at +45.0°:

2a
2a-i

C	2.637767	-1.194205	1.735848
C	3.469612	-2.322447	1.047817
C	3.07473	-2.644744	-0.403158
C	4.14673	-2.258253	-1.438143
C	4.504226	-0.759028	-1.47898
C	3.382131	0.267585	-1.46865
C	2.530132	0.252242	-0.232622
C	1.189821	0.096214	-0.390477
C	0.384209	-0.358351	0.795434
C	1.123487	-1.423245	1.608431
C	3.057966	0.204423	1.18422

C	4.555434	0.402415	1.357441
C	2.388887	1.306591	2.02663
C	0.454556	0.283058	-1.661816
C	5.395651	-3.095385	-1.280555
O	2.880667	-1.266011	3.140063
O	3.408393	-3.492989	1.84822
O	5.665048	-0.419166	-1.720172
O	3.7299	1.570787	-1.925978
O	-0.827292	-0.950398	0.264892
H	2.481737	-3.657573	2.06199
C	4.857918	2.262264	-1.574588
O	5.632058	1.828508	-0.728317
C	4.958825	3.537884	-2.345516
H	4.563643	-2.047753	1.090682
H	2.11054	-2.147379	-0.676095
H	2.728042	-0.070731	-2.346666
H	0.086279	0.512359	1.445347
H	0.672169	-1.444606	2.639217
H	0.933923	-2.425324	1.141078
H	5.169068	-0.171145	0.625908
H	4.817261	1.483337	1.237448
H	4.853361	0.094922	2.390556
H	3.153708	1.920817	2.561935
H	1.790943	1.994754	1.383348
H	1.726084	0.858392	2.806828
H	0.948444	1.04974	-2.308829
H	0.396466	-0.686939	-2.218376
H	-0.595826	0.621144	-1.462269
H	6.120438	-2.860619	-2.098136
H	5.897205	-2.88547	-0.305401
H	5.136507	-4.180407	-1.323422
H	4.001848	3.76886	-2.871445
H	5.211058	4.366505	-1.640481
H	5.778147	3.431586	-3.098388
H	3.803691	-1.518023	3.270162
C	-1.863497	-1.160051	1.120577
O	-1.765087	-0.813919	2.29988
H	3.702301	-2.467828	-2.455438
H	2.919575	-3.754589	-0.479273
C	-3.064128	-1.784551	0.428136
C	-4.322727	-0.885371	0.642913
O	-2.785429	-2.037286	-0.924755
H	-3.256019	-2.799516	0.880405
N	-4.034534	0.520698	0.783171
C	-5.439362	-1.267705	-0.293571
H	-4.674248	-1.186697	1.689108
H	-2.641721	-1.182672	-1.363265
C	-3.412051	1.344283	-0.136551
H	-4.1212	0.872988	1.710988
C	-5.44928	-0.952376	-1.653876
C	-6.52338	-1.338361	-2.458213
C	-7.594604	-2.04206	-1.913132
C	-7.590931	-2.36195	-0.55483
C	-6.523107	-1.975254	0.25044
H	-4.605553	-0.407397	-2.107157
O	-3.255129	1.02625	-1.333584

C	-2.976768	2.678909	0.373457
H	-6.517564	-1.083893	-3.52846
H	-8.439338	-2.345379	-2.548575
H	-8.432742	-2.918588	-0.11774
H	-6.536573	-2.230719	1.321055
C	-3.279999	3.818924	-0.37776
C	-2.872395.07319	0.075118	
C	-2.158043	5.188189	1.267801
C	-1.846117	4.048123	2.009684
C	-2.255156	2.790917	1.566822
H	-3.830555	3.714662	-1.325885
H	-3.112992	5.971437	-0.512683
H	-1.836695	6.178913	1.622857
H	-1.275548	4.138836	2.946009
H	-1.992401	1.891663	2.148877

2ailiz	E(RB+HF-PW91)	=	-2012.305455
SCF	GIAO	Magnetic shielding tensor (ppm):	
1	C	Isotropic=	109.4189 Anisotropy 28.6824
XX=	99.7478	YX= 2.2182	ZX= 14.8502
XY=	7.1546	YY= 105.7754	ZY= 3.0462
XZ=	8.6202	YZ= 2.627	ZZ= 122.7335
Eigenvalues:	93.8967	105.8196	128.5405
2	C	Isotropic=	112.288 Anisotropy 30.8755
XX=	94.0841	YX= 5.7573	ZX= -6.2415
XY=	-1.6057	YY= 127.3129	ZY= -4.1564
XZ=	-4.0469	YZ= -14.3822	ZZ= 115.4671
Eigenvalues:	92.9108	111.0815	132.8717
3	C	Isotropic=	142.4651 Anisotropy 20.2529
XX=	121.5185	YX= -4.5476	ZX= -0.284
XY=	3.2778	YY= 154.2462	ZY= 2.0108
XZ=	-1.0709	YZ= 3.4007	ZZ= 151.6305
Eigenvalues:	121.4931	149.9351	155.967
4	C	Isotropic=	140.1102 Anisotropy 25.1441
XX=	124.5115	YX= 1.6029	ZX= -0.3139
XY=	-10.8005	YY= 156.2191	ZY= -0.8972
XZ=	7.2356	YZ= 1.7404	ZZ= 139.5999
Eigenvalues:	123.1207	140.337	156.8729
5	C	Isotropic=	-22.171 Anisotropy 179.5062
XX=	-58.0886	YX= 31.3153	ZX= 20.0813
XY=	13.5917	YY= -103.5928	ZY= 8.782
XZ=	15.8031	YZ= 0.4446	ZZ= 95.1686
Eigenvalues:	-112.8385	-51.1742	97.4999
6	C	Isotropic=	102.2237 Anisotropy 41.166
XX=	86.3315	YX= -6.666	ZX= 1.6803
XY=	7.4518	YY= 129.0507	ZY= -6.0483
XZ=	-6.4717	YZ= -3.5955	ZZ= 91.2888
Eigenvalues:	85.3118	91.6916	129.6677
7	C	Isotropic=	44.1953 Anisotropy 157.3068
XX=	39.8136	YX= -8.7032	ZX= 16.8261
XY=	-30.0716	YY= 145.2573	ZY= 19.9282
XZ=	29.8342	YZ= 5.3813	ZZ= -52.485
Eigenvalues:	-59.4432	42.9626	149.0665
8	C	Isotropic=	41.2701 Anisotropy 156.5474
XX=	40.3881	YX= -21.0028	ZX= 8.9902

XY=	-16.8269	YY=	133.7962	ZY=	32.0109		
XZ=	-5.3899	YZ=	49.9739	ZZ=	-50.3738		
Eigenvalues:	-59.4159	37.5912	145.6351				
9	C	Isotropic=	110.6707	Anisotropy		46.8521	
XX=	126.9244	YX=	15.3132	ZX=	18.2372		
XY=	21.4732	YY=	109.1041	ZY=	-8.2725		
XZ=	18.4887	YZ=	-5.8826	ZZ=	95.9836		
Eigenvalues:	79.7214	110.3853	141.9054				
10	C	Isotropic=	148.3556	Anisotropy		41.7889	
XX=	169.3016	YX=	3.972	ZX=	12.2471		
XY=	3.562	YY=	139.4207	ZY=	-1.4379		
XZ=	20.8749	YZ=	-11.3659	ZZ=	136.3443		
Eigenvalues:	125.5515	143.3003	176.2148				
11	C	Isotropic=	148.0183	Anisotropy		13.8337	
XX=	142.9869	YX=	0.8385	ZX=	-2.0908		
XY=	-14.0706	YY=	153.6661	ZY=	-4.9916		
XZ=	1.0112	YZ=	0.0423	ZZ=	147.4019		
Eigenvalues:	139.5092	147.3048	157.2408				
12	C	Isotropic=	155.7284	Anisotropy		24.227	
XX=	165.1861	YX=	-5.6962	ZX=	-13.3733		
XY=	1.0398	YY=	158.5924	ZY=	12.5739		
XZ=	-6.5277	YZ=	6.635	ZZ=	143.4069		
Eigenvalues:	136.4383	158.8673	171.8797				
13	C	Isotropic=	148.5675	Anisotropy		54.8224	
XX=	145.7986	YX=	-21.6387	ZX=	-1.6385		
XY=	-24.9593	YY=	157.9966	ZY=	22.5059		
XZ=	2.6107	YZ=	26.034	ZZ=	141.9075		
Eigenvalues:	116.125	144.4618	185.1158				
14	C	Isotropic=	168.3921	Anisotropy		11.766	
XX=	165.0799	YX=	-9.1697	ZX=	2.7038		
XY=	3.1732	YY=	166.7711	ZY=	-1.268		
XZ=	5.8669	YZ=	-3.0472	ZZ=	173.3253		
Eigenvalues:	162.2724	166.6678	176.2361				
15	C	Isotropic=	169.4594	Anisotropy		17.1277	
XX=	174.1217	YX=	-4.7506	ZX=	-5.5984		
XY=	-6.1651	YY=	176.4426	ZY=	-1.619		
XZ=	-1.3967	YZ=	-2.5363	ZZ=	157.814		
Eigenvalues:	156.5662	170.9342	180.8779				
16	O	Isotropic=	263.0663	Anisotropy		82.3615	
XX=	313.0229	YX=	-11.695	ZX=	22.02		
XY=	-3.4484	YY=	215.3801	ZY=	55.4764		
XZ=	11.1412	YZ=	19.7565	ZZ=	260.7959		
Eigenvalues:	192.3285	278.8964	317.974				
17	O	Isotropic=	265.6569	Anisotropy		45.0519	
XX=	254.6258	YX=	20.7588	ZX=	-13.831		
XY=	-3.4011	YY=	249.871	ZY=	5.8082		
XZ=	-9.1462	YZ=	-0.1722	ZZ=	292.474		
Eigenvalues:	241.4902	259.789	295.6915				
18	O	Isotropic=	-369.7929	Anisotropy		1095.3766	
XX=	-960.2796	YX=	-140.8744	ZX=	251.804		
XY=	-120.2874	YY=	-470.7211	ZY=	88.5674		
XZ=	177.2067	YZ=	68.2371	ZZ=	321.622		
Eigenvalues:	-1031.0918	-438.7451	360.4582				
19	O	Isotropic=	95.4392	Anisotropy		127.1181	
XX=	154.4194	YX=	103.8319	ZX=	-78.0517		
XY=	-7.3763	YY=	53.5615	ZY=	41.7851		

XZ= -23.2435 YZ= 129.5828 ZZ= 78.3367
 Eigenvalues: -44.9587 151.0918 180.1846
 20 O Isotropic= 62.5427 Anisotropy 201.8835
 XX= 57.3641 YX= -62.1148 ZX= -18.1804
 XY= -81.3413 YY= 141.4068 ZY= -77.7647
 XZ= -152.3599 YZ= -118.4832 ZZ= -11.1429
 Eigenvalues: -124.32 114.8163 197.1317
 21 H Isotropic= 31.18 Anisotropy 13.4034
 XX= 36.1409 YX= 2.5969 ZX= -4.6665
 XY= 2.1921 YY= 32.522 ZY= -5.6182
 XZ= -4.534 YZ= -4.4574 ZZ= 24.8772
 Eigenvalues: 21.6664 31.7581 40.1156
 22 C Isotropic= 21.5816 Anisotropy 77.4194
 XX= 9.9386 YX= -89.2668 ZX= 13.2762
 XY= -57.2394 YY= -17.4923 ZY= 15.9472
 XZ= -4.0649 YZ= -8.9042 ZZ= 72.2986
 Eigenvalues: -78.5147 70.065 73.1946
 23 O Isotropic= -140.9032 Anisotropy 605.8041
 XX= -246.038 YX= -118.4484 ZX= -289.2785
 XY= -147.4422 YY= -139.3233 ZY= 161.3962
 XZ= -252.6616 YZ= 176.0689 ZZ= -37.3482
 Eigenvalues: -432.9864 -252.6894 262.9662
 24 C Isotropic= 166.1248 Anisotropy 37.3513
 XX= 155.7679 YX= 5.2979 ZX= 2.9505
 XY= 4.3809 YY= 182.295 ZY= -14.6835
 XZ= 4.668 YZ= -17.6309 ZZ= 160.3116
 Eigenvalues: 147.7403 159.6085 191.0257
 25 H Isotropic= 27.4494 Anisotropy 2.8038
 XX= 27.9728 YX= -0.1433 ZX= -1.3543
 XY= 0.7963 YY= 28.3831 ZY= -0.2361
 XZ= -2.0979 YZ= -0.8785 ZZ= 25.9922
 Eigenvalues: 24.9621 28.0674 29.3186
 26 H Isotropic= 28.2065 Anisotropy 8.8197
 XX= 29.4389 YX= -4.9819 ZX= -0.5084
 XY= -4.3514 YY= 29.0791 ZY= 0.9651
 XZ= -0.1888 YZ= 1.5321 ZZ= 26.1014
 Eigenvalues: 24.3257 26.2074 34.0862
 27 H Isotropic= 25.4187 Anisotropy 3.7124
 XX= 26.1423 YX= 2.1448 ZX= -1.7806
 XY= 1.5107 YY= 25.6914 ZY= 0.0487
 XZ= 1.3861 YZ= -1.654 ZZ= 24.4225
 Eigenvalues: 23.707 24.6555 27.8937
 28 H Isotropic= 25.0201 Anisotropy 7.0692
 XX= 29.4339 YX= -1.4952 ZX= 2.2232
 XY= -0.6405 YY= 24.7502 ZY= 3.3034
 XZ= 0.4066 YZ= 2.2962 ZZ= 20.8763
 Eigenvalues: 19.1405 26.1869 29.7329
 29 H Isotropic= 27.6516 Anisotropy 7.0077
 XX= 31.8004 YX= -0.7903 ZX= -1.3883
 XY= -1.6267 YY= 22.3112 ZY= -3.3843
 XZ= -1.2726 YZ= -1.1015 ZZ= 28.8431
 Eigenvalues: 21.3828 29.2486 32.3234
 30 H Isotropic= 29.6019 Anisotropy 5.5531
 XX= 32.8734 YX= -0.7023 ZX= 1.1477
 XY= -1.1275 YY= 31.1708 ZY= 0.4112
 XZ= 0.6933 YZ= 1.2703 ZZ= 24.7615

Eigenvalues:	24.5246	30.9772	33.304		
31	H	Isotropic=	29.4542	Anisotropy	8.4541
XX=	31.2603	YX=	-0.7706	ZX=	-3.2658
XY=	-1.0502	YY=	26.4998	ZY=	3.3036
XZ=	-3.5709	YZ=	2.0086	ZZ=	30.6025
Eigenvalues:	25.0871	28.1852	35.0903		
32	H	Isotropic=	29.322	Anisotropy	8.8943
XX=	29.0006	YX=	4.8356	ZX=	-1.8748
XY=	4.5599	YY=	30.7799	ZY=	-1.0409
XZ=	-1.5123	YZ=	-1.401	ZZ=	28.1856
Eigenvalues:	25.0088	27.7057	35.2516		
33	H	Isotropic=	30.3347	Anisotropy	6.7827
XX=	32.2652	YX=	1.9172	ZX=	2.8368
XY=	1.8006	YY=	27.3039	ZY=	-0.6059
XZ=	2.925	YZ=	-1.1947	ZZ=	31.4351
Eigenvalues:	26.0021	30.1455	34.8565		
34	H	Isotropic=	30.1824	Anisotropy	8.8116
XX=	30.0268	YX=	0.2702	ZX=	0.7374
XY=	1.5422	YY=	31.3062	ZY=	4.9787
XZ=	1.6033	YZ=	5.7197	ZZ=	29.2141
Eigenvalues:	24.7884	29.702	36.0568		
35	H	Isotropic=	30.4031	Anisotropy	7.3969
XX=	31.1949	YX=	-3.1277	ZX=	2.6782
XY=	-3.0744	YY=	32.9926	ZY=	0.7599
XZ=	-0.548	YZ=	1.6114	ZZ=	27.0218
Eigenvalues:	26.1205	29.7544	35.3344		
36	H	Isotropic=	28.4186	Anisotropy	6.003
XX=	28.8932	YX=	-0.1521	ZX=	-1.4612
XY=	-1.1329	YY=	27.6821	ZY=	3.8065
XZ=	-2.8978	YZ=	2.051	ZZ=	28.6805
Eigenvalues:	24.9523	27.883	32.4206		
37	H	Isotropic=	29.2763	Anisotropy	7.0511
XX=	30.6054	YX=	0.7452	ZX=	0.2322
XY=	1.7916	YY=	28.1338	ZY=	-5.5242
XZ=	-1.0303	YZ=	-4.3681	ZZ=	29.0898
Eigenvalues:	23.5773	30.2746	33.9771		
38	H	Isotropic=	29.1739	Anisotropy	6.6745
XX=	28.5498	YX=	0.2846	ZX=	0.7558
XY=	1.2322	YY=	28.4412	ZY=	3.6525
XZ=	1.3604	YZ=	3.6625	ZZ=	30.5307
Eigenvalues:	25.6818	28.2164	33.6236		
39	H	Isotropic=	28.5577	Anisotropy	10.8469
XX=	34.9488	YX=	-3.251	ZX=	-2.3957
XY=	-2.7071	YY=	23.8811	ZY=	-2.7284
XZ=	-0.4414	YZ=	-1.3981	ZZ=	26.8431
Eigenvalues:	21.9833	27.9008	35.7889		
40	H	Isotropic=	29.1842	Anisotropy	10.9188
XX=	31.9124	YX=	-0.1103	ZX=	-5.8343
XY=	-1.9028	YY=	27.0646	ZY=	-0.2894
XZ=	-5.9686	YZ=	0.6169	ZZ=	28.5756
Eigenvalues:	24.0346	27.0546	36.4634		
41	H	Isotropic=	29.6628	Anisotropy	5.8687
XX=	31.967	YX=	-1.9552	ZX=	1.8108
XY=	-2.535	YY=	26.2404	ZY=	1.0986
XZ=	1.8955	YZ=	0.7484	ZZ=	30.7809
Eigenvalues:	25.0639	30.3491	33.5752		

42	H	Isotropic=	30.4941	Anisotropy	9.7612
XX=	28.9055	YX=	-1.6632	ZX=	-1.1447
XY=	-1.7006	YY=	36.2596	ZY=	1.5491
XZ=	-1.4954	YZ=	1.9569	ZZ=	26.3171
Eigenvalues:	25.6624	28.8182	37.0015		
43	H	Isotropic=	29.2054	Anisotropy	5.3044
XX=	30.846	YX=	1.0325	ZX=	1.5612
XY=	-0.7119	YY=	29.4626	ZY=	-3.8555
XZ=	2.7362	YZ=	-2.7662	ZZ=	27.3076
Eigenvalues:	24.3705	30.504	32.7417		
44	H	Isotropic=	29.3277	Anisotropy	7.4104
XX=	26.8851	YX=	1.157	ZX=	1.0106
XY=	3.0223	YY=	33.1582	ZY=	2.4796
XZ=	0.371	YZ=	0.7329	ZZ=	27.9398
Eigenvalues:	26.2236	27.4915	34.2679		
45	H	Isotropic=	28.9794	Anisotropy	8.4895
XX=	29.9545	YX=	0.4389	ZX=	-3.648
XY=	1.6337	YY=	27.119	ZY=	-1.8287
XZ=	-4.7708	YZ=	-1.6876	ZZ=	29.8646
Eigenvalues:	25.4729	26.8261	34.639		
46	H	Isotropic=	30.687	Anisotropy	18.2233
XX=	37.8433	YX=	-4.7033	ZX=	7.5112
XY=	-3.1685	YY=	23.5571	ZY=	-3.6176
XZ=	5.4281	YZ=	-1.8446	ZZ=	30.6607
Eigenvalues:	22.3466	26.8786	42.8359		
47	C	Isotropic=	9.3501	Anisotropy	96.1462
XX=	-55.0665	YX=	-52.8082	ZX=	7.4169
XY=	-39.4893	YY=	56.0709	ZY=	-0.4938
XZ=	50.6745	YZ=	10.0287	ZZ=	27.046
Eigenvalues:	-79.5973	34.2001	73.4476		
48	O	Isotropic=	-90.3994	Anisotropy	615.1497
XX=	-165.5894	YX=	-180.1209	ZX=	28.2894
XY=	-181.1581	YY=	218.0219	ZY=	-119.4447
XZ=	74.9354	YZ=	-138.5552	ZZ=	-323.6307
Eigenvalues:	-353.6394	-237.2592	319.7004		
49	H	Isotropic=	28.7129	Anisotropy	6.5764
XX=	28.1824	YX=	-2.5309	ZX=	0.4474
XY=	-1.8951	YY=	25.402	ZY=	1.6178
XZ=	1.6955	YZ=	2.2255	ZZ=	32.5544
Eigenvalues:	23.636	29.4056	33.0972		
50	H	Isotropic=	29.474	Anisotropy	6.7119
XX=	27.6331	YX=	0.5792	ZX=	-1.4543
XY=	0.5884	YY=	33.4059	ZY=	1.2699
XZ=	-1.5547	YZ=	2.4919	ZZ=	27.3832
Eigenvalues:	25.5828	28.8907	33.9486		
51	C	Isotropic=	107.5297	Anisotropy	21.5515
XX=	109.8157	YX=	-3.8809	ZX=	3.2128
XY=	-7.5309	YY=	93.2592	ZY=	7.4582
XZ=	-2.6875	YZ=	8.4972	ZZ=	119.5142
Eigenvalues:	89.497	111.1947	121.8974		
52	C	Isotropic=	123.5153	Anisotropy	30.6775
XX=	133.4323	YX=	13.4776	ZX=	12.8577
XY=	9.6458	YY=	119.8677	ZY=	-3.1864
XZ=	10.3644	YZ=	2.9096	ZZ=	117.2459
Eigenvalues:	107.7864	118.7925	143.967		
53	O	Isotropic=	269.3813	Anisotropy	60.6475

XX= 275.3089 YX= -4.1989 ZX= -28.1712
 XY= 15.5897 YY= 293.1622 ZY= -46.6193
 XZ= 1.0684 YZ= -12.7297 ZZ= 239.6727
 Eigenvalues: 224.4218 273.909 309.8129
 54 H Isotropic= 26.5415 Anisotropy 5.6868
 XX= 25.5683 YX= 0.1977 ZX= -0.0484
 XY= -0.3836 YY= 27.9332 ZY= -3.7266
 XZ= -1.0356 YZ= -2.602 ZZ= 26.1228
 Eigenvalues: 23.614 25.6777 30.3327
 55 N Isotropic= 123.5446 Anisotropy 102.0613
 XX= 162.989 YX= 9.6448 ZX= 1.7659
 XY= 11.9905 YY= 138.6705 ZY= -46.3242
 XZ= -6.6822 YZ= -106.4239 ZZ= 68.9743
 Eigenvalues: 19.7733 159.275 191.5854
 56 C Isotropic= 56.9104 Anisotropy 177.4504
 XX= 24.5847 YX= -66.7827 ZX= -46.5539
 XY= -68.7117 YY= 137.5569 ZY= 12.6775
 XZ= -41.6425 YZ= 14.1105 ZZ= 8.5896
 Eigenvalues: -36.2894 31.8099 175.2106
 57 H Isotropic= 26.3928 Anisotropy 7.4926
 XX= 27.107 YX= 3.8409 ZX= -1.4531
 XY= 3.6962 YY= 24.53 ZY= -1.7294
 XZ= -1.9925 YZ= -1.9195 ZZ= 27.5415
 Eigenvalues: 21.7892 26.0014 31.3879
 58 H Isotropic= 28.4983 Anisotropy 13.5642
 XX= 24.2466 YX= 2.7045 ZX= -0.2867
 XY= 1.4669 YY= 31.8813 ZY= -7.2539
 XZ= -1.7699 YZ= -5.5634 ZZ= 29.3671
 Eigenvalues: 23.4406 24.5133 37.5412
 59 C Isotropic= 12.3971 Anisotropy 127.685
 XX= 60.5496 YX= -62.9177 ZX= 32.4309
 XY= -56.2784 YY= -40.9305 ZY= -6.5308
 XZ= 27.5862 YZ= 6.2071 ZZ= 17.5722
 Eigenvalues: -70.322 9.9928 97.5204
 60 H Isotropic= 25.5049 Anisotropy 5.7426
 XX= 22.8585 YX= 5.2268 ZX= -2.4183
 XY= 1.7743 YY= 27.3414 ZY= 3.2058
 XZ= -1.2293 YZ= -0.2364 ZZ= 26.3147
 Eigenvalues: 20.0824 27.0989 29.3333
 61 C Isotropic= 54.4084 Anisotropy 180.161
 XX= 22.1841 YX= -81.6355 ZX= 12.421
 XY= -82.35 YY= 121.7664 ZY= 43.4342
 XZ= 9.3683 YZ= 41.2585 ZZ= 19.2749
 Eigenvalues: -40.5783 29.2878 174.5158
 62 C Isotropic= 61.9531 Anisotropy 174.3689
 XX= 77.9562 YX= -50.697 ZX= -11.0036
 XY= -51.6262 YY= 141.0545 ZY= 41.7705
 XZ= -9.394 YZ= 44.1587 ZZ= -33.1515
 Eigenvalues: -43.1981 50.8584 178.199
 63 C Isotropic= 63.7047 Anisotropy 175.7415
 XX= 26.9663 YX= -70.6115 ZX= -50.8743
 XY= -73.9669 YY= 139.3223 ZY= 7.8206
 XZ= -51.7624 YZ= 8.9055 ZZ= 24.8256
 Eigenvalues: -38.7377 48.9862 180.8658
 64 C Isotropic= 63.6507 Anisotropy 169.8117
 XX= 26.7357 YX= -84.1334 ZX= 15.9755

XY= -85.8435 YY= 121.109 ZY= 41.0993
 XZ= 16.0209 YZ= 40.5197 ZZ= 43.1074
 Eigenvalues: -38.5107 52.6043 176.8585
 65 C Isotropic= 60.4067 Anisotropy 142.0424
 XX= 78.4347 YX= -40.3828 ZX= -5.064
 XY= -31.3003 YY= 128.4245 ZY= 39.774
 XZ= -4.9774 YZ= 40.1472 ZZ= -25.639
 Eigenvalues: -35.5099 61.6284 155.1017
 66 H Isotropic= 21.3536 Anisotropy 10.9842
 XX= 22.7384 YX= 3.9939 ZX= 5.5516
 XY= 2.7413 YY= 17.9178 ZY= -0.7196
 XZ= 4.7255 YZ= 0.2949 ZZ= 23.4047
 Eigenvalues: 15.1353 20.2491 28.6764
 67 O Isotropic= -72.9864 Anisotropy 595.6278
 XX= 200.0932 YX= -157.6103 ZX= 196.4566
 XY= -161.6044 YY= -105.3632 ZY= -66.296
 XZ= 154.3167 YZ= -73.1962 ZZ= -313.6893
 Eigenvalues: -369.6174 -173.4406 324.0987
 68 C Isotropic= 56.1929 Anisotropy 170.7185
 XX= 115.2117 YX= -13.4411 ZX= -85.2024
 XY= -26.5057 YY= -14.8598 ZY= -9.9048
 XZ= -63.4069 YZ= -17.4131 ZZ= 68.2267
 Eigenvalues: -27.7318 26.3052 170.0052
 69 H Isotropic= 23.6301 Anisotropy 5.8897
 XX= 25.862 YX= 2.8046 ZX= 1.6185
 XY= 2.6278 YY= 21.3614 ZY= -0.2777
 XZ= 1.4097 YZ= -0.2533 ZZ= 23.667
 Eigenvalues: 19.8662 23.4677 27.5566
 70 H Isotropic= 23.7552 Anisotropy 3.553
 XX= 24.4153 YX= 2.21 ZX= 0.0844
 XY= 1.862 YY= 21.633 ZY= -1.3285
 XZ= -0.1836 YZ= -1.2874 ZZ= 25.2173
 Eigenvalues: 20.2929 24.8488 26.1238
 71 H Isotropic= 23.8666 Anisotropy 4.49
 XX= 24.7932 YX= 2.1313 ZX= 1.5516
 XY= 2.0498 YY= 21.3319 ZY= -0.3168
 XZ= 1.3937 YZ= -0.5205 ZZ= 25.4747
 Eigenvalues: 20.1499 24.59 26.86
 72 H Isotropic= 24.184 Anisotropy 8.455
 XX= 28.0379 YX= 3.9454 ZX= 0.2291
 XY= 3.5429 YY= 21.9423 ZY= -0.1615
 XZ= 0.3547 YZ= -0.4177 ZZ= 22.5717
 Eigenvalues: 20.1017 22.6296 29.8206
 73 C Isotropic= 60.7434 Anisotropy 175.7794
 XX= 124.9276 YX= -10.7461 ZX= -90.3349
 XY= -14.0839 YY= 43.4202 ZY= 3.5012
 XZ= -93.4074 YZ= 3.7385 ZZ= 13.8824
 Eigenvalues: -38.0481 42.3487 177.9296
 74 C Isotropic= 61.9202 Anisotropy 177.5939
 XX= 140.9269 YX= 5.3061 ZX= -68.6659
 XY= 3.3928 YY= -8.144 ZY= 43.3197
 XZ= -68.8893 YZ= 45.6803 ZZ= 52.9778
 Eigenvalues: -40.0779 45.5224 180.3161
 75 C Isotropic= 60.8391 Anisotropy 180.8288
 XX= 137.0787 YX= -36.4844 ZX= -68.0844
 XY= -34.9105 YY= -23.9511 ZY= -18.9519

XZ= -68.0263 YZ= -17.9937 ZZ= 69.3898
 Eigenvalues: -42.8525 43.9783 181.3916
 76 C Isotropic= 62.3041 Anisotropy 177.6296
 XX= 121.4731 YX= -19.1726 ZX= -95.372
 XY= -14.9273 YY= 49.0111 ZY= 2.6144
 XZ= -97.7126 YZ= 1.3727 ZZ= 16.4282
 Eigenvalues: -41.5017 47.6902 180.7239
 77 C Isotropic= 65.8033 Anisotropy 168.7914
 XX= 136.9201 YX= 0.0901 ZX= -67.882
 XY= 6.1152 YY= 1.851 ZY= 44.2571
 XZ= -68.4176 YZ= 38.8535 ZZ= 58.6388
 Eigenvalues: -28.9758 48.0548 178.3309
 78 H Isotropic= 23.401 Anisotropy 7.8327
 XX= 20.3696 YX= -0.5084 ZX= 1.1777
 XY= 0.3554 YY= 28.4426 ZY= -1.2487
 XZ= 1.3289 YZ= -0.9763 ZZ= 21.3908
 Eigenvalues: 19.4908 22.0894 28.6228
 79 H Isotropic= 23.7576 Anisotropy 4.0306
 XX= 21.77 YX= 0.6373 ZX= 2.233
 XY= 0.6198 YY= 25.867 ZY= 0.5205
 XZ= 2.1832 YZ= 0.7521 ZZ= 23.6359
 Eigenvalues: 20.3004 24.5278 26.4447
 80 H Isotropic= 23.6876 Anisotropy 3.9488
 XX= 21.702 YX= -0.8624 ZX= 2.2262
 XY= -0.5385 YY= 25.304 ZY= -0.7834
 XZ= 2.0667 YZ= -0.7116 ZZ= 24.0569
 Eigenvalues: 20.4207 24.3221 26.3202
 81 H Isotropic= 23.7876 Anisotropy 5.6696
 XX= 21.4186 YX= -0.381 ZX= 1.2606
 XY= -0.0761 YY= 27.4853 ZY= 0.757
 XZ= 0.958 YZ= 0.5266 ZZ= 22.4588
 Eigenvalues: 20.6708 23.1246 27.5673
 82 H Isotropic= 23.4854 Anisotropy 6.8923
 XX= 22.2883 YX= 0.1136 ZX= 2.1518
 XY= 0.8821 YY= 26.4114 ZY= 3.3425
 XZ= 1.8312 YZ= 2.3713 ZZ= 21.7564
 Eigenvalues: 19.4463 22.9296 28.0802

2a-i2

C 2.66265 -1.118529 1.764125
 C 3.509365 -2.258921 1.115383
 C 3.124048 -2.631176 -0.326176
 C 4.19621 -2.266059 -1.368726
 C 4.537868 -0.765104 -1.455628
 C 3.404858 0.249154 -1.482147
 C 2.547879 0.263708 -0.249557
 C 1.209947 0.088635 -0.407796
 C 0.40431 -0.335264 0.789422
 C 1.15104 -1.366955 1.63824
 C 3.07024 0.266309 1.170358
 C 4.56472 0.487127 1.341613
 C 2.38588 1.387134 1.975103
 C 0.476485 0.235532 -1.685307
 C 5.453192 -3.08442 -1.179578
 O 2.898764 -1.148737 3.170768
 O 3.457846 -3.406348 1.949506

O	5.696154	-0.421297	-1.702794
O	3.740336	1.540901	-1.978804
O	-0.800825	-0.954202	0.274457
H	2.537419	-3.548842	2.202368
C	4.859223	2.255876	-1.64517
O	5.636801	1.854724	-0.786027
C	4.945814	3.510463	-2.451355
H	4.600157	-1.970783	1.152624
H	2.156494	-2.1521	-0.618625
H	2.757518	-0.12352	-2.351271
H	0.094874	0.552084	1.410569
H	0.696151	-1.360581	2.667905
H	0.974985	-2.385588	1.203066
H	5.187672	-0.104786	0.632914
H	4.814253	1.566196	1.183924
H	4.863246	0.220839	2.385852
H	3.141968	2.027852	2.491469
H	1.781239	2.046857	1.308638
H	1.726705	0.95664	2.768251
H	0.968652	0.985699	-2.352747
H	0.424486	-0.749191	-2.215558
H	-0.576254	0.574196	-1.497896
H	6.178886	-2.867944	-2.001422
H	5.94842	-2.838126	-0.209707
H	5.205877	-4.17299	-1.1888
H	3.991496	3.707795	-2.995592
H	5.172736	4.363652	-1.767261
H	5.776937	3.398791	-3.190382
H	3.83269	-1.349773	3.31113
C	-1.839526	-1.146251	1.133485
O	-1.722979	-0.817407	2.31524
H	3.758696	-2.512475	-2.380726
H	2.981207	-3.744462	-0.36728
C	-3.035524	-1.800853	0.468419
C	-4.310565	-0.916735	0.64981
O	-2.830695	-2.041706	-0.905075
H	-3.211477	-2.783199	0.997596
N	-4.062971	0.498364	0.742153
C	-5.401877	-1.35247	-0.293945
H	-4.662421	-1.198121	1.700592
H	-1.9333	-2.383247	-1.018486
C	-3.465515	1.345584	-0.177204
H	-4.187502	0.871916	1.657754
C	-5.375083	-1.064532	-1.66055
C	-6.428206	-1.470085	-2.482292
C	-7.510937	-2.164765	-1.947353
C	-7.539864	-2.458764	-0.583511
C	-6.493748	-2.051648	0.240767
H	-4.503228	-0.543016	-2.092287
O	-3.274106	1.053022	-1.371363
C	-3.091796	2.695429	0.351399
H	-6.397455	-1.238769	-3.557169
H	-8.340128	-2.482185	-2.596147
H	-8.390569	-3.009498	-0.156821
H	-6.532091	-2.283039	1.315953
C	-3.430106	3.826683	-0.398074

C	-3.077721	5.093933	0.064819
C	-2.382637	5.231494	1.266448
C	-2.034682	4.10093	2.006575
C	-2.388586	2.830773	1.552874
H	-3.964299	3.705143	-1.353514
H	-3.346453	5.984733	-0.522015
H	-2.105052	6.232289	1.62969
H	-1.479243	4.2094	2.949949
H	-2.097001	1.940582	2.134287

	E(RB+HF-PW91)	=	-2012.297798	
SCF	GIAO	Magnetic	shielding	tensor (ppm):
1	C	Isotropic=	109.4317	Anisotropy = 28.3646
XX=	99.3824	YX=	2.4829	ZX= 14.6957
XY=	6.723	YY=	106.3679	ZY= 3.8597
XZ=	7.9035	YZ=	3.4063	ZZ= 122.5449
Eigenvalues:	94.0566	105.8971	128.3414	
2	C	Isotropic=	112.3987	Anisotropy = 31.2663
XX=	93.9662	YX=	5.4167	ZX= -6.3916
XY=	-1.7645	YY=	126.9537	ZY= -4.9056
XZ=	-3.5154	YZ=	-14.7723	ZZ= 116.2761
Eigenvalues:	92.9137	111.0395	133.2429	
3	C	Isotropic=	142.1864	Anisotropy = 20.2155
XX=	121.1816	YX=	-5.0402	ZX= -0.4667
XY=	2.9082	YY=	153.9481	ZY= 1.9547
XZ=	-1.3198	YZ=	3.3132	ZZ= 151.4295
Eigenvalues:	121.1253	149.7705	155.6634	
4	C	Isotropic=	140.288	Anisotropy = 24.8168
XX=	124.7106	YX=	1.1611	ZX= -0.2779
XY=	-10.8768	YY=	156.0705	ZY= -1.5321
XZ=	7.4255	YZ=	1.2739	ZZ= 140.083
Eigenvalues:	123.2415	140.79	156.8326	
5	C	Isotropic=	-21.9427	Anisotropy = 179.2955
XX=	-57.9473	YX=	32.1623	ZX= 18.2279
XY=	14.4864	YY=	-102.7647	ZY= 15.2867
XZ=	14.8461	YZ=	7.0388	ZZ= 94.8838
Eigenvalues:	-112.7718	-50.644	97.5876	
6	C	Isotropic=	102.164	Anisotropy = 41.1556
XX=	86.3035	YX=	-7.1099	ZX= 2.0446
XY=	6.7807	YY=	128.614	ZY= -7.2883
XZ=	-6.5131	YZ=	-4.959	ZZ= 91.5745
Eigenvalues:	85.3514	91.5396	129.601	
7	C	Isotropic=	43.8903	Anisotropy = 157.3652
XX=	39.7106	YX=	-9.1047	ZX= 17.2651
XY=	-30.1834	YY=	145.2382	ZY= 13.7035
XZ=	31.0776	YZ=	-0.5669	ZZ= -53.2778
Eigenvalues:	-59.789	42.6595	148.8005	
8	C	Isotropic=	41.0895	Anisotropy = 155.9002
XX=	40.866	YX=	-21.7656	ZX= 10.6251
XY=	-18.3807	YY=	135.0709	ZY= 26.3342
XZ=	-4.1896	YZ=	44.2478	ZZ= -52.6685
Eigenvalues:	-59.5462	37.7916	145.023	
9	C	Isotropic=	110.0903	Anisotropy = 48.0614
XX=	126.0515	YX=	17.1078	ZX= 17.6132
XY=	23.2026	YY=	107.6408	ZY= -7.9143

XZ=	18.1102	YZ=	-6.0581	ZZ=	96.5788		
Eigenvalues:	79.0441	109.0957		142.1313			
10	C	Isotropic=	147.8983	Anisotropy	=	41.5977	
XX=	168.4755	YX=	4.5991	ZX=	12.1591		
XY=	4.1961	YY=	139.1093	ZY=	-1.0787		
XZ=	21.2204	YZ=	-10.527	ZZ=	136.1101		
Eigenvalues:	125.3961		142.6688		175.6301		
11	C	Isotropic=	148.0941	Anisotropy	=	13.8319	
XX=	143.2108	YX=	0.5955	ZX=	-2.1709		
XY=	-14.0276	YY=	153.5024	ZY=	-5.1524		
XZ=	1.3463	YZ=	-0.1342	ZZ=	147.5693		
Eigenvalues:	139.5881		147.3789		157.3154		
12	C	Isotropic=	155.7785	Anisotropy	=	24.6383	
XX=	165.3	YX=	-6.2171	ZX=	-13.3736		
XY=	0.5407	YY=	159.137	ZY=	12.0267		
XZ=	-6.6889	YZ=	6.2058	ZZ=	142.8984		
Eigenvalues:	136.4592		158.6723		172.2041		
13	C	Isotropic=	148.6929	Anisotropy	=	54.8199	
XX=	146.4907	YX=	-21.848	ZX=	-1.21		
XY=	-25.0362	YY=	159.1029	ZY=	21.842		
XZ=	2.9391	YZ=	25.4551	ZZ=	140.485		
Eigenvalues:	116.3452		144.494		185.2394		
14	C	Isotropic=	168.3237	Anisotropy	=	11.0916	
XX=	164.9037	YX=	-8.9663	ZX=	2.8439		
XY=	3.3875	YY=	166.9788	ZY=	-0.4965		
XZ=	5.7607	YZ=	-2.7106	ZZ=	173.0886		
Eigenvalues:	162.1855		167.0675		175.7181		
15	C	Isotropic=	169.4524	Anisotropy	=	17.0816	
XX=	174.2318	YX=	-4.9018	ZX=	-5.3794		
XY=	-6.1691	YY=	176.2034	ZY=	-2.2663		
XZ=	-1.1501	YZ=	-3.1656	ZZ=	157.9219		
Eigenvalues:	156.5405		170.9765		180.8401		
16	O	Isotropic=	263.4238	Anisotropy	=	83.7983	
XX=	314.4305	YX=	-8.5988	ZX=	22.1923		
XY=	-1.5885	YY=	217.6324	ZY=	57.7138		
XZ=	10.7965	YZ=	21.1369	ZZ=	258.2084		
Eigenvalues:	192.1953		278.7867		319.2893		
17	O	Isotropic=	265.4715	Anisotropy	=	45.839	
XX=	253.4348	YX=	18.4402	ZX=	-15.1217		
XY=	-5.2935	YY=	251.4867	ZY=	7.5186		
XZ=	-12.1549	YZ=	2.1493	ZZ=	291.4931		
Eigenvalues:	242.384	257.9997		296.0309			
18	O	Isotropic=	-371.248	Anisotropy	=	1097.0791	
XX=	-962.1597	YX=	-138.3867	ZX=	250.529		
XY=	-120.5401	YY=	-468.6219	ZY=	115.8177		
XZ=	175.9431	YZ=	94.5912	ZZ=	317.0377		
Eigenvalues:	-1034.0975		-439.7846		360.1381		
19	O	Isotropic=	95.3304	Anisotropy	=	127.19	
XX=	153.7141	YX=	102.5898	ZX=	-81.3228		
XY=	-7.3242	YY=	59.2441	ZY=	41.4487		
XZ=	-23.772	YZ=	129.2648	ZZ=	73.0329		
Eigenvalues:	-44.6751	150.5425		180.1237			
20	O	Isotropic=	70.4119	Anisotropy	=	196.0726	
XX=	69.3242	YX=	-62.5844	ZX=	-18.3113		
XY=	-76.7486	YY=	144.5211	ZY=	-75.6051		
XZ=	-146.3433	YZ=	-121.2095	ZZ=	-2.6097		

Eigenvalues:	-112.8996	123.0083	201.1269		
21	H	Isotropic=	31.1693	Anisotropy	= 13.3193
XX=	35.8426	YX=	2.1238	ZX=	-5.1781
XY=	1.6632	YY=	32.0269	ZY=	-5.8885
XZ=	-5.0707	YZ=	-4.8022	ZZ=	25.6383
Eigenvalues:	21.6435	31.8155	40.0488		
22	C	Isotropic=	21.5331	Anisotropy	= 77.4435
XX=	11.3197	YX=	-88.6358	ZX=	15.342
XY=	-57.0231	YY=	-18.7713	ZY=	18.4835
XZ=	-2.5689	YZ=	-6.7782	ZZ=	72.0509
Eigenvalues:	-78.5809	70.0181	73.1621		
23	O	Isotropic=	-140.6819	Anisotropy	= 605.3335
XX=	-241.4493	YX=	-127.9283	ZX=	-288.2171
XY=	-155.5277	YY=	-133.2687	ZY=	160.7871
XZ=	-250.0514	YZ=	175.1969	ZZ=	-47.3276
Eigenvalues:	-432.24	-252.6794	262.8738		
24	C	Isotropic=	166.1183	Anisotropy	= 37.3599
XX=	155.6491	YX=	5.046	ZX=	2.9323
XY=	4.1793	YY=	181.3213	ZY=	-15.4617
XZ=	4.6544	YZ=	-18.152	ZZ=	161.3844
Eigenvalues:	147.7951	159.5348	191.0248		
25	H	Isotropic=	27.4308	Anisotropy	= 2.8254
XX=	27.9304	YX=	-0.1597	ZX=	-1.3509
XY=	0.7835	YY=	28.3091	ZY=	-0.3259
XZ=	-2.0824	YZ=	-0.9581	ZZ=	26.0529
Eigenvalues:	24.9872	27.9908	29.3144		
26	H	Isotropic=	28.2704	Anisotropy	= 8.6975
XX=	29.5638	YX=	-4.8893	ZX=	-0.4034
XY=	-4.3062	YY=	29.1396	ZY=	0.8688
XZ=	-0.0616	YZ=	1.3997	ZZ=	26.1078
Eigenvalues:	24.4673	26.2751	34.0687		
27	H	Isotropic=	25.3912	Anisotropy	= 3.7479
XX=	26.0398	YX=	2.1629	ZX=	-1.8348
XY=	1.5642	YY=	25.6681	ZY=	-0.0236
XZ=	1.4071	YZ=	-1.7095	ZZ=	24.4656
Eigenvalues:	23.6277	24.6561	27.8897		
28	H	Isotropic=	25.0008	Anisotropy	= 6.9524
XX=	29.4036	YX=	-1.2052	ZX=	2.167
XY=	-0.4549	YY=	24.8319	ZY=	3.2686
XZ=	0.3896	YZ=	2.2028	ZZ=	20.767
Eigenvalues:	19.1671	26.1996	29.6358		
29	H	Isotropic=	27.5375	Anisotropy	= 7.254
XX=	31.8487	YX=	-0.6879	ZX=	-1.3572
XY=	-1.5384	YY=	21.9251	ZY=	-3.1579
XZ=	-1.3316	YZ=	-0.8304	ZZ=	28.8388
Eigenvalues:	21.1987	29.0403	32.3735		
30	H	Isotropic=	29.7428	Anisotropy	= 5.5512
XX=	33.0577	YX=	-0.6411	ZX=	1.1389
XY=	-1.0747	YY=	31.224	ZY=	0.2049
XZ=	0.7093	YZ=	1.1027	ZZ=	24.9466
Eigenvalues:	24.7558	31.029	33.4436		
31	H	Isotropic=	29.4662	Anisotropy	= 8.4953
XX=	31.2931	YX=	-0.8392	ZX=	-3.2967
XY=	-1.1114	YY=	26.6655	ZY=	3.4162
XZ=	-3.5723	YZ=	2.1237	ZZ=	30.44
Eigenvalues:	25.0764	28.1925	35.1298		

32	H	Isotropic=	29.29	Anisotropy	=	8.9341
XX=	28.8416	YX=	4.7684	ZX=	-2.0721	
XY=	4.5127	YY=	30.76	ZY=	-1.1447	
XZ=	-1.691	YZ=	-1.5022	ZZ=	28.2684	
Eigenvalues:	24.9251	27.6989	35.246			
33	H	Isotropic=	30.391	Anisotropy	=	6.7987
XX=	32.2495	YX=	2.0803	ZX=	2.7762	
XY=	1.9573	YY=	27.32	ZY=	-0.3706	
XZ=	2.8607	YZ=	-0.9711	ZZ=	31.6034	
Eigenvalues:	26.0658	30.1837	34.9234			
34	H	Isotropic=	30.1754	Anisotropy	=	8.8487
XX=	29.9886	YX=	0.2783	ZX=	0.6266	
XY=	1.5812	YY=	31.6692	ZY=	4.9347	
XZ=	1.4416	YZ=	5.6988	ZZ=	28.8686	
Eigenvalues:	24.7583	29.6934	36.0746			
35	H	Isotropic=	30.3718	Anisotropy	=	7.2477
XX=	31.1411	YX=	-2.9997	ZX=	2.6898	
XY=	-3.0203	YY=	32.9705	ZY=	0.5747	
XZ=	-0.4552	YZ=	1.3896	ZZ=	27.0039	
Eigenvalues:	26.1933	29.7186	35.2036			
36	H	Isotropic=	28.4427	Anisotropy	=	6.1057
XX=	28.9297	YX=	-0.1867	ZX=	-1.5665	
XY=	-1.1936	YY=	27.8702	ZY=	3.8327	
XZ=	-2.9707	YZ=	2.0744	ZZ=	28.5281	
Eigenvalues:	24.9222	27.8927	32.5131			
37	H	Isotropic=	29.1933	Anisotropy	=	7.1616
XX=	30.4359	YX=	0.9053	ZX=	0.3207	
XY=	1.8225	YY=	27.8268	ZY=	-5.5503	
XZ=	-0.9155	YZ=	-4.4119	ZZ=	29.317	
Eigenvalues:	23.433	30.1791	33.9677			
38	H	Isotropic=	29.3272	Anisotropy	=	6.7208
XX=	28.5948	YX=	0.4748	ZX=	0.75	
XY=	1.3877	YY=	28.7661	ZY=	3.6416	
XZ=	1.3748	YZ=	3.5899	ZZ=	30.6208	
Eigenvalues:	25.9577	28.2162	33.8078			
39	H	Isotropic=	28.2053	Anisotropy	=	10.8005
XX=	34.6183	YX=	-3.1614	ZX=	-2.2389	
XY=	-2.7384	YY=	23.3843	ZY=	-2.7451	
XZ=	-0.2561	YZ=	-1.4639	ZZ=	26.6133	
Eigenvalues:	21.5629	27.6474	35.4057			
40	H	Isotropic=	29.1781	Anisotropy	=	10.9128
XX=	31.9679	YX=	-0.2281	ZX=	-5.8106	
XY=	-2.0171	YY=	27.0281	ZY=	-0.2989	
XZ=	-5.8932	YZ=	0.5712	ZZ=	28.5381	
Eigenvalues:	24.0455	27.0354	36.4532			
41	H	Isotropic=	29.6563	Anisotropy	=	5.8555
XX=	31.9767	YX=	-1.8195	ZX=	1.8629	
XY=	-2.4112	YY=	26.2275	ZY=	1.2684	
XZ=	1.9697	YZ=	0.9231	ZZ=	30.7647	
Eigenvalues:	25.0393	30.3696	33.56			
42	H	Isotropic=	30.5051	Anisotropy	=	9.7288
XX=	28.9547	YX=	-1.7725	ZX=	-1.1011	
XY=	-1.8362	YY=	36.3144	ZY=	1.2041	
XZ=	-1.4423	YZ=	1.6082	ZZ=	26.2461	
Eigenvalues:	25.6983	28.826	36.9909			
43	H	Isotropic=	29.1666	Anisotropy	=	5.3414

XX=	30.7358	YX=	1.1435	ZX=	1.6311				
XY=	-0.5468	YY=	29.2174	ZY=	-3.9247				
XZ=	2.8752	YZ=	-2.7907	ZZ=	27.5467				
Eigenvalues:	24.3081	30.4642	32.7276						
44	H	Isotropic=	29.3087	Anisotropy	=	7.4091			
XX=	26.7611	YX=	1.0562	ZX=	0.885				
XY=	2.8731	YY=	33.3116	ZY=	2.3489				
XZ=	0.2495	YZ=	0.6238	ZZ=	27.8534				
Eigenvalues:	26.2001	27.4779	34.2481						
45	H	Isotropic=	28.9724	Anisotropy	=	8.5025			
XX=	30.002	YX=	0.3868	ZX=	-3.6282				
XY=	1.5829	YY=	27.0342	ZY=	-1.817				
XZ=	-4.7788	YZ=	-1.702	ZZ=	29.8811				
Eigenvalues:	25.4612	26.8153	34.6408						
46	H	Isotropic=	30.7461	Anisotropy	=	18.2438			
XX=	38.277	YX=	-3.6494	ZX=	7.73				
XY=	-2.2891	YY=	23.0452	ZY=	-3.2646				
XZ=	5.5565	YZ=	-1.5223	ZZ=	30.9162				
Eigenvalues:	22.2657	27.064	42.9086						
47	C	Isotropic=	11.0668	Anisotropy	=	94.8331			
XX=	-53.2571	YX=	-52.4475	ZX=	9.495				
XY=	-41.6519	YY=	56.5456	ZY=	4.3745				
XZ=	53.1825	YZ=	11.2078	ZZ=	29.912				
Eigenvalues:	-80.0357	38.9473	74.2889						
48	O	Isotropic=	-91.2693	Anisotropy	=	616.0222			
XX=	-164.0255	YX=	-184.6206	ZX=	20.0218				
XY=	-185.199	YY=	220.0728	ZY=	-99.0227				
XZ=	70.5318	YZ=	-138.0497	ZZ=	-329.8552				
Eigenvalues:	-354.6903	-238.5297	319.4121						
49	H	Isotropic=	28.7296	Anisotropy	=	6.6054			
XX=	28.2334	YX=	-2.4492	ZX=	0.4766				
XY=	-1.7986	YY=	25.4835	ZY=	1.8261				
XZ=	1.7453	YZ=	2.4566	ZZ=	32.4719				
Eigenvalues:	23.6676	29.3881	33.1332						
50	H	Isotropic=	29.4768	Anisotropy	=	6.6435			
XX=	27.6522	YX=	0.4601	ZX=	-1.5051				
XY=	0.4438	YY=	33.4917	ZY=	1.0467				
XZ=	-1.5992	YZ=	2.2618	ZZ=	27.2866				
Eigenvalues:	25.6008	28.9239	33.9058						
51	C	Isotropic=	109.299	Anisotropy	=	20.7999			
XX=	106.0806	YX=	-0.3514	ZX=	3.1379				
XY=	-2.8292	YY=	102.0953	ZY=	8.7787				
XZ=	-3.3493	YZ=	8.1782	ZZ=	119.7212				
Eigenvalues:	98.4098	106.3218	123.1656						
52	C	Isotropic=	123.2733	Anisotropy	=	28.2419			
XX=	130.7721	YX=	14.4642	ZX=	10.7686				
XY=	10.6895	YY=	121.4034	ZY=	-3.0005				
XZ=	8.8826	YZ=	1.906	ZZ=	117.6444				
Eigenvalues:	107.9554	119.7632	142.1012						
53	O	Isotropic=	280.9889	Anisotropy	=	87.8235			
XX=	337.3746	YX=	-20.8024	ZX=	-17.0927				
XY=	-1.8059	YY=	260.8222	ZY=	-11.4425				
XZ=	2.253	YZ=	7.7097	ZZ=	244.77				
Eigenvalues:	243.6983	259.7305	339.5379						
54	H	Isotropic=	26.2772	Anisotropy	=	6.0769			
XX=	24.7568	YX=	0.4897	ZX=	0.0883				

XY= -0.4731 YY= 27.1914 ZY= -3.7018
 XZ= -1.3294 YZ= -2.8049 ZZ= 26.8836
 Eigenvalues: 23.6055 24.8977 30.3285
 55 N Isotropic= 130.6982 Anisotropy = 98.8227
 XX= 165.2517 YX= 14.5383 ZX= 8.2799
 XY= 13.3184 YY= 147.534 ZY= -39.0921
 XZ= -0.9272 YZ= -105.697 ZZ= 79.3088
 Eigenvalues: 32.5475 162.967 196.5799
 56 C Isotropic= 57.594 Anisotropy = 176.6259
 XX= 26.8683 YX= -69.7417 ZX= -43.9839
 XY= -68.0752 YY= 138.735 ZY= 6.7748
 XZ= -40.3547 YZ= 7.8604 ZZ= 7.1789
 Eigenvalues: -36.1536 33.591 175.3446
 57 H Isotropic= 26.4368 Anisotropy = 7.3172
 XX= 26.8402 YX= 3.5985 ZX= -1.6021
 XY= 3.569 YY= 24.8954 ZY= -1.8199
 XZ= -2.0698 YZ= -1.7512 ZZ= 27.5749
 Eigenvalues: 22.1344 25.8612 31.315
 58 H Isotropic= 29.8554 Anisotropy = 18.5309
 XX= 40.1294 YX= -4.6353 ZX= -2.2986
 XY= -5.2314 YY= 23.5027 ZY= 5.2401
 XZ= -2.3435 YZ= 3.3313 ZZ= 25.9341
 Eigenvalues: 19.9006 27.4563 42.2093
 59 C Isotropic= 15.4464 Anisotropy = 119.5986
 XX= 61.595 YX= -60.4306 ZX= 31.2366
 XY= -53.0711 YY= -46.6385 ZY= -3.0789
 XZ= 25.8166 YZ= 14.242 ZZ= 31.3828
 Eigenvalues: -73.5801 24.7405 95.1789
 60 H Isotropic= 25.7085 Anisotropy = 6.5822
 XX= 22.5286 YX= 5.1957 ZX= -2.4235
 XY= 1.6848 YY= 28.3276 ZY= 3.6088
 XZ= -1.3188 YZ= -0.2464 ZZ= 26.2692
 Eigenvalues: 19.9981 27.0307 30.0966
 61 C Isotropic= 51.71 Anisotropy = 187.3462
 XX= 19.3496 YX= -84.3213 ZX= 10.2709
 XY= -85.8561 YY= 124.2854 ZY= 38.225
 XZ= 9.6799 YZ= 36.8608 ZZ= 11.495
 Eigenvalues: -42.6034 21.1259 176.6074
 62 C Isotropic= 62.2172 Anisotropy = 173.8728
 XX= 78.9035 YX= -51.939 ZX= -6.5936
 XY= -52.5701 YY= 142.8174 ZY= 36.0788
 XZ= -4.8031 YZ= 39.4024 ZZ= -35.0693
 Eigenvalues: -42.9618 51.481 178.1324
 63 C Isotropic= 63.9545 Anisotropy = 175.2371
 XX= 29.9124 YX= -71.8386 ZX= -49.3362
 XY= -75.1775 YY= 139.3388 ZY= 3.158
 XZ= -50.5095 YZ= 4.6453 ZZ= 22.6125
 Eigenvalues: -38.6205 49.7049 180.7793
 64 C Isotropic= 64.6935 Anisotropy = 168.1697
 XX= 27.5831 YX= -84.4871 ZX= 16.9002
 XY= -85.9557 YY= 122.5445 ZY= 36.8232
 XZ= 17.6299 YZ= 36.9995 ZZ= 43.9528
 Eigenvalues: -36.8961 54.1699 176.8066
 65 C Isotropic= 61.7544 Anisotropy = 142.2422
 XX= 79.9825 YX= -41.6812 ZX= -2.2474
 XY= -32.2104 YY= 131.5328 ZY= 34.8201

XZ= -2.4541 YZ= 35.6139 ZZ= -26.2521
 Eigenvalues: -34.03 62.7107 156.5826
 66 H Isotropic= 20.8394 Anisotropy = 10.4399
 XX= 21.5484 YX= 3.831 ZX= 5.2794
 XY= 2.5798 YY= 17.6 ZY= -0.4381
 XZ= 4.4055 YZ= 0.2894 ZZ= 23.3697
 Eigenvalues: 14.8899 19.829 27.7993
 67 O Isotropic= -105.5442 Anisotropy = 653.3611
 XX= 203.0669 YX= -157.1403 ZX= 215.9816
 XY= -164.7977 YY= -135.7922 ZY= -68.8602
 XZ= 185.9872 YZ= -65.2141 ZZ= -383.9074
 Eigenvalues: -447.1338 -199.5287 330.0299
 68 C Isotropic= 54.487 Anisotropy = 173.3126
 XX= 115.613 YX= -5.5104 ZX= -87.3937
 XY= -20.13 YY= -18.0414 ZY= -12.62
 XZ= -63.1588 YZ= -20.7923 ZZ= 65.8894
 Eigenvalues: -28.9924 22.4246 170.0287
 69 H Isotropic= 23.6457 Anisotropy = 5.8058
 XX= 25.7614 YX= 2.8032 ZX= 1.6156
 XY= 2.7033 YY= 21.4644 ZY= -0.1772
 XZ= 1.321 YZ= -0.2052 ZZ= 23.7113
 Eigenvalues: 19.9338 23.487 27.5162
 70 H Isotropic= 23.8078 Anisotropy = 3.5155
 XX= 24.449 YX= 2.212 ZX= 0.0659
 XY= 1.8599 YY= 21.653 ZY= -1.2118
 XZ= -0.2443 YZ= -1.1851 ZZ= 25.3214
 Eigenvalues: 20.3683 24.9036 26.1515
 71 H Isotropic= 23.9492 Anisotropy = 4.4383
 XX= 24.7901 YX= 2.184 ZX= 1.4661
 XY= 2.1285 YY= 21.4512 ZY= -0.1894
 XZ= 1.3143 YZ= -0.3874 ZZ= 25.6063
 Eigenvalues: 20.2459 24.6936 26.908
 72 H Isotropic= 24.2404 Anisotropy = 8.2607
 XX= 27.969 YX= 3.896 ZX= 0.2116
 XY= 3.4718 YY= 22.0828 ZY= -0.0511
 XZ= 0.4159 YZ= -0.2618 ZZ= 22.6695
 Eigenvalues: 20.2786 22.6951 29.7476
 73 C Isotropic= 60.3782 Anisotropy = 175.5712
 XX= 127.3568 YX= -6.6348 ZX= -89.1327
 XY= -10.6566 YY= 42.3582 ZY= -0.0641
 XZ= -92.2144 YZ= -0.2512 ZZ= 11.4196
 Eigenvalues: -38.4603 42.1692 177.4257
 74 C Isotropic= 61.913 Anisotropy = 176.9237
 XX= 141.6468 YX= 11.2952 ZX= -69.0927
 XY= 9.3987 YY= -7.6684 ZY= 40.7473
 XZ= -69.2513 YZ= 42.9723 ZZ= 51.7607
 Eigenvalues: -40.2022 46.0791 179.8622
 75 C Isotropic= 61.6725 Anisotropy = 179.1918
 XX= 141.3149 YX= -29.5293 ZX= -65.9288
 XY= -27.7823 YY= -25.1138 ZY= -22.576
 XZ= -65.765 YZ= -21.7419 ZZ= 68.8163
 Eigenvalues: -41.7349 45.6186 181.1337
 76 C Isotropic= 62.7793 Anisotropy = 176.421
 XX= 124.9783 YX= -15.8894 ZX= -93.5529
 XY= -11.5114 YY= 48.9769 ZY= -1.4335
 XZ= -96.1882 YZ= -2.5865 ZZ= 14.3828

Eigenvalues: -40.950848.8955 180.3933
 77 C Isotropic= 66.3783 Anisotropy = 166.7607
 XX= 138.0113 YX= 5.9238 ZX= -67.4354
 XY= 11.4621 YY= 2.3071 ZY= 41.414
 XZ= -67.7692 YZ= 35.0948 ZZ= 58.8163
 Eigenvalues: -27.758949.3416 177.5521
 78 H Isotropic= 23.3714 Anisotropy = 7.8173
 XX= 20.3069 YX= -0.8025 ZX= 1.0951
 XY= 0.1155 YY= 28.408 ZY= -1.154
 XZ= 1.2824 YZ= -0.8704 ZZ= 21.3992
 Eigenvalues: 19.537 21.9941 28.5829
 79 H Isotropic= 23.7837 Anisotropy = 4.021
 XX= 21.6933 YX= 0.5026 ZX= 2.157
 XY= 0.4727 YY= 25.9022 ZY= 0.6074
 XZ= 2.1141 YZ= 0.8513 ZZ= 23.7555
 Eigenvalues: 20.3528 24.5339 26.4643
 80 H Isotropic= 23.735 Anisotropy = 3.9297
 XX= 21.7302 YX= -0.9639 ZX= 2.2159
 XY= -0.6302 YY= 25.3266 ZY= -0.7113
 XZ= 2.0648 YZ= -0.6325 ZZ= 24.1482
 Eigenvalues: 20.4548 24.3953 26.3548
 81 H Isotropic= 23.8396 Anisotropy = 5.6758
 XX= 21.4496 YX= -0.56 ZX= 1.2941
 XY= -0.2442 YY= 27.5276 ZY= 0.7705
 XZ= 0.9658 YZ= 0.5419 ZZ= 22.5415
 Eigenvalues: 20.6708 23.2244 27.6234
 82 H Isotropic= 23.595 Anisotropy = 6.9718
 XX= 22.2742 YX= 0.072 ZX= 2.0619
 XY= 0.7783 YY= 26.5924 ZY= 3.4169
 XZ= 1.7368 YZ= 2.401 ZZ= 21.9183
 Eigenvalues: 19.5922 22.9499 28.2428

2a-ii

C	2.803352	-1.397302	1.597982
C	3.671232	-2.376699	0.746015
C	3.339631	-2.419955	-0.755087
C	4.451165	-1.846605	-1.652591
C	4.799374	-0.366774	-1.395691
C	3.670548	0.640544	-1.240129
C	2.767774	0.393706	-0.066259
C	1.436552	0.268993	-0.308039
C	0.585187	-0.396019	0.738399
C	1.297415	-1.596701	1.365973
C	3.236272	0.079997	1.337466
C	4.7238	0.241312	1.607103
C	2.525213	1.00439	2.34344
C	0.755033	0.686887	-1.553808
C	5.69825	-2.699633	-1.602521
O	2.987991	-1.734924	2.971954
O	3.584615	-3.677731	3.07149
O	5.966991	0.010857	-1.519922
O	4.028356	2.006546	-1.428019
O	-0.603258	-0.874052	0.060965
H	2.652306	-3.870441	1.465862
C	5.135151	2.618261	-0.90461
O	5.880671	2.030475	-0.128424

C	5.254391	4.019421	-1.409251
H	4.760545	-2.116134	0.885761
H	2.384293	-1.879107	-0.970258
H	3.05638	0.475274	-2.193253
H	0.259855	0.338001	1.528078
H	0.80381	-1.811372	2.354523
H	1.13436	-2.492437	0.710768
H	5.371312	-0.187657	0.808751
H	4.982435	1.325686	1.699768
H	4.981373	-0.251503	2.577324
H	3.263124	1.510567	3.012767
H	1.945063	1.79875	1.816763
H	1.837625	0.417161	3.000272
H	1.261319	1.569373	-2.017536
H	0.744138	-0.158622	-2.287907
H	-0.311543	0.965343	-1.343899
H	6.454523	-2.316542	-2.330616
H	6.157617	-2.676546	-0.58517
H	5.448585	-3.757179	-1.858475
H	4.324096	4.339711	-1.936196
H	5.45017	4.698531	-0.544481
H	6.116765	4.06723	-2.118671
H	3.911881	-1.987164	3.094446
C	-1.668819	-1.234356	0.825827
O	-1.597169	-1.162382	0.54207
H	4.05108	-1.860547	-2.70901
H	3.195612	-3.495549	-1.044782
C	-2.846501	-1.715666	0.001707
C	-4.145585	-1.024224	0.496025
O	-2.624781	-1.68067	-1.378134
H	-2.976932	-2.820308	0.230082
N	-4.239968	0.414629	0.446854
C	-5.320951	-1.690537	-0.186255
H	-4.189807	-1.287431	0.605962
H	-2.26375	-0.815812	-1.627002
C	-3.475288	1.34646	-0.217827
H	-4.934632	0.778638	1.06292
C	-5.606867	-1.43299	-1.530416
C	-6.703082	-2.042499	-2.139781
C	-7.516345	-2.909734	-1.410553
C	-7.230982	-3.169993	-0.070038
C	-6.138081	-2.559912	0.543894
H	-4.943538	-0.768862	-2.107536
O	-2.684167	1.05712	-1.140161
C	-3.685194	2.770707	0.185597
H	-6.922341	-1.840441	-3.198503
H	-8.380633	-3.390251	-1.892078
H	-7.86904	-3.856460	0.505531
H	-5.920599	-2.767174	1.602553
C	-3.858772	3.73075	-0.817136
C	-4.0424	5.068354	-0.469493
C	-4.044752	5.448293	0.872915
C	-3.861828	4.490735	1.871091
C	-3.684892	3.149795	1.531373
H	-3.836633	3.422556	-1.87422
H	-4.181355	0.823987	-1.256891

H	-4.187389	6.504908	1.145047
H	-3.855075	4.792084	2.929131
H	-3.529222	2.40134	2.323354

	E(RB+HF-PW91)	=	-2012.312295	
SCF	GIAO	Magnetic	shielding	tensor (ppm):
1	C	Isotropic=	109.3456	Anisotropy = 29.0303
XX=	98.3927	YX=	-0.2718	ZX= 13.8055
XY=	5.2328	YY=	105.1456	ZY= -0.2541
XZ=	8.752	YZ=	-1.0468	ZZ= 124.4985
Eigenvalues:	93.6294	105.7082	128.6991	
2	C	Isotropic=	112.1301	Anisotropy = 30.0088
XX=	94.5665	YX=	7.384	ZX= -5.6047
XY=	-0.6024	YY=	129.6691	ZY= -1.0854
XZ=	-4.8305	YZ=	-10.8738	ZZ= 112.1546
Eigenvalues:	93.0524	111.2019	132.1359	
3	C	Isotropic=	141.9659	Anisotropy = 20.277
XX=	121.1384	YX=	-4.7465	ZX= -2.4856
XY=	2.9582	YY=	152.4492	ZY= 2.582
XZ=	-1.2765	YZ=	3.4019	ZZ= 152.3101
Eigenvalues:	121.009	149.4048	155.4839	
4	C	Isotropic=	140.1229	Anisotropy = 24.8091
XX=	124.5358	YX=	1.5018	ZX= -0.8067
XY=	-12.0598	YY=	155.3429	ZY= 1.7039
XZ=	5.0215	YZ=	4.3728	ZZ= 140.49
Eigenvalues:	123.2656	140.4408	156.6623	
5	C	Isotropic=	-22.2741	Anisotropy = 179.8647
XX=	-59.935	YX=	28.0508	ZX= 19.2683
XY=	11.3592	YY=	-98.365	ZY= -27.9324
XZ=	12.1656	YZ=	-35.611	ZZ= 91.4777
Eigenvalues:	-112.8033	-51.6548	97.6357	
6	C	Isotropic=	101.858	Anisotropy = 40.9502
XX=	86.3352	YX=	-6.564	ZX= 0.2101
XY=	9.413	YY=	128.9514	ZY= 1.6631
XZ=	-4.5653	YZ=	3.4518	ZZ= 90.2874
Eigenvalues:	85.2441	91.1717	129.1581	
7	C	Isotropic=	44.4722	Anisotropy = 156.0023
XX=	38.9968	YX=	-13.1967	ZX= 18.0598
XY=	-37.7533	YY=	133.152	ZY= 53.1466
XZ=	26.5654	YZ=	40.083	ZZ= -38.7322
Eigenvalues:	-58.676	43.6189	148.4737	
8	C	Isotropic=	40.4055	Anisotropy = 157.5761
XX=	38.8576	YX=	-25.8262	ZX= 8.0077
XY=	-19.1851	YY=	112.4332	ZY= 62.3707
XZ=	-4.8249	YZ=	79.1819	ZZ= -30.0743
Eigenvalues:	-60.2912	36.0514	145.4562	
9	C	Isotropic=	110.6442	Anisotropy = 48.7566
XX=	126.106	YX=	12.7915	ZX= 21.7021
XY=	18.5065	YY=	109.9413	ZY= -3.7735
XZ=	23.7621	YZ=	-2.2429	ZZ= 95.8853
Eigenvalues:	80.0052	108.7788	143.1486	
10	C	Isotropic=	148.2377	Anisotropy = 41.7397
XX=	167.8707	YX=	2.2764	ZX= 13.8675
XY=	-0.6495	YY=	141.1623	ZY= -0.5366
XZ=	22.3285	YZ=	-10.5981	ZZ= 135.68

Eigenvalues:	125.6603	142.9886	176.0641		
11	C	Isotropic=	148.1159	Anisotropy	= 13.8394
XX=	143.2623	YX=	0.9566	ZX=	-2.2197
XY=	-13.3062	YY=	154.6229	ZY=	-3.5802
XZ=	-0.9766	YZ=	1.4854	ZZ=	146.4624
Eigenvalues:	140.0024	147.0031	157.3421		
12	C	Isotropic=	155.7499	Anisotropy	= 24.4342
XX=	166.0541	YX=	-3.5338	ZX=	-13.4628
XY=	1.6788	YY=	154.6891	ZY=	14.7375
XZ=	-5.7488	YZ=	8.6726	ZZ=	146.5066
Eigenvalues:	136.3136	158.8968	172.0394		
13	C	Isotropic=	148.321	Anisotropy	= 54.6207
XX=	145.6052	YX=	-21.6986	ZX=	-6.0531
XY=	-26.0714	YY=	147.8594	ZY=	23.1391
XZ=	-1.8983	YZ=	26.1193	ZZ=	151.4983
Eigenvalues:	115.7174	144.5108	184.7348		
14	C	Isotropic=	168.7407	Anisotropy	= 12.1619
XX=	164.9868	YX=	-9.2453	ZX=	1.0875
XY=	1.9214	YY=	168.4506	ZY=	-2.0089
XZ=	6.5978	YZ=	-4.671	ZZ=	172.7849
Eigenvalues:	162.386	166.9875	176.8487		
15	C	Isotropic=	169.2873	Anisotropy	= 17.19
XX=	174.3721	YX=	-3.6453	ZX=	-5.6722
XY=	-6.0899	YY=	176.2585	ZY=	1.7722
XZ=	-1.434	YZ=	0.9585	ZZ=	157.2314
Eigenvalues:	156.5159	170.5988	180.7473		
16	O	Isotropic=	262.855	Anisotropy	= 84.7125
XX=	313.1221	YX=	-15.6362	ZX=	21.945
XY=	-6.7118	YY=	202.1451	ZY=	44.392
XZ=	11.7957	YZ=	7.8408	ZZ=	273.2978
Eigenvalues:	191.4872	277.7478	319.33		
17	O	Isotropic=	265.7647	Anisotropy	= 45.4977
XX=	254.9686	YX=	22.1859	ZX=	-11.4174
XY=	-2.6539	YY=	250.8567	ZY=	-1.6098
XZ=	-12.8092	YZ=	-6.128	ZZ=	291.4688
Eigenvalues:	242.4249	258.7726	296.0965		
18	O	Isotropic=	-369.5855	Anisotropy	= 1094.5968
XX=	-974.65	YX=	-181.3978	ZX=	166.1686
XY=	-146.8337	YY=	-469.9159	ZY=	-69.7526
XZ=	95.1557	YZ=	-91.5167	ZZ=	335.8093
Eigenvalues:	-1031.1047	-437.7975	360.1456		
19	O	Isotropic=	94.6641	Anisotropy	= 127.7519
XX=	156.6963	YX=	112.9577	ZX=	-55.686
XY=	-4.521	YY=	21.7059	ZY=	31.8576
XZ=	-23.0516	YZ=	122.6476	ZZ=	105.5901
Eigenvalues:	-46.2176	150.3779	179.8321		
20	O	Isotropic=	71.5556	Anisotropy	= 191.0338
XX=	72.8424	YX=	-49.9228	ZX=	-27.2536
XY=	-46.7137	YY=	178.2541	ZY=	-32.1896
XZ=	-158.7392	YZ=	-76.8627	ZZ=	-36.4296
Eigenvalues:	-107.5128	123.2681	198.9115		
21	H	Isotropic=	31.1575	Anisotropy	= 13.4161
XX=	36.4209	YX=	3.4531	ZX=	-3.8832
XY=	3.023	YY=	33.896	ZY=	-3.7533
XZ=	-3.7556	YZ=	-2.7294	ZZ=	23.1554
Eigenvalues:	21.6654	31.7054	40.1015		

22	C	Isotropic=	21.4697	Anisotropy	=	77.8697
XX=	11.2178	YX=	-88.7573	ZX=	-6.0884	
XY=	-54.8984	YY=	-16.2156	ZY=	-3.9258	
XZ=	-17.0341	YZ=	-29.7365	ZZ=	69.407	
Eigenvalues:	-78.4233	69.4496	73.3828			
23	O	Isotropic=	-140.6745	Anisotropy	=	606.2609
XX=	-222.7598	YX=	-66.0745	ZX=	-317.6893	
XY=	-100.4731	YY=	-199.6163	ZY=	126.5319	
XZ=	-285.2639	YZ=	140.1718	ZZ=	0.3527	
Eigenvalues:	-432.9742	-252.5486	263.4995			
24	C	Isotropic=	165.813	Anisotropy	=	37.6291
XX=	155.2014	YX=	5.0516	ZX=	3.899	
XY=	3.8288	YY=	187.3452	ZY=	-9.6695	
XZ=	6.129	YZ=	-12.1655	ZZ=	154.8923	
Eigenvalues:	146.96	159.5798	190.899			
25	H	Isotropic=	27.4936	Anisotropy	=	2.9779
XX=	28.1598	YX=	0.2228	ZX=	-1.2805	
XY=	1.2806	YY=	28.5351	ZY=	0.26	
XZ=	-1.8072	YZ=	-0.4722	ZZ=	25.7859	
Eigenvalues:	25.0089	27.993	29.4789			
26	H	Isotropic=	28.1531	Anisotropy	=	8.5759
XX=	29.5185	YX=	-4.7175	ZX=	-1.4032	
XY=	-4.1915	YY=	28.4571	ZY=	1.2142	
XZ=	-0.7191	YZ=	1.5471	ZZ=	26.4837	
Eigenvalues:	24.4393	26.1496	33.8704			
27	H	Isotropic=	25.2959	Anisotropy	=	3.9517
XX=	26.0744	YX=	2.5603	ZX=	-1.1982	
XY=	1.2903	YY=	25.9291	ZY=	0.3545	
XZ=	1.9887	YZ=	-1.4277	ZZ=	23.8842	
Eigenvalues:	23.3111	24.6462	27.9304			
28	H	Isotropic=	25.1569	Anisotropy	=	7.0103
XX=	29.4168	YX=	-0.6281	ZX=	2.2017	
XY=	-0.1292	YY=	23.1304	ZY=	3.7063	
XZ=	1.1202	YZ=	1.7892	ZZ=	22.9234	
Eigenvalues:	20.0467	25.5935	29.8304			
29	H	Isotropic=	27.6393	Anisotropy	=	7.5355
XX=	32.1877	YX=	-0.209	ZX=	-1.492	
XY=	-1.0207	YY=	22.9143	ZY=	-4.418	
XZ=	-1.4632	YZ=	-2.4173	ZZ=	27.8159	
Eigenvalues:	21.0243	29.2306	32.663			
30	H	Isotropic=	29.6405	Anisotropy	=	5.6035
XX=	32.9944	YX=	-0.8372	ZX=	1.2017	
XY=	-1.2255	YY=	30.4403	ZY=	1.4825	
XZ=	0.7832	YZ=	2.0957	ZZ=	25.4868	
Eigenvalues:	24.7142	30.8311	33.3762			
31	H	Isotropic=	29.4483	Anisotropy	=	8.3676
XX=	31.498	YX=	-0.1307	ZX=	-3.3187	
XY=	-0.3886	YY=	25.7084	ZY=	2.3623	
XZ=	-3.6944	YZ=	0.9965	ZZ=	31.1384	
Eigenvalues:	25.1205	28.1977	35.0266			
32	H	Isotropic=	29.2896	Anisotropy	=	8.9856
XX=	28.8952	YX=	5.1859	ZX=	-0.8918	
XY=	4.83	YY=	31.1908	ZY=	-0.327	
XZ=	-0.5628	YZ=	-0.7184	ZZ=	27.7828	
Eigenvalues:	24.8843	27.7046	35.28			
33	H	Isotropic=	30.3318	Anisotropy	=	6.8111

XX=	31.9495	YX=	1.4777	ZX=	3.201				
XY=	1.3589	YY=	27.8025	ZY=	-1.2673				
XZ=	3.3128	YZ=	-1.812	ZZ=	31.2435				
Eigenvalues:	25.9523	30.1706	34.8726						
34	H	Isotropic=	30.2241	Anisotropy	=	9.0769			
XX=	29.6653	YX=	0.1029	ZX=	0.457				
XY=	1.1554	YY=	29.3127	ZY=	5.1349				
XZ=	1.8865	YZ=	5.6309	ZZ=	31.6942				
Eigenvalues:	24.9774	29.4195	36.2753						
35	H	Isotropic=	30.3592	Anisotropy	=	6.4227			
XX=	30.3948	YX=	-3.0192	ZX=	1.9974				
XY=	-2.7107	YY=	32.4197	ZY=	1.6973				
XZ=	-0.3438	YZ=	2.0958	ZZ=	28.2631				
Eigenvalues:	26.4694	29.9672	34.641						
36	H	Isotropic=	28.4832	Anisotropy	=	6.1925			
XX=	28.9232	YX=	0.5332	ZX=	-1.8656				
XY=	-0.3989	YY=	26.5351	ZY=	3.4662				
XZ=	-3.103	YZ=	1.4212	ZZ=	29.9913				
Eigenvalues:	24.8388	27.9993	32.6115						
37	H	Isotropic=	29.1523	Anisotropy	=	7.3196			
XX=	30.5474	YX=	0.9143	ZX=	0.8847				
XY=	2.2962	YY=	30.2262	ZY=	-5.3996				
XZ=	-0.0276	YZ=	-4.4551	ZZ=	26.6832				
Eigenvalues:	23.0005	30.4243	34.032						
38	H	Isotropic=	29.1122	Anisotropy	=	6.3303			
XX=	28.4462	YX=	0.0408	ZX=	0.6441				
XY=	0.8885	YY=	27.2322	ZY=	2.9997				
XZ=	1.5505	YZ=	2.6727	ZZ=	31.6582				
Eigenvalues:	25.8461	28.1581	33.3324						
39	H	Isotropic=	27.6158	Anisotropy	=	12.2847			
XX=	35.3788	YX=	-2.2458	ZX=	-2.6485				
XY=	-2.0429	YY=	23.735	ZY=	-3.637				
XZ=	0.0822	YZ=	-2.724	ZZ=	23.7338				
Eigenvalues:	20.1664	26.8755	35.8056						
40	H	Isotropic=	29.1959	Anisotropy	=	10.8522			
XX=	32.4078	YX=	0.9924	ZX=	-5.5754				
XY=	-0.7084	YY=	27.0744	ZY=	-0.6123				
XZ=	-5.9896	YZ=	0.3096	ZZ=	28.1056				
Eigenvalues:	24.0865	27.0706	36.4307						
41	H	Isotropic=	29.6527	Anisotropy	=	5.8534			
XX=	31.8275	YX=	-2.2266	ZX=	1.4423				
XY=	-2.8042	YY=	26.0466	ZY=	0.0737				
XZ=	1.4413	YZ=	-0.2907	ZZ=	31.0841				
Eigenvalues:	25.077	30.3261	33.555						
42	H	Isotropic=	30.4957	Anisotropy	=	9.6621			
XX=	29.0504	YX=	-1.5391	ZX=	-1.3564				
XY=	-1.4615	YY=	35.2328	ZY=	3.2063				
XZ=	-1.7013	YZ=	3.5305	ZZ=	27.2039				
Eigenvalues:	25.6945	28.8555	36.9371						
43	H	Isotropic=	29.1534	Anisotropy	=	5.4596			
XX=	30.497	YX=	0.7913	ZX=	2.0608				
XY=	-1.0102	YY=	30.6554	ZY=	-3.2633				
XZ=	3.0648	YZ=	-2.053	ZZ=	26.3077				
Eigenvalues:	24.2047	30.4624	32.7931						
44	H	Isotropic=	29.2952	Anisotropy	=	7.4852			
XX=	26.6402	YX=	0.7473	ZX=	1.0784				

XY=	2.6418	YY=	32.4024	ZY=	3.499				
XZ=	1.017	YZ=	1.689	ZZ=	28.843				
Eigenvalues:	26.1106	27.4897	34.2854						
45	H	Isotropic=	28.9664	Anisotropy	=	8.31			
XX=	30.3348	YX=	1.185	ZX=	-3.3531				
XY=	2.6844	YY=	27.9585	ZY=	-2.1039				
XZ=	-4.1185	YZ=	-2.0301	ZZ=	28.6059				
Eigenvalues:	25.5164	26.8764	34.5064						
46	H	Isotropic=	30.7493	Anisotropy	=	18.215			
XX=	37.5258	YX=	-5.5324	ZX=	6.8474				
XY=	-3.5949	YY=	24.702	ZY=	-4.9627				
XZ=	5.3324	YZ=	-3.1536	ZZ=	30.02				
Eigenvalues:	22.3757	26.9795	42.8926						
47	C	Isotropic=	10.059	Anisotropy	=	92.9366			
XX=	-56.9304	YX=	-51.1767	ZX=	-5.664				
XY=	-46.4931	YY=	53.3639	ZY=	3.5148				
XZ=	37.9118	YZ=	13.486	ZZ=	33.7435				
Eigenvalues:	-78.3649	36.5252	72.0167						
48	O	Isotropic=	-86.5357	Anisotropy	=	607.8085			
XX=	-171.5838	YX=	-172.9251	ZX=	-7.6126				
XY=	-182.4853	YY=	253.8808	ZY=	-3.4702				
XZ=	37.5599	YZ=	-17.1555	ZZ=	-341.9041				
Eigenvalues:	-343.2751	-235.0023	18.67						
49	H	Isotropic=	28.6754	Anisotropy	=	6.4758			
XX=	28.1365	YX=	-2.5669	ZX=	-0.2571				
XY=	-2.1317	YY=	24.9436	ZY=	0.0726				
XZ=	1.2009	YZ=	0.5209	ZZ=	32.946				
Eigenvalues:	23.6744	29.3591	32.9925						
50	H	Isotropic=	29.4823	Anisotropy	=	6.5627			
XX=	27.7777	YX=	0.7684	ZX=	-1.3702				
XY=	0.8277	YY=	32.4258	ZY=	2.2843				
XZ=	-1.3938	YZ=	3.3822	ZZ=	28.2434				
Eigenvalues:	25.6303	28.9591	33.8574						
51	C	Isotropic=	110.8729	Anisotropy	=	26.5443			
XX=	113.2676	YX=	-5.3712	ZX=	5.5421				
XY=	-6.4758	YY=	91.7674	ZY=	-5.9797				
XZ=	-5.5391	YZ=	-5.6813	ZZ=	127.5838				
Eigenvalues:	89.4065	114.6431	128.5691						
52	C	Isotropic=	122.836	Anisotropy	=	18.3225			
XX=	122.3541	YX=	13.7853	ZX=	8.6623				
XY=	6.8801	YY=	126.4622	ZY=	-6.2964				
XZ=	8.6705	YZ=	-5.2017	ZZ=	119.6915				
Eigenvalues:	106.0209	127.4361	135.051						
53	O	Isotropic=	285.2945	Anisotropy	=	65.6682			
XX=	284.9143	YX=	17.9959	ZX=	-18.6832				
XY=	19.5906	YY=	316.573	ZY=	-26.5617				
XZ=	-5.8113	YZ=	1.1577	ZZ=	254.396				
Eigenvalues:	249.4879	277.3222	329.0733						
54	H	Isotropic=	26.375	Anisotropy	=	4.4724			
XX=	26.5855	YX=	0.3637	ZX=	0.0049				
XY=	-1.1347	YY=	27.6391	ZY=	-2.6405				
XZ=	-1.0048	YZ=	-2.8892	ZZ=	24.9003				
Eigenvalues:	23.0721	26.6963	29.3566						
55	N	Isotropic=	121.6976	Anisotropy	=	90.5686			
XX=	113.2023	YX=	56.041	ZX=	39.5446				
XY=	41.4756	YY=	134.6925	ZY=	-26.4132				

XZ=	45.3701	YZ=	-78.3332	ZZ=	117.1981				
Eigenvalues:	25.7862	157.2299			182.0767				
56	C	Isotropic=	50.833	Anisotropy	=	185.9622			
XX=	35.4892	YX=	-91.6023	ZX=	-33.1876				
XY=	-84.4051	YY=	108.8484	ZY=	12.6472				
XZ=	-40.0385	YZ=	21.803	ZZ=	8.1614				
Eigenvalues:	-34.9367	12.628		174.8078					
57	H	Isotropic=	26.0326	Anisotropy	=	6.7743			
XX=	24.5608	YX=	2.6496	ZX=	-0.566				
XY=	1.9792	YY=	24.9837	ZY=	-2.8739				
XZ=	-0.7316	YZ=	-2.6217	ZZ=	28.5534				
Eigenvalues:	22.0889	25.4602		30.5489					
58	H	Isotropic=	26.8283	Anisotropy	=	18.0086			
XX=	23.6039	YX=	7.1606	ZX=	-1.9922				
XY=	6.6208	YY=	33.6165	ZY=	-5.1319				
XZ=	-2.5974	YZ=	-4.0998	ZZ=	23.2644				
Eigenvalues:	20.0913	21.5595		38.8341					
59	C	Isotropic=	16.0795	Anisotropy	=	120.5509			
XX=	45.3663	YX=	-31.3722	ZX=	47.0695				
XY=	-17.3782	YY=	-59.402	ZY=	-2.1253				
XZ=	33.8695	YZ=	5.8623	ZZ=	62.2742				
Eigenvalues:	-65.7672	17.559		96.4468					
60	H	Isotropic=	26.2943	Anisotropy	=	8.4232			
XX=	23.8026	YX=	3.5813	ZX=	-5.5239				
XY=	-0.0982	YY=	31.4721	ZY=	2.1094				
XZ=	-2.5672	YZ=	0.8921	ZZ=	23.6083				
Eigenvalues:	19.23	27.7432		31.9098					
61	C	Isotropic=	58.7017	Anisotropy	=	179.8834			
XX=	62.1611	YX=	-90.0906	ZX=	-0.3285				
XY=	-88.0286	YY=	90.2192	ZY=	60.3644				
XZ=	5.5429	YZ=	55.7544	ZZ=	23.7247				
Eigenvalues:	-41.7272	39.2083		178.624					
62	C	Isotropic=	62.1963	Anisotropy	=	174.6095			
XX=	90.1228	YX=	-54.7305	ZX=	-33.9036				
XY=	-54.842	YY=	122.4866	ZY=	42.9424				
XZ=	-36.2228	YZ=	43.7551	ZZ=	-26.0206				
Eigenvalues:	-41.237	49.2232		178.6026					
63	C	Isotropic=	64.2689	Anisotropy	=	174.5061			
XX=	41.5577	YX=	-86.9509	ZX=	-49.1351				
XY=	-91.3142	YY=	108.5314	ZY=	10.0149				
XZ=	-50.9572	YZ=	10.4617	ZZ=	42.7175				
Eigenvalues:	-37.1777	49.378		180.6063					
64	C	Isotropic=	63.2316	Anisotropy	=	171.0612			
XX=	63.4477	YX=	-87.4105	ZX=	5.5305				
XY=	-88.7281	YY=	90.7188	ZY=	55.7932				
XZ=	7.8765	YZ=	56.6098	ZZ=	35.5282				
Eigenvalues:	-38.1431	50.5655		177.2723					
65	C	Isotropic=	64.1702	Anisotropy	=	148.1743			
XX=	87.7006	YX=	-45.7609	ZX=	-30.2084				
XY=	-35.1776	YY=	122.3843	ZY=	38.6721				
XZ=	-30.7727	YZ=	41.0062	ZZ=	-17.5743				
Eigenvalues:	-31.5723	61.1298		162.9531					
66	H	Isotropic=	22.7973	Anisotropy	=	10.6724			
XX=	24.8667	YX=	2.5229	ZX=	5.5912				
XY=	1.0728	YY=	19.3351	ZY=	-0.4184				
XZ=	4.7544	YZ=	0.8127	ZZ=	24.1899				

Eigenvalues: 18.1598 20.3198 29.9122
 67 O Isotropic= -58.4801 Anisotropy = 572.8876
 XX= -30.2693 YX= -33.6038 ZX= 350.5005
 XY= -42.5073 YY= -142.3154 ZY= -33.8291
 XZ= 316.476 YZ= -42.5394 ZZ= -2.8557
 Eigenvalues: -350.3374 -148.5483 23.4449
 68 C Isotropic= 55.8777 Anisotropy = 171.1815
 XX= 161.1205 YX= 37.1112 ZX= -31.3895
 XY= 26.1876 YY= -17.105 ZY= -21.0441
 XZ= -7.6014 YZ= -15.3802 ZZ= 23.6175
 Eigenvalues: -27.0161 24.6504 169.9987
 69 H Isotropic= 23.7016 Anisotropy = 5.6767
 XX= 25.0495 YX= 3.4279 ZX= 1.4932
 XY= 3.0938 YY= 22.488 ZY= -0.3182
 XZ= 1.1524 YZ= -0.373 ZZ= 23.5674
 Eigenvalues: 19.9615 23.6573 27.4861
 70 H Isotropic= 23.794 Anisotropy = 3.4374
 XX= 23.7017 YX= 2.4713 ZX= 0.5258
 XY= 1.9878 YY= 22.3585 ZY= -1.4721
 XZ= 0.3347 YZ= -1.4555 ZZ= 25.3217
 Eigenvalues: 20.2899 25.0066 26.0856
 71 H Isotropic= 23.8846 Anisotropy = 4.5055
 XX= 24.3951 YX= 2.6438 ZX= 1.5429
 XY= 2.5999 YY= 22.3175 ZY= -0.3242
 XZ= 1.6236 YZ= -0.3922 ZZ= 24.9411
 Eigenvalues: 20.2243 24.5412 26.8882
 72 H Isotropic= 24.1124 Anisotropy = 8.1339
 XX= 26.3652 YX= 4.5287 ZX= -0.6125
 XY= 4.034 YY= 23.3595 ZY= -0.8581
 XZ= -0.4146 YZ= -1.0327 ZZ= 22.6125
 Eigenvalues: 20.2264 22.5758 29.535
 73 C Isotropic= 60.6028 Anisotropy = 176.528
 XX= 174.9469 YX= 22.7958 ZX= -1.5623
 XY= 18.9163 YY= 42.4069 ZY= -18.8526
 XZ= -3.7874 YZ= -17.2256 ZZ= -35.5453
 Eigenvalues: -39.5341 43.0545 178.2882
 74 C Isotropic= 61.7866 Anisotropy = 177.0576
 XX= 175.5615 YX= 26.5359 ZX= -12.183
 XY= 25.8329 YY= 10.295 ZY= 39.8673
 XZ= -12.8631 YZ= 43.2156 ZZ= -0.4968
 Eigenvalues: -40.3141 45.8488 179.8249
 75 C Isotropic= 60.9188 Anisotropy = 180.402
 XX= 176.9681 YX= 28.6567 ZX= -2.1254
 XY= 29.8429 YY= -32.3193 ZY= -21.4981
 XZ= -2.8927 YZ= -21.5779 ZZ= 38.1075
 Eigenvalues: -41.8533 43.4228 181.1868
 76 C Isotropic= 63.0908 Anisotropy = 176.2855
 XX= 178.2641 YX= 15.1814 ZX= -4.2389
 XY= 18.238 YY= 43.6907 ZY= -21.2325
 XZ= -6.2591 YZ= -25.0231 ZZ= -32.6825
 Eigenvalues: -39.1417 47.7995 180.6144
 77 C Isotropic= 66.0237 Anisotropy = 166.2468
 XX= 172.7524 YX= 22.3896 ZX= -16.624
 XY= 24.7169 YY= 18.4827 ZY= 42.1054
 XZ= -14.4596 YZ= 34.9085 ZZ= 6.836
 Eigenvalues: -29.9332 51.1494 176.8549

78	H	Isotropic=	23.317	Anisotropy	=	8.0322
XX=	20.2435	YX=	-2.1257	ZX=	0.3563	
XY=	-1.3496	YY=	27.6505	ZY=	-2.0924	
XZ=	0.4794	YZ=	-1.9177	ZZ=	22.0572	
Eigenvalues:	19.8556	21.4237	28.6719			
79	H	Isotropic=	23.7493	Anisotropy	=	4.4539
XX=	20.567	YX=	-1.0318	ZX=	0.082	
XY=	-0.9683	YY=	26.1315	ZY=	0.796	
XZ=	-0.0619	YZ=	1.1264	ZZ=	24.5493	
Eigenvalues:	20.3851	24.1441	26.7185			
80	H	Isotropic=	23.6798	Anisotropy	=	3.5651
XX=	20.5889	YX=	-1.0707	ZX=	0.3415	
XY=	-0.8126	YY=	24.6312	ZY=	-0.502	
XZ=	0.1723	YZ=	-0.4761	ZZ=	25.8192	
Eigenvalues:	20.3763	24.6065	26.0565			
81	H	Isotropic=	23.825	Anisotropy	=	5.1475
XX=	20.5345	YX=	-1.3811	ZX=	0.1295	
XY=	-1.1561	YY=	27.0122	ZY=	0.2336	
XZ=	-0.0687	YZ=	0.038	ZZ=	23.9284	
Eigenvalues:	20.294	23.9243	27.2567			
82	H	Isotropic=	23.7891	Anisotropy	=	7.9903
XX=	20.505	YX=	-0.984	ZX=	-0.1059	
XY=	-0.8852	YY=	26.5856	ZY=	3.7638	
XZ=	-0.3963	YZ=	3.0334	ZZ=	24.2767	
Eigenvalues:	20.3337	21.9175	29.116			

2a-iii

C	3.29464	1.844636	-0.010896
C	4.074777	1.717942	1.33581
C	3.659815	0.539616	2.232743
C	4.74234	-0.546144	2.370641
C	5.162743	-1.220369	1.049343
C	4.085142	-1.666454	0.073165
C	3.239062	-0.555007	-0.477047
C	1.892468	-0.648698	-0.324037
C	1.073275	0.605514	-0.454464
C	1.771509	1.806004	0.189171
C	3.771335	0.75302	-1.019975
C	5.276692	0.843286	-1.212799
C	3.15373	1.03308	-2.402893
C	1.160075	-1.888251	0.01959
C	5.955496	-0.027621	3.108783
O	3.54029	3.148535	-0.534937
O	3.967472	2.940469	2.049059
O	6.335565	-1.568450	0.893305
O	4.483741	-2.632729	-0.894063
O	-0.167577	0.367992	0.254583
H	3.039683	3.206583	2.043732
C	5.641236	-2.595806	-1.624746
O	6.405222	-1.639268	-1.556414
C	5.784762	-3.83094	-2.452544
H	5.179636	1.653853	1.113835
H	2.716264	0.06675	1.86192
H	3.414188	-2.323245	0.7299
H	0.820286	0.816701	-1.531834

H	1.324563	2.740183	-0.252135
H	1.537244	1.810665	1.286153
H	5.861854	0.440061	-0.355107
H	5.58265	0.271146	-2.124102
H	5.567694	1.911353	-1.371237
H	3.946732	1.260911	-3.156554
H	2.579396	0.150485	-2.771779
H	2.47867	1.9228	-2.360114
H	1.693653	-2.796546	-0.35559
H	1.033778	-1.965999	1.129434
H	0.13895	-1.871622	-0.439229
H	6.686015	-0.856567	3.276228
H	6.469645	0.770722	2.521529
H	5.650493	0.394758	4.096118
H	4.842755	-4.429551	-2.45269
H	6.043095	-3.53564	-3.498313
H	6.614915	-4.446853	-2.027319
H	4.460306	3.375214	-0.349281
C	-1.203557	1.227359	0.024893
O	-1.060718	2.138028	-0.789653
H	4.284981	-1.381705	2.978009
H	3.457493	0.944447	3.260732
C	-2.432814	0.853562	0.834906
C	-3.633876	0.659448	-0.153442
O	-2.18077	-0.258991	1.656702
H	-2.655508	1.694422	1.554199
N	-4.596079	-0.304189	0.319645
C	-4.254354	2.016775	-0.401078
H	-3.210578	0.264198	-1.130147
H	-1.952036	-1.005467	1.085323
C	-4.901056	-1.451282	-0.394458
H	-5.192233	-0.025221	0.62124
C	-5.054592	0.633096	0.567473
C	-5.638678	3.871897	0.308475
C	-5.425227	4.504032	-0.916696
C	-4.621406	3.896756	-1.88065
C	-4.038607	2.655313	-1.626655
H	-5.216261	2.154705	1.54505
O	-4.171034	-1.841676	-1.327133
C	-6.098822	-2.218706	0.049931
H	-6.266102	4.352095	1.073643
H	-5.886641	5.481685	-1.119472
H	-4.442201	4.396552	-2.844212
H	-3.388747	2.187963	-2.383137
C	-5.985167	-3.603751	0.212767
C	-7.093619	-4.346355	0.617224
C	-8.313525	-3.711324	0.851476
C	-8.427658	-2.331403	0.67993
C	-7.32134	-1.581235	0.282487
H	-5.022579	-4.097676	0.00719
H	-7.004742	-5.435153	0.747087
H	-9.18776	-4.299571	1.168305
H	-9.391959	-1.832380	0.856499
H	-7.421371	-0.494931	0.137543

2aiiiliz E(RB+HF-PW91) = -2012.30447

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic= 109.4059 Anisotropy 28.2154
 XX= 100.1682 YX= 12.0388 ZX= -9.1252
 XY= 4.8596 YY= 117.5968 ZY= -7.951
 XZ= -9.6517 YZ= -8.1229 ZZ= 110.4527
 Eigenvalues: 94.0413 105.9602 128.2162

2 C Isotropic= 112.1617 Anisotropy 30.3646
 XX= 94.4415 YX= -8.9996 ZX= -3.8343
 XY= -3.7792 YY= 124.3919 ZY= 14.8592
 XZ= 1.7892 YZ= 5.0114 ZZ= 117.6516
 Eigenvalues: 93.0901 110.9902 132.4048

3 C Isotropic= 142.4254 Anisotropy 20.5248
 XX= 121.2696 YX= 1.4055 ZX= 2.5018
 XY= -2.4357 YY= 150.1139 ZY= -1.5732
 XZ= -4.2472 YZ= -0.6082 ZZ= 155.8927
 Eigenvalues: 121.2374 149.9302 156.1086

4 C Isotropic= 139.9907 Anisotropy 25.1132
 XX= 124.3149 YX= -1.8003 ZX= -2.831
 XY= 11.1952 YY= 142.0765 ZY= 5.3246
 XZ= 5.1549 YZ= 7.5253 ZZ= 153.5806
 Eigenvalues: 123.1428 140.0963 156.7328

5 C Isotropic= -22.1128 Anisotropy 178.8185
 XX= -55.8597 YX= 6.0522 ZX= -36.3724
 XY= 9.8743 YY= 55.223 ZY= -75.3542
 XZ= -18.2149 YZ= -83.6449 ZZ= -65.7018
 Eigenvalues: -113.019 -50.419 97.0995

6 C Isotropic= 101.9272 Anisotropy 41.0279
 XX= 86.3689 YX= 3.3926 ZX= 3.1507
 XY= -9.5069 YY= 101.7348 ZY= 16.2609
 XZ= -6.3381 YZ= 19.0312 ZZ= 117.6779
 Eigenvalues: 85.5559 90.9465 129.2791

7 C Isotropic= 43.351 Anisotropy 158.1343
 XX= 36.3714 YX= 17.1219 ZX= -4.3665
 XY= 37.958 YY= -25.0528 ZY= 77.549
 XZ= 10.3082 YZ= 62.4994 ZZ= 118.7343
 Eigenvalues: -59.7628 41.0419 148.7738

8 C Isotropic= 42.2306 Anisotropy 154.566
 XX= 40.7667 YX= 13.2419 ZX= 9.6224
 XY= 0.24 YY= -46.7517 ZY= 36.5864
 XZ= 12.7612 YZ= 55.4364 ZZ= 132.6768
 Eigenvalues: -58.0198 39.4369 145.2746

9 C Isotropic= 111.2401 Anisotropy 47.4981
 XX= 129.3553 YX= 8.9513 ZX= -21.5504
 XY= 7.5756 YY= 104.5351 ZY= 8.2141
 XZ= -26.33 YZ= 10.7986 ZZ= 99.8298
 Eigenvalues: 80.1948 110.62 142.9055

10 C Isotropic= 148.6101 Anisotropy 41.5522
 XX= 170.2677 YX= 8.5282 ZX= -7.8176
 XY= 17.0899 YY= 142.4537 ZY= 11.0723
 XZ= -10.8169 YZ= 0.5979 ZZ= 133.1088
 Eigenvalues: 125.6475 143.8711 176.3116

11 C Isotropic= 147.8305 Anisotropy 13.7506
 XX= 141.9452 YX= -2.7061 ZX= -0.5978
 XY= 6.6955 YY= 150.0135 ZY= 2.2617
 XZ= 10.6746 YZ= 6.4805 ZZ= 151.5326

Eigenvalues:	139.783	146.7109	156.9975		
12	C	Isotropic=	155.5048	Anisotropy	24.8648
XX=	164.8203	YX=	-9.255	ZX=	10.7343
XY=	-6.6491	YY=	137.9297	ZY=	2.5737
XZ=	2.4039	YZ=	-3.7284	ZZ=	163.7644
Eigenvalues:	135.7023	158.7307	172.0814		
13	C	Isotropic=	147.9335	Anisotropy	55.221
XX=	143.0051	YX=	7.7024	ZX=	18.7077
XY=	14.0883	YY=	125.5229	ZY=	-10.3004
XZ=	20.496	YZ=	-7.7386	ZZ=	175.2724
Eigenvalues:	115.2153	143.8376	184.7475		
14	C	Isotropic=	167.8505	Anisotropy	13.2745
XX=	164.4086	YX=	6.247	ZX=	5.7308
XY=	4.1507	YY=	174.436	ZY=	0.1293
XZ=	-5.3199	YZ=	-2.0715	ZZ=	164.7068
Eigenvalues:	162.0747	164.7766	176.7001		
15	C	Isotropic=	169.3977	Anisotropy	17.0481
XX=	173.5841	YX=	-3.3858	ZX=	6.5867
XY=	1.2158	YY=	162.8199	ZY=	9.1242
XZ=	6.1096	YZ=	8.254	ZZ=	171.7891
Eigenvalues:	156.4107	171.0194	180.7631		
16	O	Isotropic=	263.0114	Anisotropy	84.8041
XX=	314.4329	YX=	28.8236	ZX=	2.7512
XY=	12.5242	YY=	222.6256	ZY=	-22.7421
XZ=	2.6354	YZ=	-58.4781	ZZ=	251.9757
Eigenvalues:	191.3258	278.1609	319.5475		
17	O	Isotropic=	265.3697	Anisotropy	45.2027
XX=	254.0902	YX=	-20.5085	ZX=	-11.753
XY=	-7.6078	YY=	281.245	ZY=	-15.4746
XZ=	9.3501	YZ=	-21.6283	ZZ=	260.774
Eigenvalues:	242.4077	258.1966	295.5049		
18	O	Isotropic=	-371.699	Anisotropy	1097.5295
XX=	-971.9124	YX=	288.8206	ZX=	-5.5758
XY=	211.7707	YY=	120.7558	ZY=	-338.3098
XZ=	8.7751	YZ=	-354.8676	ZZ=	-263.9403
Eigenvalues:	-1034.9315	-440.1528	359.9873		
19	O	Isotropic=	95.062	Anisotropy	127.8607
XX=	157.4363	YX=	-113.1922	ZX=	-59.8948
XY=	-11.9045	YY=	6.9227	ZY=	-107.8493
XZ=	18.0772	YZ=	-25.7407	ZZ=	120.8269
Eigenvalues:	-45.1444	150.0279	180.3024		
20	O	Isotropic=	74.0708	Anisotropy	179.9167
XX=	66.8065	YX=	2.2371	ZX=	54.9744
XY=	-108.2734	YY=	101.0046	ZY=	126.4634
XZ=	127.6244	YZ=	94.6064	ZZ=	54.4012
Eigenvalues:	-100.6055	128.8025	194.0152		
21	H	Isotropic=	31.1837	Anisotropy	13.6142
XX=	36.3304	YX=	-5.9672	ZX=	0.3186
XY=	-5.3343	YY=	30.1894	ZY=	5.2404
XZ=	0.6057	YZ=	6.2112	ZZ=	27.0313
Eigenvalues:	21.5952	31.696	40.2598		
22	C	Isotropic=	21.5005	Anisotropy	79.0807
XX=	3.5923	YX=	51.7157	ZX=	75.3893
XY=	21.1687	YY=	55.3186	ZY=	-22.6325
XZ=	53.6892	YZ=	-45.9264	ZZ=	5.5906
Eigenvalues:	-78.6337	68.9142	74.2209		

23	O	Isotropic=	-141.113	Anisotropy	607.0701
XX=	-261.9969	YX=	-208.4589	ZX=	220.4273
XY=	-160.2318	YY=	-187.7559	ZY=	-159.366
XZ=	229.9329	YZ=	-149.2125	ZZ=	26.4138
Eigenvalues:	-433.3396		-253.5998		263.6004
24	C	Isotropic=	165.5947	Anisotropy	38.0087
XX=	155.8763	YX=	-0.4184	ZX=	-6.605
XY=	1.7957	YY=	176.5316	ZY=	20.4904
XZ=	-6.6431	YZ=	17.9338	ZZ=	164.3761
Eigenvalues:	146.6262		159.224		190.9338
25	H	Isotropic=	27.486	Anisotropy	3.0181
XX=	28.0283	YX=	-1.389	ZX=	0.5332
XY=	-2.2741	YY=	26.883	ZY=	1.4761
XZ=	0.0744	YZ=	0.8668	ZZ=	27.5469
Eigenvalues:	25.0262	27.9338	29.4981		
26	H	Isotropic=	28.1843	Anisotropy	8.2316
XX=	29.0904	YX=	1.3372	ZX=	4.3568
XY=	1.7033	YY=	25.8182	ZY=	0.3155
XZ=	3.7376	YZ=	0.6465	ZZ=	29.6443
Eigenvalues:	24.6585	26.2223	33.672		
27	H	Isotropic=	25.3291	Anisotropy	4.1255
XX=	26.0788	YX=	-2.5347	ZX=	-1.6437
XY=	0.629	YY=	25.3656	ZY=	2.1182
XZ=	-2.1017	YZ=	0.1133	ZZ=	24.5428
Eigenvalues:	23.194	24.7139	28.0794		
28	H	Isotropic=	25.001	Anisotropy	6.6808
XX=	29.1978	YX=	0.4503	ZX=	-1.5026
XY=	0.1714	YY=	20.2019	ZY=	0.1758
XZ=	-0.3748	YZ=	-1.7821	ZZ=	25.6033
Eigenvalues:	20.0817	25.4665	29.4548		
29	H	Isotropic=	27.7865	Anisotropy	8.3193
XX=	32.5636	YX=	-1.7119	ZX=	1.4215
XY=	-0.431	YY=	29.2005	ZY=	-2.4136
XZ=	2.506	YZ=	-0.5403	ZZ=	21.5953
Eigenvalues:	21.0522	28.9745	33.3327		
30	H	Isotropic=	29.6864	Anisotropy	5.7716
XX=	33.3096	YX=	0.7309	ZX=	0.0295
XY=	1.0902	YY=	25.2581	ZY=	1.6333
XZ=	0.7024	YZ=	2.0945	ZZ=	30.4915
Eigenvalues:	24.5961	30.929	33.5341		
31	H	Isotropic=	29.4378	Anisotropy	8.321
XX=	30.9793	YX=	-2.5638	ZX=	1.9847
XY=	-2.6715	YY=	27.7719	ZY=	-2.6729
XZ=	2.4808	YZ=	-3.9994	ZZ=	29.5622
Eigenvalues:	25.0924	28.2359	34.9851		
32	H	Isotropic=	29.2394	Anisotropy	9.0861
XX=	29.0037	YX=	-4.0753	ZX=	-3.764
XY=	-3.4627	YY=	29.5994	ZY=	1.8236
XZ=	-3.4916	YZ=	1.3332	ZZ=	29.1151
Eigenvalues:	24.6489	27.7725	35.2968		
33	H	Isotropic=	30.3025	Anisotropy	6.7344
XX=	32.3334	YX=	1.6134	ZX=	-2.9138
XY=	1.8642	YY=	31.3987	ZY=	-0.7567
XZ=	-2.7717	YZ=	-1.3439	ZZ=	27.1753
Eigenvalues:	25.9028	30.2126	34.7921		
34	H	Isotropic=	30.1054	Anisotropy	9.2414

XX=	29.6032	YX=	-0.04	ZX=	-0.9786		
XY=	0.8549	YY=	25.6462	ZY=	-2.9869		
XZ=	-2.361	YZ=	-2.5626	ZZ=	35.0668		
Eigenvalues:	24.8892	29.1606	36.2664				
35	H	Isotropic=	30.193	Anisotropy		6.1164	
XX=	29.5265	YX=	2.5251	ZX=	0.6552		
XY=	0.9615	YY=	27.9637	ZY=	1.2974		
XZ=	2.2538	YZ=	1.7176	ZZ=	33.0888		
Eigenvalues:	26.7915	29.5169	34.2706				
36	H	Isotropic=	28.4223	Anisotropy		6.3885	
XX=	28.6104	YX=	-2.3723	ZX=	0.1457		
XY=	-2.3749	YY=	26.4718	ZY=	-1.5755		
XZ=	2.0759	YZ=	-3.636	ZZ=	30.1847		
Eigenvalues:	24.4149	28.1707	32.6813				
37	H	Isotropic=	28.9032	Anisotropy		7.836	
XX=	30.1821	YX=	-0.0126	ZX=	-1.7944		
XY=	-1.7001	YY=	32.7381	ZY=	2.6203		
XZ=	-1.4427	YZ=	3.5005	ZZ=	23.7895		
Eigenvalues:	22.6174	29.9651	34.1273				
38	H	Isotropic=	29.0059	Anisotropy		6.5515	
XX=	28.5572	YX=	0.5765	ZX=	-1.7448		
XY=	0.6897	YY=	27.4968	ZY=	-2.7102		
XZ=	-2.2045	YZ=	-2.8606	ZZ=	30.9637		
Eigenvalues:	25.8698	27.7742	33.3736				
39	H	Isotropic=	28.8059	Anisotropy		7.9903	
XX=	33.7803	YX=	-0.5295	ZX=	1.7089		
XY=	0.7395	YY=	29.5529	ZY=	0.7461		
XZ=	2.1266	YZ=	1.4558	ZZ=	23.0845		
Eigenvalues:	22.5875	29.6974	34.1328				
40	H	Isotropic=	29.1775	Anisotropy		10.8334	
XX=	31.753	YX=	-5.2363	ZX=	2.6492		
XY=	-4.4388	YY=	28.0526	ZY=	-1.2594		
XZ=	4.3735	YZ=	-0.3582	ZZ=	27.7268		
Eigenvalues:	24.0609	27.0717	36.3997				
41	H	Isotropic=	29.6501	Anisotropy		5.8277	
XX=	31.7731	YX=	2.5052	ZX=	1.0695		
XY=	2.9459	YY=	29.3136	ZY=	-2.007		
XZ=	1.5803	YZ=	-2.4195	ZZ=	27.8636		
Eigenvalues:	25.1253	30.2898	33.5352				
42	H	Isotropic=	30.5045	Anisotropy		9.6524	
XX=	28.8109	YX=	-0.5237	ZX=	1.5797		
XY=	-0.665	YY=	26.7937	ZY=	2.5533		
XZ=	1.7454	YZ=	2.9718	ZZ=	35.909		
Eigenvalues:	25.6696	28.9045	36.9394				
43	H	Isotropic=	29.0461	Anisotropy		5.5827	
XX=	30.3404	YX=	1.1225	ZX=	-1.7652		
XY=	2.9922	YY=	30.3312	ZY=	2.5255		
XZ=	-0.7107	YZ=	3.5373	ZZ=	26.4666		
Eigenvalues:	24.0939	30.2765	32.7679				
44	H	Isotropic=	29.1707	Anisotropy		7.6376	
XX=	26.5239	YX=	0.4595	ZX=	-1.6691		
XY=	-0.7943	YY=	27.598	ZY=	1.787		
XZ=	-3.0869	YZ=	0.0511	ZZ=	33.3904		
Eigenvalues:	25.7732	27.4765	34.2625				
45	H	Isotropic=	28.8893	Anisotropy		8.2276	
XX=	29.8916	YX=	-3.3716	ZX=	1.1503		

XY=	-4.9091	YY=	30.4939	ZY=	0.0212		
XZ=	0.4899	YZ=	0.1544	ZZ=	26.2826		
Eigenvalues:	25.4793	26.8143	34.3744				
46	H	Isotropic=	30.7449	Anisotropy	18.1805		
XX=	37.9428	YX=	8.4824	ZX=	1.141		
XY=	6.3761	YY=	31.6385	ZY=	-1.8676		
XZ=	0.7382	YZ=	0.091	ZZ=	22.6533		
Eigenvalues:	22.2911	27.0783	42.8652				
47	C	Isotropic=	10.0151	Anisotropy	92.4597		
XX=	-58.54	YX=	30.8308	ZX=	35.6544		
XY=	64.0638	YY=	28.566	ZY=	2.2518		
XZ=	5.035	YZ=	12.4598	ZZ=	60.0194		
Eigenvalues:	-81.1525	39.5429	71.6549				
48	O	Isotropic=	-99.4228	Anisotropy	606.2525		
XX=	-181.0925	YX=	90.4275	ZX=	135.3447		
XY=	111.5938	YY=	-143.0789	ZY=	313.4483		
XZ=	127.1311	YZ=	276.6049	ZZ=	25.9031		
Eigenvalues:	-365.4943	-237.5196	304.7456				
49	H	Isotropic=	28.6865	Anisotropy	6.5445		
XX=	27.973	YX=	1.5421	ZX=	1.925		
XY=	2.4635	YY=	29.8598	ZY=	-4.0346		
XZ=	0.9703	YZ=	-3.6137	ZZ=	28.2269		
Eigenvalues:	23.766	29.2441	33.0495				
50	H	Isotropic=	29.4737	Anisotropy	6.5279		
XX=	27.8111	YX=	-1.8297	ZX=	-0.263		
XY=	-1.6394	YY=	27.0004	ZY=	0.4968		
XZ=	-0.2904	YZ=	1.6115	ZZ=	33.6096		
Eigenvalues:	25.5698	29.0256	33.8257				
51	C	Isotropic=	109.6116	Anisotropy	37.4764		
XX=	107.1578	YX=	-13.3584	ZX=	18.9872		
XY=	-1.7223	YY=	117.9629	ZY=	-12.2496		
XZ=	9.3877	YZ=	-16.9848	ZZ=	103.7141		
Eigenvalues:	89.4438	104.7951	134.5959				
52	C	Isotropic=	126.6676	Anisotropy	29.0305		
XX=	130.0014	YX=	0.0438	ZX=	6.3463		
XY=	3.6285	YY=	128.3061	ZY=	-19.3874		
XZ=	6.8109	YZ=	-21.0324	ZZ=	121.6952		
Eigenvalues:	103.083	130.8985	146.0212				
53	O	Isotropic=	280.6411	Anisotropy	49.8281		
XX=	289.6648	YX=	-12.6322	ZX=	-1.7967		
XY=	-10.0587	YY=	282.3396	ZY=	22.7242		
XZ=	-6.6775	YZ=	40.5872	ZZ=	269.919		
Eigenvalues:	243.5189	284.5447	313.8598				
54	H	Isotropic=	26.6956	Anisotropy	5.4709		
XX=	26.755	YX=	-3.9947	ZX=	1.7297		
XY=	-2.3845	YY=	27.4932	ZY=	1.6065		
XZ=	0.2401	YZ=	0.6332	ZZ=	25.8385		
Eigenvalues:	23.109	26.6349	30.3428				
55	N	Isotropic=	124.428	Anisotropy	108.2108		
XX=	97.2653	YX=	-14.3445	ZX=	50.2722		
XY=	21.5456	YY=	195.9493	ZY=	-3.0284		
XZ=	71.2135	YZ=	11.0785	ZZ=	80.0696		
Eigenvalues:	27.3163	149.3991	196.5686				
56	C	Isotropic=	49.7463	Anisotropy	190.0463		
XX=	114.7813	YX=	80.2525	ZX=	42.4027		
XY=	73.9303	YY=	8.1779	ZY=	31.9423		

XZ= 49.6637 YZ= 35.4292 ZZ= 26.2796
 Eigenvalues: -33.89416.6891 176.4439
 57 H Isotropic= 25.4291 Anisotropy 2.1612
 XX= 25.1247 YX= 0.9605 ZX= -1.5718
 XY= 1.2549 YY= 25.4251 ZY= 0.17
 XZ= -0.939 YZ= 0.5988 ZZ= 25.7375
 Eigenvalues: 23.489 25.9284 26.8699
 58 H Isotropic= 30.2738 Anisotropy 14.2499
 XX= 28.5062 YX= -4.3535 ZX= -2.2469
 XY= -4.8766 YY= 36.3224 ZY= 2.5174
 XZ= -1.8282 YZ= 4.9653 ZZ= 25.9929
 Eigenvalues: 24.6413 26.4063 39.7738
 59 C Isotropic= 16.8716 Anisotropy 118.5334
 XX= 17.6236 YX= -65.8413 ZX= 15.8374
 XY= -72.1826 YY= -10.6676 ZY= -26.3009
 XZ= 12.9131 YZ= -43.5777 ZZ= 43.6587
 Eigenvalues: -70.020324.7412 95.8938
 60 H Isotropic= 26.0707 Anisotropy 6.7851
 XX= 27.7496 YX= 3.404 ZX= -4.7458
 XY= 1.6174 YY= 28.3428 ZY= 0.505
 XZ= -1.7624 YZ= 4.4204 ZZ= 22.1197
 Eigenvalues: 19.4036 28.2144 30.5941
 61 C Isotropic= 68.1153 Anisotropy 164.405
 XX= 135.6573 YX= 36.6981 ZX= 46.6814
 XY= 40.6085 YY= 64.321 ZY= 51.6043
 XZ= 47.799 YZ= 55.1479 ZZ= 4.3675
 Eigenvalues: -30.104256.7314 177.7186
 62 C Isotropic= 63.0803 Anisotropy 177.1613
 XX= 107.4835 YX= 69.6692 ZX= 72.9116
 XY= 70.6372 YY= 61.5218 ZY= -3.7085
 XZ= 77.4736 YZ= -5.9283 ZZ= 20.2357
 Eigenvalues: -41.155849.209 181.1878
 63 C Isotropic= 64.4199 Anisotropy 174.1269
 XX= 119.962 YX= 78.4978 ZX= 33.8711
 XY= 79.6333 YY= 8.2535 ZY= 39.3353
 XZ= 33.5499 YZ= 35.9705 ZZ= 65.0443
 Eigenvalues: -36.269349.0246 180.5045
 64 C Isotropic= 61.8946 Anisotropy 176.1287
 XX= 130.2831 YX= 40.6688 ZX= 54.9373
 XY= 42.8212 YY= 56.3209 ZY= 57.5116
 XZ= 52.4519 YZ= 57.1564 ZZ= -0.9202
 Eigenvalues: -40.396946.7669 179.3137
 65 C Isotropic= 55.0565 Anisotropy 158.6569
 XX= 93.7368 YX= 62.4283 ZX= 67.6597
 XY= 61.4446 YY= 54.9934 ZY= -7.6468
 XZ= 72.1018 YZ= -3.3282 ZZ= 16.4392
 Eigenvalues: -40.871245.2129 160.8277
 66 H Isotropic= 24.0058 Anisotropy 9.3633
 XX= 23.9724 YX= -3.3068 ZX= -2.2939
 XY= -4.044 YY= 26.8051 ZY= 2.1761
 XZ= -1.8461 YZ= 1.9544 ZZ= 21.2399
 Eigenvalues: 20.124 21.6454 30.248
 67 O Isotropic= -83.3684 Anisotropy 647.1667
 XX= -50.6953 YX= -127.8496 ZX= 245.5468
 XY= -113.7788 YY= -67.2715 ZY= -265.3016
 XZ= 280.7992 YZ= -256.6936 ZZ= -132.1383

Eigenvalues:	-418.339	-179.8421	348.0761		
68	C	Isotropic=	55.9395	Anisotropy	171.3731
XX=	-3.7089	YX=	-9.2393	ZX=	45.8891
XY=	-19.6743	YY=	20.7585	ZY=	29.2983
XZ=	34.6805	YZ=	54.7346	ZZ=	150.769
Eigenvalues:	-27.6763	25.3066	170.1883		
69	H	Isotropic=	23.6544	Anisotropy	4.8903
XX=	22.1999	YX=	-2.343	ZX=	-1.1121
XY=	-2.2874	YY=	25.4546	ZY=	-1.5952
XZ=	-0.9564	YZ=	-1.51	ZZ=	23.3086
Eigenvalues:	20.1251	23.9235	26.9146		
70	H	Isotropic=	23.7433	Anisotropy	3.2064
XX=	22.5438	YX=	-1.9292	ZX=	-1.7889
XY=	-1.6263	YY=	23.7803	ZY=	-0.8759
XZ=	-1.8182	YZ=	-1.0017	ZZ=	24.9056
Eigenvalues:	20.3803	24.9686	25.8808		
71	H	Isotropic=	23.7233	Anisotropy	4.8536
XX=	22.8149	YX=	-2.9253	ZX=	-1.0666
XY=	-2.726	YY=	25.0322	ZY=	-0.7254
XZ=	-1.1639	YZ=	-0.8396	ZZ=	23.3227
Eigenvalues:	20.2786	23.9322	26.959		
72	H	Isotropic=	23.5362	Anisotropy	7.9896
XX=	22.4581	YX=	-2.4349	ZX=	0.8807
XY=	-1.1982	YY=	24.3156	ZY=	-3.936
XZ=	1.0237	YZ=	-4.4007	ZZ=	23.8348
Eigenvalues:	19.7624	21.9835	28.8626		
73	C	Isotropic=	60.2184	Anisotropy	174.7714
XX=	-5.3776	YX=	41.0566	ZX=	44.1164
XY=	39.7894	YY=	24.5976	ZY=	10.4423
XZ=	49.6063	YZ=	11.8203	ZZ=	161.4353
Eigenvalues:	-39.0327	42.9553	176.7326		
74	C	Isotropic=	62.0927	Anisotropy	176.8866
XX=	54.8256	YX=	15.3395	ZX=	31.5007
XY=	12.3496	YY=	-35.8882	ZY=	27.4661
XZ=	32.3919	YZ=	27.7544	ZZ=	167.3408
Eigenvalues:	-40.5736	46.8347	180.0171		
75	C	Isotropic=	61.6655	Anisotropy	179.1633
XX=	-1.2726	YX=	-32.1215	ZX=	52.9265
XY=	-31.9118	YY=	23.4129	ZY=	31.4019
XZ=	52.3843	YZ=	30.1533	ZZ=	162.8562
Eigenvalues:	-41.3811	45.2699	181.1077		
76	C	Isotropic=	63.4262	Anisotropy	175.3732
XX=	-10	YX=	37.7718	ZX=	44.1239
XY=	41.423	YY=	32.67	ZY=	10.6957
XZ=	43.7481	YZ=	9.0418	ZZ=	167.6086
Eigenvalues:	-39.0708	49.0078	180.3417		
77	C	Isotropic=	66.1175	Anisotropy	164.3527
XX=	57.8414	YX=	10.7538	ZX=	28.0916
XY=	17.695	YY=	-23.7215	ZY=	26.0263
XZ=	28.3992	YZ=	28.0109	ZZ=	164.2327
Eigenvalues:	-28.7824	51.4489	175.686		
78	H	Isotropic=	23.3263	Anisotropy	7.8219
XX=	23.1135	YX=	2.3287	ZX=	-1.3492
XY=	2.5325	YY=	27.0575	ZY=	-1.1522
XZ=	-1.6051	YZ=	-1.1526	ZZ=	19.808
Eigenvalues:	19.237	22.201	28.5409		

79	H	Isotropic=	23.6995	Anisotropy	4.6925
XX=	26.1522	YX=	0.8231	ZX=	-1.7341
XY=	0.5438	YY=	24.3958	ZY=	-0.497
XZ=	-1.4931	YZ=	-0.3456	ZZ=	20.5504
Eigenvalues:	20.1062	24.1644	26.8278		
80	H	Isotropic=	23.6717	Anisotropy	3.8489
XX=	24.7	YX=	-0.7807	ZX=	-1.0393
XY=	-0.8366	YY=	25.8118	ZY=	-0.4054
XZ=	-0.8902	YZ=	-0.502	ZZ=	20.5033
Eigenvalues:	20.2229	24.5545	26.2377		
81	H	Isotropic=	23.8712	Anisotropy	5.4073
XX=	25.3174	YX=	1.481	ZX=	-1.5039
XY=	1.4613	YY=	25.9049	ZY=	-1.0474
XZ=	-1.0359	YZ=	-1.0183	ZZ=	20.3914
Eigenvalues:	20.0035	24.1342	27.4761		
82	H	Isotropic=	24.0403	Anisotropy	8.9253
XX=	28.9656	YX=	2.3619	ZX=	-2.2659
XY=	1.941	YY=	23.7757	ZY=	-0.6564
XZ=	-0.9835	YZ=	0.0903	ZZ=	19.3794
Eigenvalues:	19.1104	23.0199	29.9905		

2a-iii2

C	3.300796	1.835387	-0.043094
C	4.085784	1.735207	1.303027
C	3.680281	0.569446	2.220473
C	4.769371	-0.507798	2.37272
C	5.189523	-1.201245	1.061327
C	4.111471	-1.669348	0.096019
C	3.257405	-0.571859	-0.469657
C	1.911838	-0.670906	-0.310396
C	1.085082	0.576201	-0.460733
C	1.778204	1.791208	0.161637
C	3.780609	0.730262	-1.035642
C	5.284869	0.824414	-1.235083
C	3.157265	0.984488	-2.420976
C	1.187054	-1.910183	0.049578
C	5.981808	0.02992	3.098261
O	3.535839	3.133785	-0.584905
O	3.973797	2.967163	1.999557
O	6.363966	-1.544698	0.907829
O	4.512665	-2.649043	-0.856278
O	-0.154524	0.343362	0.252663
H	3.052239	3.250817	1.956179
C	5.667677	-2.617988	-1.591241
O	6.427199	-1.656806	-1.53958
C	5.814339	-3.865101	-2.400196
H	5.190266	1.672625	1.078754
H	2.739037	0.084681	1.859671
H	3.445729	-2.319020	0.765133
H	0.828227	0.768253	-1.540634
H	1.325228	2.715998	-0.293686
H	1.548074	1.813663	1.259037
H	5.874932	0.439845	-0.372195
H	5.590131	0.236668	-2.13672
H	5.571181	1.890283	-1.414916
H	3.94675	1.203924	-3.180823

H	2.586543	0.092897	-2.773552
H	2.477734	1.871317	-2.390772
H	1.726159	-2.819651	-0.31476
H	1.063034	-1.976459	1.160241
H	0.164546	-1.905679	-0.407176
H	6.716476	-0.792545	3.279097
H	6.490991	0.819448	2.49496
H	5.67741	0.469178	4.078367
H	4.873706	-4.465886	-2.391341
H	6.072104	-3.585032	-3.450296
H	6.645862	-4.472567	-1.965582
H	4.463552	3.354885	-0.434325
C	-1.196956	1.192844	0.010115
O	-1.033619	2.134016	-0.764474
H	4.31899	-1.335919	2.995253
H	3.478962	0.990286	3.242151
C	-2.428291	0.833614	0.821872
C	-3.642810	0.632438	-0.150322
O	-2.233378	-0.326761	1.601903
H	-2.634161	1.709994	1.504915
N	-4.621438	-0.313097	0.314296
C	-4.248056	1.998734	-0.399255
H	-3.220947	0.227522	-1.123675
H	-1.364759	-0.255218	2.020773
C	-4.944361	-1.455869	-0.397377
H	-5.150737	-0.072411	1.116651
C	-5.026386	2.632502	0.575621
C	-5.598503	3.876619	0.315465
C	-5.395601	4.495867	-0.918086
C	-4.615777	3.869715	-1.88964
C	-4.044788	2.623053	-1.634035
H	-5.182796	2.160098	1.556843
O	-4.224185	-1.870032	-1.326327
C	-6.161738	-2.193652	0.04836
H	-6.209125	4.370552	1.085389
H	-5.847507	5.477667	-1.122063
H	-4.446928	4.358337	-2.860735
H	-3.416922	0.139034	-2.398416
C	-6.079494	-3.580099	0.217616
C	-7.205634	-4.295952	0.621594
C	-8.411745	-3.632844	0.849246
C	-8.494255	-2.251436	0.672055
C	-7.370079	-1.528034	0.274927
H	-5.12658	-4.095206	0.018217
H	-7.141604	-5.385820	0.756321
H	-9.299916	-4.200021	0.165356
H	-9.447525	-1.730236	0.843718
H	-7.443805	-0.440152	0.12636

	E(RB+HF-PW91)	=	-2012.301627		
SCF	GIAO	Magnetic	shielding	tensor (ppm):	
1	C	Isotropic=	109.3703	Anisotropy =	
XX=	99.886	YX=	11.8558	ZX=	-9.1811
XY=	4.5283	YY=	117.3539	ZY=	-8.1494
XZ=	-9.3349	YZ=	-8.1466	ZZ=	110.8712

Eigenvalues:	94.0744	105.9862	128.0504			
2	C	Isotropic=	112.2195	Anisotropy	=	30.5935
XX=	94.5399	YX=	-9.0901	ZX=	-3.9748	
XY=	-3.6255	YY=	124.7525	ZY=	14.7745	
XZ=	1.4647	YZ=	5.1463	ZZ=	117.366	
Eigenvalues:	93.2305	110.8128	132.6151			
3	C	Isotropic=	142.148	Anisotropy	=	20.558
XX=	120.8473	YX=	1.1363	ZX=	2.7356	
XY=	-2.6732	YY=	149.9764	ZY=	-1.6418	
XZ=	-3.9935	YZ=	-0.6654	ZZ=	155.6204	
Eigenvalues:	120.8146	149.7762	155.8534			
4	C	Isotropic=	140.0163	Anisotropy	=	25.1058
XX=	124.4088	YX=	-1.8937	ZX=	-2.68	
XY=	11.2668	YY=	142.3046	ZY=	5.4773	
XZ=	5.0101	YZ=	7.8214	ZZ=	153.3355	
Eigenvalues:	123.2483	140.0472	156.7535			
5	C	Isotropic=	-21.9431	Anisotropy	=	178.6949
XX=	-55.5012	YX=	4.7081	ZX=	-35.6257	
XY=	8.8849	YY=	52.6692	ZY=	-77.6715	
XZ=	-17.7767	YZ=	-85.796	ZZ=	-62.9973	
Eigenvalues:	-112.8911	-50.1251	197.1868			
6	C	Isotropic=	101.9639	Anisotropy	=	41.0292
XX=	86.3172	YX=	3.5444	ZX=	3.1389	
XY=	-9.593	YY=	102.3791	ZY=	16.451	
XZ=	-6.1379	YZ=	19.2569	ZZ=	117.1956	
Eigenvalues:	85.5445	91.0306	129.3168			
7	C	Isotropic=	43.3935	Anisotropy	=	157.8812
XX=	36.4044	YX=	17.5417	ZX=	-4.8711	
XY=	38.5691	YY=	-22.519	ZY=	79.6296	
XZ=	9.6633	YZ=	64.8082	ZZ=	116.2949	
Eigenvalues:	-59.7662	141.299	148.6476			
8	C	Isotropic=	41.6872	Anisotropy	=	154.4651
XX=	40.0836	YX=	15.3971	ZX=	9.0819	
XY=	2.5063	YY=	-45.5944	ZY=	39.1895	
XZ=	12.7556	YZ=	58.021	ZZ=	130.5725	
Eigenvalues:	-58.4766	138.8743	144.664			
9	C	Isotropic=	110.4525	Anisotropy	=	48.7516
XX=	128.7301	YX=	7.9924	ZX=	-22.688	
XY=	7.0009	YY=	104.2224	ZY=	7.4443	
XZ=	-27.2813	YZ=	9.3025	ZZ=	98.405	
Eigenvalues:	79.4602	108.9438	142.9536			
10	C	Isotropic=	148.0697	Anisotropy	=	41.4206
XX=	169.3815	YX=	8.5686	ZX=	-8.0573	
XY=	17.5091	YY=	141.6683	ZY=	10.6528	
XZ=	-10.971	YZ=	0.5631	ZZ=	133.1592	
Eigenvalues:	125.3837	143.1419	175.6834			
11	C	Isotropic=	147.9486	Anisotropy	=	13.8266
XX=	142.0722	YX=	-2.8025	ZX=	-0.4659	
XY=	6.803	YY=	150.194	ZY=	2.3772	
XZ=	10.4605	YZ=	6.5695	ZZ=	151.5795	
Eigenvalues:	139.9281	146.7514	157.1663			
12	C	Isotropic=	155.5325	Anisotropy	=	24.9573
XX=	164.876	YX=	-8.974	ZX=	10.9817	
XY=	-6.5218	YY=	137.9146	ZY=	2.9628	
XZ=	2.5702	YZ=	-3.248	ZZ=	163.8069	
Eigenvalues:	135.7496	158.6772	172.1707			

13	C	Isotropic=	148.1353	Anisotropy	=	55.1146
XX=	143.1844	YX=	8.0591	ZX=	18.6875	
XY=	14.3754	YY=	125.6302	ZY=	-9.3926	
XZ=	20.3694	YZ=	-6.7335	ZZ=	175.5914	
Eigenvalues:	115.5485		143.9791		184.8784	
14	C	Isotropic=	167.8315	Anisotropy	=	12.4665
XX=	164.1751	YX=	6.3282	ZX=	5.4132	
XY=	3.9763	YY=	173.7998	ZY=	0.2667	
XZ=	-5.5386	YZ=	-2.5134	ZZ=	165.5197	
Eigenvalues:	161.8944		165.4577		176.1425	
15	C	Isotropic=	169.3712	Anisotropy	=	17.0362
XX=	173.5657	YX=	-3.1998	ZX=	6.551	
XY=	1.314	YY=	163.0917	ZY=	9.3319	
XZ=	6.0581	YZ=	8.4784	ZZ=	171.4562	
Eigenvalues:	156.3522		171.0327		180.7287	
16	O	Isotropic=	263.4501	Anisotropy	=	85.9636
XX=	315.4979	YX=	28.7963	ZX=	0.9925	
XY=	12.5314	YY=	221.3051	ZY=	-22.1488	
XZ=	1.716	YZ=	-58.4418	ZZ=	253.5472	
Eigenvalues:	191.4261		278.165		320.7592	
17	O	Isotropic=	265.3399	Anisotropy	=	46.0984
XX=	253.0119	YX=	-20.4475	ZX=	-9.7373	
XY=	-9.786	YY=	279.6206	ZY=	-16.011	
XZ=	12.2872	YZ=	-21.2432	ZZ=	263.3872	
Eigenvalues:	243.0009		256.9466		296.0722	
18	O	Isotropic=	-372.4263	Anisotropy	=	1098.4731
XX=	-976.4956	YX=	281.5721	ZX=	-6.3365	
XY=	204.3301	YY=	112.1602	ZY=	-345.0693	
XZ=	9.7464	YZ=	-361.9454	ZZ=	-252.9435	
Eigenvalues:	-1036.5457		-440.6223		359.8891	
19	O	Isotropic=	95.0836	Anisotropy	=	127.6781
XX=	158.0103	YX=	-113.3164	ZX=	-57.7459	
XY=	-10.7457	YY=	4.2636	ZY=	-106.4023	
XZ=	18.4603	YZ=	-23.5676	ZZ=	122.977	
Eigenvalues:	-45.0251		150.0736		180.2024	
20	O	Isotropic=	78.3991	Anisotropy	=	177.2594
XX=	72.0276	YX=	1.6498	ZX=	56.1187	
XY=	-108.3268	YY=	101.8657	ZY=	127.8945	
XZ=	122.1892	YZ=	91.7797	ZZ=	61.3041	
Eigenvalues:	-93.9381		132.5635		196.5721	
21	H	Isotropic=	31.1768	Anisotropy	=	13.5496
XX=	36.0589	YX=	-6.2008	ZX=	0.8862	
XY=	-5.5875	YY=	30.6635	ZY=	4.9836	
XZ=	1.2324	YZ=	5.887	ZZ=	26.808	
Eigenvalues:	21.5808		31.7398		40.2098	
22	C	Isotropic=	21.4099	Anisotropy	=	78.9585
XX=	3.3762	YX=	52.3642	ZX=	74.7552	
XY=	21.5334	YY=	54.5828	ZY=	-22.9878	
XZ=	53.6232	YZ=	-46.5041	ZZ=	6.2705	
Eigenvalues:	-78.6797		68.8605		74.0489	
23	O	Isotropic=	-140.9102	Anisotropy	=	606.5939
XX=	-258.3923	YX=	-205.6684	ZX=	224.9813	
XY=	-157.391	YY=	-194.1452	ZY=	-154.3651	
XZ=	233.8511	YZ=	-143.8517	ZZ=	29.8069	
Eigenvalues:	-432.8649		-253.3515		263.4857	
24	C	Isotropic=	165.6001	Anisotropy	=	38.019

XX=	155.8215	YX=	-0.5759	ZX=	-6.6686				
XY=	1.6428	YY=	177.0848	ZY=	20.3084				
XZ=	-6.7936	YZ=	17.6789	ZZ=	163.8939				
Eigenvalues:	146.622	159.2322		190.946					
25	H	Isotropic=	27.4813	Anisotropy	=	3.0556			
XX=	28.0402	YX=	-1.3835	ZX=	0.5183				
XY=	-2.2621	YY=	26.9272	ZY=	1.4834				
XZ=	0.0471	YZ=	0.8665	ZZ=	27.4766				
Eigenvalues:	25.0555	27.8701	29.5184						
26	H	Isotropic=	28.2656	Anisotropy	=	8.152			
XX=	29.1211	YX=	1.346	ZX=	4.2592				
XY=	1.7487	YY=	25.94	ZY=	0.406				
XZ=	3.7072	YZ=	0.7062	ZZ=	29.7357				
Eigenvalues:	24.7946	26.3019	33.7003						
27	H	Isotropic=	25.3154	Anisotropy	=	4.1353			
XX=	26.0344	YX=	-2.578	ZX=	-1.6539				
XY=	0.6327	YY=	25.3892	ZY=	2.1243				
XZ=	-2.1064	YZ=	0.0946	ZZ=	24.5228				
Eigenvalues:	23.1709	24.7031	28.0723						
28	H	Isotropic=	25.0065	Anisotropy	=	6.6309			
XX=	29.1207	YX=	0.4972	ZX=	-1.5904				
XY=	0.2589	YY=	20.1814	ZY=	0.2713				
XZ=	-0.4199	YZ=	-1.5962	ZZ=	25.7173				
Eigenvalues:	20.0957	25.4965	29.4271						
29	H	Isotropic=	27.6668	Anisotropy	=	8.5647			
XX=	32.6001	YX=	-1.7219	ZX=	1.3999				
XY=	-0.4986	YY=	28.9532	ZY=	-2.6173				
XZ=	2.5242	YZ=	-0.6648	ZZ=	21.4471				
Eigenvalues:	20.8544	28.7695	33.3766						
30	H	Isotropic=	29.8481	Anisotropy	=	5.7841			
XX=	33.4889	YX=	0.7245	ZX=	0.0151				
XY=	1.096	YY=	25.5289	ZY=	1.6156				
XZ=	0.6881	YZ=	2.1228	ZZ=	30.5266				
Eigenvalues:	24.8411	30.9991	33.7042						
31	H	Isotropic=	29.4473	Anisotropy	=	8.3417			
XX=	31.0184	YX=	-2.543	ZX=	2.0312				
XY=	-2.6111	YY=	27.6473	ZY=	-2.6378				
XZ=	2.555	YZ=	-3.9645	ZZ=	29.6762				
Eigenvalues:	25.0912	28.2423	35.0084						
32	H	Isotropic=	29.2177	Anisotropy	=	9.1261			
XX=	28.9737	YX=	-4.161	ZX=	-3.7159				
XY=	-3.5297	YY=	29.6289	ZY=	1.8007				
XZ=	-3.4452	YZ=	1.357	ZZ=	29.0506				
Eigenvalues:	24.6054	27.7459	35.3018						
33	H	Isotropic=	30.3531	Anisotropy	=	6.7598			
XX=	32.3399	YX=	1.5656	ZX=	-2.9737				
XY=	1.832	YY=	31.4173	ZY=	-0.881				
XZ=	-2.8218	YZ=	-1.4423	ZZ=	27.3022				
Eigenvalues:	25.9564	30.2434	34.8597						
34	H	Isotropic=	30.1065	Anisotropy	=	9.2673			
XX=	29.5711	YX=	-0.048	ZX=	-0.9706				
XY=	0.8178	YY=	25.5593	ZY=	-2.8423				
XZ=	-2.3481	YZ=	-2.3845	ZZ=	35.1891				
Eigenvalues:	24.8955	29.1393	36.2847						
35	H	Isotropic=	30.1738	Anisotropy	=	6.1409			
XX=	29.4774	YX=	2.5528	ZX=	0.5977				

XY=	1.0257	YY=	28.0327	ZY=	1.3847				
XZ=	2.2625	YZ=	1.8446	ZZ=	33.0113				
Eigenvalues:	26.7689	29.4847	34.2677						
36	H	Isotropic=	28.4417	Anisotropy	=	6.3988			
XX=	28.6349	YX=	-2.3754	ZX=	0.1841				
XY=	-2.379	YY=	26.3878	ZY=	-1.5147				
XZ=	2.1286	YZ=	-3.5364	ZZ=	30.3025				
Eigenvalues:	24.4174	28.2003	32.7076						
37	H	Isotropic=	28.8995	Anisotropy	=	7.8575			
XX=	30.0961	YX=	-0.0413	ZX=	-1.8602				
XY=	-1.6457	YY=	32.8336	ZY=	2.5215				
XZ=	-1.4372	YZ=	3.4056	ZZ=	23.769				
Eigenvalues:	22.6406	29.9201	34.1379						
38	H	Isotropic=	29.1906	Anisotropy	=	6.6763			
XX=	28.6037	YX=	0.5235	ZX=	-1.8756				
XY=	0.6663	YY=	27.7612	ZY=	-2.6403				
XZ=	-2.3152	YZ=	-2.8918	ZZ=	31.2069				
Eigenvalues:	26.0908	27.8395	33.6414						
39	H	Isotropic=	28.3707	Anisotropy	=	8.1177			
XX=	33.3963	YX=	-0.4892	ZX=	1.7571				
XY=	0.8618	YY=	29.0582	ZY=	0.7483				
XZ=	2.2204	YZ=	1.3822	ZZ=	22.6576				
Eigenvalues:	22.1515	29.178	33.7825						
40	H	Isotropic=	29.1735	Anisotropy	=	10.8468			
XX=	31.8129	YX=	-5.1809	ZX=	2.7266				
XY=	-4.357	YY=	27.9809	ZY=	-1.2469				
XZ=	4.4444	YZ=	-0.339	ZZ=	27.7266				
Eigenvalues:	24.0574	27.0583	36.4046						
41	H	Isotropic=	29.6452	Anisotropy	=	5.8235			
XX=	31.755	YX=	2.5144	ZX=	0.9984				
XY=	2.9805	YY=	29.2508	ZY=	-2.0348				
XZ=	1.5146	YZ=	-2.4459	ZZ=	27.9298				
Eigenvalues:	25.1317	30.2763	33.5275						
42	H	Isotropic=	30.5228	Anisotropy	=	9.6286			
XX=	28.845	YX=	-0.4871	ZX=	1.5836				
XY=	-0.6283	YY=	26.9204	ZY=	2.726				
XZ=	1.7683	YZ=	3.1289	ZZ=	35.8029				
Eigenvalues:	25.694	28.9324	36.9419						
43	H	Isotropic=	29.0266	Anisotropy	=	5.5911			
XX=	30.3008	YX=	1.1007	ZX=	-1.7987				
XY=	2.9911	YY=	30.4114	ZY=	2.4686				
XZ=	-0.7617	YZ=	3.4819	ZZ=	26.3675				
Eigenvalues:	24.0706	30.2552	32.754						
44	H	Isotropic=	29.1647	Anisotropy	=	7.6557			
XX=	26.5064	YX=	0.4273	ZX=	-1.693				
XY=	-0.8381	YY=	27.6232	ZY=	1.8801				
XZ=	-3.0737	YZ=	0.1327	ZZ=	33.3645				
Eigenvalues:	25.7532	27.4724	34.2685						
45	H	Isotropic=	28.8862	Anisotropy	=	8.2326			
XX=	29.9002	YX=	-3.3729	ZX=	1.1829				
XY=	-4.8977	YY=	30.4763	ZY=	-0.0349				
XZ=	0.5628	YZ=	0.0928	ZZ=	26.2821				
Eigenvalues:	25.4782	26.8059	34.3746						
46	H	Isotropic=	30.799	Anisotropy	=	18.201			
XX=	38.2345	YX=	8.2992	ZX=	0.4466				
XY=	6.2469	YY=	31.6506	ZY=	-2.1558				

XZ= 0.162 YZ= -0.1922 ZZ= 22.512
 Eigenvalues: 22.225 27.2391 42.9331
 47 C Isotropic= 11.0264 Anisotropy = 91.85
 XX= -57.4106 YX= 29.7664 ZX= 34.4938
 XY= 66.7983 YY= 28.0453 ZY= 2.588
 XZ= 5.7099 YZ= 8.9573 ZZ= 62.4444
 Eigenvalues: -80.9498 41.7692 72.2597
 48 O Isotropic= -100.6967 Anisotropy = 610.0946
 XX= -184.7554 YX= 78.3585 ZX= 140.322
 XY= 104.9576 YY= -167.5891 ZY= 319.2739
 XZ= 129.056 YZ= 262.526 ZZ= 50.2545
 Eigenvalues: -369.3047 -238.8184 306.0331
 49 H Isotropic= 28.7132 Anisotropy = 6.5568
 XX= 27.9738 YX= 1.5192 ZX= 1.9029
 XY= 2.4414 YY= 29.8088 ZY= -4.0486
 XZ= 0.9535 YZ= -3.648 ZZ= 28.357
 Eigenvalues: 23.8115 29.2437 33.0844
 50 H Isotropic= 29.5014 Anisotropy = 6.4791
 XX= 27.8649 YX= -1.8462 ZX= -0.2105
 XY= -1.6325 YY= 27.0627 ZY= 0.5885
 XZ= -0.2257 YZ= 1.7143 ZZ= 33.5766
 Eigenvalues: 25.6033 29.08 33.8208
 51 C Isotropic= 110.4991 Anisotropy = 35.413
 XX= 103.0844 YX= -16.9383 ZX= 16.6199
 XY= -5.6892 YY= 118.7729 ZY= -9.4553
 XZ= 4.8268 YZ= -13.2331 ZZ= 109.6402
 Eigenvalues: 94.7273 102.6623 134.1078
 52 C Isotropic= 128.4642 Anisotropy = 31.8433
 XX= 129.9881 YX= -1.1005 ZX= 5.9341
 XY= 2.6975 YY= 132.6969 ZY= -20.5598
 XZ= 5.5738 YZ= -21.3445 ZZ= 122.7076
 Eigenvalues: 105.1444 130.5551 149.6931
 53 O Isotropic= 287.7088 Anisotropy = 92.8543
 XX= 339.5378 YX= -9.2249 ZX= 34.3407
 XY= 0.5848 YY= 252.6418 ZY= 0.2313
 XZ= 21.7292 YZ= 8.142 ZZ= 270.9469
 Eigenvalues: 249.929 263.5858 349.6117
 54 H Isotropic= 26.5328 Anisotropy = 6.0405
 XX= 26.2857 YX= -4.1366 ZX= 1.5742
 XY= -2.7223 YY= 27.8075 ZY= 1.3719
 XZ= 0.364 YZ= 0.0788 ZZ= 25.5052
 Eigenvalues: 22.9589 26.0797 30.5598
 55 N Isotropic= 128.7461 Anisotropy = 106.8789
 XX= 105.188 YX= -13.9219 ZX= 49.8053
 XY= 23.1531 YY= 198.6843 ZY= -2.2004
 XZ= 68.3146 YZ= 15.2226 ZZ= 82.3661
 Eigenvalues: 33.5985 152.6412 199.9988
 56 C Isotropic= 49.1935 Anisotropy = 191.039
 XX= 117.5709 YX= 79.6996 ZX= 41.6319
 XY= 73.9027 YY= 6.1251 ZY= 32.3727
 XZ= 48.2429 YZ= 33.2515 ZZ= 23.8845
 Eigenvalues: -34.8473 5.875 176.5528
 57 H Isotropic= 25.1522 Anisotropy = 2.2286
 XX= 24.9846 YX= 0.947 ZX= -1.5853
 XY= 1.2742 YY= 24.86 ZY= 0.3563
 XZ= -0.9541 YZ= 0.8916 ZZ= 25.6121

Eigenvalues:	23.0896	25.7292	26.638		
58	H	Isotropic=	30.1004	Anisotropy	= 19.2389
XX=	39.9445	YX=	-0.4434	ZX=	6.2473
XY=	-0.532	YY=	22.4528	ZY=	-3.0184
XZ=	6.6265	YZ=	-4.4654	ZZ=	27.904
Eigenvalues:	20.1657	27.2092	42.9264		
59	C	Isotropic=	18.0355	Anisotropy	= 116.3422
XX=	16.3036	YX=	-66.324	ZX=	12.8034
XY=	-74.8955	YY=	-7.3644	ZY=	-25.0604
XZ=	10.0108	YZ=	-43.0694	ZZ=	45.1672
Eigenvalues:	-70.3092	28.8187	95.5969		
60	H	Isotropic=	26.1193	Anisotropy	= 6.7245
XX=	27.507	YX=	3.5221	ZX=	-4.2182
XY=	2.2733	YY=	27.8597	ZY=	0.3659
XZ=	-1.6507	YZ=	4.3656	ZZ=	22.9913
Eigenvalues:	20.0177	27.7379	30.6024		
61	C	Isotropic=	67.2411	Anisotropy	= 165.6113
XX=	137.488	YX=	37.0616	ZX=	45.9159
XY=	41.3473	YY=	62.5964	ZY=	50.2743
XZ=	46.4768	YZ=	53.7923	ZZ=	1.639
Eigenvalues:	-31.161	55.2357	177.6487		
62	C	Isotropic=	63.1775	Anisotropy	= 176.9392
XX=	111.3055	YX=	69.5271	ZX=	71.0779
XY=	70.2869	YY=	59.989	ZY=	-5.9691
XZ=	75.5284	YZ=	-8.1652	ZZ=	18.2379
Eigenvalues:	-41.0514	49.4469	181.1369		
63	C	Isotropic=	64.599	Anisotropy	= 174.0658
XX=	123.1631	YX=	78.1725	ZX=	32.5577
XY=	78.8784	YY=	7.1146	ZY=	38.1931
XZ=	32.2838	YZ=	35.0649	ZZ=	63.5193
Eigenvalues:	-36.1674	49.3215	180.6428		
64	C	Isotropic=	62.0271	Anisotropy	= 175.8983
XX=	133.0677	YX=	41.2198	ZX=	53.0482
XY=	43.0637	YY=	56.3887	ZY=	55.5675
XZ=	50.3851	YZ=	55.506	ZZ=	-3.3752
Eigenvalues:	-40.1887	46.9774	179.2926		
65	C	Isotropic=	55.4426	Anisotropy	= 158.2675
XX=	97.6779	YX=	62.4518	ZX=	66.1324
XY=	61.3512	YY=	53.5836	ZY=	-10.007
XZ=	69.6245	YZ=	-5.824	ZZ=	15.0664
Eigenvalues:	-40.4543	45.8279	160.9543		
66	H	Isotropic=	23.9741	Anisotropy	= 9.2703
XX=	23.8562	YX=	-3.1664	ZX=	-2.2062
XY=	-4.0493	YY=	26.8387	ZY=	2.2149
XZ=	-1.7526	YZ=	1.958	ZZ=	21.2274
Eigenvalues:	20.1598	21.6082	30.1543		
67	O	Isotropic=	-91.2813	Anisotropy	= 657.6239
XX=	-59.042	YX=	-131.4661	ZX=	244.4851
XY=	-114.8112	YY=	-67.7104	ZY=	-278.9675
XZ=	274.2739	YZ=	-268.169	ZZ=	-147.0913
Eigenvalues:	-434.9035	-186.0753	47.1347		
68	C	Isotropic=	55.3244	Anisotropy	= 172.6509
XX=	-5.7003	YX=	-8.0881	ZX=	46.0669
XY=	-18.5704	YY=	20.75	ZY=	28.9404
XZ=	35.2957	YZ=	54.7358	ZZ=	150.9234
Eigenvalues:	-28.2303	23.7784	170.425		

69	H	Isotropic=	23.6666	Anisotropy	=	4.8466
XX=	22.1762	YX=	-2.2997	ZX=	-1.0719	
XY=	-2.2734	YY=	25.4542	ZY=	-1.5842	
XZ=	-0.9172	YZ=	-1.4914	ZZ=	23.3695	
Eigenvalues:	20.1789	23.9233	26.8977			
70	H	Isotropic=	23.7466	Anisotropy	=	3.2068
XX=	22.4508	YX=	-1.8995	ZX=	-1.7297	
XY=	-1.6656	YY=	23.7969	ZY=	-0.8291	
XZ=	-1.7682	YZ=	-0.9038	ZZ=	24.9922	
Eigenvalues:	20.4027	24.9527	25.8845			
71	H	Isotropic=	23.7282	Anisotropy	=	4.8062
XX=	22.7176	YX=	-2.9089	ZX=	-1.0016	
XY=	-2.7224	YY=	25.0511	ZY=	-0.691	
XZ=	-1.1113	YZ=	-0.7829	ZZ=	23.4158	
Eigenvalues:	20.3037	23.9485	26.9324			
72	H	Isotropic=	23.5752	Anisotropy	=	7.9124
XX=	22.3757	YX=	-2.3212	ZX=	0.8858	
XY=	-1.2234	YY=	24.3712	ZY=	-3.9613	
XZ=	1.0194	YZ=	-4.211	ZZ=	23.9787	
Eigenvalues:	19.9407	21.9348	28.8501			
73	C	Isotropic=	59.7977	Anisotropy	=	175.6944
XX=	-4.6035	YX=	41.6824	ZX=	43.8562	
XY=	40.4166	YY=	22.2109	ZY=	10.4777	
XZ=	49.1061	YZ=	11.9157	ZZ=	161.7857	
Eigenvalues:	-39.5388	42.0046	176.9273			
74	C	Isotropic=	62.2618	Anisotropy	=	176.3419
XX=	55.663	YX=	13.4368	ZX=	31.5463	
XY=	10.5954	YY=	-36.042	ZY=	27.6251	
XZ=	32.3359	YZ=	27.9535	ZZ=	167.1644	
Eigenvalues:	-40.4193	47.3816	179.8231			
75	C	Isotropic=	62.0547	Anisotropy	=	178.1829
XX=	-2.4998	YX=	-31.654	ZX=	53.0692	
XY=	-31.4083	YY=	25.963	ZY=	30.571	
XZ=	52.5926	YZ=	29.3746	ZZ=	162.701	
Eigenvalues:	-40.9333	46.2542	180.8434			
76	C	Isotropic=	63.732	Anisotropy	=	174.3882
XX=	-8.0403	YX=	39.0805	ZX=	43.5425	
XY=	42.5592	YY=	31.7294	ZY=	10.157	
XZ=	43.1172	YZ=	8.36	ZZ=	167.5067	
Eigenvalues:	-38.7221	49.9271	179.9908			
77	C	Isotropic=	66.1116	Anisotropy	=	164.5953
XX=	57.9851	YX=	8.96	ZX=	28.5563	
XY=	15.6799	YY=	-23.9726	ZY=	26.1828	
XZ=	28.4631	YZ=	28.446	ZZ=	164.3224	
Eigenvalues:	-28.671	51.1641	175.8419			
78	H	Isotropic=	23.2541	Anisotropy	=	7.8148
XX=	23.1203	YX=	2.4186	ZX=	-1.351	
XY=	2.592	YY=	26.8816	ZY=	-1.102	
XZ=	-1.6484	YZ=	-1.1677	ZZ=	19.7605	
Eigenvalues:	19.1839	22.1146	28.464			
79	H	Isotropic=	23.7192	Anisotropy	=	4.6397
XX=	26.1872	YX=	0.7803	ZX=	-1.7104	
XY=	0.4704	YY=	24.3908	ZY=	-0.4407	
XZ=	-1.4777	YZ=	-0.3172	ZZ=	20.5797	
Eigenvalues:	20.148	24.1974	26.8124			
80	H	Isotropic=	23.7099	Anisotropy	=	3.8273

XX= 24.6935 YX= -0.7307 ZX= -1.0132
 XY= -0.7965 YY= 25.8895 ZY= -0.3988
 XZ= -0.8739 YZ= -0.5009 ZZ= 20.5466
 Eigenvalues: 20.2765 24.5917 26.2614
 81 H Isotropic= 23.9105 Anisotropy = 5.4122
 XX= 25.4107 YX= 1.5058 ZX= -1.4848
 XY= 1.487 YY= 25.878 ZY= -1.0258
 XZ= -1.0365 YZ= -1.0088 ZZ= 20.4428
 Eigenvalues: 20.0638 24.1491 27.5186
 82 H Isotropic= 24.0268 Anisotropy = 8.962
 XX= 29.0351 YX= 2.3287 ZX= -2.2093
 XY= 1.8946 YY= 23.7045 ZY= -0.6331
 XZ= -0.9294 YZ= 0.1007 ZZ= 19.3409
 Eigenvalues: 19.0921 22.9868 30.0015

2a-iv

C	-2.765221	0.096905	-1.664852
C	-3.839005	0.128371	-2.254098
C	-3.758358	-1.326806	-1.763087
C	-4.947131	-1.750788	-0.88172
C	-5.122419	-0.934742	0.414618
C	-3.901826	-0.643905	1.274097
C	-2.846076	0.185957	0.602814
C	-1.585407	-0.316909	0.545633
C	-0.636247	0.25574	-0.470721
C	-1.339011	0.540923	-1.800267
C	-3.108037	1.45173	-0.183508
C	-4.513895	2.024315	-0.097984
C	-2.168975	2.571502	0.302823
C	-1.080877	-1.438692	1.369334
C	-6.237957	-1.776523	-1.668257
O	-2.753947	2.276531	-2.466822
O	-3.774148	0.174556	-3.671112
O	-6.257731	-0.705770	0.838386
O	-4.16556	-0.276806	2.624596
O	0.383836	-0.744941	-0.698218
H	-2.848721	0.080981	-3.929135
C	-5.118567	0.618069	3.033021
O	-5.773726	1.262255	2.221412
C	-5.200283	0.661821	4.523883
H	-4.865578	0.544674	-2.037268
H	-2.807436	-1.508594	-1.20269
H	-3.467097	-1.690149	1.44507
H	-0.129883	1.18266	-0.078362
H	-0.712484	1.285296	-2.366608
H	-1.360187	-0.404254	-2.403897
H	-5.315441	1.257247	-0.196581
H	-4.661671	2.537314	0.885035
H	-4.652367	2.789019	-0.902186
H	-2.744314	3.497129	0.549782
H	-1.616489	2.261125	1.221093
H	-1.436427	2.845769	-0.495556
H	-1.599206	-1.485796	2.359059
H	-1.226375	-2.408831	0.829245
H	0.015823	-1.315973	1.557155
H	-7.066485	-2.17499	-1.032955

H	-6.523324	-0.749942	-2.001836
H	-6.123863	-2.426493	-2.568706
H	-4.349778	0.111464	4.992157
H	-5.186048	1.72865	4.854401
H	-6.164004	0.191067	4.838699
H	-3.662065	2.461226	-2.738231
C	1.530094	-0.354105	-1.338519
O	1.657404	0.826411	-1.653881
H	-4.72566-2.799422	-0.524583	
H	-3.755054	-1.994852	-2.666076
C	2.48871 -1.519537	-1.495177	
C	3.921301	-1.245166	-0.915255
O	1.925263	-2.706193	-0.990221
H	2.595445	-1.713314	-2.604271
N	4.08177 0.063239	-0.334395	
C	4.324947	-2.339811	0.048428
H	4.614287	-1.293844	-1.816514
H	1.719507	-2.57055-0.054908	
C	5.021438	0.966871	-0.814244
H	3.703135	0.210488	0.570839
C	3.783016	-2.415427	1.336838
C	4.193605	-3.418178	2.213769
C	5.145998	-4.353971	1.809921
C	5.687365	-4.283522	0.526812
C	5.281715	-3.278975	-0.351482
H	3.026499	-1.686979	1.66582
O	5.567575	0.802617	-1.921605
C	5.281459	2.168372	0.028481
H	3.76417 -3.471345	3.225055	
H	5.468499	-5.145532.502209	
H	6.438285	-5.020317	0.204557
H	5.717181	-3.226759	-1.36138
C	5.284098	3.425962	-0.584953
C	5.537423	4.566295	0.17652
C	5.795001	4.452604	1.542731
C	5.800965	3.19687 2.151041	
C	5.541348	2.052819	1.397417
H	5.092009	3.502058	-1.66711
H	5.536272	5.555796	-0.304287
H	5.996826	5.353496	2.141211
H	6.012382	3.107254	3.226675
H	5.560381	1.064845	1.8812

2aivliz E(RB+HF-PW91) = -2012.293116

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic= 109.541 Anisotropy 28.3878

XX= 95.5111 YX= -7.9235 ZX= 3.9654

XY= -5.2105 YY= 124.897 ZY= -7.5068

XZ= -2.8267 YZ= -5.7954 ZZ= 108.215

Eigenvalues: 94.0564 106.1004 128.4662

2 C Isotropic= 112.3847 Anisotropy 30.4475

XX= 96.4097 YX= 5.2477 ZX= -8.7118

XY= 7.4116 YY= 108.5921 ZY= -1.9424

XZ= 0.8087 YZ= 6.3588 ZZ= 132.1522

Eigenvalues: 93.1963 111.2748 132.683

3	C	Isotropic=	142.1631	Anisotropy	20.5324
XX=	123.2083	YX=	9.7692	ZX=	4.2554
XY=	6.4478	YY=	152.1925	ZY=	2.5325
XZ=	-1.7147	YZ=	2.4051	ZZ=	151.0883
Eigenvalues:	121.0818		149.556		155.8513
4	C	Isotropic=	140.1753	Anisotropy	24.6553
XX=	125.3467	YX=	3.6878	ZX=	0.5576
XY=	4.1434	YY=	144.0002	ZY=	8.6151
XZ=	13.7712	YZ=	3.149	ZZ=	151.1791
Eigenvalues:	123.2145		140.6993		156.6122
5	C	Isotropic=	-21.8279	Anisotropy	179.2961
XX=	-65.0613	YX=	-10.3224	ZX=	-36.7092
XY=	1.963	YY=	51.0487	ZY=	-85.2329
XZ=	-21.3892	YZ=	-79.9934	ZZ=	-51.4713
Eigenvalues:	-113.216		-49.9706		97.7028
6	C	Isotropic=	102.2472	Anisotropy	41.4607
XX=	87.5434	YX=	3.933	ZX=	9.8666
XY=	3.0605	YY=	96.1229	ZY=	14.173
XZ=	-6.2021	YZ=	15.5506	ZZ=	123.0754
Eigenvalues:	85.7393		91.1147		129.8877
7	C	Isotropic=	42.661	Anisotropy	159.3783
XX=	31.6434	YX=	-13.6573	ZX=	35.3452
XY=	-13.3244	YY=	17.9946	ZY=	82.0383
XZ=	63.4972	YZ=	89.7668	ZZ=	78.3449
Eigenvalues:	-60.845		39.9147		148.9132
8	C	Isotropic=	43.3744	Anisotropy	153.4345
XX=	48.1693	YX=	3.0911	ZX=	42.2
XY=	13.4152	YY=	34.217	ZY=	101.7385
XZ=	28.5332	YZ=	86.4329	ZZ=	47.7369
Eigenvalues:	-56.6232		41.0824		145.664
9	C	Isotropic=	111.6846	Anisotropy	46.5483
XX=	115.5147	YX=	-27.9202	ZX=	-2.7762
XY=	-31.5626	YY=	106.4432	ZY=	5.6204
XZ=	-7.5469	YZ=	3.8365	ZZ=	113.0959
Eigenvalues:	80.8921		111.4449		142.7168
10	C	Isotropic=	148.5267	Anisotropy	41.2385
XX=	160.9757	YX=	-18.6864	ZX=	1.2076
XY=	-25.9946	YY=	140.0881	ZY=	-6.5668
XZ=	8.2797	YZ=	2.4759	ZZ=	144.5164
Eigenvalues:	125.8337		143.7275		176.0191
11	C	Isotropic=	147.7933	Anisotropy	13.4563
XX=	144.4304	YX=	1.8471	ZX=	-1.1789
XY=	6.7731	YY=	145.0394	ZY=	4.2612
XZ=	11.8883	YZ=	-3.3525	ZZ=	153.9102
Eigenvalues:	139.4023		147.2135		156.7642
12	C	Isotropic=	155.8275	Anisotropy	24.2532
XX=	168.8091	YX=	11.7127	ZX=	-0.6503
XY=	2.5135	YY=	152.4717	ZY=	8.5603
XZ=	-1.0245	YZ=	14.4996	ZZ=	146.2018
Eigenvalues:	136.5904		158.896		171.9963
13	C	Isotropic=	148.4636	Anisotropy	54.5209
XX=	151.7471	YX=	16.9545	ZX=	20.6293
XY=	14.6565	YY=	162.0915	ZY=	14.9877
XZ=	25.3283	YZ=	10.6012	ZZ=	131.5521
Eigenvalues:	116.4356		144.1443		184.8108
14	C	Isotropic=	167.6682	Anisotropy	12.8515

XX=	164.3695	YX=	2.703	ZX=	6.9322		
XY=	-5.6103	YY=	168.9479	ZY=	-7.5579		
XZ=	-0.1564	YZ=	-4.2109	ZZ=	169.6871		
Eigenvalues:	162.1754		164.5933		176.2358		
15	C	Isotropic=	169.3614	Anisotropy		17.1931	
XX=	175.8991	YX=	3.8865	ZX=	2.5781		
XY=	1.0253	YY=	159.3649	ZY=	6.5391		
XZ=	6.4772	YZ=	6.5749	ZZ=	172.8203		
Eigenvalues:	156.6799		170.5808		180.8235		
16	O	Isotropic=	263.0995	Anisotropy		82.9214	
XX=	308.0424	YX=	-18.9027	ZX=	15.7183		
XY=	-12.9008	YY=	287.2538	ZY=	-25.5927		
XZ=	10.6606	YZ=	12.6121	ZZ=	194.0024		
Eigenvalues:	192.264	278.6541		318.3805			
17	O	Isotropic=	265.3214	Anisotropy		44.696	
XX=	257.4385	YX=	6.9286	ZX=	-27.7491		
XY=	16.6453	YY=	279.0074	ZY=	-14.4303		
XZ=	-3.6699	YZ=	-13.7378	ZZ=	259.5183		
Eigenvalues:	242.694	258.1515		295.1187			
18	O	Isotropic=	-371.7438	Anisotropy		1098.2854	
XX=	-956.5189	YX=	110.3662	ZX=	179.0642		
XY=	162.292	YY=	165.8342	ZY=	-378.9001		
XZ=	128.3945	YZ=	-346.9073	ZZ=	-324.5467		
Eigenvalues:	-1035.2113	-440.4666		360.4464			
19	O	Isotropic=	95.4514	Anisotropy		127.2602	
XX=	160.1558	YX=	7.1945	ZX=	-113.4576		
XY=	20.4496	YY=	140.4654	ZY=	95.4911		
XZ=	-11.6472	YZ=	-14.9742	ZZ=	-14.267		
Eigenvalues:	-44.1887	150.2514		180.2915			
20	O	Isotropic=	69.4207	Anisotropy		185.3566	
XX=	107.7597	YX=	16.16	ZX=	35.1482		
XY=	136.8983	YY=	-86.7443	ZY=	-5.1303		
XZ=	-13.2785	YZ=	46.034	ZZ=	187.2467		
Eigenvalues:	-114.0709		129.3413		192.9918		
21	H	Isotropic=	31.1139	Anisotropy		13.499	
XX=	36.6527	YX=	-0.2513	ZX=	-4.2074		
XY=	-0.2186	YY=	21.8573	ZY=	2.5657		
XZ=	-4.1086	YZ=	1.4334	ZZ=	34.8318		
Eigenvalues:	21.5454	31.6832	40.1132				
22	C	Isotropic=	21.9293	Anisotropy		79.1206	
XX=	27.1397	YX=	40.8353	ZX=	69.902		
XY=	38.3089	YY=	33.781	ZY=	-68.9297		
XZ=	39.7048	YZ=	-36.834	ZZ=	4.8674		
Eigenvalues:	-78.6637	69.7753	74.6764				
23	O	Isotropic=	-141.4623	Anisotropy		607.3423	
XX=	-104.263	YX=	352.0727	ZX=	-46.3745		
XY=	333.6531	YY=	-56.369	ZY=	41.7694		
XZ=	-4.5538	YZ=	19.7945	ZZ=	-263.7548		
Eigenvalues:	-433.2747		-254.5447		263.4326		
24	C	Isotropic=	165.8091	Anisotropy		37.7509	
XX=	152.845	YX=	-5.5859	ZX=	-2.3235		
XY=	-6.4029	YY=	153.9009	ZY=	1.8574		
XZ=	-0.062	YZ=	3.8712	ZZ=	190.6813		
Eigenvalues:	147.3293		159.1216		190.9763		
25	H	Isotropic=	27.5155	Anisotropy		3.0441	
XX=	28.4843	YX=	0.732	ZX=	-0.6031		

XY=	0.8627	YY=	25.7261	ZY=	0.626		
XZ=	-1.6514	YZ=	1.4417	ZZ=	28.3362		
Eigenvalues:	24.9865	28.0152	29.545				
26	H	Isotropic=	28.2427	Anisotropy		8.5714	
XX=	30.6607	YX=	2.4164	ZX=	4.0881		
XY=	1.8316	YY=	26.9016	ZY=	1.2086		
XZ=	3.7575	YZ=	0.6847	ZZ=	27.1657		
Eigenvalues:	24.5436	26.2275	33.9569				
27	H	Isotropic=	25.4107	Anisotropy		4.0356	
XX=	25.5361	YX=	-0.2532	ZX=	-3.0755		
XY=	-2.4899	YY=	24.3854	ZY=	-0.061		
XZ=	-0.2809	YZ=	1.1404	ZZ=	26.3108		
Eigenvalues:	23.3594	24.7717	28.1012				
28	H	Isotropic=	25.2221	Anisotropy		6.7758	
XX=	29.1971	YX=	-1.7884	ZX=	0.3885		
XY=	-1.2744	YY=	25.2871	ZY=	1.2327		
XZ=	0.4039	YZ=	3.0483	ZZ=	21.182		
Eigenvalues:	20.1628	25.7642	29.7393				
29	H	Isotropic=	27.688	Anisotropy		7.9051	
XX=	32.7807	YX=	0.2343	ZX=	-0.9416		
XY=	0.3822	YY=	24.5227	ZY=	-2.8815		
XZ=	-0.6393	YZ=	-5.1444	ZZ=	25.7604		
Eigenvalues:	21.0744	29.0314	32.958				
30	H	Isotropic=	29.6633	Anisotropy		5.613	
XX=	32.7402	YX=	-1.6608	ZX=	1.7861		
XY=	-1.1673	YY=	27.6696	ZY=	3.2458		
XZ=	1.7009	YZ=	2.5003	ZZ=	28.5801		
Eigenvalues:	24.6143	30.9703	33.4053				
31	H	Isotropic=	29.5008	Anisotropy		8.3885	
XX=	32.6525	YX=	2.9893	ZX=	-1.5249		
XY=	3.3771	YY=	30.45	ZY=	-1.0459		
XZ=	-1.0571	YZ=	0.2062	ZZ=	25.3997		
Eigenvalues:	25.1726	28.2366	35.0931				
32	H	Isotropic=	29.3118	Anisotropy		9.0512	
XX=	28.2531	YX=	-1.0017	ZX=	-5.0832		
XY=	-1.2706	YY=	28.3708	ZY=	1.4858		
XZ=	-4.4138	YZ=	1.8141	ZZ=	31.3115		
Eigenvalues:	24.7928	27.7967	35.3459				
33	H	Isotropic=	30.3328	Anisotropy		6.6745	
XX=	30.6329	YX=	-3.6406	ZX=	-0.8692		
XY=	-3.6814	YY=	31.0774	ZY=	-2.4738		
XZ=	-0.5242	YZ=	-1.9524	ZZ=	29.2881		
Eigenvalues:	25.9161	30.2999	34.7824				
34	H	Isotropic=	30.2034	Anisotropy		8.9682	
XX=	29.4398	YX=	0.7726	ZX=	0.3672		
XY=	-1.0233	YY=	35.1493	ZY=	3.5085		
XZ=	-0.0548	YZ=	2.9682	ZZ=	26.0211		
Eigenvalues:	24.9811	29.4469	36.1822				
35	H	Isotropic=	30.3962	Anisotropy		6.2285	
XX=	30.558	YX=	-0.4219	ZX=	3.4057		
XY=	1.4784	YY=	29.9719	ZY=	2.4369		
XZ=	2.6067	YZ=	2.1801	ZZ=	30.6586		
Eigenvalues:	26.9594	29.6806	34.5485				
36	H	Isotropic=	28.4872	Anisotropy		6.5867	
XX=	30.1298	YX=	2.1152	ZX=	-1.6121		
XY=	3.3955	YY=	30.103	ZY=	-0.0806		

XZ=	-0.6995	YZ=	1.7828	ZZ=	25.2289		
Eigenvalues:	24.5159	28.0675	32.8784				
37	H	Isotropic=	28.9509	Anisotropy		7.7572	
XX=	29.5559	YX=	-2.8984	ZX=	-1.4568		
XY=	-1.7212	YY=	24.3476	ZY=	-2.112		
XZ=	-2.7341	YZ=	-2.7065	ZZ=	32.9493		
Eigenvalues:	22.591	30.1393	34.1224				
38	H	Isotropic=	29.0099	Anisotropy		6.0721	
XX=	28.2351	YX=	-0.4256	ZX=	-0.1958		
XY=	-0.7462	YY=	32.9328	ZY=	0.5993		
XZ=	-0.2628	YZ=	0.5902	ZZ=	25.8617		
Eigenvalues:	25.7985	28.1732	33.0579				
39	H	Isotropic=	29.0563	Anisotropy		8.6989	
XX=	34.7074	YX=	-0.8724	ZX=	-0.3683		
XY=	-1.2286	YY=	23.7959	ZY=	-2.3284		
XZ=	0.8213	YZ=	-3.6452	ZZ=	28.6656		
Eigenvalues:	22.3184	29.9949	34.8555				
40	H	Isotropic=	29.2132	Anisotropy		10.8747	
XX=	34.0714	YX=	3.6764	ZX=	-3.012		
XY=	4.7506	YY=	26.1164	ZY=	0.4041		
XZ=	-1.7802	YZ=	-0.7531	ZZ=	27.4518		
Eigenvalues:	24.0872	27.0894	36.463				
41	H	Isotropic=	29.6792	Anisotropy		5.8036	
XX=	31.7286	YX=	-0.8299	ZX=	2.0787		
XY=	-0.5817	YY=	30.6223	ZY=	-2.3487		
XZ=	2.6529	YZ=	-2.1536	ZZ=	26.6869		
Eigenvalues:	25.107	30.3824	33.5483				
42	H	Isotropic=	30.4969	Anisotropy		9.7058	
XX=	29.8528	YX=	2.025	ZX=	1.9798		
XY=	2.4222	YY=	29.7015	ZY=	5.0502		
XZ=	1.6766	YZ=	4.7564	ZZ=	31.9363		
Eigenvalues:	25.6843	28.8389	36.9674				
43	H	Isotropic=	29.1264	Anisotropy		5.5678	
XX=	29.2245	YX=	-3.1339	ZX=	0.0063		
XY=	-3.2628	YY=	26.2051	ZY=	0.0384		
XZ=	1.8608	YZ=	-1.5242	ZZ=	31.9495		
Eigenvalues:	24.1759	30.365	32.8382				
44	H	Isotropic=	29.2263	Anisotropy		7.532	
XX=	25.9931	YX=	-0.2258	ZX=	0.1512		
XY=	-0.8099	YY=	31.3911	ZY=	2.2672		
XZ=	-1.2142	YZ=	4.3194	ZZ=	30.2945		
Eigenvalues:	25.9239	27.5073	34.2476				
45	H	Isotropic=	28.9161	Anisotropy		8.3415	
XX=	30.9993	YX=	1.8929	ZX=	-2.6344		
XY=	2.167	YY=	26.1924	ZY=	-1.3661		
XZ=	-4.2736	YZ=	-1.1072	ZZ=	29.5566		
Eigenvalues:	25.4496	26.8217	34.4771				
46	H	Isotropic=	30.7262	Anisotropy		18.1514	
XX=	36.0066	YX=	-6.093	ZX=	6.7583		
XY=	-5.2398	YY=	28.2898	ZY=	-5.132		
XZ=	4.0275	YZ=	-6.4004	ZZ=	27.8822		
Eigenvalues:	22.3158	27.0356	42.8271				
47	C	Isotropic=	14.1593	Anisotropy		87.3925	
XX=	-51.9531	YX=	40.0299	ZX=	50.7703		
XY=	-5.0783	YY=	49.0569	ZY=	9.6992		
XZ=	57.1731	YZ=	-7.452	ZZ=	45.3742		

Eigenvalues: -77.862947.9199 72.421
 48 O Isotropic= -121.5416 Anisotropy 652.622
 XX= -161.8689 YX= 35.0269 ZX= 212.4318
 XY= 17.5793 YY= -365.9312 ZY= 145.7641
 XZ= 229.9677 YZ= 188.4658 ZZ= 163.1754
 Eigenvalues: -421.453-256.7114 313.5398
 49 H Isotropic= 28.7337 Anisotropy 6.4709
 XX= 28.5443 YX= 1.7006 ZX= 1.7648
 XY= 0.248 YY= 31.9283 ZY= -2.5198
 XZ= 1.8391 YZ= -3.1566 ZZ= 25.7284
 Eigenvalues: 23.7605 29.3928 33.0476
 50 H Isotropic= 29.4742 Anisotropy 6.6695
 XX= 28.2035 YX= 1.4891 ZX= -0.3849
 XY= 1.6312 YY= 30.1304 ZY= 4.3264
 XZ= -0.7713 YZ= 3.1151 ZZ= 30.0886
 Eigenvalues: 25.5199 28.9821 33.9205
 51 C Isotropic= 115.1174 Anisotropy 32.8867
 XX= 116.9953 YX= 8.5428 ZX= 0.9941
 XY= 6.2998 YY= 131.781 ZY= -10.6377
 XZ= 1.943 YZ= -10.5933 ZZ= 96.576
 Eigenvalues: 93.1143 115.1961 137.0419
 52 C Isotropic= 129.4086 Anisotropy 36.9834
 XX= 130.6556 YX= -5.8097 ZX= 15.1023
 XY= -7.1883 YY= 143.7994 ZY= -10.0495
 XZ= 12.8701 YZ= -15.0599 ZZ= 113.7707
 Eigenvalues: 104.191 129.9705 154.0641
 53 O Isotropic= 252.8993 Anisotropy 56.6065
 XX= 271.4449 YX= -37.8944 ZX= 17.0026
 XY= -38.9308 YY= 209.9112 ZY= 31.6768
 XZ= 10.2046 YZ= 15.2843 ZZ= 277.3417
 Eigenvalues: 183.647 284.414 290.6369
 54 H Isotropic= 26.1589 Anisotropy 6.0641
 XX= 25.6262 YX= 0.4568 ZX= 0.517
 XY= 0.5069 YY= 22.7954 ZY= 1.4094
 XZ= -1.3764 YZ= 0.4494 ZZ= 30.055
 Eigenvalues: 22.5848 25.6902 30.2016
 55 N Isotropic= 123.9332 Anisotropy 98.6012
 XX= 140.7788 YX= 27.9951 ZX= 42.4983
 XY= 20.0816 YY= 159.9874 ZY= -39.6121
 XZ= 14.911 YZ= -73.8879 ZZ= 71.0333
 Eigenvalues: 31.2943 150.8379 189.6673
 56 C Isotropic= 50.9427 Anisotropy 192.7085
 XX= 88.955 YX= 84.8943 ZX= 39.3132
 XY= 73.9359 YY= 47.8312 ZY= 69.5157
 XZ= 29.2973 YZ= 63.1472 ZZ= 16.0418
 Eigenvalues: -42.292815.7059 179.415
 57 H Isotropic= 24.5335 Anisotropy 5.6842
 XX= 25.4602 YX= -0.6636 ZX= -3.5659
 XY= -0.3221 YY= 23.8904 ZY= -0.2561
 XZ= -3.2377 YZ= -0.183 ZZ= 24.25
 Eigenvalues: 21.3086 23.969 28.323
 58 H Isotropic= 30.5685 Anisotropy 12.0573
 XX= 30.5482 YX= -1.3226 ZX= -3.0247
 XY= 1.7311 YY= 24.2137 ZY= 0.391
 XZ= -3.7044 YZ= -4.0764 ZZ= 36.9436
 Eigenvalues: 23.9396 29.1592 38.6067

59 C Isotropic= 17.6237 Anisotropy 114.7045
 XX= 32.014 YX= -73.0818 ZX= 17.1364
 XY= -59.6872 YY= -26.0048 ZY= -33.4974
 XZ= 18.4497 YZ= -19.4231 ZZ= 46.8619
 Eigenvalues: -70.817 29.5948 94.0934

60 H Isotropic= 26.5687 Anisotropy 7.2674
 XX= 24.4319 YX= 6.9704 ZX= 0.0573
 XY= 1.7483 YY= 28.571 ZY= 1.2056
 XZ= -0.8557 YZ= 0.7966 ZZ= 26.7031
 Eigenvalues: 21.5275 26.7649 31.4136

61 C Isotropic= 67.2634 Anisotropy 159.8956
 XX= 79.9414 YX= 92.1153 ZX= 47.101
 XY= 88.6032 YY= 56.8837 ZY= 4.5555
 XZ= 50.1722 YZ= 2.154 ZZ= 64.9651
 Eigenvalues: -32.4705 60.4002 173.8605

62 C Isotropic= 62.6229 Anisotropy 175.7115
 XX= 102.6244 YX= 54.6666 ZX= 69.4928
 XY= 53.876 YY= 96.0184 ZY= 30.6996
 XZ= 64.3983 YZ= 30.4636 ZZ= -10.7742
 Eigenvalues: -42.0135 50.1182 179.7639

63 C Isotropic= 64.7334 Anisotropy 174.4281
 XX= 112.7532 YX= 73.6329 ZX= 17.859
 XY= 76.6925 YY= 49.9463 ZY= 64.5552
 XZ= 16.9456 YZ= 64.5726 ZZ= 31.5008
 Eigenvalues: -35.7593 48.9407 181.0189

64 C Isotropic= 60.1532 Anisotropy 177.4043
 XX= 76.203 YX= 97.1424 ZX= 49.0861
 XY= 98.6917 YY= 52.5705 ZY= 8.3918
 XZ= 51.7638 YZ= 9.2899 ZZ= 51.6861
 Eigenvalues: -42.6991 44.7359 178.4227

65 C Isotropic= 57.7462 Anisotropy 153.1142
 XX= 92.0803 YX= 48.4103 ZX= 58.9816
 XY= 44.392 YY= 94.8283 ZY= 20.4955
 XZ= 58.8468 YZ= 26.2351 ZZ= -13.67
 Eigenvalues: -40.0072 53.4235 159.8224

66 H Isotropic= 24.2802 Anisotropy 7.8315
 XX= 22.3851 YX= -0.0799 ZX= 0.4625
 XY= -0.3819 YY= 22.519 ZY= -3.0472
 XZ= 0.2193 YZ= -3.5033 ZZ= 27.9364
 Eigenvalues: 20.9745 22.3648 29.5011

67 O Isotropic= -91.3372 Anisotropy 662.9348
 XX= 6.7952 YX= -190.1102 ZX= 323.6362
 XY= -201.4911 YY= -55.113 ZY= -123.427
 XZ= 282.7364 YZ= -134.2659 ZZ= -225.6938
 Eigenvalues: -434.2335 -190.3975 350.6193

68 C Isotropic= 55.462 Anisotropy 173.5219
 XX= 158.203 YX= 1.4034 ZX= -55.4086
 XY= -18.4645 YY= -9.4352 ZY= -23.2109
 XZ= -33.6981 YZ= -26.0521 ZZ= 17.6183
 Eigenvalues: -29.353 24.5958 171.1433

69 H Isotropic= 23.6635 Anisotropy 5.7889
 XX= 22.6818 YX= -2.8608 ZX= 0.2707
 XY= -3.0128 YY= 24.261 ZY= -1.8816
 XZ= 0.2119 YZ= -2.3538 ZZ= 24.0479
 Eigenvalues: 20.0813 23.3866 27.5228

70 H Isotropic= 23.6997 Anisotropy 3.5954

XX= 23.1559 YX= -2.6554 ZX= -1.4402
 XY= -2.4678 YY= 23.4112 ZY= -0.5256
 XZ= -1.4585 YZ= -0.7567 ZZ= 24.532
 Eigenvalues: 20.199 24.8035 26.0966
 71 H Isotropic= 23.6536 Anisotropy 4.2097
 XX= 22.3453 YX= -2.2374 ZX= -0.8961
 XY= -2.0072 YY= 23.7021 ZY= -1.9663
 XZ= -0.7821 YZ= -1.9245 ZZ= 24.9134
 Eigenvalues: 20.0741 24.4266 26.4601
 72 H Isotropic= 23.7391 Anisotropy 8.3614
 XX= 23.6756 YX= -4.5775 ZX= -0.6384
 XY= -4.3191 YY= 25.735 ZY= -0.924
 XZ= -0.3387 YZ= -1.2768 ZZ= 21.8066
 Eigenvalues: 19.6126 22.2914 29.3134
 73 C Isotropic= 59.2977 Anisotropy 178.6587
 XX= 171.0694 YX= -6.2279 ZX= -35.387
 XY= -10.0723 YY= 39.3041 ZY= 11.7687
 XZ= -39.0092 YZ= 13.0584 ZZ= -32.4804
 Eigenvalues: -40.5357 40.0253 178.4034
 74 C Isotropic= 61.9338 Anisotropy 177.5362
 XX= 174.6599 YX= -9.4883 ZX= -24.7897
 XY= -11.1253 YY= -21.2643 ZY= 36.0645
 XZ= -25.0343 YZ= 38.6789 ZZ= 32.4057
 Eigenvalues: -40.461 45.971 180.2912
 75 C Isotropic= 62.2848 Anisotropy 178.5985
 XX= 172.0348 YX= -26.1787 ZX= -34.9045
 XY= -24.6287 YY= -10.3565 ZY= -36.267
 XZ= -34.3033 YZ= -36.1258 ZZ= 25.1761
 Eigenvalues: -40.4906 45.9945 181.3505
 76 C Isotropic= 64.084 Anisotropy 174.7101
 XX= 171.4025 YX= -12.6161 ZX= -39.5691
 XY= -9.7482 YY= 51.0464 ZY= 11.0919
 XZ= -41.6651 YZ= 8.6735 ZZ= -30.1968
 Eigenvalues: -38.7168 50.4115 180.5574
 77 C Isotropic= 67.2232 Anisotropy 164.3678
 XX= 171.0044 YX= -8.0104 ZX= -24.5739
 XY= -7.8503 YY= -10.0226 ZY= 39.177
 XZ= -25.5471 YZ= 32.1055 ZZ= 40.6878
 Eigenvalues: -28.5101 53.3781 176.8017
 78 H Isotropic= 23.1809 Anisotropy 7.269
 XX= 20.1935 YX= 1.3939 ZX= -0.304
 XY= 1.5743 YY= 27.7454 ZY= -0.0715
 XZ= 0.0218 YZ= 0.0336 ZZ= 21.6039
 Eigenvalues: 19.9016 21.6143 28.0269
 79 H Isotropic= 23.7412 Anisotropy 4.1639
 XX= 20.9605 YX= 1.397 ZX= 0.9437
 XY= 1.1108 YY= 25.0342 ZY= 0.7349
 XZ= 1.0094 YZ= 1.1395 ZZ= 25.229
 Eigenvalues: 20.5003 24.2062 26.5172
 80 H Isotropic= 23.7598 Anisotropy 3.6012
 XX= 20.8921 YX= 0.6243 ZX= 1.0231
 XY= 0.7058 YY= 25.2311 ZY= -1.0639
 XZ= 1.0051 YZ= -0.8465 ZZ= 25.156
 Eigenvalues: 20.5029 24.6159 26.1606
 81 H Isotropic= 23.9783 Anisotropy 5.3076
 XX= 20.9893 YX= 1.4125 ZX= 1.4799

XY=	1.2165	YY=	26.8956	ZY=	0.7537
XZ=	1.1486	YZ=	0.8535	ZZ=	24.05
Eigenvalues:	20.3556	24.0627	27.5168		
82	H	Isotropic=	24.2244	Anisotropy	8.5279
XX=	21.3473	YX=	3.1843	ZX=	2.915
XY=	1.9132	YY=	25.5142	ZY=	2.6282
XZ=	2.159	YZ=	2.8384	ZZ=	25.8117
Eigenvalues:	19.8351	22.9284	29.9097		

2a-iv2

C	-2.770965	0.995005	-1.714258
C	-3.844752	-0.004444	-2.249389
C	-3.756702	-1.433573	-1.688163
C	-4.939303	-1.817429	-0.780496
C	-5.110243	-0.939388	0.475279
C	-3.885978	-0.603141	1.312686
C	-2.836586	0.195999	0.595711
C	-1.574863	-0.306330	0.555798
C	-0.632345	0.221177	-0.490697
C	-1.343196	0.437899	-1.829355
C	-3.107064	1.420997	-0.250342
C	-4.514445	1.992294	-0.183599
C	-2.169411	2.56647	0.175039
C	-1.062499	-1.381915	1.434269
C	-6.234131	-1.88557	-1.557912
O	-2.767194	2.130592	-2.577254
O	-3.788554	-0.030952	-3.667513
O	-6.244267	-0.693750	0.892937
O	-4.143851	-0.170818	2.644798
O	0.395067	-0.781945	-0.673808
H	-2.860835	-0.08916	-3.927608
C	-5.097334	0.740223	3.014415
O	-5.761549	1.339228	2.17591
C	-5.167810	0.859704	4.501673
H	-4.871607	0.418228	-2.046722
H	-2.802791	-1.58431	-1.123892
H	-3.446349	-1.6381	1.532952
H	-0.129532	1.168803	-0.146536
H	-0.722692	1.155993	-2.435365
H	-1.365119	-0.535117	-2.386469
H	-5.313941	1.219028	-0.242492
H	-4.658282	2.54891	0.776074
H	-4.660829	2.71967	-1.020264
H	-2.746858	3.500759	0.381183
H	-1.609788	2.302797	1.103555
H	-1.443235	2.804764	-0.640538
H	-1.568896	-1.370547	2.431282
H	-1.21968	-2.380845	0.953604
H	0.037356	-1.255142	1.600168
H	-7.057887	-2.255148	-0.899336
H	-6.52481	-0.877353	-1.939483
H	-6.122744	-2.578255	-2.426262
H	-4.311891	0.336397	4.990724
H	-5.154437	1.942059	4.777206
H	-6.127558	0.402903	4.847626
H	-3.681401	2.320277	-2.823404

C	1.535167	-0.412322	-1.337101
O	1.619334	0.73119	-1.778203
H	-4.712731	-2.846622	-0.373538
H	-3.756195	-2.144674	-2.557581
C	2.515484	-1.565523	-1.450981
C	3.93968	-1.260966	-0.87007
O	2.021982	-2.714874	-0.793147
H	2.625787	-1.773104	-2.55558
N	4.059916	0.069513	-0.32918
C	4.377106	-2.323915	0.111449
H	4.631078	-1.312898	-1.773472
H	1.127956	-2.878644	-1.123153
C	4.983216	0.980357	-0.827282
H	3.689771	0.221155	0.57978
C	3.841717	-2.387634	1.402079
C	4.298189	-3.348235	2.30374
C	5.290459	-4.250809	1.921978
C	5.823429	-4.193327	0.63444
C	5.37229	-3.231536	-0.268511
H	3.033618	-1.702135	1.697443
O	5.547765	0.79528	-1.922189
C	5.2025	2.214792	-0.021171
H	3.870763	-3.395728	3.315902
H	5.650159	-5.007944	2.633879
H	6.603686	-4.905995	0.329161
H	5.803111	-3.187591	-1.280463
C	5.181423	3.451544	-0.675294
C	5.396565	4.622024	0.051301
C	5.639744	4.559249	1.423448
C	5.669539	3.324463	2.072485
C	5.448166	2.150271	1.353733
H	5.001416	3.487586	-1.761562
H	5.376861	5.595045	-0.461598
H	5.81147	5.483893	1.994437
H	5.869559	3.275046	3.1529
H	5.485934	1.179349	1.870047

E(RB+HF-PW91)		=	-2012.293387		
SCF	GIAO	Magnetic	shielding	tensor (ppm):	
1	C	Isotropic=	109.3549	Anisotropy	= 28.3864
XX=	95.3439	YX=	-7.8109	ZX=	4.5754
XY=	-5.6474	YY=	123.92	ZY=	-8.2376
XZ=	-2.659	YZ=	-6.6083	ZZ=	108.8008
Eigenvalues:	93.8031	105.9825	128.2791		
2	C	Isotropic=	112.4393	Anisotropy	= 30.8676
XX=	96.1569	YX=	4.5952	ZX=	-8.8164
XY=	6.8763	YY=	108.9153	ZY=	-0.7467
XZ=	0.6072	YZ=	7.4308	ZZ=	132.2458
Eigenvalues:	93.3054	110.9949	133.0177		
3	C	Isotropic=	141.8977	Anisotropy	= 20.5228
XX=	122.814	YX=	10.1862	ZX=	3.7871
XY=	6.505	YY=	152.3328	ZY=	2.2926
XZ=	-2.22	YZ=	2.0504	ZZ=	150.5465
Eigenvalues:	120.6165	149.4971	155.5796		
4	C	Isotropic=	140.1433	Anisotropy	= 24.843

XX=	125.439	YX=	3.6241	ZX=	0.477				
XY=	4.704	YY=	144.5414	ZY=	9.159				
XZ=	13.9678	YZ=	3.5128	ZZ=	150.4495				
Eigenvalues:	123.2131			140.5116		156.7053			
5	C	Isotropic=		-21.7259	Anisotropy	=		179.1411	
XX=	-64.6947	YX=	-12.7339	ZX=	-35.3797				
XY=	0.3029	YY=	42.515	ZY=	-90.1858				
XZ=	-21.1411	YZ=	-84.7318	ZZ=	-42.9981				
Eigenvalues:	-113.094	-49.7853	97.7015						
6	C	Isotropic=		102.1442	Anisotropy	=		41.2364	
XX=	87.503	YX=	4.4593	ZX=	9.8311				
XY=	2.9949	YY=	97.6294	ZY=	15.4492				
XZ=	-6.2051	YZ=	16.5748	ZZ=	121.3002				
Eigenvalues:	85.642	91.1554	129.6351						
7	C	Isotropic=		42.9075	Anisotropy	=		159.0165	
XX=	32.9974	YX=	-11.4704	ZX=	35.8488				
XY=	-9.6867	YY=	26.5388	ZY=	84.8249				
XZ=	63.7885	YZ=	92.5663	ZZ=	69.1864				
Eigenvalues:	-60.6977	40.5018	148.9185						
8	C	Isotropic=		42.6252	Anisotropy	=		153.4796	
XX=	47.2467	YX=	4.8551	ZX=	42.6878				
XY=	14.8546	YY=	43.22	ZY=	101.6705				
XZ=	28.9414	YZ=	86.1396	ZZ=	37.4088				
Eigenvalues:	-57.2217	40.1523	144.9449						
9	C	Isotropic=		110.9183	Anisotropy	=		47.8786	
XX=	115.2228	YX=	-28.28	ZX=	-3.0284				
XY=	-32.152	YY=	106.6112	ZY=	4.9894				
XZ=	-6.8879	YZ=	3.9742	ZZ=	110.9207				
Eigenvalues:	80.3951	109.5223		142.8373					
10	C	Isotropic=		147.9661	Anisotropy	=		41.1318	
XX=	160.703	YX=	-18.3231	ZX=	2.2136				
XY=	-25.3653	YY=	139.3007	ZY=	-5.4511				
XZ=	9.9122	YZ=	3.082	ZZ=	143.8947				
Eigenvalues:	125.4046			143.1063		175.3873			
11	C	Isotropic=		147.9922	Anisotropy	=		14.0158	
XX=	144.3216	YX=	2.1559	ZX=	-1.1382				
XY=	7.321	YY=	145.5335	ZY=	4.85				
XZ=	11.9742	YZ=	-2.5781	ZZ=	154.1215				
Eigenvalues:	139.3001			147.3404		157.336			
12	C	Isotropic=		155.8493	Anisotropy	=		24.3299	
XX=	168.7715	YX=	11.9185	ZX=	-1.2875				
XY=	2.6243	YY=	153.5831	ZY=	8.1882				
XZ=	-1.4979	YZ=	14.015	ZZ=	145.1935				
Eigenvalues:	136.6229			158.8559		172.0693			
13	C	Isotropic=		148.6152	Anisotropy	=		54.4653	
XX=	152.0441	YX=	17.9236	ZX=	19.5999				
XY=	15.9443	YY=	163.4482	ZY=	13.4565				
XZ=	24.4399	YZ=	8.9417	ZZ=	130.3532				
Eigenvalues:	116.6445			144.2756		184.9254			
14	C	Isotropic=		167.681	Anisotropy	=		12.1526	
XX=	164.106	YX=	2.9385	ZX=	6.8262				
XY=	-5.8204	YY=	168.9058	ZY=	-7.0745				
XZ=	0.0989	YZ=	-3.3229	ZZ=	170.0312				
Eigenvalues:	162.3013			164.9589		175.7827			
15	C	Isotropic=		169.345	Anisotropy	=		17.1543	
XX=	175.8962	YX=	4.1133	ZX=	2.336				

XY=	1.543	YY=	159.9279	ZY=	7.164		
XZ=	6.1897	YZ=	7.2086	ZZ=	172.2108		
Eigenvalues:	156.5821		170.6717		180.7812		
16	O	Isotropic=	263.4192	Anisotropy	=	84.3502	
XX=	309.3867	YX=	-19.2388	ZX=	15.1028		
XY=	-12.8049	YY=	286.5423	ZY=	-29.6846		
XZ=	9.844	YZ=	8.8523	ZZ=	194.3286		
Eigenvalues:	192.178	278.4269		319.6527			
17	O	Isotropic=	265.3504	Anisotropy	=	45.7643	
XX=	257.3941	YX=	6.9666	ZX=	-26.4877		
XY=	20.3182	YY=	277.5762	ZY=	-13.9785		
XZ=	-5.3707	YZ=	-13.6542	ZZ=	261.0809		
Eigenvalues:	243.1584		257.0329		295.8599		
18	O	Isotropic=	-372.4188	Anisotropy	=	1098.772	
XX=	-957.4268	YX=	113.6329	ZX=	178.4149		
XY=	164.0257	YY=	129.4518	ZY=	-401.7197		
XZ=	124.1263	YZ=	-369.1418	ZZ=	-289.2814		
Eigenvalues:	-1036.6528		-440.6994		360.0959		
19	O	Isotropic=	95.3816	Anisotropy	=	127.2116	
XX=	159.2233	YX=	1.5741	ZX=	-115.3964		
XY=	20.7192	YY=	144.2016	ZY=	86.5969		
XZ=	-13.2365	YZ=	-22.712	ZZ=	-17.2802		
Eigenvalues:	-44.2994	150.2548		180.1893			
20	O	Isotropic=	73.9944	Anisotropy	=	181.7248	
XX=	110.1497	YX=	22.9519	ZX=	35.2378		
XY=	135.2781	YY=	-73.1574	ZY=	9.1041		
XZ=	-24.3771	YZ=	68.1686	ZZ=	184.9909		
Eigenvalues:	-106.639	133.4778		195.1442			
21	H	Isotropic=	31.1043	Anisotropy	=	13.4266	
XX=	36.6068	YX=	0.2974	ZX=	-4.2744		
XY=	0.4044	YY=	21.9836	ZY=	2.8241		
XZ=	-4.1466	YZ=	1.7564	ZZ=	34.7224		
Eigenvalues:	21.502	31.7554		40.0553			
22	C	Isotropic=	21.7851	Anisotropy	=	79.0665	
XX=	27.349	YX=	44.0862	ZX=	67.7968		
XY=	39.6528	YY=	28.4601	ZY=	-70.1203		
XZ=	37.3856	YZ=	-38.2081	ZZ=	9.5462		
Eigenvalues:	-78.6073	69.4665		74.4961			
23	O	Isotropic=	-141.2949	Anisotropy	=	606.6922	
XX=	-107.4021	YX=	348.8125	ZX=	-65.6801		
XY=	332.5935	YY=	-51.1426	ZY=	27.9953		
XZ=	-22.9055	YZ=	6.2446	ZZ=	-265.34		
Eigenvalues:	-432.8192		-254.2322		263.1666		
24	C	Isotropic=	165.8451	Anisotropy	=	37.6777	
XX=	152.9449	YX=	-5.6602	ZX=	-1.7681		
XY=	-6.1045	YY=	154.2915	ZY=	3.708		
XZ=	0.5246	YZ=	5.7749	ZZ=	190.299		
Eigenvalues:	147.5226		159.0491		190.9636		
25	H	Isotropic=	27.4788	Anisotropy	=	3.0517	
XX=	28.4321	YX=	0.6944	ZX=	-0.6432		
XY=	0.7429	YY=	25.7908	ZY=	0.7084		
XZ=	-1.6925	YZ=	1.5481	ZZ=	28.2135		
Eigenvalues:	24.979	27.9442		29.5132			
26	H	Isotropic=	28.3114	Anisotropy	=	8.5209	
XX=	30.7055	YX=	2.6439	ZX=	3.8655		
XY=	2.1083	YY=	27.1136	ZY=	1.21		

XZ=	3.6172	YZ=	0.7311	ZZ=	27.115				
Eigenvalues:	24.645	26.2971	33.992						
27	H	Isotropic=	25.3891	Anisotropy	=	4.0545			
XX=	25.4898	YX=	-0.4031	ZX=	-3.0762				
XY=	-2.4948	YY=	24.4065	ZY=	0.0367				
XZ=	-0.1321	YZ=	1.273	ZZ=	26.2708				
Eigenvalues:	23.3317	24.7434	28.0921						
28	H	Isotropic=	25.2381	Anisotropy	=	6.7233			
XX=	29.1769	YX=	-1.7258	ZX=	0.496				
XY=	-1.268	YY=	25.5382	ZY=	1.1014				
XZ=	0.4429	YZ=	2.8835	ZZ=	20.9993				
Eigenvalues:	20.1424	25.8517	29.7203						
29	H	Isotropic=	27.547	Anisotropy	=	8.1351			
XX=	32.7699	YX=	0.1743	ZX=	-1.008				
XY=	0.3924	YY=	23.9434	ZY=	-2.8277				
XZ=	-0.7571	YZ=	-5.1186	ZZ=	25.9277				
Eigenvalues:	20.8318	28.8388	32.9704						
30	H	Isotropic=	29.8141	Anisotropy	=	5.6634			
XX=	32.9844	YX=	-1.4696	ZX=	1.8157				
XY=	-0.9677	YY=	28.0716	ZY=	3.202				
XZ=	1.6794	YZ=	2.4403	ZZ=	28.3864				
Eigenvalues:	24.8654	30.9872	33.5897						
31	H	Isotropic=	29.4739	Anisotropy	=	8.4371			
XX=	32.6144	YX=	2.9175	ZX=	-1.6932				
XY=	3.3611	YY=	30.38	ZY=	-1.3316				
XZ=	-1.27	YZ=	-0.0636	ZZ=	25.4274				
Eigenvalues:	25.1325	28.1906	35.0987						
32	H	Isotropic=	29.2655	Anisotropy	=	9.1069			
XX=	28.1509	YX=	-1.2319	ZX=	-5.0179				
XY=	-1.4595	YY=	28.4388	ZY=	1.6024				
XZ=	-4.3958	YZ=	1.9103	ZZ=	31.2068				
Eigenvalues:	24.7292	27.7305	35.3368						
33	H	Isotropic=	30.3556	Anisotropy	=	6.7338			
XX=	30.6727	YX=	-3.7161	ZX=	-0.6529				
XY=	-3.7452	YY=	30.8779	ZY=	-2.5066				
XZ=	-0.336	YZ=	-2.0244	ZZ=	29.5162				
Eigenvalues:	25.9386	30.2835	34.8448						
34	H	Isotropic=	30.2107	Anisotropy	=	8.9805			
XX=	29.4617	YX=	0.7919	ZX=	0.2925				
XY=	-1.0184	YY=	35.4541	ZY=	3.049				
XZ=	-0.0602	YZ=	2.5307	ZZ=	25.7162				
Eigenvalues:	24.9691	29.4652	36.1976						
35	H	Isotropic=	30.3917	Anisotropy	=	6.2565			
XX=	30.5957	YX=	-0.2313	ZX=	3.432				
XY=	1.6373	YY=	30.1832	ZY=	2.4523				
XZ=	2.5376	YZ=	2.2072	ZZ=	30.3961				
Eigenvalues:	26.9549	29.6574	34.5626						
36	H	Isotropic=	28.5181	Anisotropy	=	6.6151			
XX=	30.0998	YX=	2.0793	ZX=	-1.7275				
XY=	3.3721	YY=	30.2325	ZY=	-0.3664				
XZ=	-0.9186	YZ=	1.5198	ZZ=	25.2219				
Eigenvalues:	24.5583	28.0678	32.9281						
37	H	Isotropic=	28.963	Anisotropy	=	7.7802			
XX=	29.4153	YX=	-2.9791	ZX=	-1.2249				
XY=	-1.8917	YY=	24.1556	ZY=	-1.5915				
XZ=	-2.4989	YZ=	-2.1895	ZZ=	33.3181				

Eigenvalues:	22.6365	30.1026	34.1498			
38	H	Isotropic=	29.1939	Anisotropy	=	6.2159
XX=	28.2492	YX=	-0.4575	ZX=	-0.2357	
XY=	-0.74	YY=	33.2625	ZY=	0.1	
XZ=	-0.2171	YZ=	0.2231	ZZ=	26.07	
Eigenvalues:	26.0453	28.1985	33.3378			
39	H	Isotropic=	28.6133	Anisotropy	=	8.8476
XX=	34.3784	YX=	-0.823	ZX=	-0.3731	
XY=	-1.1606	YY=	23.0499	ZY=	-2.1317	
XZ=	0.9175	YZ=	-3.3306	ZZ=	28.4115	
Eigenvalues:	21.8512	29.4769	34.5117			
40	H	Isotropic=	29.1993	Anisotropy	=	10.8814
XX=	34.0075	YX=	3.5334	ZX=	-3.2397	
XY=	4.6875	YY=	26.1103	ZY=	0.4394	
XZ=	-2.0531	YZ=	-0.7092	ZZ=	27.4802	
Eigenvalues:	24.0697	27.0747	36.4536			
41	H	Isotropic=	29.6552	Anisotropy	=	5.8227
XX=	31.7479	YX=	-0.7505	ZX=	2.0894	
XY=	-0.4677	YY=	30.3519	ZY=	-2.5183	
XZ=	2.6757	YZ=	-2.3148	ZZ=	26.8656	
Eigenvalues:	25.0858	30.3427	33.537			
42	H	Isotropic=	30.5024	Anisotropy	=	9.6965
XX=	29.8758	YX=	2.1456	ZX=	1.8578	
XY=	2.5271	YY=	30.1819	ZY=	5.1252	
XZ=	1.5597	YZ=	4.8321	ZZ=	31.4494	
Eigenvalues:	25.6826	28.8578	36.9667			
43	H	Isotropic=	29.1091	Anisotropy	=	5.5703
XX=	29.2487	YX=	-3.135	ZX=	0.178	
XY=	-3.1571	YY=	26.1089	ZY=	0.3542	
XZ=	2.0619	YZ=	-1.1967	ZZ=	31.9696	
Eigenvalues:	24.1558	30.3488	32.8226			
44	H	Isotropic=	29.2221	Anisotropy	=	7.5352
XX=	25.9869	YX=	-0.2017	ZX=	0.1773	
XY=	-0.8653	YY=	31.7162	ZY=	2.2045	
XZ=	-1.1495	YZ=	4.2481	ZZ=	29.9632	
Eigenvalues:	25.9219	27.4989	34.2456			
45	H	Isotropic=	28.9174	Anisotropy	=	8.3492
XX=	30.9367	YX=	1.7617	ZX=	-2.7424	
XY=	1.9583	YY=	26.083	ZY=	-1.2299	
XZ=	-4.3754	YZ=	-0.9578	ZZ=	29.7327	
Eigenvalues:	25.4465	26.8222	34.4836			
46	H	Isotropic=	30.7673	Anisotropy	=	18.206
XX=	36.2856	YX=	-6.1945	ZX=	6.532	
XY=	-5.4432	YY=	27.8073	ZY=	-5.0661	
XZ=	3.8651	YZ=	-6.3791	ZZ=	28.2091	
Eigenvalues:	22.2443	27.153	42.9047			
47	C	Isotropic=	13.5275	Anisotropy	=	88.8193
XX=	-51.121	YX=	41.3976	ZX=	49.0007	
XY=	-3.5625	YY=	50.9279	ZY=	9.3629	
XZ=	63.6803	YZ=	-4.671	ZZ=	40.7755	
Eigenvalues:	-79.8625	47.7046	72.7404			
48	O	Isotropic=	-122.1591	Anisotropy	=	653.0556
XX=	-156.8229	YX=	69.5653	ZX=	203.4081	
XY=	44.7106	YY=	-325.7943	ZY=	191.9077	
XZ=	231.7627	YZ=	248.7416	ZZ=	116.1399	
Eigenvalues:	-421.8092	-257.8794	313.2113			

49	H	Isotropic=	28.7559	Anisotropy	=	6.4613
XX=	28.5801	YX=	1.7489	ZX=	1.6359	
XY=	0.3421	YY=	31.6461	ZY=	-2.815	
XZ=	1.8061	YZ=	-3.4522	ZZ=	26.0415	
Eigenvalues:	23.8031	29.4011	33.0634			
50	H	Isotropic=	29.4907	Anisotropy	=	6.5939
XX=	28.2493	YX=	1.5069	ZX=	-0.4755	
XY=	1.6223	YY=	30.4722	ZY=	4.2697	
XZ=	-0.8237	YZ=	3.0489	ZZ=	29.7505	
Eigenvalues:	25.5455	29.0399	33.8866			
51	C	Isotropic=	114.8039	Anisotropy	=	30.2036
XX=	112.5884	YX=	7.9397	ZX=	-3.6894	
XY=	5.3729	YY=	131.4899	ZY=	-5.8505	
XZ=	-2.4912	YZ=	-6.4731	ZZ=	100.3334	
Eigenvalues:	98.8964	110.5757	134.9396			
52	C	Isotropic=	129.7912	Anisotropy	=	34.5803
XX=	130.7522	YX=	-5.9542	ZX=	13.3761	
XY=	-6.7627	YY=	142.3432	ZY=	-10.0178	
XZ=	12.9996	YZ=	-13.9394	ZZ=	116.2782	
Eigenvalues:	106.8726	129.6563	152.8448			
53	O	Isotropic=	275.7522	Anisotropy	=	110.679
XX=	340.2609	YX=	-1.1912	ZX=	27.8576	
XY=	-19.9128	YY=	238.6746	ZY=	14.0943	
XZ=	31.9495	YZ=	10.2341	ZZ=	248.321	
Eigenvalues:	224.2116	253.5068	349.5382			
54	H	Isotropic=	26.1473	Anisotropy	=	6.1469
XX=	25.1741	YX=	0.3656	ZX=	0.0544	
XY=	0.6677	YY=	23.1988	ZY=	1.1904	
XZ=	-1.5491	YZ=	0.3235	ZZ=	30.0688	
Eigenvalues:	22.9525	25.2441	30.2452			
55	N	Isotropic=	122.6263	Anisotropy	=	98.2169
XX=	138.0296	YX=	28.4994	ZX=	44.6349	
XY=	19.3285	YY=	157.8687	ZY=	-40.6241	
XZ=	17.162	YZ=	-74.3549	ZZ=	71.9806	
Eigenvalues:	29.5694	150.2052	188.1042			
56	C	Isotropic=	53.3006	Anisotropy	=	188.5611
XX=	82.8086	YX=	88.6311	ZX=	29.8946	
XY=	73.9783	YY=	60.6924	ZY=	66.9406	
XZ=	21.7331	YZ=	65.1713	ZZ=	16.4007	
Eigenvalues:	-40.0804	20.9741	179.008			
57	H	Isotropic=	24.5089	Anisotropy	=	5.8705
XX=	25.538	YX=	-0.7384	ZX=	-3.5475	
XY=	-0.5289	YY=	23.7292	ZY=	-0.403	
XZ=	-3.3571	YZ=	-0.3594	ZZ=	24.2595	
Eigenvalues:	21.1948	23.9094	28.4226			
58	H	Isotropic=	30.2708	Anisotropy	=	19.3402
XX=	41.1706	YX=	3.1288	ZX=	4.895	
XY=	3.8175	YY=	27.2504	ZY=	-0.288	
XZ=	5.0853	YZ=	0.9767	ZZ=	22.3912	
Eigenvalues:	21.1018	26.5463	43.1642			
59	C	Isotropic=	17.3912	Anisotropy	=	114.5661
XX=	34.8289	YX=	-70.6054	ZX=	19.8055	
XY=	-57.0181	YY=	-31.4565	ZY=	-31.3394	
XZ=	20.478	YZ=	-17.5242	ZZ=	48.8013	
Eigenvalues:	-71.174	29.5791	93.7686			
60	H	Isotropic=	26.4282	Anisotropy	=	7.1853

XX=	23.976	YX=	6.7714	ZX=	0.0242				
XY=	1.5425	YY=	28.7058	ZY=	1.1625				
XZ=	-0.9827	YZ=	0.9117	ZZ=	26.6028				
Eigenvalues:	21.389	26.6772	31.2184						
61	C	Isotropic=	61.8012	Anisotropy	=	169.5276			
XX=	67.3392	YX=	97.833	ZX=	46.9964				
XY=	92.3808	YY=	61.6771	ZY=	11.4183				
XZ=	49.5924	YZ=	9.0136	ZZ=	56.3875				
Eigenvalues:	-38.6643	49.2483	174.8197						
62	C	Isotropic=	63.9418	Anisotropy	=	173.7228			
XX=	98.0145	YX=	55.7924	ZX=	66.5532				
XY=	54.6722	YY=	103.7284	ZY=	30.9285				
XZ=	61.5618	YZ=	29.4611	ZZ=	-9.9175				
Eigenvalues:	-39.8503	51.9186	179.757						
63	C	Isotropic=	65.0339	Anisotropy	=	173.5015			
XX=	106.4693	YX=	76.19	ZX=	12.181				
XY=	79.5742	YY=	59.8523	ZY=	64.7464				
XZ=	11.2039	YZ=	64.0001	ZZ=	28.78				
Eigenvalues:	-35.7074	50.1074	180.7015						
64	C	Isotropic=	62.3998	Anisotropy	=	173.4686			
XX=	69.5488	YX=	97.6367	ZX=	45.1737				
XY=	99.2362	YY=	63.1421	ZY=	9.5211				
XZ=	47.4994	YZ=	9.4594	ZZ=	54.5087				
Eigenvalues:	-39.6202	48.7742	178.0456						
65	C	Isotropic=	58.6946	Anisotropy	=	151.1147			
XX=	88.9198	YX=	48.8858	ZX=	56.4274				
XY=	43.5787	YY=	101.6295	ZY=	20.6817				
XZ=	55.4675	YZ=	25.3141	ZZ=	-14.4654				
Eigenvalues:	-38.9975	55.6437	159.4377						
66	H	Isotropic=	23.8288	Anisotropy	=	8.2016			
XX=	22.093	YX=	-0.493	ZX=	0.477				
XY=	-0.3956	YY=	21.6681	ZY=	-3.2579				
XZ=	0.4669	YZ=	-3.5271	ZZ=	27.7254				
Eigenvalues:	20.1255	22.0644	29.2966						
67	O	Isotropic=	-92.0563	Anisotropy	=	665.1255			
XX=	9.345	YX=	-176.5535	ZX=	339.053				
XY=	-188.398	YY=	-74.3991	ZY=	-123.8703				
XZ=	294.2981	YZ=	-132.9503	ZZ=	-211.1147				
Eigenvalues:	-436.2005	-191.3293	51.3607						
68	C	Isotropic=	55.4705	Anisotropy	=	173.746			
XX=	159.7769	YX=	4.2146	ZX=	-53.1719				
XY=	-15.1242	YY=	-11.4501	ZY=	-23.7672				
XZ=	-30.8312	YZ=	-25.9385	ZZ=	18.0847				
Eigenvalues:	-29.4065	24.5169	171.3012						
69	H	Isotropic=	23.7311	Anisotropy	=	5.6755			
XX=	23.001	YX=	-2.9689	ZX=	0.3151				
XY=	-3.0935	YY=	24.0199	ZY=	-1.8569				
XZ=	0.247	YZ=	-2.171	ZZ=	24.1724				
Eigenvalues:	20.1096	23.5689	27.5147						
70	H	Isotropic=	23.7632	Anisotropy	=	3.5166			
XX=	23.3625	YX=	-2.6872	ZX=	-1.3109				
XY=	-2.421	YY=	23.2023	ZY=	-0.4832				
XZ=	-1.3539	YZ=	-0.7482	ZZ=	24.7249				
Eigenvalues:	20.2985	24.8835	26.1077						
71	H	Isotropic=	23.7829	Anisotropy	=	4.1816			
XX=	22.6271	YX=	-2.3779	ZX=	-0.7673				

XY=	-2.1483	YY=	23.5953	ZY=	-1.9207				
XZ=	-0.6574	YZ=	-1.8673	ZZ=	25.1263				
Eigenvalues:	20.1584	24.6196	26.5706						
72	H	Isotropic=	23.805	Anisotropy	=	8.2206			
XX=	24.1334	YX=	-4.6164	ZX=	-0.4417				
XY=	-4.2585	YY=	25.3307	ZY=	-0.9858				
XZ=	-0.108	YZ=	-1.4592	ZZ=	21.951				
Eigenvalues:	19.7721	22.3576	29.2855						
73	C	Isotropic=	59.598	Anisotropy	=	178.5065			
XX=	172.5105	YX=	-4.1105	ZX=	-32.9221				
XY=	-8.2211	YY=	39.7885	ZY=	8.5933				
XZ=	-36.4219	YZ=	9.7221	ZZ=	-33.5051				
Eigenvalues:	-39.9968	40.1883	178.6023						
74	C	Isotropic=	61.9879	Anisotropy	=	177.025			
XX=	175.4402	YX=	-5.9383	ZX=	-23.5808				
XY=	-7.0876	YY=	-18.924	ZY=	36.9387				
XZ=	-23.83	YZ=	39.6891	ZZ=	29.4476				
Eigenvalues:	-40.2047	46.1639	180.0046						
75	C	Isotropic=	62.2717	Anisotropy	=	178.299			
XX=	173.8554	YX=	-22.0221	ZX=	-31.3126				
XY=	-20.4106	YY=	-13.9324	ZY=	-36.3413				
XZ=	-30.7507	YZ=	-36.1553	ZZ=	26.8921				
Eigenvalues:	-40.5784	46.2558	181.1377						
76	C	Isotropic=	63.9598	Anisotropy	=	174.8179			
XX=	172.8585	YX=	-11.0324	ZX=	-36.8565				
XY=	-7.9801	YY=	51.131	ZY=	7.3318				
XZ=	-39.0585	YZ=	4.959	ZZ=	-32.1099				
Eigenvalues:	-39.1263	50.5007	180.5051						
77	C	Isotropic=	67.1744	Anisotropy	=	165.0394			
XX=	172.2676	YX=	-4.6059	ZX=	-23.8423				
XY=	-4.8601	YY=	-8.2408	ZY=	40.1515				
XZ=	-24.7979	YZ=	32.9004	ZZ=	37.4964				
Eigenvalues:	-28.7665	53.089	177.2007						
78	H	Isotropic=	23.2059	Anisotropy	=	7.2583			
XX=	20.1501	YX=	1.1959	ZX=	-0.349				
XY=	1.4184	YY=	27.8207	ZY=	-0.2535				
XZ=	-0.0192	YZ=	-0.1279	ZZ=	21.6469				
Eigenvalues:	19.9204	21.6526	28.0448						
79	H	Isotropic=	23.7683	Anisotropy	=	4.1578			
XX=	20.9113	YX=	1.3135	ZX=	0.8396				
XY=	1.0264	YY=	25.1838	ZY=	0.7745				
XZ=	0.9004	YZ=	1.1715	ZZ=	25.2098				
Eigenvalues:	20.5298	24.2349	26.5402						
80	H	Isotropic=	23.7643	Anisotropy	=	3.5791			
XX=	20.8623	YX=	0.5635	ZX=	0.991				
XY=	0.6405	YY=	25.1951	ZY=	-1.014				
XZ=	0.9508	YZ=	-0.8234	ZZ=	25.2354				
Eigenvalues:	20.5229	24.6196	26.1503						
81	H	Isotropic=	23.9526	Anisotropy	=	5.2927			
XX=	20.8946	YX=	1.2926	ZX=	1.4028				
XY=	1.0807	YY=	26.9764	ZY=	0.7198				
XZ=	1.0508	YZ=	0.7876	ZZ=	23.9869				
Eigenvalues:	20.3468	24.03	27.4811						
82	H	Isotropic=	24.1673	Anisotropy	=	8.5227			
XX=	21.076	YX=	3.0831	ZX=	2.7498				
XY=	1.8051	YY=	25.7899	ZY=	2.7353				

XZ= 1.9695 YZ= 2.9038 ZZ= 25.6361
 Eigenvalues: 19.7604 22.8924 29.8491

2a-v

C	-3.136236	0.382028	-1.861974
C	-3.841605	-0.962081	-2.228183
C	-3.529399	-2.147745	-1.299816
C	-4.733768	-2.612941	-0.46146
C	-5.319317	-1.547797	0.48709
C	-4.371479	-0.715159	1.336474
C	-3.423177	0.147248	0.554886
C	-2.093378	0.004125	0.792819
C	-1.127168	0.50555	-0.244884
C	-1.621790.213173		-1.663693
C	-3.812905	1.027956	-0.612023
C	-5.302553	1.204502	-0.859649
C	-3.251194	2.447023	-0.40461
C	-1.509373	-0.666065	1.976456
C	-5.821131	-3.199657	-1.332609
O	-3.241835	1.250552	-2.988759
O	-3.531657	-1.294555	-3.572816
O	-6.53488-1.522729		0.693884
O	-4.951665	-0.072921	2.467369
O	0.114045	-0.210496	-0.03842
H	-2.577818	-1.202967	-3.688484
C	-6.137848	0.611445	2.471194
O	-6.761950.805994		1.433975
C	-6.496004	1.0432	3.855616
H	-4.956962	-0.792226	-2.263438
H	-2.680256	-1.906049	-0.612846
H	-3.752848	-1.517036	1.872438
H	-0.918141	1.604545	-0.110589
H	-1.085023	0.911461	-2.3647
H	-1.321564	-0.831861	-1.939267
H	-5.881306	0.254852	-0.797831
H	-5.736754	1.909683	-0.107591
H	-5.460144	1.651921	-1.872362
H	-4.053071	3.216152	-0.523797
H	-2.820628	2.562362	0.618212
H	-2.464748	2.674672	-1.165444
H	-2.177782	-0.578382.868641	
H	-1.327735	-1.748763	1.755679
H	-0.524018	-0.201788	2.234399
H	-6.641285	-3.613215	-0.696073
H	-6.262732	-2.420806	-1.999648
H	-5.403169	-4.018266	-1.966214
H	-5.642855	0.893733	4.559498
H	-6.781497	2.122808	3.833895
H	-7.370122	0.437325	4.199512
H	-4.107976	1.110834	-3.392021
C	1.240064	0.279159	-0.643053
O	1.15559 1.309841		-1.307111
H	-4.352789	-3.422726	0.228015
H	-3.212978	-3.013397	-1.941808
C	2.445985	-0.581525	-0.327763
C	3.609176	0.200918	0.372241

O	2.091917	-1.685076	0.476909
H	2.788034	-1.038508	-1.302604
N	4.882648	-0.389342	0.023391
C	3.582907	1.685922	0.108679
H	3.459753	0.037271	1.489136
H	1.669671	-1.349846	1.279772
C	5.732987	-0.907935	0.991109
H	5.270962	-0.125533	-0.852023
C	3.979978	2.219696	-1.122383
C	4.010317	3.60073	-1.311977
C	3.648934	4.458401	-0.273383
C	3.255778	3.931684	0.956695
C	3.228517	2.551591	1.150723
H	4.238034	1.553984	-1.959291
O	5.334017	-1.139778	2.148431
C	7.117736	-1.242325	0.550997
H	4.313205	4.012294	-2.286021
H	3.671107	5.547561	-0.424997
H	2.969527	4.604968	1.778122
H	2.931244	2.144922	2.129447
C	7.644524	-2.492191	0.894898
C	8.940954	-2.827465	0.506604
C	9.712733	-1.916802	-0.215332
C	9.189644	-0.667097	-0.548956
C	7.8913	-0.327635	-0.169936
H	7.032128	-3.196634	1.479795
H	9.355006	-3.810801	0.774689
H	10.736401	-2.182445	-0.518898
H	9.801756	0.053977	-1.110511
H	7.490906	0.665065	-0.425003

2avliz E(RB+HF-PW91) = -2012.296296

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic= 109.4858 Anisotropy 28.1559

XX= 99.5373 YX= -10.636 ZX= 7.2502

XY= -10.2275 YY= 114.7836 ZY= -10.1243

XZ= -0.0528 YZ= -10.2714 ZZ= 114.1366

Eigenvalues: 94.113 106.088 128.2564

2 C Isotropic= 112.4614 Anisotropy 30.7677

XX= 97.2692 YX= -3.2088 ZX= -14.5406

XY= 2.4936 YY= 112.8614 ZY= 1.3675

XZ= -8.2512 YZ= 11.346 ZZ= 127.2534

Eigenvalues: 93.2759 111.135 132.9731

3 C Isotropic= 142.688 Anisotropy 20.439

XX= 122.5512 YX= 1.326 ZX= -2.4441

XY= -4.3994 YY= 156.0459 ZY= 0.9999

XZ= -8.2641 YZ= 0.693 ZZ= 149.4668

Eigenvalues: 121.4725 150.2774 156.314

4 C Isotropic= 140.734 Anisotropy 24.1973

XX= 123.3912 YX= -3.8864 ZX= -5.8445

XY= 0.2336 YY= 149.8749 ZY= 8.7321

XZ= 8.1832 YZ= 6.1416 ZZ= 148.9359

Eigenvalues: 123.1478 142.1886 156.8655

5 C Isotropic= -22.0078 Anisotropy 179.2336

XX= -54.0796 YX= -23.4984 ZX= -10.4626

XY= -6.0224 YY= -13.7158 ZY= -106.1115
 XZ= -1.8224 YZ= -99.806 ZZ= 1.7721
 Eigenvalues: -113.046-50.458697.4813
 6 C Isotropic= 102.0263 Anisotropy 41.1798
 XX= 88.2091 YX= -0.8722 ZX= -0.2456
 XY= -6.285 YY= 106.975 ZY= 19.7627
 XZ= -14.8847 YZ= 17.9994 ZZ= 110.8948
 Eigenvalues: 85.4187 91.1806 129.4795
 7 C Isotropic= 43.2457 Anisotropy 158.8047
 XX= 28.8648 YX= -24.575 ZX= 13.7052
 XY= -14.6385 YY= 68.7571 ZY= 90.0664
 XZ= 37.3164 YZ= 103.8362 ZZ= 32.1152
 Eigenvalues: -59.881340.5028 149.1155
 8 C Isotropic= 42.7012 Anisotropy 154.5032
 XX= 38.2621 YX= -6.1507 ZX= 18.9414
 XY= -2.6132 YY= 93.3758 ZY= 98.1594
 XZ= 8.0643 YZ= 78.3738 ZZ= -3.5341
 Eigenvalues: -57.770240.1706 145.7034
 9 C Isotropic= 111.1147 Anisotropy 47.7049
 XX= 130.4185 YX= -21.5773 ZX= 5.1412
 XY= -27.5277 YY= 94.0621 ZY= 3.6766
 XZ= 2.6489 YZ= 2.5457 ZZ= 108.8634
 Eigenvalues: 80.9534 109.4727 142.9179
 10 C Isotropic= 148.8099 Anisotropy 41.1962
 XX= 167.6186 YX= -9.3806 ZX= 9.7624
 XY= -13.6175 YY= 130.7035 ZY= -5.0142
 XZ= 16.129 YZ= 6.7497 ZZ= 148.1074
 Eigenvalues: 126.365 143.7906 176.274
 11 C Isotropic= 147.671 Anisotropy 13.4258
 XX= 140.9243 YX= 0.1989 ZX= -4.8914
 XY= 7.9459 YY= 148.7875 ZY= 6.7752
 XZ= 8.4165 YZ= 1.5107 ZZ= 153.3012
 Eigenvalues: 139.1953 147.1961 156.6215
 12 C Isotropic= 155.5016 Anisotropy 24.4137
 XX= 165.6613 YX= 11.6211 ZX= -2.3177
 XY= 3.1873 YY= 161.9269 ZY= 4.1074
 XZ= -1.7539 YZ= 11.5073 ZZ= 138.9166
 Eigenvalues: 135.917 158.8104 171.7774
 13 C Isotropic= 148.405 Anisotropy 54.6962
 XX= 138.0073 YX= 14.4396 ZX= 14.0914
 XY= 13.8863 YY= 176.6432 ZY= 9.9208
 XZ= 20.6146 YZ= 7.0788 ZZ= 130.5645
 Eigenvalues: 116.4386 143.9073 184.8691
 14 C Isotropic= 167.8261 Anisotropy 12.9489
 XX= 163.2082 YX= 4.6454 ZX= 5.8922
 XY= -5.7905 YY= 166.017 ZY= -5.2278
 XZ= 0.9435 YZ= -1.9042 ZZ= 174.2532
 Eigenvalues: 162.173 164.8467 176.4587
 15 C Isotropic= 169.5562 Anisotropy 16.6553
 XX= 173.0633 YX= 5.8148 ZX= -0.756
 XY= 4.067 YY= 166.8992 ZY= 9.5993
 XZ= 3.3407 YZ= 10.9684 ZZ= 168.706
 Eigenvalues: 156.9748 171.034 180.6597
 16 O Isotropic= 263.344 Anisotropy 84.2391
 XX= 306.2015 YX= -3.1084 ZX= 44.6407
 XY= 6.5805 YY= 272.177 ZY= -42.163

XZ= 27.9171 YZ= -8.2668 ZZ= 211.6536
 Eigenvalues: 191.872 278.6566 319.5035
 17 O Isotropic= 265.4292 Anisotropy 45.0996
 XX= 258.3745 YX= -3.1063 ZX= -23.9923
 XY= 13.2399 YY= 272.6011 ZY= -23.097
 XZ= -5.1793 YZ= -19.5224 ZZ= 265.312
 Eigenvalues: 242.3251 258.4669 295.4956
 18 O Isotropic= -371.4683 Anisotropy 1097.517
 XX= -1020.8267 YX= -51.4377 ZX= 151.3303
 XY= -14.92 YY= -46.9458 ZY= -403.7124
 XZ= 80.9295 YZ= -394.0893 ZZ= -46.6323
 Eigenvalues: -1034.7029 -439.9117 360.2097
 19 O Isotropic= 95.3204 Anisotropy 127.1518
 XX= 172.2601 YX= -14.3026 ZX= -97.3957
 XY= 17.7854 YY= 148.2857 ZY= 16.9657
 XZ= 22.6158 YZ= -67.669 ZZ= -34.5846
 Eigenvalues: -44.299 150.1719 180.0882
 20 O Isotropic= 68.8622 Anisotropy 188.443
 XX= 63.3588 YX= 45.5374 ZX= 0.0717
 XY= 147.4541 YY= -0.5286 ZY= 90.2838
 XZ= -91.7964 YZ= 108.4004 ZZ= 143.7565
 Eigenvalues: -115.0883 127.1841 194.4909
 21 H Isotropic= 31.1933 Anisotropy 13.6042
 XX= 37.7508 YX= 1.76 ZX= -4.8596
 XY= 1.5767 YY= 24.2477 ZY= 4.653
 XZ= -4.4358 YZ= 3.7313 ZZ= 31.5812
 Eigenvalues: 21.5631 31.754 40.2627
 22 C Isotropic= 21.5458 Anisotropy 78.9863
 XX= -13.5586 YX= 60.5777 ZX= 65.6591
 XY= 52.038 YY= 30.9371 ZY= -45.495
 XZ= 29.8289 YZ= -21.0353 ZZ= 47.259
 Eigenvalues: -78.7279 69.162 74.2034
 23 O Isotropic= -141.1903 Anisotropy 606.0034
 XX= -241.795 YX= 271.1072 ZX= -132.4237
 XY= 264.7621 YY= 104.7967 ZY= -29.4598
 XZ= -82.8848 YZ= -38.3163 ZZ= -286.5726
 Eigenvalues: -432.6168 -253.7662 262.8119
 24 C Isotropic= 165.8359 Anisotropy 37.7197
 XX= 157.284 YX= -8.0254 ZX= -6.8559
 XY= -7.869 YY= 155.1445 ZY= 10.1358
 XZ= -4.9288 YZ= 12.8143 ZZ= 185.0792
 Eigenvalues: 147.4172 159.1081 190.9823
 25 H Isotropic= 27.4904 Anisotropy 3.0149
 XX= 28.4851 YX= 0.8547 ZX= -1.0183
 XY= 0.7122 YY= 26.887 ZY= 0.9867
 XZ= -2.1025 YZ= 1.5731 ZZ= 27.0991
 Eigenvalues: 24.9329 28.038 29.5003
 26 H Isotropic= 28.2182 Anisotropy 8.4176
 XX= 28.1597 YX= 3.8425 ZX= 2.7574
 XY= 2.8028 YY= 29.2936 ZY= 2.1079
 XZ= 2.8985 YZ= 1.9295 ZZ= 27.2013
 Eigenvalues: 24.6437 26.181 33.8299
 27 H Isotropic= 25.3564 Anisotropy 4.184
 XX= 26.553 YX= -0.8355 ZX= -2.9285
 XY= -2.1735 YY= 24.0201 ZY= -0.6169
 XZ= -0.0029 YZ= 1.5994 ZZ= 25.4963

Eigenvalues:	23.3012	24.6223	28.1458		
28	H	Isotropic=	25.5807	Anisotropy	7.5025
XX=	30.3661	YX=	-0.5535	ZX=	1.3666
XY=	-0.0797	YY=	25.8189	ZY=	-0.1265
XZ=	1.5263	YZ=	1.8933	ZZ=	20.5573
Eigenvalues:	20.1979	25.9619	30.5824		
29	H	Isotropic=	27.9852	Anisotropy	8.5805
XX=	32.6879	YX=	3.313	ZX=	-0.0077
XY=	3.0953	YY=	23.3005	ZY=	-1.9374
XZ=	0.9729	YZ=	-3.742	ZZ=	27.9672
Eigenvalues:	21.1184	29.1316	33.7055		
30	H	Isotropic=	29.758	Anisotropy	5.8304
XX=	32.8994	YX=	-0.0378	ZX=	1.7126
XY=	-0.0327	YY=	29.2105	ZY=	3.3551
XZ=	1.9342	YZ=	2.8048	ZZ=	27.1643
Eigenvalues:	24.6636	30.9655	33.645		
31	H	Isotropic=	29.4664	Anisotropy	8.4807
XX=	31.3364	YX=	2.9749	ZX=	-1.083
XY=	3.6073	YY=	31.3503	ZY=	-2.5264
XZ=	-1.1101	YZ=	-1.3096	ZZ=	25.7125
Eigenvalues:	25.1205	28.1586	35.1202		
32	H	Isotropic=	29.2907	Anisotropy	9.0768
XX=	30.6184	YX=	-2.4929	ZX=	-5.0172
XY=	-2.4334	YY=	28.2082	ZY=	0.4082
XZ=	-4.307	YZ=	1.0268	ZZ=	29.0456
Eigenvalues:	24.7316	27.7986	35.3419		
33	H	Isotropic=	30.3488	Anisotropy	6.6865
XX=	32.3189	YX=	-2.7589	ZX=	1.0241
XY=	-2.6757	YY=	27.8769	ZY=	-2.7227
XZ=	1.2682	YZ=	-2.143	ZZ=	30.8506
Eigenvalues:	25.9211	30.3188	34.8065		
34	H	Isotropic=	30.249	Anisotropy	8.9776
XX=	29.9971	YX=	-0.9414	ZX=	0.3784
XY=	-2.7049	YY=	35.6983	ZY=	0.0996
XZ=	0.8919	YZ=	-0.0868	ZZ=	25.0518
Eigenvalues:	24.966	29.547	36.2341		
35	H	Isotropic=	30.4594	Anisotropy	6.1088
XX=	29.558	YX=	-0.2018	ZX=	2.3834
XY=	1.423	YY=	31.9973	ZY=	3.2138
XZ=	1.5349	YZ=	2.5292	ZZ=	29.8229
Eigenvalues:	27.0782	29.7681	34.5319		
36	H	Isotropic=	28.6865	Anisotropy	6.479
XX=	29.6662	YX=	1.0929	ZX=	-1.4507
XY=	2.9129	YY=	31.4395	ZY=	-1.8598
XZ=	-1.0474	YZ=	0.03	ZZ=	24.9538
Eigenvalues:	24.6157	28.438	33.0058		
37	H	Isotropic=	28.9283	Anisotropy	7.9103
XX=	30.6152	YX=	-1.1396	ZX=	-1.2611
XY=	-0.8413	YY=	22.9482	ZY=	0.4407
XZ=	-2.4542	YZ=	-0.5733	ZZ=	33.2215
Eigenvalues:	22.8133	29.7698	34.2018		
38	H	Isotropic=	28.9507	Anisotropy	6.5621
XX=	28.3799	YX=	-1.3235	ZX=	0.168
XY=	-2.267	YY=	32.2556	ZY=	-1.7732
XZ=	0.3717	YZ=	-1.4757	ZZ=	26.2167
Eigenvalues:	25.7927	27.7341	33.3255		

39	H	Isotropic=	28.9729	Anisotropy	7.5517
XX=	33.287	YX=	2.9644	ZX=	-0.1318
XY=	1.9946	YY=	23.5988	ZY=	-0.2251
XZ=	1.8119	YZ=	-0.8207	ZZ=	30.0328
Eigenvalues:	22.9306	29.9807	34.0073		
40	H	Isotropic=	29.1981	Anisotropy	10.8609
XX=	32.4684	YX=	4.319	ZX=	-3.5045
XY=	5.5292	YY=	28.4266	ZY=	0.2579
XZ=	-2.2842	YZ=	-0.7036	ZZ=	26.6994
Eigenvalues:	24.1216	27.0341	36.4387		
41	H	Isotropic=	29.6986	Anisotropy	5.7733
XX=	30.8127	YX=	0.6966	ZX=	3.1883
XY=	1.109	YY=	29.3146	ZY=	-2.3027
XZ=	3.6944	YZ=	-1.9469	ZZ=	28.9685
Eigenvalues:	25.1241	30.4243	33.5474		
42	H	Isotropic=	30.496	Anisotropy	9.6645
XX=	28.7664	YX=	0.9534	ZX=	-0.1886
XY=	1.0353	YY=	33.7343	ZY=	5.1936
XZ=	-0.2788	YZ=	4.7627	ZZ=	28.9873
Eigenvalues:	25.6718	28.8772	36.939		
43	H	Isotropic=	29.1053	Anisotropy	5.5404
XX=	30.0648	YX=	-1.9201	ZX=	0.1982
XY=	-1.6831	YY=	25.1013	ZY=	1.7754
XZ=	2.4167	YZ=	0.7355	ZZ=	32.1499
Eigenvalues:	24.1909	30.3262	32.7989		
44	H	Isotropic=	29.2189	Anisotropy	7.6322
XX=	27.021	YX=	-2.2477	ZX=	-0.3709
XY=	-3.0714	YY=	32.3245	ZY=	1.0978
XZ=	-1.9689	YZ=	2.8963	ZZ=	28.3113
Eigenvalues:	25.8606	27.4892	34.307		
45	H	Isotropic=	28.9051	Anisotropy	8.2983
XX=	30.8914	YX=	2.3913	ZX=	-2.8153
XY=	2.1316	YY=	26.6836	ZY=	-0.81
XZ=	-4.4215	YZ=	-0.9396	ZZ=	29.1404
Eigenvalues:	25.442	26.8361	34.4374		
46	H	Isotropic=	30.7757	Anisotropy	18.2393
XX=	35.7379	YX=	-0.2223	ZX=	9.4352
XY=	-0.3976	YY=	23.7819	ZY=	-2.074
XZ=	7.1243	YZ=	-4.0069	ZZ=	32.8073
Eigenvalues:	22.28	27.1118	42.9353		
47	C	Isotropic=	13.954	Anisotropy	88.3356
XX=	-68.9192	YX=	25.2215	ZX=	19.5371
XY=	-17.9222	YY=	58.0096	ZY=	15.978
XZ=	43.1378	YZ=	10.2491	ZZ=	52.7717
Eigenvalues:	-76.5166	45.5342	72.8444		
48	O	Isotropic=	-125.038	Anisotropy	651.5577
XX=	-231.5261	YX=	88.0444	ZX=	82.596
XY=	56.1368	YY=	-187.05	ZY=	314.4083
XZ=	91.9683	YZ=	362.5051	ZZ=	43.4621
Eigenvalues:	-429.6753	-254.7725	309.3338		
49	H	Isotropic=	28.6995	Anisotropy	6.601
XX=	27.2567	YX=	1.9876	ZX=	1.982
XY=	0.5014	YY=	30.5775	ZY=	-3.2969
XZ=	2.7449	YZ=	-3.6291	ZZ=	28.2642
Eigenvalues:	23.7602	29.238	33.1001		
50	H	Isotropic=	29.4612	Anisotropy	6.5961

XX=	28.2974	YX=	-0.0202	ZX=	-1.8342		
XY=	-0.3929	YY=	32.5205	ZY=	3.1986		
XZ=	-1.7569	YZ=	2.182	ZZ=	27.5655		
Eigenvalues:	25.4862	29.0387	33.8586				
51	C	Isotropic=	107.9634	Anisotropy		26.6966	
XX=	112.6259	YX=	11.3954	ZX=	-2.3754		
XY=	11.9232	YY=	110.9444	ZY=	-10.032		
XZ=	0.6806	YZ=	-9.763	ZZ=	100.32		
Eigenvalues:	92.6169	105.5122	125.7612				
52	C	Isotropic=	118.3975	Anisotropy		32.389	
XX=	110.1895	YX=	21.3718	ZX=	2.9614		
XY=	12.2445	YY=	130.1112	ZY=	0.8639		
XZ=	3.1072	YZ=	2.0014	ZZ=	114.8917		
Eigenvalues:	100.3535	114.8488	139.9901				
53	O	Isotropic=	263.2169	Anisotropy		43.7901	
XX=	261.9623	YX=	15.1467	ZX=	-7.3744		
XY=	7.4163	YY=	242.1412	ZY=	27.4415		
XZ=	-7.679	YZ=	8.5047	ZZ=	285.5471		
Eigenvalues:	230.1821	267.0583	292.4102				
54	H	Isotropic=	26.7063	Anisotropy		3.2145	
XX=	26.8397	YX=	1.5589	ZX=	-0.9215		
XY=	-0.0969	YY=	25.1128	ZY=	0.7502		
XZ=	-1.3299	YZ=	0.9211	ZZ=	28.1664		
Eigenvalues:	24.4516	26.818	28.8493				
55	N	Isotropic=	117.9806	Anisotropy		101.9363	
XX=	126.9509	YX=	-12.1974	ZX=	43.7714		
XY=	-31.815	YY=	165.5081	ZY=	-0.4698		
XZ=	79.8926	YZ=	-7.3891	ZZ=	61.483		
Eigenvalues:	23.7948	144.209	185.9382				
56	C	Isotropic=	50.496	Anisotropy		195.4527	
XX=	171.3575	YX=	-0.6803	ZX=	29.6459		
XY=	7.4611	YY=	-39.7831	ZY=	9.2005		
XZ=	47.7349	YZ=	8.0691	ZZ=	19.9136		
Eigenvalues:	-41.0298	11.7201	180.7978				
57	H	Isotropic=	25.4083	Anisotropy		1.763	
XX=	25.0668	YX=	-1.4829	ZX=	0.3594		
XY=	-0.4986	YY=	24.7657	ZY=	0.1316		
XZ=	0.1137	YZ=	-0.6732	ZZ=	26.3922		
Eigenvalues:	23.9131	25.7281	26.5836				
58	H	Isotropic=	30.1481	Anisotropy		13.7939	
XX=	30.3754	YX=	-1.1096	ZX=	-6.5368		
XY=	-1.7115	YY=	25.6817	ZY=	-0.0344		
XZ=	-6.7474	YZ=	-0.6311	ZZ=	34.3872		
Eigenvalues:	24.2162	26.8841	39.344				
59	C	Isotropic=	17.1562	Anisotropy		115.7817	
XX=	-45.9926	YX=	48.8012	ZX=	-15.1791		
XY=	51.7452	YY=	74.6692	ZY=	10.9611		
XZ=	-26.852	YZ=	25.4424	ZZ=	22.7921		
Eigenvalues:	-71.3928	28.5175	94.3441				
60	H	Isotropic=	25.9262	Anisotropy		8.4391	
XX=	30.2218	YX=	-5.2994	ZX=	-2.9859		
XY=	-1.2722	YY=	23.0107	ZY=	-2.6376		
XZ=	1.3067	YZ=	-4.8327	ZZ=	24.546		
Eigenvalues:	19.0954	27.1309	31.5522				
61	C	Isotropic=	62.2859	Anisotropy		174.0344	
XX=	160.1321	YX=	16.2294	ZX=	54.8471		

XY= 19.2857 YY= 16.8014 ZY= -36.1601
 XZ= 55.2856 YZ= -41.4328 ZZ= 9.9242
 Eigenvalues: -39.8736 48.4225 178.3088
 62 C Isotropic= 62.4772 Anisotropy 177.8959
 XX= 163.2885 YX= -4.8652 ZX= 55.4447
 XY= -5.6313 YY= 36.8863 ZY= 27.4413
 XZ= 61.6922 YZ= 30.4454 ZZ= -12.7433
 Eigenvalues: -41.3694 47.7265 181.0744
 63 C Isotropic= 64.3437 Anisotropy 175.6779
 XX= 168.2811 YX= 5.509 ZX= 39.5358
 XY= 2.2242 YY= -35.2689 ZY= 10.7368
 XZ= 39.6294 YZ= 13.1952 ZZ= 60.0189
 Eigenvalues: -36.7541 48.3229 181.4623
 64 C Isotropic= 62.5958 Anisotropy 175.4601
 XX= 160.0927 YX= 18.2281 ZX= 58.0805
 XY= 17.192 YY= 15.288 ZY= -39.0621
 XZ= 55.6952 YZ= -40.0201 ZZ= 12.4068
 Eigenvalues: -40.4172 48.6354 179.5692
 65 C Isotropic= 61.7078 Anisotropy 149.9883
 XX= 146.0891 YX= -13.6644 ZX= 49.454
 XY= -6.186 YY= 47.0144 ZY= 27.7803
 XZ= 53.4139 YZ= 27.8932 ZZ= -7.9801
 Eigenvalues: -34.2912 57.7146 161.7
 66 H Isotropic= 23.7957 Anisotropy 8.3732
 XX= 22.5034 YX= 0.4544 ZX= -1.5227
 XY= 0.9094 YY= 25.6206 ZY= -4.7287
 XZ= -1.3295 YZ= -4.2554 ZZ= 23.2633
 Eigenvalues: 19.6086 22.4007 29.3779
 67 O Isotropic= -90.8223 Anisotropy 657.288
 XX= -144.7445 YX= 143.8837 ZX= 39.6716
 XY= 141.0198 YY= 261.1565 ZY= 149.8568
 XZ= 84.4265 YZ= 176.2317 ZZ= -388.8788
 Eigenvalues: -430.4754 -189.3611 347.3697
 68 C Isotropic= 55.4112 Anisotropy 172.3374
 XX= -3.1076 YX= 17.4515 ZX= 62.7565
 XY= 30.0635 YY= 32.111 ZY= 44.6353
 XZ= 59.4698 YZ= 17.5252 ZZ= 137.2301
 Eigenvalues: -28.4164 24.3471 170.3027
 69 H Isotropic= 23.6632 Anisotropy 4.3636
 XX= 21.3943 YX= 0.053 ZX= -1.5819
 XY= 0.0263 YY= 26.5709 ZY= -0.1282
 XZ= -1.2097 YZ= 0.0367 ZZ= 23.0243
 Eigenvalues: 20.593 23.8244 26.5722
 70 H Isotropic= 23.8002 Anisotropy 2.8688
 XX= 21.5237 YX= 0.6022 ZX= -1.7464
 XY= 0.2188 YY= 24.8608 ZY= 0.0253
 XZ= -1.6701 YZ= 0.3171 ZZ= 25.016
 Eigenvalues: 20.7786 24.9092 25.7127
 71 H Isotropic= 23.8844 Anisotropy 4.2931
 XX= 21.1939 YX= 0.763 ZX= -0.881
 XY= 0.6718 YY= 26.4849 ZY= -0.6624
 XZ= -1.0394 YZ= -0.4159 ZZ= 23.9743
 Eigenvalues: 20.8444 24.0623 26.7464
 72 H Isotropic= 24.1594 Anisotropy 6.8595
 XX= 21.7022 YX= -0.0613 ZX= 0.0442
 XY= -0.4802 YY= 27.5286 ZY= 2.6868

XZ= -0.2784 YZ= 2.4203 ZZ= 23.2475
 Eigenvalues: 21.6896 22.0563 28.7324
 73 C Isotropic= 60.3111 Anisotropy 177.0604
 XX= 39.9051 YX= -10.4465 ZX= 62.0221
 XY= -7.1361 YY= 23.6609 ZY= 72.5812
 XZ= 67.1002 YZ= 73.5924 ZZ= 117.3672
 Eigenvalues: -39.2615 41.8433 178.3514
 74 C Isotropic= 61.852 Anisotropy 176.2988
 XX= 52.7125 YX= 44.3715 ZX= 32.9776
 XY= 47.0682 YY= -4.7529 ZY= 62.3244
 XZ= 32.6094 YZ= 63.4287 ZZ= 137.5964
 Eigenvalues: -40.3566 46.5281 179.3846
 75 C Isotropic= 61.8751 Anisotropy 178.362
 XX= -13.2158 YX= 37.1893 ZX= 63.3971
 XY= 36.466 YY= 60.3862 ZY= 37.9455
 XZ= 61.9881 YZ= 38.3061 ZZ= 138.4548
 Eigenvalues: -41.0362 45.8783 180.783
 76 C Isotropic= 63.3581 Anisotropy 174.085
 XX= 38.147 YX= -12.8338 ZX= 63.212
 XY= -17.189 YY= 30.7065 ZY= 71.862
 XZ= 63.7099 YZ= 73.7939 ZZ= 121.2209
 Eigenvalues: -39.1628 49.8225 179.4148
 77 C Isotropic= 67.1245 Anisotropy 164.3999
 XX= 58.941 YX= 43.2622 ZX= 28.5126
 XY= 38.2412 YY= 2.4921 ZY= 58.5503
 XZ= 33.1634 YZ= 55.7191 ZZ= 139.9404
 Eigenvalues: -28.1746 52.8237 176.7245
 78 H Isotropic= 23.2292 Anisotropy 7.8232
 XX= 25.1898 YX= -3.685 ZX= -0.6524
 XY= -3.891 YY= 24.0296 ZY= -1.0853
 XZ= -0.9183 YZ= -1.1964 ZZ= 20.4682
 Eigenvalues: 19.2358 22.0072 28.4447
 79 H Isotropic= 23.723 Anisotropy 4.3955
 XX= 25.9176 YX= -0.8076 ZX= -1.9243
 XY= -0.4018 YY= 23.4524 ZY= -1.5055
 XZ= -1.8552 YZ= -1.5224 ZZ= 21.7991
 Eigenvalues: 20.2369 24.2788 26.6533
 80 H Isotropic= 23.6841 Anisotropy 3.8842
 XX= 24.0775 YX= -0.663 ZX= -1.1584
 XY= -0.5911 YY= 25.3182 ZY= -2.172
 XZ= -1.1491 YZ= -2.016 ZZ= 21.6567
 Eigenvalues: 20.2569 24.522 26.2736
 81 H Isotropic= 23.8881 Anisotropy 5.5217
 XX= 26.4516 YX= -1.9927 ZX= -1.547
 XY= -1.764 YY= 24.1997 ZY= -1.2583
 XZ= -1.0794 YZ= -1.0911 ZZ= 21.0129
 Eigenvalues: 20.0633 24.0318 27.5692
 82 H Isotropic= 24.0881 Anisotropy 8.9682
 XX= 29.5084 YX= -0.9553 ZX= -3.006
 XY= 0.1313 YY= 22.1298 ZY= -1.6081
 XZ= -1.5868 YZ= -1.7135 ZZ= 20.6262
 Eigenvalues: 19.101 23.0965 30.067

2a-v2

C -3.132196 0.310981 -1.875657
 C -3.83999-1.043994 -2.194015

C	-3.532238	-2.195742	-1.222469
C	-4.739224	-2.627383	-0.370046
C	-5.324062	-1.527076	0.537938
C	-4.375873	-0.666169	1.358251
C	-3.424141	0.165061	0.547594
C	-2.095048	0.0265	0.793079
C	-1.125674	0.490069	-0.259157
C	-1.618316	0.146861	-1.667742
C	-3.809868	1.003453	-0.651577
C	-5.298967	1.174086	-0.90652
C	-3.245582.428041	-0.495526	
C	-1.516071	-0.597093	2.004185
C	-5.826134	-3.243077	-1.221563
O	-3.231624	1.134038	-3.036463
O	-3.52834-1.429479	-3.524307	
O	-6.540012	-1.492471	0.74079
O	-4.956976	0.018171	2.463625
O	0.116733	-0.215726	-0.024162
H	-2.580975	-1.301049	-3.656794
C	-6.141431	0.704965	2.440591
O	-6.765227	0.860124	1.396481
C	-6.498616	1.19088	3.807193
H	-4.954972	-0.873476	-2.236585
H	-2.684628	-1.930493	-0.542518
H	-3.759719	-1.448755	1.924801
H	-0.916854	1.5931	-0.164577
H	-1.079152	0.818322	-2.393091
H	-1.320519	-0.907808	-1.905723
H	-5.879545	0.228093	-0.813555
H	-5.732095	1.904562	-0.17828
H	-5.456255	1.58844	-1.933167
H	-4.046052	3.193889	-0.642238
H	-2.814938	2.579358	0.522589
H	-2.458685	2.626675	-1.263991
H	-2.184138	-0.464919	2.891176
H	-1.345577	-1.690162	1.831965
H	-0.525423	-0.132805	2.241834
H	-6.648262	-3.631704	-0.571972
H	-6.265016	-2.487899	-1.917024
H	-5.40884-4.084829	-1.824514	
H	-5.643902	1.071832	4.515027
H	-6.786942.268026	3.742748	
H	-7.370554	0.597005	4.176582
H	-4.111064	1.008865	-3.414777
C	1.242549	0.254623	-0.644389
O	1.141941	1.213379	-1.40714
H	-4.36165-3.412361	0.349309	
H	-3.216773	-3.084656	-1.832221
C	2.459201	-0.582659	-0.304579
C	3.619904	0.212149	0.384065
O	2.14091	-1.599160.626956	
H	2.797293	-1.03828-1.280393	
N	4.895363	-0.379619	0.04926
C	3.575875	1.688893	0.083052
H	3.461199	0.062977	1.503273
H	1.377042	-2.083874	0.287657

C	5.749863	-0.881765	1.022773
H	5.285386	-0.127374	-0.829012
C	3.966368	2.198258	-1.160291
C	3.977353	3.574637	-1.382868
C	3.602076	4.451507	-0.365399
C	3.213936	3.948848	0.876281
C	3.205828	2.573511	1.103522
H	4.23565	1.516251	-1.980345
O	5.361492	-1.100879	2.184964
C	7.134683	-1.215864	0.579088
H	4.275879	3.967181	-2.366003
H	3.609383	5.53693	-0.542937
H	2.916313	4.637447	1.680794
H	2.910052	2.183933	2.08997
C	7.668748	-2.458688	0.936944
C	8.964766	-2.793588	0.547087
C	9.72926	-1.889278	-0.190454
C	9.199233	-0.646305	-0.537743
C	7.90119	-0.307427	-0.156941
H	7.062505	-3.157327	1.535052
H	9.384577	-3.771229	0.826667
H	10.752686	-2.154445	-0.495113
H	9.805707	0.070149	-1.111172
H	7.495713	0.680479	-0.422447

E(RB+HF-PW91)		=	-2012.297112	
SCF	GIAO	Magnetic shielding tensor (ppm):		
1	C	Isotropic=	109.3941	Anisotropy = 28.1835
XX=	99.3993	YX=	-10.2375	ZX= 7.7063
XY=	-10.1377	YY=	114.0733	ZY= -10.2372
XZ=	0.0754	YZ=	-10.3324	ZZ= 114.7099
Eigenvalues:	94.0871	105.9122	128.1831	
2	C	Isotropic=	112.5728	Anisotropy = 31.2644
XX=	97.3116	YX=	-4.1233	ZX= -14.5177
XY=	1.703	YY=	113.381	ZY= 2.0904
XZ=	-8.3401	YZ=	12.0328	ZZ= 127.0259
Eigenvalues:	93.3561	110.9466	133.4158	
3	C	Isotropic=	142.4713	Anisotropy = 20.5365
XX=	122.0159	YX=	1.4457	ZX= -2.7955
XY=	-4.3745	YY=	155.9766	ZY= 0.7601
XZ=	-7.9288	YZ=	0.4834	ZZ= 149.4215
Eigenvalues:	120.954	150.2976	156.1624	
4	C	Isotropic=	140.708	Anisotropy = 24.2787
XX=	123.5543	YX=	-4.0129	ZX= -5.6682
XY=	0.6272	YY=	150.3609	ZY= 8.941
XZ=	8.0152	YZ=	6.108	ZZ= 148.2089
Eigenvalues:	123.3296	141.9007	156.8938	
5	C	Isotropic=	-21.8469	Anisotropy = 179.3139
XX=	-53.7288	YX=	-23.0892	ZX= -9.4733
XY=	-5.6725	YY=	-21.0931	ZY= -105.4508
XZ=	-1.5511	YZ=	-99.1481	ZZ= 9.2812
Eigenvalues:	-112.8837	-50.3527	97.6957	
6	C	Isotropic=	101.9367	Anisotropy = 41.1309
XX=	88.1436	YX=	-0.8109	ZX= -0.1432
XY=	-6.8851	YY=	108.2669	ZY= 19.9197

XZ= -14.6748 YZ= 17.9973 ZZ= 109.3995
 Eigenvalues: 85.3599 91.0929 129.3572
 7 C Isotropic= 43.5527 Anisotropy = 157.998
 XX= 29.7281 YX= -24.1094 ZX= 14.9148
 XY= -13.1788 YY= 75.8735 ZY= 88.2361
 XZ= 38.21 YZ= 101.8955 ZZ= 25.0567
 Eigenvalues: -59.6946 41.4681 148.8847
 8 C Isotropic= 41.8105 Anisotropy = 154.9288
 XX= 36.41 YX= -6.0671 ZX= 20.6764
 XY= -2.699 YY= 99.0733 ZY= 94.3484
 XZ= 9.9391 YZ= 74.3871 ZZ= -10.0516
 Eigenvalues: -58.509 38.8442 145.0964
 9 C Isotropic= 110.4244 Anisotropy = 48.8779
 XX= 130.2802 YX= -22.0011 ZX= 5.0158
 XY= -27.6221 YY= 93.6747 ZY= 2.6586
 XZ= 3.3984 YZ= 2.1832 ZZ= 107.3183
 Eigenvalues: 80.5285 107.7351 143.0097
 10 C Isotropic= 148.3226 Anisotropy = 40.9899
 XX= 166.8439 YX= -9.0371 ZX= 10.1586
 XY= -12.9396 YY= 131.033 ZY= -3.9612
 XZ= 17.069 YZ= 7.4701 ZZ= 147.0909
 Eigenvalues: 126.2425 143.0761 175.6492
 11 C Isotropic= 147.755 Anisotropy = 13.7469
 XX= 141.0052 YX= 0.1472 ZX= -5.0095
 XY= 8.5255 YY= 149.1941 ZY= 7.0933
 XZ= 8.3746 YZ= 1.7992 ZZ= 153.0656
 Eigenvalues: 139.1319 147.2135 156.9196
 12 C Isotropic= 155.495 Anisotropy = 24.506
 XX= 165.6544 YX= 11.6783 ZX= -2.6702
 XY= 3.1304 YY= 162.4122 ZY= 3.3013
 XZ= -1.8886 YZ= 10.5969 ZZ= 138.4184
 Eigenvalues: 135.9481 158.7045 171.8323
 13 C Isotropic= 148.5708 Anisotropy = 54.6436
 XX= 138.2244 YX= 14.9511 ZX= 13.5754
 XY= 14.9287 YY= 177.1743 ZY= 8.2396
 XZ= 20.3558 YZ= 5.2712 ZZ= 130.3136
 Eigenvalues: 116.5495 144.163 184.9999
 14 C Isotropic= 167.9089 Anisotropy = 12.0367
 XX= 163.1065 YX= 4.4024 ZX= 5.7776
 XY= -6.0845 YY= 166.6752 ZY= -4.8241
 XZ= 1.1165 YZ= -0.9764 ZZ= 173.945
 Eigenvalues: 162.1031 165.6903 175.9333
 15 C Isotropic= 169.5495 Anisotropy = 16.6554
 XX= 173.0459 YX= 5.7133 ZX= -0.9811
 XY= 4.1843 YY= 167.6388 ZY= 9.678
 XZ= 3.1872 YZ= 11.0431 ZZ= 167.9636
 Eigenvalues: 156.9425 171.0528 180.6531
 16 O Isotropic= 263.8501 Anisotropy = 85.5918
 XX= 307.8846 YX= -2.8388 ZX= 44.4134
 XY= 7.2261 YY= 270.5135 ZY= -44.3679
 XZ= 27.2913 YZ= -10.3463 ZZ= 213.1522
 Eigenvalues: 192.0358 278.6033 320.9113
 17 O Isotropic= 265.5101 Anisotropy = 45.8971
 XX= 257.3266 YX= -2.5685 ZX= -23.352
 XY= 15.3696 YY= 272.9865 ZY= -21.5096
 XZ= -7.6398 YZ= -19.111 ZZ= 266.2172

Eigenvalues:	242.9242	257.4979	296.1082		
18	O	Isotropic=	-371.8123	Anisotropy	= 1098.263
XX=	-1022.693	YX=	-43.5849	ZX=	150.2387
XY=	-8.9659	YY=	-75.933	ZY=	-403.0501
XZ=	77.7065	YZ=	-393.3144	ZZ=	-16.8108
Eigenvalues:	-1035.8545	-439.9454	360.363		
19	O	Isotropic=	95.2834	Anisotropy	= 127.038
XX=	172.1492	YX=	-17.8142	ZX=	-96.6435
XY=	19.0601	YY=	146.3244	ZY=	10.2118
XZ=	22.411	YZ=	-74.4148	ZZ=	-32.6234
Eigenvalues:	-44.3549	150.2297	179.9754		
20	O	Isotropic=	72.0595	Anisotropy	= 185.9289
XX=	65.5344	YX=	46.1541	ZX=	-1.5309
XY=	138.0913	YY=	17.4447	ZY=	93.5631
XZ=	-101.418	YZ=	118.054	ZZ=	133.1994
Eigenvalues:	-109.0394	129.2058	196.0121		
21	H	Isotropic=	31.1977	Anisotropy	= 13.5226
XX=	37.4496	YX=	2.1847	ZX=	-5.1295
XY=	2.1166	YY=	24.7193	ZY=	4.6733
XZ=	-4.7198	YZ=	3.7943	ZZ=	31.4242
Eigenvalues:	21.5518	31.8285	40.2128		
22	C	Isotropic=	21.427	Anisotropy	= 78.8028
XX=	-13.4295	YX=	63.1491	ZX=	63.0124
XY=	53.0886	YY=	28.0811	ZY=	-44.8321
XZ=	27.5683	YZ=	-20.3984	ZZ=	49.6293
Eigenvalues:	-78.6656	68.9843	73.9622		
23	O	Isotropic=	-140.9093	Anisotropy	= 605.4233
XX=	-240.0935	YX=	266.3809	ZX=	-142.7907
XY=	261.8183	YY=	100.4726	ZY=	-44.0005
XZ=	-93.098	YZ=	-52.8525	ZZ=	-283.1071
Eigenvalues:	-432.0869	-253.3473	262.7062		
24	C	Isotropic=	165.8301	Anisotropy	= 37.7385
XX=	157.2613	YX=	-8.358	ZX=	-6.5171
XY=	-8.1251	YY=	156.1242	ZY=	11.2845
XZ=	-4.5529	YZ=	14.033	ZZ=	184.1048
Eigenvalues:	147.3455	159.1557	190.9891		
25	H	Isotropic=	27.4737	Anisotropy	= 3.0634
XX=	28.4871	YX=	0.7855	ZX=	-1.0436
XY=	0.6171	YY=	26.925	ZY=	0.9602
XZ=	-2.1591	YZ=	1.5742	ZZ=	27.0088
Eigenvalues:	24.934	27.971	29.5159		
26	H	Isotropic=	28.2942	Anisotropy	= 8.3812
XX=	28.204	YX=	3.8877	ZX=	2.5301
XY=	2.9503	YY=	29.5482	ZY=	2.0343
XZ=	2.7635	YZ=	1.8631	ZZ=	27.1304
Eigenvalues:	24.762	26.2389	33.8817		
27	H	Isotropic=	25.3375	Anisotropy	= 4.2004
XX=	26.5203	YX=	-0.9838	ZX=	-2.9171
XY=	-2.1747	YY=	24.0504	ZY=	-0.5615
XZ=	0.1011	YZ=	1.681	ZZ=	25.4419
Eigenvalues:	23.2724	24.6024	28.1378		
28	H	Isotropic=	25.6131	Anisotropy	= 7.494
XX=	30.3711	YX=	-0.5961	ZX=	1.439
XY=	-0.094	YY=	25.9599	ZY=	-0.2305
XZ=	1.5847	YZ=	1.7347	ZZ=	20.5084
Eigenvalues:	20.1725	26.0577	30.6091		

29	H	Isotropic=	27.8566	Anisotropy	=	8.826
XX=	32.715	YX=	3.3065	ZX=	-0.1117	
XY=	3.2144	YY=	22.9183	ZY=	-1.753	
XZ=	0.7953	YZ=	-3.6474	ZZ=	27.9366	
Eigenvalues:	20.9058	28.9235	33.7407			
30	H	Isotropic=	29.9395	Anisotropy	=	5.8349
XX=	33.0996	YX=	0.0543	ZX=	1.7111	
XY=	0.0871	YY=	29.6037	ZY=	3.208	
XZ=	1.8949	YZ=	2.6189	ZZ=	27.1153	
Eigenvalues:	24.9233	31.0658	33.8295			
31	H	Isotropic=	29.4733	Anisotropy	=	8.5021
XX=	31.3495	YX=	2.9366	ZX=	-1.1877	
XY=	3.6038	YY=	31.1969	ZY=	-2.715	
XZ=	-1.2583	YZ=	-1.4922	ZZ=	25.8735	
Eigenvalues:	25.1411	28.1375	35.1413			
32	H	Isotropic=	29.2652	Anisotropy	=	9.1279
XX=	30.5851	YX=	-2.6741	ZX=	-4.9551	
XY=	-2.5812	YY=	28.2078	ZY=	0.4549	
XZ=	-4.2492	YZ=	1.0537	ZZ=	29.0027	
Eigenvalues:	24.6913	27.7539	35.3505			
33	H	Isotropic=	30.3959	Anisotropy	=	6.7261
XX=	32.357	YX=	-2.7518	ZX=	1.1365	
XY=	-2.656	YY=	27.7738	ZY=	-2.598	
XZ=	1.368	YZ=	-2.059	ZZ=	31.0569	
Eigenvalues:	25.9629	30.3448	34.88			
34	H	Isotropic=	30.2582	Anisotropy	=	8.9961
XX=	30.0056	YX=	-0.9324	ZX=	0.3996	
XY=	-2.6758	YY=	35.7045	ZY=	-0.288	
XZ=	0.9686	YZ=	-0.4777	ZZ=	25.0645	
Eigenvalues:	24.9697	29.5493	36.2556			
35	H	Isotropic=	30.456	Anisotropy	=	6.125
XX=	29.5585	YX=	-0.1356	ZX=	2.396	
XY=	1.4836	YY=	32.1931	ZY=	3.153	
XZ=	1.5231	YZ=	2.4364	ZZ=	29.6164	
Eigenvalues:	27.0493	29.7794	34.5393			
36	H	Isotropic=	28.7219	Anisotropy	=	6.4867
XX=	29.6814	YX=	1.0298	ZX=	-1.4931	
XY=	2.8872	YY=	31.4214	ZY=	-2.06	
XZ=	-1.1855	YZ=	-0.183	ZZ=	25.0628	
Eigenvalues:	24.6466	28.4727	33.0464			
37	H	Isotropic=	28.9607	Anisotropy	=	7.92
XX=	30.5458	YX=	-1.2728	ZX=	-1.2236	
XY=	-0.992	YY=	23.0356	ZY=	0.9371	
XZ=	-2.3294	YZ=	-0.0961	ZZ=	33.3008	
Eigenvalues:	22.8661	29.7754	34.2407			
38	H	Isotropic=	29.1515	Anisotropy	=	6.6715
XX=	28.4578	YX=	-1.4037	ZX=	0.1615	
XY=	-2.2892	YY=	32.3408	ZY=	-2.1275	
XZ=	0.4436	YZ=	-1.716	ZZ=	26.656	
Eigenvalues:	26.0344	27.8209	33.5992			
39	H	Isotropic=	28.5208	Anisotropy	=	7.8106
XX=	32.9894	YX=	2.9843	ZX=	-0.2651	
XY=	2.1272	YY=	23.0529	ZY=	0.0289	
XZ=	1.8348	YZ=	-0.4924	ZZ=	29.5202	
Eigenvalues:	22.4103	29.4243	33.7279			
40	H	Isotropic=	29.2	Anisotropy	=	10.8585

XX=	32.5013	YX=	4.1667	ZX=	-3.6583				
XY=	5.4317	YY=	28.3924	ZY=	0.2062				
XZ=	-2.4885	YZ=	-0.744	ZZ=	26.7064				
Eigenvalues:	24.1204	27.0406	36.439						
41	H	Isotropic=	29.6969	Anisotropy	=	5.7637			
XX=	30.8048	YX=	0.7947	ZX=	3.1517				
XY=	1.2403	YY=	29.1584	ZY=	-2.3205				
XZ=	3.6435	YZ=	-1.9545	ZZ=	29.1275				
Eigenvalues:	25.1308	30.4205	33.5394						
42	H	Isotropic=	30.5172	Anisotropy	=	9.653			
XX=	28.7954	YX=	0.9401	ZX=	-0.2205				
XY=	1.0397	YY=	34.1016	ZY=	4.996				
XZ=	-0.3215	YZ=	4.5851	ZZ=	28.6546				
Eigenvalues:	25.6922	28.9069	36.9525						
43	H	Isotropic=	29.0909	Anisotropy	=	5.5472			
XX=	30.0585	YX=	-1.9162	ZX=	0.2703				
XY=	-1.5764	YY=	25.1967	ZY=	2.0729				
XZ=	2.5018	YZ=	1.0271	ZZ=	32.0174				
Eigenvalues:	24.1679	30.3157	32.789						
44	H	Isotropic=	29.2196	Anisotropy	=	7.644			
XX=	27.0262	YX=	-2.2861	ZX=	-0.2898				
XY=	-3.1638	YY=	32.4639	ZY=	0.933				
XZ=	-1.8403	YZ=	2.7387	ZZ=	28.1687				
Eigenvalues:	25.8507	27.4925	34.3156						
45	H	Isotropic=	28.9068	Anisotropy	=	8.2955			
XX=	30.8712	YX=	2.2672	ZX=	-2.933				
XY=	1.9597	YY=	26.6266	ZY=	-0.7131				
XZ=	-4.489	YZ=	-0.8447	ZZ=	29.2227				
Eigenvalues:	25.4451	26.8383	34.4371						
46	H	Isotropic=	30.8339	Anisotropy	=	18.2798			
XX=	36.2371	YX=	-0.3688	ZX=	9.1629				
XY=	-0.54	YY=	23.4209	ZY=	-1.9634				
XZ=	6.9419	YZ=	-3.9113	ZZ=	32.8437				
Eigenvalues:	22.2136	27.2677	43.0204						
47	C	Isotropic=	13.559	Anisotropy	=	89.5929			
XX=	-69.0863	YX=	24.2677	ZX=	18.9789				
XY=	-15.3165	YY=	60.8791	ZY=	13.5931				
XZ=	48.3873	YZ=	12.6876	ZZ=	48.8842				
Eigenvalues:	-78.0328	45.4221	73.2876						
48	O	Isotropic=	-124.1469	Anisotropy	=	651.234			
XX=	-232.8128	YX=	93.8464	ZX=	68.6475				
XY=	63.9937	YY=	-118.2389	ZY=	320.0074				
XZ=	86.1358	YZ=	388.2952	ZZ=	-21.3891				
Eigenvalues:	-427.6747	-254.7751	310.0091						
49	H	Isotropic=	28.7279	Anisotropy	=	6.6054			
XX=	27.2861	YX=	2.0572	ZX=	1.8659				
XY=	0.6168	YY=	30.3312	ZY=	-3.3995				
XZ=	2.7015	YZ=	-3.6989	ZZ=	28.5666				
Eigenvalues:	23.807	29.2453	33.1315						
50	H	Isotropic=	29.5001	Anisotropy	=	6.5574			
XX=	28.3572	YX=	-0.0697	ZX=	-1.8332				
XY=	-0.4221	YY=	32.7383	ZY=	2.9945				
XZ=	-1.7404	YZ=	1.9876	ZZ=	27.4047				
Eigenvalues:	25.5207	29.1078	33.8716						
51	C	Isotropic=	108.2429	Anisotropy	=	24.2277			
XX=	111.5691	YX=	7.045	ZX=	-7.4151				

XY=	8.1203	YY=	113.7553	ZY=	-7.9462			
XZ=	-5.2137	YZ=	-7.8007	ZZ=	99.4041			
Eigenvalues:	95.3208	105.0131			124.3947			
52	C	Isotropic=	121.5359	Anisotropy	=	27.6769		
XX=	116.7598	YX=	15.9963	ZX=	2.8685			
XY=	10.3312	YY=	132.0155	ZY=	2.1949			
XZ=	2.0859	YZ=	1.9872	ZZ=	115.8323			
Eigenvalues:	108.9878		115.6326		139.9871			
53	O	Isotropic=	276.9025	Anisotropy	=	85.7266		
XX=	305.9137	YX=	38.647	ZX=	14.2097			
XY=	31.3938	YY=	269.099	ZY=	11.8901			
XZ=	26.9189	YZ=	10.5031	ZZ=	255.6947			
Eigenvalues:	247.2499		249.404		334.0535			
54	H	Isotropic=	26.7015	Anisotropy	=	3.5317		
XX=	26.5143	YX=	1.1361	ZX=	-1.2463			
XY=	-0.1197	YY=	25.3244	ZY=	0.4453			
XZ=	-1.5743	YZ=	0.4521	ZZ=	28.2658			
Eigenvalues:	24.8314	26.2171	29.056					
55	N	Isotropic=	119.1536	Anisotropy	=	101.3676		
XX=	128.8735	YX=	-11.2011	ZX=	43.3228			
XY=	-30.8387	YY=	165.3796	ZY=	-1.9467			
XZ=	80.2668	YZ=	-9.3323	ZZ=	63.2077			
Eigenvalues:	25.8015	144.9273			186.732			
56	C	Isotropic=	50.6469	Anisotropy	=	195.1847		
XX=	171.1567	YX=	3.2734	ZX=	29.637			
XY=	11.4193	YY=	-39.0559	ZY=	11.7852			
XZ=	47.1342	YZ=	10.5559	ZZ=	19.8399			
Eigenvalues:	-41.1039	12.2746	180.7701					
57	H	Isotropic=	24.7694	Anisotropy	=	1.9218		
XX=	24.304	YX=	-1.126	ZX=	0.2163			
XY=	-0.5413	YY=	23.976	ZY=	0.2654			
XZ=	0.0303	YZ=	-0.4523	ZZ=	26.0281			
Eigenvalues:	23.2904	24.9672	26.0506					
58	H	Isotropic=	30.1417	Anisotropy	=	18.5452		
XX=	36.344	YX=	7.6582	ZX=	3.5361			
XY=	7.9673	YY=	31.3681	ZY=	-1.2486			
XZ=	4.0624	YZ=	0.8779	ZZ=	22.7128			
Eigenvalues:	21.0535	26.8663	42.5051					
59	C	Isotropic=	17.6604	Anisotropy	=	113.6496		
XX=	-46.9702	YX=	48.1655	ZX=	-15.7723			
XY=	50.8183	YY=	74.7908	ZY=	9.4089			
XZ=	-28.8935	YZ=	23.8829	ZZ=	25.1605			
Eigenvalues:	-71.8804	31.4348	93.4268					
60	H	Isotropic=	25.9928	Anisotropy	=	8.7461		
XX=	30.5386	YX=	-5.2332	ZX=	-2.9369			
XY=	-1.4111	YY=	22.7933	ZY=	-2.6238			
XZ=	1.3624	YZ=	-4.8827	ZZ=	24.6463			
Eigenvalues:	19.0028	27.1519	31.8235					
61	C	Isotropic=	62.1306	Anisotropy	=	174.1334		
XX=	159.1136	YX=	20.04	ZX=	55.6092			
XY=	23.2678	YY=	15.199	ZY=	-35.8411			
XZ=	55.5825	YZ=	-41.017	ZZ=	12.0792			
Eigenvalues:	-40.4763	48.6486	178.2195					
62	C	Isotropic=	62.6696	Anisotropy	=	177.5183		
XX=	163.1299	YX=	-1.8316	ZX=	55.4498			
XY=	-2.3404	YY=	38.3825	ZY=	27.2257			

XZ= 61.4923 YZ= 30.1826 ZZ= -13.5035
 Eigenvalues: -41.0579 48.0516 181.0152
 63 C Isotropic= 64.3497 Anisotropy = 175.6989
 XX= 168.0161 YX= 9.0245 ZX= 39.3659
 XY= 6.0251 YY= -34.3998 ZY= 13.7251
 XZ= 39.5443 YZ= 16.0739 ZZ= 59.4328
 Eigenvalues: -36.7191 48.2859 181.4823
 64 C Isotropic= 62.4709 Anisotropy = 175.687
 XX= 159.2885 YX= 21.7483 ZX= 58.4926
 XY= 20.6945 YY= 14.1073 ZY= -38.0154
 XZ= 56.3506 YZ= -39.1026 ZZ= 14.017
 Eigenvalues: -40.5434 48.3606 179.5956
 65 C Isotropic= 61.3262 Anisotropy = 151.8107
 XX= 146.8088 YX= -10.5849 ZX= 49.9564
 XY= -3.1298 YY= 46.0422 ZY= 26.9899
 XZ= 53.8278 YZ= 26.7244 ZZ= -8.8726
 Eigenvalues: -34.1476 55.5928 162.5333
 66 H Isotropic= 23.7901 Anisotropy = 8.3072
 XX= 22.4987 YX= 0.4328 ZX= -1.4712
 XY= 0.8539 YY= 25.4122 ZY= -4.6725
 XZ= -1.2543 YZ= -4.3613 ZZ= 23.4594
 Eigenvalues: 19.652 22.3901 29.3283
 67 O Isotropic= -96.7804 Anisotropy = 667.3873
 XX= -149.1075 YX= 145.5066 ZX= 37.0502
 XY= 143.1376 YY= 266.186 ZY= 141.1625
 XZ= 80.0732 YZ= 171.2509 ZZ= -407.4197
 Eigenvalues: -444.4627 -194.023 348.1445
 68 C Isotropic= 55.0079 Anisotropy = 173.1032
 XX= -3.0345 YX= 18.0034 ZX= 63.0943
 XY= 30.9176 YY= 32.1151 ZY= 46.4319
 XZ= 59.9886 YZ= 18.7496 ZZ= 135.9432
 Eigenvalues: -28.7959 23.4096 170.41
 69 H Isotropic= 23.6732 Anisotropy = 4.3843
 XX= 21.3957 YX= -0.0519 ZX= -1.5602
 XY= -0.0315 YY= 26.5911 ZY= -0.1975
 XZ= -1.201 YZ= -0.0691 ZZ= 23.0329
 Eigenvalues: 20.6075 23.8161 26.5961
 70 H Isotropic= 23.8002 Anisotropy = 2.8539
 XX= 21.5035 YX= 0.4946 ZX= -1.7609
 XY= 0.1637 YY= 24.8996 ZY= 0.056
 XZ= -1.6742 YZ= 0.3057 ZZ= 24.9975
 Eigenvalues: 20.7669 24.9309 25.7028
 71 H Isotropic= 23.8559 Anisotropy = 4.2818
 XX= 21.1407 YX= 0.6586 ZX= -0.8894
 XY= 0.614 YY= 26.4485 ZY= -0.6617
 XZ= -1.0389 YZ= -0.5115 ZZ= 23.9786
 Eigenvalues: 20.8094 24.0478 26.7104
 72 H Isotropic= 23.9543 Anisotropy = 6.9374
 XX= 21.457 YX= -0.1868 ZX= -0.0942
 XY= -0.5398 YY= 27.446 ZY= 2.7005
 XZ= -0.2887 YZ= 2.2832 ZZ= 22.96
 Eigenvalues: 21.4316 21.8521 28.5792
 73 C Isotropic= 60.3737 Anisotropy = 176.9137
 XX= 40.6569 YX= -9.1809 ZX= 62.17
 XY= -5.8648 YY= 25.8536 ZY= 74.0578
 XZ= 67.3075 YZ= 75.2464 ZZ= 114.6107

Eigenvalues: -39.203442.0084 178.3162
74 C Isotropic= 61.9239 Anisotropy = 176.0761
XX= 52.8162 YX= 45.4202 ZX= 32.4032
XY= 48.0287 YY= -2.6355 ZY= 64.092
XZ= 31.8981 YZ= 65.1751 ZZ= 135.5912
Eigenvalues: -40.344846.8086 179.308
75 C Isotropic= 62.1049 Anisotropy = 178.0001
XX= -12.7702 YX= 37.8709 ZX= 63.3823
XY= 37.0205 YY= 62.0966 ZY= 38.9059
XZ= 61.8131 YZ= 39.2975 ZZ= 136.9883
Eigenvalues: -40.761846.3049 180.7716
76 C Isotropic= 63.4081 Anisotropy = 173.9292
XX= 38.935 YX= -11.7289 ZX= 63.4841
XY= -16.0748 YY= 32.5476 ZY= 73.3092
XZ= 63.8819 YZ= 75.1824 ZZ= 118.7417
Eigenvalues: -39.110449.9737 179.3609
77 C Isotropic= 67.1186 Anisotropy = 164.1875
XX= 58.8753 YX= 44.1808 ZX= 28.124
XY= 39.2219 YY= 4.4015 ZY= 60.0524
XZ= 32.9089 YZ= 57.0934 ZZ= 138.0792
Eigenvalues: -28.028152.8071 176.577
78 H Isotropic= 23.2378 Anisotropy = 7.7773
XX= 25.2416 YX= -3.6568 ZX= -0.5576
XY= -3.892 YY= 23.931 ZY= -1.1188
XZ= -0.887 YZ= -1.2314 ZZ= 20.5408
Eigenvalues: 19.2772 22.0136 28.4226
79 H Isotropic= 23.7364 Anisotropy = 4.3851
XX= 25.9252 YX= -0.8113 ZX= -1.8958
XY= -0.4159 YY= 23.4048 ZY= -1.5383
XZ= -1.8523 YZ= -1.556 ZZ= 21.8794
Eigenvalues: 20.263 24.2865 26.6598
80 H Isotropic= 23.7 Anisotropy = 3.8729
XX= 24.0983 YX= -0.6758 ZX= -1.1297
XY= -0.626 YY= 25.2633 ZY= -2.219
XZ= -1.1502 YZ= -2.0695 ZZ= 21.7385
Eigenvalues: 20.2769 24.5412 26.282
81 H Isotropic= 23.898 Anisotropy = 5.5004
XX= 26.4664 YX= -1.9791 ZX= -1.5089
XY= -1.7738 YY= 24.1651 ZY= -1.2968
XZ= -1.0676 YZ= -1.1312 ZZ= 21.0626
Eigenvalues: 20.0839 24.0452 27.565
82 H Isotropic= 24.0838 Anisotropy = 8.965
XX= 29.5103 YX= -0.8986 ZX= -2.946
XY= 0.1239 YY= 22.0508 ZY= -1.6238
XZ= -1.5946 YZ= -1.7634 ZZ= 20.6903
Eigenvalues: 19.1129 23.078 30.0605

2b-i

C	3.471954	-1.390091	1.573277
C	4.21788	-2.153374	0.43342
C	3.52637	-2.132007	-0.940077
C	4.289129	-1.324711	-2.006016
C	4.492249	0.16707	-1.673632
C	3.316511	0.970803	-1.139974
C	2.780544	0.496315	0.179685
C	1.449833	0.218412	0.271003

C	1.002507	-0.667853	1.400713
C	1.996239	-1.801782	1.675695
C	3.634987	0.148653	1.381178
C	5.114126	0.498393	1.302481
C	3.103632	0.880493	2.628666
C	0.427885	0.698288	-0.679945
C	5.610065	-1.973527	-2.351894
O	4.032205	-1.801272.819685	
O	4.445497	-3.491356	0.850728
O	5.534358	0.730076	-2.018901
O	3.406015	2.376538	-1.326706
O	-0.236051	-1.378115	1.201873
H	3.60677	-3.848406	1.167763
C	4.392328	3.18479	-0.831417
O	5.38294	2.711766	-0.284562
C	4.088169	4.622855	-1.097403
H	5.264137	-1.741094	0.337809
H	2.486549	-1.727292	-0.857062
H	2.51792	0.739967	-1.93292
H	0.851206	-0.027257	2.320049
H	1.800778	-2.186543	2.713555
H	1.784446	-2.645175	0.96697
H	5.574071	0.282989	0.312142
H	5.268474	1.586155	1.512584
H	5.672187	-0.073166	2.085511
H	3.92382	1.430404	3.151857
H	2.319275	1.624953	2.353643
H	2.683139	0.151271	3.363676
H	0.832549	1.420351	-1.430637
H	-0.038869	-0.165043	-1.219669
H	-0.378171.247584		-0.122745
H	6.099252	-1.422712	-3.19222
H	6.305094	-1.955528	-1.47831
H	5.446685	-3.034709	-2.657497
H	3.144447	4.734977	-1.68285
H	3.983813	5.152313	-0.119109
H	4.938491	5.068115	-1.669269
H	4.97541	-1.958448	2.685606
C	-1.411823	-0.710894	0.980316
O	-1.610969	0.340875	1.581869
H	3.640694	-1.321012	-2.931117
H	3.454229	-3.190769	-1.307218
C	-2.35717-1.536288		0.112965
C	-3.83484-1.257428		0.486618
O	-2.051358	-1.377424	-1.248031
H	-2.160427	-2.633090.313069	
N	-4.354201	0.084027	0.366168
C	-4.732804	-2.253444	-0.217124
H	-3.876255	-1.496356	1.603153
H	-2.176054	-0.447841	-1.494391
C	-3.740197	1.245245	-0.047687
H	-5.289889	0.169783	0.698816
C	-4.77207-2.346608		-1.610897
C	-5.612663	-3.273876	-2.226915
C	-6.419255	-4.109688	-1.455602
C	-6.383867	-4.01836-0.063909	

C	-5.545873	-3.092193	0.554489
H	-4.125625	-1.697168	-2.222217
O	-2.607291.264881	-0.574585	
C	-4.526701	2.503156	0.129909
H	-5.635362	-3.345058	-3.324426
H	-7.08131-4.840717	-1.942624	
H	-7.017625	-4.677339	0.547581
H	-5.52374-3.026823	1.652949	
C	-4.595251	3.40427	-0.938306
C	-5.309514	4.592948	-0.796094
C	-5.945051	4.887158	0.410617
C	-5.864658	3.993651	1.478981
C	-5.157803	2.799186	1.341706
H	-4.072499	3.172534	-1.879315
H	-5.366065.301006	-1.636083	
H	-6.505882	5.827256	0.521651
H	-6.356058	4.231373	2.434016
H	-5.082203	2.1072	2.194181

2bi_45 E(RB+HF-PW91) = -2012.289893

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic= 110.9014 Anisotropy 30.3387
 XX= 105.3945 YX= -3.3626 ZX= 20.1294
 XY= 3.4066 YY= 107.6683 ZY= 1.214
 XZ= 14.2201 YZ= 0.2222 ZZ= 119.6414
 Eigenvalues: 93.914 107.663 131.1272

2 C Isotropic= 112.4158 Anisotropy 31.6468
 XX= 92.8982 YX= -0.6406 ZX= -0.7738
 XY= -5.5755 YY= 132.1778 ZY= 0.4342
 XZ= 0.9429 YZ= -10.103 ZZ= 112.1715
 Eigenvalues: 92.6492 111.0846 133.5137

3 C Isotropic= 141.3483 Anisotropy 20.0866
 XX= 122.4845 YX= -8.6945 ZX= 4.6171
 XY= -0.4019 YY= 150.6311 ZY= 2.4622
 XZ= 5.5465 YZ= 5.431 ZZ= 150.9295
 Eigenvalues: 120.7064 148.5992 154.7394

4 C Isotropic= 141.1985 Anisotropy 23.1142
 XX= 129.2254 YX= -1.6311 ZX= 2.1078
 XY= -15.2082 YY= 152.5661 ZY= 5.7798
 XZ= 6.2962 YZ= 5.8758 ZZ= 141.8039
 Eigenvalues: 124.4997 142.4878 156.6079

5 C Isotropic= -23.721 Anisotropy 182.298
 XX= -46.5911 YX= 16.2124 ZX= 59.8884
 XY= 2.3451 YY= -89.8531 ZY= -41.7137
 XZ= 54.7358 YZ= -51.2106 ZZ= 65.2813
 Eigenvalues: -113.8287 -55.1453 97.811

6 C Isotropic= 101.2392 Anisotropy 41.2521
 XX= 88.251 YX= -15.0385 ZX= 0.2231
 XY= 3.68 YY= 126.7889 ZY= 4.4333
 XZ= -5.0931 YZ= 8.464 ZZ= 88.6776
 Eigenvalues: 86.0189 88.958 128.7406

7 C Isotropic= 47.8675 Anisotropy 149.7484
 XX= 50.1935 YX= -12.8539 ZX= -7.4903
 XY= -29.4616 YY= 113.239 ZY= 80.5236
 XZ= -1.9301 YZ= 58.8152 ZZ= -19.83

Eigenvalues:	-49.794845.6975	147.6997		
8	C	Isotropic=	38.3228	Anisotropy 161.5824
XX=	32.4059	YX=	-9.3543	ZX= -14.2733
XY=	-10.6542	YY=	83.5799	ZY= 82.8465
XZ=	-26.7451	YZ=	101.4645	ZZ= -1.0174
Eigenvalues:	-61.644630.5686	146.0444		
9	C	Isotropic=	111.0097	Anisotropy 55.2334
XX=	131.4551	YX=	25.3937	ZX= 12.049
XY=	24.6749	YY=	104.8122	ZY= -8.3583
XZ=	19.2838	YZ=	-13.3511	ZZ= 96.7618
Eigenvalues:	75.1979	109.9992	147.8319	
10	C	Isotropic=	146.861	Anisotropy 44.1299
XX=	175.1678	YX=	5.6679	ZX= 3.2555
XY=	-0.0922	YY=	134.065	ZY= -4.6957
XZ=	10.5491	YZ=	-12.5447	ZZ= 131.3501
Eigenvalues:	123.0203	141.2817	176.2809	
11	C	Isotropic=	147.697	Anisotropy 11.6147
XX=	143.5571	YX=	0.2738	ZX= -0.477
XY=	-13.8373	YY=	151.4688	ZY= -0.8137
XZ=	-2.3538	YZ=	0.9042	ZZ= 148.0652
Eigenvalues:	139.4918	148.1592	155.4402	
12	C	Isotropic=	155.0636	Anisotropy 22.6474
XX=	159.2019	YX=	2.1112	ZX= -17.7795
XY=	6.7746	YY=	153.5816	ZY= 12.9763
XZ=	-8.7158	YZ=	7.9118	ZZ= 152.4072
Eigenvalues:	135.4092	159.6197	170.1619	
13	C	Isotropic=	148.3519	Anisotropy 54.472
XX=	148.29	YX=	-12.9371	ZX= -9.0976
XY=	-19.2613	YY=	138.4813	ZY= 26.2975
XZ=	-6.5199	YZ=	28.9201	ZZ= 158.2845
Eigenvalues:	116.3604	144.0288	184.6666	
14	C	Isotropic=	166.3013	Anisotropy 14.5642
XX=	170.8243	YX=	-9.916	ZX= 4.5883
XY=	1.4437	YY=	161.3113	ZY= 4.4242
XZ=	8.9116	YZ=	2.0654	ZZ= 166.7683
Eigenvalues:	156.3361	166.5571	176.0108	
15	C	Isotropic=	169.2364	Anisotropy 17.1967
XX=	172.6462	YX=	-2.5402	ZX= -10.0611
XY=	-5.0238	YY=	174.7663	ZY= 3.8467
XZ=	-6.1346	YZ=	2.8313	ZZ= 160.2967
Eigenvalues:	156.1888	170.8195	180.7008	
16	O	Isotropic=	263.2064	Anisotropy 82.6207
XX=	316.4509	YX=	0.156	ZX= 4.9772
XY=	19.4519	YY=	198.4985	ZY= 36.7549
XZ=	4.802	YZ=	1.8649	ZZ= 274.6696
Eigenvalues:	193.3075	278.0247	318.2868	
17	O	Isotropic=	265.5345	Anisotropy 44.8506
XX=	249.9186	YX=	22.1613	ZX= 2.0664
XY=	-0.8076	YY=	255.3257	ZY= -7.5185
XZ=	2.7398	YZ=	-17.9806	ZZ= 291.3591
Eigenvalues:	239.6623	261.5063	295.4348	
18	O	Isotropic=	-354.1343	Anisotropy 1076.2522
XX=	-735.0459	YX=	-282.0614	ZX= 425.4903
XY=	-245.5342	YY=	-513.496	ZY= -64.7406
XZ=	369.6049	YZ=	-73.7052	ZZ= 186.139
Eigenvalues:	-991.2938	-434.4763	363.3672	

19	O	Isotropic=	87.6596	Anisotropy	124.4908
XX=	99.8418	YX=	163.4988	ZX=	-53.0833
XY=	23.4815	YY=	34.0711	ZY=	16.2338
XZ=	-35.6189	YZ=	73.9246	ZZ=	129.0659
Eigenvalues:	-53.5413	145.8666		170.6535	
20	O	Isotropic=	99.2728	Anisotropy	154.0508
XX=	137.1881	YX=	-28.0111	ZX=	4.9378
XY=	-149.2312	YY=	60.1015	ZY=	-78.1448
XZ=	-88.0685	YZ=	-114.1531	ZZ=	100.5288
Eigenvalues:	-63.4427	159.2878		201.9733	
21	H	Isotropic=	31.1582	Anisotropy	13.5933
XX=	33.1635	YX=	3.5977	ZX=	-5.0565
XY=	3.0885	YY=	35.7571	ZY=	-4.041
XZ=	-4.9943	YZ=	-2.9971	ZZ=	24.5539
Eigenvalues:	21.9778	31.2764	40.2203		
22	C	Isotropic=	20.1818	Anisotropy	74.4127
XX=	39.946	YX=	-77.5559	ZX=	-10.8843
XY=	-38.0655	YY=	-44.8089	ZY=	-13.3342
XZ=	-11.9267	YZ=	-30.361	ZZ=	65.4084
Eigenvalues:	-78.3357	69.091	69.7903		
23	O	Isotropic=	-131.1637	Anisotropy	600.4122
XX=	-270.8955	YX=	-8.1566	ZX=	-293.5254
XY=	-31.1784	YY=	-255.2018	ZY=	10.3898
XZ=	-247.5188	YZ=	15.2971	ZZ=	132.6064
Eigenvalues:	-407.5349	-255.0672		269.1111	
24	C	Isotropic=	166.0829	Anisotropy	36.8924
XX=	158.5262	YX=	-4.3631	ZX=	5.9916
XY=	-4.821	YY=	188.3073	ZY=	-8.0752
XZ=	5.5648	YZ=	-6.4659	ZZ=	151.4152
Eigenvalues:	147.7244	159.8465		190.6778	
25	H	Isotropic=	27.4083	Anisotropy	2.908
XX=	26.7995	YX=	0.1416	ZX=	-1.5013
XY=	1.3876	YY=	28.8061	ZY=	0.0546
XZ=	-1.8021	YZ=	-0.4996	ZZ=	26.6192
Eigenvalues:	25.0188	27.8591	29.3469		
26	H	Isotropic=	27.954	Anisotropy	8.3017
XX=	29.7556	YX=	-3.7545	ZX=	-2.147
XY=	-3.3098	YY=	26.9548	ZY=	1.7573
XZ=	-1.7837	YZ=	2.7504	ZZ=	27.1515
Eigenvalues:	24.2434	26.1301	33.4884		
27	H	Isotropic=	25.2389	Anisotropy	3.3607
XX=	25.7988	YX=	2.0305	ZX=	-1.3531
XY=	0.4083	YY=	26.5825	ZY=	0.6674
XZ=	1.7864	YZ=	-1.4266	ZZ=	23.3352
Eigenvalues:	23.2329	25.0043	27.4793		
28	H	Isotropic=	24.507	Anisotropy	7.3939
XX=	29.1141	YX=	1.1783	ZX=	1.2529
XY=	-0.06	YY=	20.738	ZY=	3.5767
XZ=	0.7032	YZ=	2.3273	ZZ=	23.6688
Eigenvalues:	18.9075	25.1771	29.4362		
29	H	Isotropic=	28.5628	Anisotropy	6.5629
XX=	29.7486	YX=	0.6292	ZX=	-1.5007
XY=	0.1186	YY=	26.0202	ZY=	-4.4046
XZ=	-0.8166	YZ=	-3.7749	ZZ=	29.9197
Eigenvalues:	23.4244	29.3259	32.9381		
30	H	Isotropic=	29.051	Anisotropy	4.5198

XX=	32.0089	YX=	0.4568	ZX=	0.174		
XY=	0.2734	YY=	29.4675	ZY=	1.7171		
XZ=	-0.489	YZ=	2.4737	ZZ=	25.6767		
Eigenvalues:	24.7348	30.354	32.0642				
31	H	Isotropic=	29.2808	Anisotropy		8.2251	
XX=	29.0687	YX=	1.1709	ZX=	-2.9184		
XY=	1.2145	YY=	25.4596	ZY=	1.2195		
XZ=	-2.8213	YZ=	-0.4003	ZZ=	33.3141		
Eigenvalues:	24.8861	28.1921	34.7642				
32	H	Isotropic=	29.1916	Anisotropy		9.0077	
XX=	27.074	YX=	4.4866	ZX=	-0.1515		
XY=	3.8235	YY=	32.9655	ZY=	-0.7703		
XZ=	0.7007	YZ=	-1.3095	ZZ=	27.5351		
Eigenvalues:	24.7363	27.6416	35.1967				
33	H	Isotropic=	30.3762	Anisotropy		6.5795	
XX=	33.1511	YX=	1.1965	ZX=	2.8497		
XY=	1.2636	YY=	28.8706	ZY=	-1.3613		
XZ=	3.1487	YZ=	-2.0118	ZZ=	29.1068		
Eigenvalues:	26.0123	30.3537	34.7625				
34	H	Isotropic=	30.1604	Anisotropy		9.0536	
XX=	29.666	YX=	1.5398	ZX=	0.5324		
XY=	2.0319	YY=	28.7221	ZY=	4.3825		
XZ=	2.039	YZ=	5.2861	ZZ=	32.0931		
Eigenvalues:	25.164	29.1211	36.1961				
35	H	Isotropic=	30.1217	Anisotropy		6.3442	
XX=	30.7687	YX=	-2.495	ZX=	1.3182		
XY=	-2.5484	YY=	31.1258	ZY=	3.0061		
XZ=	-1.172	YZ=	2.9369	ZZ=	28.4706		
Eigenvalues:	26.0437	29.9702	34.3511				
36	H	Isotropic=	28.4325	Anisotropy		6.3408	
XX=	27.1502	YX=	1.0011	ZX=	-1.3912		
XY=	0.5043	YY=	26.4243	ZY=	2.9099		
XZ=	-2.1695	YZ=	0.5545	ZZ=	31.7229		
Eigenvalues:	25.0593	27.5784	32.6597				
37	H	Isotropic=	28.774	Anisotropy		6.757	
XX=	31.8411	YX=	0.9295	ZX=	-0.2906		
XY=	1.363	YY=	27.909	ZY=	-4.6981		
XZ=	-1.3445	YZ=	-4.5455	ZZ=	26.5719		
Eigenvalues:	22.5686	30.4747	33.2786				
38	H	Isotropic=	28.3048	Anisotropy		10.8027	
XX=	31.9264	YX=	4.3644	ZX=	1.3137		
XY=	5.4482	YY=	26.4514	ZY=	0.6209		
XZ=	3.1757	YZ=	1.6249	ZZ=	26.5365		
Eigenvalues:	23.5589	25.8489	35.5066				
39	H	Isotropic=	27.4689	Anisotropy		11.4395	
XX=	33.6915	YX=	-2.4228	ZX=	-4.0978		
XY=	-2.8285	YY=	25.4723	ZY=	-1.1037		
XZ=	-2.2951	YZ=	-1.5693	ZZ=	23.243		
Eigenvalues:	21.2978	26.0136	35.0953				
40	H	Isotropic=	29.174	Anisotropy		10.7795	
XX=	29.2618	YX=	1.9027	ZX=	-5.5213		
XY=	0.1493	YY=	27.3312	ZY=	-1.641		
XZ=	-6.1717	YZ=	-1.347	ZZ=	30.9291		
Eigenvalues:	24.1754	26.9864	36.3604				
41	H	Isotropic=	29.6234	Anisotropy		5.8981	
XX=	32.9631	YX=	-1.401	ZX=	0.9191		

XY=	-1.8444	YY=	25.355	ZY=	0.3489		
XZ=	0.9131	YZ=	-0.2128	ZZ=	30.5521		
Eigenvalues:	25.0119	30.3029	33.5555				
42	H	Isotropic=	30.4785	Anisotropy	9.5706		
XX=	28.4836	YX=	-1.2818	ZX=	-2.1344		
XY=	-1.2826	YY=	34.0841	ZY=	3.8392		
XZ=	-2.5165	YZ=	4.1528	ZZ=	28.8678		
Eigenvalues:	25.78	28.7966	36.8589				
43	H	Isotropic=	29.025	Anisotropy	5.5888		
XX=	30.3878	YX=	0.6657	ZX=	2.9415		
XY=	-1.2217	YY=	30.5866	ZY=	-2.4988		
XZ=	3.441	YZ=	-1.2174	ZZ=	26.1007		
Eigenvalues:	24.0434	30.2808	32.7509				
44	H	Isotropic=	29.2244	Anisotropy	6.7493		
XX=	26.4312	YX=	-0.9542	ZX=	-0.7603		
XY=	0.3907	YY=	31.628	ZY=	3.4202		
XZ=	-0.0825	YZ=	2.3846	ZZ=	29.6138		
Eigenvalues:	26.373	27.5762	33.7239				
45	H	Isotropic=	28.9995	Anisotropy	8.8291		
XX=	29.6074	YX=	1.75	ZX=	-2.219		
XY=	4.0099	YY=	30.2083	ZY=	-3.0343		
XZ=	-2.826	YZ=	-3.1973	ZZ=	27.1826		
Eigenvalues:	25.0834	27.0294	34.8855				
46	H	Isotropic=	30.6258	Anisotropy	17.9603		
XX=	40.6008	YX=	-5.1838	ZX=	4.091		
XY=	-3.3117	YY=	24.2545	ZY=	-3.5909		
XZ=	2.5215	YZ=	-1.7621	ZZ=	27.022		
Eigenvalues:	22.3686	26.9095	42.5993				
47	C	Isotropic=	8.3908	Anisotropy	92.7558		
XX=	-69.3853	YX=	-2.8605	ZX=	-60.6013		
XY=	29.8284	YY=	46.9003	ZY=	0.3899		
XZ=	-39.7032	YZ=	-10.7345	ZZ=	47.6573		
Eigenvalues:	-88.8069	43.7513	70.2279				
48	O	Isotropic=	-153.1488	Anisotropy	692.0613		
XX=	-259.5539	YX=	116.2759	ZX=	-165.9596		
XY=	119.7442	YY=	-291.3619	ZY=	-289.431		
XZ=	-176.6646	YZ=	-255.5491	ZZ=	91.4695		
Eigenvalues:	-438.6716	-329.0001	308.2254				
49	H	Isotropic=	28.6563	Anisotropy	6.516		
XX=	29.3226	YX=	-1.8679	ZX=	0.755		
XY=	-1.8904	YY=	24.2271	ZY=	-0.2108		
XZ=	2.0921	YZ=	0.6954	ZZ=	32.4191		
Eigenvalues:	23.5561	29.4124	33.0002				
50	H	Isotropic=	29.4437	Anisotropy	6.4988		
XX=	26.8086	YX=	0.9908	ZX=	-0.9416		
XY=	0.7704	YY=	32.192	ZY=	2.0757		
XZ=	-1.2348	YZ=	3.2186	ZZ=	29.3305		
Eigenvalues:	25.8133	28.7415	33.7762				
51	C	Isotropic=	112.1315	Anisotropy	15.3536		
XX=	122.2599	YX=	2.6187	ZX=	-0.3339		
XY=	-0.1861	YY=	97.8881	ZY=	-6.7476		
XZ=	0.0124	YZ=	-5.4742	ZZ=	116.2464		
Eigenvalues:	95.9925	118.0347	122.3673				
52	C	Isotropic=	124.2226	Anisotropy	15.6643		
XX=	115.9526	YX=	8.3994	ZX=	6.8289		
XY=	6.8097	YY=	131.2291	ZY=	-5.1103		

XZ= 5.2884 YZ= -2.9748 ZZ= 125.4862
 Eigenvalues: 109.5869 128.4154 134.6655
 53 O Isotropic= 262.1641 Anisotropy 44.2212
 XX= 261.901 YX= -3.1005 ZX= -6.1832
 XY= 8.1319 YY= 287.5123 ZY= -31.1297
 XZ= -9.1906 YZ= 3.7176 ZZ= 237.0789
 Eigenvalues: 232.0169 262.8304 291.6449
 54 H Isotropic= 26.4372 Anisotropy 5.5201
 XX= 29.4815 YX= 1.8023 ZX= 1.6323
 XY= -2.5314 YY= 26.0159 ZY= -2.8227
 XZ= 1.029 YZ= -3.0522 ZZ= 23.8141
 Eigenvalues: 21.6752 27.5191 30.1173
 55 N Isotropic= 120.1214 Anisotropy 95.7617
 XX= 49.4031 YX= 54.3047 ZX= 25.8502
 XY= 34.0233 YY= 164.4479 ZY= -3.0556
 XZ= 34.8491 YZ= -41.6549 ZZ= 146.5133
 Eigenvalues: 23.8131 152.5886 183.9626
 56 C Isotropic= 53.0154 Anisotropy 186.8095
 XX= 81.0219 YX= -101.5798 ZX= -5.7145
 XY= -97.016 YY= 74.523 ZY= -22.8358
 XZ= -10.4478 YZ= -18.6358 ZZ= 3.5013
 Eigenvalues: -33.1721 14.6633 177.5551
 57 H Isotropic= 26.5784 Anisotropy 7.3171
 XX= 24.5744 YX= 1.5403 ZX= -0.6981
 XY= 1.4357 YY= 26.3409 ZY= -3.2072
 XZ= -2.5565 YZ= -2.6604 ZZ= 28.8198
 Eigenvalues: 23.7265 24.5521 31.4565
 58 H Isotropic= 27.5777 Anisotropy 14.2504
 XX= 21.771 YX= -0.4253 ZX= -0.7932
 XY= -1.8028 YY= 36.2019 ZY= -4.0533
 XZ= -0.615 YZ= -2.2996 ZZ= 24.7602
 Eigenvalues: 21.3607 24.2944 37.078
 59 C Isotropic= 16.5088 Anisotropy 116.3569
 XX= 27.405 YX= -3.4018 ZX= 26.7047
 XY= 12.4782 YY= -64.2953 ZY= 15.3396
 XZ= 14.0446 YZ= 12.0317 ZZ= 86.4167
 Eigenvalues: -65.6084 21.0547 94.08
 60 H Isotropic= 26.4172 Anisotropy 9.6473
 XX= 25.71 YX= 0.7128 ZX= -5.1774
 XY= -1.5416 YY= 32.7641 ZY= 0.2137
 XZ= -2.7019 YZ= 0.8767 ZZ= 20.7774
 Eigenvalues: 18.5903 27.8125 32.8487
 61 C Isotropic= 59.2899 Anisotropy 179.6041
 XX= 91.5686 YX= -96.4805 ZX= 24.0379
 XY= -91.6161 YY= 77.8639 ZY= 31.3318
 XZ= 29.6452 YZ= 22.2742 ZZ= 8.4373
 Eigenvalues: -39.5378 38.3816 179.026
 62 C Isotropic= 61.9249 Anisotropy 176.3297
 XX= 119.4827 YX= -64.9312 ZX= 1.2458
 XY= -65.8108 YY= 107.9794 ZY= -4.5151
 XZ= 2.3161 YZ= -7.0644 ZZ= -41.6874
 Eigenvalues: -41.9152 48.2118 179.478
 63 C Isotropic= 63.3595 Anisotropy 176.2104
 XX= 88.2444 YX= -99.8705 ZX= -18.9073
 XY= -102.3148 YY= 70.1385 ZY= -28.9965
 XZ= -20.3362 YZ= -27.4098 ZZ= 31.6956

Eigenvalues: -38.782748.028 180.8331
 64 C Isotropic= 62.9377 Anisotropy 172.708
 XX= 89.323 YX= -94.2264 ZX= 29.6828
 XY= -94.3125 YY= 77.7923 ZY= 27.2627
 XZ= 31.8609 YZ= 28.58 ZZ= 21.6977
 Eigenvalues: -39.121449.8581 178.0764
 65 C Isotropic= 62.0951 Anisotropy 146.0036
 XX= 113.2167 YX= -50.3464 ZX= 2.8985
 XY= -46.8768 YY= 107.8704 ZY= -5.7621
 XZ= 2.7641 YZ= -6.4868 ZZ= -34.8019
 Eigenvalues: -35.068561.9229 159.4308
 66 H Isotropic= 22.521 Anisotropy 11.5522
 XX= 23.2278 YX= 4.3174 ZX= 4.6392
 XY= 3.0926 YY= 19.6756 ZY= 2.28
 XZ= 3.8079 YZ= 3.4162 ZZ= 24.6597
 Eigenvalues: 17.3368 20.0038 30.2225
 67 O Isotropic= -69.9496 Anisotropy 575.9829
 XX= -251.6276 YX= -27.167 ZX= 262.5908
 XY= -66.4117 YY= -171.3483 ZY= 62.7576
 XZ= 207.8514 YZ= 53.4253 ZZ= 213.1271
 Eigenvalues: -371.5701 -152.3177 314.039
 68 C Isotropic= 55.4585 Anisotropy 171.0421
 XX= 113.1045 YX= 87.0134 ZX= 19.6109
 XY= 79.4686 YY= 23.3538 ZY= 2.3354
 XZ= 39.3686 YZ= 18.0116 ZZ= 29.9174
 Eigenvalues: -27.118524.0075 169.4866
 69 H Isotropic= 23.7185 Anisotropy 5.6095
 XX= 23.4811 YX= 3.7326 ZX= 0.5411
 XY= 3.3946 YY= 23.8545 ZY= 0.8391
 XZ= 0.443 YZ= 0.7032 ZZ= 23.8201
 Eigenvalues: 20.0909 23.6065 27.4582
 70 H Isotropic= 23.7467 Anisotropy 3.3932
 XX= 22.7411 YX= 2.6287 ZX= -0.404
 XY= 2.2497 YY= 22.8442 ZY= -0.3694
 XZ= -0.5021 YZ= -0.2054 ZZ= 25.6548
 Eigenvalues: 20.35 24.8813 26.0089
 71 H Isotropic= 23.8121 Anisotropy 4.5458
 XX= 22.9541 YX= 3.0172 ZX= 0.5895
 XY= 2.8697 YY= 23.4065 ZY= 0.9389
 XZ= 0.5807 YZ= 1.0237 ZZ= 25.0758
 Eigenvalues: 20.216 24.3777 26.8426
 72 H Isotropic= 24.121 Anisotropy 7.9676
 XX= 24.806 YX= 4.3643 ZX= -0.8189
 XY= 4.208 YY= 25.1124 ZY= -0.7565
 XZ= -1.0242 YZ= -0.6218 ZZ= 22.4447
 Eigenvalues: 20.6496 22.2807 29.4328
 73 C Isotropic= 60.3037 Anisotropy 175.1892
 XX= 115.992 YX= 58.8661 ZX= 71.0059
 XY= 54.8389 YY= 70.8732 ZY= 8.7943
 XZ= 67.9833 YZ= 10.8408 ZZ= -5.9543
 Eigenvalues: -39.676243.4907 177.0964
 74 C Isotropic= 62.1987 Anisotropy 177.0769
 XX= 137.7442 YX= 51.9977 ZX= 34.6748
 XY= 52.9796 YY= 40.5557 ZY= 61.5663
 XZ= 32.7489 YZ= 63.7276 ZZ= 8.2963
 Eigenvalues: -40.468946.8151 180.25

75	C	Isotropic=	61.339	Anisotropy	179.4559
XX=	116.6253	YX=	87.616	ZX=	41.4703
XY=	89.5571	YY=	9.6423	ZY=	12.619
XZ=	41.1952	YZ=	11.7762	ZZ=	57.7492
Eigenvalues:	-41.386	44.4267	180.9762		
76	C	Isotropic=	63.4007	Anisotropy	175.9449
XX=	123.0226	YX=	56.55	ZX=	69.8102
XY=	58.0789	YY=	70.7704	ZY=	5.8578
XZ=	69.7613	YZ=	0.8941	ZZ=	-3.5907
Eigenvalues:	-38.7905	48.2953	180.6974		
77	C	Isotropic=	65.7712	Anisotropy	165.2201
XX=	138.8626	YX=	50.2872	ZX=	25.9327
XY=	49.2426	YY=	46.4308	ZY=	59.6429
XZ=	30.7612	YZ=	53.0046	ZZ=	12.0202
Eigenvalues:	-29.9964	51.3921	175.9179		
78	H	Isotropic=	23.3919	Anisotropy	8.2122
XX=	21.7474	YX=	-3.4328	ZX=	0.1647
XY=	-2.6486	YY=	26.3104	ZY=	-2.6342
XZ=	0.393	YZ=	-2.9494	ZZ=	22.1179
Eigenvalues:	19.6248	21.6843	28.8667		
79	H	Isotropic=	23.7504	Anisotropy	4.7517
XX=	22.4414	YX=	-2.7256	ZX=	-1.4864
XY=	-2.5753	YY=	24.9975	ZY=	-0.051
XZ=	-1.6316	YZ=	0.1032	ZZ=	23.8122
Eigenvalues:	20.278	24.0549	26.9182		
80	H	Isotropic=	23.6875	Anisotropy	3.5949
XX=	21.824	YX=	-1.7117	ZX=	-1.3801
XY=	-1.4296	YY=	23.8115	ZY=	-0.9793
XZ=	-1.4847	YZ=	-1.1674	ZZ=	25.4269
Eigenvalues:	20.3398	24.6385	26.0841		
81	H	Isotropic=	23.8043	Anisotropy	4.9888
XX=	21.9626	YX=	-2.7653	ZX=	-0.8928
XY=	-2.5766	YY=	25.7257	ZY=	-0.6066
XZ=	-1.037	YZ=	-0.9477	ZZ=	23.7248
Eigenvalues:	20.1621	24.1208	27.1302		
82	H	Isotropic=	23.7005	Anisotropy	8.531
XX=	22.3166	YX=	-3.345	ZX=	-2.4481
XY=	-3.1662	YY=	25.3775	ZY=	2.8125
XZ=	-2.6549	YZ=	1.9675	ZZ=	23.4076
Eigenvalues:	19.8726	21.8412	29.3879		

2b-ii

C	-2.962602	-2.048007	-1.266362
C	-3.564058	-2.675622	0.030802
C	-2.871861	-2.272361.343577	
C	-3.744885	-1.398223	2.261981
C	-4.190023	-0.053487	1.653141
C	-3.165123	0.801641	0.924119
C	-2.572219	0.163214	-0.298492
C	-1.215438	0.079703	-0.389357
C	-0.648185	-0.925992	-1.351841
C	-1.440042	-2.236831	-1.345906
C	-3.37268-0.546058	-1.372078	
C	-4.888674	-0.429374	-1.298316
C	-2.985332	-0.001914	-2.760335
C	-0.275268	0.855516	0.444355

C	-4.940625	-2.163539	2.781827
O	-3.460504	-2.778467	-2.385798
O	-3.575953	-4.088281	-0.108269
O	-5.305119	0.398532	1.92448
O	-3.476598	2.18474	0.836745
O	0.702095	-1.36214	-1.097583
H	-2.690077	-4.367291	-0.370886
C	-4.586824	2.713599	0.23422
O	-5.487612	1.988502	-0.17277
C	-4.522042	4.205271	0.20888
H	-4.662561	-2.422625	0.087932
H	-1.911575	-1.735322	1.141049
H	-2.334111	0.859322	1.715189
H	-0.633583	-0.466074	-2.385325
H	-1.194434	-2.792514	-2.291779
H	-1.0857	-2.869884	-0.490667
H	-5.296089	-0.510164	-0.265851
H	-5.225201	0.553073	-1.713996
H	-5.351396	-1.230785	-1.926923
H	-3.891062	0.303511	-3.339534
H	-2.324649	0.892899	-2.671741
H	-2.468663	-0.789696	-3.361609
H	-0.778492	1.677446	1.011986
H	0.242182	0.175099	1.168744
H	0.492103	1.355861	-0.202357
H	-5.504446	-1.539709	3.517952
H	-5.637666	-2.428953	1.95101
H	-4.605191	-3.103633	3.281779
H	-3.609298	4.580003	0.730457
H	-4.507976	4.544058	-0.855803
H	-5.433484	4.61065	0.712669
H	-4.355543	-3.075049	-2.176536
C	1.744874	-0.474485	-1.082711
O	1.754133	0.429221	-1.914228
H	-3.09748	-1.108713	3.141349
H	-2.626635	-3.212113	1.907483
C	2.846729	-0.933774	-0.134704
C	4.248397	-0.650585	-0.719895
O	2.590735	-0.514738	1.180019
H	2.781403	-2.067777	-0.060606
N	4.748269	0.653311	-1.068415
C	5.270536	-1.376343	0.141012
H	4.198562	-1.210639	-1.718842
H	2.352009	0.422636	1.161236
C	4.354903	1.973578	-1.066894
H	5.634303	0.546834	-1.53693
C	5.408187	-1.100379	1.503492
C	6.362465	-1.778524	2.261838
C	7.185867	-2.730919	1.662345
C	7.053892	-3.005631	0.300926
C	6.101729	-2.328886	-0.45952
H	4.751976	-0.355615	1.980631
O	5.120682	2.759722	-1.672929
C	3.211675	2.556938	-0.316409
H	6.464157	-1.559108	3.334893
H	7.938978	-3.264164	2.261036

H	7.703214	-3.754959	-0.175353
H	6.006656	-2.547543	-1.534068
C	2.447626	3.555214	-0.935413
C	1.546218	4.311205	-0.187119
C	1.446316	4.121742	1.191022
C	2.261662	3.182782	1.823488
C	3.157751	2.419298	1.076654
H	2.560118	3.726508	-2.018051
H	0.930925	5.075485	-0.685008
H	0.742682	4.726797	1.781837
H	2.217775	3.060885	2.91591
H	3.857856	1.738758	1.590351

2bii_45 E(RB+HF-PW91) = -2012.262929

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic= 110.6218 Anisotropy 30.7878
 XX= 105.9543 YX= 7.0476 ZX= 19.2953
 XY= -1.3598 YY= 108.8113 ZY= 5.0982
 XZ= 15.3843 YZ= 4.6257 ZZ= 117.0998
 Eigenvalues: 93.2919 107.4266 131.147

2 C Isotropic= 112.2116 Anisotropy 30.6055
 XX= 92.9927 YX= -4.9689 ZX= 0.8215
 XY= -0.2195 YY= 132.4442 ZY= -5.2586
 XZ= -0.2923 YZ= 5.6207 ZZ= 111.1979
 Eigenvalues: 92.8187 111.2008 132.6153

3 C Isotropic= 141.8508 Anisotropy 19.8832
 XX= 122.3946 YX= 4.7094 ZX= 4.3568
 XY= -2.4119 YY= 150.465 ZY= -1.4645
 XZ= 7.1722 YZ= -4.012 ZZ= 152.6928
 Eigenvalues: 121.244 149.2021 155.1063

4 C Isotropic= 140.7595 Anisotropy 24.3594
 XX= 127.1629 YX= -1.982 ZX= 3.5722
 XY= 12.8107 YY= 151.892 ZY= -8.5643
 XZ= 4.9833 YZ= -7.7243 ZZ= 143.2237
 Eigenvalues: 124.0614 141.2181 156.9991

5 C Isotropic= -22.9732 Anisotropy 180.7659
 XX= -42.3506 YX= 1.2625 ZX= 54.3058
 XY= 13.7052 YY= -62.7174 ZY= 76.7338
 XZ= 44.2008 YZ= 85.8193 ZZ= 36.1485
 Eigenvalues: -113.5749 -52.882 97.5374

6 C Isotropic= 101.9255 Anisotropy 41.469
 XX= 88.4586 YX= 8.663 ZX= -0.3081
 XY= -9.9343 YY= 124.1941 ZY= -11.6783
 XZ= -1.5409 YZ= -16.3161 ZZ= 93.1237
 Eigenvalues: 86.9554 89.2495 129.5714

7 C Isotropic= 45.8628 Anisotropy 154.8889
 XX= 41.6871 YX= 3.0536 ZX= 5.2715
 XY= 21.1419 YY= 86.8179 ZY= -102.7342
 XZ= 2.963 YZ= -82.8507 ZZ= 9.0832
 Eigenvalues: -53.7318 42.198 149.122

8 C Isotropic= 42.1497 Anisotropy 154.4349
 XX= 36.9707 YX= -0.9064 ZX= -4.5065
 XY= -2.3808 YY= 51.4781 ZY= -90.2742
 XZ= -13.1342 YZ= -109.5747 ZZ= 38.0001
 Eigenvalues: -56.0286 37.3713 145.1062

9	C	Isotropic=	110.3557	Anisotropy	56.1321
XX=	139.6377	YX=	-16.5474	ZX=	13.5937
XY=	-14.9798	YY=	102.6246	ZY=	10.444
XZ=	19.7503	YZ=	16.0286	ZZ=	88.8047
Eigenvalues:	73.1464	110.1436		147.7771	
10	C	Isotropic=	147.0495	Anisotropy	43.9066
XX=	175.2358	YX=	1.4581	ZX=	1.2442
XY=	8.478	YY=	138.1658	ZY=	4.1902
XZ=	5.5644	YZ=	12.9442	ZZ=	127.7469
Eigenvalues:	122.9241	141.9039		176.3206	
11	C	Isotropic=	147.306	Anisotropy	13.2064
XX=	140.6403	YX=	-1.7043	ZX=	0.4401
XY=	12.4474	YY=	153.7137	ZY=	-0.5717
XZ=	-3.9796	YZ=	-2.4107	ZZ=	147.5639
Eigenvalues:	138.562	147.2456		156.1102	
12	C	Isotropic=	154.8878	Anisotropy	22.0322
XX=	160.4469	YX=	-4.0053	ZX=	-14.5262
XY=	-7.5392	YY=	147.4864	ZY=	-14.9504
XZ=	-5.85	YZ=	-8.3668	ZZ=	156.7301
Eigenvalues:	135.0628	160.0246		169.5759	
13	C	Isotropic=	148.1586	Anisotropy	54.6485
XX=	142.8812	YX=	12.2692	ZX=	-6.523
XY=	20.5143	YY=	132.8616	ZY=	-22.7448
XZ=	-5.4504	YZ=	-24.6744	ZZ=	168.7331
Eigenvalues:	115.3215	144.5633		184.5909	
14	C	Isotropic=	168.8819	Anisotropy	16.03
XX=	170.6134	YX=	12.0422	ZX=	1.5954
XY=	3.7182	YY=	165.77	ZY=	-0.2915
XZ=	9.774	YZ=	2.7946	ZZ=	170.2624
Eigenvalues:	159.341	167.7362		179.5686	
15	C	Isotropic=	169.3184	Anisotropy	17.3614
XX=	171.5577	YX=	0.2543	ZX=	-9.5807
XY=	3.4397	YY=	173.5055	ZY=	-8.0407
XZ=	-6.5293	YZ=	-6.3891	ZZ=	162.8919
Eigenvalues:	156.3341	170.7284		180.8927	
16	O	Isotropic=	263.0313	Anisotropy	81.3197
XX=	315.3648	YX=	21.9669	ZX=	7.3922
XY=	0.8158	YY=	195.0708	ZY=	-18.7528
XZ=	4.1822	YZ=	15.0492	ZZ=	278.6584
Eigenvalues:	193.9343	277.9152		317.2445	
17	O	Isotropic=	265.6742	Anisotropy	44.5397
XX=	253.8174	YX=	-21.8517	ZX=	6.1985
XY=	1.2694	YY=	257.9406	ZY=	14.4501
XZ=	0.4433	YZ=	24.2408	ZZ=	285.2647
Eigenvalues:	239.7817	261.8737		295.3673	
18	O	Isotropic=	-356.0242	Anisotropy	1078.2583
XX=	-808.1366	YX=	315.9503	ZX=	364.8547
XY=	266.8328	YY=	-362.1319	ZY=	240.6523
XZ=	313.6037	YZ=	241.4138	ZZ=	102.1959
Eigenvalues:	-994.2619	-436.6253		362.8147	
19	O	Isotropic=	89.802	Anisotropy	123.3755
XX=	131.0703	YX=	-154.5302	ZX=	-18.323
XY=	-11.2781	YY=	-6.7797	ZY=	2.4503
XZ=	-19.3755	YZ=	-50.2043	ZZ=	145.1154
Eigenvalues:	-50.1665	147.5201		172.0524	
20	O	Isotropic=	95.2354	Anisotropy	154.8611

XX=	94.0302	YX=	37.3111	ZX=	-16.7037				
XY=	128.0935	YY=	126.3025	ZY=	72.1705				
XZ=	-136.5055	YZ=	94.5069	ZZ=	65.3736				
Eigenvalues:	-68.5832	155.8133		198.4762					
21	H	Isotropic=	31.2579	Anisotropy	13.5422				
XX=	34.3513	YX=	-4.8615	ZX=	-4.617				
XY=	-4.2806	YY=	35.5006	ZY=	1.0133				
XZ=	-4.5304	YZ=	0.0002	ZZ=	23.9218				
Eigenvalues:	22.0926	31.3951	40.286						
22	C	Isotropic=	20.4202	Anisotropy	75.1706				
XX=	18.8327	YX=	84.8848	ZX=	-29.636				
XY=	45.8375	YY=	-12.1694	ZY=	26.9547				
XZ=	-25.875	YZ=	43.7737	ZZ=	54.5974				
Eigenvalues:	-78.9729	69.6996	70.534						
23	O	Isotropic=	-132.2046	Anisotropy	600.7536				
XX=	-281.0641	YX=	-52.7042	ZX=	-280.1135				
XY=	-18.3683	YY=	-258.4637	ZY=	19.8002				
XZ=	-239.0881	YZ=	22.0101	ZZ=	142.9139				
Eigenvalues:	-407.8621		-257.0496		268.2978				
24	C	Isotropic=	166.1986	Anisotropy	36.5841				
XX=	158.2205	YX=	0.0507	ZX=	4.6142				
XY=	0.6166	YY=	190.5814	ZY=	1.1283				
XZ=	4.0443	YZ=	-0.5045	ZZ=	149.7939				
Eigenvalues:	147.9655		160.0423		190.588				
25	H	Isotropic=	27.4503	Anisotropy	2.7958				
XX=	27.2221	YX=	-0.6445	ZX=	-1.2457				
XY=	-1.7746	YY=	28.5288	ZY=	-0.7196				
XZ=	-1.4677	YZ=	-0.0549	ZZ=	26.6				
Eigenvalues:	25.1703	27.8665	29.3141						
26	H	Isotropic=	28.379	Anisotropy	8.5284				
XX=	28.895	YX=	3.8987	ZX=	-2.598				
XY=	3.5215	YY=	27.7817	ZY=	-2.053				
XZ=	-2.005	YZ=	-2.7871	ZZ=	28.4602				
Eigenvalues:	24.5419	26.5304	34.0646						
27	H	Isotropic=	25.6867	Anisotropy	3.0157				
XX=	27.1864	YX=	-1.9705	ZX=	-1.0074				
XY=	0.6165	YY=	26.6981	ZY=	-1.7158				
XZ=	1.5723	YZ=	1.1324	ZZ=	23.1756				
Eigenvalues:	23.1386	26.2244	27.6972						
28	H	Isotropic=	24.6949	Anisotropy	7.4586				
XX=	29.1753	YX=	0.5418	ZX=	2.2606				
XY=	1.7698	YY=	20.3447	ZY=	-1.9468				
XZ=	0.7413	YZ=	-1.3834	ZZ=	24.5648				
Eigenvalues:	19.5022	24.9152	29.6673						
29	H	Isotropic=	28.6692	Anisotropy	6.6593				
XX=	29.6354	YX=	-0.4186	ZX=	-2.0103				
XY=	0.3404	YY=	28.0818	ZY=	4.7956				
XZ=	-1.416	YZ=	4.104	ZZ=	28.2904				
Eigenvalues:	23.5057	29.3931	33.1087						
30	H	Isotropic=	29.2861	Anisotropy	4.2545				
XX=	32.1128	YX=	0.2127	ZX=	0.4967				
XY=	0.1416	YY=	28.8837	ZY=	-2.0711				
XZ=	-0.2186	YZ=	-2.9374	ZZ=	26.8619				
Eigenvalues:	25.1656	30.5703	32.1225						
31	H	Isotropic=	29.2982	Anisotropy	7.9534				
XX=	29.4984	YX=	-0.9919	ZX=	-2.2984				

XY=	-0.8558	YY=	25.1681	ZY=	0.0078		
XZ=	-2.6558	YZ=	1.6031	ZZ=	33.228		
Eigenvalues:	24.9667	28.3274	34.6005				
32	H	Isotropic=	29.2046	Anisotropy		8.9253	
XX=	28.7347	YX=	-5.1525	ZX=	0.9848		
XY=	-4.1228	YY=	31.7503	ZY=	-0.0623		
XZ=	1.4369	YZ=	0.5085	ZZ=	27.1289		
Eigenvalues:	24.8241	27.635	35.1549				
33	H	Isotropic=	30.2883	Anisotropy		6.8474	
XX=	33.5039	YX=	0.1951	ZX=	2.7569		
XY=	0.2985	YY=	29.4626	ZY=	1.8146		
XZ=	2.8004	YZ=	2.3024	ZZ=	27.8982		
Eigenvalues:	25.8245	30.1871	34.8532				
34	H	Isotropic=	30.1405	Anisotropy		9.0423	
XX=	30.3068	YX=	-1.1612	ZX=	1.7001		
XY=	-1.1022	YY=	26.5282	ZY=	-2.9111		
XZ=	3.282	YZ=	-3.7046	ZZ=	33.5866		
Eigenvalues:	25.216	29.0368	36.1687				
35	H	Isotropic=	30.3257	Anisotropy		6.1881	
XX=	30.1976	YX=	2.5818	ZX=	1.6669		
XY=	2.5954	YY=	30.871	ZY=	-2.8363		
XZ=	-1.0912	YZ=	-3.5366	ZZ=	29.9085		
Eigenvalues:	26.1614	30.3646	34.4511				
36	H	Isotropic=	28.5221	Anisotropy		6.1588	
XX=	27.2165	YX=	-1.0312	ZX=	-0.4176		
XY=	-0.5009	YY=	25.9616	ZY=	-1.5191		
XZ=	-1.7432	YZ=	0.4182	ZZ=	32.3881		
Eigenvalues:	25.4607	27.4776	32.6279				
37	H	Isotropic=	29.6848	Anisotropy		7.6492	
XX=	34.265	YX=	1.0872	ZX=	-1.0675		
XY=	1.7861	YY=	30.8001	ZY=	3.6371		
XZ=	-1.4856	YZ=	3.9606	ZZ=	23.9893		
Eigenvalues:	22.0407	32.2294	34.7843				
38	H	Isotropic=	29.6152	Anisotropy		7.9883	
XX=	33.5939	YX=	-0.1694	ZX=	1.7466		
XY=	-1.4539	YY=	27.5116	ZY=	-0.913		
XZ=	4.043	YZ=	-0.8102	ZZ=	27.7402		
Eigenvalues:	26.3234	27.5815	34.9407				
39	H	Isotropic=	30.6168	Anisotropy		13.3767	
XX=	34.7542	YX=	5.6737	ZX=	-2.6186		
XY=	6.1682	YY=	32.039	ZY=	2.2759		
XZ=	-2.9784	YZ=	1.773	ZZ=	25.0571		
Eigenvalues:	22.6411	29.6746	39.5346				
40	H	Isotropic=	29.2049	Anisotropy		10.745	
XX=	29.5554	YX=	-2.63	ZX=	-5.319		
XY=	-0.9076	YY=	27.4484	ZY=	1.3717		
XZ=	-6.2458	YZ=	0.9876	ZZ=	30.611		
Eigenvalues:	24.1867	27.0599	36.3683				
41	H	Isotropic=	29.6671	Anisotropy		6.1638	
XX=	32.431	YX=	2.7226	ZX=	0.4443		
XY=	3.241	YY=	26.3773	ZY=	0.5477		
XZ=	0.2758	YZ=	1.1757	ZZ=	30.193		
Eigenvalues:	25.0692	30.1558	33.7763				
42	H	Isotropic=	30.5199	Anisotropy		9.6757	
XX=	28.2851	YX=	0.0439	ZX=	-1.5343		
XY=	0.0202	YY=	32.5582	ZY=	-4.9569		

XZ=	-1.8273	YZ=	-5.2595	ZZ=	30.7165				
Eigenvalues:	25.7755	28.8138	36.9704						
43	H	Isotropic=	29.0673	Anisotropy	5.5288				
XX=	30.7622	YX=	-0.6057	ZX=	2.6644				
XY=	2.0476	YY=	31.0893	ZY=	1.796				
XZ=	2.8658	YZ=	0.6726	ZZ=	25.3504				
Eigenvalues:	24.0799	30.3689	32.7532						
44	H	Isotropic=	29.1761	Anisotropy	6.711				
XX=	26.5983	YX=	-0.1908	ZX=	-0.0072				
XY=	-0.9491	YY=	30.1416	ZY=	-3.6472				
XZ=	0.548	YZ=	-2.5932	ZZ=	30.7885				
Eigenvalues:	26.4814	27.3969	33.6501						
45	H	Isotropic=	28.9366	Anisotropy	8.883				
XX=	30.6559	YX=	-2.3702	ZX=	-2.252				
XY=	-4.3957	YY=	29.9823	ZY=	2.0155				
XZ=	-2.5282	YZ=	2.0808	ZZ=	26.1715				
Eigenvalues:	25.0284	26.9227	34.8585						
46	H	Isotropic=	30.5483	Anisotropy	18.1221				
XX=	38.376	YX=	8.5311	ZX=	1.7697				
XY=	6.5424	YY=	27.5688	ZY=	4.0306				
XZ=	0.9855	YZ=	1.6974	ZZ=	25.7002				
Eigenvalues:	22.4436	26.5717	42.6297						
47	C	Isotropic=	6.7558	Anisotropy	97.2793				
XX=	-64.73	YX=	-27.0622	ZX=	-53.7089				
XY=	-58.7116	YY=	36.1496	ZY=	-3.7417				
XZ=	-29.0618	YZ=	7.6414	ZZ=	48.8479				
Eigenvalues:	-91.0494	39.7082	71.6087						
48	O	Isotropic=	-151.0301	Anisotropy	689.304				
XX=	-222.7049	YX=	-161.9229	ZX=	-165.594				
XY=	-157.2528	YY=	-199.0799	ZY=	315.5649				
XZ=	-181.2898	YZ=	301.7837	ZZ=	-31.3055				
Eigenvalues:	-438.5928	-323.0033	308.5059						
49	H	Isotropic=	28.8237	Anisotropy	6.2278				
XX=	28.8544	YX=	2.8624	ZX=	0.1134				
XY=	3.1784	YY=	25.538	ZY=	1.5662				
XZ=	1.5276	YZ=	1.146	ZZ=	32.0787				
Eigenvalues:	23.6814	29.8142	32.9755						
50	H	Isotropic=	29.5847	Anisotropy	6.4595				
XX=	27.3955	YX=	-1.7814	ZX=	-0.2249				
XY=	-1.5865	YY=	30.8693	ZY=	-2.4638				
XZ=	-0.2694	YZ=	-3.5872	ZZ=	30.4892				
Eigenvalues:	26.1003	28.7627	33.891						
51	C	Isotropic=	111.1746	Anisotropy	16.3534				
XX=	120.0661	YX=	4.4995	ZX=	-0.159				
XY=	6.3348	YY=	102.0639	ZY=	9.6147				
XZ=	-2.1601	YZ=	11.3659	ZZ=	111.3938				
Eigenvalues:	94.2061	117.2408	122.0769						
52	C	Isotropic=	123.0061	Anisotropy	17.2968				
XX=	117.2225	YX=	-7.044	ZX=	8.9451				
XY=	-8.9148	YY=	130.7623	ZY=	5.7163				
XZ=	6.1949	YZ=	3.2572	ZZ=	121.0335				
Eigenvalues:	107.7468	126.7342	134.5372						
53	O	Isotropic=	267.4976	Anisotropy	64.0746				
XX=	287.4806	YX=	-18.914	ZX=	-0.4536				
XY=	-16.9244	YY=	293.7549	ZY=	4.6526				
XZ=	20.5339	YZ=	-16.9193	ZZ=	221.2573				

Eigenvalues:	219.5976	272.6812	310.214		
54	H	Isotropic=	26.23	Anisotropy	5.5775
XX=	29.3681	YX=	-0.7245	ZX=	1.254
XY=	2.5078	YY=	27.3707	ZY=	2.2085
XZ=	-0.6521	YZ=	3.0207	ZZ=	21.9513
Eigenvalues:	20.8951	27.8465	29.9484		
55	N	Isotropic=	122.3394	Anisotropy	111.424
XX=	96.0908	YX=	-56.9121	ZX=	25.6616
XY=	-70.7166	YY=	155.8364	ZY=	16.3735
XZ=	39.0689	YZ=	15.8211	ZZ=	115.0909
Eigenvalues:	38.5906	131.8055	196.6221		
56	C	Isotropic=	50.7616	Anisotropy	186.826
XX=	61.6113	YX=	93.7755	ZX=	-36.8573
XY=	89.7872	YY=	90.1563	ZY=	-7.2402
XZ=	-41.4251	YZ=	-14.081	ZZ=	0.5172
Eigenvalues:	-34.5774	11.5499	175.3122		
57	H	Isotropic=	26.6098	Anisotropy	6.9315
XX=	25.1267	YX=	-1.0854	ZX=	0.2914
XY=	-2.1765	YY=	27.8473	ZY=	4.0378
XZ=	-2.0518	YZ=	2.5696	ZZ=	26.8553
Eigenvalues:	23.8203	24.7782	31.2308		
58	H	Isotropic=	29.2304	Anisotropy	21.2053
XX=	22.1747	YX=	-2.2845	ZX=	-1.9063
XY=	-5.435	YY=	42.3839	ZY=	1.9969
XZ=	-0.0779	YZ=	2.4002	ZZ=	23.1325
Eigenvalues:	21.2577	23.0661	43.3672		
59	C	Isotropic=	17.6825	Anisotropy	113.9963
XX=	15.9961	YX=	39.4063	ZX=	42.778
XY=	44.4151	YY=	-35.0186	ZY=	-13.8287
XZ=	38.4117	YZ=	-16.999	ZZ=	72.0699
Eigenvalues:	-67.0007	26.3681	93.68		
60	H	Isotropic=	26.3941	Anisotropy	7.1388
XX=	28.0574	YX=	-0.1922	ZX=	-6.3064
XY=	-2.9267	YY=	27.7648	ZY=	-2.4236
XZ=	-3.5162	YZ=	-2.3812	ZZ=	23.3601
Eigenvalues:	19.2962	28.7328	31.1533		
61	C	Isotropic=	60.1271	Anisotropy	176.411
XX=	81.2743	YX=	95.2076	ZX=	-2.1593
XY=	92.5708	YY=	71.5556	ZY=	-51.2575
XZ=	1.6386	YZ=	-42.501	ZZ=	27.5513
Eigenvalues:	-36.8709	39.5177	177.7344		
62	C	Isotropic=	61.7961	Anisotropy	175.354
XX=	107.8633	YX=	60.6549	ZX=	-25.5071
XY=	60.7696	YY=	108.2892	ZY=	-40.739
XZ=	-25.3418	YZ=	-37.0209	ZZ=	-30.7641
Eigenvalues:	-41.5991	148.2887	178.6988		
63	C	Isotropic=	63.4478	Anisotropy	175.6903
XX=	67.0445	YX=	92.2976	ZX=	-49.8845
XY=	92.4181	YY=	94.555	ZY=	3.6381
XZ=	-50.6989	YZ=	3.0804	ZZ=	28.744
Eigenvalues:	-38.4049	148.1737	180.5747		
64	C	Isotropic=	62.2905	Anisotropy	173.365
XX=	76.3536	YX=	97.0689	ZX=	3.1453
XY=	96.3751	YY=	73.3767	ZY=	-45.1576
XZ=	5.8467	YZ=	-46.6746	ZZ=	37.1413
Eigenvalues:	-39.5631	148.5675	177.8672		

65 C Isotropic= 63.1667 Anisotropy 146.0828
 XX= 105.4201 YX= 47.966 ZX= -18.8359
 XY= 44.6756 YY= 107.903 ZY= -34.0893
 XZ= -18.2093 YZ= -33.727 ZZ= -23.8232
 Eigenvalues: -32.453461.3983 160.5552

66 H Isotropic= 22.3037 Anisotropy 10.7572
 XX= 24.2067 YX= -3.0398 ZX= 4.9617
 XY= -3.1325 YY= 18.5244 ZY= -0.2577
 XZ= 4.3723 YZ= -0.7904 ZZ= 24.1799
 Eigenvalues: 16.7891 20.6468 29.4751

67 O Isotropic= -145.0383 Anisotropy 586.8214
 XX= -174.2648 YX= -85.1719 ZX= 262.8098
 XY= -116.4656 YY= -358.7286 ZY= 119.0593
 XZ= 231.3468 YZ= 84.2701 ZZ= 97.8785
 Eigenvalues: -480.3756 -200.9152 246.176

68 C Isotropic= 50.4184 Anisotropy 180.824
 XX= 49.6205 YX= 108.2207 ZX= 25.8024
 XY= 77.0789 YY= 98.6834 ZY= -15.1805
 XZ= 30.4809 YZ= 3.8014 ZZ= 2.9512
 Eigenvalues: -38.1555 18.4429 170.9677

69 H Isotropic= 23.6382 Anisotropy 5.7884
 XX= 24.2788 YX= -3.456 ZX= 1.4401
 XY= -3.4744 YY= 22.8397 ZY= -0.2815
 XZ= 1.3704 YZ= -0.0749 ZZ= 23.7961
 Eigenvalues: 19.8697 23.5478 27.4971

70 H Isotropic= 23.6861 Anisotropy 3.5767
 XX= 23.1169 YX= -2.4407 ZX= 0.251
 XY= -2.4806 YY= 22.6952 ZY= 1.2394
 XZ= 0.2286 YZ= 1.2259 ZZ= 25.2462
 Eigenvalues: 20.2054 24.7824 26.0706

71 H Isotropic= 23.7632 Anisotropy 4.4636
 XX= 23.6112 YX= -2.5695 ZX= 1.4839
 XY= -2.7714 YY= 22.4596 ZY= -0.0344
 XZ= 1.4396 YZ= -0.0569 ZZ= 25.2189
 Eigenvalues: 20.1424 24.4083 26.739

72 H Isotropic= 24.1168 Anisotropy 7.9696
 XX= 25.5065 YX= -4.1285 ZX= 0.1434
 XY= -4.7247 YY= 24.4091 ZY= 0.4744
 XZ= -0.1099 YZ= 0.4242 ZZ= 22.4349
 Eigenvalues: 20.4365 22.4841 29.4299

73 C Isotropic= 53.8647 Anisotropy 186.1063
 XX= 99.7258 YX= 72.4946 ZX= 38.1217
 XY= 66.2266 YY= 95.9138 ZY= 43.4733
 XZ= 22.0696 YZ= 31.3645 ZZ= -34.0455
 Eigenvalues: -45.2035 28.862 177.9356

74 C Isotropic= 60.3742 Anisotropy 182.2178
 XX= 89.1995 YX= 97.7679 ZX= -7.1003
 XY= 101.5003 YY= 66.9314 ZY= 42.4033
 XZ= -8.1073 YZ= 43.6815 ZZ= 24.9919
 Eigenvalues: -43.1732 42.4431 181.8528

75 C Isotropic= 61.7632 Anisotropy 181.132
 XX= 82.2264 YX= 93.587 ZX= 38.786
 XY= 101.1433 YY= 83.3217 ZY= -15.4232
 XZ= 44.1899 YZ= -12.9668 ZZ= 19.7415
 Eigenvalues: -40.9358 43.7075 182.5178

76 C Isotropic= 64.2545 Anisotropy 176.0752

XX=	114.2781	YX=	64.1121	ZX=	11.3472
XY=	66.1923	YY=	113.5532	ZY=	16.6282
XZ=	19.0601	YZ=	19.7135	ZZ=	-35.0678
Eigenvalues:	-37.69	48.8155	181.638		
77	C	Isotropic=	68.4978	Anisotropy	166.8501
XX=	73.08	YX=	100.3503	ZX=	-14.304
XY=	81.4933	YY=	99.6713	ZY=	30.8201
XZ=	-12.68	YZ=	30.6625	ZZ=	32.7422
Eigenvalues:	-22.471448	2.2337	179.7312		
78	H	Isotropic=	23.034	Anisotropy	5.993
XX=	23.3967	YX=	-2.7781	ZX=	-0.6244
XY=	-2.9165	YY=	24.7515	ZY=	-0.9641
XZ=	-0.4181	YZ=	-0.9047	ZZ=	20.9539
Eigenvalues:	20.0443	22.0284	27.0293		
79	H	Isotropic=	23.6617	Anisotropy	2.8392
XX=	22.4255	YX=	-1.1213	ZX=	-1.513
XY=	-1.293	YY=	24.1651	ZY=	-0.1746
XZ=	-1.6469	YZ=	0.1124	ZZ=	24.3944
Eigenvalues:	21.1575	24.2731	25.5545		
80	H	Isotropic=	23.7492	Anisotropy	2.614
XX=	22.6298	YX=	-1.5826	ZX=	0.5806
XY=	-1.1811	YY=	24.2687	ZY=	-0.4798
XZ=	0.746	YZ=	-0.3629	ZZ=	24.3492
Eigenvalues:	21.7867	23.9691	25.4919		
81	H	Isotropic=	23.8383	Anisotropy	4.4974
XX=	23.3254	YX=	-2.6658	ZX=	0.459
XY=	-2.6687	YY=	24.1896	ZY=	1.6632
XZ=	0.1283	YZ=	1.4255	ZZ=	23.9999
Eigenvalues:	20.5929	24.0854	26.8366		
82	H	Isotropic=	23.4405	Anisotropy	5.649
XX=	21.5641	YX=	-1.257	ZX=	-0.729
XY=	-1.9283	YY=	24.2354	ZY=	2.9245
XZ=	-0.3979	YZ=	1.9061	ZZ=	24.5219
Eigenvalues:	20.7138	22.4011	27.2065		

2b-iii

C	-3.569393	-1.44271	-1.459609
C	-4.229916	-2.160411	-0.240225
C	-3.441214	-2.086612	1.07797
C	-4.126486	-1.237761	2.164067
C	-4.355540	2.240247	1.789668
C	-3.222686	1.021376	1.141889
C	-2.782467	0.495504	-0.193613
C	-1.459311	0.223171	-0.371835
C	-1.084313	-0.722146	-1.480264
C	-2.103919	-1.855536	-1.654757
C	-3.719007	0.100593	-1.316713
C	-5.187718	0.461331	-1.149033
C	-3.271323	0.779478	-2.625956
C	-0.377901	0.824201	0.435987
C	-5.418333	-1.871312	6.28232
O	-4.216347	-1.906231	-2.643702
O	-4.486351	-3.513768	-0.583719
O	-5.371055	0.817541	2.185667
O	-3.299132	2.432783	1.283084
O	0.147437	-1.451781	-1.309591

H	-3.688627	-3.872597	-0.991781
C	-4.321501	3.223349	0.831315
O	-5.344641	2.728222	0.371549
C	-4.004854	4.669673	1.026373
H	-5.266185	-1.740811	-0.084488
H	-2.411653	-1.685865	0.902851
H	-2.367491	0.81727	1.881686
H	-0.97092-0.125677	-2.43383	
H	-1.981689	-2.266934	-2.694035
H	-1.846452	-2.683476	-0.94269
H	-5.577554	0.287277	-0.121102
H	-5.352644	1.540989	-1.390967
H	-5.801637	-0.136503	-1.8679
H	-4.128003	1.297739	-3.122201
H	-2.479371.541331	-2.432943	
H	-2.887155	0.021485	-3.351676
H	-0.754289	1.543812	1.204058
H	0.231924	0.039166	0.949102
H	0.295439	1.410106	-0.244867
H	-5.847094	-1.287742	3.479429
H	-6.174085	-1.886345	1.806528
H	-5.231907	-2.920084	2.962164
H	-3.032067	4.803041	1.557169
H	-3.952244	5.161724	0.024557
H	-4.824724	5.137338	1.624465
H	-5.153632	-2.025694	-2.444614
C	1.35151 -0.804304	-1.173709	
O	1.505881	0.27801	-1.72493
H	-3.414065	-1.198847	3.039904
H	-3.341294	-3.130578	1.479284
C	2.292864	-1.63662-0.315943	
C	3.784163	-1.206691	-0.439097
O	1.881151	-1.514687	1.033357
H	2.219195	-2.70976-0.655887	
N	4.039123	0.152549	-0.051548
C	4.665461	-2.189872	0.294018
H	4.002723	-1.28029-1.554944	
H	1.06388 -2.024219	1.121538	
C	4.280773	1.162503	-0.97043
H	4.096883	0.345228	0.919386
C	4.522245	-2.421912	1.665094
C	5.35562 -3.334347	2.311522	
C	6.337193	-4.017119	1.593816
C	6.485682	-3.784878	0.22641
C	5.655071	-2.87275-0.422895	
H	3.743486	-1.887085	2.232397
O	4.111353	0.989775	-2.191117
C	4.707443	2.477104	-0.408319
H	5.236751	-3.514183	3.390103
H	6.993754	-4.736655	2.10471
H	7.260637	-4.31985-0.342201	
H	5.782024	-2.689216	-1.501082
C	4.079947	3.636636	-0.877183
C	4.465151	4.880879	-0.379864
C	5.476688	4.969569	0.576773
C	6.106328	3.813036	1.037615

C	5.721808	2.56448	0.549536
H	3.294487	3.55385	-1.645466
H	3.97232	5.793025	-0.74738
H	5.781018	5.952623	0.965758
H	6.908965	3.884139	1.78623
H	6.228684	1.656612	0.909757

2biiliz E(RB+HF-PW91) = -2012.288975

SCF GIAO Magnetic shielding tensor (ppm):

1	C	Isotropic=	111.3189	Anisotropy	30.9746
XX=	107.9555	YX=	4.2236	ZX=	20.9127
XY=	-3.5654	YY=	107.5933	ZY=	-2.3167
XZ=	15.1117	YZ=	-0.3806	ZZ=	118.4079
Eigenvalues:	94.3395	107.6484	131.9686		
2	C	Isotropic=	112.5087	Anisotropy	31.5581
XX=	93.3411	YX=	1.3294	ZX=	1.1249
XY=	5.4589	YY=	132.6427	ZY=	-1.7576
XZ=	2.6245	YZ=	8.8027	ZZ=	111.5423
Eigenvalues:	92.9159	111.0628	133.5474		
3	C	Isotropic=	141.3226	Anisotropy	19.9992
XX=	123.4041	YX=	8.4344	ZX=	6.553
XY=	0.5019	YY=	150.0043	ZY=	-2.4549
XZ=	7.6305	YZ=	-5.8905	ZZ=	150.5593
Eigenvalues:	120.6839	148.6285	154.6554		
4	C	Isotropic=	140.9589	Anisotropy	23.3796
XX=	129.7295	YX=	1.282	ZX=	2.9782
XY=	15.0163	YY=	151.7711	ZY=	-7.5068
XZ=	6.2345	YZ=	-6.7882	ZZ=	141.376
Eigenvalues:	124.3282	142.0032	156.5453		
5	C	Isotropic=	-22.9142	Anisotropy	181.0363
XX=	-36.389	YX=	-10.9753	ZX=	67.4021
XY=	2.2053	YY=	-85.0164	ZY=	47.821
XZ=	61.3155	YZ=	58.3891	ZZ=	52.6626
Eigenvalues:	-113.7847	-52.7347	97.7766		
6	C	Isotropic=	101.5072	Anisotropy	41.254
XX=	88.6882	YX=	14.8071	ZX=	0.0243
XY=	-4.0265	YY=	126.2852	ZY=	-5.7593
XZ=	-5.0919	YZ=	-11.3132	ZZ=	89.5481
Eigenvalues:	86.4549	89.0568	129.0099		
7	C	Isotropic=	45.531	Anisotropy	152.7506
XX=	44.9545	YX=	7.9543	ZX=	-10.857
XY=	22.7851	YY=	104.6785	ZY=	-92.7739
XZ=	-6.002	YZ=	-65.3079	ZZ=	-13.0399
Eigenvalues:	-52.7337	41.9621	147.3647		
8	C	Isotropic=	39.2072	Anisotropy	158.6465
XX=	31.2313	YX=	-2.9988	ZX=	-14.8049
XY=	-0.2178	YY=	69.786	ZY=	-86.3088
XZ=	-30.277	YZ=	-107.333	ZZ=	16.6044
Eigenvalues:	-61.1111	33.7612	144.9716		
9	C	Isotropic=	112.357	Anisotropy	53.8146
XX=	132.9256	YX=	-24.1885	ZX=	11.1274
XY=	-23.2772	YY=	106.9864	ZY=	7.9849
XZ=	18.8966	YZ=	13.1196	ZZ=	97.1591
Eigenvalues:	77.8036	111.034	148.2334		
10	C	Isotropic=	146.6227	Anisotropy	44.375

XX=	175.7119	YX=	-4.3041	ZX=	1.0271		
XY=	0.4799	YY=	135.2787	ZY=	3.9472		
XZ=	8.3151	YZ=	11.5546	ZZ=	128.8776		
Eigenvalues:	123.2259		140.4362		176.206		
11	C	Isotropic=	147.6075	Anisotropy		11.691	
XX=	142.8348	YX=	-0.71	ZX=	0.4282		
XY=	14.1224	YY=	151.3454	ZY=	-1.0887		
XZ=	-1.8991	YZ=	-1.7072	ZZ=	148.6422		
Eigenvalues:	139.1476		148.2733		155.4015		
12	C	Isotropic=	155.2551	Anisotropy		22.7495	
XX=	157.3617	YX=	-3.3534	ZX=	-17.7081		
XY=	-8.0757	YY=	152.7758	ZY=	-12.1513		
XZ=	-9.0545	YZ=	-7.6587	ZZ=	155.6277		
Eigenvalues:	135.7273		159.6165		170.4214		
13	C	Isotropic=	148.2729	Anisotropy		55.2346	
XX=	147.1888	YX=	10.298	ZX=	-8.685		
XY=	18.1004	YY=	135.5679	ZY=	-27.0148		
XZ=	-6.1869	YZ=	-29.1829	ZZ=	162.0619		
Eigenvalues:	115.5133		144.2093		185.0959		
14	C	Isotropic=	165.9137	Anisotropy		10.2793	
XX=	169.9564	YX=	9.5148	ZX=	1.2762		
XY=	-1.1351	YY=	161.6176	ZY=	-4.3132		
XZ=	6.533	YZ=	-2.5315	ZZ=	166.1672		
Eigenvalues:	157.3178		167.6568		172.7666		
15	C	Isotropic=	169.3847	Anisotropy		17.0529	
XX=	171.4795	YX=	1.8834	ZX=	-10.7174		
XY=	4.4788	YY=	174.6189	ZY=	-4.6811		
XZ=	-7.1162	YZ=	-3.4927	ZZ=	162.0556		
Eigenvalues:	156.4791		170.9217		180.7533		
16	O	Isotropic=	263.7056	Anisotropy		84.2973	
XX=	318.5185	YX=	-0.9766	ZX=	1.4302		
XY=	-22.9712	YY=	196.9121	ZY=	-32.6216		
XZ=	1.6398	YZ=	1.574	ZZ=	275.6863		
Eigenvalues:	192.9131		278.2999		319.9038		
17	O	Isotropic=	265.3257	Anisotropy		46.0117	
XX=	248.161	YX=	-18.3104	ZX=	5.6158		
XY=	3.1391	YY=	255.985	ZY=	7.1161		
XZ=	2.1104	YZ=	18.58	ZZ=	291.831		
Eigenvalues:	241.3834		258.5935		296.0002		
18	O	Isotropic=	-357.5313	Anisotropy		1080.4476	
XX=	-678.5848	YX=	306.1051	ZX=	477.9371		
XY=	268.0942	YY=	-512.2583	ZY=	72.837		
XZ=	421.0593	YZ=	80.2377	ZZ=	118.2492		
Eigenvalues:	-996.7896		-438.5713		362.7671		
19	O	Isotropic=	88.0735	Anisotropy		125.3453	
XX=	96.0195	YX=	-170.5685	ZX=	-42.4875		
XY=	-26.7444	YY=	31.7727	ZY=	-9.6489		
XZ=	-30.5953	YZ=	-57.7234	ZZ=	136.4283		
Eigenvalues:	-52.4581		145.0416		171.637		
20	O	Isotropic=	103.288	Anisotropy		162.7268	
XX=	149.1751	YX=	33.7163	ZX=	2.0639		
XY=	159.0238	YY=	55.8788	ZY=	64.5938		
XZ=	-78.3335	YZ=	103.0444	ZZ=	104.8101		
Eigenvalues:	-56.3972		154.4886		211.7725		
21	H	Isotropic=	31.0887	Anisotropy		13.3855	
XX=	31.8579	YX=	-3.2484	ZX=	-5.79		

XY=	-2.6681	YY=	35.7531	ZY=	4.0749		
XZ=	-5.8524	YZ=	3.1038	ZZ=	25.6551		
Eigenvalues:	21.9649	31.2888	40.0123				
22	C	Isotropic=	20.2337	Anisotropy	74.6215		
XX=	37.697	YX=	80.4224	ZX=	-11.6457		
XY=	39.8749	YY=	-42.0979	ZY=	14.8588		
XZ=	-11.7552	YZ=	28.948	ZZ=	65.102		
Eigenvalues:	-78.6676	69.3874	69.9814				
23	O	Isotropic=	-132.0297	Anisotropy	600.5866		
XX=	-307.8966	YX=	-3.7399	ZX=	-262.8007		
XY=	23.1671	YY=	-256.731	ZY=	0.8554		
XZ=	-216.7754	YZ=	-2.3752	ZZ=	168.5387		
Eigenvalues:	-408.179	-256.2714	268.3614				
24	C	Isotropic=	166.1853	Anisotropy	36.9397		
XX=	159.3017	YX=	4.8556	ZX=	5.277		
XY=	5.1925	YY=	188.9276	ZY=	6.6355		
XZ=	4.8223	YZ=	4.8647	ZZ=	150.3265		
Eigenvalues:	147.7887	159.9554	190.8117				
25	H	Isotropic=	27.3951	Anisotropy	2.8394		
XX=	26.5983	YX=	-0.1933	ZX=	-1.383		
XY=	-1.4795	YY=	28.7665	ZY=	-0.05		
XZ=	-1.7276	YZ=	0.3633	ZZ=	26.8205		
Eigenvalues:	25.078	27.8193	29.288				
26	H	Isotropic=	28.0878	Anisotropy	8.2849		
XX=	29.7249	YX=	3.2977	ZX=	-2.2594		
XY=	3.0054	YY=	26.845	ZY=	-2.0427		
XZ=	-2.1072	YZ=	-3.3044	ZZ=	27.6935		
Eigenvalues:	24.2505	26.4018	33.6111				
27	H	Isotropic=	25.4574	Anisotropy	3.3626		
XX=	25.8253	YX=	-2.023	ZX=	-1.2495		
XY=	-0.3501	YY=	26.9453	ZY=	-0.9494		
XZ=	1.375	YZ=	1.2295	ZZ=	23.6015		
Eigenvalues:	23.5887	25.0843	27.6991				
28	H	Isotropic=	24.519	Anisotropy	6.7792		
XX=	28.8548	YX=	-1.2297	ZX=	1.1036		
XY=	0.1231	YY=	20.8086	ZY=	-3.2521		
XZ=	0.0666	YZ=	-2.5051	ZZ=	23.8936		
Eigenvalues:	19.0821	25.4363	29.0385				
29	H	Isotropic=	28.4525	Anisotropy	6.4102		
XX=	29.4098	YX=	-0.4366	ZX=	-1.2826		
XY=	0.1987	YY=	26.2008	ZY=	4.5049		
XZ=	-0.7898	YZ=	3.7432	ZZ=	29.7468		
Eigenvalues:	23.447	29.1844	32.7259				
30	H	Isotropic=	29.2093	Anisotropy	4.7891		
XX=	32.3132	YX=	-0.5952	ZX=	-0.0622		
XY=	-0.4291	YY=	29.4297	ZY=	-1.8101		
XZ=	-0.8234	YZ=	-2.6974	ZZ=	25.885		
Eigenvalues:	24.739	30.4868	32.402				
31	H	Isotropic=	29.2952	Anisotropy	8.1999		
XX=	28.7054	YX=	-1.2967	ZX=	-2.43		
XY=	-1.3904	YY=	25.4777	ZY=	-0.7983		
XZ=	-2.5598	YZ=	0.7539	ZZ=	33.7027		
Eigenvalues:	24.8913	28.2326	34.7618				
32	H	Isotropic=	29.1695	Anisotropy	9.0525		
XX=	27.0829	YX=	-4.4114	ZX=	0.157		
XY=	-3.6836	YY=	33.1067	ZY=	0.7943		

XZ=	0.7678	YZ=	1.2591	ZZ=	27.3189		
Eigenvalues:	24.7469	27.5571	35.2045				
33	H	Isotropic=	30.3766	Anisotropy		6.6353	
XX=	33.5517	YX=	-0.9685	ZX=	2.7107		
XY=	-1.0241	YY=	29.0539	ZY=	1.4174		
XZ=	2.8612	YZ=	1.9523	ZZ=	28.5241		
Eigenvalues:	26.032	30.2976	34.8001				
34	H	Isotropic=	30.1078	Anisotropy		9.2121	
XX=	29.7502	YX=	-1.9391	ZX=	0.9467		
XY=	-2.1639	YY=	28.2427	ZY=	-4.1135		
XZ=	2.2495	YZ=	-5.0651	ZZ=	32.3305		
Eigenvalues:	25.0853	28.9889	36.2493				
35	H	Isotropic=	30.0934	Anisotropy		6.4027	
XX=	30.56	YX=	2.181	ZX=	1.3765		
XY=	2.4012	YY=	31.0913	ZY=	-3.1772		
XZ=	-1.6067	YZ=	-3.2653	ZZ=	28.6288		
Eigenvalues:	26.0478	29.8705	34.3618				
36	H	Isotropic=	28.4211	Anisotropy		6.297	
XX=	26.8788	YX=	-1.2356	ZX=	-0.9388		
XY=	-0.6739	YY=	26.3982	ZY=	-2.6543		
XZ=	-1.9481	YZ=	-0.3831	ZZ=	31.9865		
Eigenvalues:	25.0276	27.6167	32.6191				
37	H	Isotropic=	28.988	Anisotropy		6.9201	
XX=	31.8327	YX=	-0.8759	ZX=	-0.5787		
XY=	-1.0916	YY=	28.5046	ZY=	4.4498		
XZ=	-2.3577	YZ=	4.1518	ZZ=	26.6266		
Eigenvalues:	23.1304	30.2321	33.6014				
38	H	Isotropic=	28.5308	Anisotropy		12.4974	
XX=	32.2221	YX=	-5.7575	ZX=	1.8281		
XY=	-6.3409	YY=	27.436	ZY=	0.3309		
XZ=	3.1899	YZ=	-1.4688	ZZ=	25.9343		
Eigenvalues:	22.9745	25.7555	36.8624				
39	H	Isotropic=	28.4066	Anisotropy		9.3536	
XX=	31.7626	YX=	1.8717	ZX=	-4.0274		
XY=	2.7079	YY=	28.2664	ZY=	-0.1608		
XZ=	-4.8726	YZ=	0.3878	ZZ=	25.1908		
Eigenvalues:	22.6989	27.8786	34.6423				
40	H	Isotropic=	29.1859	Anisotropy		10.7835	
XX=	28.4809	YX=	-2.0517	ZX=	-5.2224		
XY=	-0.2713	YY=	27.449	ZY=	1.8047		
XZ=	-6.0559	YZ=	1.553	ZZ=	31.6277		
Eigenvalues:	24.197	26.9858	36.3749				
41	H	Isotropic=	29.6338	Anisotropy		5.9412	
XX=	33.1174	YX=	1.4042	ZX=	0.7521		
XY=	1.8648	YY=	25.3828	ZY=	-0.311		
XZ=	0.653	YZ=	0.2487	ZZ=	30.4012		
Eigenvalues:	25.0461	30.2607	33.5946				
42	H	Isotropic=	30.5183	Anisotropy		9.617	
XX=	28.2262	YX=	0.874	ZX=	-2.0573		
XY=	0.8867	YY=	33.8125	ZY=	-4.1335		
XZ=	-2.5102	YZ=	-4.4894	ZZ=	29.5162		
Eigenvalues:	25.7944	28.8309	36.9297				
43	H	Isotropic=	29.0678	Anisotropy		5.5634	
XX=	30.7592	YX=	-0.5636	ZX=	2.8492		
XY=	1.5795	YY=	30.7323	ZY=	2.2053		
XZ=	2.8521	YZ=	1.1845	ZZ=	25.712		

Eigenvalues:	24.1496	30.2771	32.7767		
44	H	Isotropic=	29.1758	Anisotropy	6.8074
XX=	26.3169	YX=	0.7164	ZX=	-0.499
XY=	-0.4642	YY=	31.3907	ZY=	-3.4964
XZ=	-0.1019	YZ=	-2.4971	ZZ=	29.8198
Eigenvalues:	26.2849	27.5284	33.7141		
45	H	Isotropic=	28.9716	Anisotropy	8.8806
XX=	29.3247	YX=	-1.7014	ZX=	-2.1922
XY=	-3.9128	YY=	30.4227	ZY=	3.1144
XZ=	-2.9928	YZ=	3.1939	ZZ=	27.1675
Eigenvalues:	25.0094	27.0135	34.892		
46	H	Isotropic=	30.6464	Anisotropy	18.0628
XX=	41.2909	YX=	4.8674	ZX=	3.0918
XY=	3.2232	YY=	24.3764	ZY=	3.5605
XZ=	1.477	YZ=	1.5101	ZZ=	26.2717
Eigenvalues:	22.3596	26.8913	42.6882		
47	C	Isotropic=	12.2846	Anisotropy	85.4119
XX=	-69.3178	YX=	7.4784	ZX=	-53.5673
XY=	-30.7351	YY=	52.7381	ZY=	-4.4586
XZ=	-37.4312	YZ=	4.0826	ZZ=	53.4335
Eigenvalues:	-85.2371	52.865	69.2259		
48	O	Isotropic=	-155.6066	Anisotropy	700.2625
XX=	-261.0154	YX=	-125.945	ZX=	-158.146
XY=	-104.483	YY=	-313.8589	ZY=	281.9829
XZ=	-177.8164	YZ=	259.0283	ZZ=	108.0544
Eigenvalues:	-452.6301	-325.4249	311.2351		
49	H	Isotropic=	28.7574	Anisotropy	6.4141
XX=	29.6864	YX=	1.8485	ZX=	0.922
XY=	1.944	YY=	24.332	ZY=	0.4026
XZ=	2.1294	YZ=	-0.528	ZZ=	32.2537
Eigenvalues:	23.6954	29.5433	33.0334		
50	H	Isotropic=	29.4808	Anisotropy	6.4302
XX=	26.8754	YX=	-1.2323	ZX=	-0.6434
XY=	-0.9958	YY=	31.9362	ZY=	-2.0782
XZ=	-1.006	YZ=	-3.353	ZZ=	29.6308
Eigenvalues:	25.9471	28.7277	33.7676		
51	C	Isotropic=	111.5694	Anisotropy	19.3881
XX=	123.1751	YX=	1.3186	ZX=	-4.2743
XY=	2.9911	YY=	97.1933	ZY=	1.1068
XZ=	-2.4507	YZ=	-2.4144	ZZ=	114.3398
Eigenvalues:	97.0074	113.206	124.4948		
52	C	Isotropic=	130.8813	Anisotropy	27.0229
XX=	138.9909	YX=	-9.1886	ZX=	2.3965
XY=	-12.9359	YY=	136.399	ZY=	4.0921
XZ=	-0.118	YZ=	2.7109	ZZ=	117.2542
Eigenvalues:	116.1481	127.5993	148.8966		
53	O	Isotropic=	279.0869	Anisotropy	81.3798
XX=	333.1538	YX=	12.6978	ZX=	-16.5959
XY=	-4.7499	YY=	248.224	ZY=	1.0872
XZ=	17.1258	YZ=	-1.6602	ZZ=	255.883
Eigenvalues:	248.0271	255.8936	333.3402		
54	H	Isotropic=	26.8541	Anisotropy	4.5967
XX=	29.2269	YX=	-1.7095	ZX=	1.602
XY=	2.0624	YY=	25.9698	ZY=	3.4599
XZ=	0.57	YZ=	2.6546	ZZ=	25.3656
Eigenvalues:	22.524	28.1197	29.9186		

55	N	Isotropic=	133.6763	Anisotropy	122.7106
XX=	145.9507	YX=	-26.209	ZX=	1.3381
XY=	-10.1614	YY=	175.2892	ZY=	-50.9589
XZ=	-16.7767	YZ=	-91.3305	ZZ=	79.7891
Eigenvalues:	39.6162	145.9294		215.4834	
56	C	Isotropic=	52.0307	Anisotropy	189.9289
XX=	64.8772	YX=	98.0174	ZX=	9.053
XY=	94.1329	YY=	84.1544	ZY=	43.913
XZ=	6.4812	YZ=	38.5985	ZZ=	7.0606
Eigenvalues:	-35.3227	12.7649	178.65		
57	H	Isotropic=	25.1975	Anisotropy	4.8549
XX=	24.7791	YX=	-2.5181	ZX=	-1.3604
XY=	-2.239	YY=	24.5177	ZY=	0.2925
XZ=	-2.9874	YZ=	-0.2919	ZZ=	26.2957
Eigenvalues:	21.7222	25.4362	28.4341		
58	H	Isotropic=	30.093	Anisotropy	17.8221
XX=	38.5682	YX=	7.1433	ZX=	-2.0875
XY=	6.6965	YY=	24.5914	ZY=	-2.7367
XZ=	-1.8004	YZ=	-2.885	ZZ=	27.1194
Eigenvalues:	21.126	27.1787	41.9744		
59	C	Isotropic=	20.5175	Anisotropy	112.6615
XX=	82.0452	YX=	-44.9088	ZX=	10.9533
XY=	-44.1199	YY=	-52.7218	ZY=	7.8757
XZ=	7.5294	YZ=	29.1431	ZZ=	32.2291
Eigenvalues:	-70.1595	36.0868	95.6252		
60	H	Isotropic=	26.2762	Anisotropy	7.9124
XX=	22.4393	YX=	6.4896	ZX=	1.2248
XY=	1.3221	YY=	29.7747	ZY=	0.1152
XZ=	1.0933	YZ=	-2.5077	ZZ=	26.6146
Eigenvalues:	20.3677	26.9097	31.5511		
61	C	Isotropic=	62.0529	Anisotropy	174.5974
XX=	66.7619	YX=	91.9344	ZX=	47.2372
XY=	88.759	YY=	96.3735	ZY=	-7.5509
XZ=	49.015	YZ=	-0.6929	ZZ=	23.0235
Eigenvalues:	-37.3275	45.0352	178.4512		
62	C	Isotropic=	62.4638	Anisotropy	175.5548
XX=	104.5216	YX=	60.3088	ZX=	26.5482
XY=	60.4888	YY=	116.9898	ZY=	29.7113
XZ=	27.8786	YZ=	32.7127	ZZ=	-34.12
Eigenvalues:	-42.1499	50.041	179.5004		
63	C	Isotropic=	63.9027	Anisotropy	175.5499
XX=	73.4796	YX=	97.4281	ZX=	-7.3137
XY=	96.6711	YY=	83.1256	ZY=	44.861
XZ=	-7.3328	YZ=	45.2183	ZZ=	35.1028
Eigenvalues:	-37.8988	48.6709	180.9359		
64	C	Isotropic=	62.0691	Anisotropy	174.3254
XX=	59.8372	YX=	92.2424	ZX=	48.5494
XY=	91.0556	YY=	98.1494	ZY=	-3.0285
XZ=	50.251	YZ=	-4.3047	ZZ=	28.2208
Eigenvalues:	-40.196	48.1174	178.2861		
65	C	Isotropic=	60.6032	Anisotropy	149.5227
XX=	98.9875	YX=	47.6957	ZX=	26.9124
XY=	47.8188	YY=	109.1818	ZY=	28.937
XZ=	25.7822	YZ=	28.7224	ZZ=	-26.3596
Eigenvalues:	-34.5326	56.0572	160.285		
66	H	Isotropic=	22.4927	Anisotropy	11.1998

XX= 23.1842 YX= -2.8395 ZX= 3.9146
 XY= -2.8376 YY= 19.4666 ZY= -3.2963
 XZ= 3.7293 YZ= -4.0247 ZZ= 24.8273
 Eigenvalues: 17.4198 20.0991 29.9593
 67 O Isotropic= -112.5075 Anisotropy 685.8623
 XX= 297.3161 YX= -148.8104 ZX= -35.3372
 XY= -153.3844 YY= -161.8573 ZY= 39.2951
 XZ= -38.7531 YZ= 6.1312 ZZ= -472.9813
 Eigenvalues: -475.5991 -206.6575 344.734
 68 C Isotropic= 54.912 Anisotropy 174.5837
 XX= 72.174 YX= 7.5687 ZX= -87.8092
 XY= -7.5593 YY= -14.2232 ZY= -29.2064
 XZ= -63.9512 YZ= -39.8684 ZZ= 106.7852
 Eigenvalues: -29.2645 22.6993 171.3011
 69 H Isotropic= 23.7446 Anisotropy 5.4519
 XX= 24.1897 YX= -3.2579 ZX= 0.2935
 XY= -3.291 YY= 23.3451 ZY= -1.2664
 XZ= 0.345 YZ= -1.2105 ZZ= 23.6989
 Eigenvalues: 20.3055 23.549 27.3792
 70 H Isotropic= 23.7301 Anisotropy 3.3063
 XX= 23.3448 YX= -2.2651 ZX= -1.0175
 XY= -2.3425 YY= 22.5326 ZY= -0.3426
 XZ= -1.0115 YZ= -0.3621 ZZ= 25.313
 Eigenvalues: 20.4232 24.8328 25.9343
 71 H Isotropic= 23.744 Anisotropy 4.531
 XX= 23.3014 YX= -2.813 ZX= 0.2803
 XY= -2.7333 YY= 23.0334 ZY= -1.463
 XZ= 0.2491 YZ= -1.4542 ZZ= 24.8972
 Eigenvalues: 20.2188 24.2486 26.7647
 72 H Isotropic= 23.7458 Anisotropy 8.6037
 XX= 25.2919 YX= -4.8799 ZX= -0.7231
 XY= -4.5653 YY= 24.041 ZY= 0.2183
 XZ= -0.64 YZ= 0.1168 ZZ= 21.9045
 Eigenvalues: 19.8507 21.9051 29.4816
 73 C Isotropic= 59.7801 Anisotropy 177.5085
 XX= 64.6256 YX= 10.0606 ZX= -106.7511
 XY= 7.2929 YY= 42.2818 ZY= -8.7826
 XZ= -109.8779 YZ= -10.0296 ZZ= 72.4329
 Eigenvalues: -39.8566 41.0778 178.1191
 74 C Isotropic= 62.3167 Anisotropy 176.4739
 XX= 90.6867 YX= 42.3625 ZX= -79.7672
 XY= 39.8222 YY= -9.8829 ZY= 16.3391
 XZ= -80.0655 YZ= 17.7071 ZZ= 106.1464
 Eigenvalues: -40.7044 47.6886 179.966
 75 C Isotropic= 62.5691 Anisotropy 177.0424
 XX= 102.3596 YX= -15.4911 ZX= -74.8492
 XY= -14.2979 YY= -21.4622 ZY= -35.7546
 XZ= -74.8489 YZ= -34.428 ZZ= 106.8099
 Eigenvalues: -40.1315 47.2415 180.5974
 76 C Isotropic= 63.9298 Anisotropy 174.3409
 XX= 64.1087 YX= 0.3914 ZX= -107.8312
 XY= 4.1444 YY= 50.5595 ZY= -10.1912
 XZ= -109.6154 YZ= -10.2383 ZZ= 77.1212
 Eigenvalues: -38.6255 50.2578 180.157
 77 C Isotropic= 66.3634 Anisotropy 164.3698
 XX= 89.8317 YX= 35.2535 ZX= -75.2058

XY= 40.3345 YY= -0.4001 ZY= 17.4674
 XZ= -73.6632 YZ= 12.6281 ZZ= 109.6587
 Eigenvalues: -28.8099 51.9569 175.9433
 78 H Isotropic= 23.1272 Anisotropy 7.2572
 XX= 20.9763 YX= -0.1279 ZX= 0.8099
 XY= 0.3198 YY= 27.9524 ZY= -0.5422
 XZ= 1.0682 YZ= -0.0697 ZZ= 20.4529
 Eigenvalues: 19.7287 21.6876 27.9653
 79 H Isotropic= 23.746 Anisotropy 4.7252
 XX= 23.0694 YX= 1.3625 ZX= 2.4645
 XY= 1.0558 YY= 25.6024 ZY= 0.7007
 XZ= 2.4125 YZ= 0.94 ZZ= 22.5663
 Eigenvalues: 20.358 23.9839 26.8961
 80 H Isotropic= 23.7751 Anisotropy 3.641
 XX= 23.5965 YX= -0.5226 ZX= 2.7055
 XY= -0.5166 YY= 25.0518 ZY= -0.4862
 XZ= 2.6339 YZ= -0.2687 ZZ= 22.677
 Eigenvalues: 20.4273 24.6956 26.2024
 81 H Isotropic= 23.9458 Anisotropy 5.1693
 XX= 22.8232 YX= 0.4714 ZX= 2.1489
 XY= 0.3619 YY= 27.2364 ZY= 0.4997
 XZ= 1.9145 YZ= 0.6185 ZZ= 21.7777
 Eigenvalues: 20.1976 24.2477 27.392
 82 H Isotropic= 24.0761 Anisotropy 8.6971
 XX= 23.8759 YX= 3.5659 ZX= 3.2743
 XY= 2.6869 YY= 26.601 ZY= 1.6853
 XZ= 2.7896 YZ= 1.7364 ZZ= 21.7513
 Eigenvalues: 19.5675 22.7866 29.8742

2b-iii2

C	3.531409	-1.211178	1.651652
C	4.308114	-2.063999	0.599174
C	3.645313	-2.172026	-0.784358
C	4.422622	-1.4538	-1.902256
C	4.604796	0.063722	-1.699562
C	3.410694	0.898369	-1.262958
C	2.8517	0.536615	0.082613
C	1.522085	0.254252	0.173462
C	1.059305	-0.534236	1.36803
C	2.057687	-1.628559	1.760451
C	3.6845	0.306283	1.327061
C	5.161703	0.663718	1.246805
C	3.120784	1.140032	2.493779
C	0.519543	0.63619	-0.842512
C	5.756902	-2.11544	-2.162148
O	4.069189	-1.502986	2.940451
O	4.539532	-3.357071	1.137592
O	5.647793	0.606725	-2.072447
O	3.48832	2.282656	-1.572886
O	-0.169413	-1.270329	1.208857
H	3.698806	-3.692791	1.472465
C	4.457242	3.143316	-1.131887
O	5.43894	2.730004	-0.52472
C	4.14636	4.548293	-1.531738
H	5.352252	-1.650103	0.488031
H	2.600027	-1.773972	-0.758378

H	2.632829	0.586384	-2.048639
H	0.885423	0.183356	2.224754
H	1.843916	-1.922426	2.824328
H	1.868239	-2.533409	1.12507
H	5.644141	0.366892	0.288781
H	5.302328	1.767237	1.363799
H	5.7082	0.168969	2.088172
H	3.925086	1.743094	2.981941
H	2.335262	1.848527	2.138915
H	2.69227	0.474134	3.282439
H	0.936281	1.307321	-1.633593
H	0.094907	-0.280111	-1.32726
H	-0.309433	1.209319	-0.352247
H	6.258517	-1.635857	-3.03807
H	6.433021	-2.012077	-1.279684
H	5.610195	-3.201378	-2.375326
H	3.227899	4.595333	-2.164138
H	3.992686	5.156682	-0.607225
H	5.015197	4.957871	-2.102644
H	5.01573	-1.665609	2.839837
C	-1.342263	-0.627359	0.907383
O	-1.543376	0.479923	1.396615
H	3.794248	-1.539447	-2.837153
H	3.591183	-3.259957	-1.057444
C	-2.266851	-1.525933	0.097827
C	-3.772897	-1.222	0.333786
O	-1.875789	-1.472129	-1.258806
H	-2.076733	-2.599724	0.397159
N	-4.153721	0.124387	-0.012084
C	-4.631849	-2.261309	-0.343334
H	-3.904829	-1.325889	1.461803
H	-2.074676	-0.583806	-1.585422
C	-4.400892	1.090982	0.958587
H	-4.513457	0.267664	-0.926144
C	-4.580523	-2.471784	-1.724341
C	-5.394901	-3.435942	-2.317712
C	-6.267179	-4.192933	-1.536293
C	-6.323114	-3.984761	-0.15809
C	-5.510737	-3.021438	0.437882
H	-3.881022	-1.890184	-2.34438
O	-4.129698	0.894646	2.155978
C	-4.947812	2.389928	0.471214
H	-5.344689	-3.600077	-3.404233
H	-6.908653	-4.95363	-2.005143
H	-7.009606	-4.580543	0.461624
H	-5.562952	-2.859831	1.525841
C	-4.357102	3.572416	0.930786
C	-4.852854	4.804052	0.50491
C	-5.938252	4.857079	-0.369803
C	-6.532068	3.677267	-0.819382
C	-6.037665	2.44169	-0.402778
H	-3.510489	3.516239	1.634108
H	-4.388455	5.734155	0.864711
H	-6.329683	5.830042	-0.702399
H	-7.393699	3.719893	-1.501722
H	-6.521006	1.51644	-0.750506

2biii_45 E(RB+HF-PW91) = -2012.287321

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic= 110.8129 Anisotropy 30.2348
 XX= 104.6291 YX= -1.4848 ZX= 20.1709
 XY= 4.9221 YY= 107.9319 ZY= 2.5339
 XZ= 13.3741 YZ= 1.4216 ZZ= 119.8777
 Eigenvalues: 93.8192 107.65 130.9694

2 C Isotropic= 112.3339 Anisotropy 30.8471
 XX= 93.2806 YX= -1.0385 ZX= -0.944
 XY= -5.8166 YY= 130.6158 ZY= -1.1416
 XZ= 1.1698 YZ= -11.3792 ZZ= 113.1054
 Eigenvalues: 92.9577 111.1454 132.8986

3 C Isotropic= 141.2445 Anisotropy 20.1488
 XX= 122.6053 YX= -8.628 ZX= 4.779
 XY= -0.3484 YY= 150.863 ZY= 2.4966
 XZ= 4.6391 YZ= 5.7071 ZZ= 150.2651
 Eigenvalues: 120.9461 148.1103 154.677

4 C Isotropic= 141.0792 Anisotropy 23.2583
 XX= 129.1846 YX= -1.781 ZX= 2.0702
 XY= -15.1195 YY= 153.2525 ZY= 4.5758
 XZ= 7.4062 YZ= 4.9396 ZZ= 140.8005
 Eigenvalues: 124.3236 142.3292 156.5848

5 C Isotropic= -23.2835 Anisotropy 181.3211
 XX= -48.6819 YX= 24.0712 ZX= 56.1413
 XY= 9.1194 YY= -95.3424 ZY= -26.6161
 XZ= 52.3074 YZ= -36.0803 ZZ= 74.1739
 Eigenvalues: -113.8408 -53.6069 97.5972

6 C Isotropic= 101.4484 Anisotropy 41.3512
 XX= 88.9434 YX= -15.4808 ZX= 1.8865
 XY= 2.2128 YY= 127.6603 ZY= 1.1812
 XZ= -5.6669 YZ= 4.7029 ZZ= 87.7414
 Eigenvalues: 86.2769 89.0524 129.0158

7 C Isotropic= 45.8475 Anisotropy 153.54
 XX= 47.4312 YX= -15.87 ZX= -4.18
 XY= -33.1654 YY= 123.7655 ZY= 68.5507
 XZ= 2.5189 YZ= 46.9789 ZZ= -33.6543
 Eigenvalues: -53.056 42.3909 148.2075

8 C Isotropic= 40.4718 Anisotropy 156.448
 XX= 37.0787 YX= -10.3751 ZX= -16.2034
 XY= -12.0505 YY= 99.2056 ZY= 71.0013
 XZ= -29.3075 YZ= 90.0804 ZZ= -14.8689
 Eigenvalues: -58.9384 35.5834 144.7704

9 C Isotropic= 111.2861 Anisotropy 54.3294
 XX= 130.6304 YX= 26.5533 ZX= 10.1709
 XY= 25.6877 YY= 103.8511 ZY= -7.8318
 XZ= 17.115 YZ= -12.5301 ZZ= 99.3768
 Eigenvalues: 76.6286 109.7239 147.5057

10 C Isotropic= 146.8516 Anisotropy 44.1663
 XX= 174.8323 YX= 6.7608 ZX= 3.6371
 XY= 1.4953 YY= 132.5368 ZY= -4.3471
 XZ= 11.3002 YZ= -12.4579 ZZ= 133.1858
 Eigenvalues: 123.1574 141.1017 176.2958

11 C Isotropic= 147.4806 Anisotropy 12.2728
 XX= 143.376 YX= 0.1947 ZX= -0.1901

XY=	-14.8728	YY=	151.266	ZY=	-1.0019				
XZ=	-1.4736	YZ=	0.6379	ZZ=	147.7999				
Eigenvalues:	138.9155			147.864	155.6625				
12	C	Isotropic=		155.0974	Anisotropy			22.4471	
XX=	159.7084	YX=	0.4166	ZX=	-17.678				
XY=	5.657	YY=	155.7752	ZY=	12.6874				
XZ=	-9.1732	YZ=	7.5347	ZZ=	149.8086				
Eigenvalues:	135.4253			159.8047	170.0621				
13	C	Isotropic=		148.2271	Anisotropy			54.7159	
XX=	148.9419	YX=	-14.1542	ZX=	-8.1434				
XY=	-20.9723	YY=	142.9961	ZY=	27.0618				
XZ=	-5.382	YZ=	30.0156	ZZ=	152.7432				
Eigenvalues:	116.0295			143.9473	184.7043				
14	C	Isotropic=		167.9576	Anisotropy			13.128	
XX=	171.3609	YX=	-7.9413	ZX=	3.9949				
XY=	2.904	YY=	162.6544	ZY=	3.3756				
XZ=	8.1006	YZ=	1.4741	ZZ=	169.8575				
Eigenvalues:	159.9748			167.1884	176.7096				
15	C	Isotropic=		169.2096	Anisotropy			17.3415	
XX=	173.0945	YX=	-3.4879	ZX=	-9.4893				
XY=	-5.7439	YY=	175.0763	ZY=	2.3497				
XZ=	-5.4379	YZ=	1.4839	ZZ=	159.458				
Eigenvalues:	156.1665			170.6917	180.7707				
16	O	Isotropic=		263.0757	Anisotropy			82.1801	
XX=	315.6902	YX=	1.3794	ZX=	5.7757				
XY=	19.9068	YY=	202.5641	ZY=	43.9912				
XZ=	3.3569	YZ=	8.3203	ZZ=	270.9729				
Eigenvalues:	193.1005			278.2642	317.8624				
17	O	Isotropic=		265.592	Anisotropy			44.599	
XX=	249.4812	YX=	22.4586	ZX=	-0.587				
XY=	-0.96	YY=	253.7909	ZY=	-3.6145				
XZ=	1.3001	YZ=	-13.3964	ZZ=	293.5039				
Eigenvalues:	240.0514			261.4	295.3247				
18	O	Isotropic=		-356.3469	Anisotropy			1078.7588	
XX=	-748.8208	YX=	-246.5895	ZX=	431.7428				
XY=	-215.6659	YY=	-528.6736	ZY=	-0.6237				
XZ=	370.7805	YZ=	-11.8475	ZZ=	208.4537				
Eigenvalues:	-995.0908			-436.7756	362.8256				
19	O	Isotropic=		89.0295	Anisotropy			124.6038	
XX=	101.8603	YX=	157.7131	ZX=	-66.9992				
XY=	21.0383	YY=	46.6702	ZY=	23.531				
XZ=	-37.6694	YZ=	83.5624	ZZ=	118.558				
Eigenvalues:	-51.6727	146.6625		172.0987					
20	O	Isotropic=		96.0166	Anisotropy			158.0845	
XX=	139.2267	YX=	-30.3389	ZX=	9.2757				
XY=	-157.4182	YY=	33.7464	ZY=	-72.0988				
XZ=	-70.0243	YZ=	-105.7178	ZZ=	115.0768				
Eigenvalues:	-67.8727	154.5163		201.4063					
21	H	Isotropic=		31.1108	Anisotropy			13.5843	
XX=	33.2587	YX=	3.1725	ZX=	-5.0948				
XY=	2.7082	YY=	35.0504	ZY=	-5.0195				
XZ=	-5.1326	YZ=	-3.8788	ZZ=	25.0231				
Eigenvalues:	21.9268	31.2386	40.1669						
22	C	Isotropic=		20.3489	Anisotropy			74.7209	
XX=	41.557	YX=	-77.5896	ZX=	-4.0763				
XY=	-38.8931	YY=	-48.702	ZY=	-4.5239				

XZ= -8.841 YZ= -22.5415 ZZ= 68.1917
 Eigenvalues: -78.782 69.6659 70.1629
 23 O Isotropic= -132.4541 Anisotropy 601.3128
 XX= -260.8062 YX= -34.3788 ZX= -300.8877
 XY= -55.2046 YY= -252.3558 ZY= 40.228
 XZ= -251.2772 YZ= 46.3755 ZZ= 115.7997
 Eigenvalues: -409.164 -256.6193 268.4211
 24 C Isotropic= 166.2349 Anisotropy 36.8023
 XX= 158.2924 YX= -3.8916 ZX= 6.6244
 XY= -4.1117 YY= 186.7147 ZY= -11.3984
 XZ= 5.5197 YZ= -9.7333 ZZ= 153.6974
 Eigenvalues: 148.2319 159.7029 190.7697
 25 H Isotropic= 27.399 Anisotropy 2.9056
 XX= 26.8893 YX= 0.0333 ZX= -1.4282
 XY= 1.1906 YY= 28.7621 ZY= -0.1299
 XZ= -1.9491 YZ= -0.6795 ZZ= 26.5456
 Eigenvalues: 25.0167 27.8442 29.3361
 26 H Isotropic= 28.0661 Anisotropy 8.304
 XX= 30.0687 YX= -3.939 ZX= -1.6162
 XY= -3.391 YY= 27.3285 ZY= 1.6374
 XZ= -1.5806 YZ= 2.7995 ZZ= 26.8012
 Eigenvalues: 24.2981 26.2982 33.6021
 27 H Isotropic= 25.4502 Anisotropy 3.4525
 XX= 25.9359 YX= 2.012 ZX= -1.3867
 XY= 0.5674 YY= 26.7742 ZY= 0.3835
 XZ= 1.5287 YZ= -1.4913 ZZ= 23.6405
 Eigenvalues: 23.5032 25.0955 27.7518
 28 H Isotropic= 24.401 Anisotropy 7.4511
 XX= 29.0413 YX= 1.3729 ZX= 1.3054
 XY= -0.0466 YY= 21.3646 ZY= 3.808
 XZ= 0.5038 YZ= 2.9364 ZZ= 22.7972
 Eigenvalues: 18.6332 25.2015 29.3684
 29 H Isotropic= 28.4508 Anisotropy 6.4295
 XX= 29.707 YX= 0.627 ZX= -1.4196
 XY= 0.16 YY= 25.2489 ZY= -4.0045
 XZ= -0.856 YZ= -3.2446 ZZ= 30.3964
 Eigenvalues: 23.3725 29.2428 32.7371
 30 H Isotropic= 29.0348 Anisotropy 4.5983
 XX= 32.0489 YX= 0.4193 ZX= 0.3797
 XY= 0.2251 YY= 29.8008 ZY= 1.3463
 XZ= -0.5225 YZ= 2.3036 ZZ= 25.2547
 Eigenvalues: 24.6086 30.3954 32.1003
 31 H Isotropic= 29.2689 Anisotropy 8.1871
 XX= 29.2037 YX= 0.9925 ZX= -3.0067
 XY= 0.9175 YY= 25.6094 ZY= 1.9032
 XZ= -3.1134 YZ= 0.3211 ZZ= 32.9936
 Eigenvalues: 24.8651 28.2147 34.727
 32 H Isotropic= 29.1612 Anisotropy 9.0698
 XX= 26.9787 YX= 4.4856 ZX= -0.466
 XY= 3.802 YY= 32.8479 ZY= -1.1385
 XZ= 0.2707 YZ= -1.6355 ZZ= 27.6569
 Eigenvalues: 24.7264 27.5494 35.2077
 33 H Isotropic= 30.3016 Anisotropy 6.6087
 XX= 32.947 YX= 1.5582 ZX= 2.9193
 XY= 1.5483 YY= 28.57 ZY= -1.2868
 XZ= 3.0637 YZ= -1.8718 ZZ= 29.3877

Eigenvalues:	25.9276	30.2698	34.7073		
34	H	Isotropic=	30.0697	Anisotropy	9.0637
XX=	29.4846	YX=	1.5546	ZX=	0.3892
XY=	2.109	YY=	29.6137	ZY=	4.6289
XZ=	1.6856	YZ=	5.5672	ZZ=	31.1109
Eigenvalues:	25.085	29.012	36.1122		
35	H	Isotropic=	30.0837	Anisotropy	6.5401
XX=	30.7827	YX=	-2.3203	ZX=	1.6183
XY=	-2.8224	YY=	31.6437	ZY=	2.7413
XZ=	-1.194	YZ=	2.6821	ZZ=	27.8246
Eigenvalues:	25.9632	29.8441	34.4437		
36	H	Isotropic=	28.3231	Anisotropy	6.2784
XX=	27.0944	YX=	0.9395	ZX=	-1.5183
XY=	0.2019	YY=	26.7695	ZY=	3.3493
XZ=	-2.393	YZ=	1.0418	ZZ=	31.1054
Eigenvalues:	24.9405	27.5201	32.5087		
37	H	Isotropic=	29.0544	Anisotropy	7.1738
XX=	31.8994	YX=	1.4095	ZX=	-0.1256
XY=	1.559	YY=	27.563	ZY=	-4.7198
XZ=	-1.9438	YZ=	-4.4062	ZZ=	27.7007
Eigenvalues:	23.0554	30.2708	33.8369		
38	H	Isotropic=	28.4588	Anisotropy	11.448
XX=	31.8248	YX=	4.8517	ZX=	1.2859
XY=	6.2353	YY=	26.9171	ZY=	0.9229
XZ=	2.4593	YZ=	2.4592	ZZ=	26.6344
Eigenvalues:	23.2541	26.0314	36.0908		
39	H	Isotropic=	28.6809	Anisotropy	9.8091
XX=	33.3211	YX=	-1.7182	ZX=	-3.9205
XY=	-2.3405	YY=	27.0441	ZY=	-1.3976
XZ=	-3.937	YZ=	-1.1657	ZZ=	25.6776
Eigenvalues:	23.0157	27.8068	35.2203		
40	H	Isotropic=	29.1887	Anisotropy	10.7914
XX=	29.5379	YX=	1.4512	ZX=	-5.6438
XY=	-0.3544	YY=	27.1146	ZY=	-1.3731
XZ=	-6.2519	YZ=	-1.0075	ZZ=	30.9135
Eigenvalues:	24.186	26.9971	36.383		
41	H	Isotropic=	29.6036	Anisotropy	5.9466
XX=	32.9779	YX=	-1.237	ZX=	1.1369
XY=	-1.7036	YY=	25.344	ZY=	0.768
XZ=	1.0461	YZ=	0.2734	ZZ=	30.489
Eigenvalues:	24.9768	30.266	33.568		
42	H	Isotropic=	30.4691	Anisotropy	9.5964
XX=	28.6293	YX=	-1.6232	ZX=	-1.9984
XY=	-1.6393	YY=	34.7083	ZY=	3.2429
XZ=	-2.4985	YZ=	3.6175	ZZ=	28.0698
Eigenvalues:	25.7398	28.8008	36.8667		
43	H	Isotropic=	29.0906	Anisotropy	5.4872
XX=	30.0954	YX=	1.02	ZX=	3.136
XY=	-0.9146	YY=	30.2813	ZY=	-2.8039
XZ=	3.3974	YZ=	-1.5768	ZZ=	26.8952
Eigenvalues:	24.2517	30.2714	32.7488		
44	H	Isotropic=	29.1913	Anisotropy	6.7985
XX=	26.4076	YX=	-1.1348	ZX=	-0.7937
XY=	0.0502	YY=	32.0868	ZY=	3.2085
XZ=	-0.5281	YZ=	2.1046	ZZ=	29.0794
Eigenvalues:	26.2513	27.5989	33.7236		

45	H	Isotropic=	28.9788	Anisotropy	8.8878
XX=	29.7113	YX=	1.6932	ZX=	-2.156
XY=	3.8509	YY=	29.7128	ZY=	-3.1273
XZ=	-3.2238	YZ=	-3.4373	ZZ=	27.5123
Eigenvalues:	25.0286	27.0038	34.904		
46	H	Isotropic=	30.5656	Anisotropy	17.975
XX=	40.4352	YX=	-4.6421	ZX=	4.9181
XY=	-2.9238	YY=	23.7445	ZY=	-3.3266
XZ=	3.0459	YZ=	-1.4595	ZZ=	27.5173
Eigenvalues:	22.3812	26.7668	42.549		
47	C	Isotropic=	9.7338	Anisotropy	91.7351
XX=	-64.2752	YX=	-11.6674	ZX=	-62.3549
XY=	27.3839	YY=	46.9458	ZY=	3.2978
XZ=	-49.9349	YZ=	-6.6466	ZZ=	46.5309
Eigenvalues:	-88.0735	46.3844	70.8906		
48	O	Isotropic=	-158.0069	Anisotropy	713.112
XX=	-238.3647	YX=	137.0789	ZX=	-194.431
XY=	113.0725	YY=	-355.8064	ZY=	-239.2468
XZ=	-213.9958	YZ=	-230.3875	ZZ=	120.1503
Eigenvalues:	-462.444	-328.9779	317.4011		
49	H	Isotropic=	28.7302	Anisotropy	6.4872
XX=	29.4011	YX=	-1.7288	ZX=	0.9328
XY=	-1.6248	YY=	24.3639	ZY=	0.4808
XZ=	2.0693	YZ=	1.5315	ZZ=	32.4256
Eigenvalues:	23.6293	29.5063	33.055		
50	H	Isotropic=	29.45	Anisotropy	6.5176
XX=	26.8767	YX=	0.7849	ZX=	-1.0176
XY=	0.5432	YY=	32.6527	ZY=	1.7309
XZ=	-1.4265	YZ=	3.0348	ZZ=	28.8206
Eigenvalues:	25.8317	28.7233	33.7951		
51	C	Isotropic=	111.8907	Anisotropy	14.8027
XX=	121.5971	YX=	-0.8248	ZX=	-0.0186
XY=	-3.1358	YY=	97.5066	ZY=	-2.1178
XZ=	-0.1157	YZ=	-0.5838	ZZ=	116.5683
Eigenvalues:	97.2504	116.6626	121.7592		
52	C	Isotropic=	130.7026	Anisotropy	25.9352
XX=	138.1681	YX=	7.7189	ZX=	0.903
XY=	11.3531	YY=	137.9303	ZY=	-4.7533
XZ=	-2.9299	YZ=	-3.4208	ZZ=	116.0094
Eigenvalues:	115.2468	128.8683	147.9927		
53	O	Isotropic=	274.7931	Anisotropy	38.959
XX=	285.7218	YX=	-1.9003	ZX=	30.5283
XY=	11.4295	YY=	278.9883	ZY=	-17.608
XZ=	18.9639	YZ=	-3.6995	ZZ=	259.6692
Eigenvalues:	241.1786	282.4349	300.7658		
54	H	Isotropic=	26.7125	Anisotropy	5.7976
XX=	29.6048	YX=	1.5259	ZX=	2.1405
XY=	-2.1659	YY=	25.8076	ZY=	-3.1899
XZ=	1.5249	YZ=	-2.2962	ZZ=	24.7251
Eigenvalues:	22.2604	27.2994	30.5776		
55	N	Isotropic=	135.9986	Anisotropy	135.0038
XX=	133.3126	YX=	37.6557	ZX=	1.6707
XY=	18.0883	YY=	186.4299	ZY=	55.1445
XZ=	-36.2763	YZ=	84.8085	ZZ=	88.2533
Eigenvalues:	42.907	139.0876	226.0011		
56	C	Isotropic=	52.7696	Anisotropy	189.3829

XX= 79.8405 YX= -102.4576 ZX= 5.7289
 XY= -95.5535 YY= 72.3118 ZY= -35.0288
 XZ= 3.3595 YZ= -29.6986 ZZ= 6.1565
 Eigenvalues: -33.9933 13.2772 179.0249
 57 H Isotropic= 25.1931 Anisotropy 4.756
 XX= 24.3247 YX= 2.4743 ZX= -1.0271
 XY= 1.9771 YY= 24.6988 ZY= -0.6649
 XZ= -2.7323 YZ= -0.2805 ZZ= 26.5558
 Eigenvalues: 21.9958 25.2197 28.3638
 58 H Isotropic= 30.3985 Anisotropy 10.3409
 XX= 27.8321 YX= -1.6879 ZX= -1.7762
 XY= -1.4585 YY= 33.5395 ZY= -6.1072
 XZ= -0.0995 YZ= -4.3538 ZZ= 29.8238
 Eigenvalues: 25.0917 28.8112 37.2924
 59 C Isotropic= 19.3683 Anisotropy 112.7595
 XX= 75.3543 YX= 52.6127 ZX= 6.7554
 XY= 51.4079 YY= -47.1148 ZY= -15.6515
 XZ= 7.8777 YZ= -36.9052 ZZ= 29.8654
 Eigenvalues: -73.3837 36.9473 94.5413
 60 H Isotropic= 26.7358 Anisotropy 8.2022
 XX= 24.221 YX= -7.8147 ZX= 3.6058
 XY= -1.0761 YY= 29.6277 ZY= 1.263
 XZ= 2.1906 YZ= 3.3544 ZZ= 26.3588
 Eigenvalues: 19.7028 28.3007 32.2039
 61 C Isotropic= 62.5745 Anisotropy 170.0915
 XX= 84.6581 YX= -91.0109 ZX= 42.4557
 XY= -86.7403 YY= 84.6352 ZY= 20.3024
 XZ= 43.9934 YZ= 12.3875 ZZ= 18.4304
 Eigenvalues: -37.1599 48.9146 175.9689
 62 C Isotropic= 62.4196 Anisotropy 176.4414
 XX= 116.4966 YX= -63.3605 ZX= 17.1918
 XY= -63.7407 YY= 108.4719 ZY= -22.404
 XZ= 18.0495 YZ= -25.0162 ZZ= -37.7096
 Eigenvalues: -41.8875 49.0992 180.0472
 63 C Isotropic= 63.4922 Anisotropy 176.4577
 XX= 86.7795 YX= -99.804 ZX= -8.1743
 XY= -100.6637 YY= 68.9122 ZY= -38.255
 XZ= -8.7093 YZ= -37.4734 ZZ= 34.7848
 Eigenvalues: -38.5771 47.923 181.1306
 64 C Isotropic= 61.6842 Anisotropy 175.3795
 XX= 80.7636 YX= -93.5218 ZX= 42.9068
 XY= -93.4869 YY= 84.1531 ZY= 14.9137
 XZ= 44.9274 YZ= 15.8764 ZZ= 20.1359
 Eigenvalues: -40.9763 47.425 178.6038
 65 C Isotropic= 60.0089 Anisotropy 149.5612
 XX= 108.8288 YX= -50.166 ZX= 17.5355
 XY= -50.2245 YY= 102.2812 ZY= -21.6964
 XZ= 16.4164 YZ= -21.412 ZZ= -31.0831
 Eigenvalues: -35.1238 55.4342 159.7164
 66 H Isotropic= 22.9963 Anisotropy 11.1927
 XX= 23.6349 YX= 3.4205 ZX= 3.837
 XY= 3.0349 YY= 20.3978 ZY= 3.3031
 XZ= 3.6269 YZ= 4.0347 ZZ= 24.9562
 Eigenvalues: 18.0211 20.5097 30.4581
 67 O Isotropic= -120.9541 Anisotropy 702.2171
 XX= 265.2784 YX= 179.618 ZX= -93.5246

XY=	185.9306	YY=	-153.1471	ZY=	-42.5364
XZ=	-107.6089	YZ=	-17.1342	ZZ=	-474.9935
Eigenvalues:	-488.5127		-221.5402		347.1907
68	C	Isotropic=	55.2409	Anisotropy	173.3888
XX=	61.2598	YX=	2.544	ZX=	-85.1798
XY=	16.6952	YY=	-14.9865	ZY=	19.7201
XZ=	-61.7672	YZ=	32.7589	ZZ=	119.4494
Eigenvalues:	-29.0809	23.9702	170.8334		
69	H	Isotropic=	23.7479	Anisotropy	5.45
XX=	23.6657	YX=	3.3847	ZX=	0.2364
XY=	3.393	YY=	23.8435	ZY=	1.0559
XZ=	0.285	YZ=	1.0152	ZZ=	23.7344
Eigenvalues:	20.2784	23.584	27.3812		
70	H	Isotropic=	23.6974	Anisotropy	3.3084
XX=	22.8491	YX=	2.4009	ZX=	-0.7975
XY=	2.303	YY=	22.7901	ZY=	-0.0081
XZ=	-0.7913	YZ=	0.1061	ZZ=	25.4529
Eigenvalues:	20.3971	24.792	25.9029		
71	H	Isotropic=	23.705	Anisotropy	4.584
XX=	22.8961	YX=	2.9542	ZX=	0.3837
XY=	2.7936	YY=	23.374	ZY=	1.2598
XZ=	0.3718	YZ=	1.2438	ZZ=	24.8449
Eigenvalues:	20.178	24.176	26.761		
72	H	Isotropic=	23.7343	Anisotropy	8.5877
XX=	24.4752	YX=	4.9643	ZX=	-0.8056
XY=	4.5147	YY=	24.6998	ZY=	-0.6796
XZ=	-0.7365	YZ=	-0.5742	ZZ=	22.0281
Eigenvalues:	19.8405	21.9031	29.4595		
73	C	Isotropic=	59.7767	Anisotropy	177.7992
XX=	49.5469	YX=	-5.584	ZX=	-104.8455
XY=	-2.6333	YY=	40.2828	ZY=	1.1746
XZ=	-108.787	YZ=	2.4741	ZZ=	89.5006
Eigenvalues:	-39.1947	40.2154	178.3095		
74	C	Isotropic=	61.8725	Anisotropy	177.3702
XX=	82.7686	YX=	-35.1481	ZX=	-78.3619
XY=	-32.653	YY=	-13.8998	ZY=	-22.1303
XZ=	-78.5894	YZ=	-23.5543	ZZ=	116.7485
Eigenvalues:	-41.2674	46.7656	180.1193		
75	C	Isotropic=	62.338	Anisotropy	177.9024
XX=	88.0834	YX=	27.1063	ZX=	-75.1798
XY=	26.1004	YY=	-21.3531	ZY=	25.3844
XZ=	-74.8486	YZ=	24.1735	ZZ=	120.2836
Eigenvalues:	-40.6832	46.7575	180.9396		
76	C	Isotropic=	63.723	Anisotropy	174.8241
XX=	47.1903	YX=	3.8389	ZX=	-106.0054
XY=	-0.2891	YY=	49.8001	ZY=	2.646
XZ=	-108.0626	YZ=	2.4321	ZZ=	94.1787
Eigenvalues:	-38.9973	49.8939	180.2724		
77	C	Isotropic=	67.405	Anisotropy	162.5471
XX=	83.8361	YX=	-29.6298	ZX=	-71.3373
XY=	-34.9247	YY=	-2.1009	ZY=	-22.9791
XZ=	-71.0859	YZ=	-17.7376	ZZ=	120.4798
Eigenvalues:	-27.7553	54.2006	175.7697		
78	H	Isotropic=	23.0814	Anisotropy	7.3106
XX=	21.0736	YX=	-0.3136	ZX=	0.9792
XY=	-0.6886	YY=	27.8828	ZY=	0.7858

XZ=	1.2048	YZ=	0.4096	ZZ=	20.2877		
Eigenvalues:	19.4485	21.8405	27.9551				
79	H	Isotropic=	23.7059	Anisotropy	4.7506		
XX=	23.5158	YX=	-1.6066	ZX=	2.441		
XY=	-1.2663	YY=	25.4362	ZY=	-0.421		
XZ=	2.4349	YZ=	-0.6004	ZZ=	22.1656		
Eigenvalues:	20.2658	23.9788	26.8729				
80	H	Isotropic=	23.7322	Anisotropy	3.6968		
XX=	23.8536	YX=	0.4077	ZX=	2.6081		
XY=	0.4411	YY=	25.043	ZY=	0.7054		
XZ=	2.5583	YZ=	0.4843	ZZ=	22.3		
Eigenvalues:	20.3684	24.6316	26.1967				
81	H	Isotropic=	23.9375	Anisotropy	5.1709		
XX=	23.1753	YX=	-0.8487	ZX=	2.0792		
XY=	-0.6738	YY=	27.1806	ZY=	-0.166		
XZ=	1.787	YZ=	-0.2924	ZZ=	21.4566		
Eigenvalues:	20.1932	24.2345	27.3847				
82	H	Isotropic=	24.2072	Anisotropy	8.6451		
XX=	24.8192	YX=	-3.8776	ZX=	3.066		
XY=	-3.0061	YY=	26.3593	ZY=	-1.1095		
XZ=	2.5701	YZ=	-1.1793	ZZ=	21.4432		
Eigenvalues:	19.7421	22.9089	29.9706				

2b-iv

C	-3.14414-0.051054	2.143942	
C	-3.938581	1.283774	1.98463
C	-3.478785	2.194292	0.833683
C	-4.506724	2.321439	-0.305144
C	-4.870744	0.997686	-1.006796
C	-3.756120-0.041527	-1.402411	
C	-2.9589 -0.501801	-0.252134	
C	-1.603856	-0.365445	-0.285648
C	-0.864335	-0.477694	1.01884
C	-1.626123	0.179634	2.174652
C	-3.557824	-1.055069	1.024912
C	-5.06654-1.254041-0.053372		
C	-2.95306-2.439638	1.327149	
C	-0.827136	-0.079563	-1.509466
C	-5.757163	3.035998	0.154777
O	-3.437495	-0.591609	3.431179
O	-3.901855	1.987223	3.217074
O	-6.023805	0.817272	-1.405924
O	-4.073492	-0.866931	-2.44683
O	0.422267	0.174497	1.082937
H	-2.979745	2.047843	3.495528
C	-5.079069	-1.795893	-2.415518
O	-5.886664	-1.817765	-1.493303
C	-5.036971	-2.669496	-3.625827
H	-5.035869	1.047222	1.86614
H	-2.508506	1.837945	0.405579
H	-3.065827	0.748631	-1.988649
H	-0.66949-1.571446	1.228832	
H	-1.218139	-0.235717	3.136266
H	-1.405778	1.279579	2.171709
H	-5.637745	-0.426228	0.57683
H	-5.3452 -2.199406	0.52427	

H	-5.405653	-1.355509	2.114562
H	-3.754437	-3.195828	1.514152
H	-2.337216	-2.805084	0.47145
H	-2.323671	-2.401339	2.249793
H	-1.448817	-0.125161	-2.437808
H	-0.352937	0.932657	-1.437699
H	-0.025946	-0.853231	-1.634059
H	-6.445152	3.199782	-0.71055
H	-6.303906	2.433358	0.919275
H	-5.490939	4.023991	0.601099
H	-4.251659	-2.330226	-4.342835
H	-4.817412	-3.716426	-3.30279
H	-6.036926	-2.638939	-4.123597
H	-4.350295	-0.364763	0.650559
C	1.435434	-0.176658	0.234067
O	1.539174	-1.357426	-0.090447
H	-4.017655	2.942708	-1.11204
H	-3.311651	3.222828	1.252401
C	2.346077	1.0038	-0.048487
C	3.854853	0.719733	-0.316939
O	1.728636	1.789683	-1.050013
H	2.31285	1.675045	0.867277
N	4.128637	-0.123477	-1.441494
C	4.618178	2.022361	-0.379091
H	4.196964	0.152473	0.610132
H	1.794559	1.303946	-1.884081
C	4.52072	-1.453901	-1.444254
H	4.052918	0.305619	-2.338869
C	4.321564	3.012073	-1.319962
C	5.054394	4.198743	-1.344358
C	6.089361	4.402122	-0.432627
C	6.391697	3.414846	0.50548
C	5.661466	2.228064	0.532292
H	3.501448	2.864992	-2.03902
O	4.884585	-1.912811	-2.549075
C	4.940306	-2.161282	-0.194778
H	4.812526	4.974341	-2.086028
H	6.666968	5.338043	-0.453309
H	7.209372	3.570303	1.224774
H	5.911101	1.451738	1.271703
C	6.296801	-2.540605	-0.179492
C	6.828325	-3.215257	0.914458
C	6.012873	-3.536924	2.001284
C	4.66622	-3.185625	1.979007
C	4.129361	-2.502365	0.883956
H	6.931197	-2.308671	-1.050449
H	7.890035	-3.503001	0.917217
H	6.431747	-4.073192	0.865485
H	4.012304	-3.451713	2.822799
H	3.055997	-2.272588	0.888196

2biv_45 E(RB+HF-PW91) = -2012.27348
SCF GIAO Magnetic shielding tensor (ppm):
1 C Isotropic= 111.0212 Anisotropy 30.332
XX= 100.6963 YX= 9.6104 ZX= -13.9305

XY=	10.5249	YY=	113.7629	ZY=	-8.9348		
XZ=	-5.2803	YZ=	-8.0743	ZZ=	118.6046		
Eigenvalues:	94.1958	107.6254		131.2425			
2	C	Isotropic=	112.5127	Anisotropy		31.2366	
XX=	93.7388	YX=	2.4699	ZX=	7.2971		
XY=	-2.8288	YY=	118.1784	ZY=	5.4911		
XZ=	2.4993	YZ=	15.3164	ZZ=	125.6209		
Eigenvalues:	92.8694	111.3316		133.3371			
3	C	Isotropic=	142.0204	Anisotropy		20.3994	
XX=	121.2398	YX=	-2.7579	ZX=	-3.4519		
XY=	3.637	YY=	155.5273	ZY=	-0.2136		
XZ=	1.2095	YZ=	-1.2376	ZZ=	149.294		
Eigenvalues:	121.1902	149.251		155.6199			
4	C	Isotropic=	140.6394	Anisotropy		24.2025	
XX=	125.9587	YX=	1.4657	ZX=	0.6651		
XY=	-5.9141	YY=	153.5122	ZY=	6.9433		
XZ=	-12.4137	YZ=	5.0095	ZZ=	142.4474		
Eigenvalues:	124.0767	141.0672		156.7744			
5	C	Isotropic=	-23.0957	Anisotropy		180.6534	
XX=	-56.0807	YX=	38.2034	ZX=	-10.8006		
XY=	22.0127	YY=	-65.3189	ZY=	-83.5922		
XZ=	-16.592	YZ=	-77.1377	ZZ=	52.1123		
Eigenvalues:	-113.9335	-52.6936		97.3399			
6	C	Isotropic=	101.8026	Anisotropy		40.9581	
XX=	88.4661	YX=	-6.6936	ZX=	-8.1826		
XY=	3.6538	YY=	116.5338	ZY=	19.7468		
XZ=	8.484	YZ=	18.1719	ZZ=	100.4078		
Eigenvalues:	87.1458	89.154		129.108			
7	C	Isotropic=	45.1255	Anisotropy		154.9598	
XX=	36.7026	YX=	1.3109	ZX=	-19.615		
XY=	-12.9123	YY=	122.3118	ZY=	53.9787		
XZ=	-35.127	YZ=	73.863	ZZ=	-23.6379		
Eigenvalues:	-53.8887	40.8331		148.432			
8	C	Isotropic=	41.636	Anisotropy		153.9262	
XX=	39.808	YX=	-9.8814	ZX=	-11.4358		
XY=	-15.3719	YY=	135.5059	ZY=	47.055		
XZ=	-2.7139	YZ=	26.1265	ZZ=	-50.4057		
Eigenvalues:	-57.5673	38.2219		144.2535			
9	C	Isotropic=	110.3226	Anisotropy		55.6104	
XX=	132.9027	YX=	27.7631	ZX=	3.7461		
XY=	30.3641	YY=	89.1153	ZY=	-4.6396		
XZ=	-2.3057	YZ=	1.6632	ZZ=	108.9498		
Eigenvalues:	74.5424	109.0292		147.3962			
10	C	Isotropic=	147.0103	Anisotropy		43.9137	
XX=	172.6714	YX=	7.4785	ZX=	-4.9236		
XY=	5.9004	YY=	124.1097	ZY=	-3.1		
XZ=	-14.0559	YZ=	4.5519	ZZ=	144.2498		
Eigenvalues:	123.0022	141.7427		176.2861			
11	C	Isotropic=	147.2422	Anisotropy		11.8846	
XX=	141.2645	YX=	0.5888	ZX=	2.0245		
XY=	-10.8088	YY=	149.8554	ZY=	5.1447		
XZ=	-6.341	YZ=	0.8822	ZZ=	150.6068		
Eigenvalues:	138.8409	147.7205		155.1653			
12	C	Isotropic=	154.735	Anisotropy		22.7807	
XX=	163.7259	YX=	-9.4173	ZX=	9.6481		
XY=	-1.4913	YY=	163.2863	ZY=	-2.8412		

XZ=	6.5674	YZ=	4.3741	ZZ=	137.1929				
Eigenvalues:	134.7346			159.5483		169.9222			
13	C	Isotropic=		147.8244	Anisotropy		55.7654		
XX=	144.6765	YX=	-18.1212	ZX=	-7.2123				
XY=	-21.4338	YY=	175.0825	ZY=	-7.2883				
XZ=	-14.2469	YZ=	-10.3903	ZZ=	123.7143				
Eigenvalues:	114.5759			143.896	185.0014				
14	C	Isotropic=		168.1361	Anisotropy		12.877		
XX=	168.1773	YX=	-4.3972	ZX=	-8.6907				
XY=	5.8286	YY=	167.8949	ZY=	-6.4375				
XZ=	-5.35	YZ=	-1.9638	ZZ=	168.3359				
Eigenvalues:	160.348	167.3394		176.7208					
15	C	Isotropic=		169.3159	Anisotropy		17.1292		
XX=	173.7097	YX=	-6.8267	ZX=	3.5328				
XY=	-6.4982	YY=	171.4465	ZY=	8.0098				
XZ=	-0.9113	YZ=	8.979	ZZ=	162.7915				
Eigenvalues:	156.2806			170.9317	180.7354				
16	O	Isotropic=		262.8869	Anisotropy		82.9085		
XX=	313.399	YX=	-1.7275	ZX=	-25.3825				
XY=	3.7123	YY=	251.4004	ZY=	-59.3625				
XZ=	-9.6479	YZ=	-22.4787	ZZ=	223.8612				
Eigenvalues:	192.8928			277.6086	318.1592				
17	O	Isotropic=		265.1571	Anisotropy		44.8191		
XX=	253.6795	YX=	15.5049	ZX=	20.5934				
XY=	-3.8206	YY=	258.5524	ZY=	-22.2422				
XZ=	3.4049	YZ=	-15.588	ZZ=	283.2392				
Eigenvalues:	239.3791			261.0557	295.0364				
18	O	Isotropic=		-357.3315	Anisotropy		1081.0407		
XX=	-905.7404	YX=	7.4428	ZX=	-325.7778				
XY=	-7.4094	YY=	-267.1808	ZY=	-354.7784				
XZ=	-256.6985	YZ=	-347.5957	ZZ=	100.9267				
Eigenvalues:	-997.0389			-438.3178	363.3623				
19	O	Isotropic=		89.6185	Anisotropy		124.9425		
XX=	140.4008	YX=	67.6086	ZX=	127.3888				
XY=	-10.3693	YY=	123.4024	ZY=	-19.8924				
XZ=	19.5051	YZ=	-95.6669	ZZ=	5.0522				
Eigenvalues:	-50.9448	146.8867		172.9135					
20	O	Isotropic=		86.2457	Anisotropy		157.3707		
XX=	108.4562	YX=	-24.0303	ZX=	-13.9502				
XY=	-178.9775	YY=	-26.4346	ZY=	-0.7849				
XZ=	-29.3173	YZ=	4.853	ZZ=	176.7155				
Eigenvalues:	-81.135	148.7127		191.1595					
21	H	Isotropic=		31.1554	Anisotropy		13.5466		
XX=	35.7379	YX=	0.6179	ZX=	5.5322				
XY=	0.3714	YY=	27.1866	ZY=	6.5185				
XZ=	5.0929	YZ=	5.3726	ZZ=	30.5416				
Eigenvalues:	22.0342	31.2455	40.1864						
22	C	Isotropic=		20.1271	Anisotropy		74.9215		
XX=	25.5879	YX=	-73.2268	ZX=	-43.0283				
XY=	-49.5496	YY=	-16.1067	ZY=	-51.9172				
XZ=	-15.3841	YZ=	-28.7394	ZZ=	50.9				
Eigenvalues:	-79.1545	69.461	70.0747						
23	O	Isotropic=		-131.6047	Anisotropy		599.8113		
XX=	-184.3897	YX=	-241.8464	ZX=	238.2748				
XY=	-227.3081	YY=	-63.2619	ZY=	-147.1782				
XZ=	185.0143	YZ=	-149.0229	ZZ=	-147.1624				

Eigenvalues:	-406.8985	-256.1851	268.2695		
24	C	Isotropic=	166.3514	Anisotropy	36.8101
XX=	156.2402	YX=	4.7282	ZX=	-2.8866
XY=	4.8558	YY=	164.2521	ZY=	19.0731
XZ=	-2.1863	YZ=	17.1507	ZZ=	178.562
Eigenvalues:	148.2808		159.882	190.8914	
25	H	Isotropic=	27.3798	Anisotropy	2.8356
XX=	27.6063	YX=	-0.516	ZX=	1.2881
XY=	-0.1217	YY=	27.5695	ZY=	0.8415
XZ=	2.2737	YZ=	1.4616	ZZ=	26.9636
Eigenvalues:	25.003	27.8662	29.2702		
26	H	Isotropic=	28.0428	Anisotropy	8.2399
XX=	29.292	YX=	-4.2192	ZX=	-1.8487
XY=	-3.6584	YY=	29.2936	ZY=	0.8021
XZ=	-1.8245	YZ=	-0.0997	ZZ=	25.543
Eigenvalues:	24.2638	26.3286	33.5361		
27	H	Isotropic=	25.3841	Anisotropy	3.4967
XX=	26.0724	YX=	1.3251	ZX=	2.3221
XY=	1.5515	YY=	24.9195	ZY=	0.1891
XZ=	-0.9876	YZ=	2.389	ZZ=	25.1603
Eigenvalues:	23.5331	24.9039	27.7152		
28	H	Isotropic=	24.3007	Anisotropy	7.5789
XX=	28.7484	YX=	1.3474	ZX=	-1.7713
XY=	-0.3645	YY=	24.6711	ZY=	-2.3593
XZ=	-2.2673	YZ=	-1.6801	ZZ=	19.4824
Eigenvalues:	18.4851	25.0637	29.3532		
29	H	Isotropic=	28.4638	Anisotropy	6.6006
XX=	30.3324	YX=	-0.9505	ZX=	2.0177
XY=	-1.0114	YY=	23.588	ZY=	-1.1948
XZ=	1.0097	YZ=	-1.8	ZZ=	31.4711
Eigenvalues:	23.2424	29.2848	32.8642		
30	H	Isotropic=	28.9968	Anisotropy	4.6017
XX=	31.8973	YX=	0.7654	ZX=	-1.1842
XY=	0.0085	YY=	29.8069	ZY=	1.914
XZ=	-0.854	YZ=	1.037	ZZ=	25.2863
Eigenvalues:	24.6834	30.2424	32.0646		
31	H	Isotropic=	29.245	Anisotropy	8.2415
XX=	30.2926	YX=	-1.6154	ZX=	2.7565
XY=	-2.0954	YY=	29.4203	ZY=	-4.4314
XZ=	2.6712	YZ=	-2.8959	ZZ=	28.022
Eigenvalues:	24.7946	28.201	34.7393		
32	H	Isotropic=	29.1214	Anisotropy	9.0616
XX=	28.3258	YX=	3.8734	ZX=	3.7903
XY=	3.7526	YY=	29.4534	ZY=	1.7484
XZ=	2.6668	YZ=	2.2713	ZZ=	29.585
Eigenvalues:	24.6485	27.5532	35.1625		
33	H	Isotropic=	30.2346	Anisotropy	6.626
XX=	32.4324	YX=	2.8673	ZX=	-1.735
XY=	2.8353	YY=	27.105	ZY=	-0.8034
XZ=	-1.8221	YZ=	-0.2843	ZZ=	31.1664
Eigenvalues:	25.8577	30.1942	34.6519		
34	H	Isotropic=	30.0247	Anisotropy	9.0797
XX=	29.5831	YX=	0.9858	ZX=	-0.0128
XY=	2.4846	YY=	34.9021	ZY=	-2.3379
XZ=	-0.8249	YZ=	-2.8972	ZZ=	25.5889
Eigenvalues:	24.9033	29.0929	36.0778		

35	H	Isotropic=	30.0739	Anisotropy	6.185
XX=	29.8705	YX=	-0.644	ZX=	-2.9985
XY=	-2.4738	YY=	32.8074	ZY=	1.6019
XZ=	-1.1771	YZ=	1.2184	ZZ=	27.5438
Eigenvalues:	26.2849	29.7395	34.1972		
36	H	Isotropic=	28.3955	Anisotropy	6.4629
XX=	27.9828	YX=	-0.5337	ZX=	1.8245
XY=	-2.0264	YY=	30.4686	ZY=	-3.6687
XZ=	1.8873	YZ=	-1.616	ZZ=	26.7351
Eigenvalues:	24.9166	27.5658	32.7041		
37	H	Isotropic=	28.8571	Anisotropy	7.4044
XX=	32.0967	YX=	1.178	ZX=	1.1627
XY=	0.4003	YY=	22.8506	ZY=	1.0306
XZ=	2.4281	YZ=	0.6752	ZZ=	31.6241
Eigenvalues:	22.7265	30.0514	33.7934		
38	H	Isotropic=	28.2862	Anisotropy	11.6016
XX=	32.2271	YX=	4.6014	ZX=	0.8251
XY=	6.4837	YY=	27.8526	ZY=	-1.4079
XZ=	0.3718	YZ=	-2.1079	ZZ=	24.7789
Eigenvalues:	22.599	26.2389	36.0206		
39	H	Isotropic=	28.5453	Anisotropy	8.8204
XX=	32.9928	YX=	-3.4279	ZX=	1.4587
XY=	-3.7655	YY=	25.1399	ZY=	1.2497
XZ=	0.6009	YZ=	1.3998	ZZ=	27.5033
Eigenvalues:	23.1455	28.0649	34.4256		
40	H	Isotropic=	29.1478	Anisotropy	10.8436
XX=	31.3967	YX=	-2.5916	ZX=	5.279
XY=	-4.3413	YY=	27.5059	ZY=	-0.5919
XZ=	4.5342	YZ=	-1.3838	ZZ=	28.5407
Eigenvalues:	24.1429	26.9236	36.3769		
41	H	Isotropic=	29.6197	Anisotropy	5.9448
XX=	32.0609	YX=	-0.8155	ZX=	-2.4369
XY=	-1.3436	YY=	27.7943	ZY=	-2.5922
XZ=	-2.8156	YZ=	-2.1084	ZZ=	29.0038
Eigenvalues:	25.0609	30.2153	33.5829		
42	H	Isotropic=	30.4795	Anisotropy	9.5763
XX=	28.8073	YX=	-1.803	ZX=	0.4219
XY=	-2.0592	YY=	35.7136	ZY=	2.9241
XZ=	0.6429	YZ=	2.5507	ZZ=	26.9177
Eigenvalues:	25.7457	28.8292	36.8637		
43	H	Isotropic=	29.0056	Anisotropy	5.6039
XX=	28.7697	YX=	2.9247	ZX=	-1.4924
XY=	2.0645	YY=	26.782	ZY=	2.4142
XZ=	-2.9807	YZ=	0.9402	ZZ=	31.4653
Eigenvalues:	24.1218	30.1535	32.7415		
44	H	Isotropic=	29.1468	Anisotropy	6.8597
XX=	26.3278	YX=	-1.0777	ZX=	0.3216
XY=	-0.0217	YY=	33.5642	ZY=	0.2629
XZ=	0.7423	YZ=	1.495	ZZ=	27.5485
Eigenvalues:	26.0357	27.6849	33.7199		
45	H	Isotropic=	28.9179	Anisotropy	8.9471
XX=	31.2596	YX=	0.3938	ZX=	2.8433
XY=	1.5004	YY=	25.6549	ZY=	1.4634
XZ=	4.9749	YZ=	1.9387	ZZ=	29.8393
Eigenvalues:	24.9986	26.8726	34.8826		
46	H	Isotropic=	30.4537	Anisotropy	18.0093

XX= 37.4134 YX= -1.8262 ZX= -8.7535
 XY= -1.034 YY= 22.9199 ZY= 0.1677
 XZ= -6.377 YZ= -1.8146 ZZ= 31.0278
 Eigenvalues: 22.3043 26.5968 42.4599
 47 C Isotropic= 7.5871 Anisotropy 98.7804
 XX= -41.532 YX= -40.7637 ZX= 60.8716
 XY= -5.8945 YY= 34.8697 ZY= -9.9132
 XZ= 70.5115 YZ= 6.9498 ZZ= 29.4235
 Eigenvalues: -83.8737 33.1943 73.4407
 48 O Isotropic= -140.4529 Anisotropy 694.3462
 XX= -120.5324 YX= -59.1174 ZX= 288.022
 XY= -74.0658 YY= -370.3834 ZY= -155.9188
 XZ= 287.5062 YZ= -181.9833 ZZ= 69.5571
 Eigenvalues: -433.27 -310.5333 322.4446
 49 H Isotropic= 28.6674 Anisotropy 6.5954
 XX= 28.327 YX= -1.7248 ZX= -1.7896
 XY= -0.8571 YY= 28.1571 ZY= -3.696
 XZ= -2.6605 YZ= -4.2677 ZZ= 29.5181
 Eigenvalues: 23.5496 29.3883 33.0644
 50 H Isotropic= 29.482 Anisotropy 6.423
 XX= 27.6021 YX= 0.3245 ZX= 1.4912
 XY= 0.1879 YY= 33.5348 ZY= 1.6954
 XZ= 1.5078 YZ= 0.4873 ZZ= 27.309
 Eigenvalues: 25.8939 28.788 33.764
 51 C Isotropic= 112.3986 Anisotropy 14.3276
 XX= 120.9899 YX= -1.7567 ZX= -0.503
 XY= -6.2576 YY= 105.1092 ZY= -9.9175
 XZ= -4.4665 YZ= -9.3483 ZZ= 111.0967
 Eigenvalues: 97.091 118.1545 121.9503
 52 C Isotropic= 127.4541 Anisotropy 18.2485
 XX= 127.92 YX= 6.8093 ZX= 3.9512
 XY= 4.7899 YY= 129.203 ZY= 6.5879
 XZ= 5.8564 YZ= 7.8331 ZZ= 125.2392
 Eigenvalues: 119.7094 123.033 139.6197
 53 O Isotropic= 273.4791 Anisotropy 45.2997
 XX= 278.761 YX= 20.2453 ZX= -29.2409
 XY= 25.7267 YY= 263.0411 ZY= 8.851
 XZ= -11.7473 YZ= 3.7303 ZZ= 278.6351
 Eigenvalues: 238.7416 278.0167 303.6789
 54 H Isotropic= 26.718 Anisotropy 5.678
 XX= 29.1936 YX= 3.1789 ZX= -0.7734
 XY= -1.1147 YY= 23.0005 ZY= 1.1498
 XZ= -2.8014 YZ= -0.0038 ZZ= 27.9601
 Eigenvalues: 22.6836 26.9671 30.5034
 55 N Isotropic= 135.6901 Anisotropy 140.3108
 XX= 137.5411 YX= 3.3739 ZX= 21.6382
 XY= 0.7393 YY= 223.8172 ZY= -46.6415
 XZ= 9.873 YZ= -16.37 ZZ= 45.7118
 Eigenvalues: 37.7763 140.0632 229.2306
 56 C Isotropic= 54.6457 Anisotropy 184.9906
 XX= 68.8074 YX= -65.9296 ZX= -65.9132
 XY= -62.7941 YY= 7.7585 ZY= 50.0936
 XZ= -61.2443 YZ= 43.2928 ZZ= 87.3714
 Eigenvalues: -33.3381 19.3025 177.9728
 57 H Isotropic= 26.1365 Anisotropy 7.2091
 XX= 25.4705 YX= 0.4164 ZX= 2.2398

XY=	-3.1221	YY=	29.3455	ZY=	-3.3967		
XZ=	2.5147	YZ=	-1.0758	ZZ=	23.5935		
Eigenvalues:	21.7937	25.6733	30.9426				
58	H	Isotropic=	30.2978	Anisotropy	10.755		
XX=	28.0065	YX=	-1.5246	ZX=	2.1092		
XY=	-0.6369	YY=	26.1478	ZY=	3.0105		
XZ=	0.474	YZ=	2.258	ZZ=	36.7392		
Eigenvalues:	24.9237	28.502	37.4678				
59	C	Isotropic=	12.7164	Anisotropy	119.9753		
XX=	77.0573	YX=	45.1417	ZX=	-13.3616		
XY=	49.5133	YY=	-50.5098	ZY=	37.5627		
XZ=	-8.5285	YZ=	31.0178	ZZ=	11.6018		
Eigenvalues:	-80.2542	25.7034	92.7				
60	H	Isotropic=	26.7233	Anisotropy	6.1969		
XX=	23.4439	YX=	-2.3455	ZX=	-1.578		
XY=	-0.7377	YY=	27.9319	ZY=	-5.2824		
XZ=	-0.401	YZ=	0.3908	ZZ=	28.7941		
Eigenvalues:	22.4693	26.846	30.8545				
61	C	Isotropic=	63.079	Anisotropy	171.2623		
XX=	60.951	YX=	-40.8862	ZX=	-96.5368		
XY=	-38.6033	YY=	68.4272	ZY=	24.1725		
XZ=	-94.3953	YZ=	32.5244	ZZ=	59.8589		
Eigenvalues:	-35.7441	147.7273	177.2539				
62	C	Isotropic=	62.2507	Anisotropy	175.426		
XX=	99.7745	YX=	-20.8415	ZX=	-67.6841		
XY=	-20.6312	YY=	27.7357	ZY=	74.325		
XZ=	-69.1427	YZ=	78.7798	ZZ=	59.2417		
Eigenvalues:	-41.133	48.6837	179.2013				
63	C	Isotropic=	63.1086	Anisotropy	175.7942		
XX=	79.1836	YX=	-73.8909	ZX=	-54.3654		
XY=	-74.2351	YY=	7.7235	ZY=	36.2369		
XZ=	-54.193	YZ=	36.1597	ZZ=	102.4189		
Eigenvalues:	-38.8055	47.8267	180.3048				
64	C	Isotropic=	61.5839	Anisotropy	173.9979		
XX=	53.6461	YX=	-44.0915	ZX=	-96.7234		
XY=	-42.0712	YY=	69.4453	ZY=	26.6871		
XZ=	-97.9599	YZ=	26.9152	ZZ=	61.6602		
Eigenvalues:	-41.3637	48.5328	177.5825				
65	C	Isotropic=	61.4838	Anisotropy	149.231		
XX=	94.4405	YX=	-11.4147	ZX=	-59.7174		
XY=	-12.1357	YY=	32.4983	ZY=	68.9364		
XZ=	-59.4338	YZ=	69.1412	ZZ=	57.5124		
Eigenvalues:	-33.0037	56.4839	160.9711				
66	H	Isotropic=	23.0518	Anisotropy	11.4587		
XX=	22.7897	YX=	4.5094	ZX=	-1.0385		
XY=	3.7425	YY=	26.0068	ZY=	-4.6064		
XZ=	-1.1646	YZ=	-4.3918	ZZ=	20.3589		
Eigenvalues:	17.5779	20.8866	30.691				
67	O	Isotropic=	-145.6027	Anisotropy	641.7389		
XX=	206.1436	YX=	188.1297	ZX=	92.8511		
XY=	204.7972	YY=	-251.1053	ZY=	-126.3923		
XZ=	79.4886	YZ=	-73.826	ZZ=	-391.8463		
Eigenvalues:	-488.0255	-231.0057	282.2232				
68	C	Isotropic=	57.205	Anisotropy	163.036		
XX=	32.6588	YX=	38.9153	ZX=	-9.2333		
XY=	15.752	YY=	123.329	ZY=	74.9402		

XZ= -13.8064 YZ= 78.3393 ZZ= 15.6272
 Eigenvalues: -32.4255 38.1448 165.8957
 69 H Isotropic= 23.7865 Anisotropy 5.4386
 XX= 24.0041 YX= 2.8508 ZX= 1.7422
 XY= 2.6161 YY= 25.1572 ZY= -1.0363
 XZ= 1.6484 YZ= -0.6348 ZZ= 22.1983
 Eigenvalues: 20.1275 23.8198 27.4123
 70 H Isotropic= 23.7917 Anisotropy 3.3087
 XX= 23.5467 YX= 1.0936 ZX= 2.3514
 XY= 1.0395 YY= 24.2627 ZY= -1.6258
 XZ= 2.3344 YZ= -1.4014 ZZ= 23.5658
 Eigenvalues: 20.3576 25.0201 25.9975
 71 H Isotropic= 23.9446 Anisotropy 5.2767
 XX= 23.2357 YX= 2.2168 ZX= 1.4908
 XY= 2.115 YY= 26.2556 ZY= -1.5822
 XZ= 1.4727 YZ= -1.2716 ZZ= 22.3425
 Eigenvalues: 20.2244 24.147 27.4624
 72 H Isotropic= 24.4676 Anisotropy 8.9043
 XX= 25.2121 YX= 3.7599 ZX= 3.0387
 XY= 3.3841 YY= 26.4911 ZY= 0.6611
 XZ= 3.0402 YZ= 1.5051 ZZ= 21.6996
 Eigenvalues: 19.7974 23.2016 30.4038
 73 C Isotropic= 55.296 Anisotropy 170.0646
 XX= 13.7776 YX= 17.3342 ZX= 49.9456
 XY= 14.4895 YY= 139.0899 ZY= 49.8313
 XZ= 52.6086 YZ= 64.1442 ZZ= 13.0204
 Eigenvalues: -43.2932 40.5088 168.6724
 74 C Isotropic= 62.5757 Anisotropy 173.8138
 XX= -28.685 YX= 47.2769 ZX= 15.2317
 XY= 44.9475 YY= 142.556 ZY= 48.8144
 XZ= 12.792 YZ= 48.0297 ZZ= 73.856
 Eigenvalues: -40.3428 49.6183 178.4516
 75 C Isotropic= 61.9209 Anisotropy 177.8716
 XX= 42.2704 YX= 41.2651 ZX= -11.6303
 XY= 43.9884 YY= 125.9138 ZY= 87.8714
 XZ= -11.3495 YZ= 83.0746 ZZ= 17.5785
 Eigenvalues: -41.3279 46.5887 180.5019
 76 C Isotropic= 64.016 Anisotropy 172.9131
 XX= 29.1481 YX= 10.5281 ZX= 52.919
 XY= 13.9636 YY= 142.629 ZY= 66.5312
 XZ= 55.4567 YZ= 65.6795 ZZ= 20.2709
 Eigenvalues: -39.9315 52.6881 179.2914
 77 C Isotropic= 63.0984 Anisotropy 181.6534
 XX= -19.3819 YX= 35.0404 ZX= 20.0236
 XY= 36.6114 YY= 149.0747 ZY= 54.599
 XZ= 11.1102 YZ= 59.1998 ZZ= 59.6024
 Eigenvalues: -26.9082 32.0027 184.2007
 78 H Isotropic= 23.4803 Anisotropy 7.8189
 XX= 26.0351 YX= -4.0421 ZX= 1.9018
 XY= -2.7764 YY= 21.9293 ZY= -1.5139
 XZ= 1.5081 YZ= -1.1109 ZZ= 22.4765
 Eigenvalues: 19.9554 21.7926 28.6929
 79 H Isotropic= 23.7504 Anisotropy 3.8233
 XX= 24.0763 YX= -1.4172 ZX= -0.1871
 XY= -1.4738 YY= 22.2955 ZY= -2.4352
 XZ= -0.4671 YZ= -2.0903 ZZ= 24.8794

Eigenvalues: 20.4283 24.5236 26.2992
80 H Isotropic= 23.7379 Anisotropy 3.9911
XX= 26.0387 YX= -1.3079 ZX= -0.7976
XY= -0.9436 YY= 21.6401 ZY= -1.3236
XZ= -0.837 YZ= -1.5562 ZZ= 23.5349
Eigenvalues: 20.5189 24.2962 26.3986
81 H Isotropic= 23.8977 Anisotropy 6.2661
XX= 25.8693 YX= -2.2325 ZX= 1.0338
XY= -1.9586 YY= 22.4051 ZY= -2.8839
XZ= 1.2717 YZ= -2.6499 ZZ= 23.4188
Eigenvalues: 19.9489 23.6692 28.0751
82 H Isotropic= 22.9554 Anisotropy 10.6812
XX= 25.1307 YX= -3.9943 ZX= 1.0029
XY= -3.497 YY= 21.781 ZY= -5.0062
XZ= 2.2073 YZ= -5.4445 ZZ= 21.9545
Eigenvalues: 16.3229 22.4672 30.0762

2bv

C -3.552866 1.438164 -1.376811
C -4.021469 0.322455 -2.363668
C -3.262 -1.011104 -2.263846
C -4.117157 -2.173228 -1.727257
C -4.683727 -1.965923 -0.308395
C -3.766244 -1.434696 0.782092
C -3.225783 -0.056899 0.530144
C -1.877119 0.12569 0.585299
C -1.309144 1.335486 -0.105422
C -2.032742 1.649155 -1.419626
C -4.054616 1.122521 0.064291
C -5.565833 0.943227 0.050416
C -3.788897 2.336192 0.975947
C -0.937044 -0.789539 1.264521
C -5.225018 -2.536123 -2.689833
O -4.085701 2.681381 -1.831667
O -3.960424 0.827582 -3.689045
O -5.802318 -2.405087 -0.029475
O -4.164633 -1.735196 2.112163
O 0.066748 1.230119 -0.527308
H -3.086208 1.215946 -3.817157
C -5.34398-1.357668 2.694877
O -6.225033 -0.811012 2.040245
C -5.373591 -1.741473 4.137968
H -5.125835 0.141653 -2.216391
H -2.352615 -0.904902 -1.620745
H -2.883239 -2.164702 0.694915
H -1.356071 2.212513 0.605929
H -1.825455 2.72349 -1.67756
H -1.583721 1.022775 -2.23505
H -5.89565-0.052225 -0.322511
H -5.982449 1.068538 1.080957
H -6.027191.734255 -0.591945
H -4.746171 2.774573 1.3504
H -3.179581 2.045852 1.864449
H -3.261292 3.143932 0.411989
H -1.448715 -1.634464 1.787344
H -0.19831-1.210140.534244

H	-0.382314	-0.219782	2.055728
H	-5.768954	-3.441372	-2.324424
H	-5.964167	-1.704271	-2.780595
H	-4.799828	-2.749028	-3.69982
H	-4.417084	-2.226092	4.44791
H	-5.541469	-0.821684	4.749476
H	-6.220943	-2.451798	4.300051
H	-4.955782	2.511464	-2.214406
C	1.062621	1.003661	0.381258
O	0.97121	1.502982	1.501232
H	-3.426235	-3.061457	-1.627436
H	-2.921046	-1.292795	-3.296042
C	2.222881	0.229318	-0.231911
C	3.547916	0.526247	0.528061
O	1.906214	-1.144753	-0.263529
H	2.303585	0.531248	-1.317487
N	4.650128	-0.208296	-0.053121
C	3.828097	2.010861	0.505967
H	3.405211	0.182368	1.600065
H	2.220956	-1.545249	0.561732
C	5.180157	-1.324651	0.568863
H	5.131566	0.209536	-0.812977
C	3.990851	2.689867	-0.706888
C	4.267418	4.055907	-0.712122
C	4.385663	4.74995	0.492419
C	4.224764	4.075697	1.702383
C	3.948851	2.708439	1.711958
H	3.893447	2.150371	-1.661132
O	4.602441	-1.834721	5.51116
C	6.426945	-1.896692	-0.009911
H	4.389056	4.586594	-1.667862
H	4.602022	5.828482	0.486941
H	4.311653	4.621658	2.653566
H	3.807466	2.182144	2.668763
C	6.498788	-3.279735	-0.210058
C	7.65788	-3.84255	-0.742608
C	8.744466	-3.030309	-1.067807
C	8.674525	-1.652419	-0.859512
C	7.516024	-1.081541	-0.333798
H	5.64179	-3.913940	0.066325
H	7.714559	-4.929644	-0.901876
H	9.659218	-3.47678	-1.485746
H	9.534722	-1.013489	-1.108416
H	7.472459	0.004418	-0.161158

2bv_45 E(RB+HF-PW91) = -2012.301371

SCF	GIAO	Magnetic	shielding	tensor	(ppm):
1	C	Isotropic=	111.3063	Anisotropy	30.3128
XX=	108.4614	YX=	-20.4064	ZX=	1.8953
XY=	-14.4329	YY=	118.2937	ZY=	-2.0169
XZ=	-4.8749	YZ=	-2.6166	ZZ=	107.1638
Eigenvalues:	94.7382	107.6659	131.5148		
2	C	Isotropic=	112.4765	Anisotropy	31.4587
XX=	93.8199	YX=	-0.4743	ZX=	-8.0014
XY=	0.4599	YY=	112.8885	ZY=	-12.1166

XZ=	-3.4117	YZ=	-0.4064	ZZ=	130.7209				
Eigenvalues:	92.9108	111.0697			133.4489				
3	C	Isotropic=	141.6504	Anisotropy	20.4				
XX=	122.9975	YX=	-7.2956	ZX=	0.5116				
XY=	-8.2982	YY=	149.5799	ZY=	3.793				
XZ=	-6.5402	YZ=	1.0181	ZZ=	152.3737				
Eigenvalues:	120.7138		148.987		155.2504				
4	C	Isotropic=	140.3986	Anisotropy	24.3733				
XX=	126.9776	YX=	-3.5828	ZX=	-5.2933				
XY=	-8.2541	YY=	138.6941	ZY=	3.7859				
XZ=	8.1606	YZ=	5.1957	ZZ=	155.524				
Eigenvalues:	124.2035		140.3448		156.6474				
5	C	Isotropic=	-23.3884	Anisotropy	181.7118				
XX=	-37.4628	YX=	-55.2396	ZX=	-5.7041				
XY=	-48.9775	YY=	65.1767	ZY=	-53.575				
XZ=	8.3999	YZ=	-44.264	ZZ=	-97.8792				
Eigenvalues:	-113.946	-53.9721	197.7528						
6	C	Isotropic=	101.9752	Anisotropy	41.7382				
XX=	87.9045	YX=	-1.9694	ZX=	5.4426				
XY=	3.7467	YY=	88.9286	ZY=	7.3769				
XZ=	-12.6043	YZ=	0.8807	ZZ=	129.0926				
Eigenvalues:	86.7427	89.3823	129.8007						
7	C	Isotropic=	46.6613	Anisotropy	152.5316				
XX=	42.5891	YX=	-7.8156	ZX=	-8.3674				
XY=	-8.674	YY=	-29.3643	ZY=	48.4696				
XZ=	6.6745	YZ=	75.0388	ZZ=	126.7592				
Eigenvalues:	-51.4377	43.0726	148.3491						
8	C	Isotropic=	39.4696	Anisotropy	157.5447				
XX=	34.0923	YX=	-1.6331	ZX=	-12.3761				
XY=	6.6336	YY=	-9.1378	ZY=	99.2317				
XZ=	-8.6465	YZ=	76.5824	ZZ=	93.4542				
Eigenvalues:	-60.2037	34.113	144.4994						
9	C	Isotropic=	111.0227	Anisotropy	55.9472				
XX=	143.0889	YX=	-5.362	ZX=	-16.438				
XY=	-12.0183	YY=	96.8802	ZY=	-17.3236				
XZ=	-16.0974	YZ=	-10.5078	ZZ=	93.0991				
Eigenvalues:	76.0889	108.6585	148.3208						
10	C	Isotropic=	147.2481	Anisotropy	44.4653				
XX=	175.3105	YX=	0.4723	ZX=	5.1265				
XY=	-5.2674	YY=	132.0972	ZY=	-14.4765				
XZ=	9.187	YZ=	-4.7217	ZZ=	134.3365				
Eigenvalues:	123.3746		141.4779		176.8916				
11	C	Isotropic=	147.3081	Anisotropy	11.2335				
XX=	140.4023	YX=	0.0916	ZX=	-3.432				
XY=	0.3859	YY=	147.9805	ZY=	0.8394				
XZ=	11.9248	YZ=	-0.698	ZZ=	153.5416				
Eigenvalues:	139.1445		147.9828		154.7972				
12	C	Isotropic=	154.6716	Anisotropy	22.5757				
XX=	159.5718	YX=	14.8553	ZX=	-0.4059				
XY=	7.2692	YY=	151.4226	ZY=	9.8839				
XZ=	-6.02	YZ=	16.9105	ZZ=	153.0203				
Eigenvalues:	134.4601		159.8326		169.722				
13	C	Isotropic=	147.7574	Anisotropy	55.9637				
XX=	140.301	YX=	0.892	ZX=	11.319				
XY=	-2.7549	YY=	154.434	ZY=	31.8811				
XZ=	19.1345	YZ=	30.7113	ZZ=	148.5371				

Eigenvalues:	114.3181	143.8875	185.0665		
14	C	Isotropic=	166.9616	Anisotropy	11.0043
XX=	168.8793	YX=	-3.7611	ZX=	9.365
XY=	-7.5569	YY=	167.1168	ZY=	0.4796
XZ=	-0.6474	YZ=	3.1468	ZZ=	164.8888
Eigenvalues:	159.0573	167.5296	174.2978		
15	C	Isotropic=	169.2488	Anisotropy	17.1949
XX=	169.9853	YX=	9.5105	ZX=	1.96
XY=	5.9465	YY=	160.8119	ZY=	3.2279
XZ=	4.2646	YZ=	5.0916	ZZ=	176.949
Eigenvalues:	156.1909	170.8434	180.712		
16	O	Isotropic=	263.5831	Anisotropy	83.5359
XX=	316.6789	YX=	-11.8541	ZX=	27.0822
XY=	-1.5762	YY=	271.2236	ZY=	6.8441
XZ=	5.7705	YZ=	39.1116	ZZ=	202.8467
Eigenvalues:	193.3109	278.1647	319.2736		
17	O	Isotropic=	265.1889	Anisotropy	44.9616
XX=	254.4801	YX=	-1.6426	ZX=	-20.5048
XY=	-1.1855	YY=	292.6935	ZY=	-16.5459
XZ=	2.0543	YZ=	-4.8943	ZZ=	248.3931
Eigenvalues:	239.9636	260.4398	295.1633		
18	O	Isotropic=	-354.521	Anisotropy	1077.8993
XX=	-787.9234	YX=	-477.3494	ZX=	184.8645
XY=	-417.6938	YY=	148.063	ZY=	-110.5071
XZ=	153.2156	YZ=	-116.8848	ZZ=	-423.7027
Eigenvalues:	-991.4809	-436.1606	364.0785		
19	O	Isotropic=	87.7996	Anisotropy	122.8905
XX=	135.4534	YX=	56.5607	ZX=	-138.4902
XY=	16.4799	YY=	124.175	ZY=	83.964
XZ=	0.6784	YZ=	35.9021	ZZ=	3.7705
Eigenvalues:	-52.9996	146.6719	169.7266		
20	O	Isotropic=	94.1701	Anisotropy	152.3773
XX=	84.0398	YX=	12.4497	ZX=	46.4284
XY=	102.3306	YY=	117.7046	ZY=	-90.2521
XZ=	170.8014	YZ=	-64.05	ZZ=	80.7658
Eigenvalues:	-73.7615	160.5168	195.7549		
21	H	Isotropic=	31.1471	Anisotropy	13.6657
XX=	34.1301	YX=	6.8453	ZX=	-3.1115
XY=	6.4411	YY=	25.6648	ZY=	-2.4759
XZ=	-2.8154	YZ=	-3.4704	ZZ=	33.6464
Eigenvalues:	21.8904	31.2933	40.2576		
22	C	Isotropic=	20.2131	Anisotropy	74.2731
XX=	6.3096	YX=	3.0383	ZX=	92.7692
XY=	11.3456	YY=	68.8517	ZY=	-14.92
XZ=	53.0945	YZ=	-1.3169	ZZ=	-14.522
Eigenvalues:	-78.5759	69.4867	69.7285		
23	O	Isotropic=	-130.3743	Anisotropy	599.0127
XX=	-306.8119	YX=	252.4474	ZX=	18.6246
XY=	209.7084	YY=	146.9534	ZY=	107.7425
XZ=	37.9208	YZ=	111.2575	ZZ=	-231.2643
Eigenvalues:	-405.4839	-254.6065	268.9675		
24	C	Isotropic=	166.2079	Anisotropy	36.9596
XX=	158.1822	YX=	-3.3988	ZX=	-2.7054
XY=	-3.7554	YY=	152.5185	ZY=	-10.3051
XZ=	-1.6791	YZ=	-10.7054	ZZ=	187.9229
Eigenvalues:	148.0313	159.7447	190.8476		

25	H	Isotropic=	27.4556	Anisotropy	2.9905
XX=	27.1409	YX=	1.6063	ZX=	-0.4431
XY=	2.006	YY=	26.8326	ZY=	-0.1434
XZ=	-1.6668	YZ=	0.1324	ZZ=	28.3934
Eigenvalues:	25.0175	27.9002	29.4493		
26	H	Isotropic=	27.9597	Anisotropy	8.3752
XX=	27.9354	YX=	1.6358	ZX=	3.8586
XY=	0.9963	YY=	26.9947	ZY=	3.389
XZ=	3.477	YZ=	2.2913	ZZ=	28.9491
Eigenvalues:	24.2595	26.0765	33.5432		
27	H	Isotropic=	25.3534	Anisotropy	3.5501
XX=	26.3467	YX=	1.4713	ZX=	-2.1576
XY=	-1.1484	YY=	23.6358	ZY=	-2.0708
XZ=	-0.6927	YZ=	0.7752	ZZ=	26.0776
Eigenvalues:	23.4583	24.8818	27.7201		
28	H	Isotropic=	24.7759	Anisotropy	7.9644
XX=	29.9486	YX=	-0.9517	ZX=	0.126
XY=	-0.7875	YY=	22.9735	ZY=	2.5944
XZ=	1.5681	YZ=	3.4924	ZZ=	21.4057
Eigenvalues:	18.9158	25.3264	30.0855		
29	H	Isotropic=	28.6697	Anisotropy	6.4648
XX=	30.0761	YX=	2.7149	ZX=	0.8836
XY=	1.5646	YY=	30.484	ZY=	-3.1309
XZ=	1.075	YZ=	-3.4561	ZZ=	25.449
Eigenvalues:	23.3093	29.7202	32.9796		
30	H	Isotropic=	29.0777	Anisotropy	5.0669
XX=	32.4159	YX=	0.2572	ZX=	0.1998
XY=	0.3979	YY=	25.2486	ZY=	2.3683
XZ=	0.1103	YZ=	1.4846	ZZ=	29.5685
Eigenvalues:	24.5064	30.271	32.4556		
31	H	Isotropic=	29.3208	Anisotropy	8.2466
XX=	29.1102	YX=	2.3438	ZX=	-0.2508
XY=	2.5945	YY=	33.5421	ZY=	0.7543
XZ=	-0.2718	YZ=	2.2848	ZZ=	25.31
Eigenvalues:	24.9044	28.2394	34.8185		
32	H	Isotropic=	29.2038	Anisotropy	9.1236
XX=	29.3194	YX=	0.8333	ZX=	-5.3829
XY=	0.0596	YY=	27.6842	ZY=	-1.8503
XZ=	-4.679	YZ=	-1.0318	ZZ=	30.6079
Eigenvalues:	24.7531	27.5722	35.2862		
33	H	Isotropic=	30.3619	Anisotropy	6.5757
XX=	33.8837	YX=	-2.0404	ZX=	-0.1243
XY=	-2.2106	YY=	28.9441	ZY=	-2.5867
XZ=	-0.2129	YZ=	-2.0497	ZZ=	28.2578
Eigenvalues:	25.9503	30.3896	34.7457		
34	H	Isotropic=	30.1526	Anisotropy	9.0935
XX=	30.891	YX=	-1.3599	ZX=	-1.763
XY=	-3.0812	YY=	31.2081	ZY=	4.8526
XZ=	-2.1297	YZ=	4.323	ZZ=	28.3588
Eigenvalues:	24.9671	29.2758	36.2149		
35	H	Isotropic=	30.2201	Anisotropy	6.1997
XX=	29.9508	YX=	-1.733	ZX=	1.3212
XY=	0.629	YY=	28.0146	ZY=	3.0749
XZ=	1.919	YZ=	2.4925	ZZ=	32.6949
Eigenvalues:	26.3105	29.9965	34.3533		
36	H	Isotropic=	28.5769	Anisotropy	6.1618

XX=	27.7006	YX=	0.6673	ZX=	-1.0456		
XY=	1.7338	YY=	31.5379	ZY=	1.3662		
XZ=	-0.3277	YZ=	3.5383	ZZ=	26.492		
Eigenvalues:	25.0358	28.0101	32.6847				
37	H	Isotropic=	28.9546	Anisotropy		7.2503	
XX=	31.6672	YX=	1.7951	ZX=	-0.2824		
XY=	2.9495	YY=	28.1015	ZY=	-4.0395		
XZ=	-0.1621	YZ=	-4.459	ZZ=	27.0951		
Eigenvalues:	23.0762	29.9994	33.7881				
38	H	Isotropic=	27.9435	Anisotropy		12.7829	
XX=	34.4581	YX=	-0.7176	ZX=	-4.1626		
XY=	-2.8057	YY=	25.6752	ZY=	0.5541		
XZ=	-5.1873	YZ=	-0.4191	ZZ=	23.6973		
Eigenvalues:	21.8653	25.4998	36.4655				
39	H	Isotropic=	28.642	Anisotropy		8.063	
XX=	30.3293	YX=	4.7156	ZX=	1.8045		
XY=	4.1342	YY=	26.3306	ZY=	-0.4658		
XZ=	3.0457	YZ=	0.1262	ZZ=	29.2663		
Eigenvalues:	23.1069	28.8018	34.0174				
40	H	Isotropic=	29.189	Anisotropy		10.802	
XX=	28.844	YX=	5.7274	ZX=	-1.1016		
XY=	6.13	YY=	31.7317	ZY=	0.4289		
XZ=	0.7842	YZ=	-0.0185	ZZ=	26.9912		
Eigenvalues:	24.1635	27.0132	36.3903				
41	H	Isotropic=	29.6497	Anisotropy		5.883	
XX=	32.0204	YX=	-0.9789	ZX=	2.8089		
XY=	-0.9865	YY=	30.3185	ZY=	0.0566		
XZ=	3.2777	YZ=	0.5693	ZZ=	26.6102		
Eigenvalues:	25.1506	30.2268	33.5717				
42	H	Isotropic=	30.5029	Anisotropy		9.5502	
XX=	28.088	YX=	1.1715	ZX=	-0.3969		
XY=	1.4625	YY=	28.5077	ZY=	4.2303		
XZ=	-0.3898	YZ=	3.8453	ZZ=	34.913		
Eigenvalues:	25.7631	28.8759	36.8697				
43	H	Isotropic=	29.0145	Anisotropy		5.4578	
XX=	30.6045	YX=	-1.8174	ZX=	-0.7854		
XY=	-2.6245	YY=	25.8687	ZY=	-2.2466		
XZ=	1.3267	YZ=	-3.1526	ZZ=	30.5704		
Eigenvalues:	24.0668	30.3237	32.6531				
44	H	Isotropic=	29.1929	Anisotropy		7.1506	
XX=	26.4774	YX=	-0.634	ZX=	-0.7516		
XY=	-0.8583	YY=	29.1325	ZY=	2.0811		
XZ=	-2.2459	YZ=	3.2898	ZZ=	31.9689		
Eigenvalues:	26.093	27.5258	33.96				
45	H	Isotropic=	28.932	Anisotropy		8.765	
XX=	29.9157	YX=	3.312	ZX=	-1.2457		
XY=	4.111	YY=	28.4984	ZY=	-2.5515		
XZ=	-3.1285	YZ=	-2.7379	ZZ=	28.382		
Eigenvalues:	25.1895	26.8313	34.7754				
46	H	Isotropic=	30.624	Anisotropy		18.0993	
XX=	38.2852	YX=	-2.8342	ZX=	8.3751		
XY=	-1.7793	YY=	26.9308	ZY=	-1.6637		
XZ=	6.6784	YZ=	-4.0438	ZZ=	26.6559		
Eigenvalues:	22.3633	26.8184	42.6902				
47	C	Isotropic=	7.785	Anisotropy		96.6037	
XX=	-58.5229	YX=	58.7237	ZX=	-17.0628		

XY= 40.9588 YY= 50.8284 ZY= 0.0909
 XZ= -53.6471 YZ= 9.6283 ZZ= 31.0496
 Eigenvalues: -87.9956 39.1631 72.1875
 48 O Isotropic= -143.5698 Anisotropy 696.9984
 XX= -202.6752 YX= 228.6572 ZX= -92.5685
 XY= 239.9356 YY= 139.3354 ZY= -187.8665
 XZ= -80.0849 YZ= -190.4666 ZZ= -367.3696
 Eigenvalues: -430.7026 -321.1026 321.0958
 49 H Isotropic= 28.6716 Anisotropy 6.4525
 XX= 28.4507 YX= -1.0699 ZX= 2.7082
 XY= -2.5705 YY= 32.1677 ZY= 0.6685
 XZ= 2.6135 YZ= 0.1487 ZZ= 25.3965
 Eigenvalues: 23.6605 29.3811 32.9733
 50 H Isotropic= 29.4978 Anisotropy 6.457
 XX= 27.6385 YX= 0.5248 ZX= -2.2954
 XY= 0.4308 YY= 29.0797 ZY= 3.1935
 XZ= -2.2092 YZ= 1.9069 ZZ= 31.775
 Eigenvalues: 25.8237 28.8671 33.8024
 51 C Isotropic= 108.7175 Anisotropy 22.4521
 XX= 114.2942 YX= 10.6921 ZX= 3.2251
 XY= 5.4584 YY= 116.6866 ZY= -4.0181
 XZ= 5.3706 YZ= -0.9475 ZZ= 95.1718
 Eigenvalues: 93.4322 109.0348 123.6856
 52 C Isotropic= 126.5918 Anisotropy 23.981
 XX= 126.8915 YX= 8.7532 ZX= 1.7739
 XY= 0.3197 YY= 134.2621 ZY= 9.8619
 XZ= 5.9183 YZ= 13.3084 ZZ= 118.6219
 Eigenvalues: 112.3442 124.8521 142.5792
 53 O Isotropic= 271.7425 Anisotropy 48.1892
 XX= 287.4884 YX= 12.9732 ZX= 35.3232
 XY= 2.5079 YY= 264.6317 ZY= -12.9108
 XZ= 14.4288 YZ= -31.2043 ZZ= 263.1074
 Eigenvalues: 231.6434 279.7154 303.8687
 54 H Isotropic= 26.6585 Anisotropy 4.1149
 XX= 27.4244 YX= 1.9559 ZX= 0.3007
 XY= 0.9871 YY= 26.0384 ZY= -3.1772
 XZ= 1.2155 YZ= -2.8066 ZZ= 26.5127
 Eigenvalues: 22.7288 27.8449 29.4018
 55 N Isotropic= 120.4434 Anisotropy 124.3993
 XX= 94.7867 YX= -14.3996 ZX= 43.8234
 XY= -46.359 YY= 194.2073 ZY= 10.2339
 XZ= 63.2216 YZ= 2.9654 ZZ= 72.3362
 Eigenvalues: 25.3154 132.6385 203.3763
 56 C Isotropic= 52.1167 Anisotropy 190.5703
 XX= 170.4281 YX= -44.3825 ZX= -4.5251
 XY= -40.5224 YY= -27.5025 ZY= 2.7152
 XZ= 1.901 YZ= -0.0701 ZZ= 13.4246
 Eigenvalues: -36.2449 13.4315 179.1636
 57 H Isotropic= 25.035 Anisotropy 2.5027
 XX= 23.5743 YX= -0.4355 ZX= -0.1018
 XY= -1.4715 YY= 24.9637 ZY= 0.3959
 XZ= -0.2152 YZ= 0.3703 ZZ= 26.5671
 Eigenvalues: 23.0889 25.3126 26.7035
 58 H Isotropic= 29.4437 Anisotropy 14.2045
 XX= 28.0669 YX= -1.4421 ZX= 4.7639
 XY= -0.9501 YY= 30.4554 ZY= -6.6189

XZ= 5.7369 YZ= -7.0073 ZZ= 29.8089
 Eigenvalues: 21.5966 27.8212 38.9134
 59 C Isotropic= 15.9722 Anisotropy 120.5881
 XX= -0.2503 YX= 69.2869 ZX= 20.1255
 XY= 72.6532 YY= 7.5007 ZY= 22.4676
 XZ= 17.7815 YZ= 37.0776 ZZ= 40.6662
 Eigenvalues: -67.8999 19.4522 96.3643
 60 H Isotropic= 26.4595 Anisotropy 8.7696
 XX= 28.5636 YX= -6.0657 ZX= -4.5985
 XY= -2.1407 YY= 27.7859 ZY= -1.8318
 XZ= -0.5879 YZ= -4.6479 ZZ= 23.0289
 Eigenvalues: 19.3649 27.7076 32.3059
 61 C Isotropic= 67.3854 Anisotropy 166.5815
 XX= 173.9152 YX= -24.2411 ZX= -6.6226
 XY= -25.904 YY= 39.323 ZY= -36.5698
 XZ= -5.1336 YZ= -39.9425 ZZ= -11.082
 Eigenvalues: -33.1255 56.842 178.4397
 62 C Isotropic= 62.6256 Anisotropy 176.8837
 XX= 174.6937 YX= -29.3987 ZX= 9.471
 XY= -28.9494 YY= 34.2506 ZY= 35.0188
 XZ= 10.3648 YZ= 37.8316 ZZ= -21.0675
 Eigenvalues: -41.4075 48.7362 180.548
 63 C Isotropic= 63.7467 Anisotropy 176.6017
 XX= 173.197 YX= -41.2983 ZX= 3.0807
 XY= -41.9852 YY= -29.4538 ZY= -0.9894
 XZ= 2.6307 YZ= 0.3887 ZZ= 47.4969
 Eigenvalues: -37.6777 47.4366 181.4811
 64 C Isotropic= 61.0427 Anisotropy 177.5779
 XX= 173.9777 YX= -27.9513 ZX= -0.7457
 XY= -28.291 YY= 30.6929 ZY= -36.6502
 XZ= -3.2881 YZ= -38.1621 ZZ= -21.5426
 Eigenvalues: -42.0892 45.7893 179.4279
 65 C Isotropic= 56.7579 Anisotropy 160.5521
 XX= 158.7965 YX= -25.4814 ZX= 11.961
 XY= -25.0405 YY= 32.3773 ZY= 33.2081
 XZ= 11.0041 YZ= 34.5515 ZZ= -20.9001
 Eigenvalues: -39.7014 46.1825 163.7926
 66 H Isotropic= 24.0399 Anisotropy 8.6896
 XX= 22.1388 YX= 1.421 ZX= -1.146
 XY= 2.1582 YY= 26.9282 ZY= -4.0953
 XZ= -0.7052 YZ= -3.6217 ZZ= 23.0528
 Eigenvalues: 20.6502 21.6366 29.833
 67 O Isotropic= -73.2148 Anisotropy 618.3385
 XX= -47.0852 YX= 129.7729 ZX= 204.7026
 XY= 123.2029 YY= -50.1604 ZY= 286.2028
 XZ= 228.5417 YZ= 259.4232 ZZ= -122.3989
 Eigenvalues: -387.5888 -171.0666 339.0108
 68 C Isotropic= 56.8812 Anisotropy 171.5463
 XX= 4.2486 YX= -0.6946 ZX= 65.0157
 XY= 12.6806 YY= 26.9018 ZY= -25.8508
 XZ= 58.5773 YZ= -50.1536 ZZ= 139.4932
 Eigenvalues: -27.4368 26.8351 171.2454
 69 H Isotropic= 23.7772 Anisotropy 4.8305
 XX= 21.1077 YX= 1.6298 ZX= -0.2086
 XY= 1.6433 YY= 26.5014 ZY= 0.455
 XZ= -0.017 YZ= 0.3442 ZZ= 23.7225

Eigenvalues:	20.6347	23.6993	26.9976		
70	H	Isotropic=	23.7483	Anisotropy	2.9792
XX=	20.9939	YX=	1.2147	ZX=	-0.1138
XY=	1.1587	YY=	24.551	ZY=	0.2338
XZ=	-0.0844	YZ=	0.1551	ZZ=	25.6999
Eigenvalues:	20.6298	24.8805	25.7344		
71	H	Isotropic=	23.7273	Anisotropy	4.4688
XX=	21.0014	YX=	1.6722	ZX=	0.1115
XY=	1.5797	YY=	26.1898	ZY=	-0.2847
XZ=	-0.1338	YZ=	-0.47	ZZ=	23.9907
Eigenvalues:	20.5314	23.944	26.7065		
72	H	Isotropic=	23.4785	Anisotropy	8.0721
XX=	21.0538	YX=	1.7784	ZX=	0.8557
XY=	1.7896	YY=	25.9682	ZY=	3.8235
XZ=	0.4177	YZ=	3.2067	ZZ=	23.4137
Eigenvalues:	20.2729	21.3028	28.86		
73	C	Isotropic=	60.2978	Anisotropy	176.6572
XX=	17.3265	YX=	-45.3731	ZX=	58.6752
XY=	-43.792	YY=	11.6586	ZY=	-3.3012
XZ=	63.8931	YZ=	-4.2108	ZZ=	151.9084
Eigenvalues:	-39.2975	42.1217	178.0693		
74	C	Isotropic=	61.7957	Anisotropy	176.8354
XX=	64.5327	YX=	-4.7396	ZX=	45.4447
XY=	-2.1885	YY=	-36.9278	ZY=	-26.8997
XZ=	46.4832	YZ=	-25.8376	ZZ=	157.7822
Eigenvalues:	-40.5086	46.2097	179.6859		
75	C	Isotropic=	61.3299	Anisotropy	179.356
XX=	2.5944	YX=	23.2621	ZX=	73.3479
XY=	23.0449	YY=	32.6744	ZY=	-28.5101
XZ=	72.5306	YZ=	-27.3218	ZZ=	148.7208
Eigenvalues:	-41.6613	44.7503	180.9005		
76	C	Isotropic=	63.2122	Anisotropy	175.2297
XX=	12.5711	YX=	-43.5137	ZX=	59.6729
XY=	-47.5319	YY=	20.241	ZY=	-2.6682
XZ=	59.1231	YZ=	-0.5537	ZZ=	156.8246
Eigenvalues:	-39.4137	49.0183	180.032		
77	C	Isotropic=	66.609	Anisotropy	165.1658
XX=	67.7552	YX=	-1.9331	ZX=	41.5525
XY=	-8.2459	YY=	-25.4465	ZY=	-25.2439
XZ=	39.8299	YZ=	-27.8351	ZZ=	157.5185
Eigenvalues:	-29.2237	52.3312	176.7196		
78	H	Isotropic=	23.2795	Anisotropy	7.9266
XX=	23.3599	YX=	-2.7873	ZX=	-1.7475
XY=	-2.9772	YY=	26.1638	ZY=	1.3101
XZ=	-2.1822	YZ=	1.4259	ZZ=	20.3147
Eigenvalues:	19.3512	21.9233	28.5639		
79	H	Isotropic=	23.7099	Anisotropy	4.5674
XX=	25.8607	YX=	-0.5295	ZX=	-2.222
XY=	-0.2157	YY=	24.2146	ZY=	0.3024
XZ=	-2.0485	YZ=	0.313	ZZ=	21.0543
Eigenvalues:	20.2367	24.1381	26.7548		
80	H	Isotropic=	23.6829	Anisotropy	3.7379
XX=	24.2285	YX=	0.5823	ZX=	-1.3499
XY=	0.6672	YY=	25.9735	ZY=	0.2651
XZ=	-1.2983	YZ=	0.4662	ZZ=	20.8467
Eigenvalues:	20.3359	24.538	26.1748		

81	H	Isotropic=	23.8987	Anisotropy	5.3537
XX=	25.4742	YX=	-1.4831	ZX=	-1.9986
XY=	-1.3368	YY=	25.3274	ZY=	0.9676
XZ=	-1.6854	YZ=	1.1466	ZZ=	20.8944
Eigenvalues:	20.1856	24.0426	27.4678		
82	H	Isotropic=	24.108	Anisotropy	8.9022
XX=	29.2431	YX=	-1.5956	ZX=	-2.7809
XY=	-0.8667	YY=	22.9372	ZY=	0.1708
XZ=	-1.9489	YZ=	0.3305	ZZ=	20.1438
Eigenvalues:	19.5652	22.7161	30.0428		

2b-vi

C	3.364179	-2.056717	-0.337472
C	4.00883	-1.506956	-1.64914
C	3.274691	-0.323716	-2.301918
C	4.061473	0.998468	-2.251371
C	4.391861	1.507745	-0.834111
C	3.301466	1.4983	0.226118
C	2.775327	0.13536	0.57177
C	1.429821	-0.069743	0.509
C	0.947283	-1.488777	0.38216
C	1.864782	-2.3431	-0.501444
C	3.639403	-1.079030	0.843201
C	5.137287	-0.845814	0.976476
C	3.20302	-1.739415	2.165613
C	0.423843	1.009988	0.582871
C	5.315621	0.928507	-3.092809
O	3.931072	-3.338675	-0.072079
O	4.147263	-2.572958	-2.576134
O	5.462247	2.085072	-0.628936
O	3.491343	2.405879	1.301901
O	-0.336744	-1.669818	-0.252066
H	3.302895	-3.038288	-2.621311
C	4.555974	2.407301	2.163171
O	5.516493	1.66847	1.977057
C	4.364599	3.415836	3.247605
H	5.079675	-1.218059	-1.439057
H	2.273989	-0.166295	-1.827574
H	2.459731	2.05328	-0.325113
H	0.852968	-1.929504	1.418668
H	1.675106	-3.422133	-0.248559
H	1.566899	-2.200705	-1.573652
H	5.546786	-0.125029	0.233772
H	5.38057	-0.451091	1.994522
H	5.675794	-1.819459	0.861412
H	4.080314	-1.913435	2.835626
H	2.47815	-1.094693	2.716767
H	2.739852	-2.738066	1.9733
H	0.878247	2.023824	0.705371
H	-0.230933	1.018649	-0.324699
H	-0.219961	0.840322	1.486669
H	5.81686	1.927083	-3.116957
H	6.039621	0.190636	-2.670967
H	5.060243	0.623303	-4.135808
H	3.413158	3.982983	3.110071
H	4.342463	2.884133	4.230091

H	5.228107	4.125033	3.2315
H	4.857491	-3.318287	-0.344105
C	-1.472051	-1.105685	0.266107
O	-1.558758	-0.939543	1.478742
H	3.385339	1.792622	-2.685379
H	3.107856	-0.57514	-3.383555
C	-2.468239	-0.790648	-0.842604
C	-3.901163	-0.555228	-0.264533
O	-2.033819	0.358708	-1.534181
H	-2.491138	-1.680093	-1.538344
N	-4.868386	-0.255071	-1.283922
C	-4.315722	-1.787677	0.509774
H	-3.823161	0.332193	0.435556
H	-1.309519	0.079913	-2.111503
C	-5.429603	0.97323	-1.584473
H	-5.21597	-1.033137	-1.802357
C	-4.402055	-3.035355	-0.117674
C	-4.805051	-4.156039	0.606593
C	-5.127449	-4.036091	1.958653
C	-5.045723	-2.793139	2.585477
C	-4.643153	-1.669291	1.864107
H	-4.1567	-3.138501	-1.185375
O	-6.391527	0.968422	-2.382832
C	-5.074072	2.21428	-0.842128
H	-4.869607	-5.135191	0.109632
H	-5.445421	-4.921304	2.529024
H	-5.297528	-2.695944	3.651949
H	-4.56765	-0.692216	2.365512
C	-6.140777	2.925653	-0.269979
C	-5.900835	4.118292	0.407364
C	-4.601805	4.620398	0.500611
C	-3.546663	9.29791	-0.092322
C	-3.780438	2.730151	-0.767344
H	-7.166335	2.536067	-0.370851
H	-6.738513	4.668178	0.861054
H	-4.413448	5.563676	1.034331
H	-2.524148	4.330796	-0.034853
H	-2.941949	2.209645	-1.253209

2	bviliz	E(RB+HF-PW91)	=	-2012.286132
SCF	GIAO	Magnetic shielding	tensor (ppm):	
1	C	Isotropic=	111.4746	Anisotropy 30.7261
XX=	107.0436	YX=	-19.065	ZX= 8.1003
XY=	-10.1773	YY=	116.2985	ZY= -4.5197
XZ=	11.4369	YZ=	-5.9871	ZZ= 111.0818
Eigenvalues:	94.6271	107.838	131.9587	
2	C	Isotropic=	112.2273	Anisotropy 31.1186
XX=	92.7633	YX=	0.4691	ZX= 1.5156
XY=	-2.7928	YY=	121.6611	ZY= 16.3629
XZ=	-1.6501	YZ=	5.6198	ZZ= 122.2576
Eigenvalues:	92.7112	110.9977	132.9731	
3	C	Isotropic=	141.1599	Anisotropy 19.9706
XX=	122.2281	YX=	-8.0652	ZX= -2.2368
XY=	-4.9183	YY=	147.2107	ZY= -2.8764
XZ=	4.8903	YZ=	0.4086	ZZ= 154.0408

Eigenvalues:	120.6122	148.3938	154.4737	
4	C	Isotropic=	140.6391	Anisotropy 24.0754
XX=	128.1677	YX=	-2.1984	ZX= 1.9161
XY=	-12.7407	YY=	138.3479	ZY= 3.4702
XZ=	-7.6936	YZ=	3.093	ZZ= 155.4016
Eigenvalues:	124.1844	141.0435	156.6894	
5	C	Isotropic=	-22.6564	Anisotropy 180.8679
XX=	-39.6969	YX=	-43.924	ZX= 42.3456
XY=	-46.4515	YY=	65.2552	ZY= -40.6284
XZ=	27.3162	YZ=	-50.6252	ZZ= -93.5275
Eigenvalues:	-113.8213	-52.0701	97.9222	
6	C	Isotropic=	101.8384	Anisotropy 41.3794
XX=	88.1705	YX=	-7.4505	ZX= -9.9213
XY=	7.1077	YY=	94.189	ZY= 11.9688
XZ=	2.9167	YZ=	17.0134	ZZ= 123.1556
Eigenvalues:	86.8585	89.232	129.4247	
7	C	Isotropic=	45.1382	Anisotropy 154.2621
XX=	41.9185	YX=	-1.5836	ZX= -5.8253
XY=	-13.4863	YY=	-48.8991	ZY= 42.082
XZ=	-17.3253	YZ=	14.5277	ZZ= 142.3953
Eigenvalues:	-53.3551	40.7902	147.9796	
8	C	Isotropic=	40.1991	Anisotropy 155.9602
XX=	34.9765	YX=	8.152	ZX= -2.5306
XY=	17.9225	YY=	-57.6442	ZY= -19.5925
XZ=	-11.5305	YZ=	2.1817	ZZ= 143.2649
Eigenvalues:	-59.7345	36.1592	144.1725	
9	C	Isotropic=	111.49	Anisotropy 55.6078
XX=	136.043	YX=	3.4896	ZX= 24.8761
XY=	-3.6302	YY=	108.6737	ZY= 10.075
XZ=	28.8827	YZ=	3.448	ZZ= 89.7534
Eigenvalues:	76.2474	109.6608	148.5618	
10	C	Isotropic=	146.78	Anisotropy 44.5683
XX=	175.8191	YX=	-0.4728	ZX= 2.2462
XY=	-9.099	YY=	139.3905	ZY= 9.8094
XZ=	2.5328	YZ=	1.2088	ZZ= 125.1305
Eigenvalues:	122.9718	140.8761	176.4922	
11	C	Isotropic=	147.4126	Anisotropy 11.5625
XX=	141.8462	YX=	0.4395	ZX= 1.5266
XY=	-5.967	YY=	148.5946	ZY= 0.8633
XZ=	-12.0737	YZ=	2.3493	ZZ= 151.797
Eigenvalues:	139.1688	147.948	155.1209	
12	C	Isotropic=	155.0553	Anisotropy 22.5458
XX=	159.1469	YX=	15.2405	ZX= -7.0917
XY=	10.8847	YY=	142.9754	ZY= -2.289
XZ=	1.4803	YZ=	-8.0731	ZZ= 163.0436
Eigenvalues:	135.3274	159.7527	170.0859	
13	C	Isotropic=	148.4158	Anisotropy 55.2642
XX=	145.7696	YX=	-0.8084	ZX= -13.9625
XY=	-7.5899	YY=	127.6075	ZY= -22.1327
XZ=	-18.85	YZ=	-20.1356	ZZ= 171.8703
Eigenvalues:	115.4873	144.5015	185.2586	
14	C	Isotropic=	165.9157	Anisotropy 10.4099
XX=	168.8986	YX=	-6.749	ZX= -6.8147
XY=	-5.7581	YY=	162.7074	ZY= -1.3664
XZ=	5.0312	YZ=	-4.0822	ZZ= 166.1411
Eigenvalues:	157.8826	167.0089	172.8556	

15	C	Isotropic=	169.3606	Anisotropy	17.0152
XX=	171.5015	YX=	7.2607	ZX=	-7.2274
XY=	3.1115	YY=	161.6882	ZY=	5.5426
XZ=	-7.3595	YZ=	4.1041	ZZ=	174.892
Eigenvalues:	156.3491		171.0286		180.704
16	O	Isotropic=	263.5508	Anisotropy	84.5745
XX=	319.4143	YX=	-10.2037	ZX=	-4.3398
XY=	4.6951	YY=	235.861	ZY=	-25.2258
XZ=	11.9511	YZ=	-59.9024	ZZ=	235.3769
Eigenvalues:	193.0497		277.6689		319.9337
17	O	Isotropic=	265.2424	Anisotropy	45.8655
XX=	250.3368	YX=	8.866	ZX=	18.9752
XY=	-1.3102	YY=	292.0677	ZY=	-7.1483
XZ=	-1.5607	YZ=	-17.9934	ZZ=	253.3225
Eigenvalues:	240.5289		259.3788		295.8194
18	O	Isotropic=	-357.9595	Anisotropy	1082.1927
XX=	-752.9185	YX=	-525.7199	ZX=	15.0618
XY=	-456.2439	YY=	62.3196	ZY=	-243.9006
XZ=	13.5154	YZ=	-248.1236	ZZ=	-383.2796
Eigenvalues:	-998.0524		-439.3284		363.5023
19	O	Isotropic=	88.5962	Anisotropy	124.3874
XX=	114.6809	YX=	126.2053	ZX=	108.5606
XY=	32.7486	YY=	57.8925	ZY=	-95.5444
XZ=	0.9931	YZ=	-41.6656	ZZ=	93.2151
Eigenvalues:	-51.2968		145.5642		171.5211
20	O	Isotropic=	98.7061	Anisotropy	155.9599
XX=	129.3373	YX=	-15.0425	ZX=	-32.174
XY=	-14.1488	YY=	173.0238	ZY=	31.5801
XZ=	-184.7203	YZ=	-2.6549	ZZ=	-6.2428
Eigenvalues:	-66.475		159.914		202.6794
21	H	Isotropic=	31.1469	Anisotropy	13.6422
XX=	33.1069	YX=	6.8951	ZX=	-0.3305
XY=	6.5047	YY=	31.1098	ZY=	5.502
XZ=	-0.431	YZ=	6.391	ZZ=	29.2239
Eigenvalues:	21.8954		31.3036		40.2417
22	C	Isotropic=	20.1929	Anisotropy	74.8301
XX=	28.3734	YX=	-37.0111	ZX=	-77.9141
XY=	-13.2492	YY=	54.7605	ZY=	-28.9215
XZ=	-45.7341	YZ=	-44.7464	ZZ=	-22.5553
Eigenvalues:	-78.8355		69.3345		70.0796
23	O	Isotropic=	-131.3218	Anisotropy	599.8652
XX=	-287.8574	YX=	232.1775	ZX=	-154.4659
XY=	180.3193	YY=	-3.0129	ZY=	-197.7556
XZ=	-151.2996	YZ=	-196.2117	ZZ=	-103.0952
Eigenvalues:	-406.4411		-256.1126		268.5883
24	C	Isotropic=	166.2523	Anisotropy	36.9951
XX=	158.1249	YX=	-5.3304	ZX=	0.879
XY=	-5.4039	YY=	169.2658	ZY=	19.5805
XZ=	0.4385	YZ=	20.9238	ZZ=	171.3664
Eigenvalues:	148.1049		159.7364		190.9157
25	H	Isotropic=	27.3991	Anisotropy	3.0618
XX=	26.9153	YX=	1.4582	ZX=	-0.5422
XY=	2.3714	YY=	27.3633	ZY=	1.3237
XZ=	0.4278	YZ=	0.7125	ZZ=	27.9188
Eigenvalues:	25.0242		27.7328		29.4403
26	H	Isotropic=	28.1021	Anisotropy	8.2098

XX=	29.3243	YX=	-0.2546	ZX=	-4.3137		
XY=	-0.3472	YY=	25.1897	ZY=	-1.398		
XZ=	-3.6594	YZ=	-0.386	ZZ=	29.7923		
Eigenvalues:	24.5122	26.2188	33.5753				
27	H	Isotropic=	25.402	Anisotropy		3.5905	
XX=	25.9698	YX=	2.2111	ZX=	1.1735		
XY=	-1.178	YY=	24.8523	ZY=	2.9438		
XZ=	1.3899	YZ=	0.4443	ZZ=	25.3839		
Eigenvalues:	23.3138	25.0965	27.7957				
28	H	Isotropic=	24.8298	Anisotropy		7.6562	
XX=	29.7636	YX=	-0.212	ZX=	1.1521		
XY=	-0.9438	YY=	20.3526	ZY=	-1.9967		
XZ=	0.1734	YZ=	-3.0411	ZZ=	24.3732		
Eigenvalues:	19.135	25.4205	29.9339				
29	H	Isotropic=	28.5993	Anisotropy		6.4745	
XX=	30.088	YX=	1.7313	ZX=	-1.1273		
XY=	0.7153	YY=	32.3566	ZY=	-0.3325		
XZ=	-0.5774	YZ=	0.0178	ZZ=	23.3532		
Eigenvalues:	23.247	29.6352	32.9156				
30	H	Isotropic=	29.2304	Anisotropy		5.0061	
XX=	32.5451	YX=	0.2194	ZX=	-0.1015		
XY=	0.5917	YY=	24.9854	ZY=	0.5568		
XZ=	0.1019	YZ=	1.1991	ZZ=	30.1606		
Eigenvalues:	24.8198	30.3035	32.5678				
31	H	Isotropic=	29.3003	Anisotropy		8.1391	
XX=	29.0946	YX=	2.758	ZX=	-0.5711		
XY=	2.8333	YY=	30.7012	ZY=	-3.0452		
XZ=	-0.5696	YZ=	-4.7097	ZZ=	28.105		
Eigenvalues:	24.9107	28.2637	34.7264				
32	H	Isotropic=	29.1736	Anisotropy		9.1782	
XX=	27.7896	YX=	2.8202	ZX=	4.0936		
XY=	1.6869	YY=	29.8059	ZY=	3.0073		
XZ=	3.9786	YZ=	2.4092	ZZ=	29.9254		
Eigenvalues:	24.6776	27.5508	35.2924				
33	H	Isotropic=	30.3406	Anisotropy		6.7418	
XX=	33.5658	YX=	-1.8167	ZX=	2.0767		
XY=	-1.9776	YY=	30.4718	ZY=	1.1296		
XZ=	2.3486	YZ=	0.5443	ZZ=	26.9842		
Eigenvalues:	25.8827	30.3041	34.8351				
34	H	Isotropic=	30.1681	Anisotropy		9.2473	
XX=	30.0912	YX=	0.1684	ZX=	2.0093		
XY=	-1.1015	YY=	26.8079	ZY=	-4.079		
XZ=	3.2697	YZ=	-3.3481	ZZ=	33.6051		
Eigenvalues:	25.0792	29.0921	36.3329				
35	H	Isotropic=	30.2658	Anisotropy		6.1146	
XX=	30.4263	YX=	-2.1874	ZX=	-0.8867		
XY=	-0.4312	YY=	26.765	ZY=	0.0734		
XZ=	-2.3608	YZ=	0.1799	ZZ=	33.6061		
Eigenvalues:	26.324	30.1312	34.3422				
36	H	Isotropic=	28.6035	Anisotropy		6.1887	
XX=	27.5239	YX=	1.6375	ZX=	0.3832		
XY=	1.8876	YY=	28.6407	ZY=	-2.0608		
XZ=	-0.4068	YZ=	-4.4937	ZZ=	29.6458		
Eigenvalues:	25.055	28.0262	32.7293				
37	H	Isotropic=	28.8431	Anisotropy		6.9481	
XX=	31.7818	YX=	1.2189	ZX=	0.4534		

XY=	1.8497	YY=	31.3392	ZY=	2.3877				
XZ=	0.2561	YZ=	2.429	ZZ=	23.4083				
Eigenvalues:	22.7336	30.3204	33.4751						
38	H	Isotropic=	28.3907	Anisotropy	12.7764				
XX=	32.8845	YX=	1.4741	ZX=	5.5684				
XY=	-0.3171	YY=	26.4864	ZY=	-0.0623				
XZ=	7.7019	YZ=	0.773	ZZ=	25.8014				
Eigenvalues:	21.8218	26.4421	36.9083						
39	H	Isotropic=	28.519	Anisotropy	7.2527				
XX=	30.9209	YX=	2.8638	ZX=	-3.4364				
XY=	1.3593	YY=	27.0887	ZY=	2.0316				
XZ=	-3.6818	YZ=	0.8807	ZZ=	27.5473				
Eigenvalues:	23.6333	28.5695	33.3541						
40	H	Isotropic=	29.1386	Anisotropy	10.8354				
XX=	29.0003	YX=	5.663	ZX=	-1.4968				
XY=	5.2987	YY=	31.0745	ZY=	-1.5316				
XZ=	-3.3464	YZ=	-1.165	ZZ=	27.3411				
Eigenvalues:	24.0827	26.9709	36.3622						
41	H	Isotropic=	29.6099	Anisotropy	5.9712				
XX=	32.7867	YX=	-1.7442	ZX=	-1.2017				
XY=	-1.9778	YY=	28.999	ZY=	-1.7779				
XZ=	-1.542	YZ=	-2.3867	ZZ=	27.044				
Eigenvalues:	25.1054	30.1336	33.5907						
42	H	Isotropic=	30.4541	Anisotropy	9.5796				
XX=	28.1808	YX=	1.1966	ZX=	-1.5755				
XY=	1.5317	YY=	26.6732	ZY=	0.4899				
XZ=	-1.7323	YZ=	0.8392	ZZ=	36.5081				
Eigenvalues:	25.6779	28.8439	36.8404						
43	H	Isotropic=	29.0195	Anisotropy	5.6123				
XX=	30.3691	YX=	-1.8778	ZX=	2.078				
XY=	-3.5053	YY=	29.2136	ZY=	2.5186				
XZ=	0.6983	YZ=	3.6541	ZZ=	27.4758				
Eigenvalues:	23.9364	30.361	32.761						
44	H	Isotropic=	29.1822	Anisotropy	7.0332				
XX=	26.1788	YX=	0.068	ZX=	-0.4528				
XY=	0.216	YY=	27.5177	ZY=	0.2526				
XZ=	0.9714	YZ=	-0.8184	ZZ=	33.8501				
Eigenvalues:	26.1531	27.5225	33.871						
45	H	Isotropic=	28.9226	Anisotropy	8.8624				
XX=	29.7339	YX=	3.083	ZX=	0.1167				
XY=	4.7594	YY=	30.7418	ZY=	2.3684				
XZ=	1.5848	YZ=	2.324	ZZ=	26.2922				
Eigenvalues:	25.0371	26.8999	34.8309						
46	H	Isotropic=	30.5806	Anisotropy	18.1863				
XX=	40.2401	YX=	-6.2523	ZX=	-3.5813				
XY=	-4.1867	YY=	28.6127	ZY=	-0.6013				
XZ=	-2.5832	YZ=	1.4759	ZZ=	22.8891				
Eigenvalues:	22.3148	26.7223	42.7048						
47	C	Isotropic=	10.419	Anisotropy	91.2537				
XX=	-63.5404	YX=	53.2564	ZX=	-30.5069				
XY=	54.1501	YY=	48.9556	ZY=	4.1928				
XZ=	12.0964	YZ=	-6.3221	ZZ=	45.8418				
Eigenvalues:	-85.5662	45.5685	71.2548						
48	O	Isotropic=	-146.3953	Anisotropy	692.773				
XX=	-224.3458	YX=	233.7135	ZX=	-8.6736				
XY=	234.1684	YY=	199.4544	ZY=	-99.8848				

XZ= -20.2036 YZ= -94.0728 ZZ= -414.2946
 Eigenvalues: -432.9321 -321.7072 315.4534
 49 H Isotropic= 28.7062 Anisotropy 6.3308
 XX= 29.1631 YX= -1.8914 ZX= -1.4233
 XY= -2.9686 YY= 30.0789 ZY= -3.7741
 XZ= -0.7188 YZ= -3.0303 ZZ= 26.8766
 Eigenvalues: 23.7697 29.4222 32.9268
 50 H Isotropic= 29.4532 Anisotropy 6.302
 XX= 27.0326 YX= 1.4596 ZX= 0.7581
 XY= 1.524 YY= 27.7656 ZY= -0.5038
 XZ= 0.6719 YZ= 0.7789 ZZ= 33.5613
 Eigenvalues: 25.833 28.872 33.6545
 51 C Isotropic= 110.6922 Anisotropy 23.586
 XX= 119.9526 YX= 7.2307 ZX= -9.7721
 XY= 3.4644 YY= 113.0011 ZY= -5.3044
 XZ= -4.1956 YZ= -9.7891 ZZ= 99.1231
 Eigenvalues: 94.9972 110.6632 126.4162
 52 C Isotropic= 126.585 Anisotropy 17.1993
 XX= 124.6451 YX= 1.9059 ZX= -0.9823
 XY= -1.9957 YY= 121.1443 ZY= -6.5871
 XZ= 1.3824 YZ= -10.0278 ZZ= 133.9655
 Eigenvalues: 117.0613 124.6425 138.0512
 53 O Isotropic= 271.4821 Anisotropy 75.8758
 XX= 317.9949 YX= 6.7346 ZX= -39.9179
 XY= -17.2167 YY= 259.6912 ZY= 1.6507
 XZ= 5.6461 YZ= 8.3773 ZZ= 236.7602
 Eigenvalues: 232.7276 259.6527 322.066
 54 H Isotropic= 26.7012 Anisotropy 6.2658
 XX= 27.4431 YX= 2.2095 ZX= -1.7016
 XY= 1.5418 YY= 29.782 ZY= 2.1553
 XZ= -1.365 YZ= 0.9735 ZZ= 22.8785
 Eigenvalues: 21.8636 27.3616 30.8784
 55 N Isotropic= 126.6399 Anisotropy 127.7068
 XX= 90.3855 YX= -43.7615 ZX= -44.6096
 XY= -13.9538 YY= 201.6427 ZY= -15.8525
 XZ= -39.8081 YZ= -42.0386 ZZ= 87.8914
 Eigenvalues: 36.7795 131.3624 211.7777
 56 C Isotropic= 51.607 Anisotropy 189.2075
 XX= 157.2517 YX= -38.5224 ZX= 50.1212
 XY= -39.8933 YY= -14.4614 ZY= 12.541
 XZ= 45.9927 YZ= 13.685 ZZ= 12.0306
 Eigenvalues: -36.5936 13.6692 177.7453
 57 H Isotropic= 25.9 Anisotropy 5.3555
 XX= 23.6337 YX= -1.032 ZX= -1.2429
 XY= -1.9512 YY= 29.076 ZY= 1.3477
 XZ= 0.5126 YZ= -2.0201 ZZ= 24.9905
 Eigenvalues: 23.1475 25.0822 29.4704
 58 H Isotropic= 29.7104 Anisotropy 17.1184
 XX= 34.5538 YX= -3.3634 ZX= -9.0113
 XY= -2.6158 YY= 25.1411 ZY= 0.3544
 XZ= -7.7771 YZ= -0.5038 ZZ= 29.4362
 Eigenvalues: 22.0212 25.9873 41.1226
 59 C Isotropic= 14.5121 Anisotropy 116.9411
 XX= 58.8721 YX= 21.826 ZX= -28.0694
 XY= 16.9458 YY= -71.8585 ZY= -17.7413
 XZ= -34.7215 YZ= -9.6896 ZZ= 56.5228

Eigenvalues: -75.335626.3992 92.4729
 60 H Isotropic= 26.8038 Anisotropy 6.9309
 XX= 24.8742 YX= -1.5831 ZX= 4.4407
 XY= 2.5657 YY= 30.6631 ZY= 3.0084
 XZ= 3.0404 YZ= 0.0071 ZZ= 24.8742
 Eigenvalues: 21.0782 27.9088 31.4244
 61 C Isotropic= 67.5837 Anisotropy 165.4878
 XX= 164.18 YX= -16.255 ZX= 45.5023
 XY= -16.8139 YY= 60.0219 ZY= -14.0097
 XZ= 45.8421 YZ= -12.3023 ZZ= -21.4509
 Eigenvalues: -32.9801 57.8223 177.9089
 62 C Isotropic= 62.8848 Anisotropy 176.9692
 XX= 168.6622 YX= -26.9307 ZX= 28.2411
 XY= -26.8986 YY= -16.444 ZY= -40.7493
 XZ= 28.0648 YZ= -44.4599 ZZ= 36.4363
 Eigenvalues: -40.6413 48.4315 180.8643
 63 C Isotropic= 64.0248 Anisotropy 176.0595
 XX= 161.7214 YX= -44.3655 ZX= 43.7191
 XY= -42.9282 YY= -2.0775 ZY= 29.9559
 XZ= 43.3761 YZ= 28.2301 ZZ= 32.4305
 Eigenvalues: -36.7534 47.43 181.3978
 64 C Isotropic= 61.3974 Anisotropy 177.6916
 XX= 163.4346 YX= -21.9328 ZX= 48.3779
 XY= -20.7587 YY= 49.4857 ZY= -16.4024
 XZ= 49.912 YZ= -14.7853 ZZ= -28.7281
 Eigenvalues: -41.7342 46.068 179.8585
 65 C Isotropic= 56.8753 Anisotropy 159.3225
 XX= 153.5483 YX= -23.1639 ZX= 23.3128
 XY= -21.7902 YY= -15.257 ZY= -40.6294
 XZ= 23.2926 YZ= -42.0495 ZZ= 32.3344
 Eigenvalues: -39.4926 47.0282 163.0903
 66 H Isotropic= 24.1288 Anisotropy 9.2098
 XX= 22.0359 YX= 2.3534 ZX= -0.1021
 XY= 2.8598 YY= 29.4428 ZY= 0.8539
 XZ= -0.4876 YZ= -0.5334 ZZ= 20.9076
 Eigenvalues: 20.6961 21.4215 30.2686
 67 O Isotropic= -130.1079 Anisotropy 620.0387
 XX= -104.9674 YX= 59.8858 ZX= -351.7299
 XY= 100.0155 YY= -211.1028 ZY= -5.2988
 XZ= -372.583 YZ= -39.397 ZZ= -74.2534
 Eigenvalues: -459.4882 -214.0867 283.2513
 68 C Isotropic= 58.7136 Anisotropy 167.7828
 XX= 41.2565 YX= -22.9638 ZX= 9.3609
 XY= -33.2117 YY= 26.7778 ZY= -79.3761
 XZ= 26.2301 YZ= -94.6979 ZZ= 108.1065
 Eigenvalues: -31.558 37.13 170.5687
 69 H Isotropic= 23.8133 Anisotropy 4.9686
 XX= 21.3849 YX= 1.7791 ZX= -1.5399
 XY= 1.8456 YY= 25.3527 ZY= -0.8955
 XZ= -1.5759 YZ= -1.2208 ZZ= 24.7022
 Eigenvalues: 20.3876 23.9265 27.1257
 70 H Isotropic= 23.8378 Anisotropy 3.0031
 XX= 21.2142 YX= 0.8809 ZX= -1.3202
 XY= 1.105 YY= 25.0579 ZY= 0.7204
 XZ= -1.4114 YZ= 0.5326 ZZ= 25.2412
 Eigenvalues: 20.5111 25.1623 25.8399

71	H	Isotropic=	23.8927	Anisotropy	5.0491
XX=	21.3527	YX=	1.3625	ZX=	-1.5653
XY=	1.6574	YY=	26.2979	ZY=	-0.8497
XZ=	-1.526	YZ=	-0.9093	ZZ=	24.0274
Eigenvalues:	20.4569	23.9624	27.2587		
72	H	Isotropic=	23.9315	Anisotropy	8.7225
XX=	21.6118	YX=	0.9054	ZX=	-2.6815
XY=	1.4407	YY=	23.2045	ZY=	-2.8837
XZ=	-2.7376	YZ=	-3.2313	ZZ=	26.9782
Eigenvalues:	20.475	21.573	29.7465		
73	C	Isotropic=	57.3903	Anisotropy	175.3646
XX=	-32.8993	YX=	-34.8387	ZX=	10.3023
XY=	-30.6859	YY=	70.77	ZY=	-56.2457
XZ=	5.4463	YZ=	-66.2367	ZZ=	134.3003
Eigenvalues:	-42.9946	40.8655	174.3001		
74	C	Isotropic=	62.8471	Anisotropy	174.8442
XX=	-2.1219	YX=	24.272	ZX=	42.963
XY=	22.7095	YY=	62.3411	ZY=	-73.4077
XZ=	44.4271	YZ=	-73.933	ZZ=	128.322
Eigenvalues:	-39.6196	48.751	179.4099		
75	C	Isotropic=	62.0678	Anisotropy	178.0007
XX=	46.6569	YX=	-23.0948	ZX=	8.4238
XY=	-24.5594	YY=	15.0517	ZY=	-95.6506
XZ=	9.7374	YZ=	-90.6542	ZZ=	124.4948
Eigenvalues:	-41.2965	46.765	180.7349		
76	C	Isotropic=	64.719	Anisotropy	172.8844
XX=	-22.2261	YX=	-41.5396	ZX=	11.1161
XY=	-40.6317	YY=	72.13	ZY=	-58.2973
XZ=	9.7659	YZ=	-55.7916	ZZ=	144.2531
Eigenvalues:	-38.2757	52.4574	179.9753		
77	C	Isotropic=	60.9561	Anisotropy	182.7604
XX=	-3.7706	YX=	2.8362	ZX=	39.7525
XY=	10.8448	YY=	64.52	ZY=	-77.6574
XZ=	42.0842	YZ=	-81.5775	ZZ=	122.1188
Eigenvalues:	-29.9277	29.9996	182.7963		
78	H	Isotropic=	23.3435	Anisotropy	7.2957
XX=	23.4809	YX=	-3.0276	ZX=	-0.8908
XY=	-2.0067	YY=	24.8945	ZY=	2.9598
XZ=	-0.8713	YZ=	3.2005	ZZ=	21.6552
Eigenvalues:	19.6889	22.1344	28.2073		
79	H	Isotropic=	23.7215	Anisotropy	3.6028
XX=	24.9269	YX=	0.4245	ZX=	0.0655
XY=	0.4884	YY=	24.9298	ZY=	2.3272
XZ=	0.264	YZ=	1.968	ZZ=	21.3078
Eigenvalues:	20.3092	24.7319	26.1234		
80	H	Isotropic=	23.7332	Anisotropy	4.3974
XX=	26.132	YX=	-0.6196	ZX=	-0.9598
XY=	-0.6088	YY=	23.6577	ZY=	1.5484
XZ=	-0.9944	YZ=	1.8427	ZZ=	21.41
Eigenvalues:	20.44	24.0949	26.6648		
81	H	Isotropic=	23.8895	Anisotropy	6.0952
XX=	24.2321	YX=	-1.2369	ZX=	-0.7458
XY=	-1.2606	YY=	26.3417	ZY=	2.6289
XZ=	-1.1045	YZ=	2.3723	ZZ=	21.0946
Eigenvalues:	20.0535	23.6619	27.9529		
82	H	Isotropic=	22.2592	Anisotropy	9.2894

XX= 22.8087 YX= -1.31 ZX= 0.3267
 XY= -1.5291 YY= 27.7459 ZY= 2.2595
 XZ= 0.128 YZ= 1.9863 ZZ= 16.2231
 Eigenvalues: 15.8117 22.5138 28.4522

2b-vi2

C	-3.383149	-2.010949	0.118136
C	-4.102567	-1.634559	1.451947
C	-3.441044	-0.510096	2.26626
C	-4.273486	0.783351	2.32779
C	-4.562385	1.439304	0.962722
C	-3.428585	1.58523	-0.040444
C	-2.838130.287908		-0.511847
C	-1.491342	0.113919	-0.401658
C	-0.972067	-1.297076	-0.437376
C	-1.882488	-2.265588	0.323692
C	-3.647182	-0.913117	-0.958252
C	-5.147414	-0.715702	-1.123941
C	-3.142647	-1.403719	-2.32888
C	-0.527989	1.214504	-0.190747
C	-5.559019	0.578513	3.096721
O	-3.890639	-3.269797	-0.320315
O	-4.238014	-2.804728	2.24398
O	-5.643026	2.003257	0.774223
O	-3.604416	2.600986	-1.017377
O	0.315213	-1.521911	0.174862
H	-3.37006-3.222419		2.305605
C	-4.629784	2.665168	-1.922947
O	-5.570858	1.881757	-1.864151
C	-4.428073.794128		-2.879271
H	-5.174477	-1.360757	1.22827
H	-2.42665-0.267057		1.861849
H	-2.635369	2.103111	0.609691
H	-0.858734	-1.610493	-1.518241
H	-1.642697	-3.307785	-0.023078
H	-1.630459	-2.216032	1.4155
H	-5.610674	-0.097444	-0.322915
H	-5.369875	-0.217906	-2.100644
H	-5.651509	-1.714284	-1.138684
H	-3.986764	-1.508665	-3.053793
H	-2.408676	-0.686888	-2.76756
H	-2.669756	-2.412099	-2.236151
H	-0.990929	2.223993	-0.323365
H	-0.090151.146048		0.838086
H	0.294342	1.150549	-0.948452
H	-6.095841	1.551891	3.211936
H	-6.237898	-0.126982	2.560083
H	-5.337375	0.162273	4.108577
H	-3.481905	4.344967	-2.662396
H	-4.390069	3.381415	-3.91687
H	-5.295308	4.49368	-2.792426
H	-4.819642	-3.324907	-0.061996
C	1.429986	-0.873222	-0.275343
O	1.547775	-0.657413	-1.480283
H	-3.646005	1.544101	2.878937
H	-3.311119	-0.876944	3.319724

C	2.446816	-0.645110	0.836995
C	3.894019	-0.599806	0.256833
O	2.08354	0.494521	1.578571
H	2.359299	-1.493565	1.580459
N	4.906893	-0.386741	1.255192
C	4.159284	-1.893267	-0.483845
H	3.925372	0.266992	-0.473041
H	2.021838	1.23346	0.955566
C	5.631968	0.756735	1.532211
H	5.133926	-1.184012	1.812181
C	4.096247	-3.123393	0.180003
C	4.361041	-4.304806	-0.510785
C	4.693888	-4.263647	-1.864977
C	4.760942	-3.038582	-2.527832
C	4.497252	-1.854179	-1.840112
H	3.839381	-3.164751	1.249305
O	6.590947	0.63077	2.32387
C	5.452034	2.020287	0.765609
H	4.307788	-5.269821	0.014455
H	4.902677	-5.196754	-2.408825
H	5.021195	-3.003354	-3.596096
H	4.539319	-0.890296	-2.369935
C	6.593665	2.57155	0.165308
C	6.50913	3.791007	-0.503257
C	5.299776	4.486185	-0.542175
C	4.181691	3.971832	0.113128
C	4.26264	2.74997	0.781617
H	7.551713	2.030961	0.22624
H	7.402484	4.211334	-0.988775
H	5.233759	5.447589	-1.072945
H	3.238173	4.537038	0.118786
H	3.410082	2.394832	1.37587

2bvi_45	E(RB+HF-PW91)	=	-2012.283065
SCF	GIAO	Magnetic shielding tensor (ppm):	
1	C	Isotropic=	111.036 Anisotropy 30.138
XX=	105.0333	YX=	17.0786 ZX= 9.6822
XY=	8.3682	YY=	116.2605 ZY= 5.7395
XZ=	12.3849	YZ=	6.0317 ZZ= 111.8141
Eigenvalues:	94.1004	107.8796	131.1279
2	C	Isotropic=	112.4857 Anisotropy 31.1846
XX=	93.0738	YX=	-1.9958 ZX= 0.8221
XY=	1.72	YY=	124.5644 ZY= -16.3859
XZ=	-2.7405	YZ=	-5.2553 ZZ= 119.8188
Eigenvalues:	93.0293	111.1523	133.2754
3	C	Isotropic=	141.6079 Anisotropy 19.727
XX=	122.1861	YX=	6.9916 ZX= -2.866
XY=	2.9305	YY=	147.9833 ZY= 1.9339
XZ=	3.9433	YZ=	-0.5765 ZZ= 154.6542
Eigenvalues:	121.26	148.8044	154.7592
4	C	Isotropic=	140.9159 Anisotropy 23.8845
XX=	127.8455	YX=	1.869 ZX= 1.1426
XY=	13.4656	YY=	140.5055 ZY= -4.5475
XZ=	-7.2118	YZ=	-4.8735 ZZ= 154.3967
Eigenvalues:	124.2138	141.695	156.8389

5	C	Isotropic=	-22.9794	Anisotropy	180.9827
XX=	-46.6441	YX=	32.6492	ZX=	47.2739
XY=	37.5816	YY=	55.1797	ZY=	60.238
XZ=	32.3001	YZ=	69.7221	ZZ=	-77.4738
Eigenvalues:	-113.9584		-52.6556	97.6757	
6	C	Isotropic=	101.9924	Anisotropy	41.8413
XX=	88.5506	YX=	8.647	ZX=	-9.3344
XY=	-6.9498	YY=	97.7836	ZY=	-15.9021
XZ=	1.8637	YZ=	-19.6009	ZZ=	119.6429
Eigenvalues:	86.9539	89.1367	129.8866		
7	C	Isotropic=	44.6275	Anisotropy	155.9013
XX=	42.6271	YX=	6.7467	ZX=	-8.7441
XY=	21.0982	YY=	-39.3181	ZY=	-62.9303
XZ=	-20.8322	YZ=	-42.0423	ZZ=	130.5737
Eigenvalues:	-55.135	40.4558	148.5618		
8	C	Isotropic=	42.4821	Anisotropy	152.553
XX=	39.8257	YX=	-6.9245	ZX=	-12.0747
XY=	-15.1151	YY=	-52	ZY=	-13.2261
XZ=	-18.715	YZ=	-32.3145	ZZ=	139.6205
Eigenvalues:	-56.3725	39.6347	144.1841		
9	C	Isotropic=	110.3213	Anisotropy	56.8347
XX=	135.123	YX=	-5.9818	ZX=	25.6547
XY=	0.6383	YY=	108.7885	ZY=	-7.9648
XZ=	29.5864	YZ=	-1.8825	ZZ=	87.0523
Eigenvalues:	74.1425	108.6103	148.2111		
10	C	Isotropic=	147.312	Anisotropy	44.2201
XX=	175.9016	YX=	0.0371	ZX=	4.4584
XY=	9.0624	YY=	142.001	ZY=	-7.3607
XZ=	4.2248	YZ=	1.2001	ZZ=	124.0336
Eigenvalues:	123.0347	142.1093	176.7921		
11	C	Isotropic=	147.0105	Anisotropy	12.3483
XX=	141.8626	YX=	-0.9981	ZX=	0.6457
XY=	7.1497	YY=	149.4195	ZY=	-1.7093
XZ=	-12.18	YZ=	-3.4845	ZZ=	149.7493
Eigenvalues:	138.5885	147.2002	155.2427		
12	C	Isotropic=	154.7254	Anisotropy	22.3982
XX=	160.2722	YX=	-14.0467	ZX=	-8.9653
XY=	-9.9095	YY=	140.5378	ZY=	-1.1454
XZ=	-0.1279	YZ=	4.5813	ZZ=	163.3664
Eigenvalues:	134.8807	159.638	169.6576		
13	C	Isotropic=	148.3253	Anisotropy	54.8437
XX=	146.8034	YX=	2.4931	ZX=	-15.5576
XY=	9.2341	YY=	123.659	ZY=	16.0276
XZ=	-19.3732	YZ=	13.2379	ZZ=	174.5135
Eigenvalues:	115.9298	144.1583	184.8878		
14	C	Isotropic=	168.2947	Anisotropy	13.654
XX=	170.8457	YX=	7.8365	ZX=	-4.4847
XY=	6.0763	YY=	167.1861	ZY=	2.826
XZ=	7.2984	YZ=	4.9454	ZZ=	166.8523
Eigenvalues:	160.874	166.6128	177.3974		
15	C	Isotropic=	169.2642	Anisotropy	17.154
XX=	172.5466	YX=	-5.8326	ZX=	-7.978
XY=	-1.5102	YY=	162.4703	ZY=	-7.1762
XZ=	-7.5106	YZ=	-5.9407	ZZ=	172.7756
Eigenvalues:	156.2654	170.8269	180.7002		
16	O	Isotropic=	263.1758	Anisotropy	81.732

XX=	316.1632	YX=	11.9859	ZX=	-0.7385		
XY=	-2.5704	YY=	226.9052	ZY=	23.7808		
XZ=	12.612	YZ=	59.4035	ZZ=	246.459		
Eigenvalues:	193.9563		277.9073		317.6638		
17	O	Isotropic=	265.1851	Anisotropy		44.6153	
XX=	251.162	YX=	-13.3491	ZX=	18.6696		
XY=	2.0428	YY=	288.3584	ZY=	11.1226		
XZ=	0.152	YZ=	20.6563	ZZ=	256.0349		
Eigenvalues:	239.4425		261.1842		294.9286		
18	O	Isotropic=	-357.0808	Anisotropy		1081.0649	
XX=	-785.8656	YX=	482.1108	ZX=	42.9252		
XY=	413.2342	YY=	30.7862	ZY=	308.9469		
XZ=	34.9768	YZ=	316.5654	ZZ=	-316.1631		
Eigenvalues:	-997.0121		-437.8595		363.6291		
19	O	Isotropic=	89.7529	Anisotropy		121.7099	
XX=	115.7261	YX=	-136.4817	ZX=	89.0785		
XY=	-34.0124	YY=	37.5855	ZY=	91.6074		
XZ=	-3.4715	YZ=	28.964	ZZ=	115.9471		
Eigenvalues:	-49.9982		148.3641		170.8929		
20	O	Isotropic=	93.2331	Anisotropy		153.794	
XX=	117.8993	YX=	17.9783	ZX=	-31.0784		
XY=	18.3986	YY=	180.4275	ZY=	-18.8764		
XZ=	-184.3615	YZ=	15.3637	ZZ=	-18.6275		
Eigenvalues:	-78.0955		162.0323		195.7624		
21	H	Isotropic=	31.1551	Anisotropy		13.7486	
XX=	33.994	YX=	-6.3137	ZX=	-0.3127		
XY=	-6.0508	YY=	31.4946	ZY=	-5.6893		
XZ=	-0.2708	YZ=	-6.6017	ZZ=	27.9767		
Eigenvalues:	21.8603		31.2843		40.3208		
22	C	Isotropic=	20.3999	Anisotropy		75.1346	
XX=	32.3772	YX=	42.4458	ZX=	-72.3845		
XY=	16.3813	YY=	47.7076	ZY=	35.0781		
XZ=	-43.4405	YZ=	53.6398	ZZ=	-18.8853		
Eigenvalues:	-78.95		69.66		70.4896		
23	O	Isotropic=	-131.8515	Anisotropy		600.2941	
XX=	-258.1065	YX=	-228.2383	ZX=	-195.3176		
XY=	-180.5235	YY=	-61.0939	ZY=	190.8287		
XZ=	-188.0803	YZ=	184.7283	ZZ=	-76.354		
Eigenvalues:	-407.2927		-256.6063		268.3446		
24	C	Isotropic=	166.5471	Anisotropy		36.6518	
XX=	157.703	YX=	5.76	ZX=	1.4551		
XY=	6.1208	YY=	174.0488	ZY=	-18.9837		
XZ=	0.8835	YZ=	-19.6896	ZZ=	167.8894		
Eigenvalues:	148.7688		159.8907		190.9816		
25	H	Isotropic=	27.3782	Anisotropy		3.039	
XX=	27.0463	YX=	-1.399	ZX=	-0.7915		
XY=	-2.4253	YY=	27.4328	ZY=	-1.4703		
XZ=	0.034	YZ=	-0.8293	ZZ=	27.6556		
Eigenvalues:	24.9029		27.8276		29.4042		
26	H	Isotropic=	28.1243	Anisotropy		8.2538	
XX=	29.5672	YX=	0.8401	ZX=	-4.5947		
XY=	0.7804	YY=	25.3197	ZY=	0.7982		
XZ=	-3.5772	YZ=	-0.1269	ZZ=	29.4861		
Eigenvalues:	24.5623		26.1838		33.6268		
27	H	Isotropic=	25.427	Anisotropy		3.6776	
XX=	26.1373	YX=	-2.4222	ZX=	0.8815		

XY=	1.0057	YY=	25.2129	ZY=	-2.8123		
XZ=	1.5682	YZ=	-0.6462	ZZ=	24.9307		
Eigenvalues:	23.2619	25.1403	27.8787				
28	H	Isotropic=	24.7513	Anisotropy		8.3481	
XX=	30.0688	YX=	-0.0202	ZX=	1.493		
XY=	0.9312	YY=	19.4834	ZY=	1.4091		
XZ=	0.5378	YZ=	2.4886	ZZ=	24.7016		
Eigenvalues:	18.8348	25.1024	30.3167				
29	H	Isotropic=	28.6927	Anisotropy		6.5576	
XX=	30.4995	YX=	-1.8615	ZX=	-1.1726		
XY=	-0.8526	YY=	32.1581	ZY=	1.1123		
XZ=	-0.3788	YZ=	0.7295	ZZ=	23.4206		
Eigenvalues:	23.2677	29.746	33.0644				
30	H	Isotropic=	29.0985	Anisotropy		4.7789	
XX=	32.2717	YX=	-0.0482	ZX=	-0.1214		
XY=	-0.5345	YY=	25.0675	ZY=	-1.0287		
XZ=	0.1048	YZ=	-1.6521	ZZ=	29.9564		
Eigenvalues:	24.7134	30.2977	32.2845				
31	H	Isotropic=	29.2709	Anisotropy		8.1656	
XX=	29.3637	YX=	-2.9221	ZX=	-1.0443		
XY=	-2.8976	YY=	29.5435	ZY=	3.0614		
XZ=	-1.0725	YZ=	4.7532	ZZ=	28.9054		
Eigenvalues:	24.8946	28.2034	34.7146				
32	H	Isotropic=	29.1704	Anisotropy		9.2001	
XX=	27.6757	YX=	-3.267	ZX=	3.7701		
XY=	-2.0557	YY=	30.2759	ZY=	-2.9289		
XZ=	3.7837	YZ=	-2.4058	ZZ=	29.5597		
Eigenvalues:	24.6709	27.5366	35.3038				
33	H	Isotropic=	30.3204	Anisotropy		6.6364	
XX=	33.2265	YX=	1.579	ZX=	2.4975		
XY=	1.791	YY=	30.7316	ZY=	-0.6265		
XZ=	2.7735	YZ=	-0.0147	ZZ=	27.003		
Eigenvalues:	25.8683	30.3482	34.7446				
34	H	Isotropic=	30.1495	Anisotropy		9.0529	
XX=	29.9515	YX=	-0.4814	ZX=	1.6618		
XY=	0.6203	YY=	25.9754	ZY=	3.138		
XZ=	3.112	YZ=	2.3402	ZZ=	34.5214		
Eigenvalues:	25.0887	29.175	36.1847				
35	H	Isotropic=	30.288	Anisotropy		6.2428	
XX=	30.6834	YX=	2.294	ZX=	-0.8987		
XY=	0.7489	YY=	26.8419	ZY=	-0.8836		
XZ=	-2.4705	YZ=	-0.9185	ZZ=	33.3387		
Eigenvalues:	26.2984	30.1158	34.4499				
36	H	Isotropic=	28.5692	Anisotropy		6.0931	
XX=	27.66	YX=	-1.8715	ZX=	-0.0253		
XY=	-1.9105	YY=	27.8049	ZY=	1.7915		
XZ=	-0.8214	YZ=	4.1031	ZZ=	30.2427		
Eigenvalues:	25.0643	28.012	32.6312				
37	H	Isotropic=	28.8732	Anisotropy		7.4044	
XX=	31.8707	YX=	-1.0835	ZX=	0.8192		
XY=	-2.012	YY=	31.9656	ZY=	-1.9205		
XZ=	0.5069	YZ=	-2.147	ZZ=	22.7833		
Eigenvalues:	22.3414	30.4687	33.8095				
38	H	Isotropic=	28.6541	Anisotropy		10.0517	
XX=	32.3486	YX=	-1.1244	ZX=	3.5897		
XY=	-0.2746	YY=	25.9509	ZY=	1.1302		

XZ=	6.0185	YZ=	0.3286	ZZ=	27.6628				
Eigenvalues:	24.124	26.4831	35.3552						
39	H	Isotropic=	28.7696	Anisotropy	8.6625				
XX=	32.9168	YX=	-2.8864	ZX=	-3.6523				
XY=	-1.0269	YY=	28.311	ZY=	-1.146				
XZ=	-3.1153	YZ=	-0.8467	ZZ=	25.081				
Eigenvalues:	23.281	28.4832	34.5446						
40	H	Isotropic=	29.1586	Anisotropy	10.8485				
XX=	29.6105	YX=	-5.5368	ZX=	-2.1691				
XY=	-4.9785	YY=	30.4259	ZY=	1.6476				
XZ=	-3.8797	YZ=	1.2396	ZZ=	27.4394				
Eigenvalues:	24.1188	26.9661	36.3909						
41	H	Isotropic=	29.6106	Anisotropy	5.9334				
XX=	32.7441	YX=	1.8824	ZX=	-0.8629				
XY=	2.1424	YY=	28.636	ZY=	2.0609				
XZ=	-1.1759	YZ=	2.6371	ZZ=	27.4518				
Eigenvalues:	25.0665	30.1992	33.5662						
42	H	Isotropic=	30.4214	Anisotropy	9.5945				
XX=	28.3707	YX=	-0.8722	ZX=	-2.0661				
XY=	-1.2276	YY=	26.8677	ZY=	-1.6751				
XZ=	-2.2055	YZ=	-2.0015	ZZ=	36.0258				
Eigenvalues:	25.6485	28.798	36.8177						
43	H	Isotropic=	29.063	Anisotropy	5.6061				
XX=	30.3152	YX=	1.7525	ZX=	2.326				
XY=	3.4522	YY=	29.8779	ZY=	-2.151				
XZ=	1.1312	YZ=	-3.376	ZZ=	26.9961				
Eigenvalues:	24.0048	30.3839	32.8004						
44	H	Isotropic=	29.1981	Anisotropy	7.073				
XX=	26.1715	YX=	0.0632	ZX=	-0.6235				
XY=	-0.2905	YY=	27.5414	ZY=	-1.0259				
XZ=	0.833	YZ=	0.1456	ZZ=	33.8815				
Eigenvalues:	26.1616	27.5193	33.9135						
45	H	Isotropic=	28.9227	Anisotropy	8.8432				
XX=	29.7402	YX=	-3.0947	ZX=	-0.119				
XY=	-4.865	YY=	31.1711	ZY=	-1.8558				
XZ=	1.0733	YZ=	-1.7355	ZZ=	25.8569				
Eigenvalues:	25.0889	26.8611	34.8181						
46	H	Isotropic=	30.5629	Anisotropy	18.0521				
XX=	39.7105	YX=	7.1761	ZX=	-2.5969				
XY=	4.8908	YY=	29.0482	ZY=	1.2801				
XZ=	-1.6742	YZ=	-0.6058	ZZ=	22.9301				
Eigenvalues:	22.4085	26.6826	42.5976						
47	C	Isotropic=	7.9936	Anisotropy	97.4248				
XX=	-63.687	YX=	-54.5197	ZX=	-36.3799				
XY=	-58.2213	YY=	47.7557	ZY=	-3.4276				
XZ=	4.3102	YZ=	5.706	ZZ=	39.912				
Eigenvalues:	-88.8331	139.8704	72.9434						
48	O	Isotropic=	-148.9409	Anisotropy	707.9466				
XX=	-218.9942	YX=	-244.3657	ZX=	-19.0657				
XY=	-247.1179	YY=	182.0225	ZY=	131.8235				
XZ=	-31.141	YZ=	139.6803	ZZ=	-409.8509				
Eigenvalues:	-445.29	-324.5561	323.0235						
49	H	Isotropic=	28.6632	Anisotropy	6.4005				
XX=	29.0151	YX=	1.8621	ZX=	-1.3526				
XY=	2.859	YY=	29.3385	ZY=	4.2892				
XZ=	-0.3797	YZ=	3.408	ZZ=	27.636				

Eigenvalues: 23.6494 29.41 32.9302
 50 H Isotropic= 29.4001 Anisotropy 6.4576
 XX= 26.9521 YX= -1.4866 ZX= 0.2759
 XY= -1.6467 YY= 27.6911 ZY= -0.2358
 XZ= 0.2715 YZ= -1.3972 ZZ= 33.557
 Eigenvalues: 25.7008 28.7943 33.7051
 51 C Isotropic= 108.9301 Anisotropy 18.5713
 XX= 116.6768 YX= -2.0259 ZX= -9.5657
 XY= 1.7028 YY= 114.787 ZY= 6.8516
 XZ= -5.8036 YZ= 11.1936 ZZ= 95.3266
 Eigenvalues: 89.8864 115.593 121.311
 52 C Isotropic= 124.5979 Anisotropy 16.0354
 XX= 122.4899 YX= -4.8526 ZX= -3.112
 XY= 0.5332 YY= 119.6967 ZY= 5.6689
 XZ= 1.0913 YZ= 8.8003 ZZ= 131.6072
 Eigenvalues: 115.9194 122.5862 135.2882
 53 O Isotropic= 254.224 Anisotropy 50.7571
 XX= 268.6358 YX= 10.5413 ZX= -1.8281
 XY= 10.7932 YY= 262.5385 ZY= -26.4293
 XZ= 16.13 YZ= -46.5587 ZZ= 231.4977
 Eigenvalues: 205.1392 269.4707 288.0621
 54 H Isotropic= 26.5136 Anisotropy 5.2828
 XX= 27.3038 YX= -1.3384 ZX= -2.1368
 XY= -0.4767 YY= 29.4583 ZY= -2.3007
 XZ= -1.0873 YZ= -1.4074 ZZ= 22.7787
 Eigenvalues: 21.7229 27.7825 30.0355
 55 N Isotropic= 123.9505 Anisotropy 127.7985
 XX= 97.6017 YX= 55.4567 ZX= -46.4434
 XY= 26.2005 YY= 191.8259 ZY= 19.2439
 XZ= -37.493 YZ= 43.9734 ZZ= 82.4239
 Eigenvalues: 31.3895 131.3125 209.1495
 56 C Isotropic= 52.0216 Anisotropy 189.0079
 XX= 164.2954 YX= 17.7123 ZX= 48.2349
 XY= 19.6207 YY= -21.6628 ZY= -17.2956
 XZ= 43.5457 YZ= -18.9769 ZZ= 13.4323
 Eigenvalues: -36.2247 14.2627 178.0269
 57 H Isotropic= 26.3792 Anisotropy 4.9127
 XX= 24.7223 YX= 2.1034 ZX= -1.1671
 XY= 2.3437 YY= 28.6259 ZY= -1.0008
 XZ= 0.7513 YZ= 1.8209 ZZ= 25.7893
 Eigenvalues: 23.6548 25.8284 29.6543
 58 H Isotropic= 30.3676 Anisotropy 13.889
 XX= 27.4359 YX= -1.7421 ZX= -0.2106
 XY= -0.3362 YY= 37.8246 ZY= -4.6185
 XZ= 1.7914 YZ= -4.9496 ZZ= 25.8424
 Eigenvalues: 24.1163 27.3596 39.627
 59 C Isotropic= 15.7052 Anisotropy 116.5515
 XX= 52.1945 YX= -38.8329 ZX= -23.6683
 XY= -34.4246 YY= -61.1307 ZY= 25.8249
 XZ= -31.8442 YZ= 20.2554 ZZ= 56.0517
 Eigenvalues: -73.6069 27.3164 93.4062
 60 H Isotropic= 26.7509 Anisotropy 7.0389
 XX= 24.6886 YX= 2.6299 ZX= 3.927
 XY= -1.542 YY= 30.5386 ZY= -3.779
 XZ= 3.065 YZ= -0.7682 ZZ= 25.0255
 Eigenvalues: 20.9462 27.8629 31.4435

61 C Isotropic= 67.5613 Anisotropy 167.1756
 XX= 167.5308 YX= 4.8979 ZX= 47.4541
 XY= 5.7985 YY= 56.2988 ZY= 6.5845
 XZ= 46.8692 YZ= 5.0567 ZZ= -21.1458
 Eigenvalues: -32.4997 56.1719 179.0116

62 C Isotropic= 62.7118 Anisotropy 177.0408
 XX= 172.4563 YX= 5.4608 ZX= 32.2658
 XY= 4.704 YY= -17.6192 ZY= 37.7268
 XZ= 33.1012 YZ= 42.2722 ZZ= 33.2984
 Eigenvalues: -40.2019 47.5984 180.7391

63 C Isotropic= 63.8849 Anisotropy 175.9624
 XX= 169.7287 YX= 24.5551 ZX= 38.9089
 XY= 23.0588 YY= -12.3765 ZY= -33.6504
 XZ= 38.631 YZ= -31.9855 ZZ= 34.3024
 Eigenvalues: -36.875 47.3365 181.1931

64 C Isotropic= 61.4037 Anisotropy 177.5881
 XX= 167.1061 YX= 9.4929 ZX= 49.0339
 XY= 7.9673 YY= 47.0768 ZY= 7.9344
 XZ= 50.7448 YZ= 6.5328 ZZ= -29.9717
 Eigenvalues: -42.1639 46.5792 179.7958

65 C Isotropic= 57.5063 Anisotropy 159.3818
 XX= 157.2503 YX= 2.5754 ZX= 27.7135
 XY= 2.6023 YY= -15.522 ZY= 39.2726
 XZ= 27.7875 YZ= 40.9887 ZZ= 30.7907
 Eigenvalues: -39.4115 48.1696 163.7608

66 H Isotropic= 24.0709 Anisotropy 9.0389
 XX= 21.5805 YX= -1.4425 ZX= -0.0639
 XY= -1.7838 YY= 29.773 ZY= -1.1314
 XZ= -0.3339 YZ= 0.2361 ZZ= 20.8592
 Eigenvalues: 20.7052 21.4107 30.0968

67 O Isotropic= -136.1772 Anisotropy 623.0209
 XX= -140.8527 YX= -80.7493 ZX= -349.5853
 XY= -117.3344 YY= -185.1942 ZY= 58.9274
 XZ= -365.5749 YZ= 90.1848 ZZ= -82.4848
 Eigenvalues: -472.3036 -215.3981 279.17

68 C Isotropic= 57.5728 Anisotropy 171.2088
 XX= 50.5742 YX= 25.1413 ZX= 25.3614
 XY= 34.3188 YY= 18.6617 ZY= 73.4227
 XZ= 46.3754 YZ= 92.2389 ZZ= 103.4824
 Eigenvalues: -32.6014 33.6078 171.712

69 H Isotropic= 23.8133 Anisotropy 4.8945
 XX= 21.1081 YX= -1.3142 ZX= -1.3772
 XY= -1.3408 YY= 25.7366 ZY= 1.0227
 XZ= -1.3964 YZ= 1.3636 ZZ= 24.5953
 Eigenvalues: 20.4678 23.8958 27.0763

70 H Isotropic= 23.8487 Anisotropy 2.9673
 XX= 21.1365 YX= -0.4628 ZX= -1.3861
 XY= -0.639 YY= 25.1606 ZY= -0.5754
 XZ= -1.4396 YZ= -0.3618 ZZ= 25.2492
 Eigenvalues: 20.6005 25.1187 25.8269

71 H Isotropic= 23.8997 Anisotropy 4.9338
 XX= 21.1617 YX= -0.7446 ZX= -1.4682
 XY= -0.9999 YY= 26.5844 ZY= 0.9324
 XZ= -1.3961 YZ= 1.0066 ZZ= 23.953
 Eigenvalues: 20.5255 23.9847 27.1889

72 H Isotropic= 24.0224 Anisotropy 8.5284

XX=	21.5452	YX=	-0.5678	ZX=	-2.2956		
XY=	-1.2313	YY=	23.6666	ZY=	3.1948		
XZ=	-2.3399	YZ=	3.5164	ZZ=	26.8556		
Eigenvalues:	20.5949	21.7644	29.7081				
73	C	Isotropic=	57.03	Anisotropy		176.9435	
XX=	-20.2886	YX=	51.2176	ZX=	23.8789		
XY=	44.289	YY=	58.2528	ZY=	52.4842		
XZ=	18.8305	YZ=	65.9631	ZZ=	133.1259		
Eigenvalues:	-43.0927	39.1904	174.9924				
74	C	Isotropic=	61.2803	Anisotropy		177.0582	
XX=	-5.1118	YX=	-10.7873	ZX=	59.0968		
XY=	-8.7687	YY=	64.616	ZY=	67.5918		
XZ=	59.7405	YZ=	66.6508	ZZ=	124.3368		
Eigenvalues:	-41.0883	45.6102	179.3191				
75	C	Isotropic=	61.9545	Anisotropy		178.5857	
XX=	55.103	YX=	20.4691	ZX=	27.4104		
XY=	23.1266	YY=	7.1732	ZY=	92.8602		
XZ=	28.4183	YZ=	84.1654	ZZ=	123.5872		
Eigenvalues:	-40.9468	45.7986	181.0116				
76	C	Isotropic=	64.589	Anisotropy		172.7448	
XX=	-2.5692	YX=	57.5136	ZX=	29.7194		
XY=	57.9664	YY=	54.4143	ZY=	52.9346		
XZ=	30.8818	YZ=	46.376	ZZ=	141.922		
Eigenvalues:	-38.466	52.4809	179.7522				
77	C	Isotropic=	64.363	Anisotropy		169.8064	
XX=	10.6158	YX=	8.6382	ZX=	62.6943		
XY=	1.0558	YY=	75.6067	ZY=	63.5121		
XZ=	66.6692	YZ=	69.0726	ZZ=	106.8667		
Eigenvalues:	-29.6738	45.1956	177.5673				
78	H	Isotropic=	23.314	Anisotropy		7.2702	
XX=	24.0464	YX=	3.0675	ZX=	-1.4899		
XY=	1.9615	YY=	24.2481	ZY=	-2.827		
XZ=	-1.5021	YZ=	-2.8764	ZZ=	21.6476		
Eigenvalues:	19.8101	21.9712	28.1608				
79	H	Isotropic=	23.6828	Anisotropy		3.6365	
XX=	24.6173	YX=	-0.5134	ZX=	-0.4649		
XY=	-0.5752	YY=	25.1369	ZY=	-2.2194		
XZ=	-0.1173	YZ=	-1.8241	ZZ=	21.2942		
Eigenvalues:	20.3713	24.5699	26.1071				
80	H	Isotropic=	23.69	Anisotropy		4.1847	
XX=	25.9502	YX=	0.0094	ZX=	-1.3614		
XY=	0.1263	YY=	23.5003	ZY=	-1.2599		
XZ=	-1.4877	YZ=	-1.8704	ZZ=	21.6194		
Eigenvalues:	20.4614	24.1287	26.4798				
81	H	Isotropic=	23.8951	Anisotropy		5.8173	
XX=	24.1803	YX=	1.0985	ZX=	-1.2479		
XY=	1.1643	YY=	26.2066	ZY=	-2.4523		
XZ=	-1.5361	YZ=	-2.032	ZZ=	21.2985		
Eigenvalues:	20.2102	23.7019	27.7734				
82	H	Isotropic=	23.4972	Anisotropy		7.6294	
XX=	24.1535	YX=	1.31	ZX=	0.5383		
XY=	1.3442	YY=	28.0427	ZY=	-1.2654		
XZ=	-0.2355	YZ=	-1.2524	ZZ=	18.2954		
Eigenvalues:	18.1183	23.7898	28.5835				

2b-vii

C	-2.880047	0.346291	1.825217
C	-3.758199	1.614942	1.585098
C	-3.703148	2.19856	0.163305
C	-5.022992.057886		-0.616426
C	-5.502283	0.60849	-0.832469
C	-4.500202	-0.439218	-1.292119
C	-3.374696	-0.693717	-0.331719
C	-2.104912	-0.558405	-0.795706
C	-0.99998-0.365483		0.205064
C	-1.428459	0.544619	1.358453
C	-3.535095	-0.903442	1.159422
C	-4.952936	-1.074634	1.683196
C	-2.770911	-2.169347	1.59088
C	-1.721859	-0.526548	-2.224895
C	-6.122624	2.891096	0.00178
O	-2.763193	0.154054	3.234249
O	-3.409287	2.60506	2.540002
O	-6.709231	0.355555	-0.810819
O	-5.064106	-1.575538	-1.932953
O	0.091867	0.293578	-0.481478
H	-2.448017	2.691643	2.539752
C	-5.9628 -2.442959		-1.37297
O	-6.462922	-2.213275	-0.277388
C	-6.232166	-3.595024	-2.284465
H	-4.828054	1.373835	1.853371
H	-2.878863	1.730073	-0.43033
H	-4.042908	0.067199	-2.217022
H	-0.635402	-1.360169	0.590792
H	-0.740425	0.346652	2.226239
H	-1.276961.612236		1.04933
H	-5.689248	-0.387262	1.20906
H	-5.309183	-2.120376	1.507851
H	-4.964469	-0.901908	2.788209
H	-3.425017	-2.847049	2.192189
H	-2.412393	-2.743245	0.703815
H	-1.898615	-1.902987	2.236918
H	-2.433051	-1.118501	-2.852843
H	-1.696704	0.530339	-2.593942
H	-0.697363	-0.956821	-2.358503
H	-7.041935	2.843478	-0.631855
H	-6.386183	2.514102	1.019111
H	-5.794024	3.954472	0.088355
H	-5.669017	-3.493598	-3.242753
H	-5.924756	-4.537648	-1.769455
H	-7.328497	-3.632161	-2.497733
H	-3.593430.428208		3.644263
C	1.361612	0.039166	-0.051448
O	1.539751	-0.72	0.899232
H	-4.824255	2.446585	-1.658378
H	-3.480441	3.296032	0.250193
C	2.392157	0.802018	-0.868867
C	3.709708	0.975682	-0.050478
O	2.569043	0.196666	-2.131555
H	1.976728	1.825257	-1.111167
N	4.642842	-0.102345	-0.244516

C	4.294113	2.324836	-0.40899
H	3.427454	0.983177	1.050207
H	2.756701	-0.741514	-1.993878
C	5.314295	-0.701186	0.811486
H	4.880477	-0.341316	-1.176818
C	4.647828	2.613553	-1.731346
C	5.206912	3.849215	-2.051064
C	5.418071	4.799708	-1.051312
C	5.070496	4.511766	0.268063
C	4.51349	3.274486	0.592644
H	4.462007	1.864837	-2.517794
O	5.282533	-0.216836	1.957767
C	6.079414	-1.942069	0.497275
H	5.481638	4.074249	-3.091928
H	5.860285	5.774595	-1.303968
H	5.240856	5.258026	1.058096
H	4.258767	3.042968	1.638612
C	5.967426	-3.026411	1.375274
C	6.676076	-4.199725	1.120778
C	7.501885	-4.289404	0.000029
C	7.623017	-3.203241	-0.867089
C	6.912207	-2.028614	-0.622282
H	5.325604	-2.938282	2.266454
H	6.58586	-5.053008	1.809307
H	8.062212	-5.215368	-0.197788
H	8.282877	-3.270259	-1.744585
H	7.029823	-1.171525	-1.302142

2bvii_45E(RB+HF-PW91) = -2012.304912

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic= 109.7681 Anisotropy 28.0988
 XX= 96.4531 YX= 4.2458 ZX= -7.1539
 XY= 7.4916 YY= 108.0786 ZY= -7.9035
 XZ= -0.3513 YZ= -6.6753 ZZ= 124.7726
 Eigenvalues: 93.9895 106.8141 128.5007

2 C Isotropic= 112.1188 Anisotropy 30.3932
 XX= 99.2076 YX= 9.3777 ZX= 12.8729
 XY= 0.4364 YY= 122.926 ZY= 5.58
 XZ= 9.6083 YZ= 13.4781 ZZ= 114.223
 Eigenvalues: 93.1969 110.7786 132.3809

3 C Isotropic= 141.9823 Anisotropy 19.6778
 XX= 123.5527 YX= -3.6117 ZX= 6.6426
 XY= 3.6836 YY= 154.465 ZY= -2.3505
 XZ= 9.0399 YZ= -1.3117 ZZ= 147.9292
 Eigenvalues: 121.2391 149.607 155.1008

4 C Isotropic= 140.2473 Anisotropy 24.9258
 XX= 123.8756 YX= 2.8209 ZX= 5.7487
 XY= -7.0821 YY= 155.9343 ZY= 5.9078
 XZ= -4.5093 YZ= 1.2772 ZZ= 140.9321
 Eigenvalues: 123.6912 140.1862 156.8645

5 C Isotropic= -23.1525 Anisotropy 181.0842
 XX= -56.1637 YX= 20.132 ZX= 22.9506
 XY= 2.7797 YY= -97.0532 ZY= -47.5428
 XZ= 22.6207 YZ= -45.7803 ZZ= 83.7595
 Eigenvalues: -113.3105 -53.7172 97.5703

6	C	Isotropic=	101.8947	Anisotropy	42.3253
XX=	88.7384	YX=	-2.3734	ZX=	-3.8449
XY=	10.6267	YY=	125.7388	ZY=	11.2664
XZ=	9.5598	YZ=	12.9286	ZZ=	91.207
Eigenvalues:	86.2602	89.3123	130.1116		
7	C	Isotropic=	43.636	Anisotropy	158.1406
XX=	18.6136	YX=	6.3073	ZX=	-36.0039
XY=	-15.5194	YY=	143.7641	ZY=	22.9288
XZ=	-51.4771	YZ=	32.3581	ZZ=	-31.4699
Eigenvalues:	-59.1653	41.0102	149.063		
8	C	Isotropic=	40.6681	Anisotropy	157.141
XX=	30.4107	YX=	-16.829	ZX=	-34.2046
XY=	-12.9102	YY=	143.4542	ZY=	8.4793
XZ=	-19.7573	YZ=	-9.1418	ZZ=	-51.8607
Eigenvalues:	-60.0234	36.599	145.4288		
9	C	Isotropic=	112.6626	Anisotropy	48.3145
XX=	122.037	YX=	23.3309	ZX=	-18.0091
XY=	28.2821	YY=	103.0527	ZY=	5.5156
XZ=	-18.0928	YZ=	5.3464	ZZ=	112.8981
Eigenvalues:	78.2998	114.8158	144.8723		
10	C	Isotropic=	148.2465	Anisotropy	44.3759
XX=	161.7541	YX=	10.2265	ZX=	-16.4385
XY=	6.4865	YY=	132.6935	ZY=	1.3301
XZ=	-25.1382	YZ=	9.9286	ZZ=	150.2918
Eigenvalues:	123.8869	143.0222	177.8304		
11	C	Isotropic=	147.8483	Anisotropy	12.3264
XX=	142.5483	YX=	1.7198	ZX=	4.516
XY=	-10.5542	YY=	152.2081	ZY=	8.3597
XZ=	-1.7325	YZ=	0.8504	ZZ=	148.7885
Eigenvalues:	139.7396	147.7393	156.0659		
12	C	Isotropic=	155.3971	Anisotropy	21.9988
XX=	167.1778	YX=	-6.8383	ZX=	3.4803
XY=	-1.7647	YY=	162.7458	ZY=	-8.0369
XZ=	-1.4359	YZ=	0.0888	ZZ=	136.2678
Eigenvalues:	135.6794	160.449	170.063		
13	C	Isotropic=	148.0638	Anisotropy	55.3086
XX=	139.9345	YX=	-24.9203	ZX=	-4.1831
XY=	-26.826	YY=	168.205	ZY=	-11.5945
XZ=	-10.0685	YZ=	-15.4275	ZZ=	136.0518
Eigenvalues:	115.8043	143.4508	184.9362		
14	C	Isotropic=	167.9273	Anisotropy	12.7345
XX=	162.4257	YX=	-6.7274	ZX=	-1.7376
XY=	4.0085	YY=	165.3618	ZY=	-1.507
XZ=	-1.9931	YZ=	3.9017	ZZ=	175.9943
Eigenvalues:	161.7673	165.5975	176.417		
15	C	Isotropic=	169.2932	Anisotropy	17.154
XX=	174.0082	YX=	-3.7597	ZX=	0.9465
XY=	-4.8897	YY=	175.2197	ZY=	6.3424
XZ=	-3.8282	YZ=	7.2124	ZZ=	158.6517
Eigenvalues:	156.232	170.9184	180.7292		
16	O	Isotropic=	262.6006	Anisotropy	82.1839
XX=	298.0304	YX=	-15.5055	ZX=	-38.8133
XY=	-18.8246	YY=	229.9744	ZY=	-58.8998
XZ=	-27.1153	YZ=	-20.1104	ZZ=	259.7971
Eigenvalues:	192.144	278.268	317.3899		
17	O	Isotropic=	265.7157	Anisotropy	44.5102

XX=	263.5329	YX=	14.9212	ZX=	23.6743		
XY=	-8.5633	YY=	252.5851	ZY=	-12.4853		
XZ=	15.0161	YZ=	-12.4466	ZZ=	281.0289		
Eigenvalues:	241.6489		260.1089		295.3891		
18	O	Isotropic=	-358.6346	Anisotropy		1082.3558	
XX=	-972.3057	YX=	-127.0577	ZX=	62.1657		
XY=	-121.4836	YY=	-410.7831	ZY=	-187.9037		
XZ=	133.7999	YZ=	-178.6207	ZZ=	307.1851		
Eigenvalues:	-1001.2792		-437.5605		362.9359		
19	O	Isotropic=	91.5744	Anisotropy		118.2639	
XX=	167.0154	YX=	52.4437	ZX=	66.3491		
XY=	-21.3119	YY=	92.9459	ZY=	-42.6137		
XZ=	-22.0914	YZ=	-142.8195	ZZ=	14.762		
Eigenvalues:	-50.1353	154.4415		170.4171			
20	O	Isotropic=	71.4522	Anisotropy		162.9295	
XX=	110.516	YX=	-20.8446	ZX=	0.0016		
XY=	-84.7027	YY=	75.3207	ZY=	119.7375		
XZ=	117.0414	YZ=	131.8025	ZZ=	28.5201		
Eigenvalues:	-104.8055		139.0904		180.0719		
21	H	Isotropic=	31.1649	Anisotropy		13.9616	
XX=	38.5344	YX=	2.9592	ZX=	2.386		
XY=	2.8681	YY=	29.9779	ZY=	5.8233		
XZ=	2.2961	YZ=	4.7367	ZZ=	24.9822		
Eigenvalues:	21.6279	31.3941	40.4726				
22	C	Isotropic=	20.2207	Anisotropy		74.9258	
XX=	19.5296	YX=	-81.0626	ZX=	-8.8351		
XY=	-59.6747	YY=	-28.6976	ZY=	-13.5699		
XZ=	12.2342	YZ=	17.1807	ZZ=	69.8301		
Eigenvalues:	-79.0101	169.501	70.1713				
23	O	Isotropic=	-132.0844	Anisotropy		601.9801	
XX=	-32.3794	YX=	-212.8046	ZX=	275.7137		
XY=	-211.4362	YY=	-133.459	ZY=	-96.1984		
XZ=	223.9864	YZ=	-97.1611	ZZ=	-230.4149		
Eigenvalues:	-408.7684		-256.7205		269.2357		
24	C	Isotropic=	166.4669	Anisotropy		36.9429	
XX=	155.1475	YX=	9.3963	ZX=	0.464		
XY=	9.329	YY=	174.598	ZY=	17.932		
XZ=	0.9522	YZ=	16.4111	ZZ=	169.6554		
Eigenvalues:	148.6477		159.6576		191.0955		
25	H	Isotropic=	27.4792	Anisotropy		3.1045	
XX=	28.8199	YX=	0.1717	ZX=	0.7785		
XY=	0.6472	YY=	28.1106	ZY=	0.3628		
XZ=	1.7727	YZ=	1.1615	ZZ=	25.5072		
Eigenvalues:	24.9593	27.9295	29.5489				
26	H	Isotropic=	28.2727	Anisotropy		7.9248	
XX=	28.7681	YX=	-4.427	ZX=	-1.0223		
XY=	-3.7588	YY=	29.7271	ZY=	0.7643		
XZ=	-1.1663	YZ=	0.4014	ZZ=	26.3231		
Eigenvalues:	24.9713	26.2909	33.5559				
27	H	Isotropic=	25.4074	Anisotropy		4.2991	
XX=	26.1735	YX=	2.7277	ZX=	1.7789		
XY=	1.8729	YY=	25.5131	ZY=	-0.2445		
XZ=	-1.3971	YZ=	1.7181	ZZ=	24.5354		
Eigenvalues:	23.3505	24.5981	28.2734				
28	H	Isotropic=	24.7318	Anisotropy		7.1029	
XX=	28.8858	YX=	0.6246	ZX=	-2.6072		

XY=	-0.5466	YY=	24.1279	ZY=	-2.86		
XZ=	-1.5351	YZ=	-1.2606	ZZ=	21.1817		
Eigenvalues:	19.7506	24.9776	29.4671				
29	H	Isotropic=	28.1718	Anisotropy	6.9061		
XX=	32.5155	YX=	-0.8627	ZX=	1.0736		
XY=	-1.045	YY=	22.5271	ZY=	1.8332		
XZ=	0.5924	YZ=	0.1161	ZZ=	29.4729		
Eigenvalues:	22.2827	29.4569	32.7759				
30	H	Isotropic=	29.5928	Anisotropy	5.5018		
XX=	32.3405	YX=	0.2936	ZX=	-2.9434		
XY=	-0.3444	YY=	30.9236	ZY=	0.8381		
XZ=	-2.3539	YZ=	0.0838	ZZ=	25.5141		
Eigenvalues:	24.5782	30.9395	33.2606				
31	H	Isotropic=	29.2896	Anisotropy	8.3612		
XX=	32.1607	YX=	-1.5966	ZX=	2.4866		
XY=	-2.5327	YY=	27.5743	ZY=	-3.6662		
XZ=	2.595	YZ=	-2.4128	ZZ=	28.1339		
Eigenvalues:	24.7956	28.2095	34.8638				
32	H	Isotropic=	29.2322	Anisotropy	9.2721		
XX=	29.8726	YX=	5.1597	ZX=	2.4876		
XY=	4.6491	YY=	30.4503	ZY=	0.133		
XZ=	1.5769	YZ=	0.5303	ZZ=	27.3737		
Eigenvalues:	24.6214	27.6615	35.4136				
33	H	Isotropic=	30.2699	Anisotropy	6.4221		
XX=	31.1291	YX=	2.5304	ZX=	-2.185		
XY=	2.243	YY=	27.0441	ZY=	-0.3367		
XZ=	-2.2609	YZ=	0.1201	ZZ=	32.6364		
Eigenvalues:	25.8326	30.4257	34.5513				
34	H	Isotropic=	30.0874	Anisotropy	9.1889		
XX=	29.003	YX=	-0.4401	ZX=	-0.6094		
XY=	1.0509	YY=	33.226	ZY=	-4.7579		
XZ=	-1.698	YZ=	-4.8976	ZZ=	28.0333		
Eigenvalues:	24.9727	29.0762	36.2134				
35	H	Isotropic=	30.2935	Anisotropy	6.2135		
XX=	28.9741	YX=	-1.3619	ZX=	-2.5824		
XY=	-2.1438	YY=	33.6873	ZY=	0.8744		
XZ=	-0.2953	YZ=	0.2863	ZZ=	28.2192		
Eigenvalues:	27.0429	29.4017	34.4359				
36	H	Isotropic=	28.3918	Anisotropy	6.4932		
XX=	29.8863	YX=	-0.3311	ZX=	1.6822		
XY=	-2.3388	YY=	28.8074	ZY=	-3.7785		
XZ=	2.3997	YZ=	-2.2143	ZZ=	26.4816		
Eigenvalues:	24.2525	28.2022	32.7206				
37	H	Isotropic=	29.0545	Anisotropy	7.9725		
XX=	30.4084	YX=	2.7544	ZX=	-0.2546		
XY=	3.238	YY=	26.13	ZY=	4.6396		
XZ=	1.4563	YZ=	3.7942	ZZ=	30.6249		
Eigenvalues:	22.8813	29.9126	34.3695				
38	H	Isotropic=	29.1278	Anisotropy	6.8907		
XX=	27.6933	YX=	0.6315	ZX=	-0.5629		
XY=	1.2287	YY=	29.8401	ZY=	-3.7818		
XZ=	-0.7212	YZ=	-3.561	ZZ=	29.8501		
Eigenvalues:	26.1435	27.5184	33.7216				
39	H	Isotropic=	29.0098	Anisotropy	7.6538		
XX=	33.7492	YX=	-1.2124	ZX=	0.0155		
XY=	-1.2455	YY=	24.149	ZY=	3.3149		

XZ=	-1.1879	YZ=	2.3951	ZZ=	29.1311		
Eigenvalues:	22.7801	30.1368	34.1123				
40	H	Isotropic=	29.1953	Anisotropy		10.9104	
XX=	34.3497	YX=	-1.4968	ZX=	4.1555		
XY=	-3.0156	YY=	27.2634	ZY=	0.5991		
XZ=	3.9287	YZ=	-0.7005	ZZ=	25.9728		
Eigenvalues:	24.1112	27.0058	36.4689				
41	H	Isotropic=	29.6293	Anisotropy		5.774	
XX=	30.6096	YX=	-1.8976	ZX=	-2.2715		
XY=	-2.5712	YY=	26.7934	ZY=	-1.2433		
XZ=	-2.3907	YZ=	-0.983	ZZ=	31.4848		
Eigenvalues:	25.1016	30.3077	33.4786				
42	H	Isotropic=	30.5107	Anisotropy		9.5383	
XX=	29.2016	YX=	-1.3954	ZX=	0.0097		
XY=	-1.4151	YY=	36.5821	ZY=	0.8192		
XZ=	0.4288	YZ=	0.4142	ZZ=	25.7484		
Eigenvalues:	25.6868	28.9758	36.8696				
43	H	Isotropic=	29.0835	Anisotropy		5.6927	
XX=	27.5466	YX=	2.7857	ZX=	-1.3824		
XY=	1.9281	YY=	28.042	ZY=	3.1141		
XZ=	-2.618	YZ=	1.3151	ZZ=	31.6619		
Eigenvalues:	24.2355	30.1363	32.8786				
44	H	Isotropic=	29.2324	Anisotropy		7.0238	
XX=	26.5824	YX=	-0.629	ZX=	0.6998		
XY=	0.1183	YY=	33.8268	ZY=	-1.4867		
XZ=	0.9818	YZ=	0.1067	ZZ=	27.288		
Eigenvalues:	26.0196	27.7627	33.915				
45	H	Isotropic=	28.9442	Anisotropy		8.818	
XX=	33.021	YX=	1.5038	ZX=	1.6475		
XY=	2.8137	YY=	26.6842	ZY=	1.3951		
XZ=	3.3994	YZ=	2.172	ZZ=	27.1274		
Eigenvalues:	25.108	26.9018	34.8229				
46	H	Isotropic=	30.5794	Anisotropy		18.0252	
XX=	33.4537	YX=	-3.5374	ZX=	-8.6605		
XY=	-1.8805	YY=	23.076	ZY=	3.0364		
XZ=	-6.5268	YZ=	1.4577	ZZ=	35.2085		
Eigenvalues:	22.3928	26.7492	42.5962				
47	C	Isotropic=	11.5227	Anisotropy		88.657	
XX=	-79.5239	YX=	-26.1811	ZX=	15.5843		
XY=	1.1775	YY=	58.2265	ZY=	13.0499		
XZ=	-10.3496	YZ=	13.2452	ZZ=	55.8655		
Eigenvalues:	-80.7552	44.6959	70.6274				
48	O	Isotropic=	-101.085	Anisotropy		631.5088	
XX=	-256.7714	YX=	-20.7677	ZX=	-43.7522		
XY=	-23.782	YY=	77.0634	ZY=	287.7268		
XZ=	-57.6094	YZ=	360.248	ZZ=	-123.547		
Eigenvalues:	-369.3626	-253.8134	319.9209				
49	H	Isotropic=	28.718	Anisotropy		6.5883	
XX=	27.4885	YX=	-2.9913	ZX=	0.0832		
XY=	-2.0633	YY=	26.4949	ZY=	-2.2817		
XZ=	-1.0173	YZ=	-2.5817	ZZ=	32.1704		
Eigenvalues:	23.8318	29.2119	33.1101				
50	H	Isotropic=	29.5293	Anisotropy		6.4364	
XX=	28.6765	YX=	0.4597	ZX=	1.2101		
XY=	0.665	YY=	33.6973	ZY=	-0.2585		
XZ=	1.3709	YZ=	-1.3623	ZZ=	26.2141		

Eigenvalues: 25.547 29.2207 33.8203
 51 C Isotropic= 108.9322 Anisotropy 22.9014
 XX= 119.9281 YX= -0.0423 ZX= 9.6106
 XY= 2.2026 YY= 98.1438 ZY= 5.3894
 XZ= 5.5459 YZ= 5.2495 ZZ= 108.7247
 Eigenvalues: 95.754 106.8428 124.1998
 52 C Isotropic= 131.6408 Anisotropy 19.8054
 XX= 135.2323 YX= 5.1877 ZX= -2.6401
 XY= 7.7507 YY= 139.9596 ZY= 6.7687
 XZ= -4.0524 YZ= 4.8657 ZZ= 119.7303
 Eigenvalues: 116.7856 133.2923 144.8443
 53 O Isotropic= 295.3862 Anisotropy 24.1167
 XX= 289.4666 YX= 2.8364 ZX= -13.8001
 XY= -1.7053 YY= 306.8405 ZY= -14.3234
 XZ= -12.0005 YZ= -1.1057 ZZ= 289.8515
 Eigenvalues: 275.9097 298.785 311.464
 54 H Isotropic= 26.3635 Anisotropy 6.3456
 XX= 30.3734 YX= 2.6212 ZX= -0.0188
 XY= -0.6769 YY= 26.1601 ZY= -0.2352
 XZ= 0.2699 YZ= 1.2878 ZZ= 22.5569
 Eigenvalues: 22.4815 26.015 30.5939
 55 N Isotropic= 138.6152 Anisotropy 115.4863
 XX= 149.1418 YX= 6.0348 ZX= -4.2047
 XY= 11.9928 YY= 160.6509 ZY= -68.3573
 XZ= 59.3927 YZ= -84.3307 ZZ= 106.0528
 Eigenvalues: 44.8591 155.3804 215.606
 56 C Isotropic= 46.7195 Anisotropy 196.2741
 XX= 144.1756 YX= -73.4503 ZX= 24.9233
 XY= -72.3344 YY= -6.4084 ZY= -1.8893
 XZ= 29.7549 YZ= -2.0317 ZZ= 2.3913
 Eigenvalues: -37.8369 0.4265 177.5689
 57 H Isotropic= 25.2295 Anisotropy 2.5202
 XX= 24.8396 YX= 0.2405 ZX= -1.2479
 XY= 2.1447 YY= 24.1573 ZY= 0.8978
 XZ= 0.0355 YZ= 0.3797 ZZ= 26.6915
 Eigenvalues: 23.0477 25.7311 26.9096
 58 H Isotropic= 30.2202 Anisotropy 14.184
 XX= 25.8524 YX= -2.9016 ZX= 1.7651
 XY= -3.5351 YY= 38.6345 ZY= 3.5185
 XZ= 0.2595 YZ= 0.9166 ZZ= 26.1738
 Eigenvalues: 23.9549 27.0295 39.6762
 59 C Isotropic= 18.0599 Anisotropy 114.3471
 XX= 31.5683 YX= 72.2263 ZX= -39.124
 XY= 67.5157 YY= -4.3826 ZY= 5.0979
 XZ= -40.599 YZ= 24.5647 ZZ= 26.994
 Eigenvalues: -72.1656 32.0539 94.2913
 60 H Isotropic= 26.2292 Anisotropy 7.8568
 XX= 27.3696 YX= -8.7533 ZX= -1.2191
 XY= -2.5321 YY= 23.6899 ZY= -0.2163
 XZ= 0.009 YZ= -1.761 ZZ= 27.6281
 Eigenvalues: 19.4318 27.7888 31.4671
 61 C Isotropic= 65.6494 Anisotropy 168.3933
 XX= 155.2288 YX= -51.4418 ZX= 13.7629
 XY= -49.6936 YY= 31.5954 ZY= -50.007
 XZ= 8.3005 YZ= -48.5191 ZZ= 10.1241
 Eigenvalues: -32.7562 51.7928 177.9116

62 C Isotropic= 62.045 Anisotropy 177.3358
 XX= 153.4873 YX= -48.5696 ZX= 39.6561
 XY= -48.2219 YY= 64.6712 ZY= 5.5657
 XZ= 40.4977 YZ= 8.3278 ZZ= -32.0235
 Eigenvalues: -43.139 49.0051 180.2689

63 C Isotropic= 64.8146 Anisotropy 174.3795
 XX= 145.612 YX= -75.6401 ZX= 25.8851
 XY= -75.5736 YY= -0.3466 ZY= 8.8647
 XZ= 27.3621 YZ= 9.6244 ZZ= 49.1785
 Eigenvalues: -36.7163 50.0925 181.0676

64 C Isotropic= 61.9057 Anisotropy 174.8633
 XX= 154.8122 YX= -54.1984 ZX= 8.9194
 XY= -53.6844 YY= 26.2886 ZY= -49.2037
 XZ= 8.6787 YZ= -51.9949 ZZ= 4.6163
 Eigenvalues: -40.497 47.7329 178.4812

65 C Isotropic= 61.2972 Anisotropy 152.7444
 XX= 141.9198 YX= -40.6809 ZX= 30.0087
 XY= -41.0158 YY= 65.9436 ZY= 10.983
 XZ= 33.0421 YZ= 8.588 ZZ= -23.9717
 Eigenvalues: -32.9469 53.7118 163.1268

66 H Isotropic= 23.1067 Anisotropy 10.464
 XX= 21.6423 YX= 3.7447 ZX= -3.0566
 XY= 3.6407 YY= 24.1245 ZY= -3.797
 XZ= -2.6283 YZ= -3.5541 ZZ= 23.5533
 Eigenvalues: 18.9732 20.2642 30.0827

67 O Isotropic= -105.8314 Anisotropy 673.8388
 XX= 151.7973 YX= 217.4317 ZX= -183.0226
 XY= 242.8603 YY= -74.4721 ZY= -171.5165
 XZ= -86.869 YZ= -107.4625 ZZ= -394.8194
 Eigenvalues: -451.7579 -209.1307 343.3945

68 C Isotropic= 54.3581 Anisotropy 171.98
 XX= 87.3067 YX= 44.9508 ZX= 83.7715
 XY= 57.7293 YY= -2.7751 ZY= 23.0233
 XZ= 60.7455 YZ= 7.9285 ZZ= 78.5426
 Eigenvalues: -29.5188 23.5817 169.0114

69 H Isotropic= 23.6961 Anisotropy 5.135
 XX= 21.4684 YX= 2.3983 ZX= -0.8263
 XY= 2.4546 YY= 26.0498 ZY= -0.0721
 XZ= -0.7239 YZ= 0.1192 ZZ= 23.5702
 Eigenvalues: 20.2643 23.7046 27.1195

70 H Isotropic= 23.7822 Anisotropy 3.2124
 XX= 21.3539 YX= 1.7107 ZX= -0.8199
 XY= 1.5494 YY= 24.3268 ZY= 0.6323
 XZ= -0.8004 YZ= 0.6267 ZZ= 25.666
 Eigenvalues: 20.4441 24.9788 25.9238

71 H Isotropic= 23.7634 Anisotropy 4.7092
 XX= 21.5011 YX= 2.4455 ZX= -1.0215
 XY= 2.2951 YY= 25.3532 ZY= -0.5597
 XZ= -1.0556 YZ= -0.6785 ZZ= 24.4358
 Eigenvalues: 20.2606 24.1267 26.9028

72 H Isotropic= 23.6318 Anisotropy 8.0126
 XX= 21.1472 YX= 2.8672 ZX= 0.6463
 XY= 2.544 YY= 27.3265 ZY= 2.2094
 XZ= 0.4993 YZ= 1.6996 ZZ= 22.4218
 Eigenvalues: 20.1172 21.8047 28.9735

73 C Isotropic= 60.743 Anisotropy 176.5913

XX= 100.152 YX= 34.9121 ZX= 90.559
 XY= 39.0974 YY= 56.9382 ZY= 22.7623
 XZ= 95.2069 YZ= 23.5155 ZZ= 25.1387
 Eigenvalues: -37.551441.3098 178.4705
 74 C Isotropic= 61.852 Anisotropy 177.8749
 XX= 125.2275 YX= 28.0173 ZX= 61.1995
 XY= 30.3737 YY= 11.4991 ZY= 66.4462
 XZ= 60.623 YZ= 67.9816 ZZ= 48.8293
 Eigenvalues: -40.965646.0864 180.4352
 75 C Isotropic= 62.7205 Anisotropy 177.71
 XX= 102.6384 YX= 74.2838 ZX= 63.6813
 XY= 72.4858 YY= 2.6201 ZY= 12.0927
 XZ= 63.2772 YZ= 13.1147 ZZ= 82.9031
 Eigenvalues: -39.565746.5335 181.1938
 76 C Isotropic= 63.9102 Anisotropy 174.9987
 XX= 94.6873 YX= 40.3226 ZX= 94.3312
 XY= 36.9398 YY= 65.8557 ZY= 21.6112
 XZ= 97.4735 YZ= 20.4645 ZZ= 31.1875
 Eigenvalues: -38.410549.565 180.576
 77 C Isotropic= 68.4253 Anisotropy 161.3724
 XX= 123.6525 YX= 26.034 ZX= 55.935
 XY= 21.7006 YY= 21.5572 ZY= 65.8172
 XZ= 57.4231 YZ= 59.5472 ZZ= 60.066
 Eigenvalues: -26.464755.7336 176.0069
 78 H Isotropic= 23.1845 Anisotropy 7.5154
 XX= 20.9902 YX= -2.4291 ZX= -0.0788
 XY= -2.7198 YY= 26.5895 ZY= -2.1853
 XZ= -0.3185 YZ= -2.0841 ZZ= 21.9737
 Eigenvalues: 19.5238 21.8349 28.1947
 79 H Isotropic= 23.7136 Anisotropy 4.5388
 XX= 23.0077 YX= -2.5621 ZX= -1.9643
 XY= -2.2839 YY= 24.6013 ZY= -0.3183
 XZ= -2.0595 YZ= -0.1042 ZZ= 23.5316
 Eigenvalues: 20.2626 24.1387 26.7394
 80 H Isotropic= 23.7319 Anisotropy 3.7131
 XX= 22.5142 YX= -0.9872 ZX= -2.1742
 XY= -1.0647 YY= 24.3165 ZY= -1.6604
 XZ= -2.1469 YZ= -1.4673 ZZ= 24.365
 Eigenvalues: 20.3302 24.6583 26.2073
 81 H Isotropic= 23.8866 Anisotropy 5.0805
 XX= 22.8495 YX= -2.4288 ZX= -1.7877
 XY= -2.2998 YY= 25.9979 ZY= -1.0964
 XZ= -1.4602 YZ= -1.0741 ZZ= 22.8124
 Eigenvalues: 20.1573 24.2289 27.2736
 82 H Isotropic= 24.0558 Anisotropy 8.7214
 XX= 25.1016 YX= -4.5692 ZX= -3.481
 XY= -3.6739 YY= 24.4338 ZY= 0.8086
 XZ= -2.4856 YZ= 0.3795 ZZ= 22.6319
 Eigenvalues: 19.5618 22.7354 29.87

2b-viii

C	-2.483497	-1.077174	1.44642
C	-3.184683	-0.049648	2.390248
C	-3.206828	1.403376	1.886891
C	-4.613538	1.912847	1.524457
C	-5.324844	1.125562	0.405808

C	-4.549318	0.768296	-0.852785
C	-3.371584	-0.13517-0.627851	
C	-2.157495	0.287287	-1.067832
C	-0.929679	-0.353724	-0.483946
C	-1.081928	-0.612792	1.016663
C	-3.389536	-1.392599	0.216172
C	-4.747694	-1.881305	0.696462
C	-2.779096	-2.561304	-0.580107
C	-1.939666	1.378056	-2.04399
C	-5.498571	2.01079 2.746231	
O	-2.233718	-2.263664	2.198773
O	-2.584772	-0.119522	3.674505
O	-6.545383	0.957179	0.460035
O	-5.345509	0.508119	-2.000672
O	0.164807	0.581189	-0.64957
H	-1.62825-0.067264	3.557791	
C	-6.293398	-0.473727	-2.108441
O	-6.624202	-1.140051	-1.133864
C	-6.833938	-0.543841	-3.498833
H	-4.240508	-0.397472.587646	
H	-2.535345	1.530978	1.001364
H	-4.130504	1.791933	-1.165709
H	-0.678278	-1.304539	-1.035085
H	-0.335959	-1.402883	1.306819
H	-0.810788	0.322984	1.57263
H	-5.422504	-1.062467	1.033492
H	-5.273933	-2.434102	-0.121361
H	-4.607054	-2.598419	1.543178
H	-3.454451	-3.451527	-0.566877
H	-2.613782	-2.277227	-1.646328
H	-1.809128	-2.883256	-0.127834
H	-2.797324	1.467095	-2.756109
H	-1.802435	2.352402	-1.509531
H	-1.011541.183686	-2.638593	
H	-6.481488	2.466386	2.471897
H	-5.696513	1.00073 3.178819	
H	-5.007925	2.643375	3.524266
H	-6.378172	0.239295	-4.150593
H	-6.609968	-1.554704	-3.918777
H	-7.941217	-0.398381	-3.458679
H	-2.966104	-2.386568	2.816087
C	1.422255	0.07381 -0.79678	
O	1.582683	-1.145787	-0.774637
H	-4.479918	2.950085	1.097174
H	-2.814776	2.058926	2.710375
C	2.446329	1.183682	-0.958152
C	3.886195	0.731902	-0.54642
O	2.368023	1.726884	-2.258169
H	2.140167	2.042445	-0.287009
N	4.636104	0.175661	-1.637769
C	4.573648	1.925574	0.081193
H	3.760721	-0.070615	0.244651
H	2.516123	1.01439 -2.895327	
C	5.41076 -0.975275	-1.630966	
H	4.806298	0.801517	-2.397832
C	4.756045	3.101403	-0.654544

C	5.407264	4.190895	-0.079146
C	5.878284	4.110572	1.231953
C	5.696312	2.939451	1.96692
C	5.047999	1.845559	1.393306
H	4.366491	3.163833	-1.683643
O	6.128659	-1.167761	-2.634642
C	5.473807	-1.891093	-0.461197
H	5.549765	5.113782	-0.660532
H	6.393613	4.970342	1.685069
H	6.067895	2.874242	3.000242
H	4.916128	0.920863	1.975351
C	6.751051	-2.264697	-0.016871
C	6.885662	-3.162033	1.039798
C	5.751624	-3.711056	1.640107
C	4.483387	-3.3683	1.174065
C	4.341414	-2.464836	0.119671
H	7.641223	-1.848376	-0.514444
H	7.888322	-3.445523	1.392235
H	5.859545	-4.422327	2.472421
H	3.587722	-3.816845	1.629078
H	3.335992	-2.232021	-0.267034

2bviii_45	E(RB+HF-PW91)	=	-2012.301776	
SCF GIAO	Magnetic shielding	tensor (ppm):		
1 C	Isotropic=	109.6226	Anisotropy	= 27.6172
XX=	97.492	YX= 7.0656	ZX= 0.5194	
XY=	4.2412	YY= 124.0528	ZY= -8.3364	
XZ=	7.4305	YZ= -8.5319	ZZ= 107.323	
Eigenvalues:	93.7091	107.1247	128.0341	
2 C	Isotropic=	112.3337	Anisotropy	= 30.5282
XX=	104.323	YX= -2.4508	ZX= 20.7389	
XY=	-7.3757	YY= 109.0564	ZY= -0.0299	
XZ=	11.2849	YZ= 7.0818	ZZ= 123.6217	
Eigenvalues:	93.0219	111.2933	132.6858	
3 C	Isotropic=	141.7135	Anisotropy	= 19.6764
XX=	126.1728	YX= -6.2382	ZX= 6.2571	
XY=	-3.4605	YY= 152.4276	ZY= 3.6893	
XZ=	13.0487	YZ= 5.2265	ZZ= 146.5402	
Eigenvalues:	121.1079	149.2016	154.8311	
4 C	Isotropic=	140.44	Anisotropy	= 24.5668
XX=	124.3794	YX= -1.1916	ZX= 11.3389	
XY=	0.7525	YY= 144.2702	ZY= 8.7533	
XZ=	-3.0407	YZ= 4.7752	ZZ= 152.6705	
Eigenvalues:	123.7105	140.7917	156.8179	
5 C	Isotropic=	-22.8792	Anisotropy	= 181.0053
XX=	-47.929	YX= -18.0523	ZX= 26.0975	
XY=	-29.117	YY= 52.0218	ZY= -80.6769	
XZ=	12.8681	YZ= -80.8788	ZZ= -72.7305	
Eigenvalues:	-113.2362	-53.1924	97.7909	
6 C	Isotropic=	101.6413	Anisotropy	= 42.0827
XX=	91.6994	YX= 4.478	ZX= 1.8625	
XY=	2.96	YY= 93.736	ZY= 14.5669	
XZ=	19.8726	YZ= 15.1003	ZZ= 119.4884	
Eigenvalues:	86.356	88.8715	129.6964	
7 C	Isotropic=	43.419	Anisotropy	= 158.2652

XX=	10.5004	YX=	47.3008	ZX=	-1.5832				
XY=	42.3897	YY=	16.1402	ZY=	71.9435				
XZ=	-28.4169	YZ=	81.5322	ZZ=	103.6163				
Eigenvalues:	-59.3485	40.6763	148.9291						
8	C	Isotropic=	41.0549	Anisotropy	=	155.7405			
XX=	21.5278	YX=	31.4633	ZX=	-26.6746				
XY=	26.9612	YY=	33.5949	ZY=	101.6946				
XZ=	-14.5987	YZ=	83.1154	ZZ=	68.0419				
Eigenvalues:	-58.9784	37.2611	144.8819						
9	C	Isotropic=	112.3788	Anisotropy	=	48.2739			
XX=	125.0195	YX=	27.1055	ZX=	3.3099				
XY=	30.2028	YY=	101.9629	ZY=	-12.1132				
XZ=	6.8771	YZ=	-11.6094	ZZ=	110.1541				
Eigenvalues:	77.6457	114.9293	144.5614						
10	C	Isotropic=	148.155	Anisotropy	=	44.3654			
XX=	159.185	YX=	17.3242	ZX=	-5.4754				
XY=	19.5696	YY=	136.3671	ZY=	-18.1198				
XZ=	-14.3489	YZ=	-8.6991	ZZ=	148.913				
Eigenvalues:	123.7306	143.0025	177.7319						
11	C	Isotropic=	147.9201	Anisotropy	=	12.6602			
XX=	141.851	YX=	-2.8028	ZX=	7.2347				
XY=	-4.879	YY=	145.9267	ZY=	5.9012				
XZ=	-6.5163	YZ=	-1.984	ZZ=	155.9826				
Eigenvalues:	139.4343	147.9658	156.3603						
12	C	Isotropic=	155.2163	Anisotropy	=	22.124			
XX=	165.3644	YX=	-3.7489	ZX=	-6.0928				
XY=	1.5558	YY=	151.4643	ZY=	9.6245				
XZ=	-5.861	YZ=	18.7727	ZZ=	148.8201				
Eigenvalues:	135.4176	160.2656	169.9656						
13	C	Isotropic=	147.894	Anisotropy	=	55.2129			
XX=	130.6651	YX=	-9.6561	ZX=	-19.1938				
XY=	-5.615	YY=	163.6816	ZY=	21.2211				
XZ=	-25.1439	YZ=	18.293	ZZ=	149.3351				
Eigenvalues:	115.4175	143.5618	184.7026						
14	C	Isotropic=	167.8239	Anisotropy	=	13.2105			
XX=	161.8218	YX=	-3.191	ZX=	-4.0872				
XY=	2.9186	YY=	169.9499	ZY=	-9.2762				
XZ=	3.9272	YZ=	-2.203	ZZ=	171.7001				
Eigenvalues:	161.8142	165.0266	176.631						
15	C	Isotropic=	169.3045	Anisotropy	=	16.9286			
XX=	172.4567	YX=	-1.7852	ZX=	-1.7465				
XY=	0.6186	YY=	159.3666	ZY=	6.7274				
XZ=	-5.5629	YZ=	8.3092	ZZ=	176.0902				
Eigenvalues:	156.4458	170.8774	180.5902						
16	O	Isotropic=	263.0308	Anisotropy	=	82.4347			
XX=	282.9199	YX=	21.0774	ZX=	-52.8886				
XY=	1.401	YY=	285.675	ZY=	-28.2772				
XZ=	-47.4291	YZ=	6.0555	ZZ=	220.4974				
Eigenvalues:	192.4337	278.6714	317.9872						
17	O	Isotropic=	265.5323	Anisotropy	=	45.1068			
XX=	268.3438	YX=	-10.0108	ZX=	23.9255				
XY=	-18.6788	YY=	281.5051	ZY=	-10.0316				
XZ=	-0.0269	YZ=	-11.1965	ZZ=	246.7479				
Eigenvalues:	240.9596	260.0337	295.6034						
18	O	Isotropic=	-359.3448	Anisotropy	=	1084.9068			
XX=	-965.4432	YX=	-175.8577	ZX=	72.1299				

XY=	-228.624	YY=	180.6396	ZY=	-299.6051				
XZ=	123.7983	YZ=	-300.28	ZZ=	-293.2307				
Eigenvalues:	-1003.4299		-438.5308		363.9264				
19	O	Isotropic=	92.1053	Anisotropy	=	118.052			
XX=	170.0237	YX=	-14.5983	ZX=	45.4812				
XY=	22.4363	YY=	141.2509	ZY=	97.1424				
XZ=	-70.0296	YZ=	2.6806	ZZ=	-34.9586				
Eigenvalues:	-48.8704	154.3796		170.8067					
20	O	Isotropic=	67.4872	Anisotropy	=	166.0193			
XX=	104.3945	YX=	-15.0691	ZX=	-1.2408				
XY=	-143.1432	YY=	-77.5584	ZY=	26.9096				
XZ=	26.5841	YZ=	16.0535	ZZ=	175.6255				
Eigenvalues:	-109.2588		133.5537		178.1667				
21	H	Isotropic=	31.2183	Anisotropy	=	13.9706			
XX=	39.81	YX=	0.2586	ZX=	2.6538				
XY=	0.2848	YY=	21.958	ZY=	2.2465				
XZ=	2.2315	YZ=	1.2209	ZZ=	31.8867				
Eigenvalues:	21.6629	31.4599	40.532						
22	C	Isotropic=	20.2507	Anisotropy	=	75.3779			
XX=	-1.0376	YX=	-52.3896	ZX=	-64.1014				
XY=	-60.0485	YY=	26.3234	ZY=	-53.5141				
XZ=	-34.1896	YZ=	-23.7069	ZZ=	35.4662				
Eigenvalues:	-79.2627	69.5121	70.5026						
23	O	Isotropic=	-132.3742	Anisotropy	=	601.2517			
XX=	-46.196	YX=	-330.3512	ZX=	-20.6412				
XY=	-290.9962	YY=	-85.4797	ZY=	118.3668				
XZ=	-53.5363	YZ=	124.5793	ZZ=	-265.447				
Eigenvalues:	-409.0496		-256.5333		268.4602				
24	C	Isotropic=	166.1552	Anisotropy	=	37.2462			
XX=	159.1819	YX=	5.6645	ZX=	13.2978				
XY=	6.1152	YY=	154.014	ZY=	-0.4009				
XZ=	13.5458	YZ=	-1.8366	ZZ=	185.2697				
Eigenvalues:	147.878	159.6017		190.986					
25	H	Isotropic=	27.4576	Anisotropy	=	3.0995			
XX=	29.1791	YX=	-0.249	ZX=	0.435				
XY=	-0.7924	YY=	25.8953	ZY=	0.9283				
XZ=	1.3163	YZ=	1.5816	ZZ=	27.2983				
Eigenvalues:	24.9665	27.8823	29.5239						
26	H	Isotropic=	28.276	Anisotropy	=	7.7909			
XX=	27.3614	YX=	-1.8342	ZX=	-3.5457				
XY=	-1.36	YY=	27.3076	ZY=	2.0054				
XZ=	-3.3267	YZ=	1.8251	ZZ=	30.1589				
Eigenvalues:	25.0057	26.3523	33.4699						
27	H	Isotropic=	25.399	Anisotropy	=	4.2524			
XX=	26.8029	YX=	0.7486	ZX=	3.1148				
XY=	1.9856	YY=	24.2246	ZY=	-1.1435				
XZ=	0.3176	YZ=	1.1627	ZZ=	25.1695				
Eigenvalues:	23.2827	24.6804	28.2339						
28	H	Isotropic=	24.6019	Anisotropy	=	6.9649			
XX=	28.0827	YX=	2.7438	ZX=	-2.1285				
XY=	0.8334	YY=	24.2225	ZY=	0.449				
XZ=	-2.6503	YZ=	1.8302	ZZ=	21.5006				
Eigenvalues:	20.0496	24.511	29.2452						
29	H	Isotropic=	28.1848	Anisotropy	=	7.5583			
XX=	32.551	YX=	-2.3937	ZX=	-0.7698				
XY=	-2.1704	YY=	25.3409	ZY=	-2.6822				

XZ=	-1.7184	YZ=	-4.2113	ZZ=	26.6625				
Eigenvalues:	21.8802	29.4506	33.2237						
30	H	Isotropic=	29.5691	Anisotropy	=	5.4327			
XX=	31.6726	YX=	2.6651	ZX=	-1.9604				
XY=	1.6749	YY=	27.4105	ZY=	2.5411				
XZ=	-2.4455	YZ=	1.7637	ZZ=	29.6241				
Eigenvalues:	24.7748	30.7415	33.1909						
31	H	Isotropic=	29.2756	Anisotropy	=	8.3737			
XX=	31.8369	YX=	-2.7678	ZX=	-0.8478				
XY=	-3.6729	YY=	31.0067	ZY=	0.1517				
XZ=	-1.5618	YZ=	1.2469	ZZ=	24.9833				
Eigenvalues:	24.7731	28.1957	34.8581						
32	H	Isotropic=	29.2017	Anisotropy	=	9.332			
XX=	31.7557	YX=	1.7485	ZX=	5.1927				
XY=	2.0815	YY=	28.305	ZY=	0.8457				
XZ=	4.0976	YZ=	1.2901	ZZ=	27.5445				
Eigenvalues:	24.544	27.6381	35.423						
33	H	Isotropic=	30.2914	Anisotropy	=	6.4161			
XX=	31.3175	YX=	2.7532	ZX=	0.1338				
XY=	2.4918	YY=	30.2418	ZY=	-3.5822				
XZ=	-0.2582	YZ=	-3.1344	ZZ=	29.315				
Eigenvalues:	25.82	30.4855	34.5688						
34	H	Isotropic=	30.0354	Anisotropy	=	9.0854			
XX=	28.7801	YX=	0.7989	ZX=	-1.0218				
XY=	2.6355	YY=	34.9561	ZY=	2.7704				
XZ=	-0.7685	YZ=	2.9589	ZZ=	26.37				
Eigenvalues:	24.9937	29.0203	36.0923						
35	H	Isotropic=	30.2064	Anisotropy	=	6.0509			
XX=	28.1386	YX=	1.4819	ZX=	-1.7585				
XY=	-0.5315	YY=	29.8527	ZY=	2.9836				
XZ=	-0.9612	YZ=	2.0016	ZZ=	32.6279				
Eigenvalues:	27.0866	29.2922	34.2403						
36	H	Isotropic=	28.3821	Anisotropy	=	6.283			
XX=	29.866	YX=	-1.0627	ZX=	0.2401				
XY=	-3.1059	YY=	30.4012	ZY=	1.1648				
XZ=	-1.0227	YZ=	2.3796	ZZ=	24.879				
Eigenvalues:	24.35	28.2255	32.5707						
37	H	Isotropic=	28.9898	Anisotropy	=	8.1429			
XX=	31.278	YX=	1.3923	ZX=	2.1907				
XY=	0.466	YY=	24.4155	ZY=	-2.6365				
XZ=	3.5316	YZ=	-3.6221	ZZ=	31.276				
Eigenvalues:	22.7494	29.8016	34.4184						
38	H	Isotropic=	29.1041	Anisotropy	=	6.9467			
XX=	27.709	YX=	1.1103	ZX=	-0.0114				
XY=	1.3683	YY=	33.4771	ZY=	-0.0692				
XZ=	0.115	YZ=	0.3626	ZZ=	26.1262				
Eigenvalues:	26.1228	27.4544	33.7353						
39	H	Isotropic=	28.8733	Anisotropy	=	7.4055			
XX=	32.8071	YX=	-1.3564	ZX=	-1.4385				
XY=	-0.4809	YY=	24.044	ZY=	-2.5827				
XZ=	-2.5271	YZ=	-3.1393	ZZ=	29.7687				
Eigenvalues:	22.5995	30.21	33.8103						
40	H	Isotropic=	29.1771	Anisotropy	=	10.9379			
XX=	34.3142	YX=	-4.1368	ZX=	0.1986				
XY=	-4.7668	YY=	26.6669	ZY=	2.1246				
XZ=	-1.1529	YZ=	0.7773	ZZ=	26.5503				

Eigenvalues:	24.0932	26.9691	36.469			
41	H	Isotropic=	29.6302	Anisotropy	=	5.7695
XX=	29.3245	YX=	0.0617	ZX=	-3.2113	
XY=	-0.3908	YY=	30.5474	ZY=	-2.2869	
XZ=	-3.8824	YZ=	-2.0799	ZZ=	29.0188	
Eigenvalues:	25.074	30.3402	33.4765			
42	H	Isotropic=	30.4985	Anisotropy	=	9.5219
XX=	28.9598	YX=	0.0565	ZX=	-0.2768	
XY=	-0.282	YY=	29.8775	ZY=	5.5956	
XZ=	-0.102	YZ=	5.1969	ZZ=	32.6583	
Eigenvalues:	25.6952	28.954	36.8465			
43	H	Isotropic=	29.0105	Anisotropy	=	5.779
XX=	27.8087	YX=	2.2657	ZX=	1.9661	
XY=	2.9774	YY=	27.754	ZY=	-1.8327	
XZ=	0.4687	YZ=	-3.4939	ZZ=	31.4689	
Eigenvalues:	24.1095	30.0589	32.8632			
44	H	Isotropic=	29.1719	Anisotropy	=	6.9958
XX=	26.7589	YX=	-0.1263	ZX=	0.7283	
XY=	-0.1405	YY=	30.7466	ZY=	2.5749	
XZ=	1.4389	YZ=	4.1878	ZZ=	30.0101	
Eigenvalues:	25.9374	27.7425	33.8357			
45	H	Isotropic=	28.9122	Anisotropy	=	8.8023
XX=	34.0068	YX=	-0.3509	ZX=	1.2076	
XY=	-0.8861	YY=	25.157	ZY=	-0.6923	
XZ=	3.34	YZ=	-0.047	ZZ=	27.5727	
Eigenvalues:	25.0905	26.8656	34.7804			
46	H	Isotropic=	30.5529	Anisotropy	=	18.0248
XX=	31.1174	YX=	2.8352	ZX=	-8.3715	
XY=	2.4188	YY=	27.4542	ZY=	-6.1164	
XZ=	-5.8456	YZ=	-7.7778	ZZ=	33.0871	
Eigenvalues:	22.1849	26.9043	42.5695			
47	C	Isotropic=	10.053	Anisotropy	=	90.9427
XX=	-74.8544	YX=	-26.3243	ZX=	18.5963	
XY=	12.2158	YY=	36.7042	ZY=	-3.799	
XZ=	18.5208	YZ=	6.4689	ZZ=	68.3093	
Eigenvalues:	-77.6701	37.1477	70.6815			
48	O	Isotropic=	-90.5418	Anisotropy	=	600.0245
XX=	-236.8463	YX=	33.4806	ZX=	66.9958	
XY=	23.0953	YY=	-334.6791	ZY=	12.2775	
XZ=	51.1205	YZ=	72.1694	ZZ=	299.8999	
Eigenvalues:	-343.3463	-237.7537	309.4745			
49	H	Isotropic=	28.7148	Anisotropy	=	6.6827
XX=	26.6099	YX=	-2.4104	ZX=	-2.1739	
XY=	-0.9802	YY=	32.1897	ZY=	-2.2371	
XZ=	-2.3021	YZ=	-2.2327	ZZ=	27.3448	
Eigenvalues:	23.8073	29.1672	33.1699			
50	H	Isotropic=	29.5348	Anisotropy	=	6.3824
XX=	29.1864	YX=	0.044	ZX=	1.3717	
XY=	0.1044	YY=	30.3272	ZY=	4.332	
XZ=	1.4467	YZ=	3.3093	ZZ=	29.0907	
Eigenvalues:	25.5409	29.2738	33.7897			
51	C	Isotropic=	109.0014	Anisotropy	=	21.924
XX=	121.4059	YX=	-5.5435	ZX=	5.006	
XY=	-3.2996	YY=	99.658	ZY=	-6.6837	
XZ=	2.5152	YZ=	-4.4009	ZZ=	105.9403	
Eigenvalues:	96.2659	107.121	123.6174			

52	C	Isotropic=	128.704	Anisotropy	=	16.1684
XX=	124.8914	YX=	3.8421	ZX=	2.2285	
XY=	-0.6781	YY=	124.5237	ZY=	4.4584	
XZ=	0.6152	YZ=	7.7472	ZZ=	136.6969	
Eigenvalues:	121.7087		124.9204		139.4829	
53	O	Isotropic=	293.2015	Anisotropy	=	19.3251
XX=	288.0268	YX=	11.4445	ZX=	-8.8508	
XY=	4.4465	YY=	302.5224	ZY=	-0.4594	
XZ=	-9.6256	YZ=	10.3979	ZZ=	289.0553	
Eigenvalues:	276.0778		297.4419		306.0849	
54	H	Isotropic=	26.5027	Anisotropy	=	6.6149
XX=	30.7465	YX=	2.7916	ZX=	1.4106	
XY=	-0.7065	YY=	24.1887	ZY=	0.5947	
XZ=	-1.5023	YZ=	2.1196	ZZ=	24.5728	
Eigenvalues:	22.923	25.6724	30.9126			
55	N	Isotropic=	135.8642	Anisotropy	=	121.498
XX=	128.439	YX=	-19.1311	ZX=	42.5377	
XY=	-16.4136	YY=	213.0722	ZY=	-6.6269	
XZ=	40.0815	YZ=	12.5095	ZZ=	66.0814	
Eigenvalues:	44.8344	145.8953		216.8629		
56	C	Isotropic=	46.6625	Anisotropy	=	194.3327
XX=	127.4529	YX=	-65.5282	ZX=	-61.3501	
XY=	-67.3331	YY=	-1.4509	ZY=	7.6379	
XZ=	-57.408	YZ=	7.6613	ZZ=	13.9856	
Eigenvalues:	-37.1911	10.961	176.2177			
57	H	Isotropic=	25.6576	Anisotropy	=	7.1718
XX=	24.544	YX=	0.301	ZX=	0.8649	
XY=	-1.8	YY=	29.3093	ZY=	-4.0341	
XZ=	0.8916	YZ=	-1.1959	ZZ=	23.1194	
Eigenvalues:	22.0282	24.5057	30.4388			
58	H	Isotropic=	29.7152	Anisotropy	=	13.8429
XX=	24.95	YX=	-2.4708	ZX=	0.6743	
XY=	-1.864	YY=	28.571	ZY=	6.7198	
XZ=	-1.5294	YZ=	4.6688	ZZ=	35.6246	
Eigenvalues:	23.3982	26.8036	38.9438			
59	C	Isotropic=	13.7969	Anisotropy	=	115.6725
XX=	53.6278	YX=	57.025	ZX=	3.1945	
XY=	57.3065	YY=	-36.4089	ZY=	46.1326	
XZ=	8.5766	YZ=	38.0119	ZZ=	24.1718	
Eigenvalues:	-76.914	27.3928	90.9119			
60	H	Isotropic=	26.5343	Anisotropy	=	6.8211
XX=	24.8913	YX=	-2.1029	ZX=	-2.8119	
XY=	0.6458	YY=	28.0074	ZY=	-5.3295	
XZ=	-2.0918	YZ=	-1.629	ZZ=	26.7041	
Eigenvalues:	21.8968	26.6243	31.0817			
61	C	Isotropic=	66.0066	Anisotropy	=	170.1688
XX=	141.2874	YX=	-40.4202	ZX=	-61.086	
XY=	-34.6896	YY=	66.3777	ZY=	19.523	
XZ=	-62.6927	YZ=	23.0505	ZZ=	-9.6453	
Eigenvalues:	-32.3888	50.9561	179.4524			
62	C	Isotropic=	61.0006	Anisotropy	=	178.7187
XX=	148.1932	YX=	-47.7658	ZX=	-34.5234	
XY=	-48.8637	YY=	1.8026	ZY=	55.343	
XZ=	-33.2458	YZ=	58.6033	ZZ=	33.006	
Eigenvalues:	-43.594	46.4494	180.1464			
63	C	Isotropic=	64.343	Anisotropy	=	174.8536

XX= 131.0802 YX= -71.0698 ZX= -56.3852
 XY= -71.7601 YY= 13.3045 ZY= -13.1937
 XZ= -55.4432 YZ= -12.3471 ZZ= 48.6443
 Eigenvalues: -36.964 49.081 180.9121
 64 C Isotropic= 62.1225 Anisotropy = 174.5886
 XX= 138.0999 YX= -38.1385 ZX= -66.5301
 XY= -36.85 YY= 63.6883 ZY= 22.0635
 XZ= -66.244 YZ= 19.6149 ZZ= -15.4205
 Eigenvalues: -40.581 48.4337 178.5149
 65 C Isotropic= 64.4234 Anisotropy = 149.1938
 XX= 138.9744 YX= -35.7739 ZX= -27.6407
 XY= -39.45 YY= 11.3399 ZY= 53.3008
 XZ= -26.8908 YZ= 51.154 ZZ= 42.9558
 Eigenvalues: -28.7184 58.1026 163.8859
 66 H Isotropic= 23.0587 Anisotropy = 10.7861
 XX= 21.8547 YX= 4.9545 ZX= 0.9275
 XY= 4.3657 YY= 27.6589 ZY= -1.1649
 XZ= 0.8328 YZ= -0.1942 ZZ= 19.6624
 Eigenvalues: 18.3467 20.5799 30.2494
 67 O Isotropic= -134.2657 Anisotropy = 633.4267
 XX= 1.2311 YX= 219.184 ZX= 259.9693
 XY= 264.7719 YY= -118.6334 ZY= 16.9963
 XZ= 260.622 YZ= 66.3222 ZZ= -285.3948
 Eigenvalues: -467.9698 -222.8461 288.0188
 68 C Isotropic= 58.487 Anisotropy = 166.3763
 XX= 40.2589 YX= 0.0492 ZX= -7.6766
 XY= -17.5338 YY= 89.0133 ZY= 92.2974
 XZ= -18.5539 YZ= 103.1705 ZZ= 46.1889
 Eigenvalues: -32.7631 38.8197 169.4045
 69 H Isotropic= 23.7125 Anisotropy = 5.1054
 XX= 22.066 YX= 2.4028 ZX= 1.8562
 XY= 2.298 YY= 24.9048 ZY= 0.3888
 XZ= 1.9565 YZ= 0.9935 ZZ= 24.1668
 Eigenvalues: 20.2451 23.7764 27.1161
 70 H Isotropic= 23.8674 Anisotropy = 3.1635
 XX= 21.7403 YX= 1.4417 ZX= 1.4783
 XY= 1.4307 YY= 24.8637 ZY= -1.1923
 XZ= 1.4612 YZ= -0.8869 ZZ= 24.9983
 Eigenvalues: 20.4966 25.1293 25.9765
 71 H Isotropic= 24.0609 Anisotropy = 5.4611
 XX= 21.9698 YX= 2.2403 ZX= 1.5172
 XY= 2.3396 YY= 26.4559 ZY= 0.3413
 XZ= 1.5776 YZ= 0.5827 ZZ= 23.7569
 Eigenvalues: 20.5053 23.9757 27.7016
 72 H Isotropic= 24.6974 Anisotropy = 8.0947
 XX= 22.5906 YX= 1.5483 ZX= 3.223
 XY= 1.2033 YY= 25.6659 ZY= 2.5399
 XZ= 2.8704 YZ= 3.4462 ZZ= 25.8357
 Eigenvalues: 20.723 23.2754 30.0939
 73 C Isotropic= 58.8258 Anisotropy = 176.1408
 XX= -16.8767 YX= -25.5303 ZX= 26.831
 XY= -22.0498 YY= 113.509 ZY= 72.2081
 XZ= 30.6387 YZ= 83.3404 ZZ= 79.845
 Eigenvalues: -40.8767 41.101 176.253
 74 C Isotropic= 62.5417 Anisotropy = 175.5191
 XX= -27.0829 YX= 17.4003 ZX= -26.6928

XY= 15.4392 YY= 118.7352 ZY= 71.6275
 XZ= -27.4809 YZ= 70.7063 ZZ= 95.9728
 Eigenvalues: -40.1575 48.2281 179.5544
 75 C Isotropic= 61.8185 Anisotropy = 178.5165
 XX= 45.8672 YX= 1.4309 ZX= -8.167
 XY= 1.8775 YY= 84.3091 ZY= 112.8161
 XZ= -8.3877 YZ= 107.0833 ZZ= 55.2792
 Eigenvalues: -41.7209 46.3469 180.8295
 76 C Isotropic= 63.8095 Anisotropy = 174.2009
 XX= -7.3139 YX= -34.3643 ZX= 27.3971
 XY= -32.487 YY= 108.5092 ZY= 81.2412
 XZ= 28.0847 YZ= 78.3831 ZZ= 90.2333
 Eigenvalues: -39.1896 50.6748 179.9434
 77 C Isotropic= 62.5013 Anisotropy = 182.6963
 XX= -18.1898 YX= -0.2874 ZX= -21.8903
 XY= 4.6157 YY= 121.2205 ZY= 75.694
 XZ= -26.5876 YZ= 81.1772 ZZ= 84.4734
 Eigenvalues: -27.3673 30.5724 184.2989
 78 H Isotropic= 23.5166 Anisotropy = 7.1509
 XX= 24.9938 YX= -3.4329 ZX= 1.758
 XY= -2.1601 YY= 22.5908 ZY= -2.4588
 XZ= 1.5796 YZ= -2.4064 ZZ= 22.9652
 Eigenvalues: 20.0609 22.205 28.2839
 79 H Isotropic= 23.7529 Anisotropy = 3.6429
 XX= 24.6104 YX= -0.3603 ZX= -0.3378
 XY= -0.202 YY= 23.3517 ZY= -3.0331
 XZ= -0.5856 YZ= -2.6608 ZZ= 23.2966
 Eigenvalues: 20.4112 24.666 26.1815
 80 H Isotropic= 23.6648 Anisotropy = 4.2977
 XX= 26.4536 YX= -0.462 ZX= 0.3041
 XY= -0.1039 YY= 22.2382 ZY= -1.7165
 XZ= 0.3339 YZ= -2.0484 ZZ= 22.3027
 Eigenvalues: 20.3877 24.0769 26.5299
 81 H Isotropic= 23.6543 Anisotropy = 6.0661
 XX= 25.0842 YX= -1.4641 ZX= 1.344
 XY= -1.1415 YY= 23.3582 ZY= -3.3187
 XZ= 1.6301 YZ= -3.1965 ZZ= 22.5206
 Eigenvalues: 19.6415 23.6231 27.6984
 82 H Isotropic= 21.7115 Anisotropy = 6.7918
 XX= 24.2624 YX= -1.5496 ZX= -0.3341
 XY= -0.5946 YY= 22.9817 ZY= -4.6091
 XZ= 0.5852 YZ= -4.7042 ZZ= 17.8905
 Eigenvalues: 15.1078 23.7874 26.2394