Electronic Supplementary Information

Interactions between alkanes and aromatic molecules: a rotational study of pyridine –methane

*Qian Gou, Lorenzo Spada, Montserrat Vallejo-López, Alberto Lesarri, Emilio J. Cocinero, Walther Caminati**

Content:

1) Completion of Reference [17].

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2) Table 1S: Experimental transition frequencies of PYR(^{14}N)-CH_4 and PYR(^{15}N)-CH_4

$J'(K'_aK'_c)$-$J''(K''_aK''_c)$	PYR(^{14}N)-CH_4				PYR(^{15}N)-CH_4	
	F'	F''	ν/MHz	$\Delta\nu$/kHz	ν/MHz	$\Delta\nu$/kHz
2_{12}-1_{01}	3	2	8556.0310	0.4	8477.5846	-0.7
	2	1	8554.5914	-0.3		
	1	0	8557.7500	-1.8		
	2	2	8555.5674	0.4		
	1	1	8555.3134	-0.3		
2_{21}-1_{10}	3	2	10840.4374	1.1	10721.9009	-3.5
	2	1	10838.9595	0.8		
	1	0	10841.6687	2.4		
	2	2	10839.3897	-1.6		
	1	1	10840.5863	1.7		
2_{20}-1_{11}	3	2	10860.2293	2.8	10755.9710	0.5
	2	1	10860.6072	0.0		
	1	0	10858.6850	-0.3		
	2	2	10859.1982	-0.9		
	1	1	10862.2064	0.5		
3_{13}-2_{02}	4	3	12252.4981	-2.5	12138.4172	-2.8
	3	2	12251.2566	-1.0		
	2	1	12253.1441	-3.2		
	3	2	12252.2799	-5.2		
	2	1	12251.5494	0.4		
3_{03}-2_{12}	4	3	10075.9565	-0.4	10074.0245	0.9
	3	2	10077.4586	-4.3		
	2	1	10075.3345	-0.7		
3_{31}-2_{20}	4	3	16840.5774	1.4	16659.6700	-0.1
	3	2	16840.2565	2.1		
	2	1	16840.4762	-0.9		
3_{30}-2_{21}	4	3	16840.8346	-0.3	16660.4329	-0.5
	3	2	16840.5321	1.1		
	2	1	16840.7212	-5.1		
4_{14}-3_{03}	5	4	15939.0041	0.4	15783.3855	-2.3
	4	3	15937.8464	-0.6		
	3	2	15939.3968	-1.0		
4_{04}-3_{13}	5	4	13829.6330	-1.8	13827.6878	-3.0
	4	3	13830.8830	7.4		
	3	2	13829.2975	2.1		
4_{23}-3_{12}	5	4	18240.8320	5.1	18057.3264	5.1
	4	3	18239.4386	2.5		
	3	2	18241.3572	2.6		
4_{22}-3_{13}	5	4	18363.1822	-0.2	18268.3989	0.2
	4	3	18363.9201	-7.5		
	3	2	18362.9725	-0.1		
5_{05}-4_{14}	6	5	17590.5262	-2.9	17591.1536	0.0
	5	4	17591.6382	-3.6		
	4	3	17590.2994	3.6		
3_{03}-2_{02}	4	3	11178.8330	5.0	11130.0850	-0.5
	3	2	11178.8330	-6.0		
	2	1	11179.0362	0.8		
3_{13}-2_{12}	4	3	11149.6327	3.1	11082.3611	3.0
	3	2	11149.8752	-2.5		
	2	1	11149.4465	-0.6		
3_{12}-2_{11}	4	3	11209.0332	1.9	11182.2433	-0.2
	3	2	11209.3532	0.7		
	2	1	11209.2331	4.1		
2_{02}-1_{01}	2	1	7453.1600	0.4	7421.5213	-1.4
	1	0	7453.2078	-4.0		
2_{12}-1_{11}					7388.7543	1.6
2_{11}-1_{10}					7455.3722	3.8

3) Table 2S. MP2/6-311++G(d,p) geometry of the observed species of PYR-CH_4. See the figure below for the atom numbering.

bond lengths/Å		angles/°		dihedral angles/°	
C2C1	1.398				
C3C2	1.400	C3C2C1	118.6		
N4C3	1.345	N4C3C2	123.8	N4C3C2C1	0.1
C5N4	1.345	C5N4N4	116.8	C5N4C3C2	-0.1
C6C5	1.400	C6C5C1	123.8	C6C5C1C3	0.1
C7N4	3.836	C7N4C3	80.9	C7N4C3C2	74.8
H8C3	1.088	H8C3N4	115.8	H8C3N4C5	180.0
H9C5	1.088	H9C5N4	115.8	H9C5N4C3	180.0
H10C2	1.086	H10C2C3	120.1	H10C2C3N4	179.9
H11C6	1.086	H11C6C5	120.1	H11C6C5N4	-179.9
H12C1	1.086	H12C1C2	120.9	H12C1C2C3	180.0
H13C7	1.090	H13C7N4	28.2	H13C7N4C3	-59.6
H14C7	1.091	H13C7N4	81.0	H13C7N4C3	120.4
H15C7	1.091	H13C7N4	121.2	H13C7N4C3	-132.2
H16C7	1.091	H13C7N4	121.2	H13C7N4C3	13.0