

Supplementary Information Available for:

“Quantification of the magnetotropy of inorganic unsaturated planar rings”

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Basis sets used in the calculations

All the basis sets are completely uncontracted, i.e., the coefficients are always 1.0

Boron atoms

s functions exponents

33360.216573
4972.095217
1125.641723
316.491356
102.007256
36.295873
13.971410
5.741156
2.496268
1.114202
0.421549
0.169633
0.068535

p functions exponents

880.000000
220.000000
55.000000
13.366101
4.135394
1.481256
0.602136
0.255634
0.111151
0.047648

d functions exponents

3.330000
1.110000
0.402000
0.145000
0.048333

f functions exponents

0.882000
0.311000

Nitrogen atoms

s functions	exponents
	74761.715106
	11123.653813
	2512.685697
	703.777285
	225.478793
	79.615810
	30.237283
	12.263622
	5.265086
	2.333471
	0.901856
	0.358336
p functions	0.141093
	exponents
	2282.781623
	537.728660
	126.666567
	29.837389
	9.394038
	3.405104
	1.350000
	0.557696
	0.232449
	0.094264
d functions	exponents
	8.314630
	2.837000
	0.968000
	0.335000
	0.115930
f functions	exponents
	2.666000
	0.685000

Phosphorous atoms

s functions	exponents
	77492.400000
	11605.800000
	2645.960000
	753.980000
	248.755000
	91.156500
	36.225700
	15.211300
	4.752400
	1.790200
	0.324700
	0.104100
	0.033375
p functions	exponents
	7616.969912
	1845.288657
	447.040000
	108.300000
	34.767000
	12.583000
	4.631500
	1.702600
	0.367400
	0.087200
d functions	exponents
	5.940668
	1.968074
	0.652000
	0.216000
	0.077500
f functions	exponents
	0.452000
	0.165000

Oxygen atoms

s functions	exponents
	105374.945317
	15679.240331
	3534.544676
	987.365160
	315.978752
	111.654281
	42.699451
	17.395596
	7.438309
	3.222862
	1.253877
	0.495155
	0.191665
p functions	exponents
	3694.545000
	859.598000
	200.000000
	46.533367
	14.621809
	5.313064
	2.102525
	0.850223
	0.337597
	0.128892
d functions	exponents
	10.962000
	3.775000
	1.300000
	0.444000
	0.152000
f functions	exponents
	2.666000
	0.859000

Silicon atoms

s functions	exponents
	471908.259426
	69989.300000
	10380.200000
	2330.010000
	657.470000
	214.000000
	77.606000
	30.640000
	12.816000
	3.927100
	1.452200
	0.257600
	0.094400
p functions	exponents
	7124.226523
	1691.486031
	401.605000
	95.352000
	30.334000
	10.944000
	4.041700
	1.461500
	0.330200
	0.095200
d functions	exponents
	32.013000
	10.671000
	3.308000
	0.481000
	0.159000
	0.055600
f functions	exponents
	7.001000
	0.336000
	0.125000

Aluminum atoms

s functions	exponents
	55112.700000
	8204.660000
	1863.560000
	530.195000
	174.895000
	64.009000
	25.323100
	10.563900
	3.212600
	1.154300
	0.178100
	0.065900
p functions	exponents
	352.546000
	83.016000
	26.004000
	9.232100
	3.355000
	1.188300
	0.276200
	0.072800
d functions	exponents
	8.646000
	2.634000
	0.333000
	0.109000
	0.035600
f functions	exponents
	0.244000
	5.686000
	0.085800

Hydrogen atoms

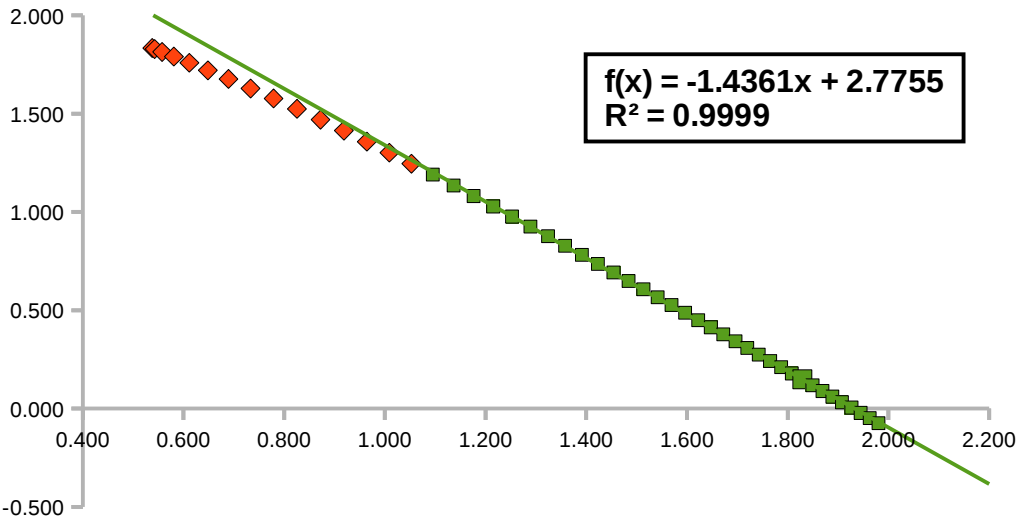
s functions	exponents
	402.009948
	60.241959
	13.732173
	3.904505
	1.282709
	0.465544
	0.181120
	0.072791
p functions	exponents
	6.269000
	2.292000
	0.838000
	0.292000
d function	exponents
	1.057000

**The Arrighini-Maestro-Moccia sum rules
for charge conservation and gauge invariance**

molecule	$n\ e^-$	xx	yy	zz
H₆	6	5.89801	5.89801	5.55344
N₆	42	41.97573	41.97573	41.95820
N₄²⁻	30	29.94231	29.94231	29.90190
P₆	90	87.51086	87.51086	87.47229
Al₄²⁻	54	52.44405	52.44405	52.87942
Si₆H₆	90	88.28716	88.28716	88.28418
B₃N₃H₆	42	41.98264	41.98264	41.96002
B₃O₃H₃	42	41.98255	41.98255	41.96106

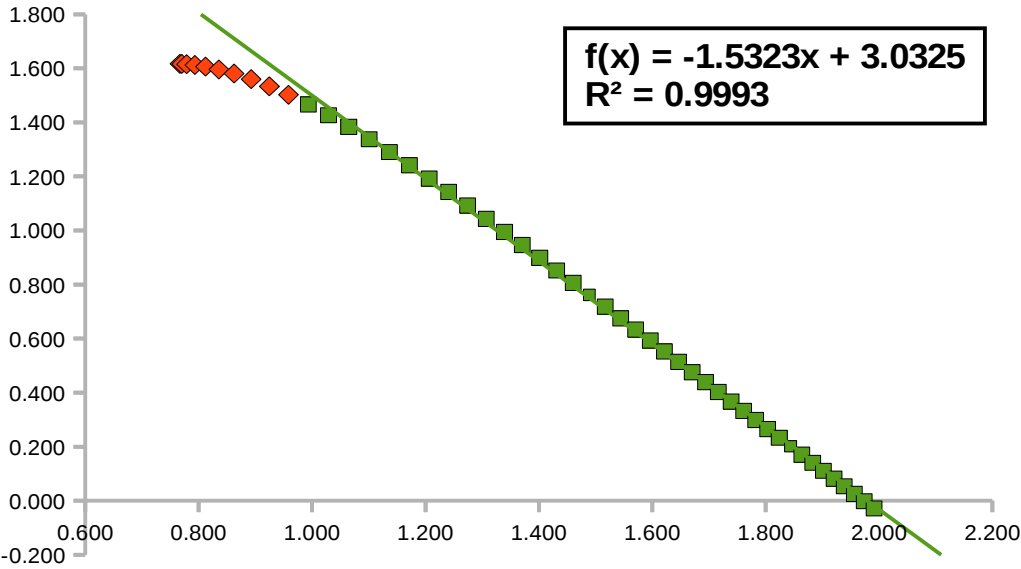
h and s are expressed in bohr all over the S.I.A.

H₆				
h	sigma_zz	s	log(s²+h²)	log(sigma_zz)
0.00000	68.20703	1.85763	0.53791	1.83383
0.20000	67.42460		0.54292	1.82882
0.40000	65.17089		0.55760	1.81405
0.60000	61.69727		0.58101	1.79027
0.80000	57.34857		0.61180	1.75852
1.00000	52.49924		0.64843	1.72015
1.20000	47.46658		0.68938	1.67639
1.40000	42.50701		0.73326	1.62846
1.60000	37.79378		0.77893	1.57742
1.80000	33.43151		0.82547	1.52416
2.00000	29.47240		0.87220	1.46942
2.20000	25.92641		0.91859	1.41374
2.40000	22.78262		0.96430	1.35760
2.60000	20.01600		1.00906	1.30138
2.80000	17.59400		1.05272	1.24536
3.00000	15.48172		1.09520	1.18982
3.20000	13.64453		1.13643	1.13496
3.40000	12.04987		1.17640	1.08098
3.60000	10.66623		1.21513	1.02801
3.80000	9.46653		1.25263	0.97619
4.00000	8.42534		1.28894	0.92559
4.20000	7.52055		1.32409	0.87625
4.40000	6.73297		1.35814	0.82821
4.60000	6.04568		1.39112	0.78145
4.80000	5.44452		1.42309	0.73596
5.00000	4.91714		1.45409	0.69171
5.20000	4.45315		1.48417	0.64867
5.40000	4.04369		1.51336	0.60678
5.60000	3.68131		1.54171	0.56600
5.80000	3.35978		1.56927	0.52631
6.00000	3.07329		1.59606	0.48760
6.20000	2.81769		1.62212	0.44989
6.40000	2.58888		1.64749	0.41311
6.60000	2.38364		1.67220	0.37724
6.80000	2.19896		1.69628	0.34222
7.00000	2.03246		1.71975	0.30802
7.20000	1.88198		1.74265	0.27462
7.40000	1.74568		1.76500	0.24196
7.60000	1.62197		1.78683	0.21004
7.80000	1.50939		1.80815	0.17880
8.00000	1.40685		1.82899	0.14825
8.20000	1.31331		1.84936	0.11837
8.40000	1.22767		1.86929	0.08908
8.60000	1.14920		1.88880	0.06039
8.80000	1.07716		1.90790	0.03228
9.00000	1.01094		1.92660	0.00472
9.20000	0.94995		1.94493	-0.02230
9.40000	0.89371		1.96289	-0.04880
9.60000	0.84177		1.98051	-0.07481



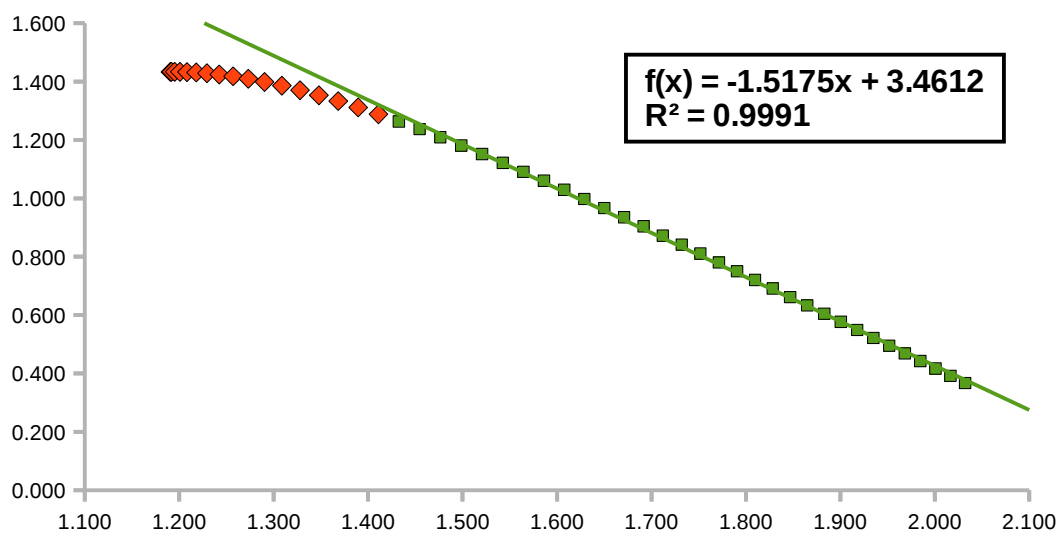
Chi_graph = -298.16729 ppm au
Chi_calc = -402.33904 ppm au
J-suscept. = -37.11300 au
H min 3.00000 au
H max 9.60000 au
s 1.85763 au
sigma_zz(CM) 68.20700 ppm

N₆				
h	sigma_zz	s	log(s2+h2)	log(sigma_zz)
0.00000	41.36302	2.41865	0.76715	1.61661
0.20000	41.33562		0.77011	1.61632
0.40000	41.23494		0.77886	1.61527
0.60000	40.95902		0.79308	1.61235
0.80000	40.39501		0.81224	1.60633
1.00000	39.44932		0.83568	1.59604
1.20000	38.07560		0.86272	1.58065
1.40000	36.29096		0.89264	1.55980
1.60000	34.15887		0.92479	1.53350
1.80000	31.77583		0.95856	1.50210
2.00000	29.25289		0.99343	1.46617
2.20000	26.68511		1.02897	1.42627
2.40000	24.16745		1.06483	1.38323
2.60000	21.75974		1.10071	1.33765
2.80000	19.50858		1.13640	1.29023
3.00000	17.43920		1.17172	1.24153
3.20000	15.56290		1.20655	1.19209
3.40000	13.87887		1.24080	1.14235
3.60000	12.37707		1.27439	1.09262
3.80000	11.04413		1.30728	1.04313
4.00000	9.86998		1.33945	0.99432
4.20000	8.83267		1.37088	0.94609
4.40000	7.91878		1.40157	0.89866
4.60000	7.11356		1.43152	0.85209
4.80000	6.40353		1.46075	0.80642
5.00000	5.77710		1.48925	0.76171
5.20000	5.22356		1.51706	0.71797
5.40000	4.73349		1.54419	0.67518
5.60000	4.29926		1.57066	0.63339
5.80000	3.91393		1.59649	0.59261
6.00000	3.57064		1.62169	0.55275
6.20000	3.26456		1.64630	0.51382
6.40000	2.99100		1.67034	0.47582
6.60000	2.74600		1.69381	0.43870
6.80000	2.52614		1.71675	0.40246
7.00000	2.32839		1.73918	0.36706
7.20000	2.15013		1.76110	0.33246
7.40000	1.98915		1.78254	0.29867
7.60000	1.84345		1.80352	0.26563
7.80000	1.71130		1.82406	0.23333
8.00000	1.59128		1.84417	0.20175
8.20000	1.48192		1.86386	0.17083
8.40000	1.38219		1.88315	0.14057
8.60000	1.29108		1.90206	0.11095
8.80000	1.20771		1.92059	0.08196
9.00000	1.13124		1.93877	0.05356
9.20000	1.06101		1.95660	0.02572
9.40000	0.99639		1.97410	-0.00157
9.60000	0.93686		1.99127	-0.02832



Chi_graph	-538.84022 ppm au
Chi_calc	-425.31292 ppm au
Jsuscept	-23.14263 au
Hmin	2.00000 au
Hmax	9.60000 au
s(AV)	2.41865 au
sigma_zz(CM)	41.36302 ppm

		P₆		
h	sigma_zz	s	log(s2+h2)	log(sigma_zz)
0.00000	27.11660	3.93884	1.19074	1.43324
0.20000	27.12758		1.19185	1.43341
0.40000	27.13319		1.19519	1.43350
0.60000	27.12995		1.20070	1.43345
0.80000	27.09357		1.20829	1.43287
1.00000	27.00261		1.21786	1.43141
1.20000	26.83605		1.22928	1.42872
1.40000	26.56871		1.24240	1.42437
1.60000	26.18839		1.25707	1.41811
1.80000	25.68310		1.27310	1.40965
2.00000	25.05632		1.29036	1.39892
2.20000	24.31391		1.30866	1.38585
2.40000	23.47453		1.32786	1.37060
2.60000	22.54054		1.34781	1.35296
2.80000	21.54181		1.36837	1.33328
3.00000	20.49723		1.38942	1.31170
3.20000	19.42486		1.41085	1.28836
3.40000	18.33934		1.43256	1.26338
3.60000	17.26342		1.45446	1.23713
3.80000	16.20457		1.47646	1.20964
4.00000	15.17692		1.49851	1.18118
4.20000	14.18542		1.52054	1.15184
4.40000	13.23924		1.54251	1.12186
4.60000	12.34111		1.56436	1.09135
4.80000	11.49345		1.58607	1.06045
5.00000	10.69725		1.60761	1.02927
5.20000	9.95236		1.62895	0.99793
5.40000	9.25848		1.65006	0.96654
5.60000	8.61381		1.67094	0.93520
5.80000	8.01333		1.69156	0.90381
6.00000	7.45302		1.71193	0.87233
6.20000	6.94416		1.73203	0.84162
6.40000	6.46903		1.75185	0.81084
6.60000	6.03104		1.77140	0.78039
6.80000	5.62618		1.79067	0.75021
7.00000	5.25219		1.80966	0.72034
7.20000	4.90726		1.82837	0.69084
7.40000	4.58772		1.84680	0.66160
7.60000	4.29363		1.86495	0.63282
7.80000	4.02293		1.88283	0.60454
8.00000	3.77199		1.90045	0.57657
8.20000	3.53997		1.91779	0.54900
8.40000	3.32526		1.93487	0.52183
8.60000	3.12624		1.95170	0.49502
8.80000	2.94118		1.96827	0.46852
9.00000	2.77147		1.98459	0.44271
9.20000	2.61288		2.00067	0.41712
9.40000	2.46535		2.01651	0.39188
9.60000	2.32856		2.03211	0.36709



Chi_graph = -1446.00570 ppm au

Chi_calc = -1143.76358 ppm au

J-suscept. = -23.46652 au

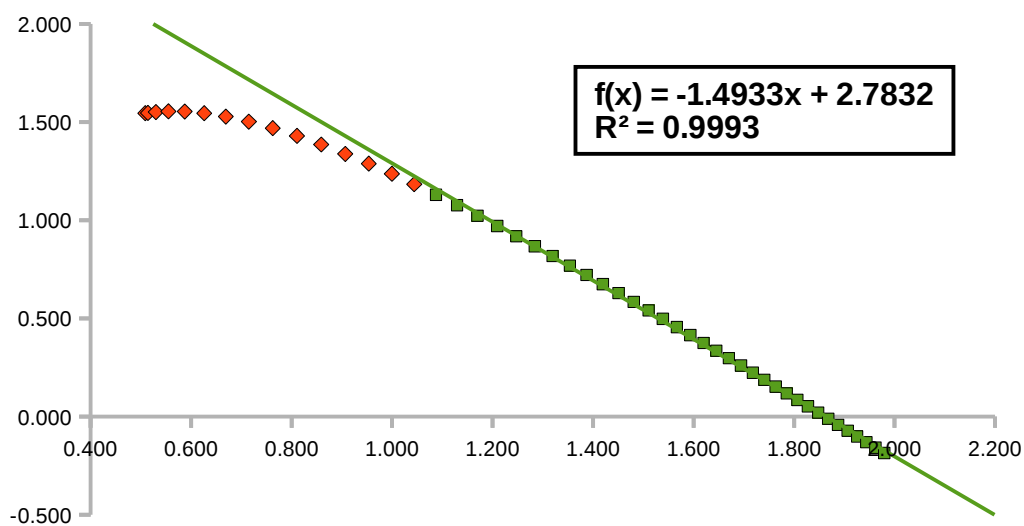
H min 3.40000 au

H max 9.60000 au

s 3.93884 au

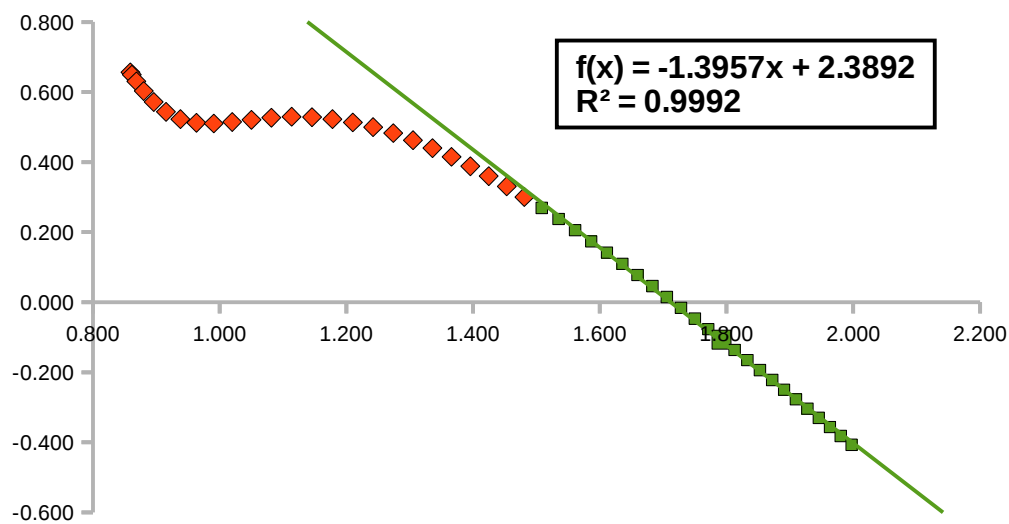
sigma_zz(Cl 27.11660 ppm

h	sigma_zz	N_4^{2-}	log(s2+h2)	log(sigma_zz)
		s		
0.00000	35.07555	1.79655	0.50888	1.54500
0.20000	35.21856		0.51423	1.54677
0.40000	35.57422		0.52989	1.55114
0.60000	35.86415		0.55480	1.55466
0.80000	35.77709		0.58744	1.55361
1.00000	35.09079		0.62609	1.54519
1.20000	33.73245		0.66909	1.52805
1.40000	31.79118		0.71497	1.50231
1.60000	29.44529		0.76250	1.46902
1.80000	26.89556		0.81074	1.42968
2.00000	24.30072		0.85899	1.38562
2.20000	21.76049		0.90674	1.33767
2.40000	19.42159		0.95364	1.28828
2.60000	17.23854		0.99946	1.23650
2.80000	15.26072		1.04405	1.18357
3.00000	13.49012		1.08734	1.13002
3.20000	11.92192		1.12929	1.07635
3.40000	10.54298		1.16990	1.02296
3.60000	9.33653		1.20918	0.97019
3.80000	8.28455		1.24718	0.91827
4.00000	7.36785		1.28392	0.86734
4.20000	6.56857		1.31947	0.81747
4.40000	5.87056		1.35387	0.76868
4.60000	5.26027		1.38717	0.72101
4.80000	4.72464		1.41942	0.67437
5.00000	4.25344		1.45067	0.62874
5.20000	3.83768		1.48098	0.58407
5.40000	3.47046		1.51038	0.54039
5.60000	3.14483		1.53892	0.49760
5.80000	2.85572		1.56664	0.45572
6.00000	2.59856		1.59359	0.41473
6.20000	2.36939		1.61980	0.37464
6.40000	2.16475		1.64530	0.33541
6.60000	1.98178		1.67013	0.29705
6.80000	1.81783		1.69432	0.25955
7.00000	1.67070		1.71790	0.22290
7.20000	1.53840		1.74090	0.18707
7.40000	1.41920		1.76334	0.15204
7.60000	1.31162		1.78524	0.11781
7.80000	1.21431		1.80664	0.08433
8.00000	1.12618		1.82755	0.05161
8.20000	1.04611		1.84799	0.01958
8.40000	0.97338		1.86798	-0.01172
8.60000	0.90704		1.88755	-0.04237
8.80000	0.84601		1.90670	-0.07262
9.00000	0.79109		1.92545	-0.10177
9.20000	0.74040		1.94383	-0.13054
9.40000	0.69387		1.96184	-0.15872
9.60000	0.65113		1.97949	-0.18633



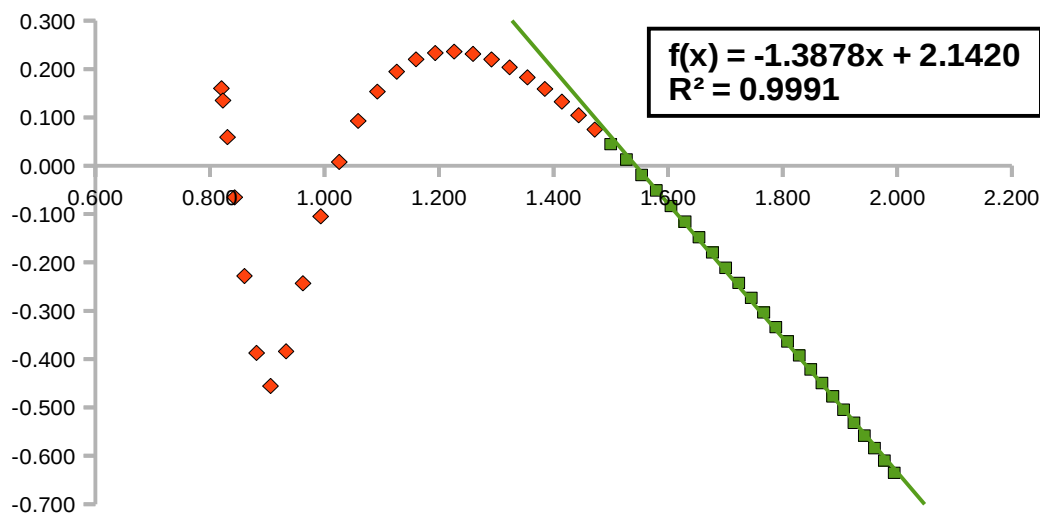
Chi_graph	-303.54005 ppm au
Chi_calc	-278.10098 ppm au
Jsuscept	-27.42675 au
Hmin	3.00000 au
Hmax	9.60000 au
s	1.79655 au
sigma_zz(CM)	35.07555 ppm

B₃N₃H₆				
h	sigma_zz	s	log(s2+h2)	log(sigma_zz)
0.00000	4.52951	2.68867	0.85908	0.65605
0.20000	4.46001		0.86147	0.64934
0.40000	4.26899		0.86858	0.63033
0.60000	4.00590		0.88018	0.60270
0.80000	3.72999		0.89592	0.57171
1.00000	3.49462		0.91534	0.54340
1.20000	3.33172		0.93797	0.52267
1.40000	3.25113		0.96327	0.51203
1.60000	3.23743		0.99074	0.51020
1.80000	3.27015		1.01990	0.51457
2.00000	3.31745		1.05034	0.52080
2.20000	3.36169		1.08167	0.52656
2.40000	3.38312		1.11357	0.52932
2.60000	3.37458		1.14579	0.52822
2.80000	3.33272		1.17808	0.52280
3.00000	3.25972		1.21029	0.51318
3.20000	3.15950		1.24227	0.49962
3.40000	3.03860		1.27390	0.48267
3.60000	2.90118		1.30511	0.46257
3.80000	2.75347		1.33584	0.43988
4.00000	2.60043		1.36603	0.41505
4.20000	2.44465		1.39566	0.38822
4.40000	2.29072		1.42470	0.35997
4.60000	2.14048		1.45315	0.33051
4.80000	1.99586		1.48100	0.30013
5.00000	1.85808		1.50825	0.26907
5.20000	1.72785		1.53490	0.23751
5.40000	1.60557		1.56097	0.20563
5.60000	1.49139		1.58646	0.17359
5.80000	1.38542		1.61139	0.14158
6.00000	1.28697		1.63577	0.10957
6.20000	1.19603		1.65962	0.07774
6.40000	1.11204		1.68295	0.04612
6.60000	1.03467		1.70577	0.01480
6.80000	0.96340		1.72810	-0.01619
7.00000	0.89790		1.74996	-0.04677
7.20000	0.83735		1.77136	-0.07709
7.40000	0.78176		1.79231	-0.10693
7.60000	0.73050		1.81284	-0.13638
7.80000	0.68330		1.83295	-0.16539
8.00000	0.63977		1.85266	-0.19398
8.20000	0.59963		1.87198	-0.22212
8.40000	0.56255		1.89092	-0.24984
8.60000	0.52831		1.90950	-0.27711
8.80000	0.49666		1.92772	-0.30394
9.00000	0.46736		1.94561	-0.33035
9.20000	0.44016		1.96317	-0.35639
9.40000	0.41498		1.98041	-0.38198
9.60000	0.39160		1.99734	-0.40716



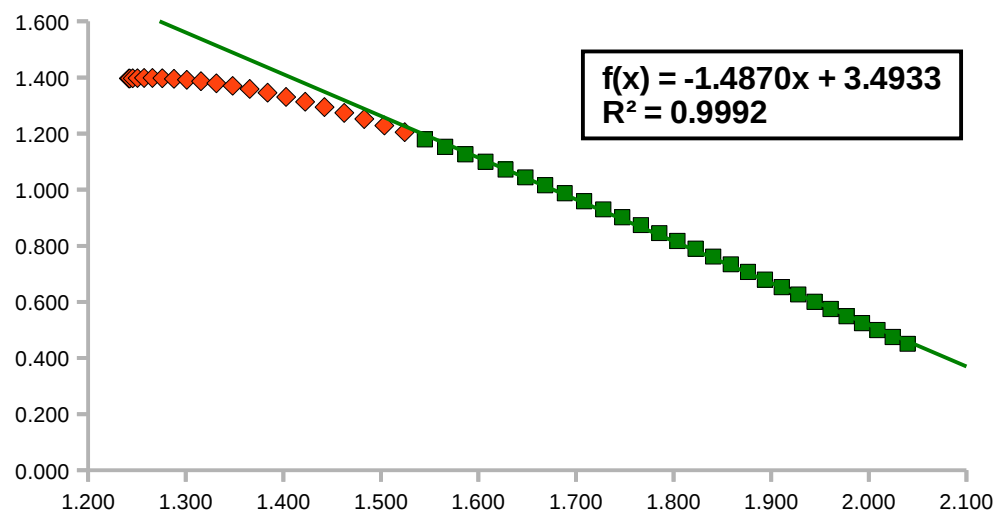
Chi_graph	-122.49941 ppm au
Chi_calc	-190.19112 ppm au
Jsuscept	-8.37460 au
Hmin	5.00000 au
Hmax	9.60000 au
s(AV)	2.68867 au
sigma_zz(CM)	4.52951 ppm

B₃O₃H₃				
h	sigma_zz	s	log(s2+h2)	log(sigma_zz)
0.00000	1.44644	2.57088	0.82016	0.16030
0.20000	1.36458		0.82278	0.13500
0.40000	1.14598		0.83055	0.05918
0.60000	0.86022		0.84320	-0.06539
0.80000	0.59166		0.86030	-0.22792
1.00000	0.40999		0.88135	-0.38723
1.20000	0.35030		0.90576	-0.45556
1.40000	0.41309		0.93295	-0.38395
1.60000	0.57132		0.96234	-0.24312
1.80000	0.78600		0.99341	-0.10458
2.00000	1.01845		1.02569	0.00794
2.20000	1.23775		1.05878	0.09263
2.40000	1.42350		1.09235	0.15336
2.60000	1.56537		1.12611	0.19462
2.80000	1.66036		1.15985	0.22020
3.00000	1.71109		1.19339	0.23327
3.20000	1.72320		1.22659	0.23634
3.40000	1.70378		1.25934	0.23141
3.60000	1.65956		1.29158	0.21999
3.80000	1.59799		1.32324	0.20357
4.00000	1.52378		1.35429	0.18292
4.20000	1.44233		1.38470	0.15906
4.40000	1.35754		1.41446	0.13275
4.60000	1.27216		1.44357	0.10454
4.80000	1.18825		1.47202	0.07491
5.00000	1.10832		1.49982	0.04466
5.20000	1.03010		1.52698	0.01288
5.40000	0.95714		1.55351	-0.01903
5.60000	0.88892		1.57943	-0.05114
5.80000	0.82532		1.60476	-0.08338
6.00000	0.76636		1.62951	-0.11556
6.20000	0.71162		1.65369	-0.14775
6.40000	0.66162		1.67733	-0.17939
6.60000	0.61510		1.70044	-0.21106
6.80000	0.57242		1.72304	-0.24228
7.00000	0.53326		1.74515	-0.27306
7.20000	0.49710		1.76678	-0.30356
7.40000	0.46381		1.78795	-0.33366
7.60000	0.43321		1.80868	-0.36331
7.80000	0.40511		1.82898	-0.39242
8.00000	0.37917		1.84886	-0.42116
8.20000	0.35527		1.86835	-0.44944
8.40000	0.33323		1.88745	-0.47726
8.60000	0.31290		1.90617	-0.50459
8.80000	0.29406		1.92453	-0.53157
9.00000	0.27664		1.94255	-0.55809
9.20000	0.26051		1.96023	-0.58418
9.40000	0.24560		1.97758	-0.60978
9.60000	0.23174		1.99462	-0.63500



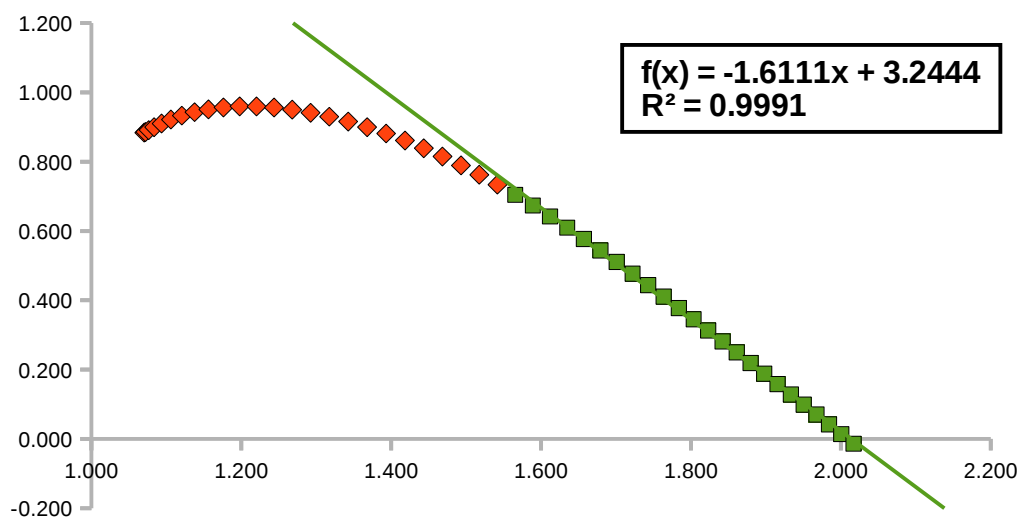
Chi_graph	-69.34258 ppm au
Chi_calc	-113.09264 ppm au
Jsuscept	-5.44654 au
Hmin	5.00000 au
Hmax	9.60000 au
s(AV)	2.57088 au
sigma_zz(CM)	1.44644 ppm

Si ₆ H ₆				
h	sigma_zz	s	log(s2+h2)	log(sigma_zz)
0.00000	24.91796	4.17661	1.24165	1.39651
0.20000	24.92532		1.24264	1.39664
0.40000	24.95635		1.24561	1.39718
0.60000	24.99195		1.25052	1.39780
0.80000	25.02112		1.25730	1.39831
1.00000	25.02013		1.26586	1.39829
1.20000	24.97030		1.27610	1.39742
1.40000	24.85219		1.28789	1.39536
1.60000	24.65606		1.30112	1.39192
1.80000	24.35488		1.31564	1.38659
2.00000	23.95619		1.33131	1.37942
2.20000	23.45373		1.34799	1.37021
2.40000	22.85482		1.36556	1.35898
2.60000	22.16654		1.38389	1.34570
2.80000	21.40157		1.40285	1.33045
3.00000	20.57482		1.42233	1.31334
3.20000	19.70382		1.44223	1.29455
3.40000	18.79698		1.46246	1.27409
3.60000	17.87238		1.48293	1.25218
3.80000	16.94445		1.50357	1.22903
4.00000	16.03003		1.52432	1.20493
4.20000	15.12062		1.54511	1.17957
4.40000	14.22918		1.56590	1.15318
4.60000	13.38428		1.58663	1.12660
4.80000	12.58009		1.60728	1.09968
5.00000	11.80715		1.62782	1.07214
5.20000	11.06840		1.64820	1.04408
5.40000	10.37244		1.66842	1.01588
5.60000	9.71678		1.68846	0.98752
5.80000	9.09264		1.70829	0.95869
6.00000	8.51562		1.72790	0.93022
6.20000	7.98269		1.74729	0.90215
6.40000	7.47806		1.76644	0.87379
6.60000	7.00836		1.78536	0.84562
6.80000	6.56873		1.80403	0.81748
7.00000	6.15773		1.82246	0.78942
7.20000	5.77663		1.84063	0.76167
7.40000	5.42230		1.85856	0.73418
7.60000	5.09248		1.87624	0.70693
7.80000	4.78563		1.89367	0.67994
8.00000	4.50002		1.91086	0.65321
8.20000	4.23475		1.92780	0.62683
8.40000	3.98785		1.94450	0.60074
8.60000	3.75732		1.96097	0.57488
8.80000	3.54338		1.97719	0.54942
9.00000	3.34391		1.99319	0.52425
9.20000	3.15808		2.00896	0.49942
9.40000	2.98474		2.02450	0.47491
9.60000	2.82313		2.03983	0.45073



Chi_graph	-1556.93329 ppm au
Chi_calc	-1412.45341 ppm au
Jsuscept	-25.77368 au
Hmin	4.20000 au
Hmax	9.60000 au
s	4.17661 au
sigma_zz(CM)	24.91796 ppm

Al₄²⁻				
h	sigma_zz	s	log(s2+h2)	log(sigma_zz)
0.00000	7.65275	3.42995	1.07058	0.88382
0.20000	7.68591		1.07205	0.88570
0.40000	7.78441		1.07644	0.89123
0.60000	7.93860		1.08367	0.89974
0.80000	8.13297		1.09358	0.91025
1.00000	8.35142		1.10601	0.92176
1.20000	8.56667		1.12072	0.93281
1.40000	8.76626		1.13750	0.94281
1.60000	8.93109		1.15608	0.95090
1.80000	9.04815		1.17622	0.95656
2.00000	9.10732		1.19768	0.95939
2.20000	9.10455		1.22023	0.95926
2.40000	9.03915		1.24365	0.95613
2.60000	8.91440		1.26775	0.95009
2.80000	8.73388		1.29236	0.94121
3.00000	8.50680		1.31732	0.92977
3.20000	8.23857		1.34251	0.91585
3.40000	7.93716		1.36781	0.89966
3.60000	7.60907		1.39313	0.88133
3.80000	7.26116		1.41838	0.86101
4.00000	6.89953		1.44349	0.83882
4.20000	6.52951		1.46842	0.81488
4.40000	6.15622		1.49310	0.78931
4.60000	5.78407		1.51752	0.76223
4.80000	5.41800		1.54164	0.73384
5.00000	5.06051		1.56543	0.70419
5.20000	4.71521		1.58888	0.67350
5.40000	4.38454		1.61198	0.64192
5.60000	4.07025		1.63472	0.60962
5.80000	3.77426		1.65710	0.57683
6.00000	3.49715		1.67911	0.54371
6.20000	3.23884		1.70074	0.51039
6.40000	2.99911		1.72201	0.47699
6.60000	2.77786		1.74292	0.44371
6.80000	2.57352		1.76346	0.41053
7.00000	2.38654		1.78365	0.37777
7.20000	2.21435		1.80349	0.34525
7.40000	2.05632		1.82298	0.31309
7.60000	1.91117		1.84214	0.28130
7.80000	1.77798		1.86096	0.24993
8.00000	1.65561		1.87947	0.21896
8.20000	1.54310		1.89765	0.18839
8.40000	1.43963		1.91553	0.15825
8.60000	1.34434		1.93311	0.12851
8.80000	1.25666		1.95039	0.09922
9.00000	1.17583		1.96738	0.07034
9.20000	1.10127		1.98410	0.04189
9.40000	1.03244		2.00054	0.01387
9.60000	0.96884		2.01672	-0.01375



Chi_graph	-877.76044 ppm au
Chi_calc	-373.34273 ppm au
Jsuscept	-10.10142 au
Hmin	5.00000 au
Hmax	9.60000 au
s	3.42995 au
sigma_zz(CM)	7.65275 ppm