## **Contents**

1	Ato	mic Bells and Frequency Finders	l
	1.1	Chemical Choirs	1
	1.2	Essentials of Electromagnetism	3
	1.3	Electromagnetic Microsensors	5
	1.4	Frequency Finders	8
	1.5	Basics of One-Dimensional NMR	16
	Furt	ther Reading	18
2	Bon	ded Bells and Two-Dimensional Spectra	19
	2.1	Introduction to Coupling	19
	2.2	Bonded Bells: J-Coupling	22
	2.3	NMR Maps: Two-Dimensional Spectra	27
	2.4	The <sup>1</sup> H– <sup>15</sup> N HSQC: Our Bread and Butter	34
	2.5	Hidden Notes: Creating Two-Dimensional Spectra	37
	Refe	erences and Further Reading	42
3	Neighboring Bells and Structure Bundles		
	3.1	Bumping Bells: Dipole-Dipole Coupling	44
	3.2	Atomic Meter Stick: The NOE	51
	3.3	Into "Three-D"	57
	3.4	Adult "Connect-the-Dots:" HNCA	62
	3.5	Putting the Pieces Together: A Quick Review	66



x Contents

	3.6	a Three-Dimensional Structure	69	
	Refe	erences and Further Reading	73	
4	Silencing of the Bells: Relaxation Theory Part One			
_	4.1	Nothing Rings Forever: Two Paths to Relax	75 76	
	4.2	Relaxation: Ticket to the Protein Prom	81	
	4.3		84	
	4.4	Blowing Off Steam and Returning to Equilibrium: T <sub>1</sub>	92	
	4.5	Loosing Lock-Step: Coherence and $T_2$	97	
		erences and Further Reading	105	
_				
5		axation Theory Part Two: Moving Atoms	105	
		Changing Notes	107	
	5.1	Keeping the Terms Straight	108	
	5.2	NMR Dynamics in a Nutshell: The Rules of Exchange	111	
	5.3	,		
		Lane of Exchange	113	
	5.4	Two States, Two Peaks: Atoms in the Slow		
		Lane of Exchange	116	
	5.5	Two States, One Strange Peak: Atoms		
		in Intermediate Exchange	117	
	5.6	Tumbling Together: Rotational Correlation Time $(\tau_c)$	123	
	5.7	Summary	128	
	Furt	her Reading	129	
6	Protein Dynamics			
	6.1	Dynamics Analysis by NMR: Multi-channel		
		Metronomes, Not a GPS	132	
	6.2	Elegant Simplicity: Lipari and Szabo Throw		
		Out the Models	133	
	6.3	Wagging Tails and Wiggling Bottoms: Local		
		Versus Global Motion	135	
	6.4	Measuring Fast Motion: Model Free Analysis	137	
	6.5	Changing Directions on the Track: Refocusing Pulses	146	

Contents xi

6.6	Measuring Intermediate Motion: CPMG	
	Relaxation Dispersion Analysis	148
6.7	Measuring Slow Motion: Z-Exchange Spectroscopy .	151
6.8	Measuring Motion Summary	154
Refe	rences and Further Reading	155
Index .		157