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

![Figure 16](image)

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

When we change three $\tau$ of complex 1 using the second way, the variations in the calculated $\Delta_{ij}$ are small resulting in the small variations in $J_a$. However, the variations in the calculated $\Delta_{ij}$ corresponding to $J_a$ are also small when we change one $\tau$ using the second way for 1, but the variations in $J_a$ are large (see Figure 11). The above results show that distorting one $\tau$ 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 $\tau$ using the third way, the calculated $\Delta_{ij}$ 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 $\tau$ 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.