Supplementary Material for Perkin Transactions 1
This journal is © The Royal Society of Chemistry 2002

Supplementary data

Electronic Supplementary Information

Paper Ref.: B205613P

Title: Origins of stereoselectivity in the chelation-controlled addition of alkyl radicals to \( \alpha \)-methylene-\( \gamma \)-oxocarboxylic acid esters.

Hajime Nagano,* Satoko Toi, Mikako Matsuda, Tamano Hirasawa, Satomi Hirasawa and Tomoko Yajima

Department of Chemistry, Faculty of Science, Ochanomizu University, Otsuka, Bunkyo-ku, Tokyo 112-8610, Japan.


\[
\begin{align*}
51A-1 & \ (-236.6), \ 51A-2 \ (-235.3), \ 51A-3 \ (-234.5), \\
53A-1 & \ (-241.1), \ 53A-2 \ (-241.0), \ 53A-3 \ (-240.5) \\
54A-1 & \ (-184.7), \ 54A-2 \ (-183.4) \\
56B-1 & \ (-196.4) \\
57B-1 & \ (-261.5), \ 57B-2 \ (-260.5), \ 57B-3 \ (-260.0) \\
58B-1 & \ (-264.6), \ 58B-2 \ (-264.0), \ 58B-3 \ (-263.1) \\
59B-1 & \ (-146.4), \ 59B-2 \ (-146.2), \ 59B-3 \ (-135.4) \\
66B-1 & \ (-140.1), \ 66B-2 \ (-139.5) \\
67B-1 & \ (-216.3), \ 67B-2 \ (-216.1), \ 67B-3 \ (-216.0), \ 67B-4 \ (-215.9)
\end{align*}
\]

[2] Low energy conformers and their heats of formation (kcal mol\(^{-1}\)) for 46A (Fig. S1), 46B–46D (Fig. S2), 47A (Fig. S3), 48B (Fig. S4), 49B (Fig. S5), 50A/50B (Fig. S6), 51A-3 (Fig. S7), 52A (Fig. S8), 55B (Fig. S9), 68B (Fig. S10) and 69B (Fig. S11).

Global minimum energy conformers for the intermediate model in the ethyl...
Supplementary data

radical addition to compound 4 (Fig. S12).
Fig. S1  Low energy conformers of 46A and their heats of formation (kcal mol\(^{-1}\))

Supplementary data
Fig. S2  Low energy conformers of 46B, 46C and 46D and their heats of formation (kcal mol$^{-1}$)
Supplementary data

Fig. S3  Low energy conformers of 47A and their heats of formation (kcal mol$^{-1}$)

![Diagram of 47A with structures 47A-1, 47A-2, 47A-3, and 47A-4 showing their heats of formation: 47A-1 (-235.8), 47A-2 (-234.2), 47A-3 (-233.6), 47A-4 (-231.1)]
Fig. S4  Low energy conformers of 48B and their heats of formation (kcal mol$^{-1}$)
Supplementary data

Fig. S5  Low energy conformers of 49B and their heats of formation (kcal mol\(^{-1}\))

49B

49B-1 (-183.6)

49B-2 (-182.6)

49B-3 (-182.3)
Fig. S6  Low energy conformers of 50A and 50B and their heats of formation (kcal mol\textsuperscript{-1})
Supplementary data

Fig. S7  Low energy conformer 52A-3 and its heat of formation (kcal mol$^{-1}$)
Supplementary data
Supplementary data

Fig. S8  Low energy conformers of 52A and their heats of formation (kcal mol$^{-1}$)

52A

52A-3 (-226.6)

52A-1 (-227.5)  52A-2 (-226.9)
Supplementary data

Fig. S9  Global minimum energy conformers of 55B and its heat of formation (kcal mol$^{-1}$)

55B

55B-1 (-192.0)
Supplementary data

Fig. S10  Low energy conformers of 68B and their heats of formation (kcal mol⁻¹)

\[ \omega = \text{-120.1°} \]
\[ \theta = \text{107.0°} \]
\[ \text{68B-3 (-210.6)} \]

\[ \omega = \text{-120.1°} \]
\[ \text{68B-1 (-211.4)} \]

\[ \omega = \text{-124.1°} \]
\[ \theta = \text{107.6°} \]
\[ \text{68B-2 (-210.9)} \]

\[ \omega = \text{-119.7°} \]
\[ \theta = \text{110.1°} \]
\[ \text{68B-4 (-210.4)} \]
Fig. S11 Global minimum conformer 69B-1 and its heat of formation (kca mol$^{-1}$)
Fig. S12. Global minimum energy conformers for the model in the ethyl radical addition to compound 4

-221.8 kcal mol\(^{-1}\)

\(\omega = -93.8^\circ\)