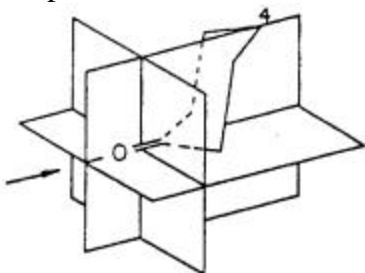


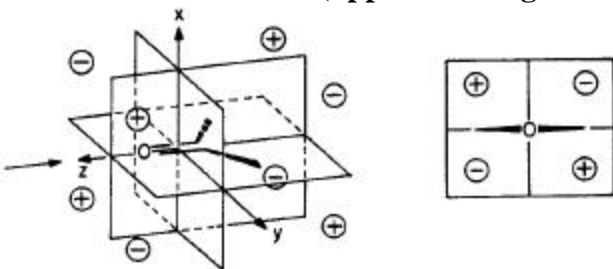
### 3. Sign of the CE and Octant Rule

according to Djerassi, 1960

- view ketone along the O=C bond (in the direction of the ring), upward position
- a Cartesian set through the molecule defines 8 sectors (octants): the origin is the C=O bond midpoint, the z-axis is collinear with the C=O bond

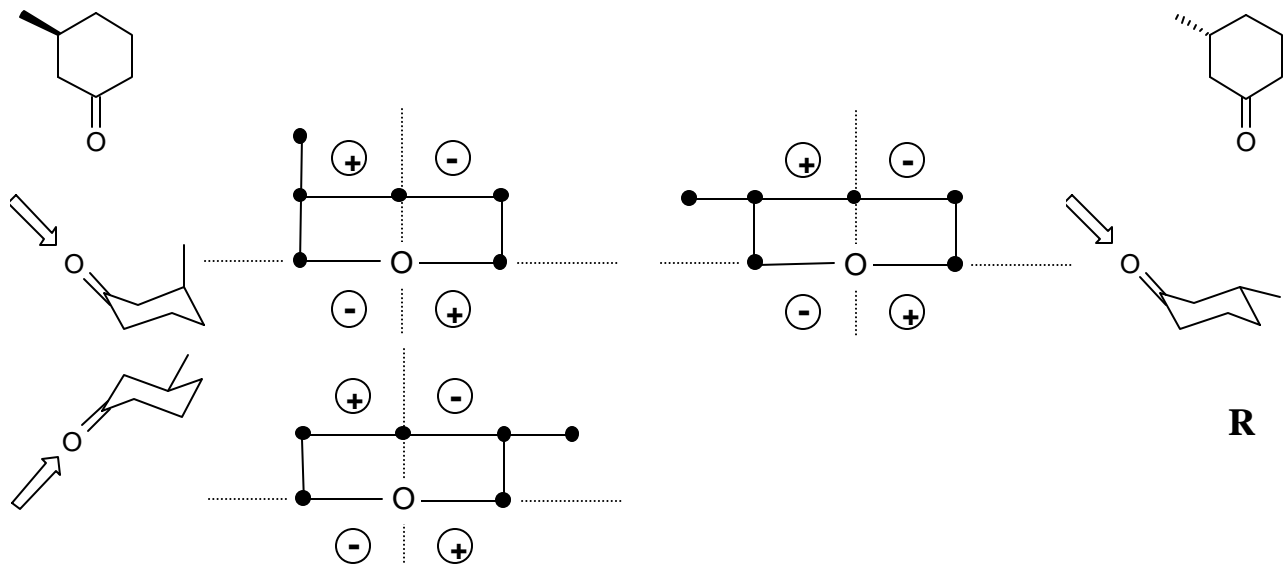


front and back octants (upper-front-right octant is positive, others alternate):

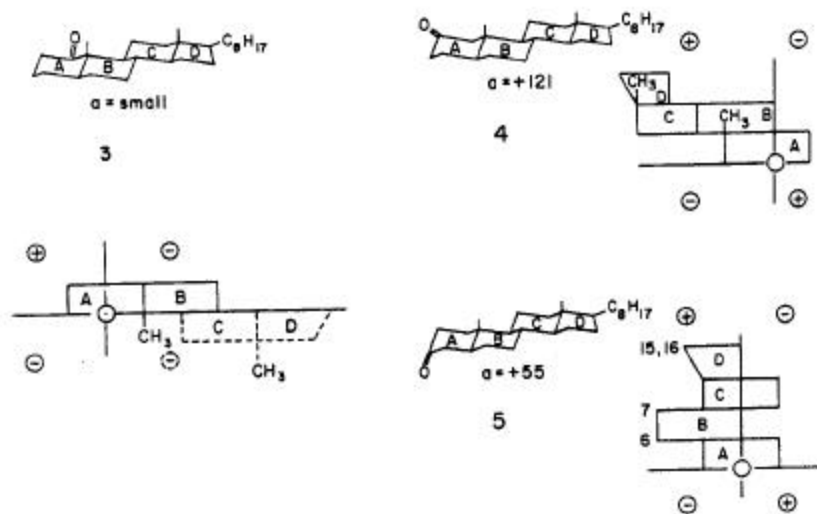


- three kinds of substituents:  
C, X: a substituent in a positive (negative) sector makes a positive (negative) contribution  
O, N: inverse behaviour  
substituents on or near nodes make no contribution

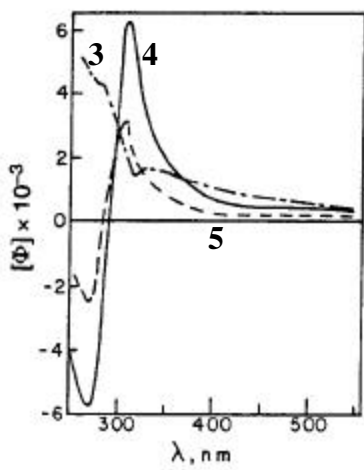
ex.: (+)-3-methylcyclohexanone exhibits a positive CE. Is it R or S configured?



Cholestanones: semiquantitative assessment of the CE (sign and magnitude)



ORD



CD

