Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary data to the manuscript "Infrared Absorption Spectra of 2-(Hydroxyimino)propanohydroxamic and Oxalodihydroxamic Acids Isolated in Argon Matrices" by A. Kaczor, J.Szczepanski, M. Vala, H. Kozłowski and L. Proniewicz

Geometry (Bond Lengths in Å, Angles in °) of the two most stable **hpha** structures.

Parameter	zEe-keto[a]	zEe-keto[b]	zEz-keto[a]
C_1-C_2	1.501	1.493	1.506
C_1-C_6	1.498	1.492	1.504
C_1-N_7	1.285	1.296	1.286
C_2-N_4	1.361	1.364	1.354
C_2-O_3	1.234	1.240	1.239
C_6-H_{11}	1.095	1.094	1.092
C_6-H_{12}	1.090	1.089	1.095
C_6-H_{13}	1.096	1.094	1.095
N_4-H_9	1.013	1.016	1.011
N_4-O_5	1.402	1.412	1.394
N_7-O_8	1.392	1.400	1.407
O_5-H_{10}	0.985	0.987	0.987
O_8-H_{14}	0.971	0.975	0.970
O_3···H_{10}	2.000	2.008	1.961
C_1-C_2-O_3	122.9	122.9	122.8
C_1-C_6-H_{11}	110.3	109.9	109.9
C_1-C_6-H_{12}	109.8	109.7	110.4
C_1-C_6-H_{13}	110.2	109.9	110.4
C_1-N_7-O_8	111.9	110.7	114.3
C_2-N_4-H_9	120.2	118.7	123.6
C_2-N_4-O_5	115.8	114.9	116.2
C_6-C_1-N_7	126.0	125.5	129.1
N_4-O_5-H_{10}	100.8	100.6	100.6

N_7-O_8-H_{14}	102.8	102.2	102.4
O_3-C_2-N_4	120.6	121.1	119.7
O_3···H_{10}-O_5	119.1	119.3	119.8
C_1-C_2-N_4-H_9	-27.5	-31.5	-23.4
C_1-N_7-O_8-H_{14}	-178.7	-178.7	179.0
C_2-C_1-C_6-H_{11}	-125.8	-122.8	-179.0
C_2-C_1-C_6-H_{12}	-4.5	-1.8	-57.8
C_2-C_1-C_6-H_{13}	116.4	119.4	59.9
C_2-C_1-N_7-O_8	179.5	179.1	-1.4
C_2-N_4-O_5-H_{10}	-10.9	-13.8	-6.6
O_3-C_2-C_1-N_7	-166.1	-160.4	-172.0
O_3-C_2-N_4-O_5	15.5	18.1	9.7
C_2-O_3···H_{10}-O_5	2.4	-179.0	1.5

[a] B3LYP/6- 31G(d), [b] MP2/6-31G(d)

Geometry (Bond Lengths in Å, Angles in °) of the two most stable **oxha** structures.

Parameter	zEz-keto[a]	zEz-keto[b]	eEz-keto[a]
C_2-C_3	1.515	1.508	1.522
C_2-N_5	1.340	1.340	1.346
C_3-N_9	1.340	1.340	1.330
C_2-O_1	1.236	1.244	1.233
C_3-O_4	1.236	1.244	1.249
N_5-H_{12}	1.011	1.014	1.012
N_9-H_8	1.011	1.014	1.011
N_5-O_6	1.388	1.396	1.397
N_9-O_{10}	1.388	1.396	1.383
O_6-H_7	0.984	0.987	0.992
O_{10}-H_{11}	0.984	0.987	0.984
O_1···H_7	2.088	2.087	3.684
O_4···H_{11}	2.088	2.087	2.093
C_2-C_3-N_9	112.8	112.6	112.2

C_3-C_2-N_5	112.8	112.6	115.3
C_2-C_3-O_4	124.3	124.2	126.1
C_3-C_2-O_1	124.3	124.2	120.7
C_2-N_5-H_{12}	123.9	123.0	119.7
C_3-N_9-H_8	123.9	123.0	124.0
C_2-N_5-O_6	118.4	117.8	127.6
C_3-N_9-O_{10}	118.4	117.8	119.8
N_5-C_2-O_1	122.9	123.2	123.9
N_9-C_3-O_4	122.9	123.2	121.7
N_5-O_6-H_7	101.3	101.1	103.3
N_9-O_{10}-H_{11}	101.3	101.1	101.7
O_6-N_5-H_{12}	114.5	113.7	112.0
O_{10}-N_9-H_8	114.5	113.7	115.9
O_1···H_7-O_6	117.0	117.6	76.6
O_4···H_{11}-O_{10}	117.0	117.6	116.3
C_2-C_3-N_9-O_{10}	173.0	171.4	177.9
C_3-C_2-N_5-O_6	173.0	171.4	-7.4
C_2-N_5-O_6-H_7	5.8	8.3	11.7
C_3-N_9-O_{10}-H_{11}	5.8	8.3	1.4
O_1-C_2-C_3-O_4	173.5	170.6	177.3
O_1-C_2-N_5-H_{12}	-166.8	-163.0	4.4
O_4-C_3-N_9-H_8	-166.8	-163.0	-176.0
C_2-O_1···H_7-O_6	179.3	179.6	177.7
C_3-O_4···H_{11}-O_{10}	179.3	179.6	179.5

[a] B3LYP/6- 31G(d), [b] MP2/6-31G(d)