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Supplementary Information

Characterisation of the paramagnetic [2Fe-2S] centre in palustrisredoxin-B (PuxB) from *Rhodopseudomonas palustris* CGA009: g-matrix determination and spin coupling analysis

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Table S1: A list of parameters for the 13 protons of the EPR model 3. The columns correspond to residue and reference number, the distance from the nearest Fe ion, and the experimental isotropic a_{iso} and dipolar T_i hyperfine couplings [MHz], and full matrix **T** relative to the '3HUI.pdb' frame.

Residue	No.	r_{Fe-H} [Å]	a_{iso} [MHz]	T1	T2	T3	**T**		
Cys85	1	*2.825*	2.90	9.67	-4.28	-5.43	4.7249	-4.6777	4.939
							-4.6733	-1.868	-2.7118
							4.9323	-2.7153	-2.8879
Cys48	2	*3.2*	3.29	7.02	-4.46	-2.55	-2.545	3.0104	-2.4732
							2.985	3.828	-3.3986
							-2.423	-3.3669	-1.2739
Cys39	3	*3.78*	-4.10	-1.79	0.69	1.03	0.6029	-0.1785	-0.5619
							-0.1811	0.9567	-0.2976
							-0.5312	-0.2697	-1.6243
Cys45	4	*3.853*	-3.22	-1.69	0.60	1.03	-0.9435	0.2219	-1.0456
							0.2497	0.8553	0.3883
							-1.0846	0.369	0.0335
Cys85	5	*3.889*	3.28	4.31	-1.80	-2.52	3.861	-1.5518	0.4163
							-1.5395	-1.3811	-0.1209
							0.4007	-0.1279	-2.4927
Cys48	6	*4.048*	2.80	3.96	-2.27	-1.69	-2.0792	0.0225	-0.4264
							0.0148	0.8107	-2.8995
							-0.4079	-2.8867	1.2636
Cys45	7	*4.527*	-3.81	-1.11	0.38	0.72	-1.0596	0.2561	-0.0024
							0.2972	0.4346	0.1674
							-0.0413	0.1568	0.6193
Cys39	8	*4.555*	-2.46	-1.05	0.55	0.49	0.41	-0.0044	0.4078
							0.0043	0.4968	-0.116
							0.4424	-0.0771	-0.9195
Gly41	9	*3.406*	-	5.95	-4.04	-1.92	2.2336	-1.5932	-4.4065
							-1.5377	-1.3549	1.3438
							-4.4514	1.3369	-0.8897
Leu83	10	*3.447*	-	5.55	-3.03	-2.54	-2.7522	-0.9246	-0.9657
							-0.9261	2.2071	3.8799
							-0.9689	3.8759	0.5233
Cys39	11	*3.005*	-	-4.01	1.42	2.52	1.5944	-1.0069	0.0534
							-1.0663	-2.4738	-2.4932
							-0.032	-2.614	0.8042
Ala44	12	*3.232*	-	-3.69	0.75	3.08	0.5937	-0.9502	0.9043
							-1.0631	-2.9136	1.555
							1.0037	1.5768	2.4645
Gly41	13	*3.361*	-	-4.46	-0.39	4.77	-2.8685	1.0023	-2.2945
							1.0783	-0.5236	2.2761
							-2.3169	2.3042	3.3136

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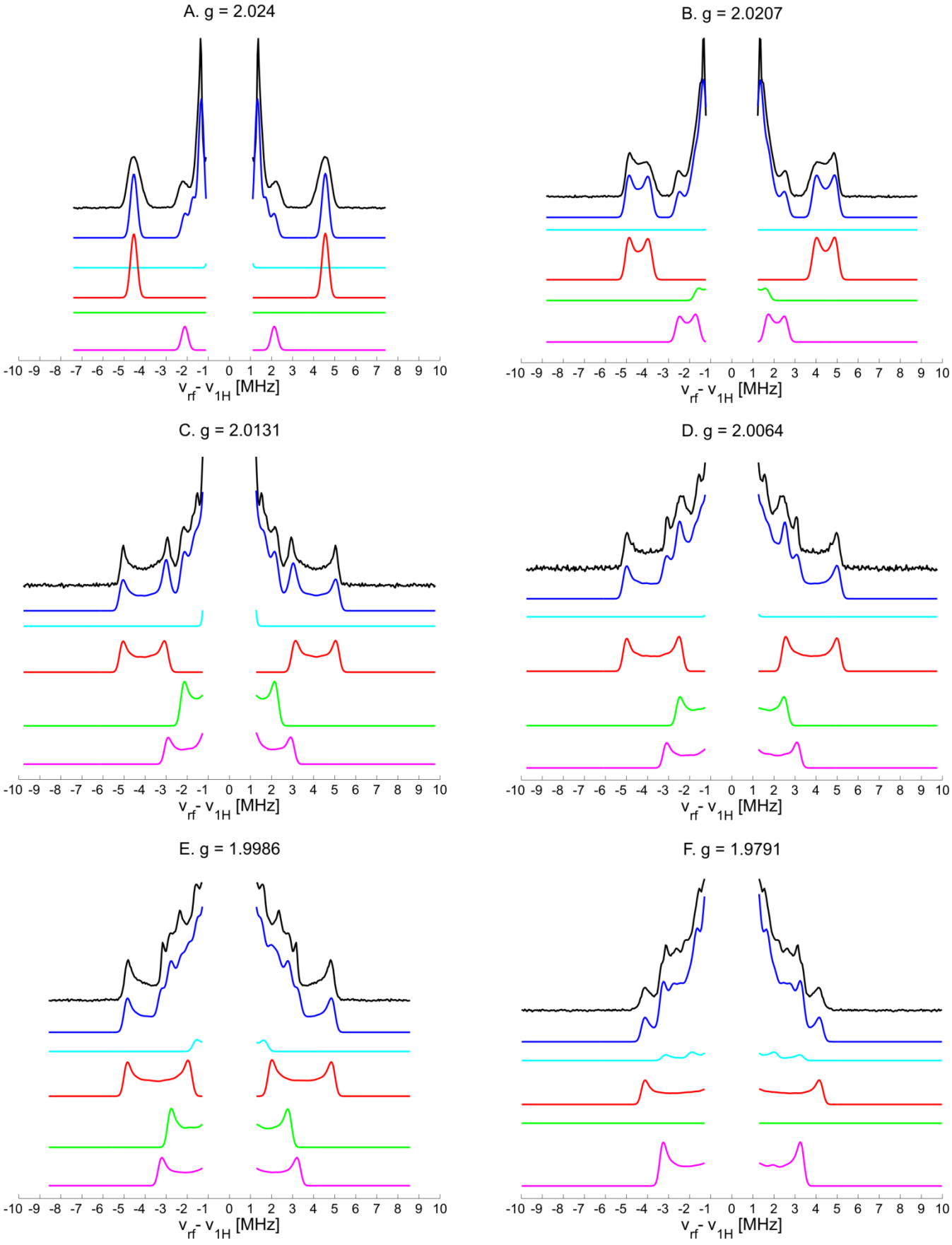

Figure S1: W-band (≅93.83GHz) ENDOR spectra of PuxB (continued next page)

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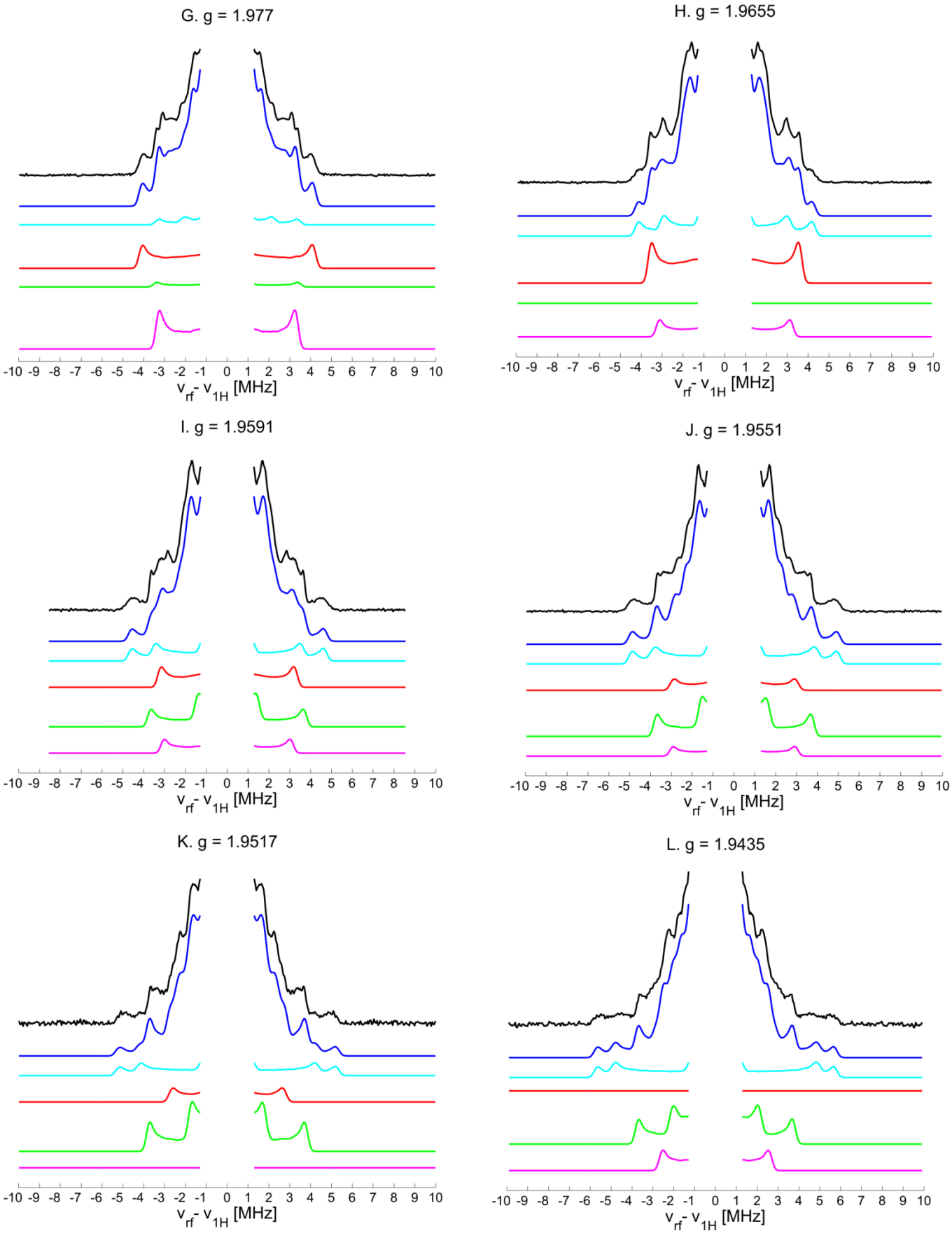

Figure S1: W-band (≅93.83GHz) ENDOR spectra of PuxB (continued next page)

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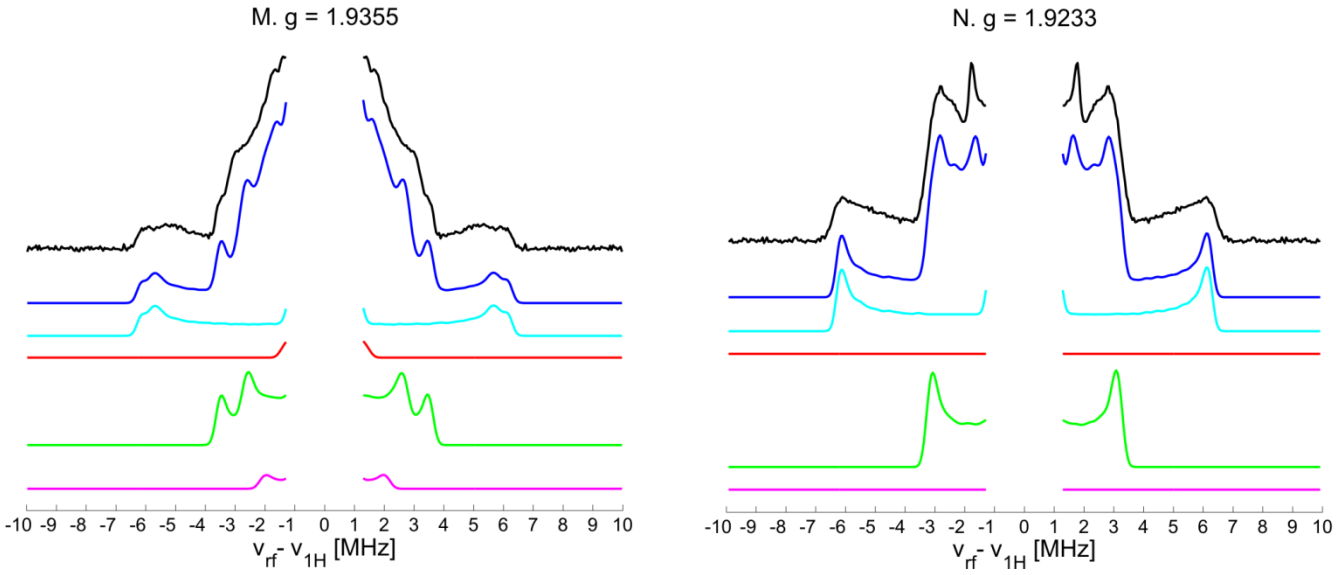

Figure S1: W-band (≅93.83GHz) ENDOR spectra of PuxB recorded at 20K at the g-value positions indicated. At each field the traces from top to bottom are: experiment, total simulation (sum of the 13 protons) and individual simulations for protons 1 (turquoise), 2 (red), 5 (green), 6 (magenta). The hyperfine couplings for the simulations are given in Table S1 (and Table 1).

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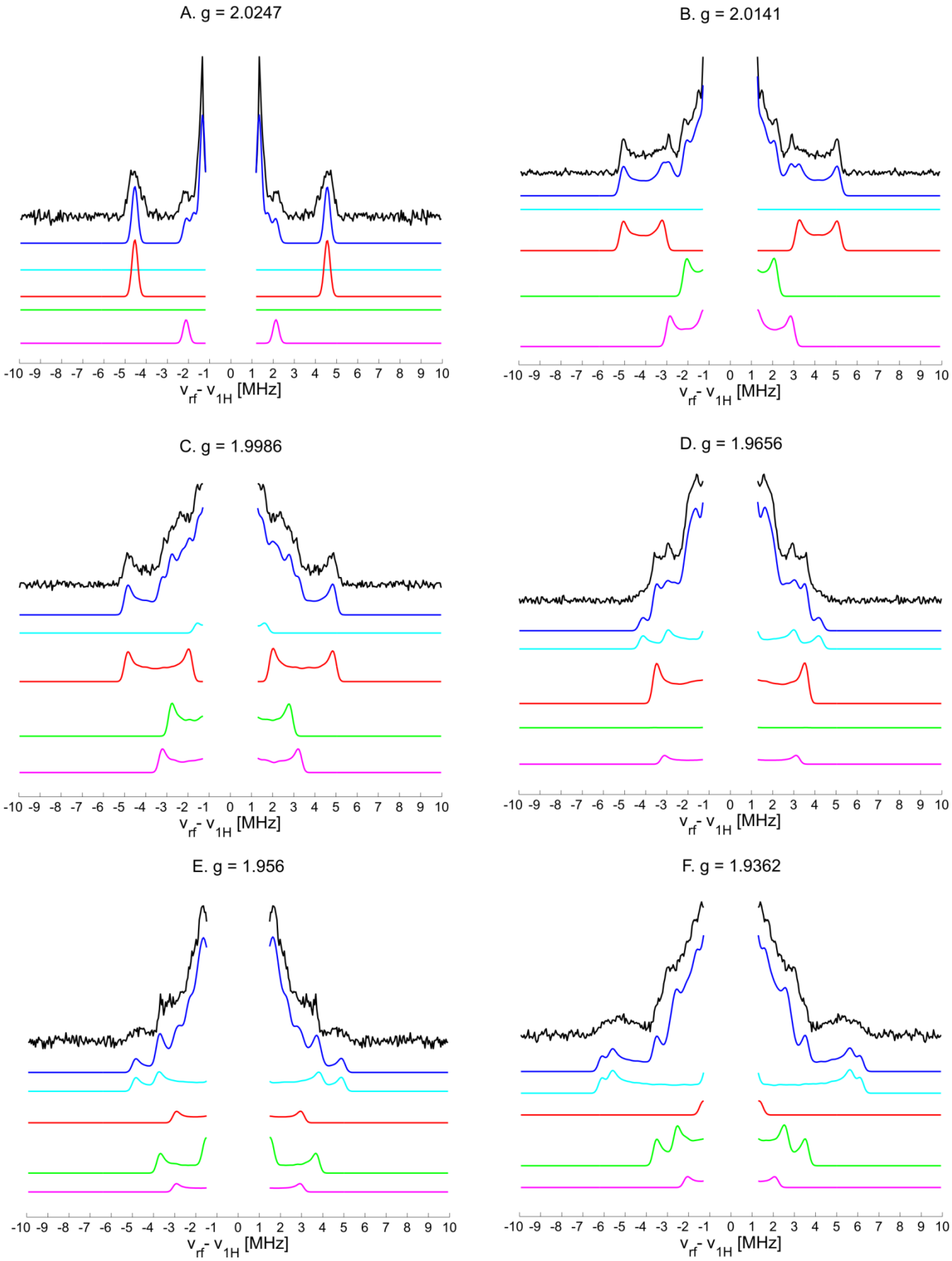

Figure S2: W-band (≅93.83GHz) ENDOR spectra of the PuxB-PuR complex (continued next page)

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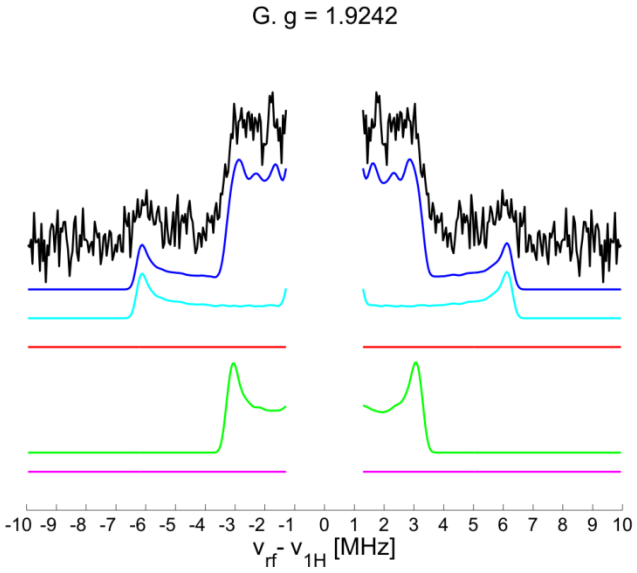

Figure S2: W-band (≅93.83GHz) ENDOR spectra of the PuxB-PuR complex recorded at 20K at the g-value positions indicated. At each field the traces from top to bottom are: experiment, total simulation (sum of the 13 protons) and individual simulations for protons 1 (turquoise), 2 (red), 5 (green), 6 (magenta). The hyperfine couplings for the simulations are given in Table S1 (and Table 1).