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Faculty of Sciences

Solid State Sciences

Fourth stable radical species in X-ray irradiated sucrose

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Introduction

Sucrose is present in nearly every household as the main component of table sugar or as an ingredient of sugar-containing foodstuffs. The EPR spectrum of radicals induced by irradiation of this carbohydrate is detectable at room temperature and has several properties that make it relevant for dosimetric applications: long term stability of radicals, considerable linear dose response range and a relatively low detection limit. It is likely that dose assessment protocols could be improved if the spectrum was completely understood. Additionally, thorough characterisation of radicals enables their identification, which in turn may provide insight into the radiation chemistry of more complex sugar-containing and biologically relevant systems, e.g. DNA.

X-ray induced radicals in sucrose

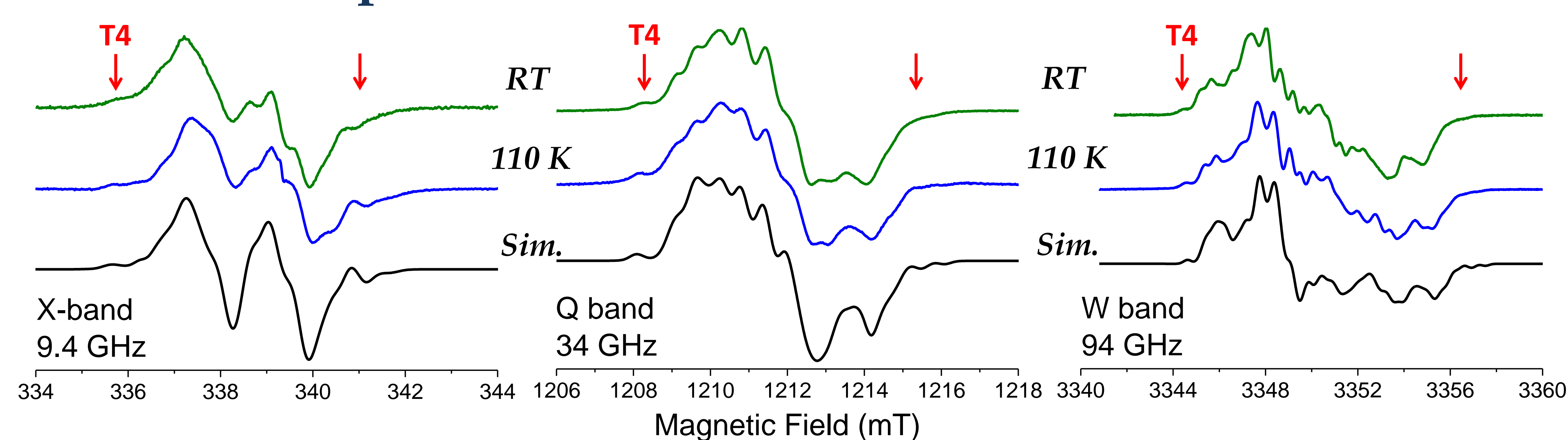### Field-Frequency ENDOR at $B_0 \| b$
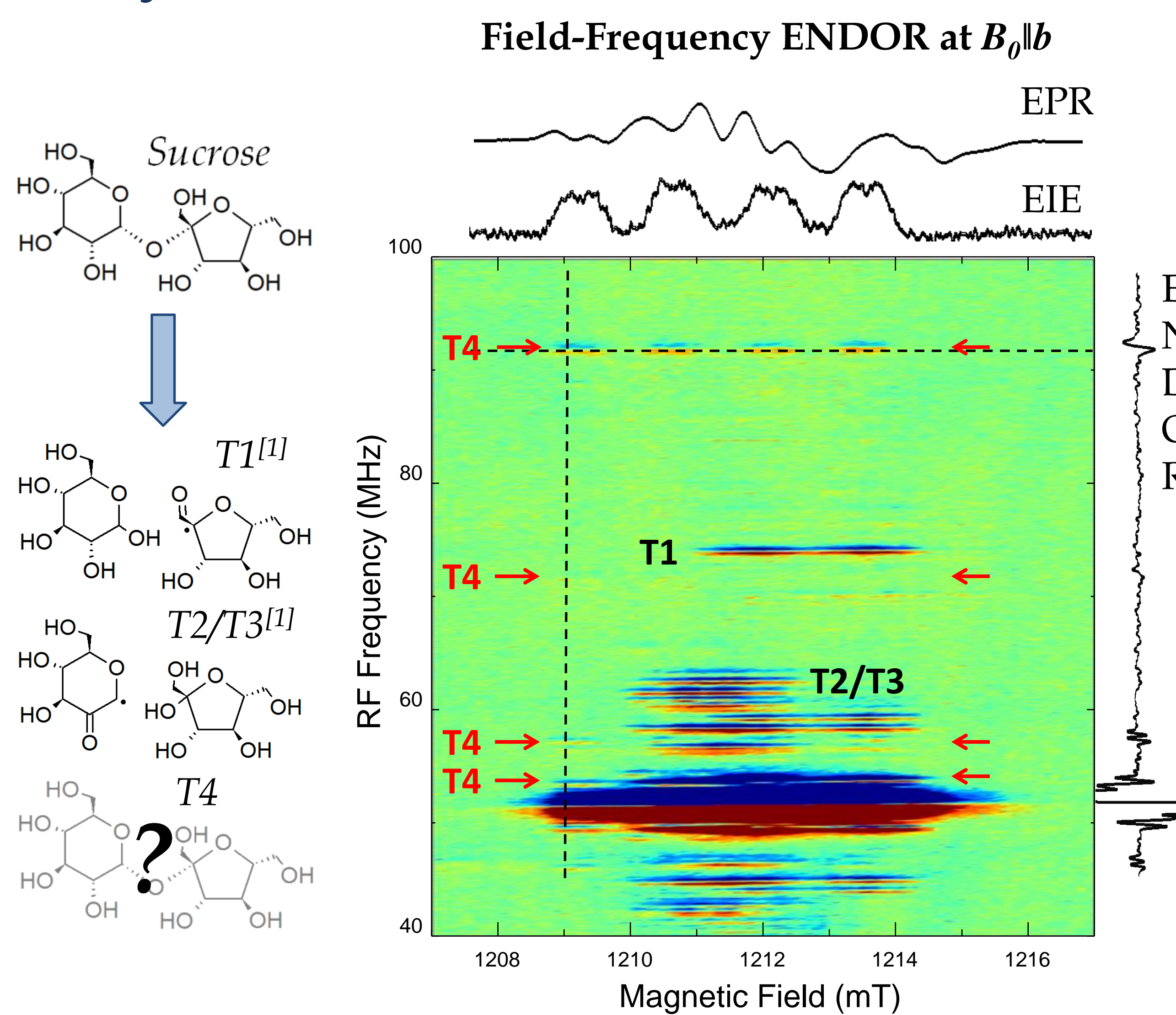
Characterisation of T4

ENDOR and EIE angular variations
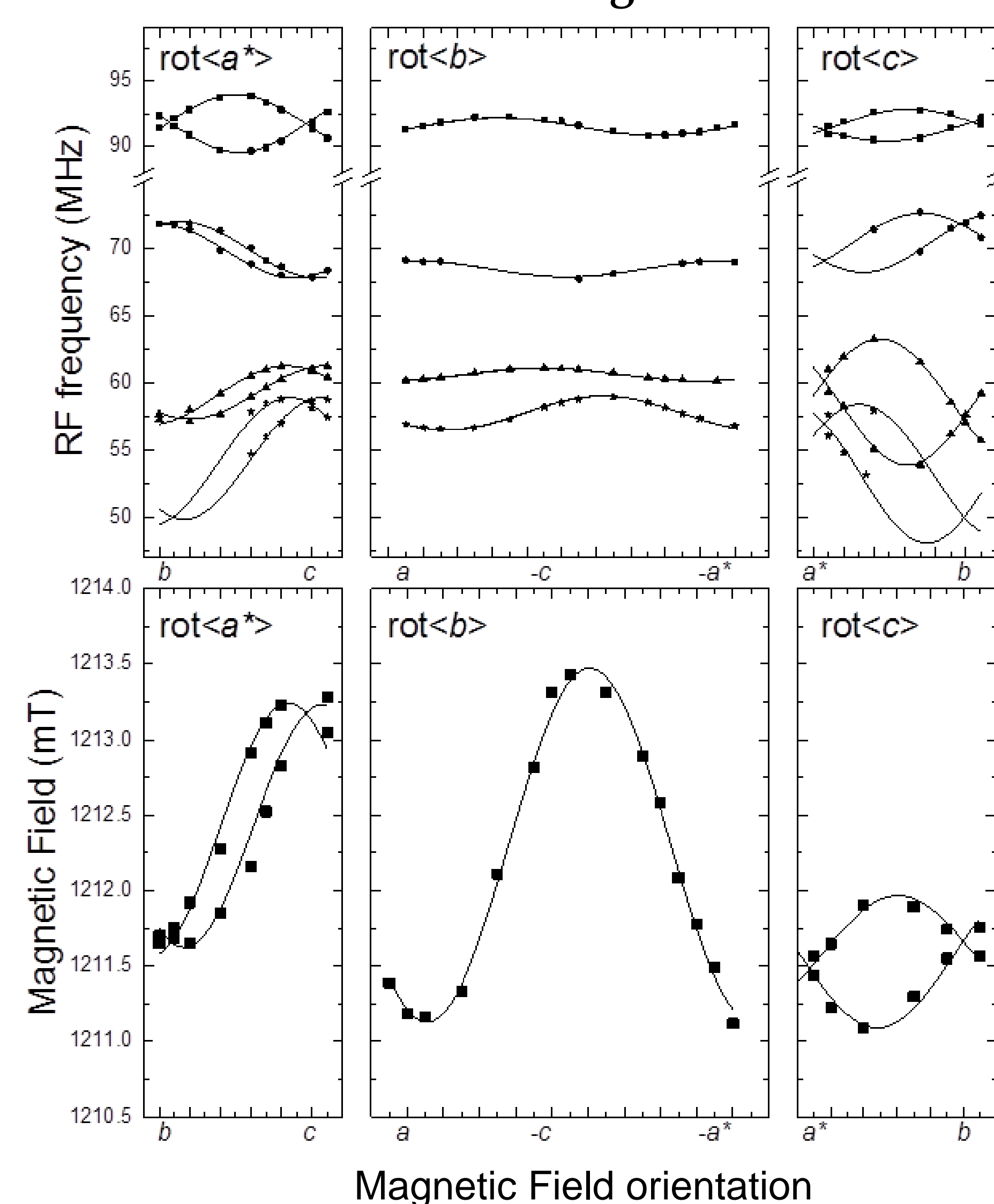
Spectra were measured in Q band, at 110 K and in four rotation planes (to solve the Schonland ambiguity).

		Δg (ppt)	a*	b	c
g_x	2.0019	-0.4	0.370	0.080	0.926
g_y	2.0044	2.1	0.510	-0.851	-0.130
g_z	2.0065	4.2	-0.777	-0.520	0.355

	iso	aniso	a*	b	c
		-4.31	-0.198	0.721	0.664
HF1	80.12	-1.45	-0.918	0.102	-0.384
		5.76	0.344	0.685	-0.642
		-3.84	0.432	-0.279	0.858
HF2	36.22	-2.42	-0.794	0.334	0.508
		6.26	0.428	0.901	0.077
		-8.09	0.758	0.582	-0.296
HF3	-15.78	-3.07	0.304	0.086	0.949
		11.16	-0.578	0.809	0.112
		-7.96	0.419	0.011	0.908
HF4	-7.07	-6.56	0.820	-0.434	-0.373
		14.52	0.390	0.901	-0.191

Powder EPR spectrum simulations

X-band 9.4 GHz

Q band 34 GHz

W band 94 GHz

Ranges of values for intensity relations of T1, T2 and T3 were determined from a single crystal analysis in Ref. [2]. Relations used here: (T2+T3)/T1=1.2 and T2/T3=1.5. Determined relative double integral intensities in powder spectra:
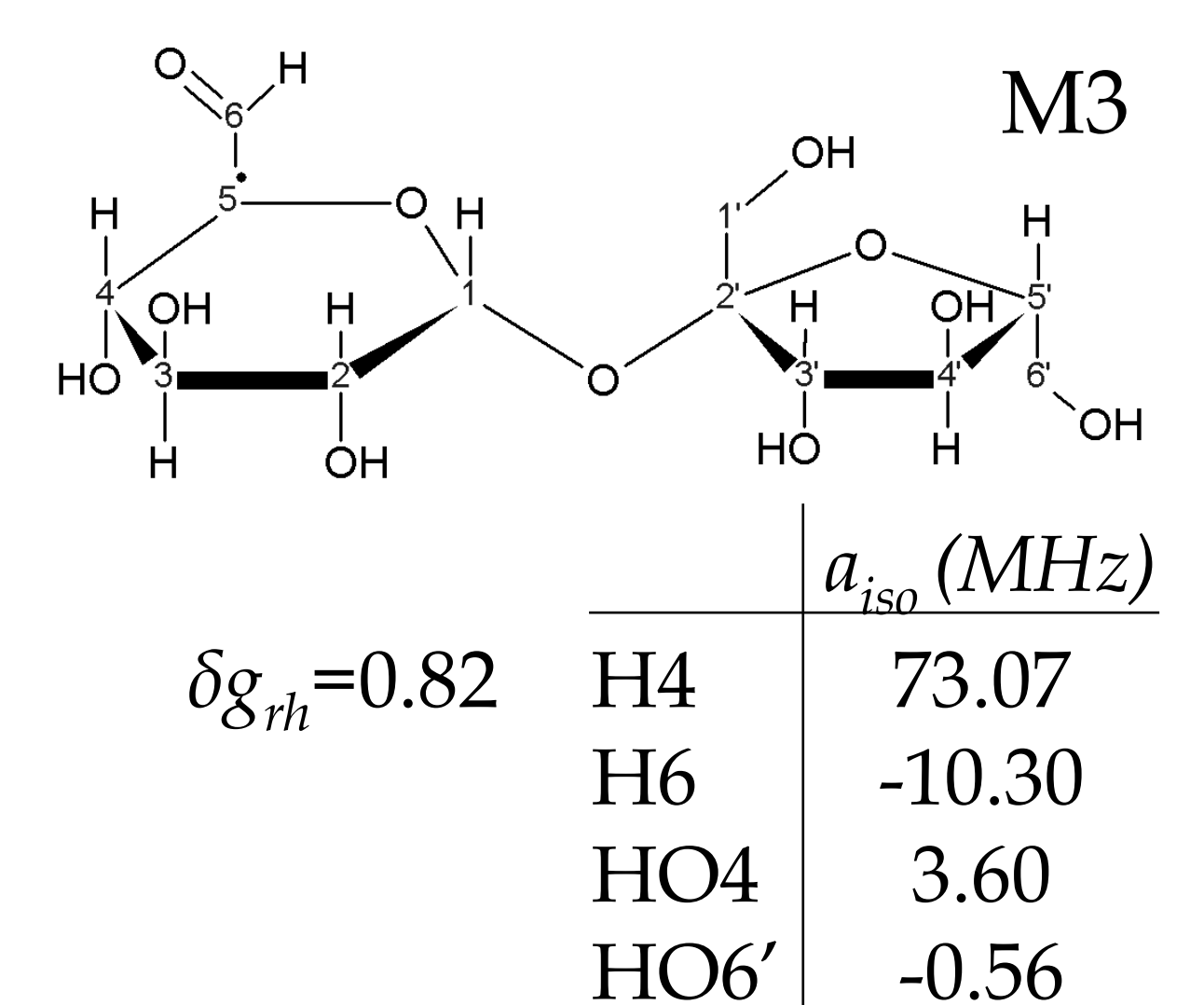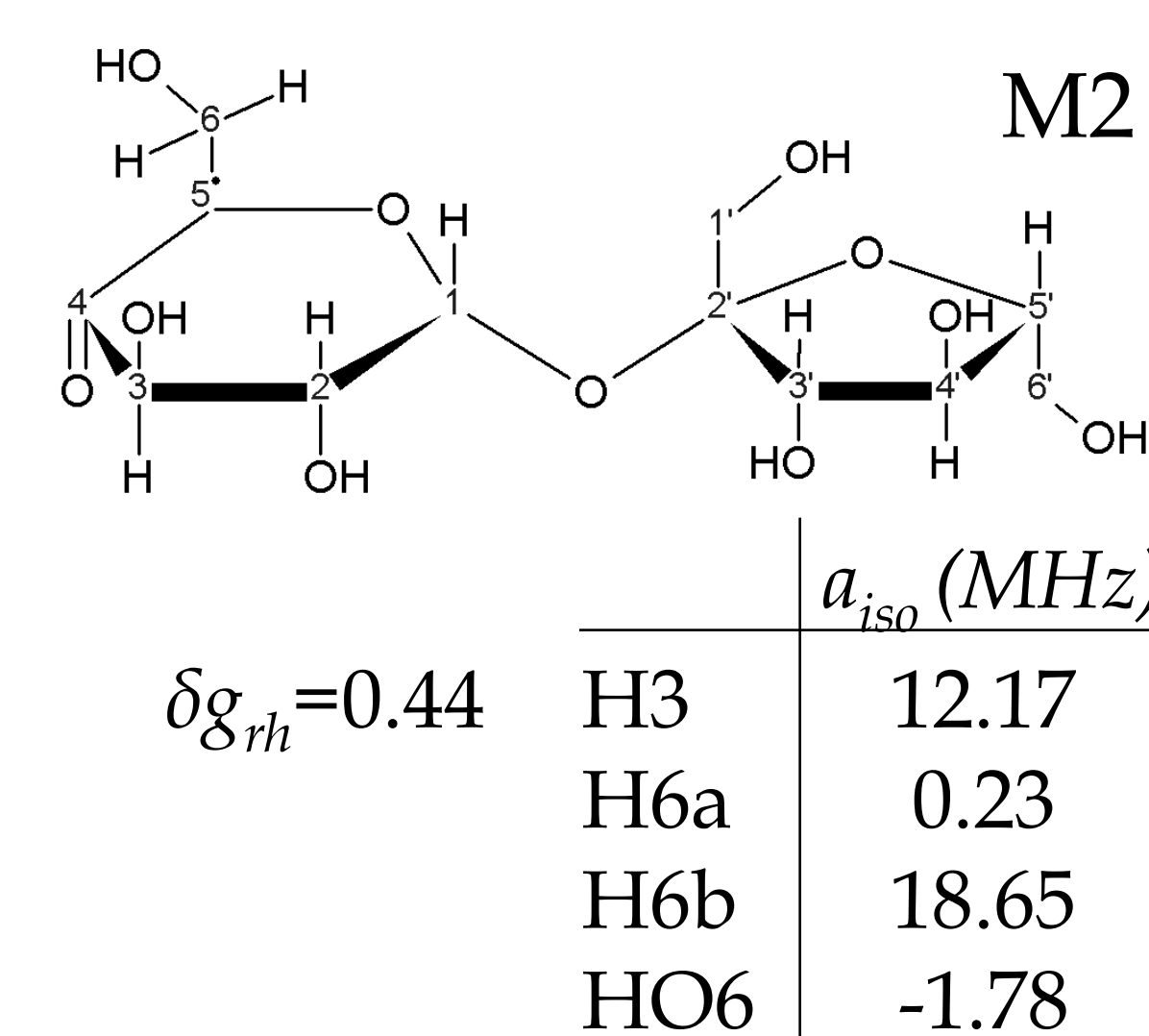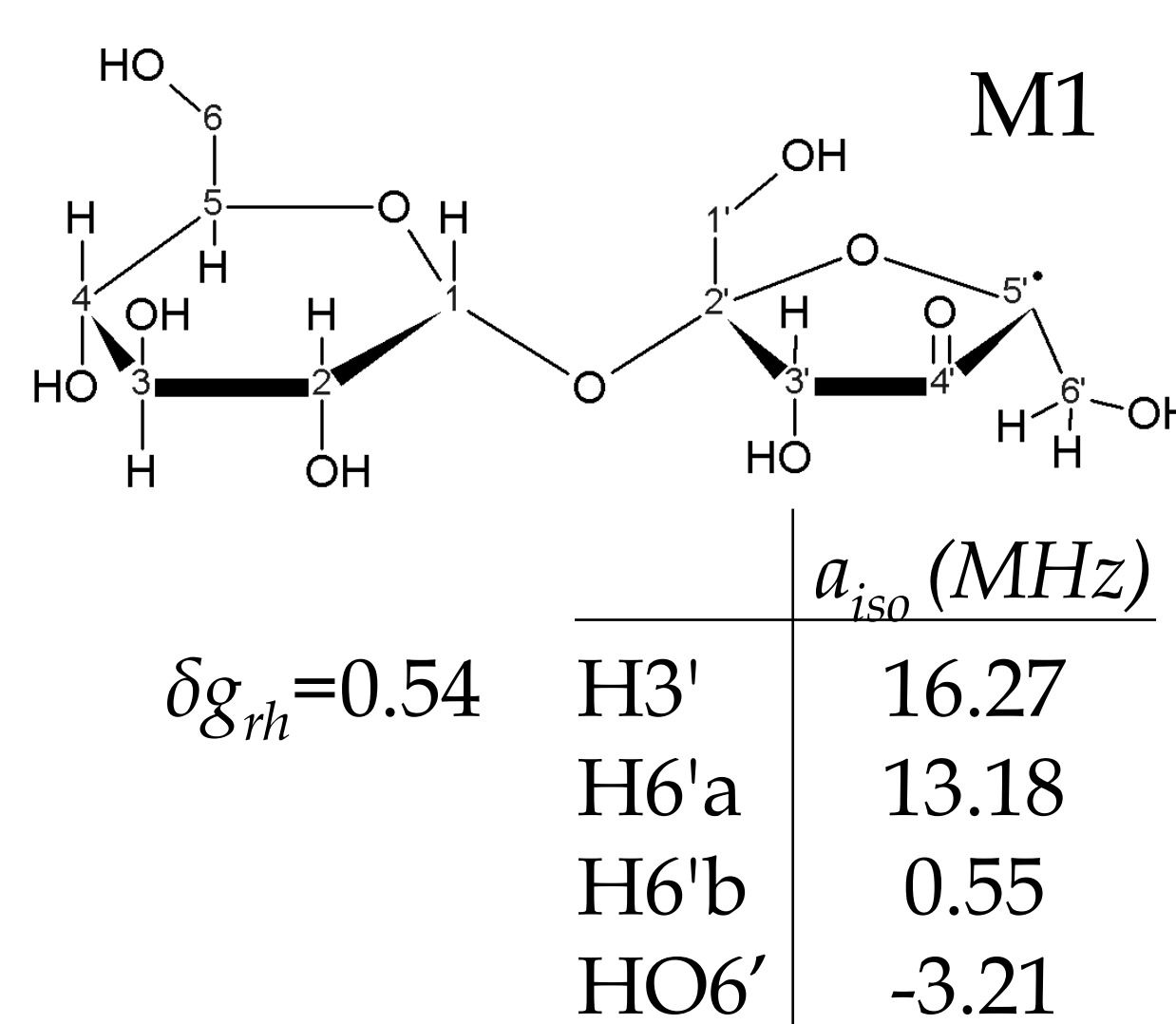
39%×T1 + 28%×T2 + 18%×T3 + 15%×T4.

Possible radical models

Inspection of the *g* tensor suggests that LEO should be located between a C=O group and a ring O. Its relative rhombicity $\delta g_{rh} \approx 0.80$, is more similar to T1's (0.70) than T2's (0.47) or T3's (0.44) [2].

A set of possible models has been devised by comparing experimental g_x and A_z directions to the crystallographic data.

Experimental results could not be reproduced by DFT calculations, but δg_{rh}'s of calculated *g* tensors and a large β-H interaction suggest that M3 is so far the best.

M1

		a_{iso} (MHz)
δg_{rh}=0.54	H3'	16.27
	H6'a	13.18
	H6'b	0.55
	HO6'	-3.21

M2

		a_{iso} (MHz)
δg_{rh}=0.44	H3	12.17
	H6a	0.23
	H6b	18.65
	HO6	-1.78

M3

		a_{iso} (MHz)
δg_{rh}=0.82	H4	73.07
	H6	-10.30
	HO4	3.60
	HO6'	-0.56

EPRc for Android™

I have also made a f-B_0-g calculator for Android. It is based on eprconvert from the EasySpin package (http://easyspin.org) and is something I made for my own use and would like to share it. You can get it at http://goo.gl/ZzYTak or by using the QR code.
Hope this will be useful and best of luck!
Jevgenij K.

ANDROID APP ON
Google play

Conclusions

- Fourth radical species is well characterised.
- The powder spectrum of sucrose can be rather thoroughly understood.
- The model of T4 is not clear yet.

References

1. H. De Cooman et al., Phys. Chem. Chem. Phys., 2009, 11, 1105−1114.
2. H. De Cooman et al., J. Phys. Chem. B, 2013, 117, 7169-7178.