The dependence of J on Δ_{ij} for complex **1** through distorting τ using the second or third way, respectively, which are shown in Figure 16.

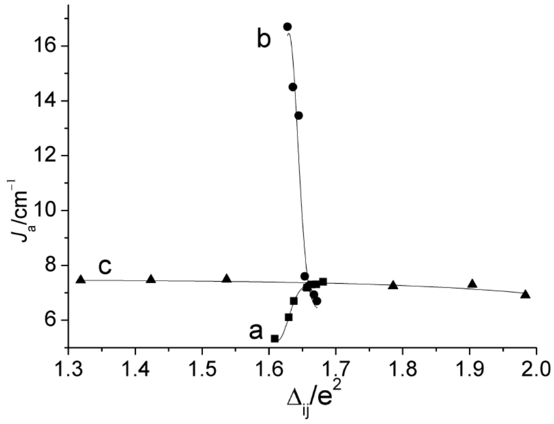

Figure 16. Dependence of the exchange coupling constants J_a on the Δ_{ij} for **1**: [a] distorting three τ using the second way (■); [b] distorting one τ using the second way (●); [c] distorting three τ using the third way (▲) .

When we change three τ of complex **1** using the second way, the variations in the calculated Δ_{ij} are small resulting in the small variations in J_a. However, the variations in the calculated Δ_{ij} corresponding to J_a are also small when we change one τ using the second way for **1**, but the variations in J_a are large (see Figure 11). The above results show that distorting one τ using the second way for **1** have a small influence on the overlap integrals S_{ij}, and which have no way to rationalize the variations in J. As our previous papers indicated,[25(a–b)] S_{ij} can not always be used to rationalize the variations in J especially when the magnetic interactions are ferromagnetic. When we decrease three τ using the third way, the calculated Δ_{ij} corresponding to J_a increase largely (see Figure 16) which should decrease J_a. However, Figure 12 shows that the variations in J_a for **1** are very small. The above result also shows that distorting τ using the third way has a large influence on S_{ij}, but a small on J_a because the variations in S_{ij} are no longer the dominant factor to influence J_a at this time.