Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
This journal is © The Owner Societies 2012

Theoretical study of the gauche-trans equilibrium with and without an intramolecular hydrogen bond for $^{+}H_3NCH_2CH_2X$ systems (X=OH, NH_2, COO^-) in solution

Peter I. Nagy

Center for Drug Design and Development, The University of Toledo, Toledo, OH, 43606-3390; e-mail: pnagy@utnet.utoledo.edu

Supplementary Information

This journal is © The Owner Societies 2012

Table S1. Major geometric parameters for the $^{+}H_3N$-CH_2-CH_2-X ions and H_2N-CH_2-CH_2-COOH molecule optimized at the IEF-PCM/B97D/aug-cc-pvtz level in water and chloroform

	water		chloroform	
	gauche	trans	gauche	trans
X = OH				
O-H	0.965	0.966	0.966	0.966
N-H^+	1.024,1.020,1.021	1.024,1.023,1.024	1.025,1.022,1.024	1.023,1.025,1.025
O-C	1.433	1.428	1.430	1.422
N-C	1.512	1.510	1.519	1.514
HOC	108.2	107.5	108.6	108.2
OCC	107.0	106.4	106.9	105.9
NCC	109.5	109.6	109.7	109.6
HOCC	168.5	180.1	173.6	179.9
NCCO	-60.7	180.0	-59.7	180.0
H^+NCC	48.1, 168.0, -71.1	60.0,179.8, -60.3	53.1, 173.3, -66.0	60.1,180.0, -60.1
H^+…O	2.378		2.405	
N-H^+…O	104.7		102.6	
X=NH_2				
N-H	1.015,1.016	1.017	1.016, 1.014	1.016
N^+-H	1.030,1.021,1.022	1.023	1.038,1.021,1.022	1.024
N-C	1.472	1.463	1.471	1.457
N^+-C	1.513	1.518	1.515	1.525
HNC	110.1, 110.4	110.1	110.9, 110.9	111.1
NCC	109.2	113.0	108.7	113.5
N^+CC	108.8	110.9	107.7	110.6
HNCC	-80.2, 161.8	-59.2, 58.2	-84.0, 156.8	-60.1, 59.6
N^+CCN	-56.4	179.9	-51.1	179.6
H^+NCC	45.1, 165.3, -73.1	59.7,179.8, -60.2	39.6,159.5, -78.0	59.4,179.7, -60.2
H^+…N	2.319		2.148	
NH^+…N	109.4		114.8	

Distances in Å, angles in deg. One of the antipodes for the gauche conformers. Trans conformers are of nearly C_s symmetry from symmetry unrestricted optimizations.

This journal is © The Owner Societies 2012

Table 1, continued

	water		chloroform	
	gauche	trans	gauche	trans
X=COO^-				
N-H^+	1.092, 1.017, 1.019	1.023		1.023
N-C	1.507	1.523		1.534
C-C_{carb}	1.554	1.562		1.576
C-O	1.287, 1.248	1.263, 1.262		1.261,1.255
NCC	108.9	110.5		110.4
CCC	114.5	113.2		112.2
CCO	116.4, 118.1	117.5, 115.2		116.3, 114.7
OCO	125.5	127.3		129.0
H^+NCC	42.3, 162.8, -74.9	61.0, 181.2, -58.7		60.3, 180.9, -58.7
NCCC	-54.2	-179.4		179.6
CCCO	30.7, -151.0	2.3, -177.9		1.2, -178.8
H^+…O	1.561			
N-H^+…O	150.0			
$H_2NCH_2CH_2COOH$[a]				
N-H	1.015, 1.016	1.018	1.014, 1.015	1.016
N-C	1.485(1.473)	1.465	1.483	1.461
C-C_{carb}	1.532(1.512)	1.508	1.533	1.507
C-O	1.223, 1.339(1.357)	1.219,1.360	1.218, 1.343	1.216,1.362
O-H	1.042(0.972)	0.974	1.025	0.973
NCC	109.6	114.1	109.9	114.2
CCC	114.7	110.5	115.1	110.5
CCO	122.8, 116.0	125.3, 112.0	122.7, 115.9	125.4, 111.9
OCO	121.2	122.7	121.4	122.6
HOC	107.3	108.2	107.7	107.6
NCCC	-55.6(-61.1)	178.5	-57.0	179.4
CCCO	-147.1, 34.5	-90.6, 86.3	-147.1, 34.5	-88.3, 88.4
H…N	1.605		1.658	
N…H-O	156.1		155.3	

[a]Data for the gauche $H_2NCH_2CH_2COOH$ refer to the –COOH anti conformation. For the more stable syn conformer in aqueous solution, some key geometric parameters are provided in parentheses.

This journal is © The Owner Societies 2012

Table S2. Calculated IEF-PCM/B97D/aug-cc-pvtz ELPO fitted CHELPG charges[a]

	Water		Chloroform	
	gauche	trans	gauche	trans
$^{+}H_3NCH_2CH_2OH$				
N	-0.24	-0.58	-0.27	-0.59
H^{+}	0.30, 0.32	0.39, 0.41	0.31, 0.33	0.39, 0.41
O	-0.63	-0.70	-0.61	-0.66
(O)H	0.43	0.45	0.43	0.44
DM(QM)	16.12	20.33	15.84	19.90
DM(ELPO)	15.90	20.30	15.75	19.88
$^{+}H_3NCH_2CH_2NH_2$				
N^{+}	-0.10	-0.40	-0.14	-0.38
H^{+}	0.22, 0.29	0.34, 0.38	0.21, 0.29	0.33, 0.37
N	-0.89	-1.00	-0.83	-0.92
(N)H	0.35, 0.36	0.37	0.35	0.36
DM(QM)	14.06	19.36	13.49	18.79
DM(ELPO)	14.01	19.24	13.36	18.81
$^{+}H_3NCH_2CH_2COO^{-}$				
N	-0.52	-0.46		-0.48
H^{+}	0.35, 0.37	0.36		0.35
C	0.88	0.91		0.89
O	-0.81, -0.82	-0.86, -0.87		-0.82, -0.83
DM(QM)	14.02	21.18		19.74
DM(ELPO)	13.87	21.00		19.55
$H_2NCH_2CH_2COOH$				
N	-0.74	-1.05	-0.72	-1.00
(N)H	0.32	0.38	0.31	0.36
O=	-0.67	-0.62	-0.63	-0.59
O(H)	-0.64	-0.58	-0.60	-0.57
(O)H	0.36	0.43	0.34	0.42
DM(QM)	9.04	2.57	8.20	2.37
DM(ELPO)	8.96	2.57	8.14	2.37

[a]Atomic charges in charge units, dipole moments in D.