MQMAS spectra dependent on static magnetic fields B_0 and RF fields B_1

Recent developments of high magnetic fields and high-quality probes permit easy measurements of half-integer quadrupolar nuclei, especially in MQMAS experiments.

Sensitivity of MQMAS spectra is governed by
(1) Quadrupolar coupling constant C_Q,
(2) Static magnetic field strength B_0,
(3) RF magnetic field strength B_1.

In this Note, we treat three compounds, $RbNO_3$, $Na_4P_2O_7$, and Na_2HPO_4, having maximum C_Q of 1.94, 3.22, and 3.70 MHz, respectively. Since quadrupolar broadenings are proportional to $C_Q^2/\gamma B_0$, signal sensitivities are estimated as follows:

	$RbNO_3$	$Na_4P_2O_7$	Na_2HPO_4
21.9 T	37.6	10.9	8.28
14.1 T	12.5	3.64	2.76
9.4 T	4.54	1.32	1

Clearly from the above table, high magnetic fields are very effective in achieving high sensitivity.

The effects of RF fields B_1 on signal sensitivities are demonstrated experimentally, using MQMAS probe (B_1=150-250 kHz) and standard CPMAS probe (B_1=50-150 kHz) at B_0=14.1 T, in the following: Strong RF fields excite MQMAS signals efficiently, leading to high sensitivity.

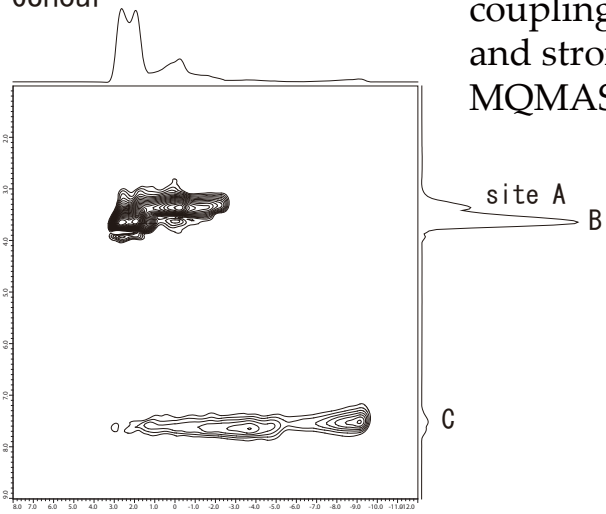
* Experiments at B_0 =21.9 T were conducted with cooperation of Dr. T. Shimizu of National Institute of Materials Science (NIMS).

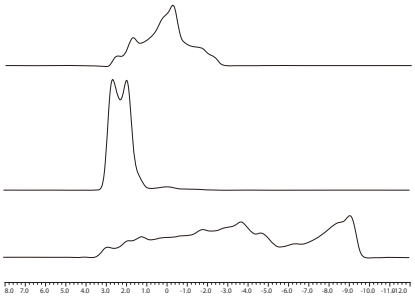
JEOL RESONANCE

Na_2HPO_4

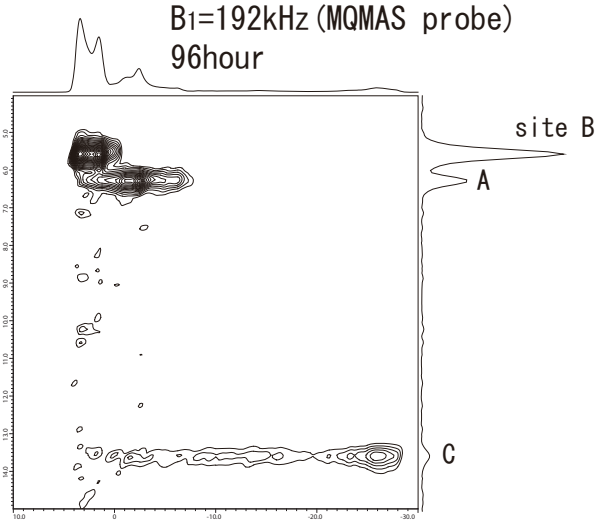
B0=21.9T (ECA930)
B1=227kHz (MQMAS probe)
68hour

The compound has large quadrupolar couplings so that only high magnetic field and strong RF field give high sensitivity MQMAS spectra.

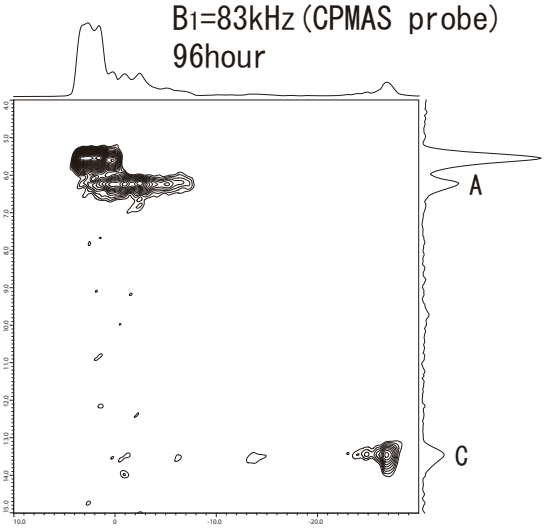




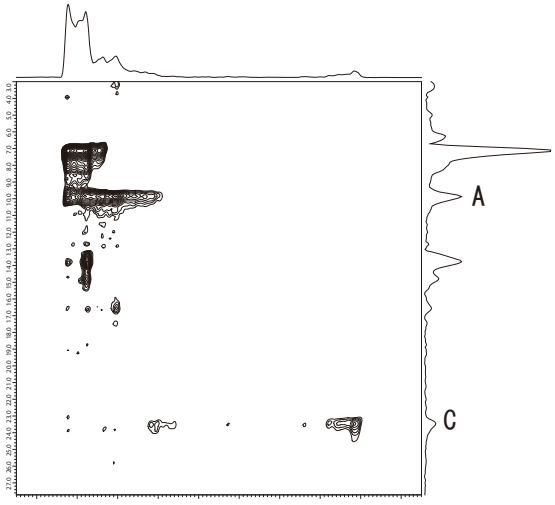
B0=14.1T (ECA600)
B1=192kHz (MQMAS probe)
96hour



B0=14.1T (ECA600)
B1=83kHz (CPMAS probe)
96hour



B0=9.4T (ECX400)
B1=100kHz (CPMAS probe)
195hour

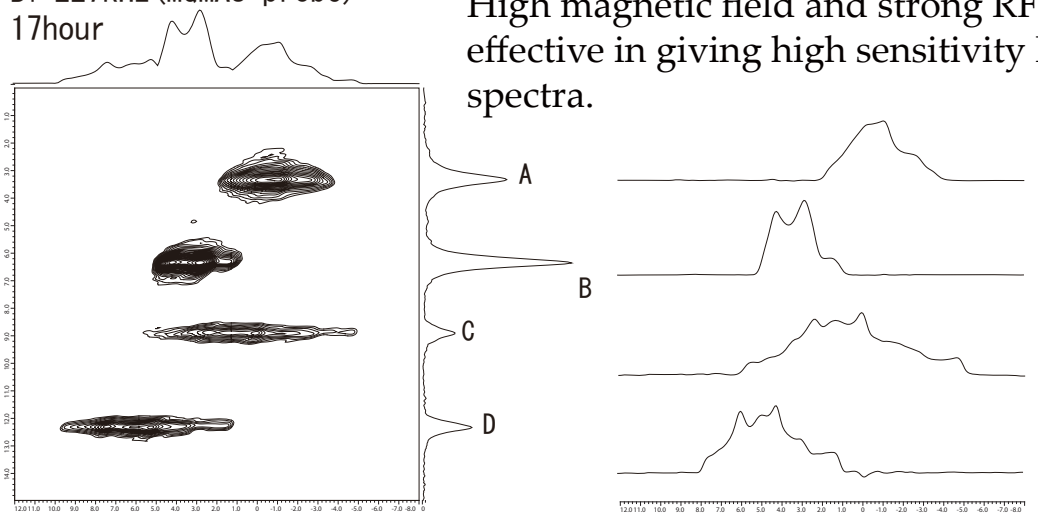


JEOL RESONANCE

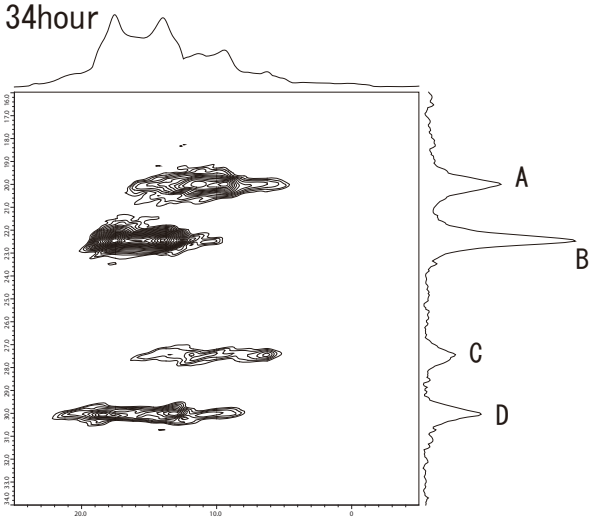
$Na_4P_2O_7$

High magnetic field and strong RF field are effective in giving high sensitivity MQMAS spectra.

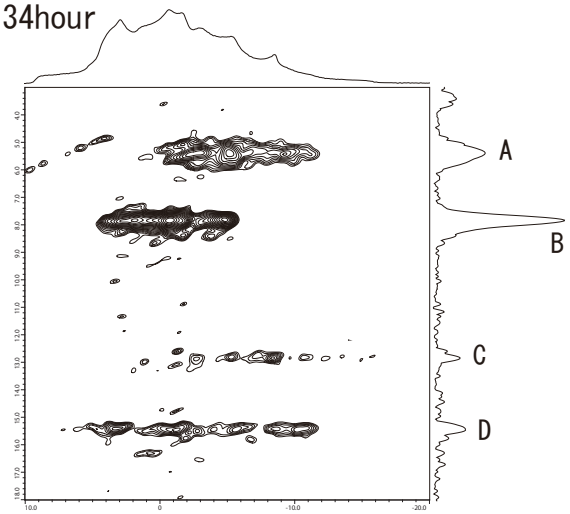
B0=21.9T (ECA930)
B1=227kHz (MQMAS probe)
17hour



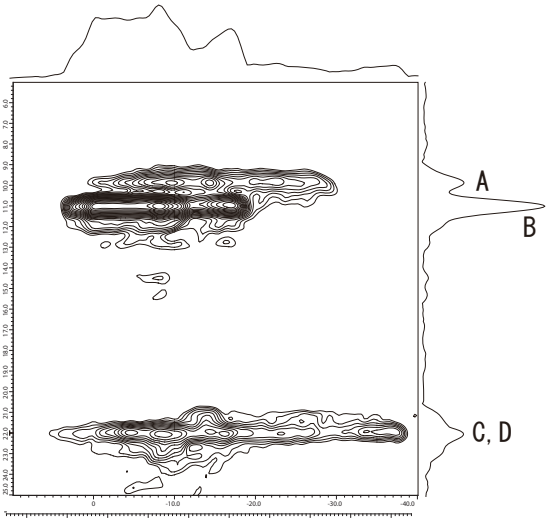
B0=14.1T (ECA600)
B1=192kHz (MQMAS probe)
34hour



B0=14.1T (ECA600)
B1=83kHz (CPMAS probe)
34hour



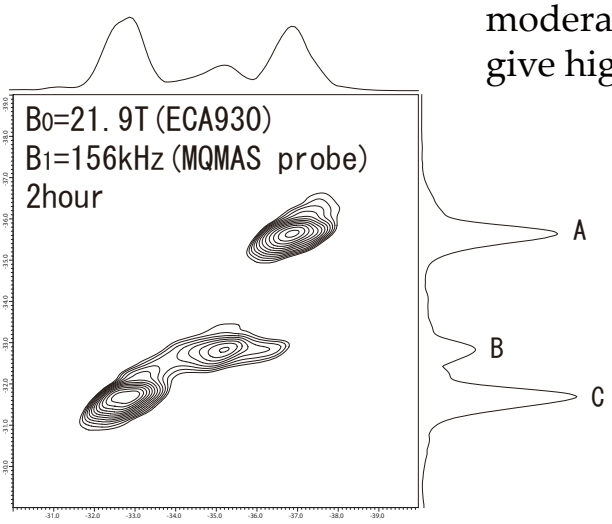
B0=9.4T (ECX400)
B1=114kHz (CPMAS probe)
68hour

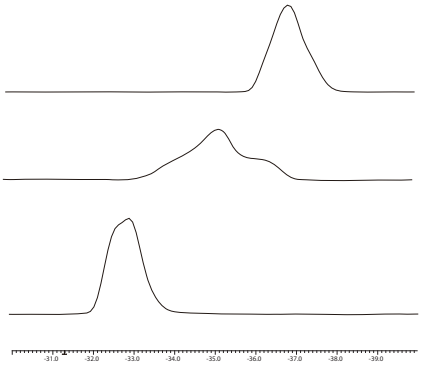


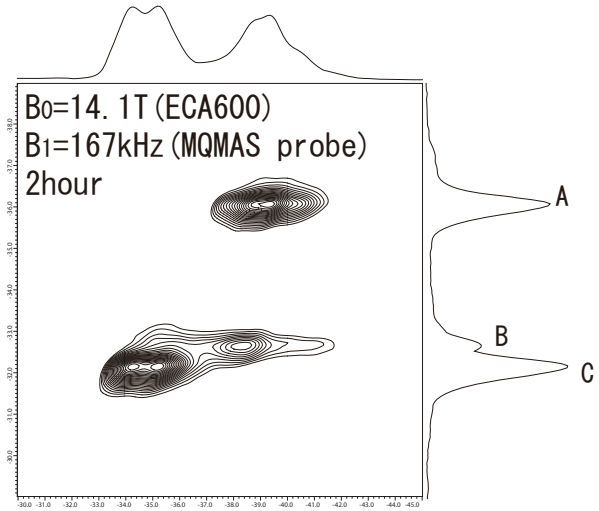
JEOL RESONANCE

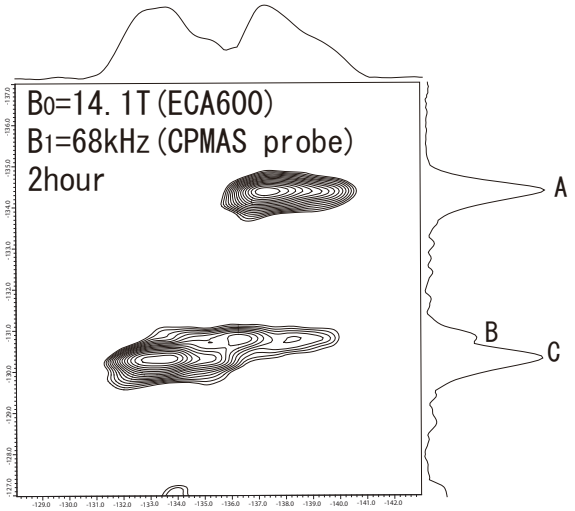
$RbNO_3$

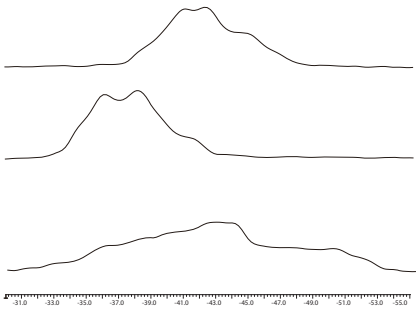
Because of small quadrupolar couplings, moderate magnetic field and RF field can give high sensitivity MQMAS spectra.

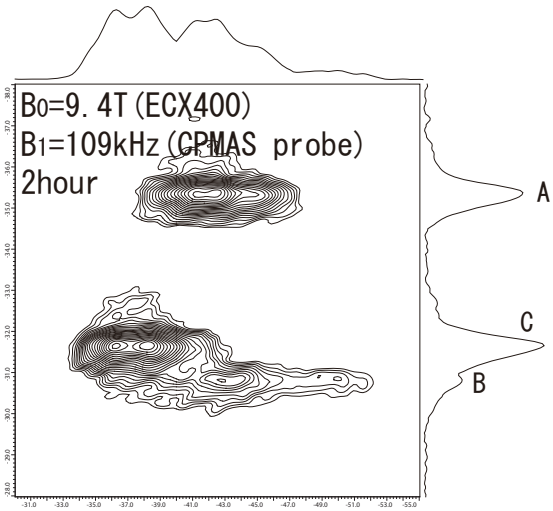












JEOL RESONANCE