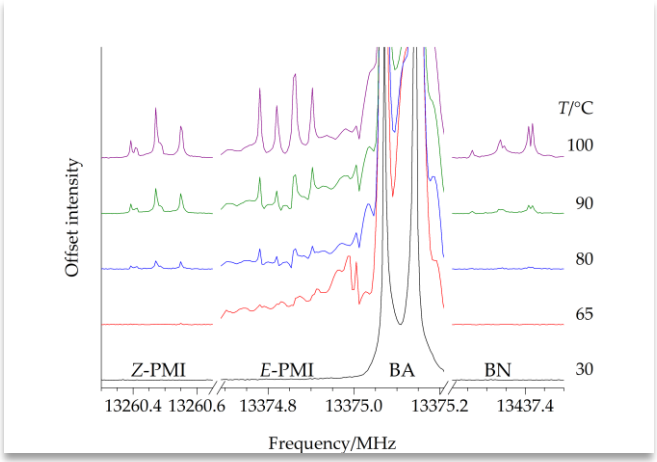
P5414: SPECTROSCOPIC CHARACTERIZATION OF *E*- AND *Z*-PHENYLMETHANIMINE

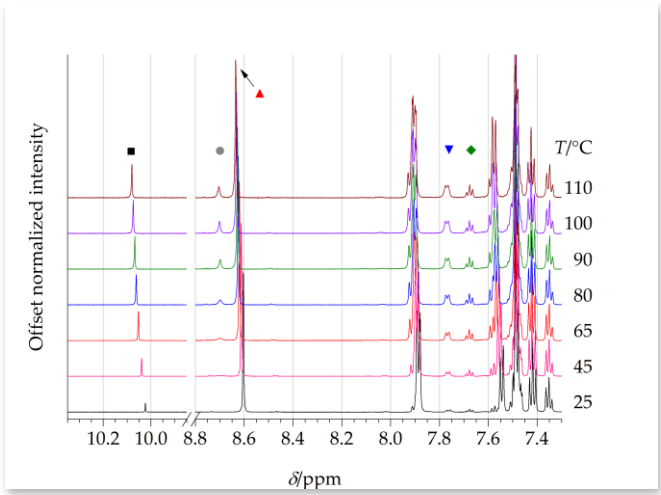
Alessio Melli, et al. Scuola Normale Superiore, Pisa (IT) and University of Bologna, Bologna (IT).

- We relied on an approach which involves organic synthesis, NMR, rotational spectroscopy and quantum chemistry;
- We recorded the rotational spectrum of *E*- and *Z*-PMI, a prerequisite for a possible radio astronomical detection;

	E-phenylmethanimine		*Z*-phenylmethanimine	
	exp.	best theo.	exp.	best theo.
A_0	5217.29202(11)	5216.95	5200.81278(16)	5200.42
B_0	1565.283633(28)	1564.68	1548.969349(92)	1548.76
C_0	1204.540307(14)	1204.05	1194.842313(78)	1194.30
D_J	$5.775(11) \times 10^{-5}$	5.57×10^{-5}	$5.643(35) \times 10^{-5}$	5.28×10^{-5}
D_K	$7.65(11) \times 10^{-4}$	7.07×10^{-3}	7.06×10^{-3}	7.06×10^{-3}
D_{JK}	$1.678(37) \times 10^{-4}$	1.81×10^{-4}	$1.445(47) \times 10^{-4}$	1.57×10^{-4}
d_1	$-1.6941(55) \times 10^{-5}$	-1.63×10^{-5}	$-1.542(44) \times 10^{-5}$	-1.51×10^{-5}
d_2	$-3.162(23) \times 10^{-6}$	-3.00×10^{-6}	-2.68×10^{-6}	-2.68×10^{-6}
$1.5\chi_{aa}$	1.5271(14)	1.61	−5.8871(23)	−6.05
$0.25(\chi_{bb} - \chi_{cc})$	−1.70630(38)	−1.83	0.4954(15)	−0.55
# lines	180		118	
rms $\times 10^3$	4.56		1.38	
σ	0.65		0.69	



- We proposed an easy and accessible hydrolytic formation pathway in which water is expected to play a crucial role;
- Its dependency from the temperature has been studied by both rotational and NMR spectroscopy.



A. Melli et al., *Chem. Eur. J.* **2020**, 26, 15016-15022.