Gas Phase and Solution Conformations of α -L-Iduronic Acid Structural Unit of Heparin

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Supporting Information

Table A. B3LYP/6-311++G(d,p) Optimized Relevant Bond Lengths (Å), Bond Angles (deg) and Dihedral Angles (deg) for the Functional Groups of the 1,4-DiOMe IdoA2S Species Studied

Parameters	1,4-DiOMe IdoA2S					
	4C_1		1C_4		2S_0	
	gas phase	in water	gas phase	in water	gas phase	in water
$d[\text{O}(2)\text{--S}]$	1.642	1.618	1.627	1.615	1.646	1.628
$d[\text{S--O(a)}]$	1.605	1.581	1.610	1.596	1.605	1.576
$d[\text{S--O(b)}]$	1.451	1.451	1.451	1.451	1.449	1.452
$d[\text{S--O(c)}]$	1.434	1.444	1.440	1.444	1.435	1.446
$d[\text{O(a)} \cdots \text{H}]$	0.988	1.020	0.971	0.977	0.990	1.033
$d[\text{C}(5)\text{--C}(6)]$	1.535	1.531	1.522	1.520	1.528	1.520
$d[\text{C}(6)\text{--O(d)}]$	1.350	1.334	1.341	1.329	1.342	1.329
$d[\text{C}(6)\text{--O(e)}]$	1.202	1.210	1.206	1.211	1.205	1.211
$d[\text{O(d)} \cdots \text{H}]$	0.970	0.977	0.970	0.976	0.969	0.977
$\theta[\text{C}(2)\text{--O}(2)\text{--S}]$	119.7	119.3	117.2	119.6	119.1	118.6
$\theta[\text{O}(2)\text{--S--O(a)}]$	101.3	102.5	96.5	101.1	101.9	102.6
$\theta[\text{S--O(a)} \cdots \text{H}]$	108.6	111.5	110.0	113.5	109.0	111.1
$\theta[\text{C}(5)\text{--C}(6)\text{--O(d)}]$	113.5	114.6	114.4	115.6	113.1	115.6
$\theta[\text{C}(6)\text{--O(d)} \cdots \text{H}]$	107.8	109.9	106.6	109.3	107.4	109.4
$\phi[\text{C}(1)\text{--O}(5)\text{--C}(5)\text{--C}(4)]$	51.5	50.3	−58.7	−66.7	−39.2	−66.3
$\phi[\text{O}(5)\text{--C}(5)\text{--C}(4)\text{--C}(3)]$	−49.5	−57.0	52.1	57.1	−23.1	30.9
$\phi[\text{C}(5)\text{--C}(4)\text{--C}(3)\text{--C}(2)]$	54.1	61.1	−47.3	−40.1	65.0	33.1
$\phi[\text{C}(1)\text{--C}(2)\text{--O}(2)\text{--S}]$	141.8	135.3	93.3	89.0	148.6	143.7
$\phi[\text{C}(2)\text{--O}(2)\text{--S--O(a)}]$	87.6	73.5	−175.9	−130.8	81.9	75.2
$\phi[\text{O}(2)\text{--S--O(a)} \cdots \text{H}]$	−48.3	−25.1	66.9	74.5	−56.4	−21.2
$\phi[\text{O}(5)\text{--C}(5)\text{--C}(6)\text{--O(d)}]$	47.2	33.6	0.9	2.2	42.1	2.7
$\phi[\text{C}(5)\text{--C}(6)\text{--O(d)} \cdots \text{H}]$	−179.3	179.4	179.9	179.7	178.3	179.9
$\phi[\text{C}(2)\text{--C}(3)\text{--O--H}]$	173.8	173.2	40.4	−169.3	167.1	−136.8

Table A. – Continued

Parameters	Dianion of 1,4-DiOMe IdoA2S					
	$^4\text{C}_1$		$^1\text{C}_4$		$^2\text{S}_0$	
	gas phase	in water	gas phase	in water	gas phase	in water
$d[\text{O}(2)\text{--S}]$	1.688	1.643	1.705	1.647	1.708	1.660
$d[\text{S--O(a)}]$	1.491	1.482	1.472	1.471	1.479	1.473
$d[\text{S--O(b)}]$	1.480	1.469	1.482	1.476	1.483	1.470
$d[\text{S--O(c)}]$	1.468	1.468	1.482	1.470	1.472	1.473
$d[\text{O(a)} \cdots \text{H}]$						
$d[\text{C}(5)\text{--C}(6)]$	1.575	1.532	1.576	1.531	1.577	1.519
$d[\text{C}(6)\text{--O(d)}]$	1.250	1.254	1.245	1.250	1.241	1.250
$d[\text{C}(6)\text{--O(e)}]$	1.258	1.253	1.257	1.255	1.264	1.254
$d[\text{O(d)} \cdots \text{H}]$						
$\theta[\text{C}(2)\text{--O}(2)\text{--S}]$	119.2	117.3	115.7	118.7	118.0	117.8
$\theta[\text{O}(2)\text{--S--O(a)}]$	104.0	104.5	101.2	101.2	105.2	106.4
$\theta[\text{S--O(a)} \cdots \text{H}]$						
$\theta[\text{C}(5)\text{--C}(6)\text{--O(d)}]$	117.4	117.8	117.7	119.3	118.3	119.2
$\theta[\text{C}(6)\text{--O(d)} \cdots \text{H}]$						
$\phi[\text{C}(1)\text{--O}(5)\text{--C}(5)\text{--C}(4)]$	57.8	53.8	−60.3	−58.6	−45.6	−68.5
$\phi[\text{O}(5)\text{--C}(5)\text{--C}(4)\text{--C}(3)]$	−49.0	−51.4	57.0	51.7	−15.7	30.3
$\phi[\text{C}(5)\text{--C}(4)\text{--C}(3)\text{--C}(2)]$	48.8	54.1	−50.2	−48.4	61.7	35.8
$\phi[\text{C}(1)\text{--C}(2)\text{--O}(2)\text{--S}]$	136.2	131.8	121.6	170.0	82.4	93.3
$\phi[\text{C}(2)\text{--O}(2)\text{--S--O(a)}]$	70.3	70.5	−178.9	−161.4	49.8	28.4
$\phi[\text{O}(2)\text{--S--O(a)} \cdots \text{H}]$						
$\phi[\text{O}(5)\text{--C}(5)\text{--C}(6)\text{--O(d)}]$	43.7	44.4	−12.6	3.0	31.2	4.2
$\phi[\text{C}(5)\text{--C}(6)\text{--O(d)} \cdots \text{H}]$						
$\phi[\text{C}(2)\text{--C}(3)\text{--O--H}]$	−34.1	−38.7	41.9	41.4	164.1	−157.7

Table B. B3LYP/6-311++G(d,p) Optimized Relevant Bond Lengths (Å), Bond Angles (deg) and Dihedral Angles (deg) for the Functional Groups of the 1,4-DiOMe IdoA2S Sodium Salt Species Studied

Parameters	1,4-DiOMe IdoA2S sodium salt					
	⁴ C ₁		¹ C ₄		² S ₀	
	gas phase	in water	gas phase	in water	gas phase	in water
<i>d</i> [O(2)–S]	1.694	1.662	1.684	1.658	1.735	1.661
<i>d</i> [S–O(a)]	1.498	1.484	1.498	1.484	1.488	1.468
<i>d</i> [S–O(b)]	1.490	1.487	1.498	1.477	1.480	1.483
<i>d</i> [S–O(c)]	1.449	1.477	1.446	1.468	1.452	1.471
<i>d</i> [O(a) ⋯Na]	2.334	2.718	2.277	2.425	2.466	4.608
<i>d</i> [O(b) ⋯Na]	2.314	2.636	2.303	2.704	2.424	2.377
<i>d</i> [C(5)–C(6)]	1.542	1.544	1.536	1.532	1.543	1.531
<i>d</i> [C(6)–O(d)]	1.263	1.262	1.257	1.251	1.258	1.254
<i>d</i> [C(6)–O(e)]	1.263	1.262	1.268	1.259	1.267	1.253
<i>d</i> [O(d) ⋯Na]	2.214	2.464	2.216	2.492	2.211	2.462
<i>d</i> [O(e) ⋯Na]	2.232	2.521	2.220	2.528	2.228	2.653
∠[C(2)–O(2)–S]	125.2	125.5	117.1	118.8	119.1	117.2
∠[O(2)–S–O(a)]	104.4	107.6	104.3	106.1	97.1	101.6
∠[S–O(a) ⋯Na]	87.8	91.0	92.7	100.9	80.9	43.5
∠[O(a) ⋯Na⋯O(b)]	63.2	54.8	64.0	56.7	60.1	16.3
∠[C(5)–C(6)–O(d)]	119.5	119.5	119.4	119.6	118.9	119.3
∠[C(6)–O(d) ⋯Na]	87.8	92.1	87.5	91.9	87.8	95.9
∠[O(d) ⋯Na⋯O(e)]	60.3	53.3	60.5	52.7	60.5	51.4
∠[C(1)–O(5)–C(5)–C(4)]	55.4	56.4	–62.9	–73.1	–35.4	–64.0
∠[O(5)–C(5)–C(4)–C(3)]	–47.3	–53.6	65.7	37.0	–27.5	37.1
∠[C(5)–C(4)–C(3)–C(2)]	49.8	57.8	–39.4	26.5	68.9	26.7
∠[C(1)–C(2)–O(2)–S]	–63.9	–54.9	81.3	87.5	100.5	130.6
∠[C(2)–O(2)–S–O(a)]	25.2	15.7	44.1	31.8	154.7	–160.7
∠[O(2)–S–O(a) ⋯Na]	75.5	84.3	–94.2	–103.5	–58.2	–92.3
∠[S–O(a) ⋯Na⋯O(b)]	19.9	16.4	–11.7	–7.2	–28.8	–42.5
∠[O(5)–C(5)–C(6)–O(d)]	34.5	29.7	–20.0	7.6	42.0	–4.1
∠[C(5)–C(6)–O(d) ⋯Na]	170.4	171.7	177.3	–178.5	–178.2	–170.6
∠[C(6)–O(d) ⋯Na⋯O(e)]	4.3	3.7	2.9	0.1	–1.5	–4.0
∠[C(2)–C(3)–O–H]	–176.1	170.7	–172.3	–157.4	156.7	–151.0

Table B. – Continued

Parameters	Dianions of 1,4-DiOMe IdoA2S sodium salt					
	${}^4\text{C}_1$		${}^1\text{C}_4$		${}^2\text{S}_0$	
	gas phase	in water	gas phase	in water	gas phase	in water
$d[\text{O}(2)\text{--S}]$	1.723	1.653	1.708	1.647	1.708	1.656
$d[\text{S--O(a)}]$	1.475	1.469	1.483	1.472	1.479	1.472
$d[\text{S--O(b)}]$	1.476	1.474	1.483	1.472	1.473	1.471
$d[\text{S--O(c)}]$	1.477	1.471	1.469	1.475	1.482	1.471
$d[\text{O(a)} \cdots \text{Na}]$						
$d[\text{O(b)} \cdots \text{Na}]$						
$d[\text{C}(5)\text{--C}(6)]$	1.575	1.526	1.576	1.531	1.578	1.519
$d[\text{C}(6)\text{--O(d)}]$	1.244	1.252	1.256	1.255	1.241	1.249
$d[\text{C}(6)\text{--O(e)}]$	1.262	1.254	1.248	1.250	1.264	1.254
$d[\text{O(d)} \cdots \text{Na}]$						
$d[\text{O(e)} \cdots \text{Na}]$						
$\theta[\text{C}(2)\text{--O}(2)\text{--S}]$	125.7	123.2	116.6	118.8	118.0	116.8
$\theta[\text{O}(2)\text{--S--O(a)}]$	105.5	107.4	105.0	107.1	105.2	106.5
$\theta[\text{S--O(a)} \cdots \text{Na}]$						
$\theta[\text{O(a)} \cdots \text{Na} \cdots \text{O(b)}]$						
$\theta[\text{C}(5)\text{--C}(6)\text{--O(d)}]$	117.8	117.9	112.0	114.3	118.3	119.4
$\theta[\text{C}(6)\text{--O(d)} \cdots \text{Na}]$						
$\theta[\text{O(d)} \cdots \text{Na} \cdots \text{O(e)}]$						
$\phi[\text{C}(1)\text{--O}(5)\text{--C}(5)\text{--C}(4)]$	56.0	55.0	−60.0	−58.3	−45.6	−68.4
$\phi[\text{O}(5)\text{--C}(5)\text{--C}(4)\text{--C}(3)]$	−47.6	−48.9	57.8	51.0	−15.7	29.9
$\phi[\text{C}(5)\text{--C}(4)\text{--C}(3)\text{--C}(2)]$	50.8	52.6	−51.2	−47.8	61.7	35.9
$\phi[\text{C}(1)\text{--C}(2)\text{--O}(2)\text{--S}]$	−68.1	−68.4	144.3	169.7	82.4	114.3
$\phi[\text{C}(2)\text{--O}(2)\text{--S--O(a)}]$	70.2	51.2	71.2	80.1	49.8	35.0
$\phi[\text{O}(2)\text{--S--O(a)} \cdots \text{Na}]$						
$\phi[\text{S--O(a)} \cdots \text{Na} \cdots \text{O(b)}]$						
$\phi[\text{O}(5)\text{--C}(5)\text{--C}(6)\text{--O(d)}]$	35.6	42.3	175.4	−177.6	31.2	5.9
$\phi[\text{C}(5)\text{--C}(6)\text{--O(d)} \cdots \text{Na}]$						
$\phi[\text{C}(6)\text{--O(d)} \cdots \text{Na} \cdots \text{O(e)}]$						
$\phi[\text{C}(2)\text{--C}(3)\text{--O--H}]$	−176.9	−177.5	41.7	41.5	164.1	−162.6