

DISCRETE SUMMATION OF INTER-MOLECULAR CONTRIBUTION
TO INDUCED FIELDS WITHIN INNER VOLUME ELEMENTS AND THE
CONVERGENCE CHARACTERISTICS AT OFF-CENTRE PROTON
SITES WITHIN THE I.V.E

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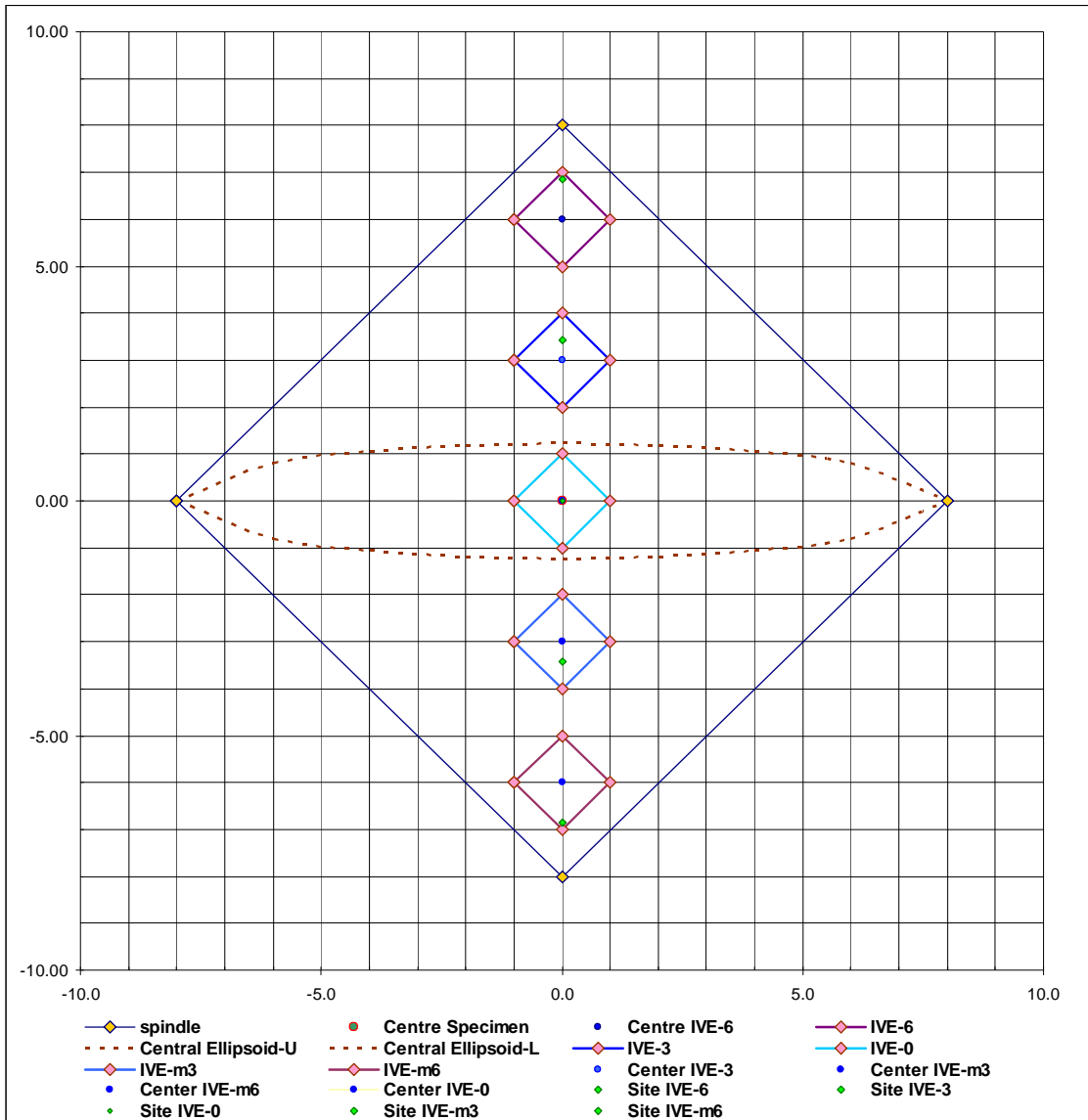
When the shape of a magnetized material is a non-spheroid, the bulk susceptibility-induced field distribution is inhomogeneous within the medium. However if the shape is a regular shape, even if non-spheroid, then it has been noted that an inner volume element of shape similar to the external macroscopic shape within which a special position can be found such that at that point the induced field from the external bulk can be zero¹. This situation was remarked to be similar to the case of spherical inner and outer shapes.

In the case of the spherical shape, this situation of zero induced fields within the IVE turned out to be advantageous for HR PMR measurement of chemical shift tensor parameters because of the convergence characteristics² of discretely summed intermolecular contributions to induced field at the centre of IVE.

But in the case of non-spheroid regular shapes, the zero induced field positions need not be the central points within the IVEs described. Then, it becomes imperative to find out the convergence characteristics of discrete summations to enable the possibility of applying a correction.

Such consideration would make it possible to envisage a protocol of procedure to extract the intra molecular Shielding Tensor Parameters of Protons in organic molecular single crystal by the HR PMR techniques in solids.

1. a) <http://nehuacin.tripod.com/id3.html> Sheet-11 of the poster at 4th Alpine Conference on SSNMR, held at Chamonix Mont Blanc, France; Sept. 11-15, 2005.
b) <http://nehuacin.tripod.com/id1.html> Sheets 18 and 19 of the Poster presentation at the EUROMAR2006, held at York University, York, UK; July, 16-21, 2006.
2. <http://nehuacin.tripod.com/id3.html> [same as Ref. 1.a) above] Sheets 6-8 of the same poster.



0.00	6.00	6.857
0.00	5.00	5.714
0.00	4.00	4.571
0.00	3.00	3.429
0.00	2.00	2.286
0.00	1.00	1.143
0.00	0.00	0
0.00	-1.00	-1.143
0.00	-2.00	-2.286
0.00	-3.00	-3.429
0.00	-4.00	-4.571
0.00	-5.00	-5.714
0.00	-6.00	-6.857

1	2	3	4	5	6	7
S.No	Center of inner Cavity	Series 1	Series 2	Coordinate of SITE	Series 3	Series-4
1	6.00	-3.600761	-5.379115	6.857	-5.674923	-9.158108E-03
2	5.00	-2.207148	-3.152036	5.714	-4.218981	-9.157889E-03
3	4.00	-1.173087	-1.728898	4.571	-2.968869	-9.157839E-03
4	3.00	-0.384413	-0.695102	3.429	-1.888949	-9.159081E-03
5	2.00	0.184228	0.043739	2.286	-0.876701	-9.157531E-03
6	1.00	0.534325	0.497607	1.143	-0.213899	-9.158962E-03
7	0.00	0.653988	0.653988	0.000	-0.009159	-9.159081E-03
8	-1.00	0.534322	0.497600	-1.143	-0.213903	-9.159088E-03
9	-2.00	0.184220	0.043727	-2.286	-0.876709	-9.158664E-03
10	-3.00	-0.384428	-0.695118	-3.429	-1.888960	-9.158962E-03
11	-4.00	-1.173105	-1.728915	-4.571	-2.968877	-9.157813E-03
12	-5.00	-2.207167	-3.152055	-5.714	-4.218988	-9.157280E-03
13	-6.00	-3.600782	-5.379138	-6.857	-5.674924	-9.159162E-03

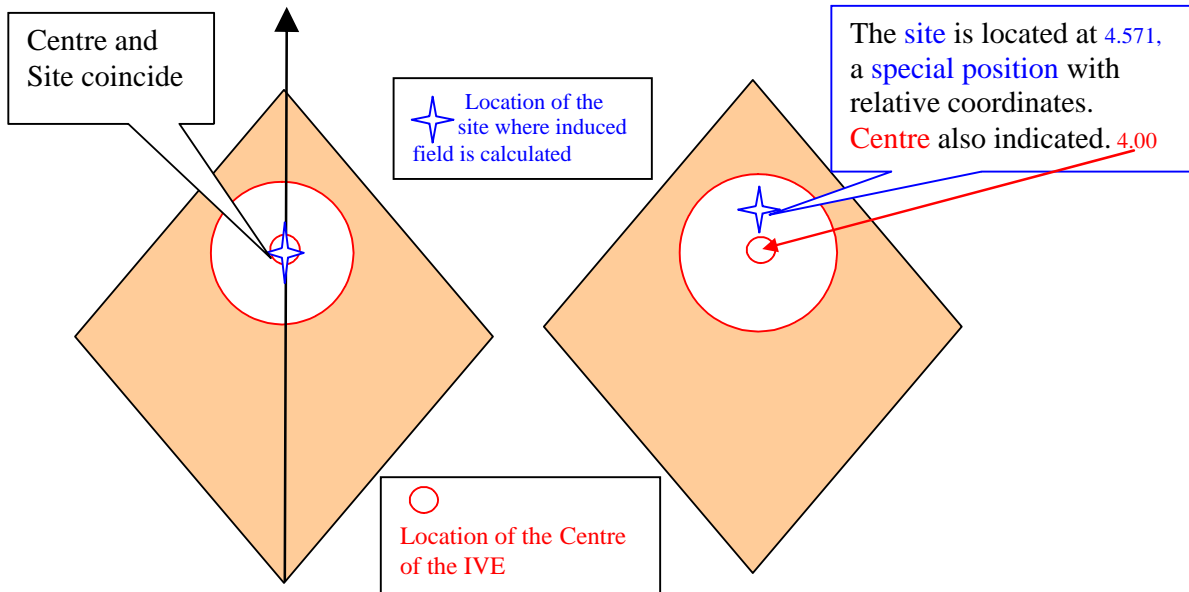
Series-1: Calculated for Spindle shaped specimen with spherical Inner Volume (CAVITY) Element around the site. But the site coordinates are NOT THE SAME as that of the CENTER (Col.2) of the INNER SPHERE. The site coordinates are inside the IVE with recalculated coordinate values (Col.5) for the site location inside the IVE.

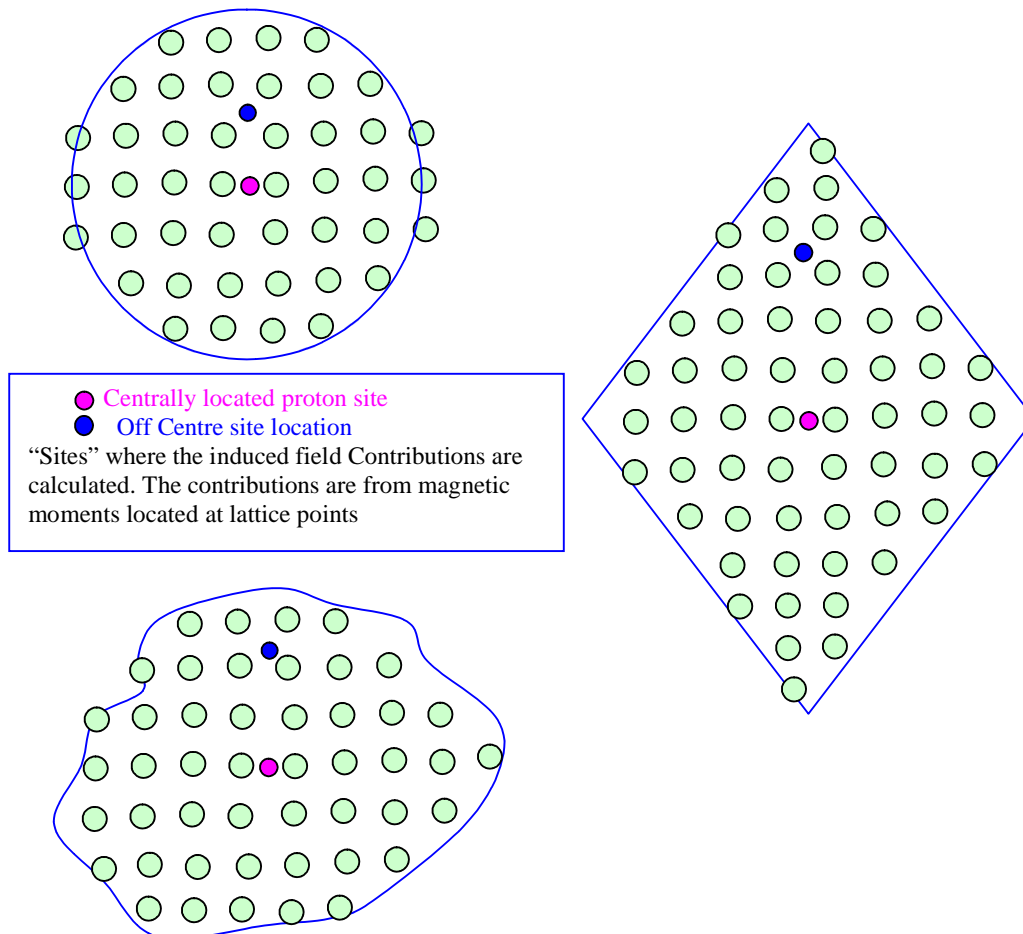
Series-2: The same case above but the site locations are at the same coordinate values as that of the center of the Spherical IVE.

In Column 6 and 7 of the Table, the calculated values are for the spindle shaped specimen with correspondingly similar spindle shaped cavity inside as the INNER VOLUME ELEMENT

Series-3: Calculated for the spindle shaped IVE at a site coinciding with center of IVE.

In column 7 the calculations are same as for Col.6 but the site is located inside IVE at a specially recalculated value. The last coordinate are all the same for induced fields as if it is a homogeneously magnetized specimen (homogeneity indicated for Homogeneous specimen of spindle shape)



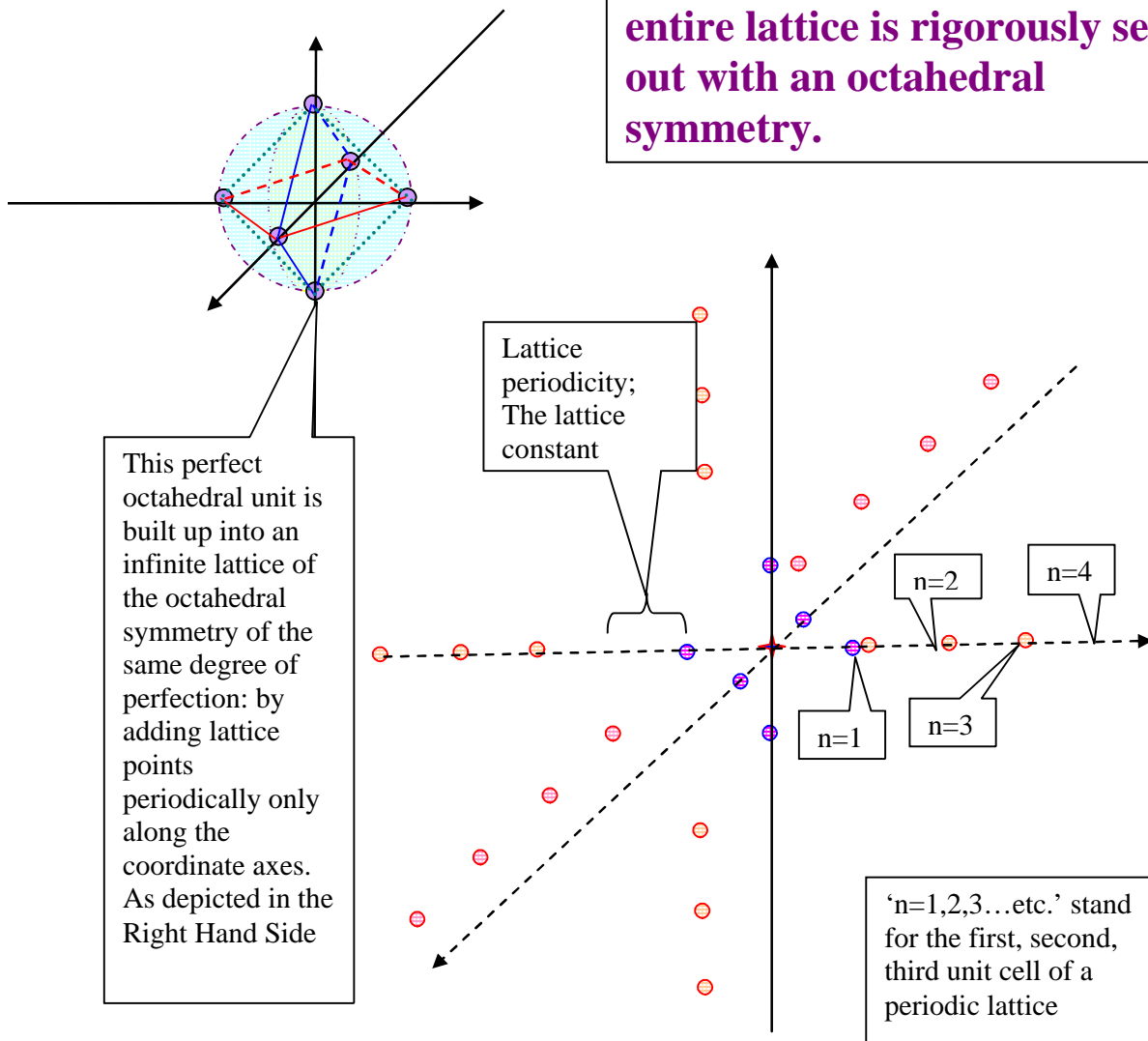


Considering the two types of Sites in a lattice where the induced field contributions are calculated by discrete summation from the moments at the lattice points, the following question is to be answered.

Will the induced field contributions would converge as it happens for the spherical shape?

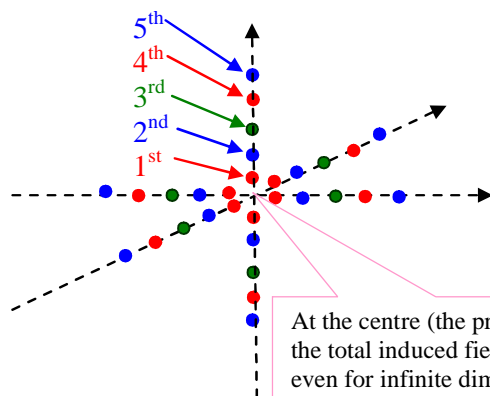
And, to get an answer it is necessary to examine the trends of the contributions from nearby to farther points. The Highly symmetric octahedral point group symmetry is evidently a choice for exemplifying typically text-book case.

A depiction of the hypothetical periodic lattice, where the entire lattice is rigorously set out with an octahedral symmetry.



The trends of induced field values when the proton location is varied along the coordinate axis are displayed in the following sheets.

Calculation for First coordinate sphere n=1						
n	Proton Position coordinates			Distance	angle	Induced field
1.0	3.0	0.0	0.0	3.0	89.96	1.1111E-07
1.0	-3.0	0.0	0.0	3.0	89.96	1.1111E-07
1.0	0.0	3.0	0.0	3.0	89.96	1.1111E-07
1.0	0.0	-3.0	0.0	3.0	89.96	1.1111E-07
1.0	0.0	0.0	3.0	3.0	0	-2.2222E-07
1.0	0.0	0.0	-3.0	3.0	0	-2.2222E-07
						Total=0.0
Calculation of coordinate sphere n=2						
2.0	6.0	0.0	0.0	6.0	89.96	1.3889E-08
2.0	-6.0	0.0	0.0	6.0	89.96	1.3889E-08
2.0	0.0	6.0	0.0	6.0	89.96	1.3889E-08
2.0	0.0	-6.0	0.0	6.0	89.96	1.3889E-08
2.0	0.0	0.0	6.0	6.0	0	-2.7778E-08
2.0	0.0	0.0	-6.0	6.0	0	-2.7778E-08
						Total=0.0
Calculation of to coordinate sphere n=3						
3.0	9.0	0.0	0.0	9.0	89.96	4.1152E-09
3.0	-9.0	0.0	0.0	9.0	89.96	4.1152E-09
3.0	0.0	9.0	0.0	9.0	89.96	4.1152E-09
3.0	0.0	-9.0	0.0	9.0	89.96	4.1152E-09
3.0	0.0	0.0	9.0	9.0	0	-8.2305E-09
3.0	0.0	0.0	-9.0	9.0	0	-8.2305E-09
						Total=0.0
Calculation of to coordinate sphere n=4						
4.0	12.0	0.0	0.0	12.0	89.96	1.7361E-09
4.0	-12.0	0.0	0.0	12.0	89.96	1.7361E-09
4.0	0.0	12.0	0.0	12.0	89.96	1.7361E-09
4.0	0.0	-12.0	0.0	12.0	89.96	1.7361E-09
4.0	0.0	0.0	12.0	12.0	0	-3.4722E-09
4.0	0.0	0.0	-12.0	12.0	0	-3.4722E-09
						Total=0.0
Calculation of coordinate sphere n=5						
5.0	15.0	0.0	0.0	15.0	89.96	8.8889E-10
5.0	-15.0	0.0	0.0	15.0	89.96	8.8889E-10
5.0	0.0	15.0	0.0	15.0	89.96	8.8889E-10
5.0	0.0	-15.0	0.0	15.0	89.96	8.8889E-10
5.0	0.0	0.0	15.0	15.0	0	-1.7778E-09
5.0	0.0	0.0	-15.0	15.0	0	-1.7778E-09
						Total=0.0



At the centre (the proton position) the total induced field value is zero even for infinite dimensions.

A typical text-book case of discrete summation of induced fields. At the centre of octahedral-surrounding, the discretely summed value for the induced field results in exact zero.

What would be the trend if the proton is located at a general point-not at any of the periodic lattice points?

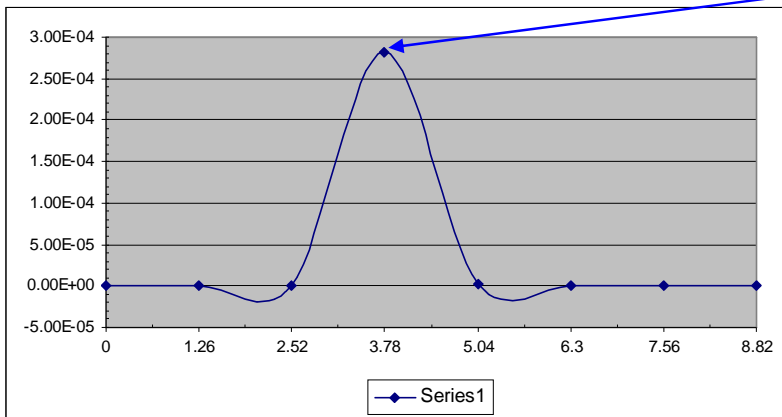
CALCULATION FOR OCTAHEDRAL SYMMETRY

LATTICE Constant = 4.

N	FLDR	FLDRT	RIA	RIAN	RIB	RIBN	RIC	RICN
1	0.00000E+00	0.00000E+00	4.000	4.000	4.000	4.000	4.000	4.000
1	0.85105E-07	0.85105E-07	2.740	5.260	4.194	4.194	4.194	4.194
1	0.87945E-06	0.87945E-06	1.480	6.520	4.728	4.728	4.728	4.728
1	0.28171E-03	0.28171E-03	0.220	7.780	5.503	5.503	5.503	5.503
1	0.26485E-05	0.26485E-05	1.040	9.040	6.434	6.434	6.434	6.434
1	0.23488E-06	0.23488E-06	2.300	10.300	7.463	7.463	7.463	7.463
1	0.58845E-07	0.58845E-07	3.560	11.560	8.553	8.553	8.553	8.553
1	0.21609E-07	0.21609E-07	4.820	12.820	9.685	9.685	9.685	9.685

N	PA	PB	PC	FLDR	FLDRT
1	0.000	0.000	0.000	0.00000E+00	0.00000E+00
1	1.260	0.000	0.000	0.85105E-07	0.85105E-07
1	2.520	0.000	0.000	0.87945E-06	0.87945E-06
1	3.780	0.000	0.000	0.28171E-03	0.28171E-03
1	5.040	0.000	0.000	0.26485E-05	0.26485E-05
1	6.300	0.000	0.000	0.23488E-06	0.23488E-06
1	7.560	0.000	0.000	0.58845E-07	0.58845E-07
1	8.820	0.000	0.000	0.21609E-07	0.21609E-07

The magnetic moments are at the lattice points. When the proton site is located at 3.78,0,0 the nearest moment is at 4, 0, 0. And the distance is 0.220(RIA). For this distance the induced field is of the order of 10^{-4}



CALCULATION FOR OCTAHEDRAL SYMMETRY

LATTICE Constant = 5.

N	FLDR	FLDRT	RIA	RIAN	RIB	RIBN	RIC	RICN
1	0.00000E+00	0.00000E+00	5.000	5.000	5.000	5.000	5.000	5.000
1	0.25810E-07	0.25810E-07	3.740	6.260	5.156	5.156	5.156	5.156
1	0.16956E-06	0.16956E-06	2.480	7.520	5.599	5.599	5.599	5.599
1	0.16322E-05	0.16322E-05	1.220	8.780	6.268	6.268	6.268	6.268
1	0.46875E-01	0.46875E-01	0.040	10.040	7.099	7.099	7.099	7.099
1	0.13560E-05	0.13560E-05	1.300	11.300	8.043	8.043	8.043	8.043
1	0.17227E-06	0.17227E-06	2.560	12.560	9.064	9.064	9.064	9.064
1	0.49198E-07	0.49198E-07	3.820	13.820	10.139	10.139	10.139	10.139
1	0.19547E-07	0.19547E-07	5.080	15.080	11.252	11.252	11.252	11.252

N	PA	PB	PC	FLDR	FLDRT
1	0.000	0.000	0.000	0.00000E+00	0.00000E+00
1	1.260	0.000	0.000	0.25810E-07	0.25810E-07
1	2.520	0.000	0.000	0.16956E-06	0.16956E-06
1	3.780	0.000	0.000	0.16322E-05	0.16322E-05
1	5.040	0.000	0.000	0.46875E-01	0.46875E-01
1	6.300	0.000	0.000	0.13560E-05	0.13560E-05
1	7.560	0.000	0.000	0.17227E-06	0.17227E-06
1	8.820	0.000	0.000	0.49198E-07	0.49198E-07
1	10.080	0.000	0.000	0.19547E-07	0.19547E-07

CALCULATION FOR OCTAHEDRAL SYMMETRY

LATTICE Constant = 6.

N	FLDR	FLDRT	RIA	RIAN	RIB	RIBN	RIC	RICN
1	0.00000E+00	0.00000E+00	6.000	6.000	6.000	6.000	6.000	6.000
1	0.99733E-08	0.99733E-08	4.740	7.260	6.131	6.131	6.131	6.131
1	0.54265E-07	0.54265E-07	3.480	8.520	6.508	6.508	6.508	6.508
1	0.26058E-06	0.26058E-06	2.220	9.780	7.091	7.091	7.091	7.091
1	0.33806E-05	0.33806E-05	0.960	11.040	7.836	7.836	7.836	7.836
1	0.11110E-03	0.11110E-03	0.300	12.300	8.700	8.700	8.700	8.700
1	0.78475E-06	0.78475E-06	1.560	13.560	9.652	9.652	9.652	9.652
1	0.12975E-06	0.12975E-06	2.820	14.820	10.667	10.667	10.667	10.667
1	0.41176E-07	0.41176E-07	4.080	16.080	11.731	11.731	11.731	11.731
1	0.17435E-07	0.17435E-07	5.340	17.340	12.829	12.829	12.829	12.829
1	0.86936E-08	0.86936E-08	6.600	18.600	13.956	13.956	13.956	13.956

N	PA	PB	PC	FLDR	FLDRT
1	0.000	0.000	0.000	0.00000E+00	0.00000E+00
1	1.260	0.000	0.000	0.99733E-08	0.99733E-08
1	2.520	0.000	0.000	0.54265E-07	0.54265E-07
1	3.780	0.000	0.000	0.26058E-06	0.26058E-06
1	5.040	0.000	0.000	0.33806E-05	0.33806E-05
1	6.300	0.000	0.000	0.11110E-03	0.11110E-03
1	7.560	0.000	0.000	0.78475E-06	0.78475E-06
1	8.820	0.000	0.000	0.12975E-06	0.12975E-06
1	10.080	0.000	0.000	0.41176E-07	0.41176E-07
1	11.340	0.000	0.000	0.17435E-07	0.17435E-07
1	12.600	0.000	0.000	0.86936E-08	0.86936E-08

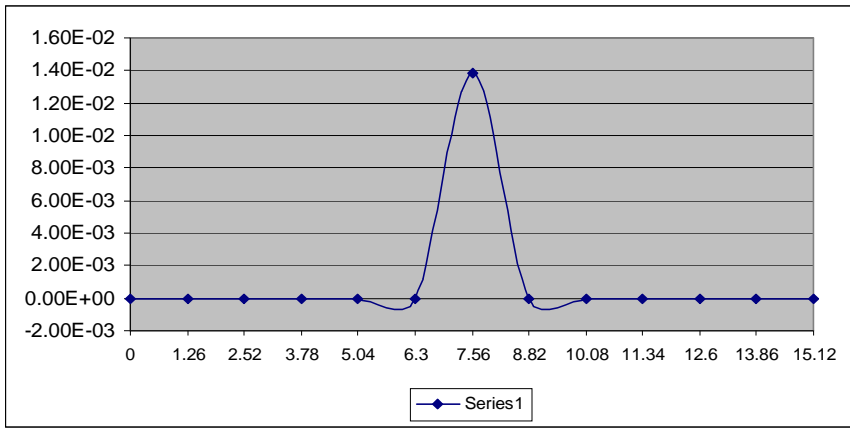
CALCULATION FOR OCTAHEDRAL SYMMETRY

LATTICE Constant = 7.5

N	FLDR	FLDRT	RIA	RIAN	RIB	RIBN	RIC	RICN
1	0.00000E+00	0.00000E+00	7.500	7.500	7.500	7.500	7.500	7.500
1	0.31693E-08	0.31693E-08	6.240	8.760	7.605	7.605	7.605	7.605
1	0.15158E-07	0.15158E-07	4.980	10.020	7.912	7.912	7.912	7.912
1	0.50239E-07	0.50239E-07	3.720	11.280	8.399	8.399	8.399	8.399
1	0.19491E-06	0.19491E-06	2.460	12.540	9.036	9.036	9.036	9.036
1	0.17309E-05	0.17309E-05	1.200	13.800	9.795	9.795	9.795	9.795
1	0.13889E-01	0.13889E-01	0.060	15.060	10.649	10.649	10.649	10.649
1	0.13012E-05	0.13012E-05	1.320	16.320	11.578	11.578	11.578	11.578
1	0.17221E-06	0.17221E-06	2.580	17.580	12.564	12.564	12.564	12.564
1	0.51043E-07	0.51043E-07	3.840	18.840	13.596	13.596	13.596	13.596
1	0.21082E-07	0.21082E-07	5.100	20.100	14.663	14.663	14.663	14.663
1	0.10436E-07	0.10436E-07	6.360	21.360	15.759	15.759	15.759	15.759
1	0.57917E-08	0.57917E-08	7.620	22.620	16.878	16.878	16.878	16.878

N	PA	PB	PC	FLDR	FLDRT
1	0.000	0.000	0.000	0.00000E+00	0.00000E+00
1	1.260	0.000	0.000	0.31693E-08	0.31693E-08
1	2.520	0.000	0.000	0.15158E-07	0.15158E-07
1	3.780	0.000	0.000	0.50239E-07	0.50239E-07
1	5.040	0.000	0.000	0.19491E-06	0.19491E-06
1	6.300	0.000	0.000	0.17309E-05	0.17309E-05
1	7.560	0.000	0.000	0.13889E-01	0.13889E-01
1	8.820	0.000	0.000	0.13012E-05	0.13012E-05
1	10.080	0.000	0.000	0.17221E-06	0.17221E-06
1	11.340	0.000	0.000	0.51043E-07	0.51043E-07
1	12.600	0.000	0.000	0.21082E-07	0.21082E-07
1	13.860	0.000	0.000	0.10436E-07	0.10436E-07
1	15.120	0.000	0.000	0.57917E-08	0.57917E-08

The magnetic moments are at the lattice points. When the proton site is located at **7.56,0,0** the nearest moment is at **7.5, 0, 0**. And the distance is **0.060** (RIA). For this distance the induced field is of the order of **10⁻⁰²**



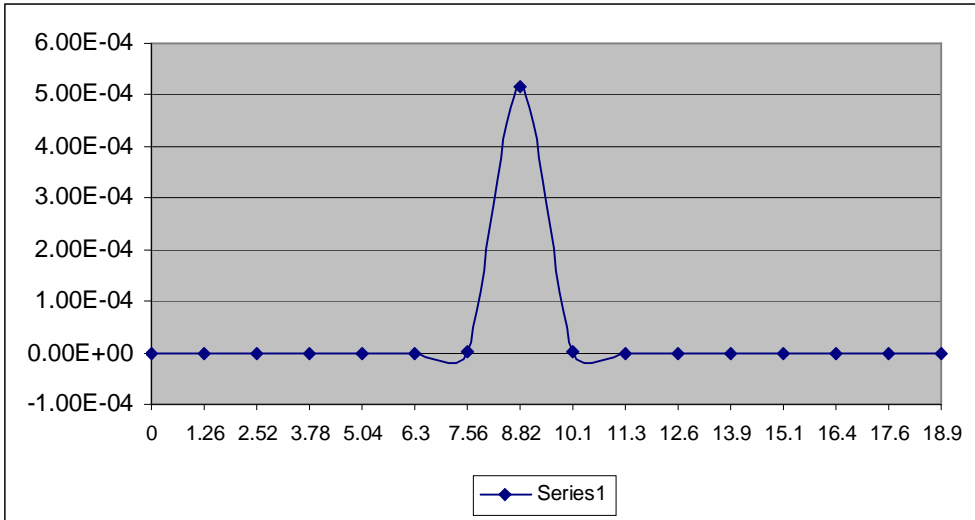
CALCULATION FOR OCTAHEDRAL SYMMETRY

LATTICE Constant = 9.

N	FLDR	FLDRT	RIA	RIAN	RIB	RIBN	RIC	RICN
1	0.00000E+00	0.00000E+00	9.000	9.000	9.000	9.000	9.000	9.000
1	0.12533E-08	0.12533E-08	7.740	10.260	9.088	9.088	9.088	9.088
1	0.56383E-08	0.56383E-08	6.480	11.520	9.346	9.346	9.346	9.346
1	0.16078E-07	0.16078E-07	5.220	12.780	9.762	9.762	9.762	9.762
1	0.43927E-07	0.43927E-07	3.960	14.040	10.315	10.315	10.315	10.315
1	0.14873E-06	0.14873E-06	2.700	15.300	10.986	10.986	10.986	10.986
1	0.10017E-05	0.10017E-05	1.440	16.560	11.754	11.754	11.754	11.754
1	0.51441E-03	0.51441E-03	0.180	17.820	12.601	12.601	12.601	12.601
1	0.23795E-05	0.23795E-05	1.080	19.080	13.513	13.513	13.513	13.513
1	0.23252E-06	0.23252E-06	2.340	20.340	14.477	14.477	14.477	14.477
1	0.62982E-07	0.62982E-07	3.600	21.600	15.484	15.484	15.484	15.484
1	0.25056E-07	0.25056E-07	4.860	22.860	16.526	16.526	16.526	16.526
1	0.12200E-07	0.12200E-07	6.120	24.120	17.596	17.596	17.596	17.596
1	0.67281E-08	0.67281E-08	7.380	25.380	18.690	18.690	18.690	18.690
1	0.40375E-08	0.40375E-08	8.640	26.640	19.803	19.803	19.803	19.803
1	0.25759E-08	0.25759E-08	9.900	27.900	20.933	20.933	20.933	20.933

N	PA	PB	PC	FLDR	FLDRT
1	0.000	0.000	0.000	0.00000E+00	0.00000E+00
1	1.260	0.000	0.000	0.12533E-08	0.12533E-08
1	2.520	0.000	0.000	0.56383E-08	0.56383E-08
1	3.780	0.000	0.000	0.16078E-07	0.16078E-07
1	5.040	0.000	0.000	0.43927E-07	0.43927E-07
1	6.300	0.000	0.000	0.14873E-06	0.14873E-06
1	7.560	0.000	0.000	0.10017E-05	0.10017E-05
1	8.820	0.000	0.000	0.51441E-03	0.51441E-03
1	10.080	0.000	0.000	0.23795E-05	0.23795E-05
1	11.340	0.000	0.000	0.23252E-06	0.23252E-06
1	12.600	0.000	0.000	0.62982E-07	0.62982E-07
1	13.860	0.000	0.000	0.25056E-07	0.25056E-07
1	15.120	0.000	0.000	0.12200E-07	0.12200E-07
1	16.380	0.000	0.000	0.67281E-08	0.67281E-08
1	17.640	0.000	0.000	0.40375E-08	0.40375E-08
1	18.900	0.000	0.000	0.25759E-08	0.25759E-08

The magnetic moments are at the lattice points. When the proton site is located at **8.82,0,0** the nearest moment is at **9.0, 0, 0**. And the distance is **0.180** (RIA). For this distance the induced field is of the order of **10⁻⁰⁴**



CALCULATION FOR OCTAHEDRAL SYMMETRY

LATTICE Constant = 10.

N	FLDR	FLDRT	RIA	RIAN	RIB	RIBN	RIC	RICN
1	0.00000E+00	0.00000E+00	10.000	10.000	10.000	10.000	10.000	10.000
1	0.73501E-09	0.73501E-09	8.740	11.260	10.079	10.079	10.079	10.079
1	0.32263E-08	0.32263E-08	7.480	12.520	10.313	10.313	10.313	10.313
1	0.87024E-08	0.87024E-08	6.220	13.780	10.691	10.691	10.691	10.691
1	0.21195E-07	0.21195E-07	4.960	15.040	11.198	11.198	11.198	11.198
1	0.56285E-07	0.56285E-07	3.700	16.300	11.819	11.819	11.819	11.819
1	0.20402E-06	0.20402E-06	2.440	17.560	12.536	12.536	12.536	12.536
1	0.18238E-05	0.18238E-05	1.180	18.820	13.334	13.334	13.334	13.334
1	0.58592E-02	0.58592E-02	0.080	20.080	14.199	14.199	14.199	14.199
1	0.12454E-05	0.12454E-05	1.340	21.340	15.119	15.119	15.119	15.119
1	0.16951E-06	0.16951E-06	2.600	22.600	16.086	16.086	16.086	16.086
1	0.51182E-07	0.51182E-07	3.860	23.860	17.091	17.091	17.091	17.091
1	0.21534E-07	0.21534E-07	5.120	25.120	18.128	18.128	18.128	18.128
1	0.10867E-07	0.10867E-07	6.380	26.380	19.191	19.191	19.191	19.191
1	0.61497E-08	0.61497E-08	7.640	27.640	20.277	20.277	20.277	20.277
1	0.37661E-08	0.37661E-08	8.900	28.900	21.382	21.382	21.382	21.382
1	0.24434E-08	0.24434E-08	10.160	30.160	22.504	22.504	22.504	22.504

N	PA	PB	PC	FLDR	FLDRT
1	0.000	0.000	0.000	0.00000E+00	0.00000E+00
1	1.260	0.000	0.000	0.73501E-09	0.73501E-09
1	2.520	0.000	0.000	0.32263E-08	0.32263E-08
1	3.780	0.000	0.000	0.87024E-08	0.87024E-08
1	5.040	0.000	0.000	0.21195E-07	0.21195E-07
1	6.300	0.000	0.000	0.56285E-07	0.56285E-07
1	7.560	0.000	0.000	0.20402E-06	0.20402E-06
1	8.820	0.000	0.000	0.18238E-05	0.18238E-05
1	10.080	0.000	0.000	0.58592E-02	0.58592E-02
1	11.340	0.000	0.000	0.12454E-05	0.12454E-05
1	12.600	0.000	0.000	0.16951E-06	0.16951E-06
1	13.860	0.000	0.000	0.51182E-07	0.51182E-07
1	15.120	0.000	0.000	0.21534E-07	0.21534E-07
1	16.380	0.000	0.000	0.10867E-07	0.10867E-07
1	17.640	0.000	0.000	0.61497E-08	0.61497E-08
1	18.900	0.000	0.000	0.37661E-08	0.37661E-08
1	20.160	0.000	0.000	0.24434E-08	0.24434E-08

SITE Location			Total InducedField
a	b	c	
-1	0	0	2.6974E-07
-0.9	0	0	2.1070E-07
-0.8	0	0	1.6157E-07
-0.7	0	0	1.2071E-07
-0.6	0	0	8.6958E-08
-0.5	0	0	5.9453E-08
-0.4	0	0	3.7595E-08
-0.3	0	0	2.0960E-08
-0.2	0	0	9.2586E-09
-0.1	0	0	2.3064E-09
0	0	0	0.0000E+00
0.1	0	0	2.3064E-09
0.2	0	0	9.2587E-09
0.3	0	0	2.0960E-08
0.4	0	0	3.7595E-08
0.5	0	0	5.9453E-08
0.6	0	0	8.6958E-08
0.7	0	0	1.2071E-07
0.8	0	0	1.6157E-07
0.9	0	0	2.1070E-07
1	0	0	2.6974E-07
1.1	0	0	3.4095E-07
1.2	0	0	4.2745E-07
1.3	0	0	5.3367E-07
1.4	0	0	6.6582E-07
1.5	0	0	8.3289E-07
1.6	0	0	1.0481E-06
1.7	0	0	1.3311E-06
1.8	0	0	1.7126E-06
1.9	0	0	2.2413E-06
2	0	0	2.9982E-06
2.1	0	0	4.1243E-06
2.2	0	0	5.8794E-06
2.3	0	0	8.7774E-06
2.4	0	0	1.3931E-05
2.5	0	0	2.4053E-05
2.6	0	0	4.6940E-05
2.7	0	0	1.1119E-04
2.8	0	0	3.7508E-04
2.9	0	0	3.0000E-03
3	0	0	6.4537E+11
3.1	0	0	3.0003E-03
3.2	0	0	3.7516E-04
3.3	0	0	1.1128E-04
3.4	0	0	4.7068E-05
3.5	0	0	2.4217E-05
3.6	0	0	1.4134E-05
3.7	0	0	9.0239E-06
3.8	0	0	6.1750E-06
3.9	0	0	4.4758E-06
4	0	0	3.4145E-06
4.1	0	0	2.7336E-06

For Lattice constant=3.0

Table of computed data on the Left Hand Side.

For varying the proton location. Since the X-axis value 3.0 corresponds to the location of proton site at 3 units, the moment located at the 3 units distance is very close to the proton site, as close as zero.

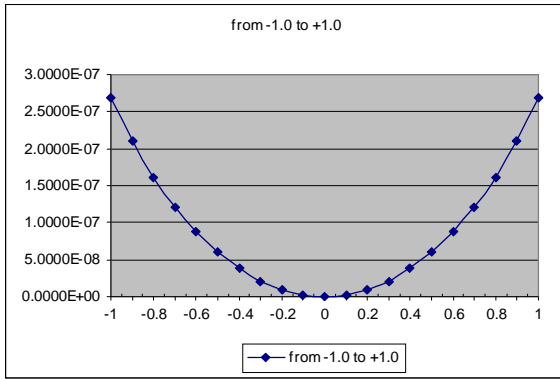
Hence the induced field contribution is significantly very high compared to other locations away from the point at 3units.

If, in the computer program, a control statement is introduced to skip the calculations if the distance factor is close to zero value, this sharp increased value in the total induced field contribution will not appear in listed out data and even at the 3 units distance, the program would have skipped a calculation step , and would not add to the total.

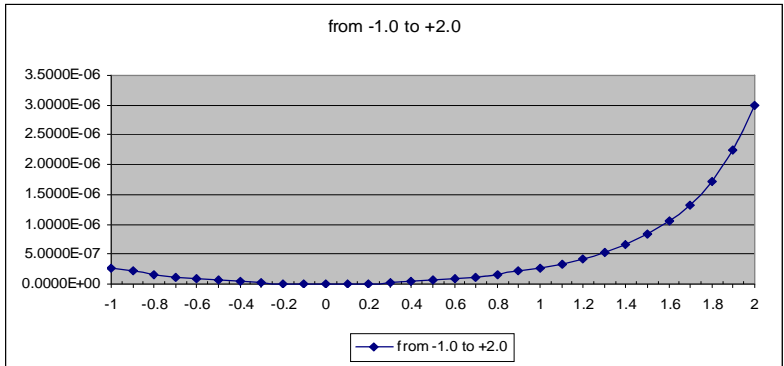
These considerations are depicted in the Graphical plot of these data in the next sheet on display.

Since the Lattice is periodic, the characteristics described for the trends within a unit cell would repeat for the remaining part of the lattice.

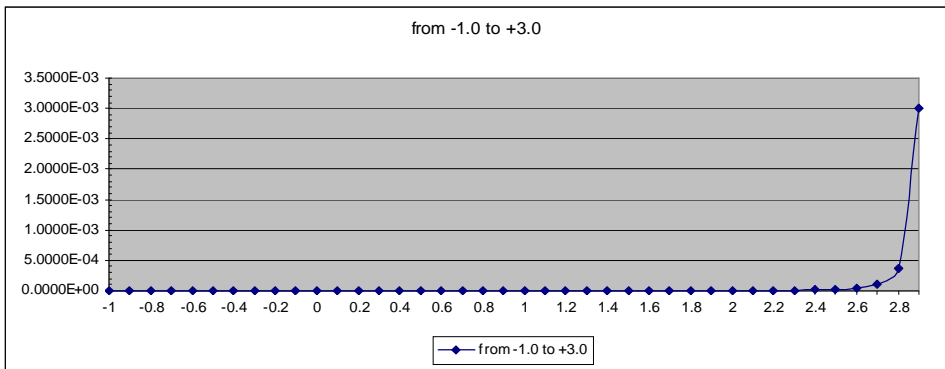
Thus the inferences from the Graphical plots of this data can be considered for indicating the trends for a Unit cell



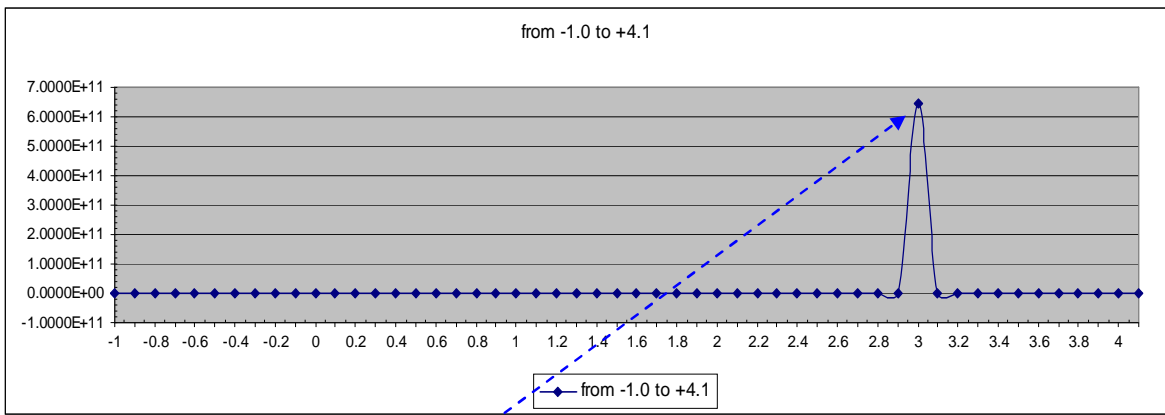
From the table in previous sheet, the region from -1 to +1 is plotted. The corresponding y-axis values are mostly in the range from 0 up to 10^{-7}



The same table is the data source.
X-axis from -1.0 to +2.0
The corresponding y-values are up to 10^{-6}



Plot X-axis -1 to +3
Y-values range up to 10^{-3}



Plot X-axis -1 up to +4 the Y-values sharply raise near '+3' and range up to 10^{+11}
This trend of appearance of sharp raise in the induced field contributions occur whenever the proton sites are closer to the moments (in this instance moments are located at the lattice points).
This had been already elaborated in the preceding sheets #05, 06, 07 &08

