A study of radiation damage in plastic scintillators using magnetic resonance techniques for the upgrade of the ATLAS detector

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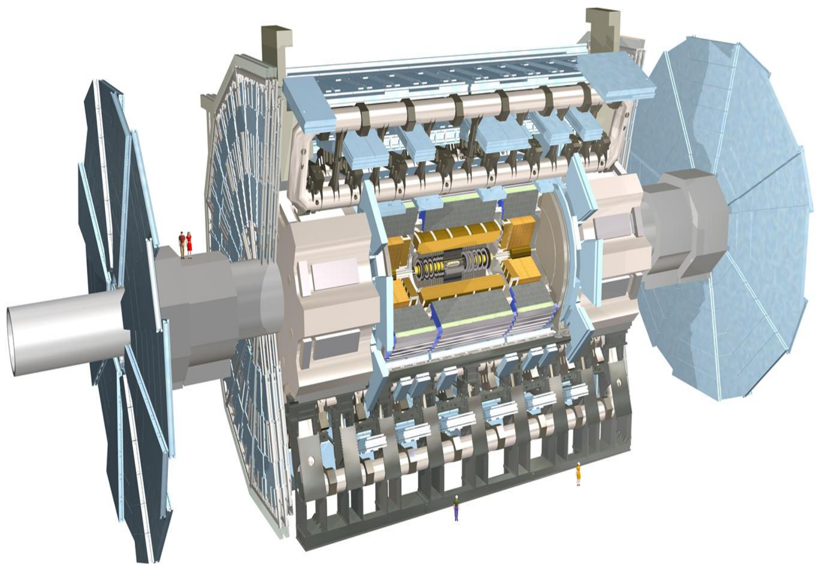
Outline of presentation

- The ATLAS detector
- MBTS plastics
- Aims
- Plastic structure
- EPR
- Results and Summary

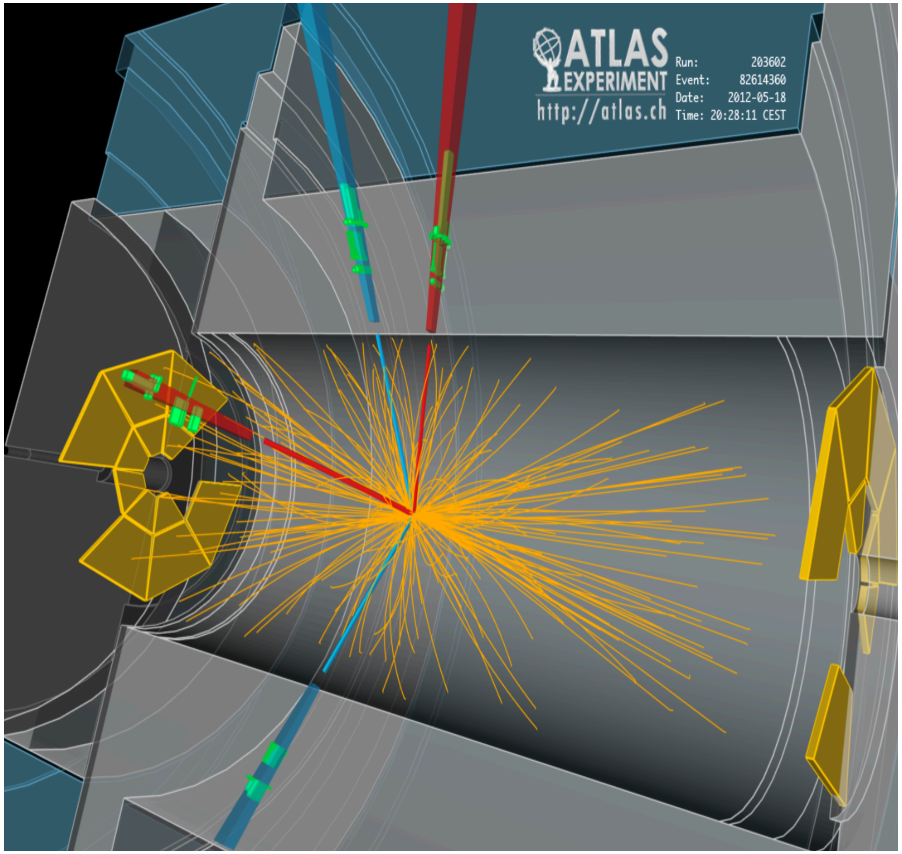
The ATLAS Detector



- Largest of 4 detectors in the LHC
- Tile Calorimeter (TileCal) situated in the inner detector
- Able to detect energetic particles: hadrons, quarks, jets…

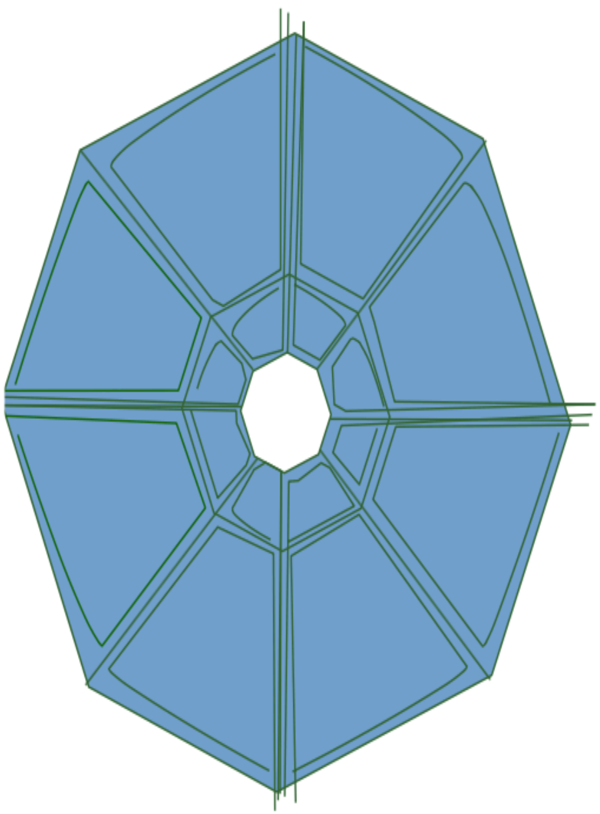
The Minium Bias Trigger Scintillator plastics

- Located on EndCaps of ATLAS detector
- Installed at 2.08<|η|<3.75 around beam pipe
- Part of the Level 1 Trigger system
- 32 in total, 16 on both EndCaps
- Track trajectories of energetic particles



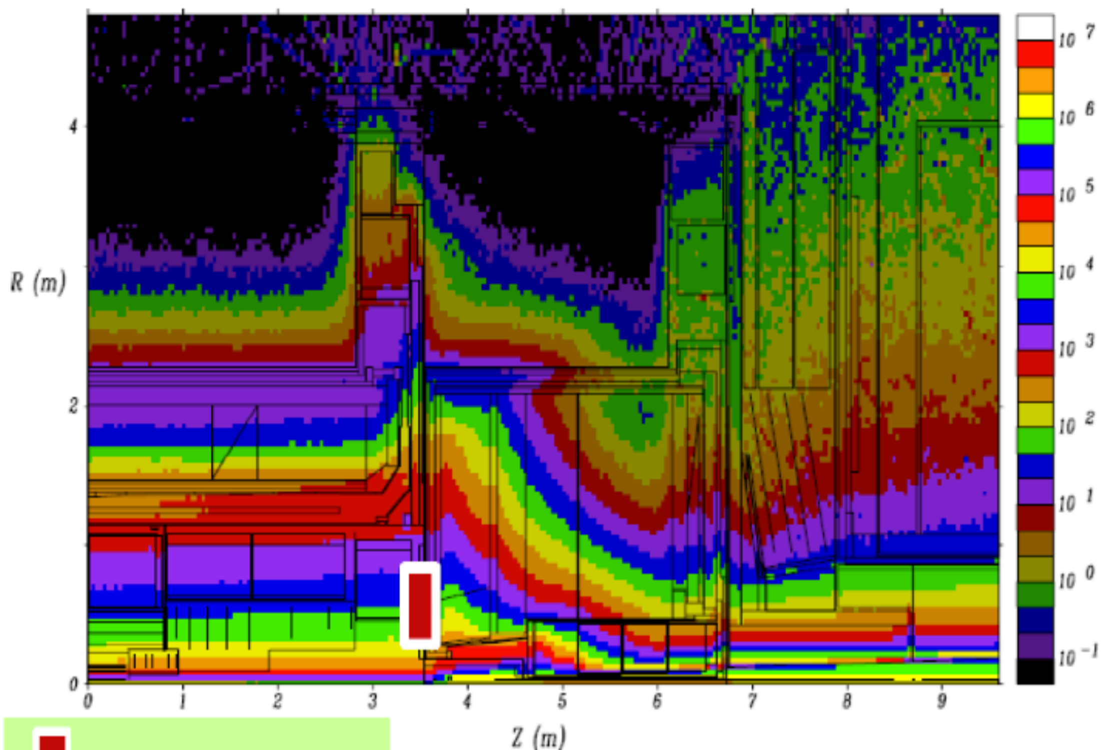
http://www.atlas.ch/photos/atlas_photos/selected-photos/events/run203602_evt82614360_VP1DetailFull.png

MBTS Continued



- 2 cm thick
- Polystyrene base plastics
- Susceptible to radiation damage due to low to medium energy particle interaction
- Due to be replaced because of lack of efficiency

Radiation Environment



@10^4 Gy → ~50% Loss Light Transmission

MBTS position

Ionization dose (Gy) prediction after 1 year at 10^{34} $cm^{-2}s^{-1}$ at $\sqrt{s}$=14 TeV

In Run I MBTS accumulated ~0.21 x (0.5-2.0)x 10^4 Gy = [0.1~0.4] x 10^4 Gy

A. Sidoti 2014 *JINST* **9** C10020

Our aims are then to:

Find a replacement

- From 6 plastic grades, which one is best?

Polyvinyl-toluene (PVT) based Eljen samples:

- EJ200
- EJ208
- EJ260
- Bicron

Polystyrene based samples

- Dubna
- Protvino

Understand the damage

- How can we characterize damage to the different plastics?

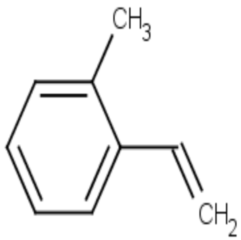
Using electron paramagnetic resonance (EPR)

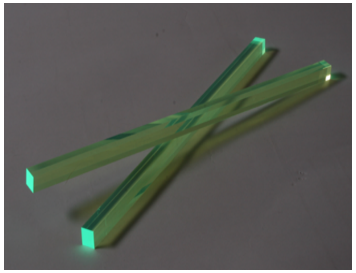
Post density functional theory (DFT) calculations

The plastics

The PVT samples

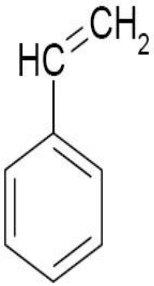
- Two blue and one green emitting scintillator: EJ200, EJ208, EJ260, Bicron
- Organic dopants

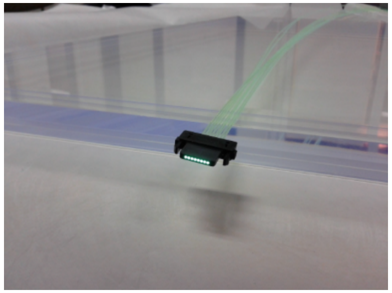




The polystyrene samples

- Three blue emitting scintillators: Dubna, Protvino
- Organic dopants: POPOP, p-TP

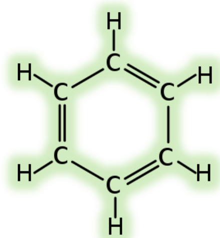




C-H bonds are most likely to break in both samples[1,2]

[1] Torrisi L 1998 *Radiation Effects and Defects in Solids* **145** 271–284 ISSN 1042-0150
[2] Torrisi L 2002 *Radiation Physics and Chemistry* **63** 89–92 ISSN 0969806X

DFT Set Up



VASP

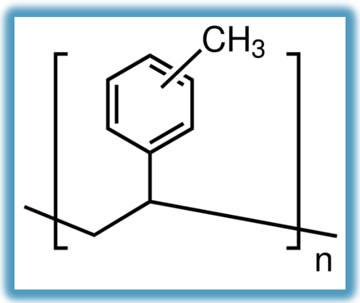
PHYSICAL REVIEW VOLUME 140, NUMBER 4A 15 NOVEMBER 1965

Self-Consistent Equations Including Exchange and Correlation Effects

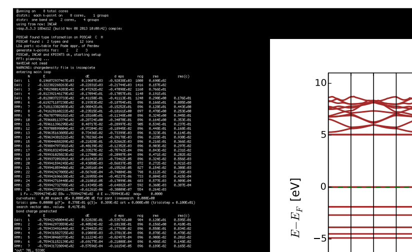
W. Kohn and L. J. Sham

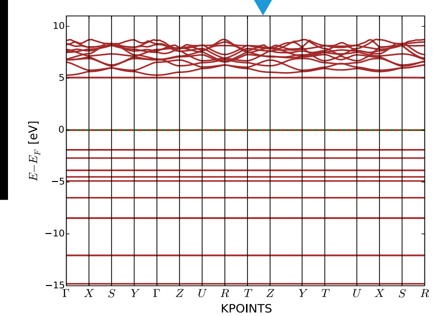
University of California, San Diego, La Jolla, California

$$E=\sum_{1}^{N}\epsilon_i-\frac{1}{2}\int\int\frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}\,d\mathbf{r}'+\int n(\mathbf{r})[\epsilon_{xc}(n(\mathbf{r}))-\mu_{xc}(n(\mathbf{r}))]\,d\mathbf{r}.$$



Quantum Espresso

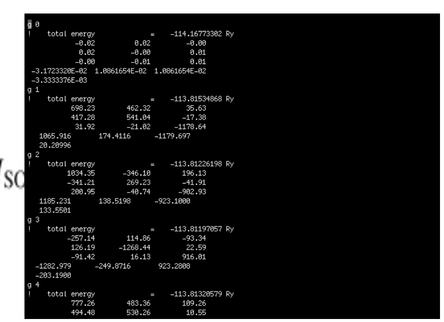




First-Principles Theory of the EPR g Tensor in Solids: Defects in Quartz

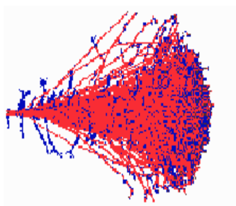
Chris J. Pickard

$$H=\sum_i\left\{\frac{[\mathbf{p}_i+\alpha\mathbf{A}(\mathbf{r}_i)]^2}{2}-\sum_I\frac{Z_I}{|\mathbf{r}_i-\mathbf{R}_I|}+\sum_{j\neq i}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}\right\}+H_Z+H_{Z\text{-KE}}+H_{SO}$$



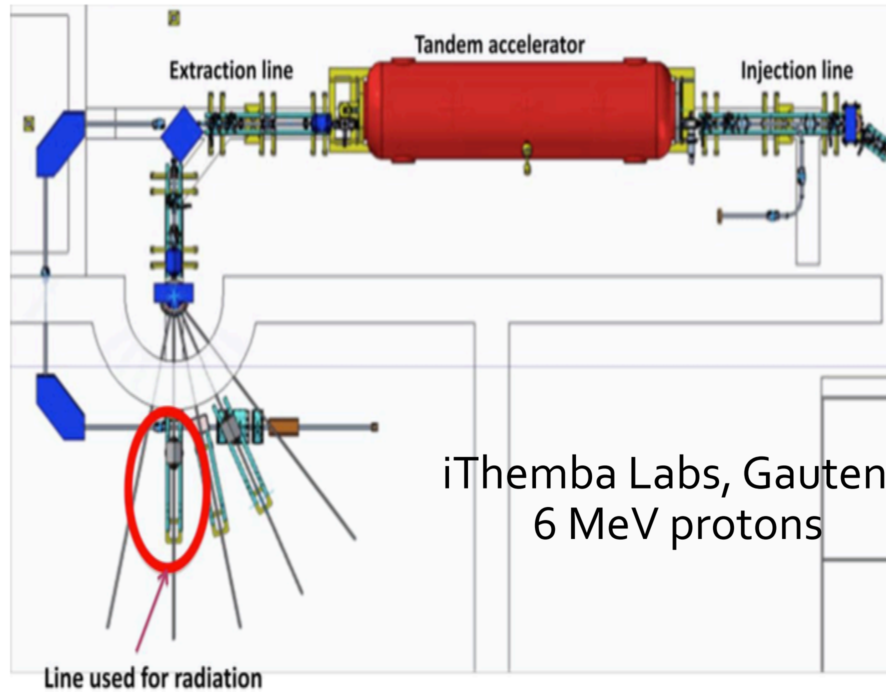
Sample preparation

SRIM (Stopping Range of Ions in Matter)



~470μm

~250μm



iThemba Labs, Gauteng
6 MeV protons

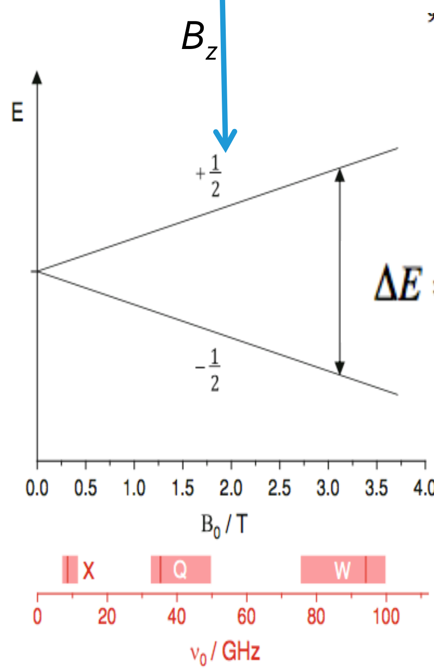
Irradiated sample

All six plastics to be irradiated to 6 different doses and compared to an un-irradiated sample

Electron Paramagnetic Resonance

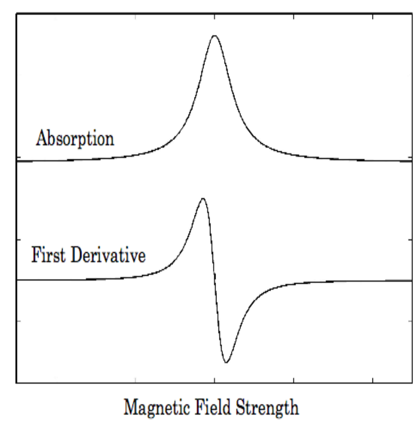
EPR probes the electronic structure of the samples by looking at their unpaired electrons and ions

$$\mathcal{H} = \beta \mathbf{B} \cdot \mathbf{g} \cdot \mathbf{S} + \sum_{l} \mathbf{S} \cdot \mathbf{A}_l \cdot \mathbf{I}_l$$



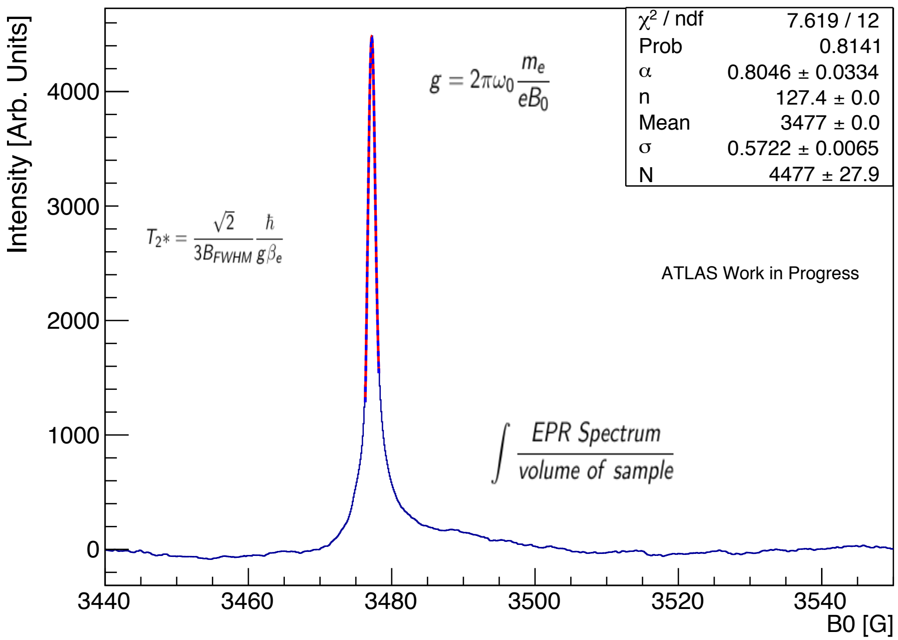
$$\Delta E = \hbar\omega_0 = g\beta_e B_0.$$

NMR Lab, University of Witwatersrand



Sample Spectra and Analysis

EJ260 with dosage 8 MGy at 80K

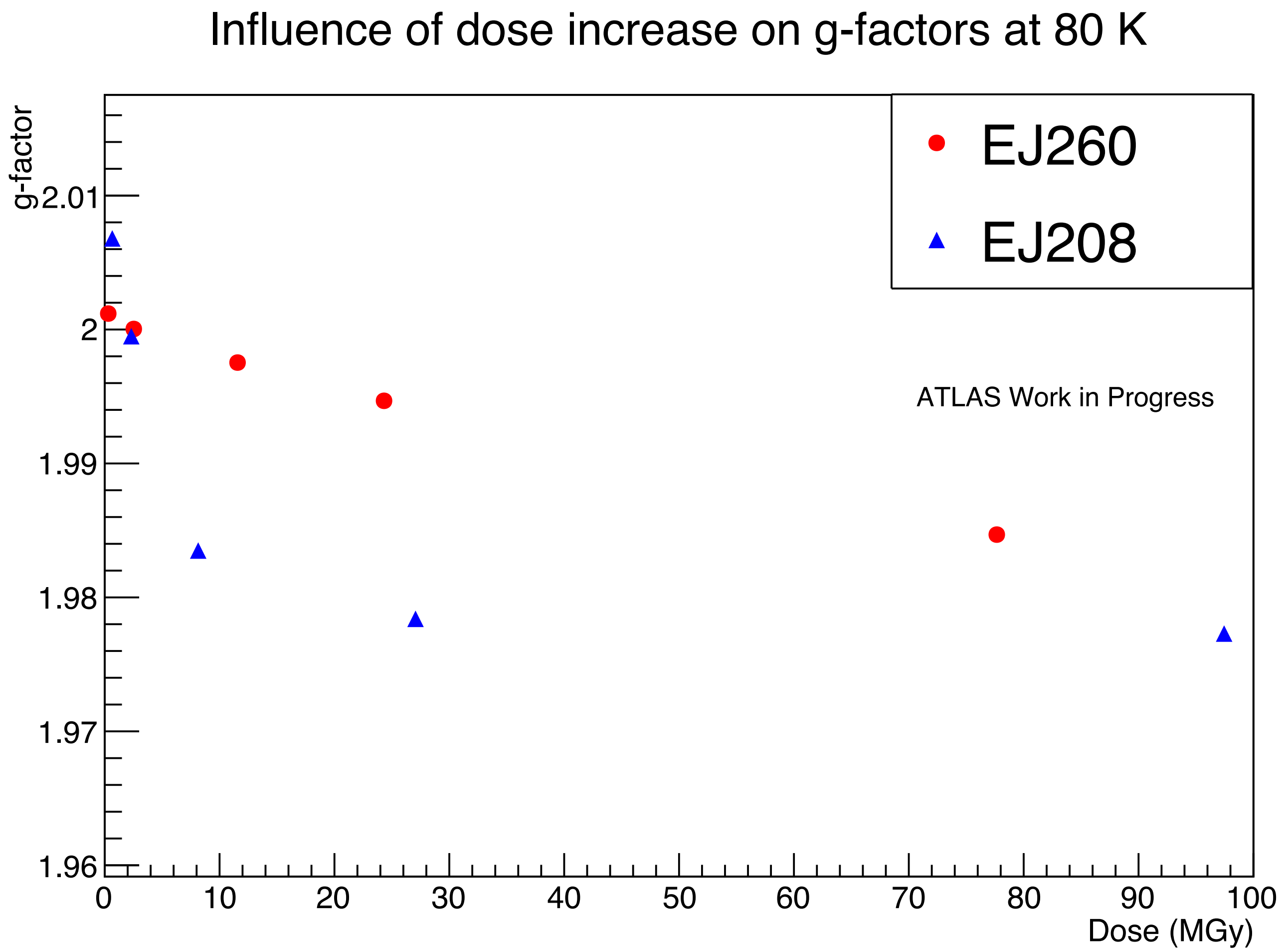


$$f(x;\alpha,n,\bar{x},\sigma) = N \cdot \begin{cases} \exp(-\frac{(x-\bar{x})^2}{2\sigma^2}), & \text{for } \frac{x-\bar{x}}{\sigma} > -\alpha \\ A \cdot (B - \frac{x-\bar{x}}{\sigma})^{-n}, & \text{for } \frac{x-\bar{x}}{\sigma} \leqslant -\alpha \end{cases}$$

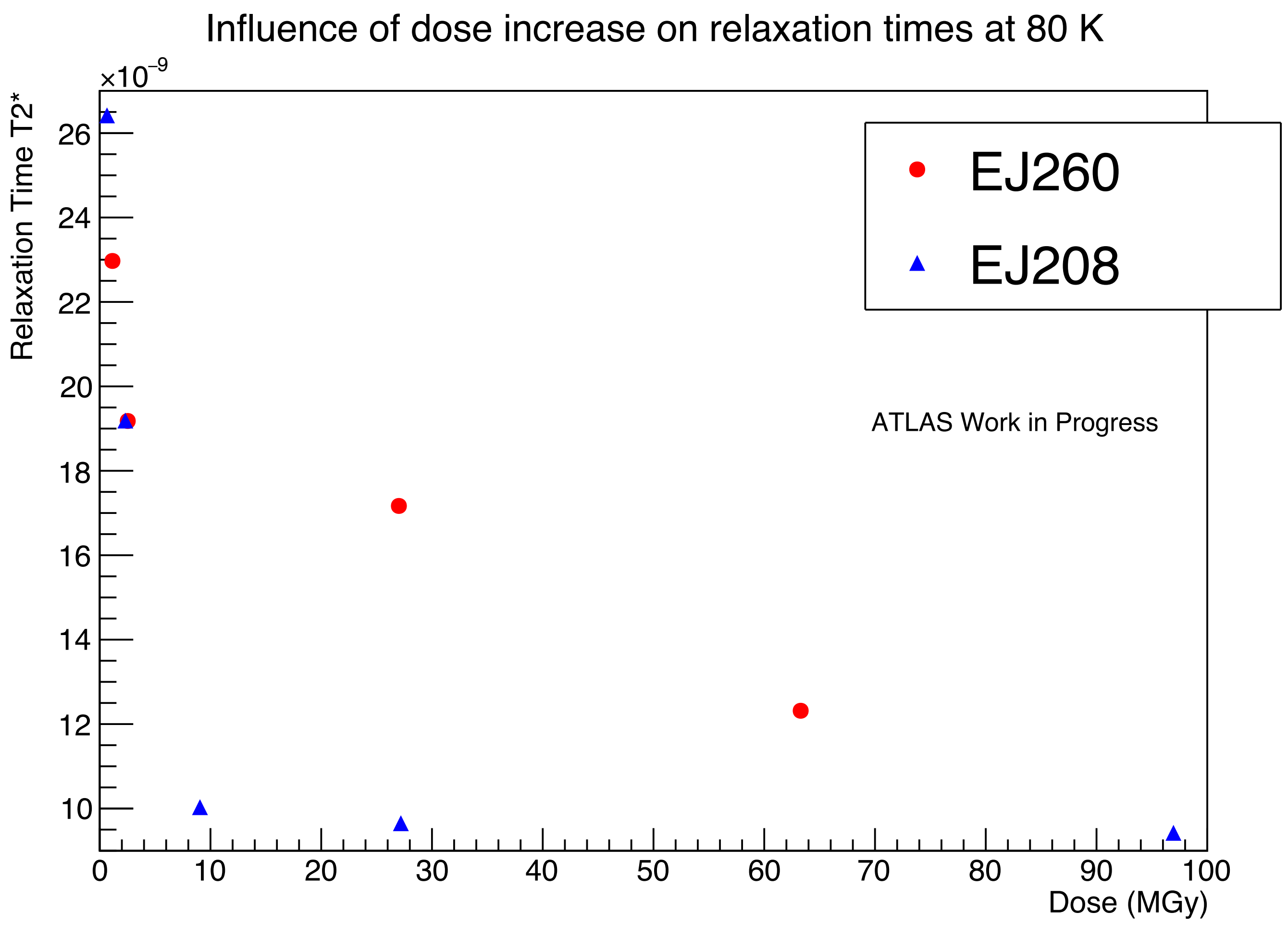
Variable Name	Parameter(s) Used	Symbol
Intensity	Peak Height (N)	I
Peak Magnetic Field	Mean	B_0
Magnetic Field at FWHM	σ, α	B_{FWHM}
Integral	σ, α	$\int \frac{EPR\ Spectrum}{volume\ of\ sample}$

- g-factor: gives information about environment spins see
- $T_2{}^*$: spin-spin relaxation time
- Spin density: number of spins per sample

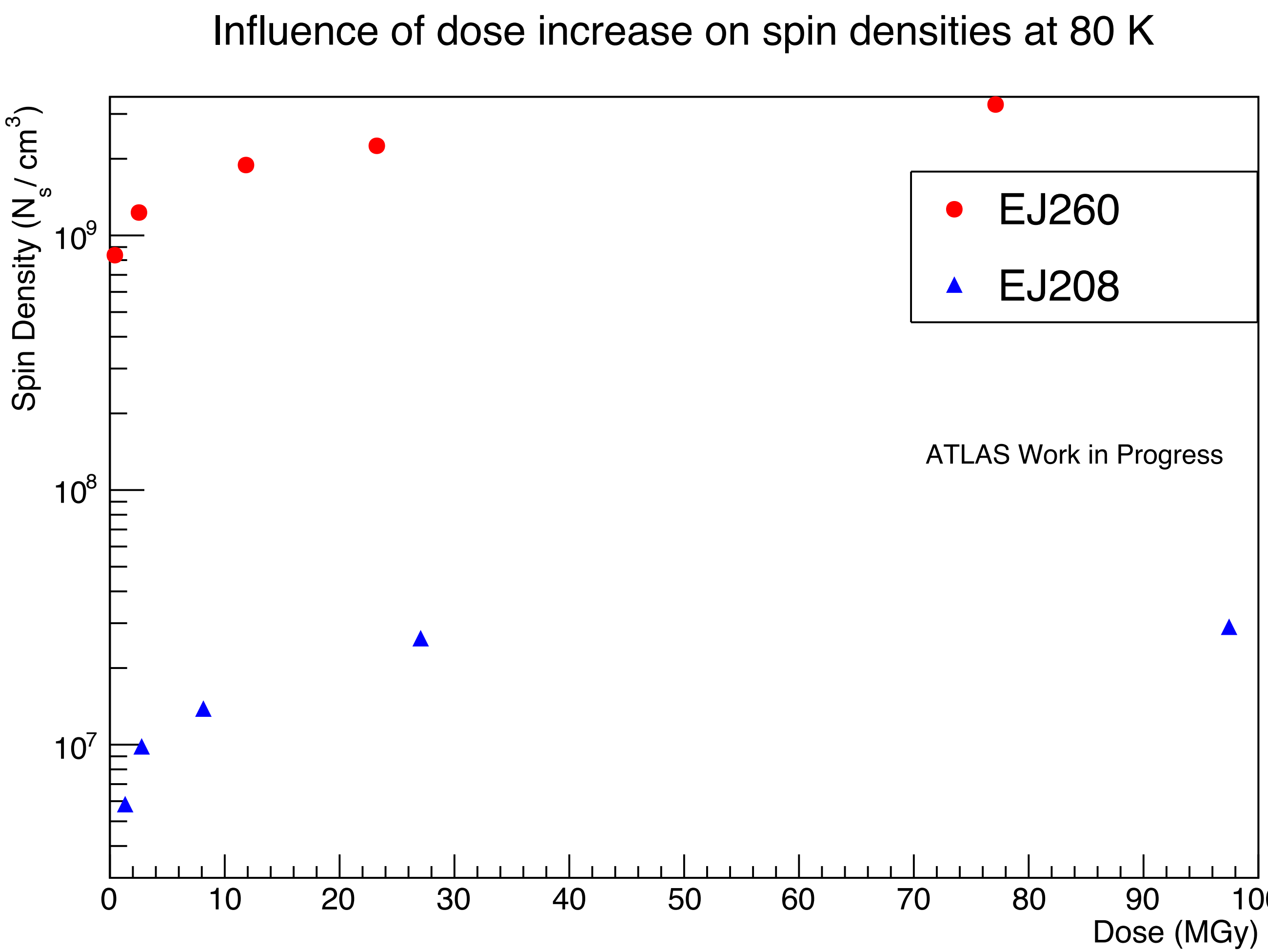
Results: g-factor



Results: Relaxation Time



Results: Spin density



DFT Results

Analysis of 1-ethenyl-2methylbezene: an isomer of the PVT molecule

Hydrogens removed	Δg (ppm)			Total Energy (Ry)
	g_{xx}	g_{yy}	g_{zz}	
0	**-0.031**	**0.010**	**0.010**	**-114.167**
1	1065.91	174.41	-1179.69	-113.816
2	1185.23	138.51	-923.10	-113.815
3	-1282.97	-249.87	923.28	-113.811
4	67.25	-657.46	-679.41	-113.813
5	**-0.17**	**0.052**	**0.052**	**-114.064**
6	71.83	-651.25	-677.79	-113.884
7	71.83	-651.25	-677.7996	-113.884
8	**-0.11**	**-0.052**	**0.033**	**-114.171**

- Hyperfine tensor principle components change as samples are damaged effecting principle components of the g-tensor

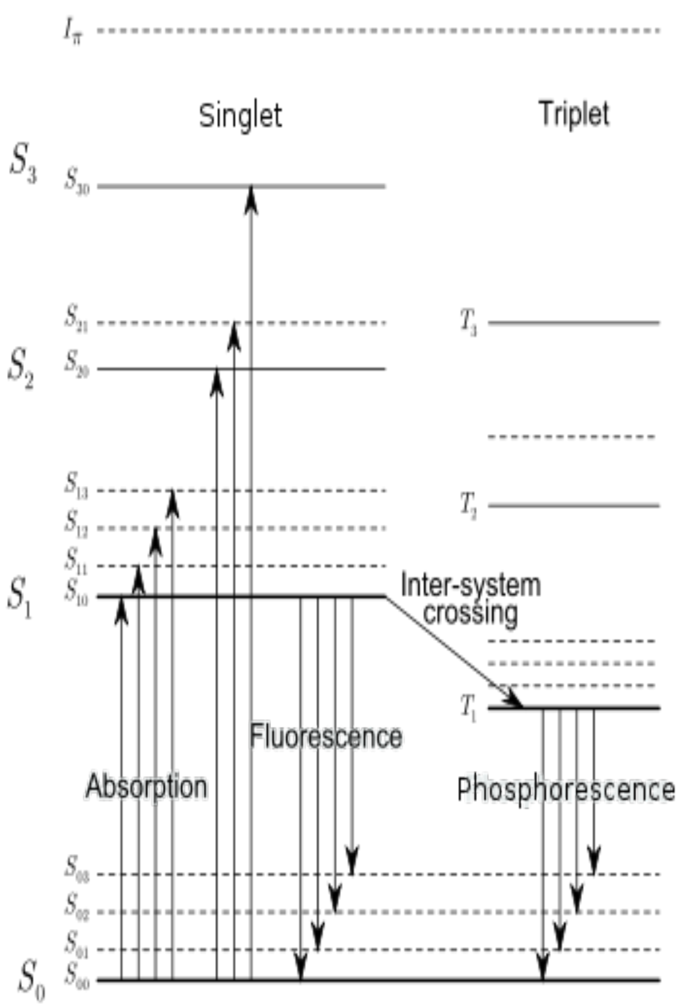
In summary…

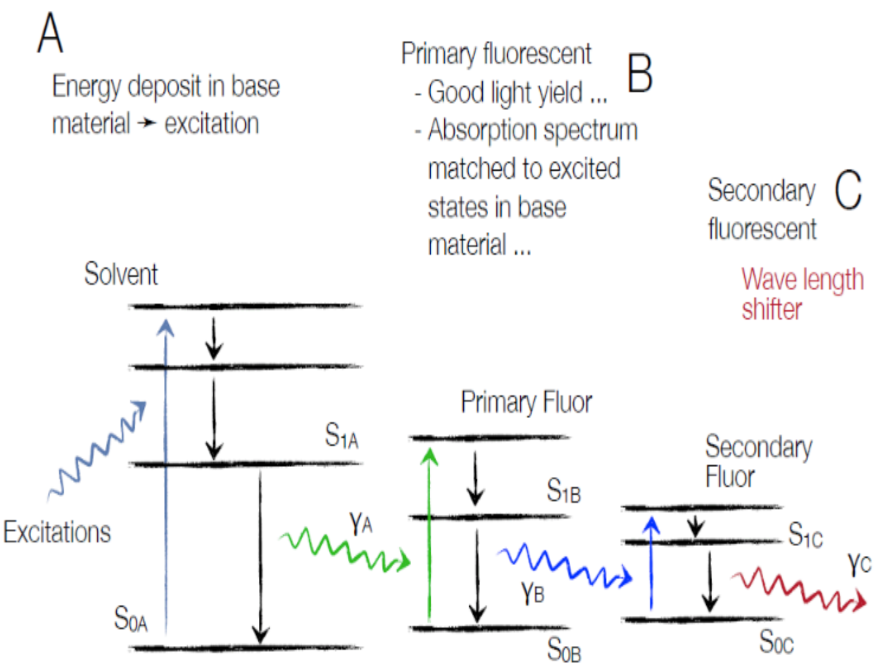
- Structural damage to plastic scintillators cause them to deteriorate
- C-H bonds are most likely to break causing a shift in the g-factor away from the free electron, a decrease in relaxation time due to hyperfine parameters, and an increase in spin density
- All six plastic scintillators to be tested

Thank you to

- SA CERN
- NRF
- iThemba LABS, Gauteng

Back Up: The Scintillation Mechanism

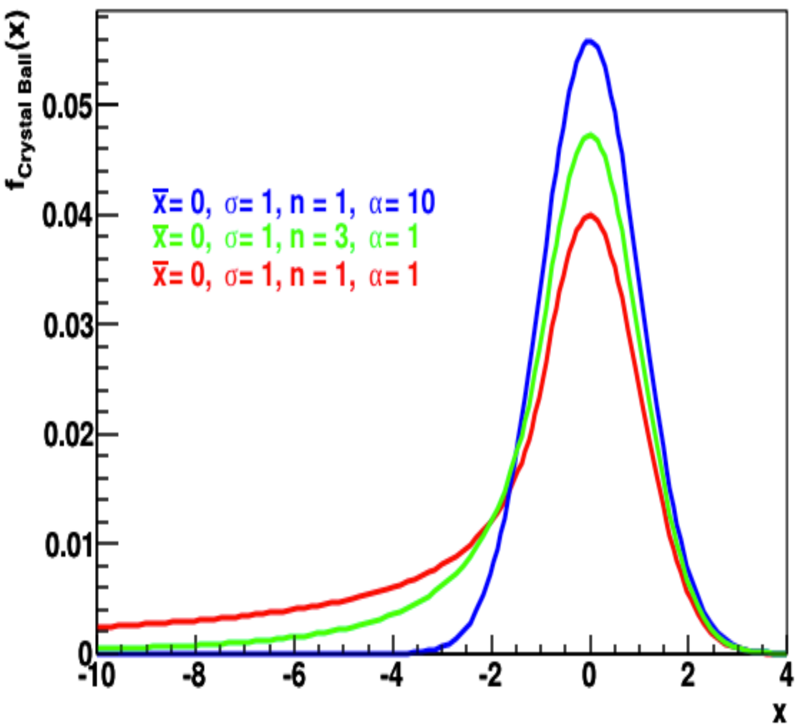




Back Up: The Crystal Ball Fit

$$f(x;\alpha,n,\bar{x},\sigma) = N \cdot \begin{cases} \exp(-\frac{(x-\bar{x})^2}{2\sigma^2}), & \text{for } \frac{x-\bar{x}}{\sigma} > -\alpha \\ A \cdot (B - \frac{x-\bar{x}}{\sigma})^{-n}, & \text{for } \frac{x-\bar{x}}{\sigma} \leqslant -\alpha \end{cases}$$

My Parameters



Variable Name	Parameter(s) Used	Symbol
Intensity	Peak Height (N)	I
Peak Magnetic Field	Mean	B_0
Magnetic Field at FWHM	σ, α	B_{FWHM}
Integral	σ, α	$\int \frac{EPR\ Spectrum}{volume\ of\ sample}$

Back Up: post DFT details

- QE-GIPAW (Gauge-Including Projector-Augmented Wave) used to calculate EPR parameters

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All-electron magnetic response with pseudopotentials: NMR chemical shifts

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$$\bar{H}=\frac{1}{2}\mathbf{p}^2+V^{\mathrm{loc}}(\mathbf{r})+\sum_{\mathbf{R}} e^{(i/2c)\mathbf{r}\cdot\mathbf{R}\times\mathbf{B}}V_{\mathbf{R}}^{\mathrm{nl}}e^{-(i/2c)\mathbf{r}\cdot\mathbf{R}\times\mathbf{B}} + \frac{1}{2c}\mathbf{L}\cdot\mathbf{B}+\frac{1}{8c^2}(\mathbf{B}\times\mathbf{r})^2.$$

First-Principles Theory of the EPR *g* Tensor in Solids: Defects in Quartz

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$$H=\sum_i\left\{\frac{[\mathbf{p}_i+\alpha\mathbf{A}(\mathbf{r}_i)]^2}{2}-\sum_I\frac{Z_I}{|\mathbf{r}_i-\mathbf{R}_I|}+\sum_{j\neq i}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}\right\}+H_{\mathrm{Z}}+H_{\mathrm{Z\text{-}KE}}+H_{\mathrm{SO}}+H_{\mathrm{SOO}}.$$

C. J. Pickard and F. Mauri, Phys. Rev. B 63, 245101 (2001)
J. R. Yates, C. J. Pickard and F. Mauri, Phys. Rev. B 76, 024401 (2007)
C. J. Pickard and F. Mauri, Phys. Rev. Lett. 88, 086403 (2002)
M. S. Bahramy, M. H. F. Sluiter and Y. Kawazoe, Phys. Rev. B 76, 035124 (2007)