Supplementary Material (ESI) for Chemical Communications

A Synthetic Receptor for Hydrogen-bonding to Fluorines of Trifluroborates

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Electronic Supplementary Information

General Information	S1
Synthesis of receptor **1** and fluoroborates **5**-**9**	S2-S11
Titration experiments of receptor **1** and fluoroborates **5**-**9**	S12-S16
Computational study of fluoroborate **5** bound in **1**	S17-S36

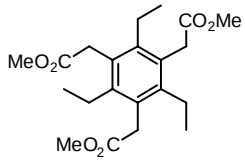
1. General Information

^{1}H NMR spectra were recorded on a Bruker DRX-600 spectrometer with a 5mm QNP probe. Proton chemical shifts are reported in parts per million with respect to tetramethylsilane (TMS $\delta = 0$, ^{1}H and ^{13}C NMR) or fluorotrichloromethane (^{19}F NMR, $\delta = 0$. Deuterated NMR solvents were obtained from Cambridge Isotope Laboratories, Inc., Andover, MA, and used without further purification. All chemicals were purchased from commercial suppliers and used without further purification.

2. Synthesis of receptor 1 and fluoroborates 5-9

2.1 Synthesis of receptor 1

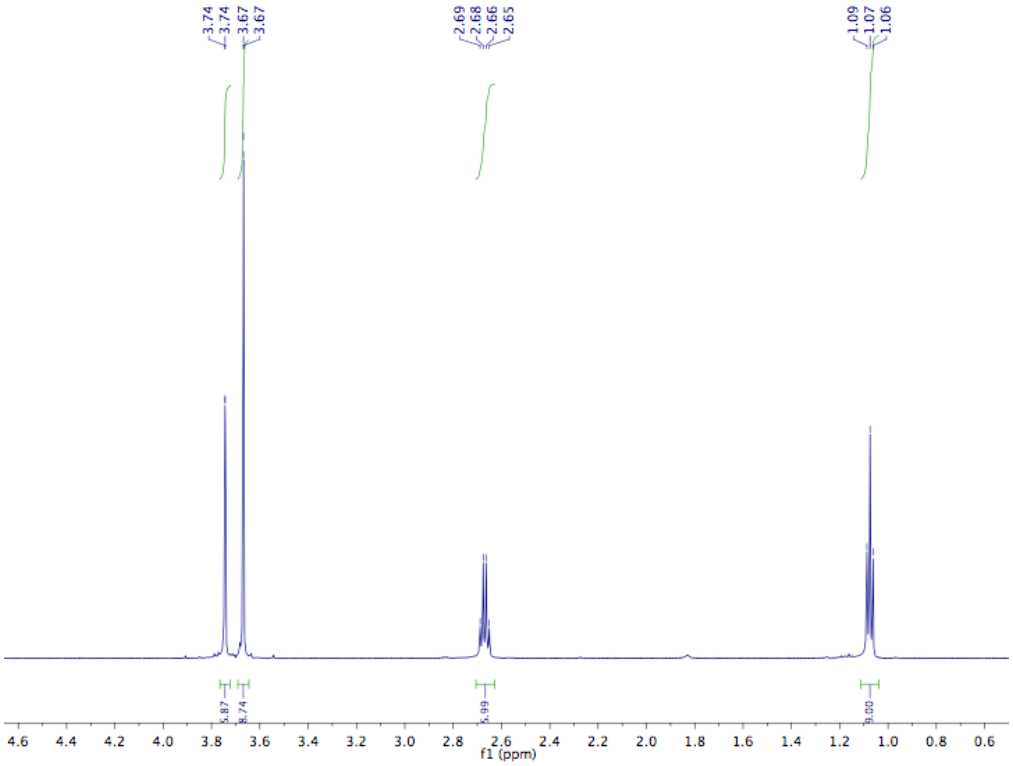
Triester 2

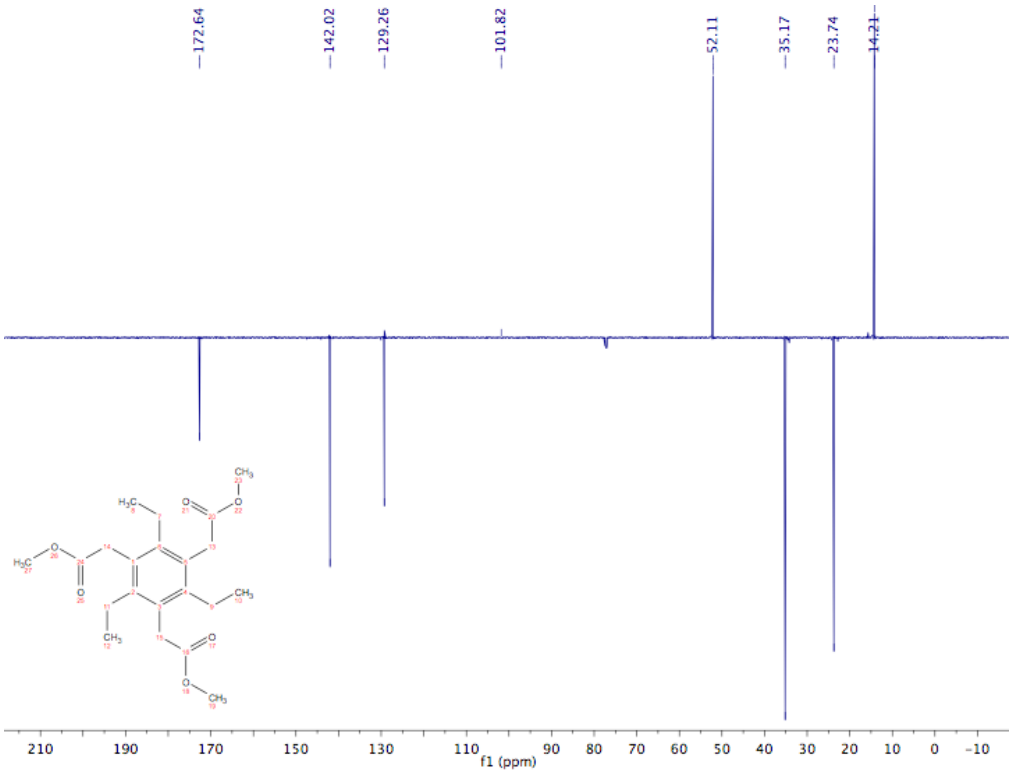


3

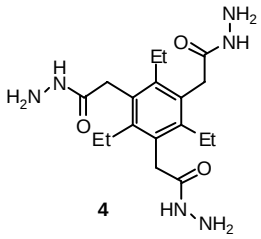
Triacid, **2**[1] (2.688 g, 8.0 mmol) was dissolved in 100 mL dry methanol. The mixture was stirred while conc. sulfuric acid (2 mL) was added dropwise. The reaction was refluxed for 16h and cooled to room temperature and the solvent was removed *in vacuo*. The resulting oil was dissolved in CH_2Cl_2 (100 mL) and washed with brine (50 mL) and water (50 mL). The organic phase was dried (Na_2SO_4) and the solvent was removed *in vacuo* to yield a yellow oil. Flash chromatography of the residue (SiO_2, CH_2Cl_2) yielded **3** as a white solid. Yield 1.977 g (65 %). ^{1}H NMR ($CDCl_3$, 600 MHz) δ 3.74 (s, 6H), 3.67 (s, 9H), 2.67 (q, J = 10.0 Hz, 6 H), 1.07 (t, J = 10.0 Hz, 9H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 172.64, 142.02, 129.26, 52.11, 35.17, 23.74, 14.21. MS (ESI) m/z (%) 401 (100) [M + Na] $^{+}$

[1] O'Leary, Brendan M.; Szabo, Tomas; Svenstrup, Niels; Schalley, Christoph A.; Luetzen, Arne; Schaefer, Mathias; Rebek, Julius, Jr. *J. Am. Chem. Soc.* **2001**, *123*, 11519-11533.


3.74
3.74
3.67
3.67
2.69
2.68
2.66
2.65
1.09
1.07
1.06
5.87
6.74
5.99
9.00
4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6
f1 (ppm)

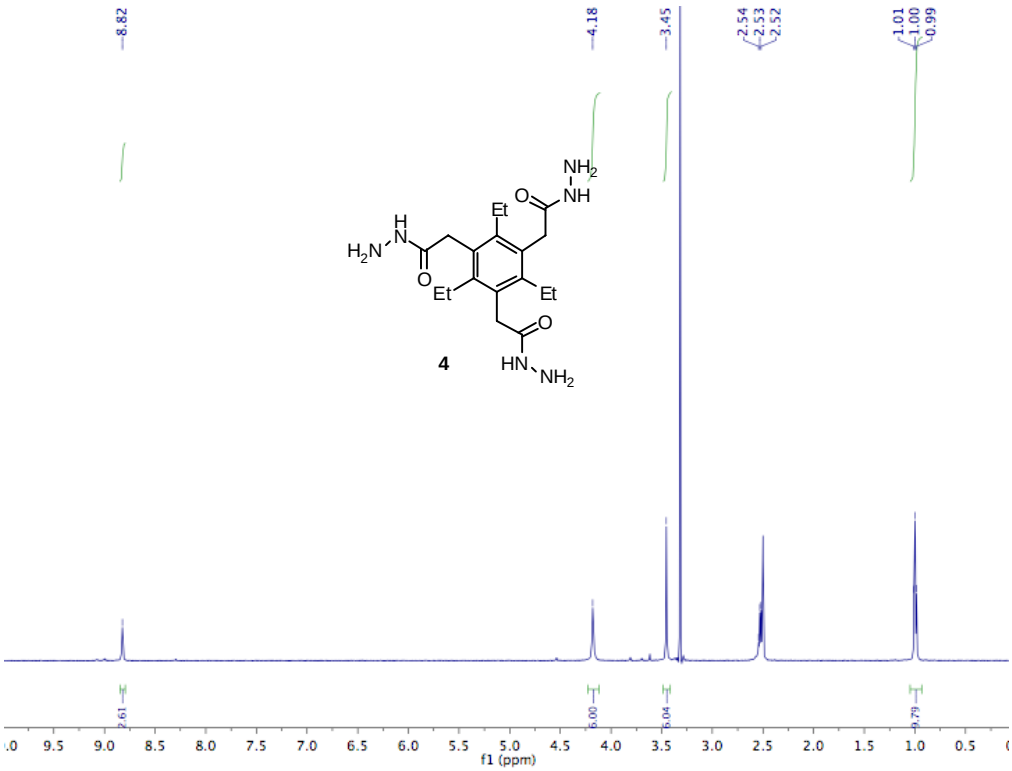

172.64
142.02
129.26
101.82
52.11
35.17
23.74
14.21
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Trihydrazide (4)

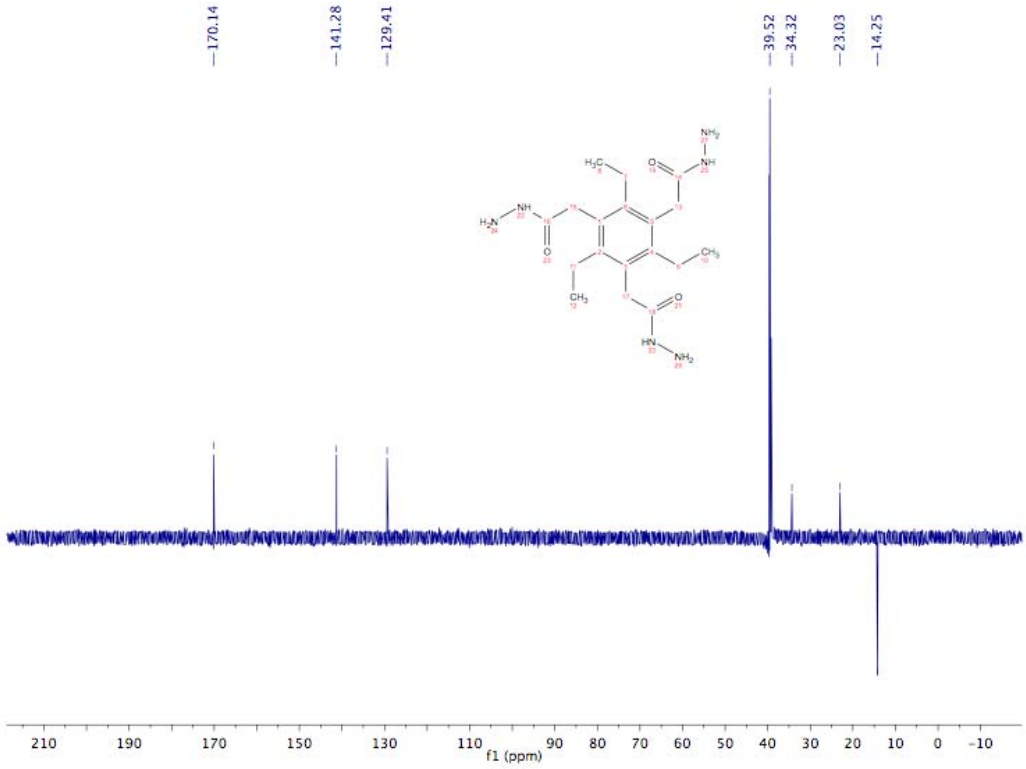


4

Trimethylester, **3** (0.50g, 1.32 mmol) was dissolved in EtOH (20 mL). The solution was heated to 60°C, hydrazine hydrate (1 mL, 0.17 mmol) was added dropwise and the solution was heated to reflux. After refluxing for 12h more hydrazine hydrate (1 mL, 0.17 mmol) was added and refluxing was continued for 9h. The suspension was cooled in an ice bath and filtered to give **4** as a white solid. Yield 0.284 g (57 %). ^{1}H NMR (DMSO-d_6, 600 MHz): δ 8.82 (s, 3H), 4.18 (s, 6H), 3.45 (s, 6H), 2.53 (q, J = 10.0 Hz, 6H), 1.00 (t, J = 10.0 Hz, 9H); ^{13}C NMR (DMSO-d_6, 150 MHz): δ (ppm) 170.13, 141.27, 129.40, 34.31, 23.02, 14.24. MS (ESI) m/z (%) 379 (100) $[M + H]^+$



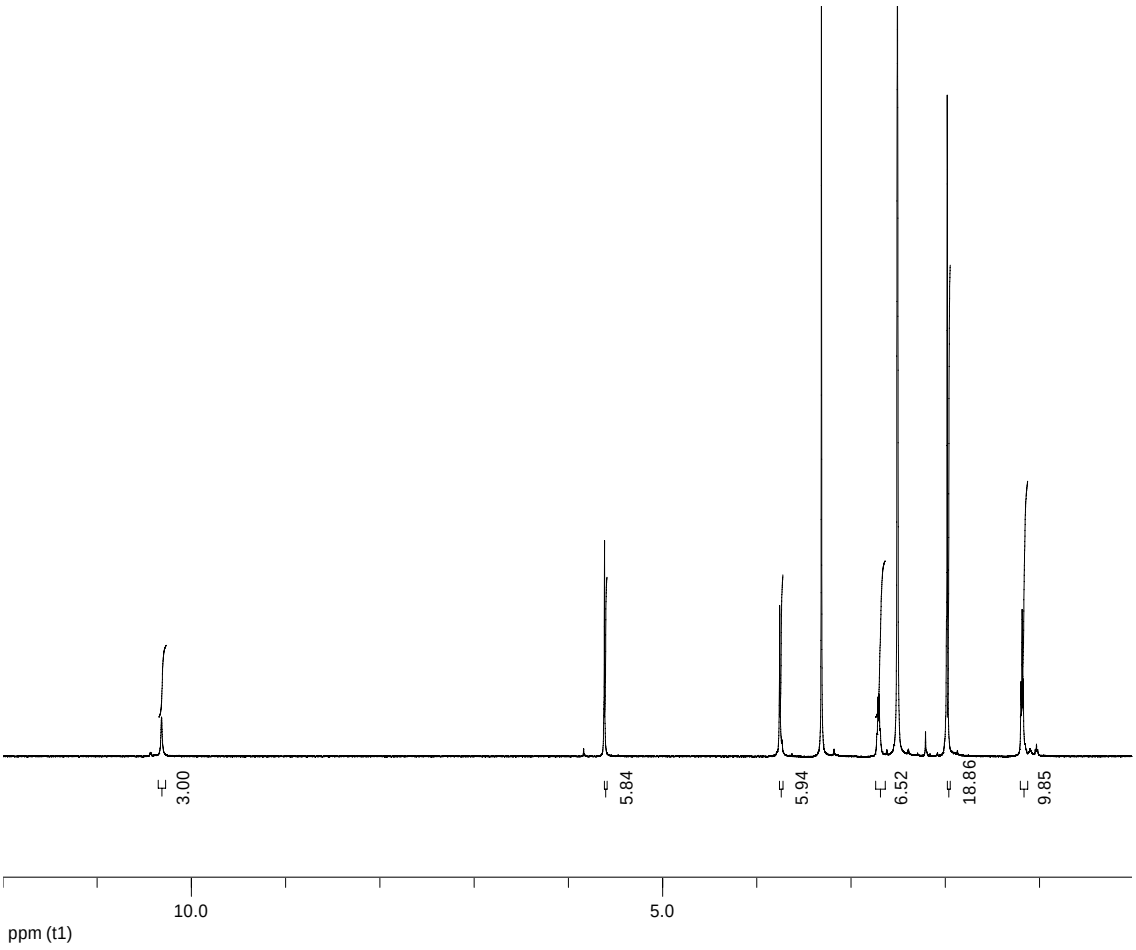
4

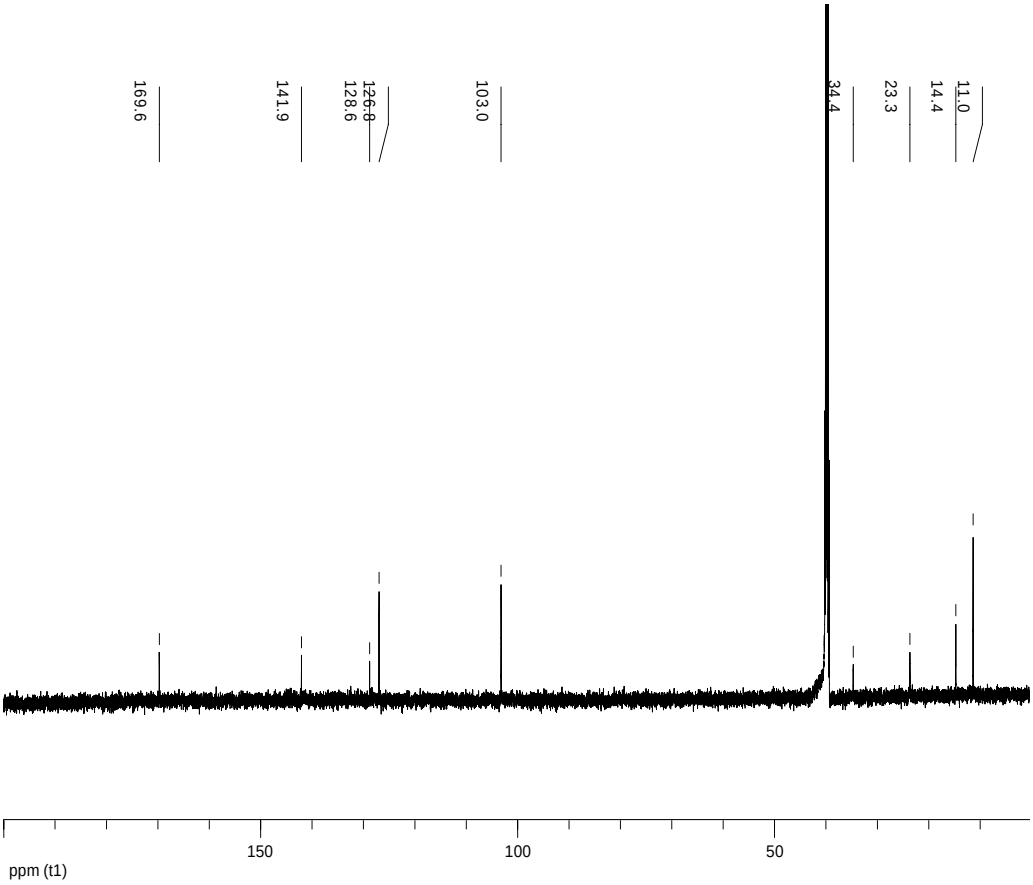

170.14
141.28
129.41
39.52
34.32
23.03
14.25
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Receptor 1

A suspension of trihydrazide **4** (50 mg, 0.14 mmol), 2,5-hexadione (165 μL, 1.4 mmol) in MeOH (4mL) and glacial acetic acid (100 μL) was heated to reflux for 3h. The white precipitate was filtered and washed several times with MeOH and hexanes to give a **1** (84 mg, 96%) as a white powder.

^{1}H NMR (DMSO-d_6, 600 MHz): δ 10.31 (s, 3H), 5.60 (s, 6H), 3.74 (s, 6H), 2.70 (q, J = 7.8 Hz, 6H), 1.96 (s, 18H), 1.16 (t, J = 7.8 Hz, 9H); ^{13}C NMR (DMSO-d_6, 150 MHz): δ 169.6, 141.9, 128.6, 126.8, 103.0, 34.4, 23.3, 14.4, 11.0. MS (ESI) m/z (%) 635 (100) [M + Na]$^{+}$





2.1 Synthesis of the fluoroborate salts 5-9

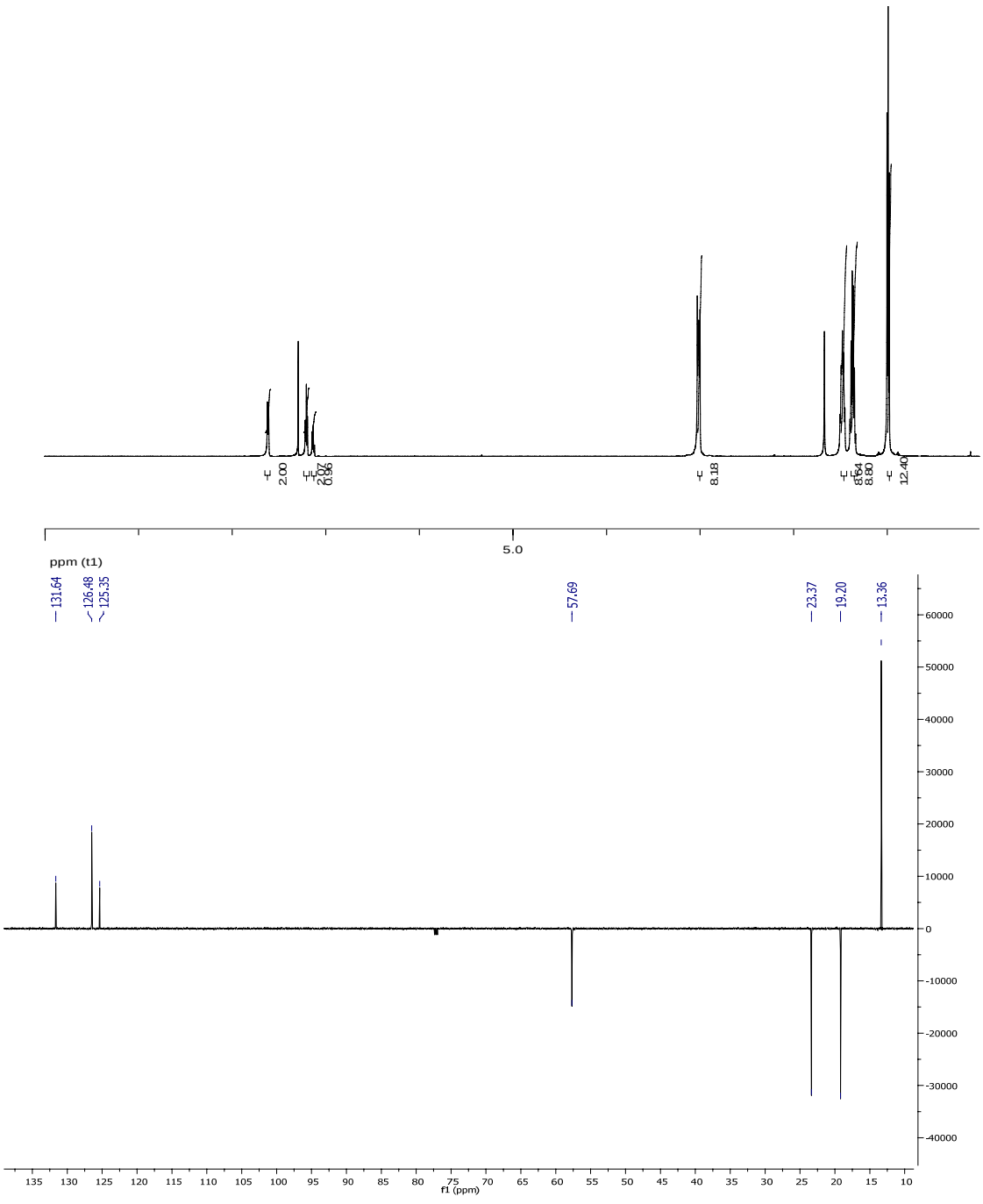
The tetra-*n*-butylammonium fluoroborates **5-8** were prepared from the corresponding commercially available potassium salts by ion-exchange according to the general procedure:

To a suspension of the potassium fluoroborate salt (2.2 mmol, 1 equiv.) in CH_2Cl_2 (15 mL) was added NBu_4OH (1.54 M in H_2O, 1.51 mL, 1 equiv.) and the solution was stirred for 30 minutes. The organic phase was separated and washed with H_2O (2x15 mL), dried (Na_2SO_4), filtered and evaporated. The tetra-*n*-butyl ammonium salts of phenylfluoroborate **5**[2], methylfluoroborate **6** and *p*-tolylfluoroborate **8** and *p*-methoxy-phenylfluoroborate **9** were received as white solids; *p*-nitro-phenylfluoroborate **7** was isolated as a yellowish solid all in quantitative yields.

[2] Batey, R. A.; Quach T. D. *Tet. Lett.* **2001**, *42*, 9099-9103.

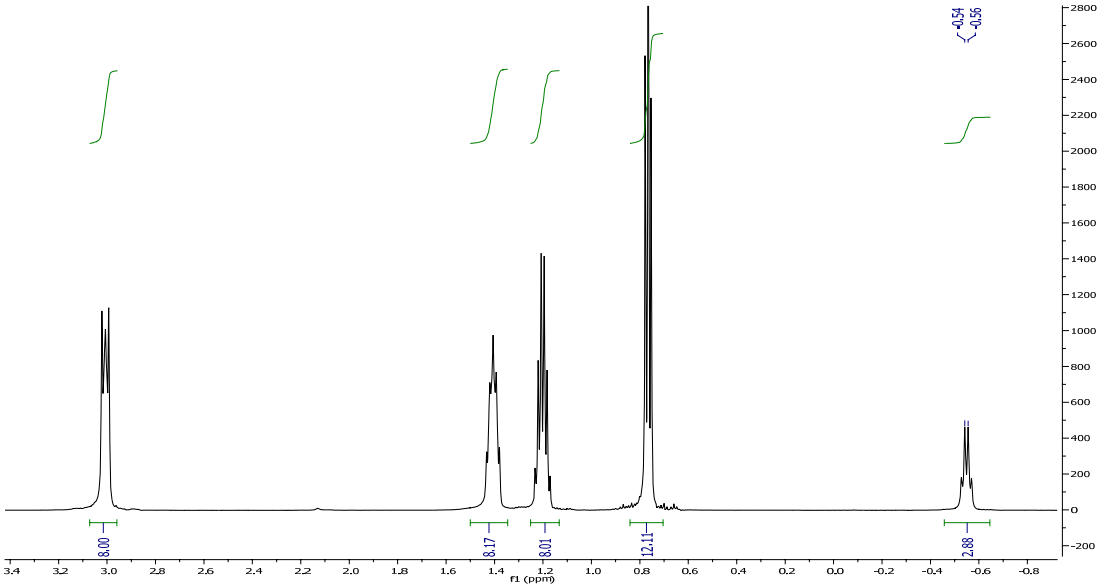
Tetra-*n*-butylammonium phenylfluoroborate **5**

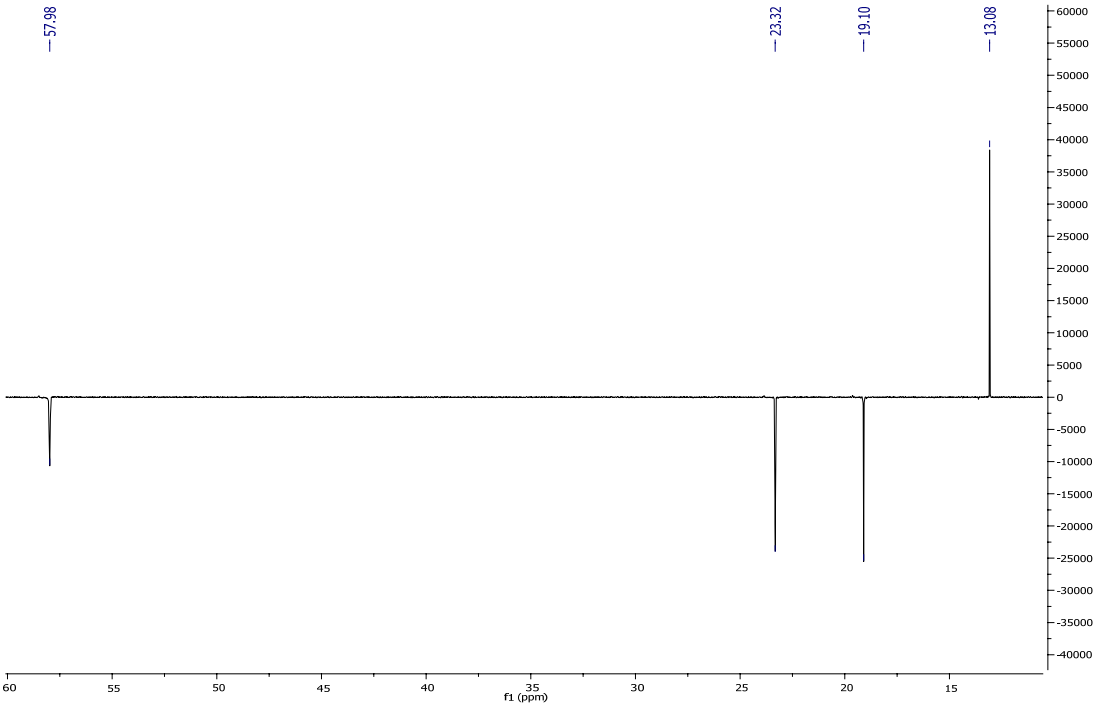
^{1}H NMR ($CDCl_3$, 600 MHz) δ 7.44 (d, *J* = 6.8 Hz, 2H), 7.06 (d, *J* = 7.3 Hz, 2H), 6.99 (t, *J* = 7.2 Hz, 1H), 2.72 (m, 8H), 1.20 (m, 8H), 1.17 (m, 8H), 0.82 (t, *J* = 7.2 Hz, 12H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ 131.6, 126.4, 125.3, 57.6, 23.3, 19.2, 13.3 (one signal missing); ^{19}F NMR ($CDCl_3$, 565 MHz) δ -142.03 (s, b).



Tetra-*n*-butylammonium methylfluoroborate **6**

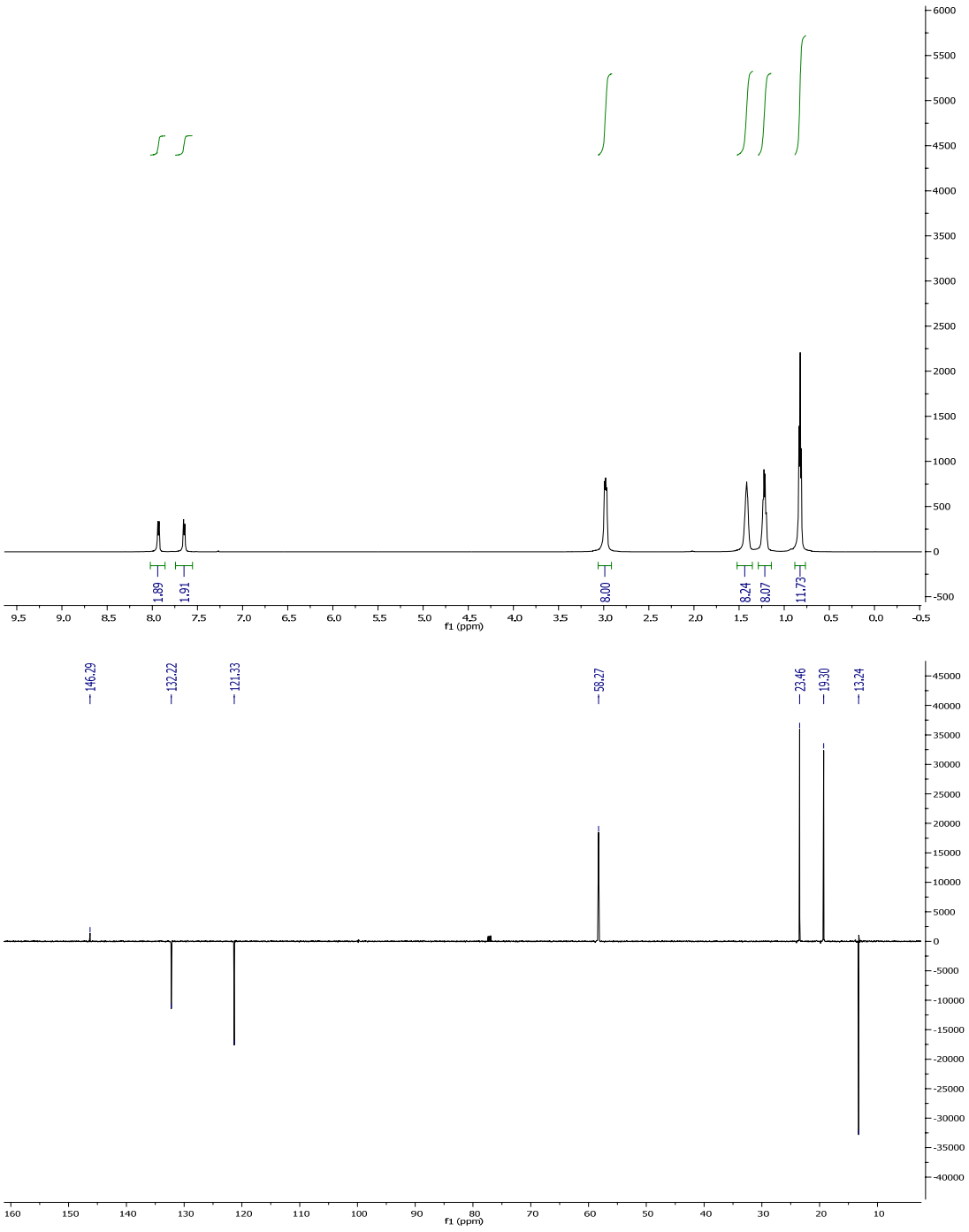
^{1}H NMR ($CDCl_3$, 600 MHz) δ 3.24 (m, 8H), 1.63 (m, 8H), 1.43 (hextett, J = 7.8 Hz, 8H), 1.01 (t, J = 7.8 Hz, 12H), -0.55 (q, J = 8.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ 57.9, 23.3, 19.1, 13.1 (one signal missing); ^{19}F NMR ($CDCl_3$, 565 MHz) δ -134.9.





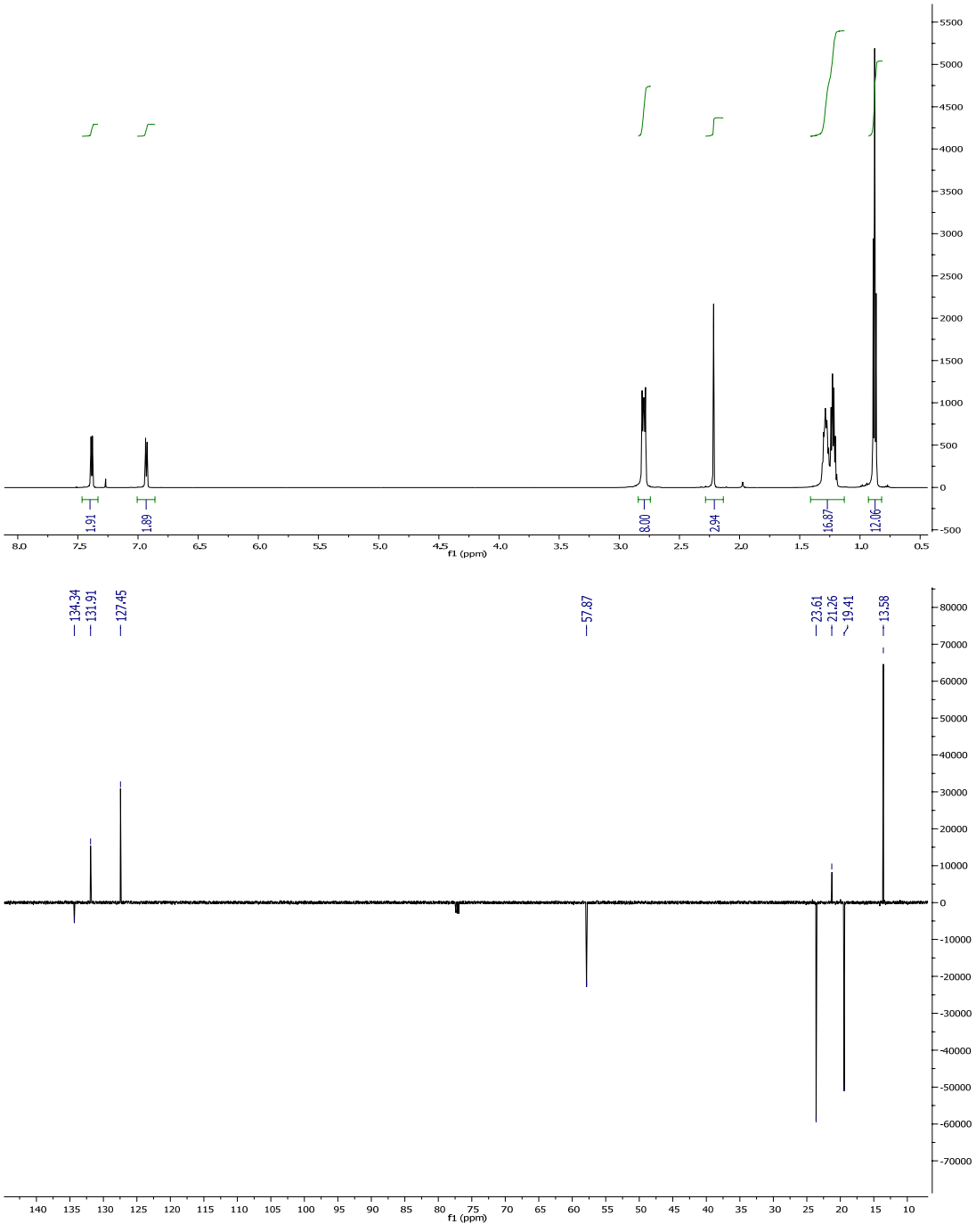
Tetra-*n*-butylammonium *p*-nitro-phenylfluoroborate **7**

^{1}H NMR ($CDCl_3$, 600 MHz) δ 7.93 (d, *J* = 7.8 Hz, 2H), 7.65 (d, *J* = 7.7 Hz, 2H), 2.98 (m, 8H), 1.42 (m, 8H), 1.22 (hextett, *J* = 7.1 Hz, 8H), 0.82 (t, *J* = 7.2 Hz, 12H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ 146.3, 132.2, 121.3, 58.3, 23.5, 19.3, 13.2 (one signal missing); ^{19}F NMR ($CDCl_3$, 565 MHz) δ -143.0.



Tetra-*n*-butylammonium *p*-tolylfluoroborate **8**

^{1}H NMR ($CDCl_3$, 600 MHz) δ 7.39 (d, J = 7.6 Hz, 2H), 6.93 (d, J = 7.4 Hz, 2H), 2.80 (m, 8H), 2.22 (s, 3H), 1.29 (m, 8H), 1.22 (hextett, J = 7.2 Hz, 8H), 0.88 (t, J = 7.2 Hz, 12H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ 134.3, 131.9, 127.4, 57.8, 23.6, 21.26, 19.4, 13.6 (one signal missing); ^{19}F NMR (DMSO-d_6 565 MHz) δ -138.3.



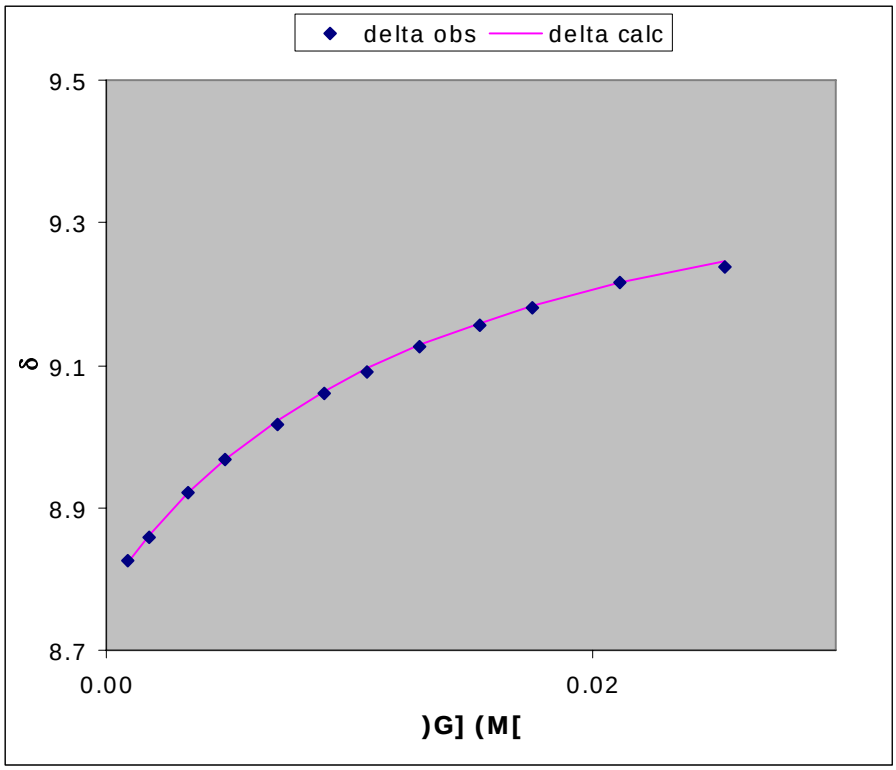
3. NMR titration experiments

The anion stock solutions were prepared by diluting the fluoroborate salt with a known amount of receptor stock solution in $CDCl_3$:MeCN (97:3) such that a constant receptor concentration is maintained throughout the titration. Aliquots from the guest stock solution were then added to the initial solution of receptor (c:a 0.5 mM) and the chemical shift of the acyl-hydrazide NH protons of **1** were measured at different guest concentrations. The reported association constants were calculated from the hydrazide NH protons of receptor **1**. These peaks were chosen for analysis for their sensitivity since they exhibits the largest change throughout the titration. Association constants were determined by fitting the data to 1:1 binding isotherms using Excel (see: http://www.dur.ac.uk/j.m.sanderson/science/downloads.html) and are presented as an average of two or three measurements. Due to the low solubility of receptor **1** the receptor concentration was determined by integrating the receptor signals and comparing them to the internal standard trifluorobenzene (1.47 mM). The $CDCl_3$ was passed through a short plug of activated basic Al_2O_3 to remove water and acidic impurities prior to the NMR titrations. All additions were done through septa with Hamilton gas tight syringes to minimize evaporation. All proton signals were referenced to the residual solvent peak $CDCl_3$ (7.27 ppm).

3.1 Titration experiments of phenylfluoroborate 5 and receptor 1

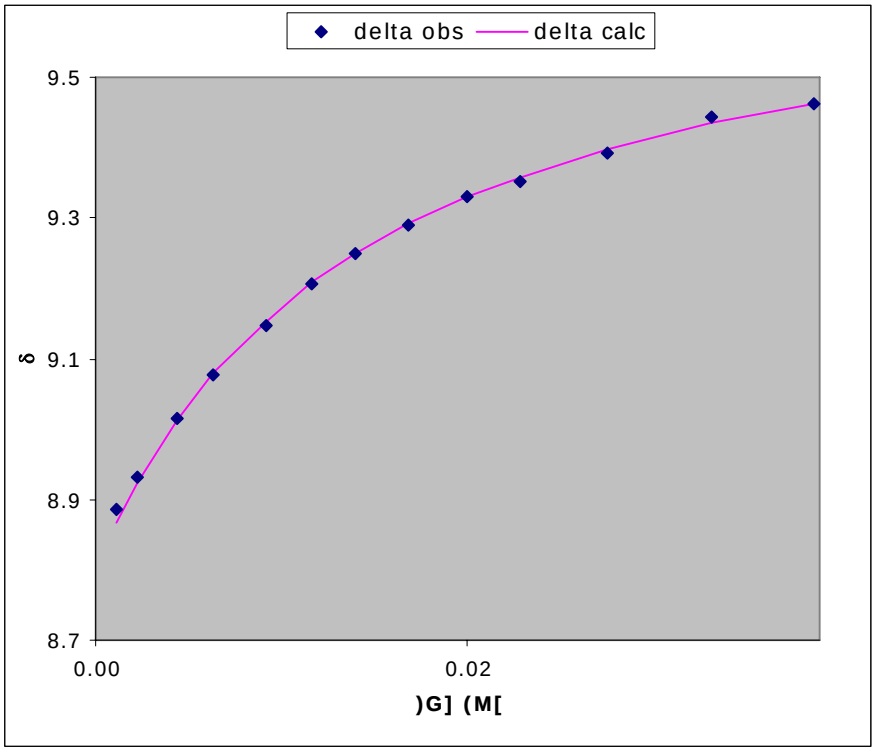
Addition	Vol Guest Added (L)	Total Volume in tube (L)	[Guest] (M)	Equiv. Guest	[Host] (M)	NH peak (ppm)
0	0	0.0006	0	0	0.000221627	8.78
1	0.00001	0.00061	0.000880253	3.971776927	0.000221627	8.825
2	0.00002	0.00062	0.001732111	7.815432018	0.000221627	8.8592
3	0.00004	0.00064	0.003355965	15.14239953	0.000221627	8.9202
4	0.00006	0.00066	0.004881403	22.02530841	0.000221627	8.9671
5	0.00009	0.00069	0.007003752	31.60152946	0.000221627	9.0175
6	0.00012	0.00072	0.008949239	40.37973209	0.000221627	9.0606
7	0.00015	0.00075	0.010739087	48.45567851	0.000221627	9.0908
8	0.00019	0.00079	0.012914092	58.26948682	0.000221627	9.1247
9	0.00024	0.00084	0.015341552	69.22239787	0.000221627	9.155
10	0.00029	0.00089	0.017496265	78.94464476	0.000221627	9.1817
11	0.00039	0.00099	0.021152746	95.44300313	0.000221627	9.2165
12	0.00054	0.00114	0.025434679	114.7634491	0.000221627	9.2383

ss residuals	0.000148587
weighted ss	1.77262E-06
Ka	**73 M^{-1}**



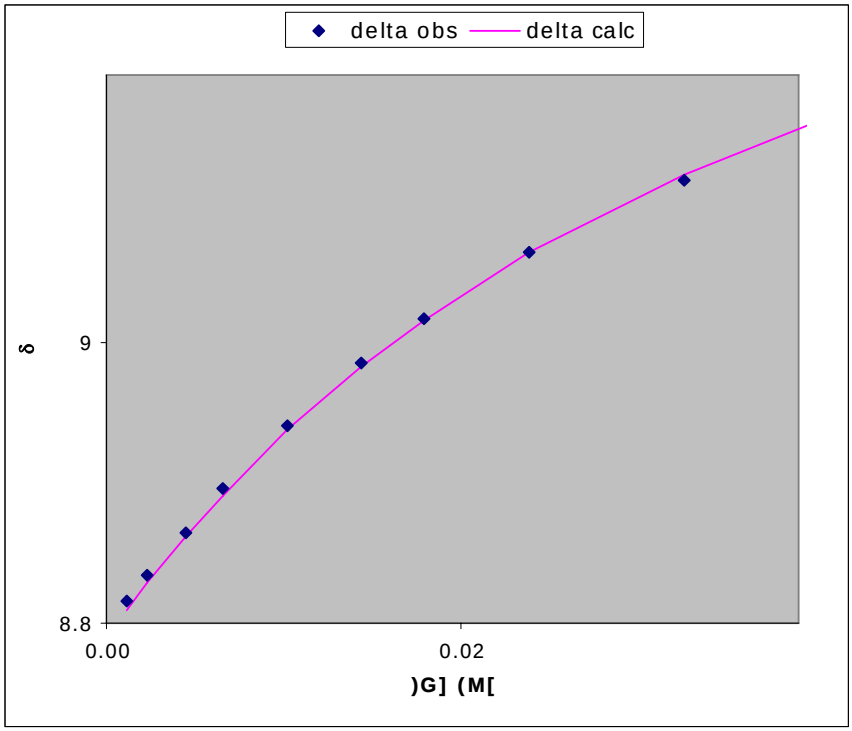
3.2 Titration experiments of methylfluoroborate 6 and receptor 1

Addition	Vol Guest Added (L)	Total Volume in tube (L)	[Guest] (M)	Equiv. Guest	[Host] (M)	NH peak (ppm)
0	0	0.0006	0	0	0.000739	8.8009
1	0.00001	0.00061	0.001149	1.555795772	0.000739	8.8849
2	0.00002	0.00062	0.0022609	3.061404583	0.000739	8.9327
3	0.00004	0.00064	0.0043805	5.93147138	0.000739	9.0142
4	0.00006	0.00066	0.0063717	8.627594734	0.000739	9.0777
5	0.00009	0.00069	0.0091419	12.37872288	0.000739	9.1476
6	0.00012	0.00072	0.0116814	15.81725701	0.000739	9.2065
7	0.00015	0.00075	0.0140176	18.98070842	0.000739	9.2493
8	0.00019	0.00079	0.0168567	22.82490253	0.000739	9.289
9	0.00024	0.00084	0.0200252	27.11529774	0.000739	9.3304
10	0.00029	0.00089	0.0228377	30.92362607	0.000739	9.3507
11	0.00039	0.00099	0.0276105	37.38624385	0.000739	9.3914
12	0.00054	0.00114	0.0331997	44.95430941	0.000739	9.444
13	0.0074	0.00134	0.0387054	52.40941876	0.000739	9.4619
		ss residuals	0.0006529			
		weighted ss	7.946E-06			
		Ka	**73 M^{-1}**			

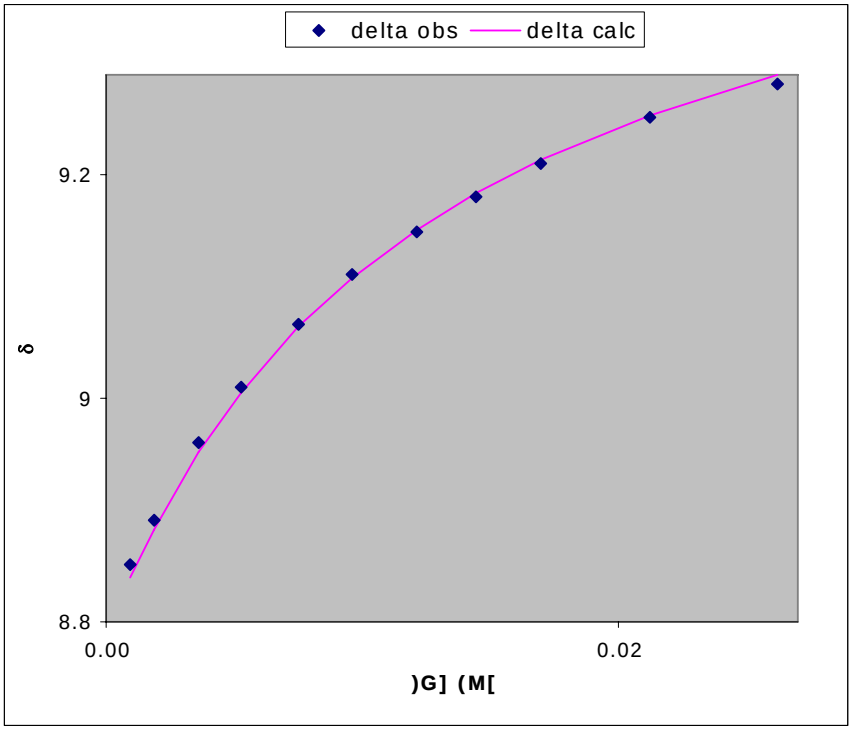


3.3 Titration experiments of *p*-NO_2-phenylfluoroborate 7 and receptor 1

Addition	Vol Guest Added (L)	Total Volume in tube (L)	[Guest] (M)	Equiv. Guest	[Host] (M)	NH peak (ppm)
0	0	0.0006	0	0	0.000739	8.7886
1	0.00001	0.00061	0.0011735	1.588959806	0.000739	8.8164
2	0.00002	0.00062	0.0023091	3.126662843	0.000739	8.8335
3	0.00004	0.00064	0.0044739	6.057909259	0.000739	8.8647
4	0.00006	0.00066	0.0065075	8.811504377	0.000739	8.896
5	0.00009	0.00069	0.010226	13.84664973	0.000739	8.9403
6	0.00012	0.00072	0.0143164	19.38530963	0.000739	8.9846
7	0.00015	0.00075	0.0178956	24.23163704	0.000739	9.017
8	0.00019	0.00079	0.0238607	32.30884938	0.000739	9.0634
9	0.00024	0.00084	0.0325374	44.05752188	0.000739	9.1155
10	0.00029	0.00089	0.041962	56.81901098	0.000739	9.1577
11	0.00039	0.00099	0.0459408	62.2065906	0.000739	9.1725
		ss residuals	0.0003315			
		weighted ss	4.051E-06			
		Ka	**25 M^{-1}**			



3.4 Titration experiments of *p*-tolylfluoroborate 8 and receptor 1

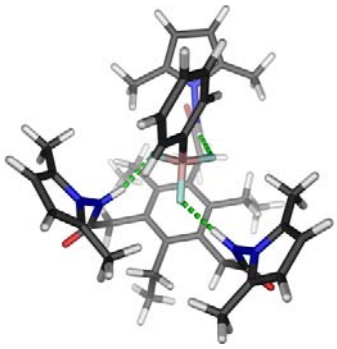


Addition	Vol Guest Added (L)	Total Volume in tube (L)	[Guest] (M)	Equiv. Guest	[Host] (M)	NH peak (ppm)
0	0	0.0006	0	0	0.00038403	8.7901
1	0.00001	0.00061	0.00094546	2.4619411	0.00038403	8.8514
2	0.00002	0.00062	0.001860422	4.8444709	0.00038403	8.8918
3	0.00004	0.00064	0.003604568	9.3861623	0.00038403	8.96
4	0.00006	0.00066	0.005243008	13.6526	0.00038403	9.0103
5	0.00009	0.00069	0.007522577	19.588513	0.00038403	9.0673
6	0.00012	0.00072	0.009612181	25.029766	0.00038403	9.1105
7	0.00016	0.00076	0.012141702	31.616547	0.00038403	9.1497
8	0.0002	0.0008	0.014418272	37.544649	0.00038403	9.181
9	0.00025	0.00085	0.016962673	44.170176	0.00038403	9.2106
10	0.00035	0.00095	0.021247979	55.328957	0.00038403	9.2525
11	0.0005	0.0011	0.026215039	68.262999	0.00038403	9.2821
			0.00036439			
		ss residuals				
			4.5266E-06			
		weighted ss				
		Ka	**80 M^{-1}**			

4. Computational Methods

Complete list of author for Guassian, Inc., Pittsburgh, PA, 2003:
Gaussian 03, Revision B.05,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,
A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 2003.

All calculations were performed using Gaussian 03. Geometries of stationary points were fully optimized using the B3LYP method and 6-31G* basis set. Vibrational frequencies were computed at the same level as the optimizations, in order to verify that stationary points were minima (zero imaginary frequencies), and to obtain unscaled zero-point energies (ZPEs) for correction of relative energies.
In order to obtain more reliable relative energies, single point energies were computed at the B3LYP /6-311+G(2d,p).The NMR calculation also performed at B3LYP/6-311+G(2d,p).



x –

B3LYP/6-311+G(2d,p)// B3LYP/6-31G(d)

E_{abs} = -2551.2854303 au

Charge = -1 Multiplicity = 1

C	-1.40437	-2.28517	1.16984
C	1.20963	-1.75515	2.11971
C	-0.28033	-2.84586	0.51816
C	-1.2142	-1.42604	2.27949
C	0.09603	-1.13138	2.72133
C	1.01654	-2.62862	1.03235
C	-2.40819	-0.82559	3.01535
H	-2.24778	0.25012	3.15493
H	-3.30843	-0.89579	2.40477
C	-2.71552	-1.47493	4.38181
H	-1.89662	-1.35497	5.09822
H	-3.61308	-1.02376	4.82199
C	2.60825	-1.51795	2.67565
H	3.34304	-1.54628	1.86492
H	2.68767	-0.51243	3.09371
C	3.01313	-2.52693	3.76915
H	3.00639	-3.55702	3.39513
H	2.32435	-2.48702	4.62039
H	4.02058	-2.30865	4.14242
C	-0.42455	-3.6938	-0.74231
H	0.49716	-3.63003	-1.32448
H	-1.1832	-3.25505	-1.39847
C	-0.7466	-5.18031	-0.49824
H	-0.79759	-5.72419	-1.44903
H	-1.70411	-5.31231	0.01666
H	0.02159	-5.65874	0.11988
C	-2.80808	-2.69898	0.69519
C	-3.777	-1.59067	0.22481
C	0.33309	-0.1925	3.89889
H	-0.60821	0.05893	4.38893
H	0.93956	-0.67759	4.66881
C	1.02333	1.16612	3.67953
C	2.19016	-3.41496	0.46159
H	1.88647	-4.44056	0.23733
H	2.97446	-3.52329	1.21486
C	2.93868	-2.96628	-0.80729
O	-4.96604	-1.60061	0.51489
O	1.71026	1.66299	4.56144
O	3.70867	-3.73773	-1.36152
N	0.75356	1.78966	2.49101
H	0.23683	1.3567	1.7214
N	-3.22486	-0.67187	-0.62981
H	-2.22119	-0.60291	-0.8124
H	-2.66601	-3.27757	-0.21962
H	-2.89536	-2.54911	4.27881
N	2.7355	-1.67687	-1.22031
H	2.06387	-1.03248	-0.79784
N	1.24807	3.05594	2.24829
C	2.52029	3.33896	1.77169
C	0.53249	4.22392	2.46928

C	1.36221	5.26311	2.11668
H	1.09682	6.31194	2.15696
C	2.60416	4.71032	1.68155
H	3.47287	5.25702	1.33728
C	3.50902	2.26272	1.4685
H	3.81778	1.72868	2.37712
H	3.09634	1.53126	0.76512
C	-0.87233	4.20256	2.97284
H	-1.24636	5.2279	3.05252
H	-0.9485	3.73846	3.96543
H	-1.54201	3.65181	2.29954
N	-4.03066	0.23068	-1.29467
C	-4.43224	1.4666	-0.80895
C	-4.57232	-0.00538	-2.55187
C	-5.31731	1.10657	-2.87075
H	-5.86469	1.24496	-3.79472
C	-5.23082	2.02446	-1.78125
H	-5.6967	2.99939	-1.71623
C	-4.31125	-1.27317	-3.29603
H	-3.23947	-1.44569	-3.46064
H	-4.79713	-1.227	-4.27559
H	-4.70675	-2.15119	-2.76709
C	-4.00264	1.969	0.52905
H	-4.43834	1.37483	1.3436
H	-4.3345	3.00459	0.65228
H	-2.9129	1.93777	0.63219
N	3.38732	-1.20534	-2.34277
C	4.67214	-0.68197	-2.34122
C	2.85286	-1.20182	-3.62393
C	3.8142	-0.65435	-4.44242
H	3.70425	-0.4959	-5.50763
C	4.9509	-0.33131	-3.6421
H	5.87828	0.1133	-3.9807
C	5.48866	-0.59406	-1.09528
H	5.67768	-1.58563	-0.66309
H	5.00546	0.01819	-0.32246
H	6.4562	-0.13736	-1.32582
C	1.48489	-1.72595	-3.91379
H	1.42148	-2.81104	-3.74898
H	1.23976	-1.53438	-4.96308
H	0.71901	-1.24928	-3.29201
C	-3.54107	-3.64518	1.667
H	-3.9508	-3.11574	2.52777
H	-2.85539	-4.42002	2.02554
H	-4.38333	-4.12395	1.15914
H	4.40286	2.70597	1.01863
C	-0.07346	2.14021	-2.01338
C	-0.23052	4.33098	-3.80362
C	0.77817	3.25082	-1.88777
C	-1.00511	2.16272	-3.06423
C	-1.08878	3.23959	-3.94959
C	0.70505	4.33329	-2.76654
H	1.51162	3.27321	-1.08501
H	-1.68108	1.32045	-3.19139
H	-1.82534	3.22744	-4.75092
H	1.37843	5.17936	-2.64186
H	-0.29068	5.17301	-4.49098
B	-0.01406	0.91761	-0.97535
F	1.31713	0.61994	-0.54553
F	-0.76832	1.17934	0.22452
F	-0.56477	-0.28826	-1.53381

SCF GIAO Magnetic shielding tensor (ppm):
1 C Isotropic = 35.3922 Anisotropy = 170.2721
XX= -40.9979 YX= 8.2252 ZX= -21.7985
XY= 8.2582 YY= 91.8756 ZY= 75.4038
XZ= -22.3350 YZ= 70.1749 ZZ= 55.2989
Eigenvalues: -51.3653 8.6350 148.9069
2 C Isotropic = 31.1176 Anisotropy = 187.2914
XX= -55.2358 YX= 2.5570 ZX= -31.0741

XY= 1.8617 YY= 93.2083 ZY= 75.9646
XZ= -29.7902 YZ= 80.0700 ZZ= 55.3803
Eigenvalues: -67.0258 4.4001 155.9786
3 C Isotropic = 30.5893 Anisotropy = 184.5694
XX= -1.9124 YX= -7.0014 ZX= -14.6513
XY= -4.8255 YY= 78.5457 ZY= 109.3357
XZ= -7.5873 YZ= 92.8890 ZZ= 15.1348
Eigenvalues: -59.6486 -2.2190 153.6356
4 C Isotropic = 31.8894 Anisotropy = 185.1077
XX= -36.9885 YX= -23.8898 ZX= 18.3718
XY= -24.7250 YY= 83.7621 ZY= 85.9974
XZ= 16.6991 YZ= 87.8424 ZZ= 48.8947
Eigenvalues: -59.7104 0.0841 155.2945
5 C Isotropic = 44.0898 Anisotropy = 164.7618
XX= 35.3881 YX= 0.1618 ZX= -13.8051
XY= -0.6525 YY= 73.5417 ZY= 94.7511
XZ= -15.5160 YZ= 108.6810 ZZ= 23.3397
Eigenvalues: -57.7262 36.0646 153.9310
6 C Isotropic = 43.9931 Anisotropy = 161.8560
XX= -16.8742 YX= -45.9190 ZX= 16.1359
XY= -41.0221 YY= 80.3964 ZY= 75.6028
XZ= 18.7630 YZ= 73.7140 ZZ= 68.4572
Eigenvalues: -52.9686 33.0509 151.8972
7 C Isotropic = 153.7888 Anisotropy = 17.1371
XX= 156.4892 YX= 5.4756 ZX= -6.3876
XY= 5.3873 YY= 149.4495 ZY= 0.2071
XZ= -9.8898 YZ= -0.4963 ZZ= 155.4276
Eigenvalues: 144.5734 151.5794 165.2135
8 H Isotropic = 28.8007 Anisotropy = 4.6012
XX= 27.9670 YX= -0.4937 ZX= -0.6504
XY= -0.2632 YY= 31.8298 ZY= -1.3604
XZ= 0.3249 YZ= 1.1424 ZZ= 26.6052
Eigenvalues: 26.5815 27.9523 31.8682
9 H Isotropic = 28.9100 Anisotropy = 8.9787
XX= 29.0462 YX= -0.8908 ZX= 3.1345
XY= 1.0541 YY= 25.1773 ZY= -1.5352
XZ= 4.0116 YZ= -1.4000 ZZ= 32.5064
Eigenvalues: 24.6932 27.1409 34.8958
10 C Isotropic = 164.0912 Anisotropy = 31.4483
XX= 159.6029 YX= -0.6251 ZX= -10.0104
XY= -5.6549 YY= 155.1117 ZY= 6.7361
XZ= -13.2566 YZ= 6.4509 ZZ= 177.5589
Eigenvalues: 153.3175 153.8994 185.0567
11 H Isotropic = 30.4703 Anisotropy = 7.0304
XX= 31.4291 YX= -2.1547 ZX= 1.1275
XY= -3.2057 YY= 25.3139 ZY= 2.1415
XZ= 1.5736 YZ= -0.1614 ZZ= 34.6679
Eigenvalues: 24.1173 32.1364 35.1572
12 H Isotropic = 30.5905 Anisotropy = 11.8714
XX= 32.5388 YX= 1.7049 ZX= -4.9458
XY= 0.6629 YY= 26.1929 ZY= -0.3728
XZ= -6.1452 YZ= -1.2981 ZZ= 33.0399
Eigenvalues: 25.9683 27.2984 38.5048
13 C Isotropic = 154.1695 Anisotropy = 18.2800
XX= 161.5469 YX= -1.5473 ZX= 5.7051
XY= 3.9374 YY= 148.9357 ZY= 3.9074
XZ= 10.0070 YZ= 2.3151 ZZ= 152.0258
Eigenvalues: 145.9206 150.2317 166.3562
14 H Isotropic = 28.7277 Anisotropy = 6.0439
XX= 29.3095 YX= 0.1745 ZX= -1.9762
XY= -1.9271 YY= 25.3459 ZY= 0.0170
XZ= -2.1203 YZ= -0.4623 ZZ= 31.5277
Eigenvalues: 25.0870 28.3391 32.7570
15 H Isotropic = 28.6713 Anisotropy = 7.3133
XX= 27.7729 YX= 1.5158 ZX= 0.9045
XY= 0.6407 YY= 33.1114 ZY= -2.2938
XZ= -0.4032 YZ= -0.6052 ZZ= 25.1295
Eigenvalues: 24.8083 27.6587 33.5468
16 C Isotropic = 167.4633 Anisotropy = 27.3260
XX= 167.0509 YX= 0.9342 ZX= 10.0439

XY= 4.5891 YY= 165.6041 ZY= 12.4631
XZ= 11.9311 YZ= 11.5674 ZZ= 169.7350
Eigenvalues: 153.0435 163.6657 185.6807
17 H Isotropic = 30.7218 Anisotropy = 7.4708
XX= 26.8160 YX= 1.9474 ZX= 1.2951
XY= 3.6877 YY= 34.6393 ZY= -0.2740
XZ= 3.0241 YZ= 0.6459 ZZ= 30.7101
Eigenvalues: 25.1764 31.2867 35.7024
18 H Isotropic = 30.7165 Anisotropy = 7.7117
XX= 29.4014 YX= 2.0435 ZX= -1.8725
XY= 3.0675 YY= 27.6157 ZY= 3.5077
XZ= -0.8444 YZ= 1.1324 ZZ= 35.1325
Eigenvalues: 25.0869 31.2050 35.8577
19 H Isotropic = 30.6801 Anisotropy = 11.9719
XX= 34.6696 YX= 0.5535 ZX= 4.8739
XY= 1.7334 YY= 26.9609 ZY= 1.6801
XZ= 6.1242 YZ= 0.7153 ZZ= 30.4099
Eigenvalues: 26.3476 27.0314 38.6614
20 C Isotropic = 151.5628 Anisotropy = 18.5699
XX= 143.9663 YX= -3.0831 ZX= 1.8357
XY= -3.6950 YY= 156.7979 ZY= -10.4474
XZ= 0.2527 YZ= -5.3800 ZZ= 153.9241
Eigenvalues: 143.0064 147.7393 163.9427
21 H Isotropic = 28.8802 Anisotropy = 7.6779
XX= 31.7771 YX= -2.4320 ZX= -1.9156
XY= -3.9385 YY= 26.6197 ZY= 1.2892
XZ= -2.5079 YZ= -1.3089 ZZ= 28.2438
Eigenvalues: 24.7908 27.8510 33.9988
22 H Isotropic = 28.6663 Anisotropy = 5.1474
XX= 28.5874 YX= 2.0385 ZX= 0.7906
XY= 2.6079 YY= 28.3420 ZY= 1.9800
XZ= 2.8155 YZ= -0.0473 ZZ= 29.0695
Eigenvalues: 26.0086 27.8924 32.0979
23 C Isotropic = 166.9979 Anisotropy = 26.9200
XX= 156.2407 YX= -5.0438 ZX= 0.8120
XY= -6.0934 YY= 183.4836 ZY= -5.0437
XZ= -2.2424 YZ= -1.2357 ZZ= 161.2695
Eigenvalues: 154.8668 161.1824 184.9446
24 H Isotropic = 30.5458 Anisotropy = 11.7450
XX= 26.7172 YX= -1.4274 ZX= 0.5478
XY= -1.3789 YY= 34.2308 ZY= -6.2639
XZ= 0.2971 YZ= -4.6800 ZZ= 30.6895
Eigenvalues: 26.1441 27.1175 38.3759
25 H Isotropic = 30.5386 Anisotropy = 6.9668
XX= 32.6475 YX= -0.8543 ZX= -3.5123
XY= -2.3445 YY= 32.4818 ZY= -1.0118
XZ= -4.4997 YZ= -0.0381 ZZ= 26.4866
Eigenvalues: 24.3403 32.0924 35.1831
26 H Isotropic = 30.6205 Anisotropy = 7.9172
XX= 30.8499 YX= 1.0973 ZX= 2.1141
XY= 2.1251 YY= 34.6093 ZY= 0.9841
XZ= 2.5588 YZ= 2.6324 ZZ= 26.4021
Eigenvalues: 25.2777 30.6850 35.8986
27 C Isotropic = 136.2501 Anisotropy = 25.1900
XX= 137.6781 YX= 7.0679 ZX= 10.0371
XY= 4.6070 YY= 140.7440 ZY= 13.5692
XZ= 1.6569 YZ= 10.7336 ZZ= 130.3282
Eigenvalues: 122.1036 133.6032 153.0434
28 C Isotropic = 2.1776 Anisotropy = 118.4008
XX= 13.6882 YX= -13.4072 ZX= 10.0774
XY= -21.6312 YY= -27.7570 ZY= -78.0860
XZ= -4.3745 YZ= -79.1720 ZZ= 20.6015
Eigenvalues: -87.3759 12.7972 81.1114
29 C Isotropic = 138.9230 Anisotropy = 42.5281
XX= 125.8499 YX= -23.8073 ZX= 9.4389
XY= -13.6071 YY= 158.4947 ZY= 3.0467
XZ= 1.8405 YZ= 8.7784 ZZ= 132.4244
Eigenvalues: 114.1668 135.3270 167.2751
30 H Isotropic = 27.6142 Anisotropy = 6.9215
XX= 31.1811 YX= -2.8165 ZX= -0.1882

```
  XY=   -2.8437   YY=   24.5522   ZY=   -1.7220
  XZ=   -1.3138   YZ=   -1.5980   ZZ=   27.1093
  Eigenvalues:   22.7503   27.8638   32.2286
31 H   Isotropic =   28.1370   Anisotropy =    4.7776
  XX=   27.6351   YX=    1.5428   ZX=    0.8606
  XY=    2.4133   YY=   26.5159   ZY=    1.2745
  XZ=    2.8847   YZ=   -1.9943   ZZ=   30.2599
  Eigenvalues:   24.6382   28.4507   31.3220
32 C   Isotropic =    5.8792   Anisotropy =  115.5892
  XX=   56.4950   YX=   28.6754   ZX=  -19.3383
  XY=   39.6725   YY=  -38.9870   ZY=  -51.1340
  XZ=   -8.9782   YZ=  -65.2412   ZZ=    0.1298
  Eigenvalues:  -83.6847   18.3837   82.9387
33 C   Isotropic =  139.1922   Anisotropy =   40.8789
  XX=  136.7893   YX=    4.0530   ZX=  -16.2349
  XY=   -0.9191   YY=  132.4748   ZY=    8.7144
  XZ=  -29.5769   YZ=    1.4279   ZZ=  148.3123
  Eigenvalues:  117.6373  133.4944  166.4447
34 H   Isotropic =   28.0638   Anisotropy =    4.3905
  XX=   30.3001   YX=   -0.8109   ZX=   -0.3730
  XY=    0.3474   YY=   30.4522   ZY=   -3.0669
  XZ=    1.2051   YZ=   -0.3230   ZZ=   23.4393
  Eigenvalues:   23.0338   30.1668   30.9909
35 H   Isotropic =   27.8917   Anisotropy =    5.4327
  XX=   27.0497   YX=    1.6865   ZX=    1.6174
  XY=    3.6588   YY=   26.2634   ZY=   -2.4540
  XZ=    2.3746   YZ=   -1.8806   ZZ=   30.3621
  Eigenvalues:   22.8070   29.3546   31.5135
36 C   Isotropic =    7.5805   Anisotropy =  112.4681
  XX=   50.7466   YX=   -1.6645   ZX=   41.6867
  XY=    8.8175   YY=  -21.0788   ZY=  -67.4551
  XZ=   46.5392   YZ=  -50.5981   ZZ=   -6.9263
  Eigenvalues:  -81.6204   21.8027   82.5592
37 O   Isotropic =  -72.8455   Anisotropy =  634.8557
  XX= -323.7384   YX=  -38.3357   ZX=  127.6513
  XY=  -11.5745   YY=   -5.2902   ZY= -265.5332
  XZ=  172.1008   YZ= -264.7957   ZZ=  110.4922
  Eigenvalues: -382.5067  -186.4214   350.3917
38 O   Isotropic =  -73.6060   Anisotropy =  592.0322
  XX=   96.2380   YX=  201.4704   ZX= -248.1954
  XY=  176.8612   YY=  -91.1492   ZY=  -83.2078
  XZ= -232.2592   YZ=  -54.7067   ZZ= -225.9069
  Eigenvalues: -358.0654  -183.8347   321.0821
39 O   Isotropic =  -68.1521   Anisotropy =  595.1016
  XX=   52.5522   YX= -190.9601   ZX=  246.7184
  XY= -195.7209   YY= -234.5254   ZY=  -59.3298
  XZ=  247.8538   YZ=  -64.9919   ZZ=  -22.4833
  Eigenvalues: -347.2282  -185.8104   328.5822
40 N   Isotropic =   98.5897   Anisotropy =  110.5183
  XX=   80.5230   YX=   63.9689   ZX=  -17.2815
  XY=   27.0661   YY=   92.2222   ZY=   35.2977
  XZ=  -37.5633   YZ=   89.0471   ZZ=  123.0238
  Eigenvalues:    6.0744  117.4260  172.2685
41 H   Isotropic =   21.8672   Anisotropy =   12.4322
  XX=   18.1183   YX=   -4.4127   ZX=    4.7702
  XY=   -4.2291   YY=   23.0039   ZY=   -3.6162
  XZ=    6.4062   YZ=   -0.6805   ZZ=   24.4794
  Eigenvalues:   13.9710   21.4753   30.1553
42 N   Isotropic =   99.7106   Anisotropy =  113.3512
  XX=   16.6636   YX=  -55.2001   ZX=  -35.2986
  XY=   -6.7754   YY=  139.6866   ZY=   23.4280
  XZ=   14.2156   YZ=   33.7450   ZZ=  142.7815
  Eigenvalues:    9.1944  114.6593  175.2781
43 H   Isotropic =   21.6690   Anisotropy =   12.0959
  XX=   29.7286   YX=   -0.7234   ZX=   -0.8431
  XY=    0.5521   YY=   17.6510   ZY=    4.4793
  XZ=    0.4893   YZ=    3.1076   ZZ=   17.6276
  Eigenvalues:   13.8456   21.4286   29.7330
44 H   Isotropic =   27.4214   Anisotropy =    6.9226
  XX=   28.2584   YX=    0.6174   ZX=   -2.5100
```

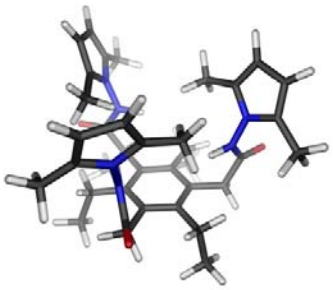
XY= 2.2286 YY= 26.0565 ZY= -2.3856
XZ= -3.2801 YZ= -1.8128 ZZ= 27.9493
Eigenvalues: 24.6042 25.6235 32.0365
45 H Isotropic = 30.8236 Anisotropy = 6.4077
XX= 27.3975 YX= -2.8556 ZX= -0.0558
XY= -4.2913 YY= 32.9116 ZY= 0.5748
XZ= -1.4705 YZ= 1.1663 ZZ= 32.1616
Eigenvalues: 25.6270 31.7484 35.0953
46 N Isotropic = 95.7213 Anisotropy = 112.1066
XX= 62.7088 YX= -13.0319 ZX= 55.4084
XY= -50.9553 YY= 144.9951 ZY= 76.3551
XZ= 38.5972 YZ= 18.6516 ZZ= 79.4600
Eigenvalues: 1.8616 114.8432 170.4590
47 H Isotropic = 21.8363 Anisotropy = 10.8025
XX= 21.5654 YX= 5.5554 ZX= -4.0685
XY= 3.4695 YY= 23.5923 ZY= 0.2436
XZ= -6.2470 YZ= -1.4840 ZZ= 20.3511
Eigenvalues: 14.8989 21.5720 29.0380
48 N Isotropic = 61.6138 Anisotropy = 73.8480
XX= 87.6289 YX= 42.2749 ZX= 4.3256
XY= 45.0919 YY= -3.9878 ZY= -22.2182
XZ= 0.8323 YZ= -22.4434 ZZ= 101.2004
Eigenvalues: -25.2070 99.2026 110.8458
49 C Isotropic = 45.1655 Anisotropy = 109.4140
XX= -8.7463 YX= -18.2889 ZX= 43.3391
XY= -12.3396 YY= 42.2055 ZY= -2.1650
XZ= 45.4464 YZ= 0.2876 ZZ= 102.0374
Eigenvalues: -27.2289 44.6173 118.1082
50 C Isotropic = 48.8581 Anisotropy = 105.4364
XX= 12.9338 YX= -28.3668 ZX= 37.0844
XY= -37.2172 YY= 30.3185 ZY= 7.6297
XZ= 43.4974 YZ= 4.1705 ZZ= 103.3222
Eigenvalues: -22.7315 50.1568 119.1491
51 C Isotropic = 75.5105 Anisotropy = 113.5476
XX= 73.7625 YX= -28.2113 ZX= 26.5008
XY= -31.3557 YY= 11.6109 ZY= 3.3507
XZ= 28.4399 YZ= 5.2357 ZZ= 141.1583
Eigenvalues: -1.8399 77.1626 151.2089
52 H Isotropic = 26.1865 Anisotropy = 3.6616
XX= 26.1505 YX= -0.7096 ZX= -1.3279
XY= -0.9716 YY= 28.3408 ZY= -0.9338
XZ= -0.9163 YZ= 0.0176 ZZ= 24.0682
Eigenvalues: 23.4589 26.4730 28.6276
53 C Isotropic = 75.5658 Anisotropy = 112.7894
XX= 24.2398 YX= 22.1549 ZX= 48.1151
XY= 23.9613 YY= 69.1337 ZY= -14.6838
XZ= 44.9364 YZ= -12.3164 ZZ= 133.3239
Eigenvalues: -2.5764 78.5150 150.7588
54 H Isotropic = 26.0170 Anisotropy = 4.5590
XX= 25.7200 YX= -0.4429 ZX= -0.3234
XY= -1.1156 YY= 28.8653 ZY= -0.7445
XZ= -0.6717 YZ= 0.0657 ZZ= 23.4657
Eigenvalues: 23.3154 25.6792 29.0563
55 C Isotropic = 169.0243 Anisotropy = 25.2421
XX= 171.0285 YX= 12.3732 ZX= -4.6125
XY= 12.3296 YY= 171.4835 ZY= -8.3352
XZ= -3.3851 YZ= -3.1579 ZZ= 164.5610
Eigenvalues: 158.5666 162.6540 185.8524
56 H Isotropic = 29.6957 Anisotropy = 5.5519
XX= 30.1762 YX= 1.8875 ZX= 1.5712
XY= 0.5092 YY= 30.0977 ZY= 1.7599
XZ= 1.2658 YZ= 3.9066 ZZ= 28.8130
Eigenvalues: 26.5083 29.1817 33.3969
57 H Isotropic = 28.9839 Anisotropy = 10.7675
XX= 28.3523 YX= -1.8349 ZX= 0.8317
XY= -3.3604 YY= 30.7740 ZY= -5.8991
XZ= 0.2626 YZ= -5.9916 ZZ= 27.8254
Eigenvalues: 22.9006 27.8889 36.1623
58 C Isotropic = 169.6063 Anisotropy = 23.1769
XX= 183.0042 YX= 2.7859 ZX= -5.7685

```
  XY=    2.0421   YY=   159.6335   ZY=    -2.4098
  XZ=    -5.5407   YZ=    -1.5741   ZZ=   166.1813
  Eigenvalues:   159.0419   164.7195   185.0576
59 H   Isotropic =    30.1583   Anisotropy =     9.3476
  XX=    30.2989   YX=     3.6902   ZX=    -2.2456
  XY=     2.0312   YY=    34.3040   ZY=    -1.8443
  XZ=    -1.6933   YZ=    -1.7230   ZZ=    25.8721
  Eigenvalues:    25.0658    29.0192    36.3901
60 H   Isotropic =    29.8688   Anisotropy =     6.8512
  XX=    27.8939   YX=     0.2854   ZX=    -3.2288
  XY=     1.0313   YY=    29.1377   ZY=     0.0038
  XZ=    -3.6483   YZ=     1.7537   ZZ=    32.5748
  Eigenvalues:    25.7791    29.3910    34.4363
61 H   Isotropic =    29.8159   Anisotropy =     9.3528
  XX=    32.7231   YX=    -2.5551   ZX=     2.3165
  XY=    -0.9696   YY=    29.7220   ZY=    -4.6457
  XZ=     3.8739   YZ=    -3.6159   ZZ=    27.0026
  Eigenvalues:    23.7353    29.6612    36.0511
62 N   Isotropic =    62.2986   Anisotropy =    71.8361
  XX=    57.8217   YX=   -51.5373   ZX=   -32.0575
  XY=   -47.7978   YY=    52.2766   ZY=   -42.0648
  XZ=   -35.6125   YZ=   -44.4414   ZZ=    76.7975
  Eigenvalues:   -24.3182   101.0247   110.1894
63 C   Isotropic =    44.4449   Anisotropy =   113.4352
  XX=    95.3882   YX=   -31.0114   ZX=   -18.1754
  XY=   -28.7962   YY=    14.0454   ZY=    48.9117
  XZ=   -24.8331   YZ=    45.9985   ZZ=    23.9010
  Eigenvalues:   -29.2859    42.5522   120.0683
64 C   Isotropic =    49.7235   Anisotropy =   101.0708
  XX=    94.9338   YX=   -10.7219   ZX=   -34.0396
  XY=   -17.2551   YY=    39.4465   ZY=    40.3488
  XZ=   -28.8037   YZ=    46.1280   ZZ=    14.7901
  Eigenvalues:   -20.4691    52.5356   117.1040
65 C   Isotropic =    75.4365   Anisotropy =   112.3792
  XX=   109.6529   YX=   -23.1224   ZX=   -58.3039
  XY=   -22.6852   YY=    90.1007   ZY=    13.9719
  XZ=   -55.6396   YZ=    13.2760   ZZ=    26.5559
  Eigenvalues:    -2.4440    78.3975   150.3559
66 H   Isotropic =    25.9634   Anisotropy =     3.8269
  XX=    25.9611   YX=     1.2345   ZX=     2.0322
  XY=     2.2715   YY=    26.1882   ZY=    -0.0413
  XZ=     1.9151   YZ=    -0.3006   ZZ=    25.7408
  Eigenvalues:    23.2160    26.1594    28.5146
67 C   Isotropic =    76.2879   Anisotropy =   113.6565
  XX=   116.7469   YX=   -54.0045   ZX=   -16.1964
  XY=   -49.0258   YY=    25.0588   ZY=    28.6051
  XZ=   -18.9363   YZ=    28.1602   ZZ=    87.0579
  Eigenvalues:    -2.2265    79.0312   152.0589
68 H   Isotropic =    26.3310   Anisotropy =     4.1846
  XX=    26.5811   YX=     1.2417   ZX=     1.8520
  XY=     2.5523   YY=    25.9638   ZY=    -0.1736
  XZ=     1.9624   YZ=     0.2625   ZZ=    26.4481
  Eigenvalues:    23.7087    26.1636    29.1207
69 C   Isotropic =   168.6905   Anisotropy =    23.8934
  XX=   162.2622   YX=     0.0083   ZX=    -3.2186
  XY=     2.3867   YY=   174.8238   ZY=   -12.6802
  XZ=    -2.3077   YZ=   -11.4220   ZZ=   168.9855
  Eigenvalues:   158.8515   162.6005   184.6194
70 H   Isotropic =    29.3861   Anisotropy =     6.7979
  XX=    33.0276   YX=     2.5144   ZX=     0.2349
  XY=     2.5365   YY=    25.9200   ZY=    -1.2260
  XZ=    -0.0838   YZ=    -3.1664   ZZ=    29.2107
  Eigenvalues:    24.2123    30.0279    33.9180
71 H   Isotropic =    29.8025   Anisotropy =     9.6794
  XX=    27.3792   YX=     0.9906   ZX=     3.8321
  XY=     0.5656   YY=    28.1736   ZY=    -2.2389
  XZ=     4.9467   YZ=    -1.2470   ZZ=    33.8546
  Eigenvalues:    24.5382    28.6138    36.2554
72 H   Isotropic =    29.6262   Anisotropy =     6.6297
  XX=    26.8214   YX=    -3.6427   ZX=     1.6891
```

XY= -1.7647 YY= 33.0272 ZY= 1.0677
XZ= 1.6442 YZ= 0.5419 ZZ= 29.0301
Eigenvalues: 24.9712 29.8615 34.0461
73 C Isotropic = 169.2852 Anisotropy = 23.4033
XX= 164.2752 YX= -6.3862 ZX= 4.0008
XY= -3.1840 YY= 164.1843 ZY= -8.0662
XZ= 5.1455 YZ= -8.5410 ZZ= 179.3961
Eigenvalues: 158.8642 164.1040 184.8874
74 H Isotropic = 29.9621 Anisotropy = 5.9461
XX= 27.7374 YX= -0.0825 ZX= -2.5665
XY= 1.3836 YY= 29.1852 ZY= 1.3196
XZ= -1.0336 YZ= 1.9224 ZZ= 32.9639
Eigenvalues: 26.6430 29.3172 33.9262
75 H Isotropic = 30.3974 Anisotropy = 8.0136
XX= 28.5016 YX= 2.0437 ZX= 1.3988
XY= 4.2507 YY= 33.7773 ZY= -2.2115
XZ= 1.1623 YZ= -2.8622 ZZ= 28.9132
Eigenvalues: 25.4492 30.0032 35.7398
76 H Isotropic = 29.1818 Anisotropy = 11.5536
XX= 36.2872 YX= 0.7076 ZX= 1.9963
XY= 1.6026 YY= 26.0989 ZY= -3.3661
XZ= 3.0735 YZ= -0.7116 ZZ= 25.1592
Eigenvalues: 22.9837 27.6774 36.8842
77 N Isotropic = 62.6244 Anisotropy = 74.4844
XX= 75.7819 YX= 17.5611 ZX= 51.1244
XY= 14.8712 YY= 88.8333 ZY= -38.6339
XZ= 53.8435 YZ= -37.6762 ZZ= 23.2580
Eigenvalues: -24.0818 99.6743 112.2806
78 C Isotropic = 47.6224 Anisotropy = 107.8343
XX= 5.1266 YX= 39.6144 ZX= -36.3128
XY= 45.4027 YY= 100.1331 ZY= -3.2268
XZ= -28.9864 YZ= -4.7535 ZZ= 37.6074
Eigenvalues: -24.9911 48.3463 119.5119
79 C Isotropic = 46.4586 Anisotropy = 105.6767
XX= 26.4090 YX= 34.6558 ZX= -36.2733
XY= 34.0424 YY= 99.8049 ZY= -2.9429
XZ= -47.0876 YZ= -2.5093 ZZ= 13.1621
Eigenvalues: -25.9189 48.3850 116.9097
80 C Isotropic = 75.5269 Anisotropy = 112.8365
XX= 86.1409 YX= 24.3453 ZX= -23.6003
XY= 26.9856 YY= 135.2101 ZY= -15.9437
XZ= -26.4824 YZ= -18.0528 ZZ= 5.2297
Eigenvalues: -2.5688 78.3983 150.7512
81 H Isotropic = 26.4637 Anisotropy = 4.3688
XX= 27.7167 YX= -0.8430 ZX= -1.4716
XY= -1.2691 YY= 23.9498 ZY= 0.4704
XZ= -1.5739 YZ= -0.2091 ZZ= 27.7247
Eigenvalues: 23.6551 26.3598 29.3763
82 C Isotropic = 76.0398 Anisotropy = 113.4323
XX= 23.2489 YX= 54.7500 ZX= 5.8035
XY= 53.1942 YY= 126.0948 ZY= -17.0264
XZ= 6.4283 YZ= -17.0433 ZZ= 78.7758
Eigenvalues: -1.7903 78.2484 151.6614
83 H Isotropic = 26.3360 Anisotropy = 3.6617
XX= 27.0989 YX= -0.6083 ZX= -0.5853
XY= -0.9656 YY= 23.9484 ZY= 0.5574
XZ= -1.4152 YZ= 0.4872 ZZ= 27.9605
Eigenvalues: 23.7428 26.4880 28.7771
84 C Isotropic = 169.1570 Anisotropy = 23.8387
XX= 170.2060 YX= 0.0797 ZX= 11.7945
XY= -0.0982 YY= 162.6021 ZY= -2.7629
XZ= 12.2931 YZ= -4.6494 ZZ= 174.6629
Eigenvalues: 158.6511 163.7704 185.0495
85 H Isotropic = 29.6744 Anisotropy = 6.1728
XX= 30.8160 YX= 1.3277 ZX= 2.4488
XY= 0.7613 YY= 30.2994 ZY= 3.8794
XZ= 1.0503 YZ= 2.6776 ZZ= 27.9078
Eigenvalues: 25.4705 29.7632 33.7897
86 H Isotropic = 29.6206 Anisotropy = 9.2792
XX= 29.9446 YX= 0.5073 ZX= -1.8013

XY= -0.1326 YY= 27.8274 ZY= -5.6984
XZ= -3.3000 YZ= -4.8644 ZZ= 31.0898
Eigenvalues: 23.6168 29.4383 35.8067
87 H Isotropic = 30.0676 Anisotropy = 9.4235
XX= 35.1210 YX= -3.4397 ZX= -0.8595
XY= -3.5064 YY= 26.3410 ZY= 0.7749
XZ= 0.2057 YZ= -0.2079 ZZ= 28.7409
Eigenvalues: 25.1261 28.7268 36.3499
88 C Isotropic = 169.2842 Anisotropy = 23.2909
XX= 182.3613 YX= -2.1041 ZX= 4.5452
XY= -9.1085 YY= 164.0000 ZY= 0.2052
XZ= 3.8589 YZ= -3.6586 ZZ= 161.4912
Eigenvalues: 160.4812 162.5599 184.8115
89 H Isotropic = 29.8936 Anisotropy = 6.1267
XX= 27.6715 YX= -1.7368 ZX= -0.2610
XY= -3.7388 YY= 32.7655 ZY= 0.7614
XZ= 0.1545 YZ= -1.4818 ZZ= 29.2437
Eigenvalues: 26.4657 29.2370 33.9780
90 H Isotropic = 30.3464 Anisotropy = 8.2320
XX= 29.8296 YX= -0.0492 ZX= 2.4602
XY= -1.3014 YY= 25.8372 ZY= 1.0672
XZ= 0.8376 YZ= -0.0888 ZZ= 35.3723
Eigenvalues: 25.6645 29.5402 35.8344
91 H Isotropic = 29.1165 Anisotropy = 12.3103
XX= 32.3509 YX= 4.3704 ZX= -4.5934
XY= 3.1786 YY= 24.5731 ZY= -1.7932
XZ= -3.4721 YZ= -4.0604 ZZ= 30.4254
Eigenvalues: 22.7837 27.2424 37.3233
92 C Isotropic = 160.9379 Anisotropy = 21.6939
XX= 165.0111 YX= -6.8454 ZX= -2.4744
XY= -7.8377 YY= 162.2399 ZY= 6.0416
XZ= -5.9635 YZ= 12.0377 ZZ= 155.5627
Eigenvalues: 149.2202 158.1929 175.4005
93 H Isotropic = 29.8709 Anisotropy = 6.2179
XX= 28.7165 YX= -1.2642 ZX= -1.9529
XY= -2.7966 YY= 28.5222 ZY= -2.0159
XZ= -3.5568 YZ= -2.0862 ZZ= 32.3739
Eigenvalues: 25.0162 30.5802 34.0162
94 H Isotropic = 31.0582 Anisotropy = 6.4525
XX= 30.1061 YX= 1.1207 ZX= -0.6040
XY= -0.2437 YY= 34.2122 ZY= 2.0155
XZ= -1.8878 YZ= 3.4450 ZZ= 28.8563
Eigenvalues: 27.1264 30.6884 35.3599
95 H Isotropic = 30.0500 Anisotropy = 10.7662
XX= 32.6777 YX= -4.8558 ZX= 1.5617
XY= -5.7299 YY= 30.8610 ZY= -0.4054
XZ= 0.1437 YZ= -0.5683 ZZ= 26.6111
Eigenvalues: 26.2740 26.6484 37.2275
96 H Isotropic = 30.0022 Anisotropy = 7.9847
XX= 33.4937 YX= -2.3694 ZX= -3.1823
XY= -1.0046 YY= 30.2920 ZY= -0.8762
XZ= -3.7567 YZ= 0.4218 ZZ= 26.2209
Eigenvalues: 24.7006 29.9806 35.3253
97 C Isotropic = 31.5108 Anisotropy = 236.1021
XX= 66.5702 YX= 63.1190 ZX= -89.6610
XY= 63.4167 YY= -7.3911 ZY= -75.1826
XZ= -88.3161 YZ= -73.8709 ZZ= 35.3535
Eigenvalues: -63.7205 -30.6593 188.9123
98 C Isotropic = 54.1972 Anisotropy = 174.7618
XX= 103.0945 YX= 30.8567 ZX= -52.3513
XY= 31.2243 YY= 9.0212 ZY= -84.1430
XZ= -52.5427 YZ= -84.2868 ZZ= 50.4760
Eigenvalues: -57.4293 49.3158 170.7051
99 C Isotropic = 45.2009 Anisotropy = 193.3932
XX= 47.2789 YX= 43.0347 ZX= -107.1213
XY= 44.3074 YY= 62.1351 ZY= -34.7188
XZ= -107.4312 YZ= -40.3858 ZZ= 26.1887
Eigenvalues: -71.0788 32.5518 174.1297
100 C Isotropic = 46.2441 Anisotropy = 191.0359
XX= 57.7128 YX= 96.5488 ZX= -60.0088

XY= 90.4926 YY= -0.7166 ZY= -26.0950
XZ= -63.1266 YZ= -27.4739 ZZ= 81.7362
Eigenvalues: -71.1697 36.3006 173.6014
101 C Isotropic = 52.8133 Anisotropy = 176.0865
XX= 51.6329 YX= 37.5384 ZX= -104.3788
XY= 33.9110 YY= 73.3286 ZY= -32.6543
XZ= -103.7957 YZ= -29.6119 ZZ= 33.4783
Eigenvalues: -61.9380 50.1736 170.2042
102 C Isotropic = 52.5553 Anisotropy = 176.9132
XX= 60.2438 YX= 88.2314 ZX= -56.6915
XY= 91.4258 YY= 5.4385 ZY= -20.4171
XZ= -55.9546 YZ= -23.0058 ZZ= 91.9837
Eigenvalues: -62.9572 50.1257 170.4975
103 H Isotropic = 25.1729 Anisotropy = 8.2223
XX= 20.6540 YX= -2.4708 ZX= 1.2066
XY= -2.5342 YY= 28.5821 ZY= 2.5158
XZ= -0.5454 YZ= 2.6721 ZZ= 26.2825
Eigenvalues: 19.7484 25.1158 30.6544
104 H Isotropic = 25.0870 Anisotropy = 8.7253
XX= 25.3281 YX= 0.9330 ZX= 1.0950
XY= 0.7212 YY= 22.8958 ZY= 5.9623
XZ= 1.4505 YZ= 4.2808 ZZ= 27.0372
Eigenvalues: 19.4420 24.9151 30.9039
105 H Isotropic = 25.0487 Anisotropy = 7.3703
XX= 23.5266 YX= -2.4679 ZX= -0.1823
XY= -1.9616 YY= 27.1963 ZY= 3.6049
XZ= 0.4139 YZ= 3.1365 ZZ= 24.4234
Eigenvalues: 21.2380 23.9460 29.9622
106 H Isotropic = 25.0505 Anisotropy = 7.5276
XX= 22.9347 YX= 0.1726 ZX= 2.7223
XY= -0.0663 YY= 25.2339 ZY= 3.0284
XZ= 2.1205 YZ= 3.5524 ZZ= 26.9830
Eigenvalues: 21.1531 23.9295 30.0689
107 H Isotropic = 25.0506 Anisotropy = 4.0737
XX= 25.0501 YX= -2.0189 ZX= 2.4554
XY= -1.9769 YY= 25.2953 ZY= 0.9132
XZ= 2.3718 YZ= 0.8298 ZZ= 24.8066
Eigenvalues: 21.4334 25.9521 27.7664
108 B Isotropic = 97.2443 Anisotropy = 5.9137
XX= 96.8042 YX= -3.1438 ZX= 4.2797
XY= -2.6517 YY= 98.4698 ZY= 2.7624
XZ= 4.7549 YZ= 2.7319 ZZ= 96.4588
Eigenvalues: 90.1889 100.3572 101.1867
109 F Isotropic = 322.9822 Anisotropy = 54.3012
XX= 336.1255 YX= 23.6611 ZX= 14.8000
XY= 37.0426 YY= 315.9831 ZY= -17.8518
XZ= 25.7019 YZ= -17.6046 ZZ= 316.8381
Eigenvalues: 276.7306 333.0330 359.1831
110 F Isotropic = 304.7991 Anisotropy = 51.1228
XX= 313.1897 YX= -22.4437 ZX= 0.9555
XY= -23.2268 YY= 262.3853 ZY= 1.5314
XZ= -2.8197 YZ= -5.5446 ZZ= 338.8225
Eigenvalues: 253.5731 321.9434 338.8810
111 F Isotropic = 321.6408 Anisotropy = 47.9183
XX= 340.0774 YX= -5.0841 ZX= -27.1196
XY= -10.7318 YY= 330.9357 ZY= -27.4121
XZ= -29.2532 YZ= -13.4901 ZZ= 293.9093
Eigenvalues: 272.3884 338.9477 353.5864



x –
B3LYP/6-311+G(2d,p)// B3LYP/6-31G(d)
E_{abs} = -1994.7601374 au
Charge = 0 Multiplicity = 1

C	1.29607	-1.36805	-1.77012
C	-1.18493	-0.14877	-2.41173
C	0.08698	-2.0889	-1.61628
C	1.26333	-0.03016	-2.24405
C	0.02169	0.5762	-2.53763
C	-1.14402	-1.48577	-1.96969
C	2.55117	0.76213	-2.4584
H	2.43685	1.77637	-2.05729
H	3.37202	0.3293	-1.88696
C	2.98559	0.86016	-3.93636
H	2.24304	1.37537	-4.55406
H	3.92976	1.41027	-4.01708
C	-2.50876	0.50633	-2.79608
H	-3.31713	0.13593	-2.158
H	-2.47432	1.58194	-2.60843
C	-2.88685	0.27535	-4.2726
H	-2.98596	-0.79172	-4.50037
H	-2.12375	0.68134	-4.94567
H	-3.83843	0.76426	-4.50757
C	0.07076	-3.52991	-1.10717
H	-0.89367	-3.75702	-0.64925
H	0.79267	-3.66579	-0.29434
C	0.34576	-4.57459	-2.20583
H	0.29249	-5.5888	-1.79536
H	1.33595	-4.44023	-2.65364
H	-0.39069	-4.49815	-3.01342
C	2.6253	-2.05123	-1.40132
C	3.36392	-1.39439	-0.21488
C	-0.05413	2.03561	-2.97203
H	0.91332	2.3956	-3.32571
H	-0.74064	2.17104	-3.80939
C	-0.51967	3.04108	-1.90439
C	-2.42925	-2.29525	-1.84603
H	-2.29597	-3.31669	-2.20598
H	-3.21887	-1.87164	-2.47167
C	-3.02304	-2.44007	-0.43343
O	4.55525	-1.14532	-0.21317
O	-1.24537	3.98307	-2.16253
O	-3.62462	-3.43506	-0.07537
N	0.00266	2.81306	-0.64763
H	0.60042	2.0139	-0.47326
N	2.55187	-1.16975	0.88404
H	1.58578	-1.47629	0.87098
H	2.37285	-3.0414	-1.01785
H	3.13339	-0.13194	-4.37199
N	-2.855	-1.32868	0.36704
H	-2.31695	-0.53557	0.03963
N	-0.2318	3.66453	0.40672
C	-1.20887	3.46772	1.37945

C	0.48759	4.82982	0.65608
C	-0.03745	5.36639	1.80763
H	0.2941	6.28601	2.27166
C	-1.09332	4.51742	2.25879
H	-1.70974	4.66341	3.13605
C	-2.13426	2.29751	1.35103
H	-2.84547	2.36936	2.17786
H	-2.71037	2.25285	0.41713
C	1.56578	5.30516	-0.25997
H	2.36941	4.56673	-0.38394
H	2.01386	6.21561	0.14753
H	1.17459	5.54009	-1.25817
N	3.06778	-0.79729	2.10488
C	3.01919	0.49537	2.6191
C	3.70816	-1.65846	2.99294
C	4.05638	-0.89755	4.08284
H	4.57799	-1.26634	4.95628
C	3.62655	0.44402	3.8506
H	3.75005	1.28692	4.51772
C	3.93145	-3.10031	2.67837
H	2.9946	-3.63846	2.47773
H	4.4135	-3.58711	3.53063
H	4.58302	-3.23051	1.80485
C	2.38402	1.62261	1.8771
H	2.49777	2.55002	2.44422
H	1.30504	1.47161	1.72948
H	2.84287	1.77486	0.89077
N	-3.34381	-1.26891	1.65102
C	-4.64099	-0.8936	1.98632
C	-2.59894	-1.55145	2.79329
C	-3.43699	-1.33959	3.86156
H	-3.16443	-1.47063	4.90054
C	-4.70948	-0.93131	3.35876
H	-5.59093	-0.70212	3.94298
C	-5.66542	-0.57546	0.94861
H	-6.59921	-0.28355	1.43704
H	-5.87626	-1.44182	0.30876
H	-5.35909	0.25267	0.29522
C	-1.17451	-1.99275	2.72499
H	-1.05654	-2.91026	2.13373
H	-0.80821	-2.19575	3.73487
H	-0.51499	-1.22679	2.28928
C	3.60089	-2.31549	-2.56359
H	4.12609	-1.41833	-2.88937
H	3.06102	-2.73686	-3.41748
H	4.36325	-3.03258	-2.24592
H	-1.60627	1.33977	1.46809

SCF GIAO Magnetic shielding tensor (ppm):
1 C Isotropic = 34.8752 Anisotropy = 172.4347
XX= -37.7742 YX= -18.7576 ZX= -30.4170
XY= -18.0380 YY= 11.0841 ZY= -52.6595
XZ= -17.7825 YZ= -43.9734 ZZ= 131.3156
Eigenvalues: -52.8499 7.6438 149.8316
2 C Isotropic = 32.1428 Anisotropy = 184.9577
XX= -42.3766 YX= -15.6295 ZX= -19.4819
XY= -15.0199 YY= 1.3991 ZY= -51.9130
XZ= -15.9266 YZ= -51.1444 ZZ= 137.4058
Eigenvalues: -53.7932 -5.2264 155.4479
3 C Isotropic = 33.2021 Anisotropy = 180.9144
XX= -0.9200 YX= 2.3878 ZX= -13.4045
XY= 6.0568 YY= -25.8370 ZY= -70.9186
XZ= -12.9149 YZ= -65.8687 ZZ= 126.3635
Eigenvalues: -52.0664 -2.1389 153.8117
4 C Isotropic = 32.5925 Anisotropy = 182.4046
XX= -36.6682 YX= 29.7592 ZX= -8.0163
XY= 27.7021 YY= -3.5245 ZY= -51.3836
XZ= -8.1097 YZ= -44.9137 ZZ= 137.9702
Eigenvalues: -55.0650 -1.3530 154.1956
5 C Isotropic = 41.5141 Anisotropy = 170.4575

XX= 25.2180 YX= 2.9186 ZX= -9.6679
XY= 3.1137 YY= -31.7570 ZY= -56.0766
XZ= -10.3547 YZ= -75.4180 ZZ= 131.0813
Eigenvalues: -54.9917 24.3815 155.1524
6 C Isotropic = 41.6588 Anisotropy = 166.0114
XX= -27.3856 YX= 33.2665 ZX= -6.5465
XY= 33.5579 YY= 15.4479 ZY= -43.3091
XZ= -17.8410 YZ= -39.4891 ZZ= 136.9142
Eigenvalues: -46.1779 18.8213 152.3331
7 C Isotropic = 154.4397 Anisotropy = 18.5697
XX= 158.6204 YX= -7.3123 ZX= -3.3665
XY= -8.7721 YY= 151.6174 ZY= 2.3744
XZ= -8.6809 YZ= 2.3145 ZZ= 153.0812
Eigenvalues: 145.9785 150.5210 166.8195
8 H Isotropic = 28.8718 Anisotropy = 6.6944
XX= 27.8742 YX= 0.2270 ZX= -1.7046
XY= 0.8339 YY= 31.6669 ZY= -2.1914
XZ= -0.2006 YZ= -3.9007 ZZ= 27.0743
Eigenvalues: 25.3962 27.8844 33.3347
9 H Isotropic = 28.6840 Anisotropy = 9.7373
XX= 28.2271 YX= 2.5503 ZX= 2.0127
XY= 1.0319 YY= 29.1836 ZY= 5.2624
XZ= 3.4883 YZ= 4.2949 ZZ= 28.6414
Eigenvalues: 23.9436 26.9330 35.1755
10 C Isotropic = 164.2356 Anisotropy = 30.8263
XX= 162.8928 YX= -4.3010 ZX= -9.6969
XY= -1.6158 YY= 154.7433 ZY= 5.5876
XZ= -16.5277 YZ= 5.7303 ZZ= 175.0707
Eigenvalues: 153.1803 154.7400 184.7864
11 H Isotropic = 30.5563 Anisotropy = 7.0912
XX= 30.6008 YX= 2.4677 ZX= -0.0990
XY= 3.3342 YY= 27.9807 ZY= 2.6257
XZ= -0.7860 YZ= 4.8110 ZZ= 33.0875
Eigenvalues: 24.7001 31.6850 35.2838
12 H Isotropic = 30.4906 Anisotropy = 11.9811
XX= 33.7547 YX= -3.8891 ZX= -3.4103
XY= -3.6850 YY= 28.4963 ZY= 2.2058
XZ= -5.1207 YZ= 3.2080 ZZ= 29.2210
Eigenvalues: 26.1265 26.8674 38.4780
13 C Isotropic = 154.4659 Anisotropy = 22.5632
XX= 161.1864 YX= 5.8212 ZX= 6.4338
XY= 3.3751 YY= 147.4607 ZY= 0.4229
XZ= 13.1417 YZ= 4.6734 ZZ= 154.7506
Eigenvalues: 145.9982 147.8915 169.5081
14 H Isotropic = 28.8934 Anisotropy = 7.0054
XX= 29.9880 YX= -1.0671 ZX= -1.9481
XY= 0.2885 YY= 27.0727 ZY= 3.1867
XZ= -3.5989 YZ= 3.0100 ZZ= 29.6194
Eigenvalues: 24.6596 28.4569 33.5637
15 H Isotropic = 28.6949 Anisotropy = 7.5691
XX= 28.5033 YX= -1.5960 ZX= 2.6899
XY= -1.9593 YY= 32.2526 ZY= -1.3908
XZ= 0.4651 YZ= -2.8392 ZZ= 25.3288
Eigenvalues: 24.4291 27.9146 33.7410
16 C Isotropic = 166.4933 Anisotropy = 28.5088
XX= 164.3592 YX= 4.6774 ZX= 9.2977
XY= 3.1454 YY= 155.9384 ZY= -2.2985
XZ= 13.7693 YZ= -0.2889 ZZ= 179.1822
Eigenvalues: 152.7997 161.1810 185.4991
17 H Isotropic = 30.7532 Anisotropy = 7.4274
XX= 27.2739 YX= -1.4944 ZX= 2.1866
XY= -2.2614 YY= 32.8933 ZY= -1.3532
XZ= 4.2532 YZ= -1.9882 ZZ= 32.0924
Eigenvalues: 25.5321 31.0227 35.7048
18 H Isotropic = 30.6459 Anisotropy = 7.5341
XX= 29.7894 YX= -2.5972 ZX= -0.6334
XY= -2.5789 YY= 27.2712 ZY= 1.1398
XZ= 0.1501 YZ= 3.4115 ZZ= 34.8769
Eigenvalues: 25.3015 30.9675 35.6686
19 H Isotropic = 30.4936 Anisotropy = 12.1277

XX= 33.7212 YX= 2.9740 ZX= 4.5591
XY= 2.4092 YY= 27.3341 ZY= 1.3893
XZ= 6.0479 YZ= 2.3342 ZZ= 30.4255
Eigenvalues: 26.3354 26.5668 38.5787
20 C Isotropic = 153.2642 Anisotropy = 18.8012
XX= 146.0811 YX= 2.9956 ZX= -0.5977
XY= 1.0709 YY= 165.5708 ZY= 2.8713
XZ= -0.6616 YZ= -3.8675 ZZ= 148.1409
Eigenvalues: 145.7330 148.2614 165.7984
21 H Isotropic = 28.6254 Anisotropy = 8.7016
XX= 32.5877 YX= 2.0591 ZX= -3.4314
XY= 1.4463 YY= 27.5266 ZY= -0.5850
XZ= -3.8028 YZ= 1.7883 ZZ= 25.7619
Eigenvalues: 23.7674 27.6824 34.4265
22 H Isotropic = 28.7669 Anisotropy = 5.6965
XX= 28.9727 YX= -1.4509 ZX= 2.6373
XY= -0.4906 YY= 27.5850 ZY= -0.2031
XZ= 3.7262 YZ= 1.6803 ZZ= 29.7430
Eigenvalues: 25.4572 28.2789 32.5645
23 C Isotropic = 166.3132 Anisotropy = 28.5751
XX= 154.6200 YX= 3.4688 ZX= -2.3312
XY= 1.4991 YY= 179.8812 ZY= -7.6578
XZ= -3.7579 YZ= -12.7232 ZZ= 164.4383
Eigenvalues: 153.7428 159.8335 185.3633
24 H Isotropic = 30.4177 Anisotropy = 12.2130
XX= 26.4792 YX= 0.4427 ZX= -0.2683
XY= -0.0517 YY= 38.5558 ZY= 0.7764
XZ= -0.4277 YZ= -0.9508 ZZ= 26.2180
Eigenvalues: 25.9768 26.7166 38.5597
25 H Isotropic = 30.5421 Anisotropy = 6.9097
XX= 33.2365 YX= -0.7706 ZX= -2.5765
XY= -0.5953 YY= 30.7178 ZY= -2.6547
XZ= -4.5114 YZ= -3.7769 ZZ= 27.6721
Eigenvalues: 24.3381 32.1397 35.1486
26 H Isotropic = 30.6579 Anisotropy = 7.5997
XX= 30.5884 YX= 0.5940 ZX= 2.3481
XY= -0.2356 YY= 30.0741 ZY= -3.0160
XZ= 3.8433 YZ= -4.7833 ZZ= 31.3111
Eigenvalues: 25.6839 30.5654 35.7243
27 C Isotropic = 136.3710 Anisotropy = 25.5242
XX= 134.2521 YX= 2.4408 ZX= 10.6662
XY= 0.8401 YY= 125.8176 ZY= -9.5213
XZ= 2.5049 YZ= -6.7045 ZZ= 149.0434
Eigenvalues: 122.1232 133.6027 153.3871
28 C Isotropic = 4.5437 Anisotropy = 115.1355
XX= 23.5551 YX= 4.1011 ZX= 27.3750
XY= 7.3918 YY= 61.6276 ZY= 50.0378
XZ= 7.6737 YZ= 52.6457 ZZ= -71.5516
Eigenvalues: -90.9542 23.2845 81.3007
29 C Isotropic = 140.0769 Anisotropy = 40.3423
XX= 123.6407 YX= 15.7786 ZX= -2.0514
XY= 6.6984 YY= 148.2121 ZY= -15.5080
XZ= -0.4921 YZ= -18.1267 ZZ= 148.3780
Eigenvalues: 118.2116 135.0474 166.9718
30 H Isotropic = 27.6858 Anisotropy = 5.8966
XX= 30.5868 YX= 1.9132 ZX= -1.6548
XY= 1.4520 YY= 27.2150 ZY= 1.6145
XZ= -2.6516 YZ= 1.9135 ZZ= 25.2556
Eigenvalues: 23.2180 28.2225 31.6168
31 H Isotropic = 28.0179 Anisotropy = 4.4083
XX= 28.3958 YX= -1.1294 ZX= 1.6396
XY= -1.2395 YY= 27.8786 ZY= 0.3120
XZ= 3.9218 YZ= 3.5256 ZZ= 27.7792
Eigenvalues: 24.0090 29.0879 30.9568
32 C Isotropic = 9.3319 Anisotropy = 113.0925
XX= 62.5264 YX= -19.1287 ZX= -25.9985
XY= -26.1510 YY= 37.3940 ZY= 31.0170
XZ= -9.7067 YZ= 50.0440 ZZ= -71.9247
Eigenvalues: -85.9901 29.2588 84.7269
33 C Isotropic = 139.6760 Anisotropy = 38.5990

XX= 134.2505 YX= -5.9925 ZX= -15.4246
XY= -9.2268 YY= 131.8547 ZY= -0.4745
XZ= -22.9704 YZ= 0.2298 ZZ= 152.9226
Eigenvalues: 118.8801 134.7392 165.4086
34 H Isotropic = 28.2026 Anisotropy = 4.2072
XX= 29.6594 YX= 0.6315 ZX= -0.5478
XY= -0.0788 YY= 30.4105 ZY= -0.1789
XZ= 1.4778 YZ= -3.7042 ZZ= 24.5380
Eigenvalues: 23.9063 29.6942 31.0074
35 H Isotropic = 27.8933 Anisotropy = 5.2495
XX= 27.6221 YX= -0.1511 ZX= 2.1779
XY= -1.2905 YY= 29.0815 ZY= 2.8138
XZ= 3.1276 YZ= 2.9095 ZZ= 26.9763
Eigenvalues: 23.3644 28.9225 31.3930
36 C Isotropic = 9.4976 Anisotropy = 114.2710
XX= 68.5328 YX= 12.6064 ZX= 29.3706
XY= 6.3701 YY= 14.4606 ZY= 62.1224
XZ= 38.3923 YZ= 39.3802 ZZ= -54.5008
Eigenvalues: -85.7228 28.5373 85.6782
37 O Isotropic = -95.3243 Anisotropy = 681.2184
XX= -389.0085 YX= 132.4427 ZX= 58.7132
XY= 110.2229 YY= 275.1302 ZY= 174.6805
XZ= 101.9683 YZ= 164.9214 ZZ= -172.0946
Eigenvalues: -422.4610 -222.3332 358.8213
38 O Isotropic = -94.8025 Anisotropy = 633.0100
XX= 63.6847 YX= -326.5321 ZX= -139.9293
XY= -303.2214 YY= -124.8750 ZY= 24.0344
XZ= -152.7822 YZ= 3.4481 ZZ= -223.2171
Eigenvalues: -397.7046 -213.9070 327.2042
39 O Isotropic = -93.0339 Anisotropy = 639.3429
XX= 155.9539 YX= 237.1081 ZX= 165.0059
XY= 262.6879 YY= -284.8321 ZY= 50.3421
XZ= 167.3530 YZ= 71.1099 ZZ= -150.2235
Eigenvalues: -398.4803 -213.8162 333.1947
40 N Isotropic = 106.6215 Anisotropy = 114.6032
XX= 104.4724 YX= -53.7068 ZX= 51.4785
XY= -35.7205 YY= 44.7173 ZY= 22.9672
XZ= 5.7583 YZ= -19.8447 ZZ= 170.6747
Eigenvalues: 19.3024 117.5385 183.0236
41 H Isotropic = 25.1555 Anisotropy = 10.3864
XX= 21.4984 YX= 4.9435 ZX= 0.0580
XY= 3.3441 YY= 27.1701 ZY= -2.8142
XZ= 2.5812 YZ= -6.4218 ZZ= 26.7980
Eigenvalues: 17.9060 25.4807 32.0798
42 N Isotropic = 106.2750 Anisotropy = 117.8510
XX= 44.8591 YX= 30.1518 ZX= -80.0033
XY= 10.8265 YY= 107.8849 ZY= 16.4290
XZ= -22.2810 YZ= -6.2232 ZZ= 166.0810
Eigenvalues: 21.0852 112.8976 184.8423
43 H Isotropic = 25.1213 Anisotropy = 9.9534
XX= 26.4516 YX= -1.6627 ZX= 2.1954
XY= -3.3173 YY= 19.9076 ZY= -4.5118
XZ= 3.3584 YZ= -0.3306 ZZ= 29.0046
Eigenvalues: 18.8427 24.7642 31.7569
44 H Isotropic = 27.4758 Anisotropy = 7.4824
XX= 29.4530 YX= -1.7677 ZX= -1.7712
XY= -3.9610 YY= 28.0484 ZY= 1.5951
XZ= -1.8210 YZ= 1.6011 ZZ= 24.9260
Eigenvalues: 24.1499 25.8134 32.4641
45 H Isotropic = 30.7178 Anisotropy = 6.2974
XX= 27.4489 YX= 2.0684 ZX= -1.8127
XY= 2.4395 YY= 32.4406 ZY= -0.5120
XZ= -3.9785 YZ= -1.0537 ZZ= 32.2639
Eigenvalues: 25.6386 31.5987 34.9161
46 N Isotropic = 105.6975 Anisotropy = 114.1882
XX= 87.1318 YX= 33.0045 ZX= 33.4040
XY= 51.9430 YY= 112.6866 ZY= -96.3774
XZ= 19.8611 YZ= -34.4306 ZZ= 117.2741
Eigenvalues: 15.5920 119.6775 181.8230
47 H Isotropic = 24.7669 Anisotropy = 11.6926

XX= 22.0609 YX= -3.0736 ZX= -3.7033
XY= -2.0662 YY= 23.1766 ZY= -0.0123
XZ= -8.1749 YZ= -0.6822 ZZ= 29.0632
Eigenvalues: 17.6166 24.1221 32.5619
48 N Isotropic = 68.0455 Anisotropy = 81.9664
XX= 114.4351 YX= -21.6456 ZX= 6.6096
XY= -19.6601 YY= 61.4092 ZY= 52.8113
XZ= 15.7190 YZ= 58.2588 ZZ= 28.2921
Eigenvalues: -16.5829 98.0296 122.6898
49 C Isotropic = 49.5458 Anisotropy = 102.6254
XX= 34.7285 YX= 56.3756 ZX= 45.2856
XY= 46.0435 YY= 58.4418 ZY= 4.0088
XZ= 49.1403 YZ= 1.1585 ZZ= 55.4671
Eigenvalues: -23.5777 54.2524 117.9627
50 C Isotropic = 47.5336 Anisotropy = 103.2084
XX= 45.4792 YX= 54.8979 ZX= 35.5906
XY= 60.3416 YY= 31.8352 ZY= 7.5879
XZ= 31.7717 YZ= 10.2839 ZZ= 65.2865
Eigenvalues: -22.4579 48.7195 116.3392
51 C Isotropic = 71.8075 Anisotropy = 117.2978
XX= 91.8667 YX= 54.4601 ZX= 17.8487
XY= 56.2267 YY= 36.6600 ZY= 42.6818
XZ= 18.7699 YZ= 40.4222 ZZ= 86.8958
Eigenvalues: -5.6469 71.0635 150.0060
52 H Isotropic = 25.8639 Anisotropy = 3.5912
XX= 24.8736 YX= -0.6794 ZX= -1.9100
XY= -0.9474 YY= 26.7413 ZY= -1.5103
XZ= -1.7650 YZ= -1.9775 ZZ= 25.9768
Eigenvalues: 22.7532 26.5805 28.2580
53 C Isotropic = 72.4368 Anisotropy = 121.0086
XX= 73.5734 YX= 29.2211 ZX= 67.8891
XY= 29.6535 YY= 93.5946 ZY= 22.4735
XZ= 67.4021 YZ= 21.4528 ZZ= 50.1425
Eigenvalues: -6.8458 71.0470 153.1092
54 H Isotropic = 26.0118 Anisotropy = 4.9659
XX= 24.8268 YX= -0.9783 ZX= -1.1556
XY= -0.9578 YY= 27.7904 ZY= -2.4829
XZ= -1.3492 YZ= -2.3950 ZZ= 25.4183
Eigenvalues: 22.7152 25.9978 29.3224
55 C Isotropic = 169.5779 Anisotropy = 25.6676
XX= 172.1460 YX= -10.9081 ZX= 0.0870
XY= -11.8214 YY= 177.7202 ZY= 3.6181
XZ= 1.5621 YZ= 0.8090 ZZ= 158.8674
Eigenvalues: 158.0333 164.0107 186.6896
56 H Isotropic = 30.3578 Anisotropy = 7.4900
XX= 30.3243 YX= -2.1537 ZX= -5.5342
XY= -3.0304 YY= 31.3153 ZY= -0.2585
XZ= -4.8272 YZ= -2.5860 ZZ= 29.4339
Eigenvalues: 23.6461 32.0762 35.3511
57 H Isotropic = 30.1866 Anisotropy = 5.9642
XX= 30.7856 YX= -3.4878 ZX= 2.2862
XY= -2.1136 YY= 28.9239 ZY= -0.1129
XZ= 0.9229 YZ= -2.6795 ZZ= 30.8503
Eigenvalues: 26.8917 29.5054 34.1627
58 C Isotropic = 170.2996 Anisotropy = 24.2846
XX= 177.8938 YX= -5.4619 ZX= -7.6145
XY= -5.2527 YY= 165.8757 ZY= 8.1536
XZ= -9.7582 YZ= 8.0591 ZZ= 167.1292
Eigenvalues: 158.0897 166.3197 186.4893
59 H Isotropic = 29.7706 Anisotropy = 6.6063
XX= 32.6652 YX= 1.9137 ZX= -2.8261
XY= 1.0864 YY= 31.2884 ZY= -0.6421
XZ= -0.9783 YZ= -1.5641 ZZ= 25.3580
Eigenvalues: 24.8091 30.3279 34.1748
60 H Isotropic = 29.7144 Anisotropy = 9.7887
XX= 28.4908 YX= -5.1336 ZX= -0.3874
XY= -4.1853 YY= 33.1507 ZY= -2.4729
XZ= -1.0801 YZ= -1.5692 ZZ= 27.5017
Eigenvalues: 24.5821 28.3209 36.2402
61 H Isotropic = 29.6051 Anisotropy = 6.9792

XX= 26.1971 YX= -1.5566 ZX= 0.8883
XY= -2.2948 YY= 29.7466 ZY= 3.3315
XZ= 0.5528 YZ= 1.6411 ZZ= 32.8716
Eigenvalues: 24.9711 29.5863 34.2579
62 N Isotropic = 67.1103 Anisotropy = 80.1308
XX= 81.1714 YX= 9.8181 ZX= -35.1989
XY= 15.4382 YY= 108.6470 ZY= 33.4003
XZ= -36.4488 YZ= 38.5151 ZZ= 11.5127
Eigenvalues: -15.3001 96.1002 120.5309
63 C Isotropic = 49.2037 Anisotropy = 101.2125
XX= 102.2240 YX= -22.9636 ZX= -19.5092
XY= -31.4367 YY= -16.9042 ZY= 0.4040
XZ= -22.7275 YZ= 8.1883 ZZ= 62.2914
Eigenvalues: -22.8219 53.7543 116.6787
64 C Isotropic = 48.1012 Anisotropy = 104.8878
XX= 93.8879 YX= -37.9764 ZX= -29.1066
XY= -36.7319 YY= -2.2063 ZY= -11.9971
XZ= -35.9936 YZ= -15.4538 ZZ= 52.6220
Eigenvalues: -22.9160 49.1932 118.0264
65 C Isotropic = 72.6204 Anisotropy = 119.4450
XX= 115.3088 YX= -32.7902 ZX= -60.1574
XY= -32.9393 YY= 55.7692 ZY= -20.0889
XZ= -55.7677 YZ= -20.5445 ZZ= 46.7832
Eigenvalues: -5.7137 71.3246 152.2504
66 H Isotropic = 25.9775 Anisotropy = 3.3763
XX= 24.1823 YX= 0.5843 ZX= 1.7518
XY= 0.4649 YY= 26.6910 ZY= -0.9583
XZ= 2.3208 YZ= -0.4910 ZZ= 27.0591
Eigenvalues: 22.9552 26.7488 28.2283
67 C Isotropic = 72.4279 Anisotropy = 118.6969
XX= 133.5553 YX= -12.1587 ZX= -31.9183
XY= -12.2190 YY= 16.1201 ZY= 41.3187
XZ= -30.2531 YZ= 40.7033 ZZ= 67.6084
Eigenvalues: -6.7059 72.4306 151.5592
68 H Isotropic = 26.0591 Anisotropy = 4.9905
XX= 24.6411 YX= 0.6190 ZX= 2.8297
XY= 0.8951 YY= 26.1507 ZY= 0.2149
XZ= 3.1195 YZ= 0.1367 ZZ= 27.3855
Eigenvalues: 22.6521 26.1391 29.3861
69 C Isotropic = 170.0352 Anisotropy = 24.1168
XX= 164.7090 YX= 4.1121 ZX= -3.2078
XY= 3.5563 YY= 185.2337 ZY= -0.7407
XZ= -2.2060 YZ= -2.7300 ZZ= 160.1628
Eigenvalues: 158.9011 165.0914 186.1131
70 H Isotropic = 29.8332 Anisotropy = 6.7211
XX= 30.3666 YX= -2.8621 ZX= 2.5818
XY= -3.0060 YY= 31.9455 ZY= -0.0231
XZ= 2.7900 YZ= 2.0218 ZZ= 27.1875
Eigenvalues: 24.8294 30.3563 34.3140
71 H Isotropic = 29.7042 Anisotropy = 9.9215
XX= 26.8328 YX= 2.5943 ZX= 3.8049
XY= 3.2812 YY= 31.2329 ZY= 3.4584
XZ= 3.7954 YZ= 2.1014 ZZ= 31.0467
Eigenvalues: 24.3527 28.4413 36.3185
72 H Isotropic = 29.6561 Anisotropy = 6.1680
XX= 28.7972 YX= 4.2714 ZX= -2.7496
XY= 3.2215 YY= 28.6862 ZY= -0.4826
XZ= -1.4016 YZ= 0.0343 ZZ= 31.4850
Eigenvalues: 24.7322 30.4680 33.7681
73 C Isotropic = 169.4730 Anisotropy = 25.8474
XX= 168.6683 YX= 9.3200 ZX= 3.1228
XY= 8.6796 YY= 175.3282 ZY= 8.3807
XZ= 5.4994 YZ= 11.5106 ZZ= 164.4225
Eigenvalues: 158.4036 163.3108 186.7046
74 H Isotropic = 30.3431 Anisotropy = 7.1858
XX= 27.3347 YX= 2.5487 ZX= 3.1092
XY= 1.5538 YY= 34.4220 ZY= -2.7051
XZ= 4.9847 YZ= -1.0328 ZZ= 29.2726
Eigenvalues: 23.4441 32.4515 35.1336
75 H Isotropic = 30.9832 Anisotropy = 11.1910

XX= 35.3870 YX= 4.4598 ZX= 3.3519
XY= 2.5946 YY= 30.1217 ZY= 0.4917
XZ= 4.3464 YZ= 0.8583 ZZ= 27.4409
Eigenvalues: 25.7335 28.7722 38.4438
76 H Isotropic = 30.2125 Anisotropy = 5.8908
XX= 27.0919 YX= 1.2122 ZX= -1.8560
XY= 1.0587 YY= 30.4180 ZY= 2.2690
XZ= 1.5294 YZ= 1.5617 ZZ= 33.1275
Eigenvalues: 26.6501 29.8476 34.1397
77 N Isotropic = 67.5287 Anisotropy = 80.4672
XX= 98.2706 YX= 6.0770 ZX= 40.2714
XY= 8.9675 YY= 103.9576 ZY= 16.2685
XZ= 44.1222 YZ= 6.4158 ZZ= 0.3580
Eigenvalues: -15.8577 97.2703 121.1735
78 C Isotropic = 47.3199 Anisotropy = 105.6171
XX= -10.2357 YX= -37.1473 ZX= -15.4103
XY= -38.3517 YY= 106.5496 ZY= -6.4556
XZ= -8.6620 YZ= -4.2513 ZZ= 45.6458
Eigenvalues: -23.8307 48.0591 117.7313
79 C Isotropic = 50.2083 Anisotropy = 99.5668
XX= 12.4275 YX= -34.3840 ZX= -27.8259
XY= -40.8173 YY= 103.0092 ZY= -9.4870
XZ= -36.1056 YZ= -12.6145 ZZ= 35.1883
Eigenvalues: -21.3693 55.4081 116.5862
80 C Isotropic = 71.9933 Anisotropy = 120.6961
XX= 63.3115 YX= -28.7299 ZX= -27.5633
XY= -27.2995 YY= 143.3372 ZY= -17.0379
XZ= -29.6335 YZ= -13.9558 ZZ= 9.3312
Eigenvalues: -7.3914 70.9139 152.4573
81 H Isotropic = 26.0124 Anisotropy = 4.7081
XX= 27.0771 YX= 0.8388 ZX= -1.6702
XY= 0.4648 YY= 23.2371 ZY= -0.1086
XZ= -1.7628 YZ= 0.7717 ZZ= 27.7231
Eigenvalues: 23.0383 25.8478 29.1512
82 C Isotropic = 72.9130 Anisotropy = 119.1608
XX= 17.2437 YX= -39.6938 ZX= 26.9492
XY= -37.6156 YY= 141.0956 ZY= 2.4280
XZ= 25.7580 YZ= 4.3423 ZZ= 60.3996
Eigenvalues: -4.4812 70.8666 152.3535
83 H Isotropic = 25.8740 Anisotropy = 3.5055
XX= 26.6893 YX= 0.5131 ZX= -0.4680
XY= 0.4155 YY= 23.0651 ZY= 0.4294
XZ= -0.9585 YZ= 0.4330 ZZ= 27.8675
Eigenvalues: 22.9509 26.4600 28.2110
84 C Isotropic = 170.0714 Anisotropy = 23.6218
XX= 175.1655 YX= 3.2615 ZX= 11.9404
XY= 2.6039 YY= 166.7757 ZY= 3.4671
XZ= 12.6012 YZ= 5.5560 ZZ= 168.2730
Eigenvalues: 158.5160 165.8789 185.8193
85 H Isotropic = 29.7169 Anisotropy = 9.7531
XX= 35.1090 YX= 2.5962 ZX= -2.4493
XY= 2.7802 YY= 25.2535 ZY= -0.5308
XZ= -1.0540 YZ= -0.1056 ZZ= 28.7884
Eigenvalues: 24.5641 28.3677 36.2190
86 H Isotropic = 29.5799 Anisotropy = 6.9719
XX= 31.2353 YX= -1.3201 ZX= 2.5880
XY= -1.3321 YY= 28.2881 ZY= -4.2668
XZ= 1.0061 YZ= -3.3157 ZZ= 29.2164
Eigenvalues: 24.9257 29.5862 34.2278
87 H Isotropic = 29.6953 Anisotropy = 6.7223
XX= 30.0253 YX= 0.3878 ZX= -0.1176
XY= 0.6674 YY= 29.6916 ZY= 5.2744
XZ= -1.8042 YZ= 3.9718 ZZ= 29.3691
Eigenvalues: 24.6942 30.2149 34.1769
88 C Isotropic = 169.0752 Anisotropy = 23.6317
XX= 183.7901 YX= 3.8993 ZX= 0.7448
XY= 5.1959 YY= 164.9188 ZY= 0.6008
XZ= -0.8555 YZ= 1.2978 ZZ= 158.5168
Eigenvalues: 158.3567 164.0393 184.8297
89 H Isotropic = 29.8631 Anisotropy = 6.3293

XX= 29.2533 YX= 2.2841 ZX= -0.7576
XY= 3.6357 YY= 30.4487 ZY= -3.4395
XZ= -1.2258 YZ= -0.7353 ZZ= 29.8873
Eigenvalues: 26.7016 28.8050 34.0826
90 H Isotropic = 30.0175 Anisotropy = 7.5557
XX= 31.4851 YX= 1.3261 ZX= 2.6373
XY= 1.5376 YY= 25.0346 ZY= 2.3075
XZ= 0.2382 YZ= 2.5071 ZZ= 33.5328
Eigenvalues: 24.2503 30.7475 35.0547
91 H Isotropic = 30.5901 Anisotropy = 10.4026
XX= 35.1456 YX= -3.1896 ZX= -1.9737
XY= -3.8592 YY= 27.7909 ZY= 1.6003
XZ= -2.3963 YZ= 2.9142 ZZ= 28.8337
Eigenvalues: 25.6888 28.5563 37.5251
92 C Isotropic = 161.9176 Anisotropy = 20.9280
XX= 167.3236 YX= 4.9343 ZX= -5.6833
XY= 5.6106 YY= 155.8731 ZY= -5.2416
XZ= -9.5923 YZ= -6.1786 ZZ= 162.5560
Eigenvalues: 152.5270 157.3562 175.8696
93 H Isotropic = 29.7242 Anisotropy = 6.2053
XX= 29.8554 YX= -0.7165 ZX= -2.0736
XY= 0.0522 YY= 31.7038 ZY= 2.5728
XZ= -4.1295 YZ= 2.6371 ZZ= 27.6134
Eigenvalues: 24.8493 30.4621 33.8611
94 H Isotropic = 30.8194 Anisotropy = 6.8456
XX= 29.6447 YX= -0.4644 ZX= -0.0304
XY= 0.0655 YY= 29.9312 ZY= -3.1384
XZ= -1.5521 YZ= -4.1339 ZZ= 32.8823
Eigenvalues: 27.3213 29.7538 35.3831
95 H Isotropic = 30.1216 Anisotropy = 10.6974
XX= 32.7869 YX= 5.2030 ZX= -0.4054
XY= 5.4376 YY= 30.6261 ZY= -0.4491
XZ= -1.8377 YZ= -0.2847 ZZ= 26.9516
Eigenvalues: 26.0492 27.0623 37.2532
96 H Isotropic = 31.0052 Anisotropy = 10.3867
XX= 28.4423 YX= 0.0022 ZX= -1.2289
XY= -1.1934 YY= 37.7993 ZY= 1.3511
XZ= -1.9657 YZ= 0.4606 ZZ= 26.7740
Eigenvalues: 25.78