

# COMPUTER MODELLING AND FORECASTING OF PHYSICAL AND CHEMICAL PROPERTIES OF LACTOSE

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**Table 1 - Dependence of valent angles values in the method of optimization of  $\alpha$ -lactose molecule**

Angle	Experiment by K. Hirotsu and A. Shimada	PM3	AM1
Galactose residue	110,9	113,8	112,3
C(1')-C(2')-C(3')	110,9	110,2	113,8
C(2')-C(3')-C(4')	108,9	112,9	109,9
C(3')-C(4')-C(5')	109,0	112,2	110,0
C(4')-C(5')-O(5')	112,2	120,3	114,9
C(5')-O(5')-C(1')	111,2	117,6	113,6
O(5')-C(1')-C(2')	107,0	102,7	108,2
O(5')-C(1')-O(1')	107,7	109,3	105,6
C(2')-C(1')-O(1')	108,8	110,0	110,1
C(1')-C(2')-O(2')	110,5	111,6	110,7
C(3')-C(2')-O(2')	108,1	111,8	109,7
C(2')-C(3')-O(3')	111,4	113,9	109,7
C(4')-C(3')-O(3')	110,0	113,1	110,1
C(3')-C(4')-O(4')	108,4	112,1	112,7
C(5')-C(4')-O(4')	112,0	116,4	114,3
C(4')-C(5')-C(6')	106,8	112,7	104,5
O(5')-C(5')-C(6')	110,3	115,3	109,9
C(5')-C(6')-O(6')	117,1	117,0	117,5
Glycosidic lincage			
C(1')-O(1')-C(4)			

**Table 1 - Dependence of valent angles values in the method of optimization of  $\alpha$ -lactose molecule (continue)**

Angle	Experiment by K. Hirotsu and A. Shimada	PM3	AM1
Glucose residue	110,9	112,2	108,9
C(1)-C(2)-C(3)	110,3	110,5	108,9
C(2)-C(3)-C(4)	111,1	111,2	109,6
C(3)-C(4)-C(5)	107,9	111,9	112,1
C(4)-C(5)-O(5)	114,1	116,3	114,3
C(5)-O(5)-C(1)	109,7	113,0	112,0
O(5)-C(1)-C(2)	111,5	107,9	103,6
O(5)-C(1)-O(1)	108,8	109,3	110,9
C(2)-C(1)-O(1)	111,1	112,3	112,2
C(1)-C(2)-O(2)	112,7	111,6	110,9
C(3)-C(2)-O(2)	107,0	110,1	112,5
C(2)-C(3)-O(3)	111,6	106,3	109,0
C(4)-C(3)-O(3)	110,6	109,6	112,6
C(3)-C(4)-O(1')	107,0	104,4	105,3
C(5)-C(4)-O(1')	113,7	111,7	111,0
C(4)-C(5)-C(6)	107,2	104,6	106,5
O(5)-C(5)-C(6)	111,2	112,2	111,3
C(5)-C(6)-O(6)			

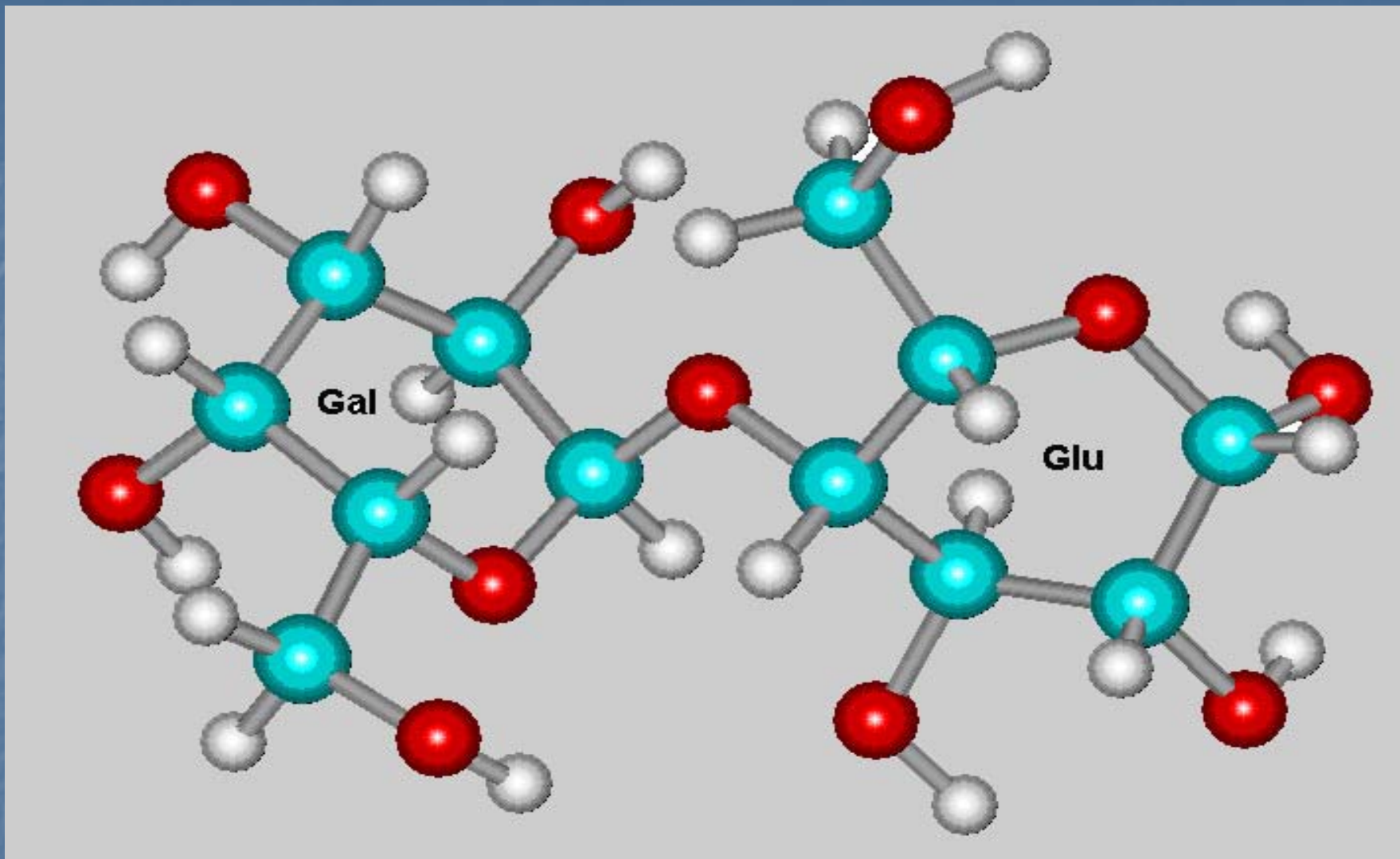


Fig 1 Alpha-lactose molecule after semiempirical method optimization in AM1 parametrization on Polak-Ribiere algorithm

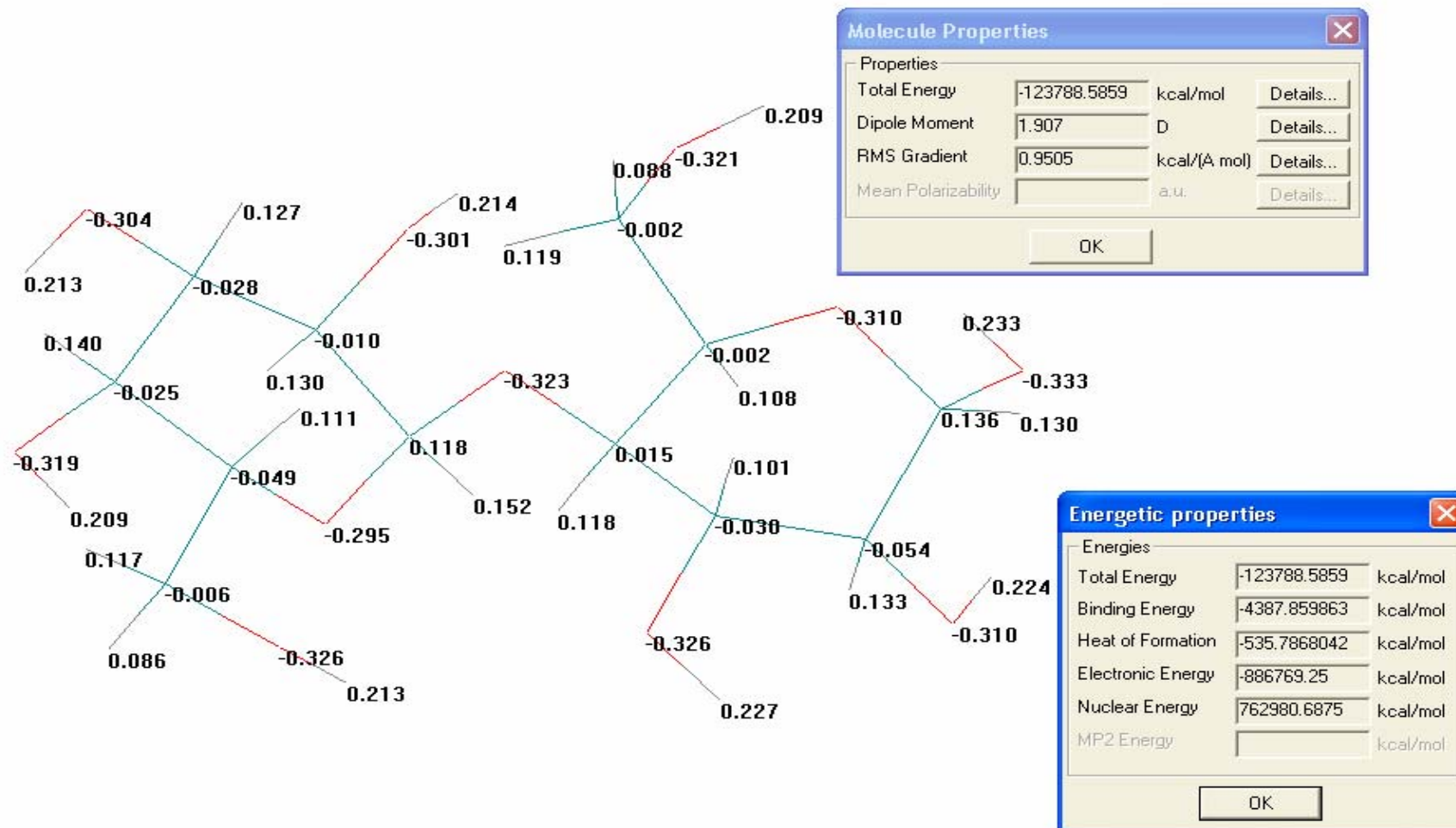


Fig 2. Values of an effective charge of alpha-lactose molecule atoms and its formation heat after geometrical optimization by means of semiempirical method in AM1 parametrization on Polak-Ribiere algorithm

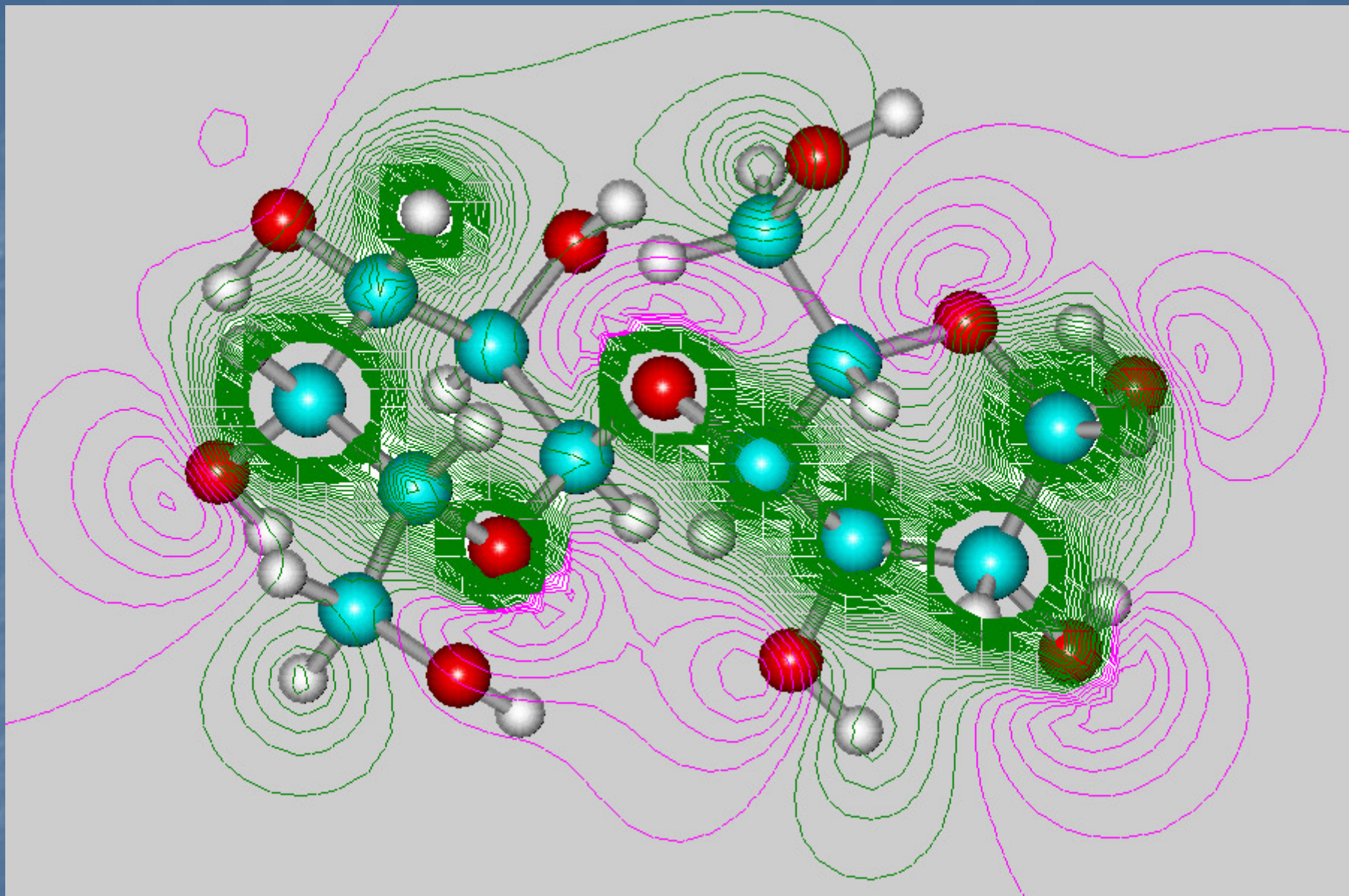


Fig. 3 Map of distribution of molecular electrostatic potential of  $\alpha$ -lactose molecule

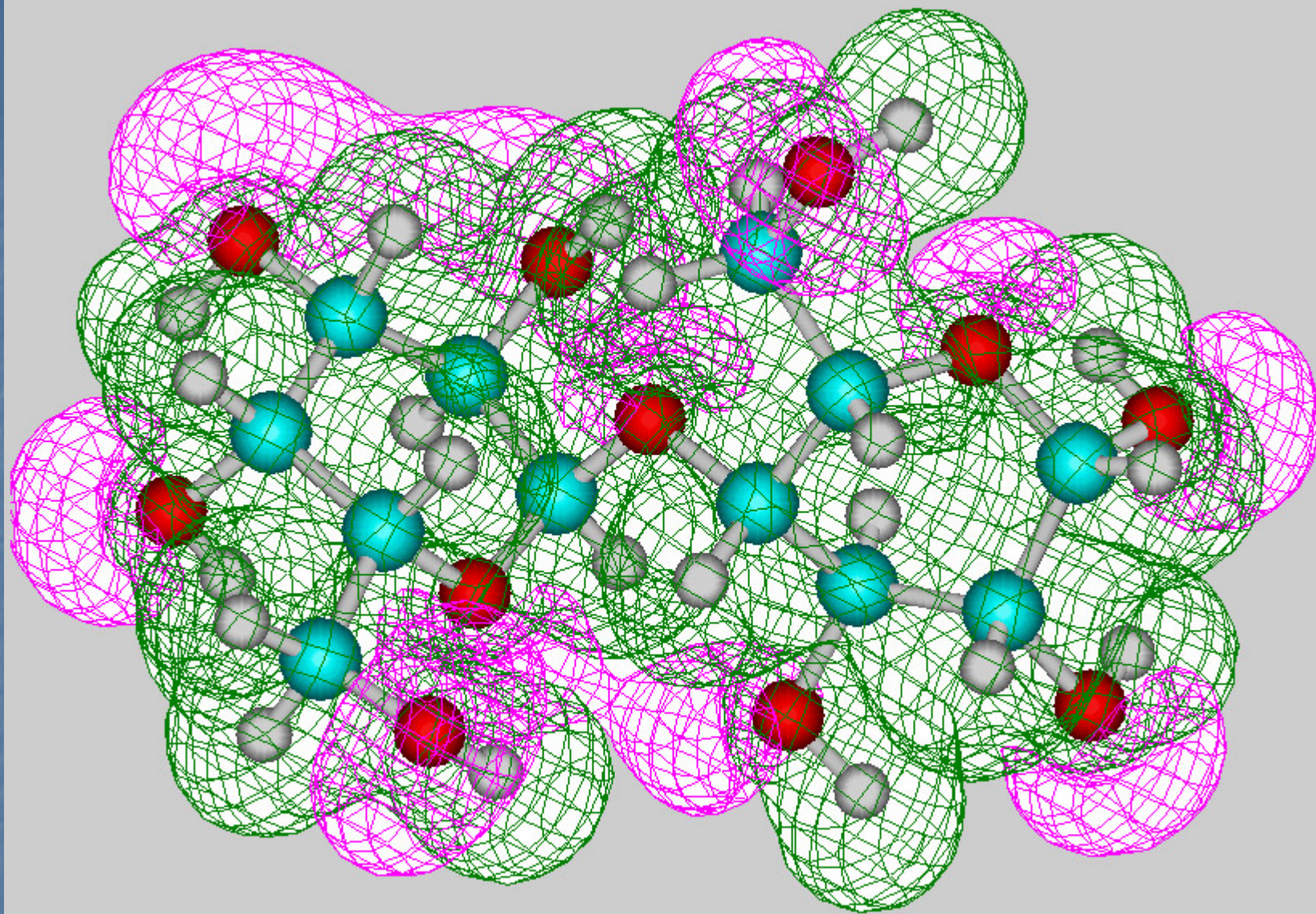


Fig. 4 Map of three-dimensional distribution of molecular electrostatic potential of  $\alpha$ -lactose molecule

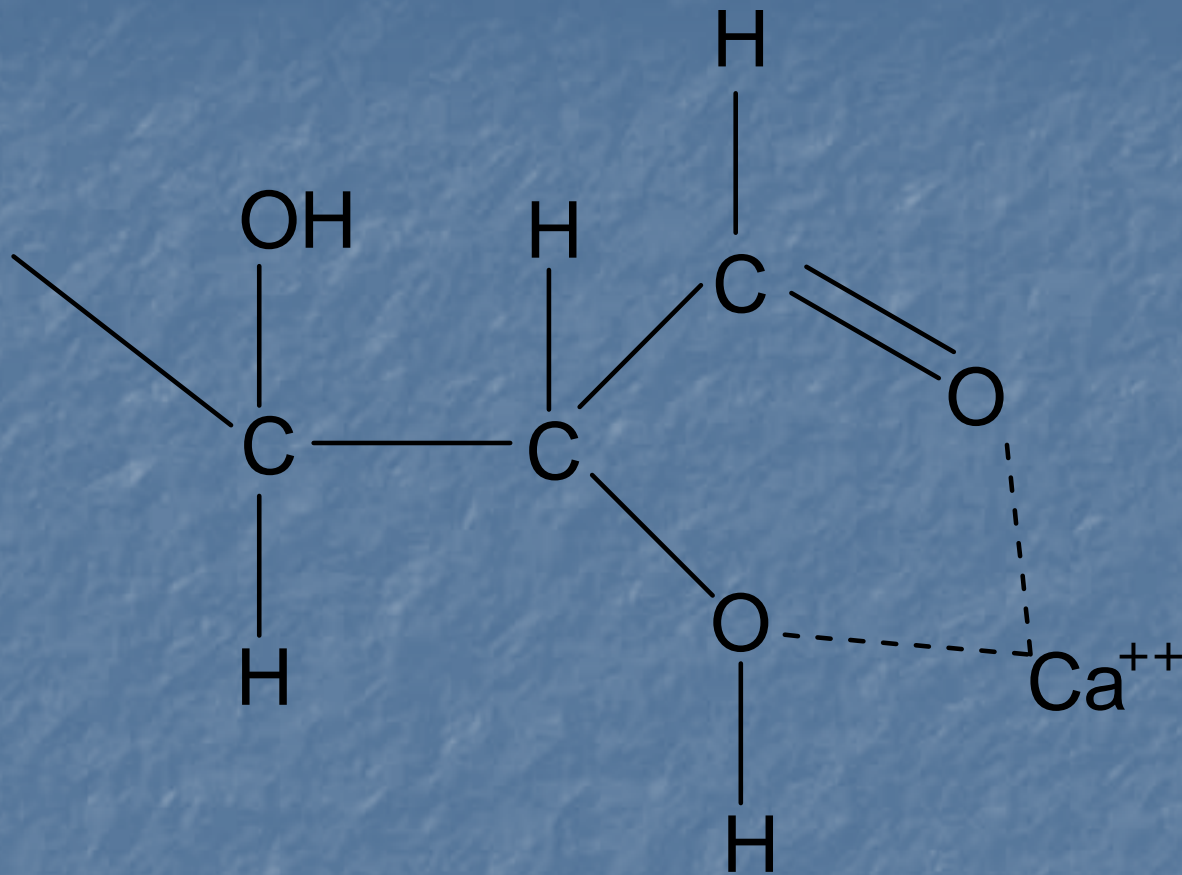


Fig 5 Metal-organic complex

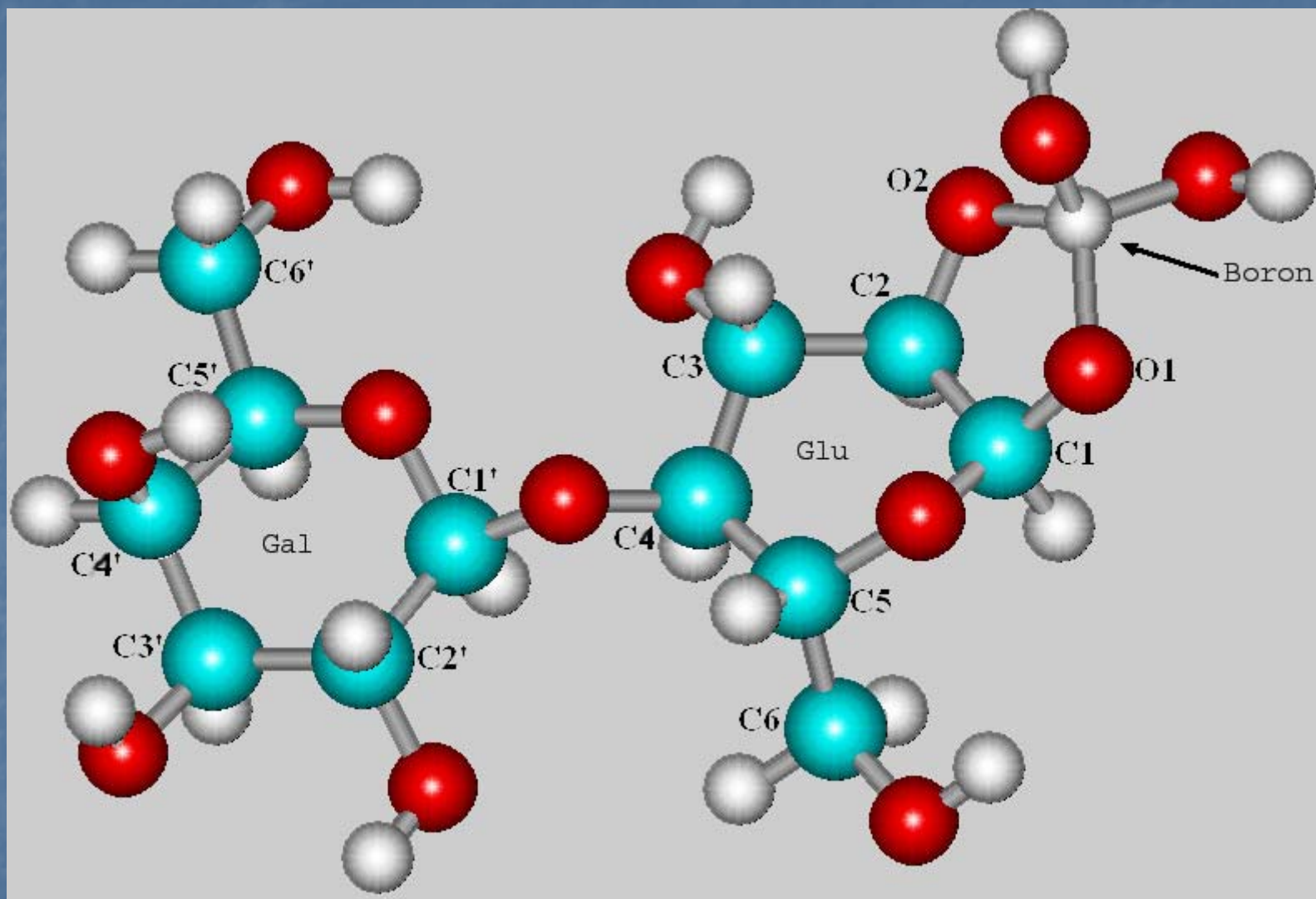


Figure 6 - Structure of complex tetrahydroxoborate-lactose

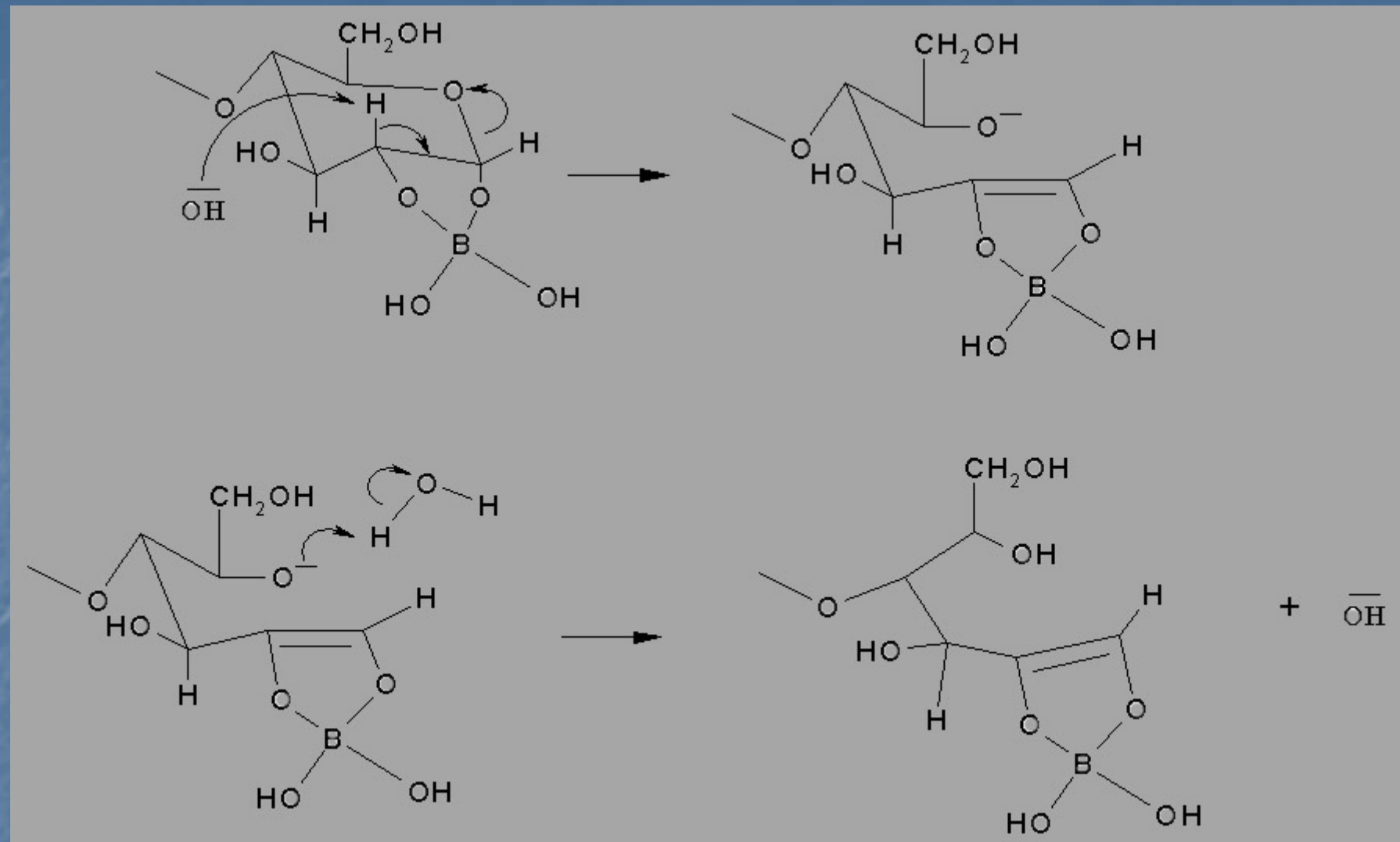


Fig. 7 - Possible isomerization mechanism of lactose at presence of a tetrahydroborate-ion

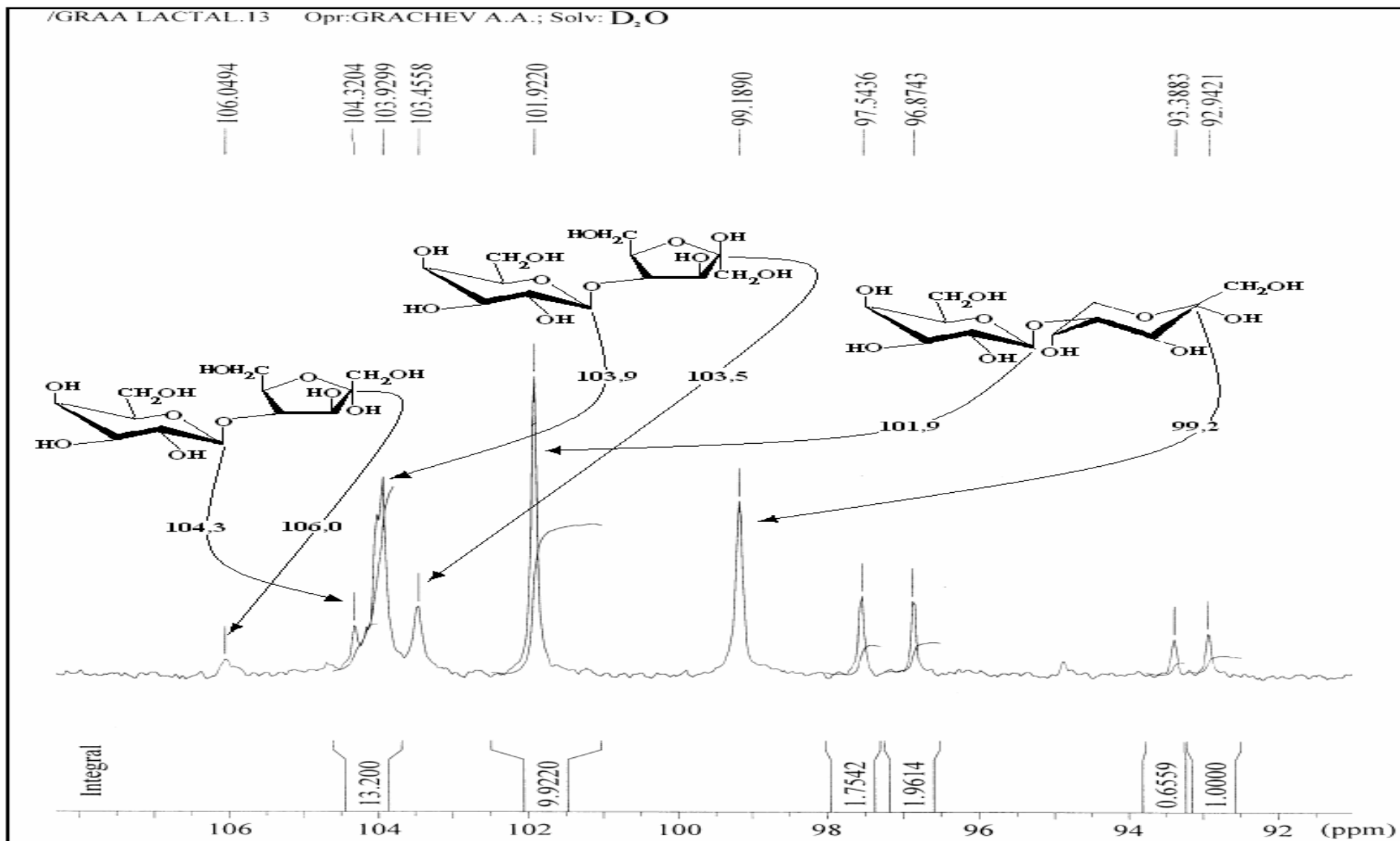


Figure 8 - Spectrum of the <sup>13</sup>C nuclear magnetic resonance of anomeric centers in the equilibrium lactulose solution