Electronic Supplementary Information

New Journal of Chemistry

Solvent effects on the nitrogen NMR chemical shifts in 1-methylazoles – a theoretical study

Agnieszka Brzyska, Piotr Borowski, Krzysztof Woliński

Table 1S The experimental nitrogen chemical shifts (in ppm) of azole molecules (II-X) referred to nitromethane [1-4].

Exp.	I	II	III		IV		V			VI			VII			VIII			IX			X			
	N1	N1	N1	N2	N1	N3	N 1	N 2	N 3	N 1	N 2	N 4	N 1	N 3,4	N 3,4	N 1	N 2,5	N 2,5	N 1	N 2	N 3	N 4	N 1	N 2	N 3	N5
c-hexane	238.77	235.19	181.28	65.69	225.02	111.50	149.50	7.51	20.58	176.07	78.95	122.91	226.00	47.00	47.00	133.07	47.97	47.97	159.55	8.42	-23.31	43.23	106.99	-3.41	41.30	73.09
dioxane	232.14	231.69	178.50	68.93	220.87	115.85	144.88	12.13	25.16	172.93	80.75	125.88	220.69	54.77	54.77	131.11	48.97	48.97	153.99	10.06	-16.40	47.96	103.34	-0.53	44.94	73.43
CC_{l4}	237.81	234.14	180.93	68.84	223.48	114.71	147.61	11.59	24.31	175.47	80.24	124.53	224.23	50.04	50.04	133.22	48.72	48.72	157.47	9.29	-18.82	45.63	106.63	-1.89	42.96	73.18
C_6H_6	235.87	232.88	179.72	68.57	222.56	115.41	146.52	11.36	24.51	174.29	80.55	125.35	222.51	52.71	52.71	132.16	48.98	48.98	155.94	9.37	-17.96	46.62	104.97	-1.64	43.76	73.27
Et_2O	231.16	233.62	180.24	67.25	223.05	114.06	147.15	10.72	24.05	174.45	80.45	124.98	223.40	51.21	51.21	132.52	48.87	48.87	156.47	9.42	-19.11	45.94	105.08	-1.95	43.27	73.39
CHC_{l3}	234.73	230.80	179.36	73.74	220.52	122.54	145.49	15.28	30.36	173.55	83.56	129.81	220.49	59.39	59.39	132.40	51.33	51.33	154.63	9.91	-14.61	49.71	104.52	-0.28	47.31	73.66
CH_2Cl_2	234.34	230.74	178.76	71.67	220.23	120.25	145.05	14.06	28.58	173.10	82.40	128.66	219.94	58.96	58.96	131.84	50.74	50.74	154.28	9.81	-14.46	49.24	104.00	-0.12	46.90	73.63
$(CH_3)_2CO$	230.29	231.36	178.51	70.05	220.23	117.16	144.52	12.85	26.18	172.39	80.99	126.73	219.45	56.41	56.41	131.52	49.36	49.36	153.10	9.93	-15.27	48.61	102.93	-0.50	45.47	72.86
EtOH	228.81	232.14	180.03	82.82	218.72	131.15	143.97	17.25	37.84	171.68	84.60	136.18	216.69	72.01	72.01	132.48	52.01	52.01	152.71	10.96	-8.78	55.63	103.47	0.30	49.50	73.42
MeOH	229.85	231.37	179.74	84.48	216.21	133.74	143.30	17.84	39.97	171.28	85.56	137.28	216.21	73.10	73.10	132.35	53.20	53.20	151.99	10.35	-8.28	56.35	102.78	0.68	51.41	73.35
DMSO	224.17	229.33	177.00	70.26	218.02	117.52	142.32	14.83	27.22	170.85	81.28	126.99	216.82	59.33	59.33	130.68	48.94	48.94	150.92	10.35	-13.00	50.18	101.51	0.38	46.14	72.58
H_2O	226.50	226.89	178.20	87.98	215.35	135.56	141.71	27.49	42.63	171.28	92.06	138.72	214.33	77.71	77.71	132.88	58.85	58.85	150.34	14.06	1.75	60.33	102.34	6.00	56.36	77.56

Table 2SA The solvent effect on the bond lengths in 1-methyl-1,2,3,4-tetrazole (the atoms numbering see Figure 1S)

R [Å]	gas	c-hexane	dioxane	CCl_4	C_6H_6	Et_2O	$CHCl_3$	CH_2Cl_2	$(CH_3)_2CO$	EtOH	MeOH	DMSO	H_2O
N_2N_1	1.3516	1.3390	1.3398	1.3387	1.3387	1.3374	1.3372	1.3363	1.3358	1.3357	1.3356	1.3355	1.3353
N_3N_2	1.2881	1.2910	1.2908	1.2911	1.2912	1.2920	1.2919	1.2925	1.2928	1.2929	1.2930	1.2929	1.2932
N_4N_3	1.3611	1.3592	1.3591	1.3590	1.3590	1.3580	1.3581	1.3575	1.3573	1.3572	1.3571	1.3571	1.3569
C_5N_1	1.3468	1.3532	1.3524	1.3529	1.3529	1.3515	1.3514	1.3506	1.3501	1.3500	1.3498	1.3499	1.3496
C_5N_4	1.3133	1.3148	1.3154	1.3152	1.3152	1.3167	1.3168	1.3177	1.3182	1.3184	1.3186	1.3185	1.3188
C_6N_1	1.4549	1.4562	1.4567	1.4564	1.4564	1.4580	1.4581	1.4590	1.4597	1.4598	1.4599	1.4599	1.4600
H_7C_5	1.0776	1.0773	1.0775	1.0773	1.0773	1.0773	1.0773	1.0773	1.0773	1.0773	1.0773	1.0773	1.0774
H_8C_6	1.0909	1.0897	1.0909	1.0885	1.0885	1.0881	1.0880	1.0878	1.0876	1.0876	1.0876	1.0876	1.0876
H_9C_6	1.0909	1.0886	1.0892	1.0897	1.0897	1.0893	1.0894	1.0892	1.0890	1.0890	1.0890	1.0890	1.0889
$H_{10}C_6$	1.0877	1.0895	1.0880	1.0894	1.0894	1.0892	1.0892	1.0890	1.0889	1.0889	1.0889	1.0889	1.0890
R^{gas}-R^{medium}													
N_2N_1		0.0136	0.0127	0.0138	0.0139	0.0152	0.0154	0.0162	0.0168	0.0169	0.0170	0.0170	0.0173
N_3N_2		-0.0029	-0.0028	-0.0031	-0.0031	-0.0039	-0.0039	-0.0044	-0.0047	-0.0048	-0.0049	-0.0049	-0.0051
N_4N_3		0.0019	0.0020	0.0021	0.0021	0.0031	0.0030	0.0036	0.0038	0.0040	0.0040	0.0040	0.0042
C_5N_1		-0.0065	-0.0056	-0.0061	-0.0061	-0.0047	-0.0046	-0.0038	-0.0034	-0.0032	-0.0031	-0.0031	-0.0029
C_5N_4		-0.0016	-0.0022	-0.0019	-0.0019	-0.0034	-0.0035	-0.0045	-0.0050	-0.0052	-0.0053	-0.0053	-0.0055
C_6N_1		-0.0012	-0.0018	-0.0015	-0.0015	-0.0030	-0.0032	-0.0041	-0.0047	-0.0048	-0.0049	-0.0050	-0.0051
H_7C_5		0.0002	0.0001	0.0003	0.0002	0.0003	0.0003	0.0003	0.0003	0.0002	0.0002	0.0002	0.0002
H_8C_6		0.0012	0.0000	0.0024	0.0025	0.0028	0.0029	0.0031	0.0033	0.0033	0.0033	0.0034	0.0034
H_9C_6		0.0024	0.0018	0.0012	0.0012	0.0016	0.0015	0.0018	0.0019	0.0019	0.0019	0.0019	0.0020
$H_{10}C_6$		-0.0018	-0.0003	-0.0017	-0.0017	-0.0015	-0.0015	-0.0014	-0.0012	-0.0012	-0.0013	-0.0012	-0.0013

Table 2SB The solvent effect on the bond angles in 1-methyl-1,2,3,4-tetrazole (the atoms numbering see Figure 1S)

α [°]	gas	c-hexane	dioxane	CCl_4	C_6H_6	Et_2O	$CHCl_3$	CH_2Cl_2	$(CH_3)_2CO$	EtOH	MeOH	DMSO	H_2O
$N_3N_2N_1$	106.71	106.90	106.90	106.90	106.90	106.91	106.91	106.92	106.93	106.93	106.93	106.93	106.93
$N_4N_3N_2$	111.11	111.04	111.02	111.03	111.03	110.99	110.99	110.95	110.94	110.93	110.92	110.93	110.91
$N_2N_1C_5$	107.53	107.83	107.83	107.84	107.85	107.93	107.94	107.99	108.01	108.03	108.03	108.03	108.05
$N_1C_5N_4$	109.13	108.70	108.69	108.69	108.69	108.64	108.64	108.60	108.58	108.58	108.57	108.57	108.56
C_5N4N_3	105.52	105.53	105.55	105.53	105.53	105.54	105.53	105.54	105.53	105.54	105.54	105.53	105.54
$N_2N_1C_6$	121.27	122.04	122.08	122.06	122.05	122.17	122.20	122.26	122.32	122.33	122.34	122.35	122.36
$C_5N_1C_6$	131.19	130.14	130.04	130.10	130.10	129.90	129.87	129.75	129.66	129.64	129.62	129.62	129.59
$H_7C_5N_1$	124.49	124.71	124.77	124.71	124.71	124.70	124.69	124.68	124.66	124.66	124.65	124.65	124.62
$H_7C_5N_4$	126.38	126.59	126.53	126.60	126.60	126.66	126.67	126.72	126.76	126.76	126.78	126.77	126.82
$H_8C_6N_1$	110.42	109.49	110.24	108.98	108.97	108.85	108.81	108.76	108.70	108.70	108.69	108.67	108.66
$H_9C_6N_1$	110.42	109.03	109.59	109.50	109.50	109.35	109.39	109.30	109.26	109.25	109.22	109.24	109.16
$H_8C_6H_9$	109.83	109.67	109.90	109.68	109.68	109.74	109.75	109.79	109.81	109.82	109.83	109.82	109.85
$H_{10}C_6N_1$	107.08	109.27	107.69	109.25	109.26	109.22	109.18	109.15	109.14	109.11	109.11	109.13	109.13
$H_8C_6H_{10}$	109.52	109.72	109.69	109.67	109.67	109.73	109.74	109.78	109.80	109.81	109.82	109.81	109.85
$H_9C_6H_{10}$	109.52	109.66	109.70	109.75	109.75	109.92	109.95	110.04	110.11	110.12	110.14	110.15	110.17
α^{gas}-α^{medium}													
$N_3N_2N_1$		-0.19	-0.19	-0.19	-0.19	-0.20	-0.20	-0.21	-0.22	-0.22	-0.22	-0.22	-0.22
$N_4N_3N_2$		0.07	0.09	0.08	0.08	0.12	0.12	0.16	0.17	0.18	0.19	0.18	0.20
$N_2N_1C_5$		-0.29	-0.30	-0.31	-0.31	-0.40	-0.40	-0.45	-0.48	-0.49	-0.50	-0.50	-0.52
$N_1C_5N_4$		0.42	0.43	0.44	0.44	0.49	0.49	0.53	0.54	0.55	0.56	0.55	0.57
C_5N4N_3		-0.01	-0.04	-0.01	-0.02	-0.02	-0.01	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02
$N_2N_1C_6$		-0.77	-0.81	-0.78	-0.78	-0.90	-0.92	-0.99	-1.05	-1.06	-1.07	-1.08	-1.09
$C_5N_1C_6$		1.06	1.16	1.10	1.10	1.29	1.33	1.44	1.53	1.55	1.57	1.57	1.61
$H_7C_5N_1$		-0.21	-0.28	-0.22	-0.22	-0.21	-0.20	-0.19	-0.16	-0.17	-0.16	-0.16	-0.13
$H_7C_5N_4$		-0.21	-0.15	-0.22	-0.22	-0.28	-0.30	-0.34	-0.38	-0.38	-0.40	-0.40	-0.44
$H_8C_6N_1$		0.93	0.18	1.44	1.45	1.57	1.61	1.66	1.72	1.72	1.73	1.75	1.76
$H_9C_6N_1$		1.39	0.83	0.92	0.92	1.07	1.03	1.12	1.16	1.17	1.20	1.18	1.26
$H_8C_6H_9$		0.17	-0.07	0.15	0.15	0.09	0.08	0.04	0.02	0.01	0.00	0.01	-0.02
$H_{10}C_6N_1$		-2.19	-0.60	-2.17	-2.17	-2.14	-2.09	-2.07	-2.05	-2.03	-2.03	-2.04	-2.04
$H_8C_6H_{10}$		-0.20	-0.17	-0.15	-0.15	-0.21	-0.22	-0.26	-0.28	-0.29	-0.30	-0.29	-0.33
$H_9C_6H_{10}$		-0.14	-0.18	-0.23	-0.23	-0.40	-0.43	-0.52	-0.59	-0.60	-0.62	-0.63	-0.65

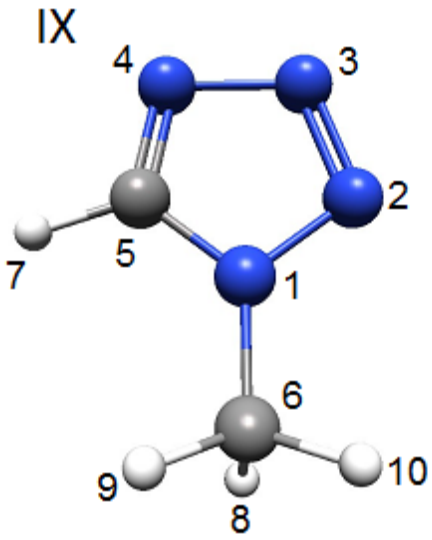

Figure 1S. The atoms numbering in 1-methyl-1,2,3,4-tetrazole.