Supplementary Material for Perkin Transactions 1

Supplementary data

Electonic Supplementary Information

Paper Ref.: B205613P

Title : Origins of stereoselectivity in the chelation-controlled addition of alkyl radicals to α-methylene-γ-oxycarboxylic acid esters.

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[1] The heats of formation (kcal mol^{-1}) for **51**, **53**–**59**, **66**, and **67**.

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)

[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

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radical addition to compound **4** (Fig. S12).

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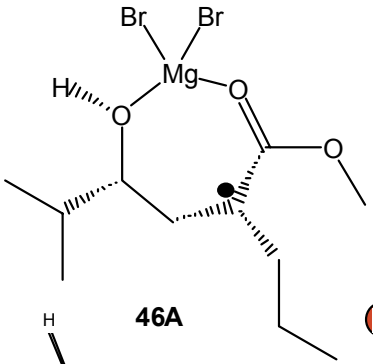
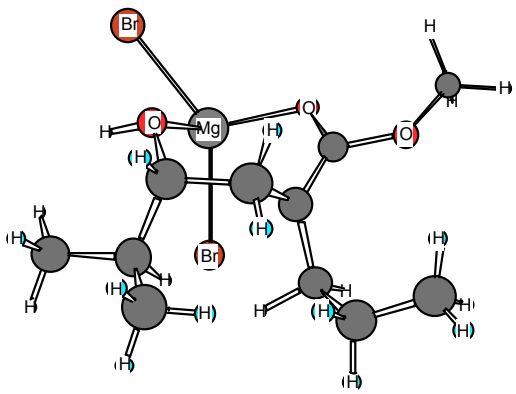
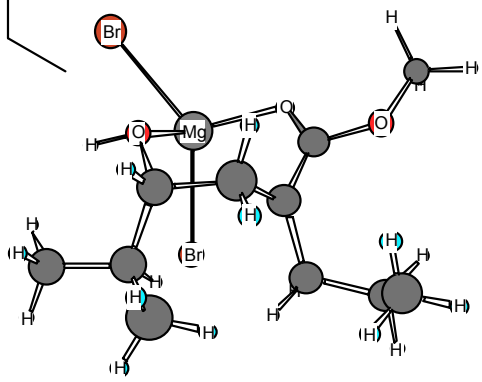
Fig. S1 Low energy conformers of **46A** and their heats of formation (kcal mol^{-1})



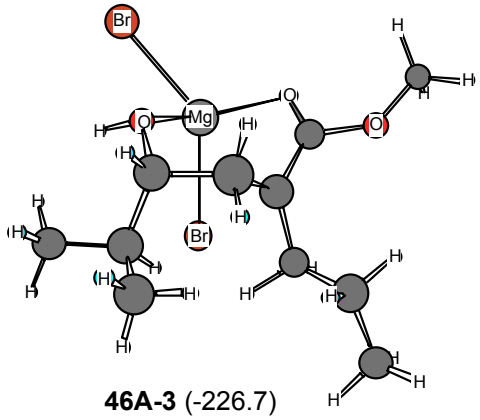
46A



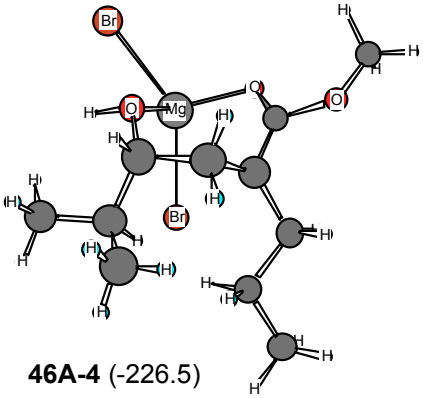
46A-5 (-225.9)



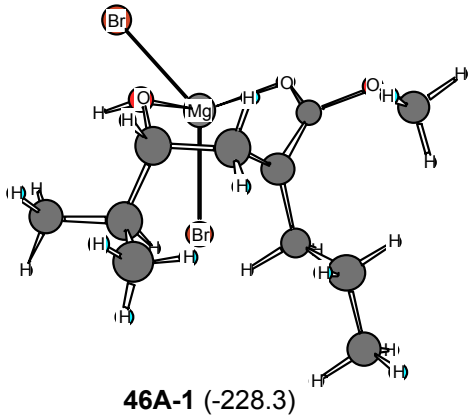
46A-6 (-225.9)



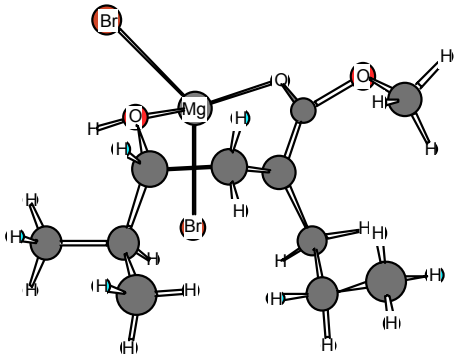
46A-3 (-226.7)



46A-4 (-226.5)



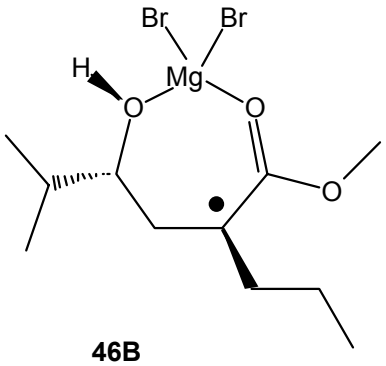
46A-1 (-228.3)



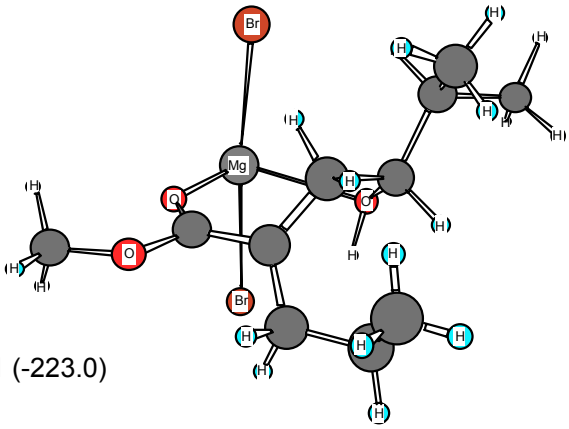
46A-2 (-227.6)

Supplementary data

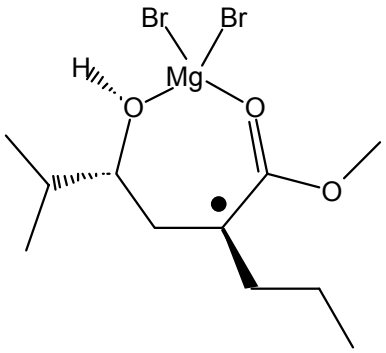
Fig. S2 Low energy conformers of **46B**, **46C** and **46D** and their heats of formation (kcal mol^{-1})



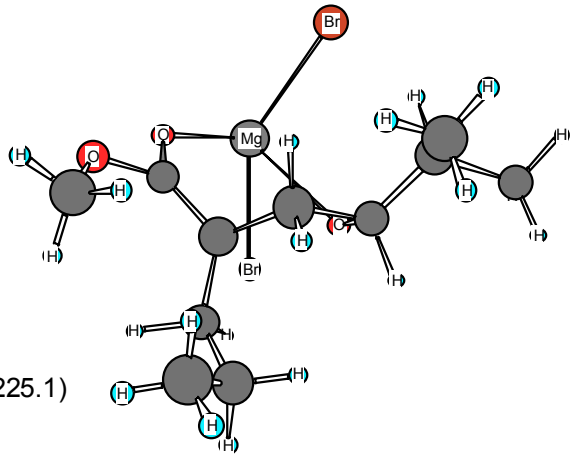
46B



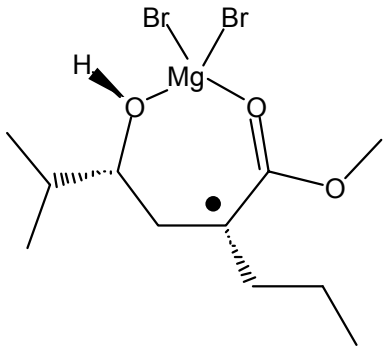
46B-1 (-223.0)



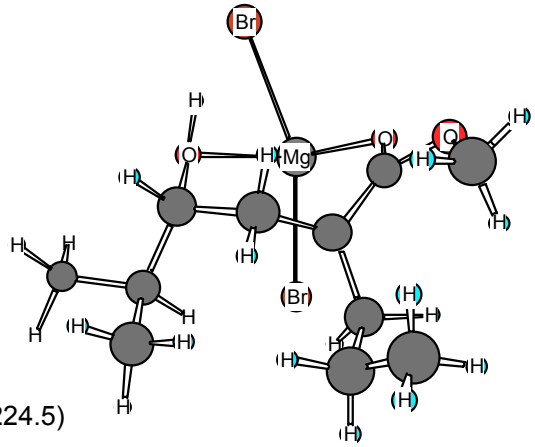
46C



46C-1 (-225.1)



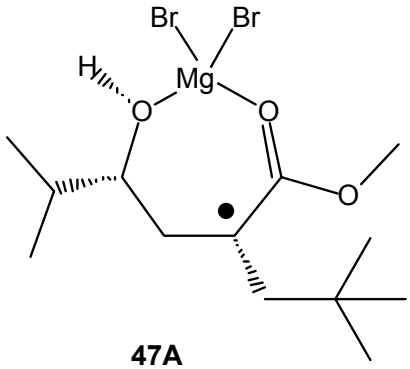
46D



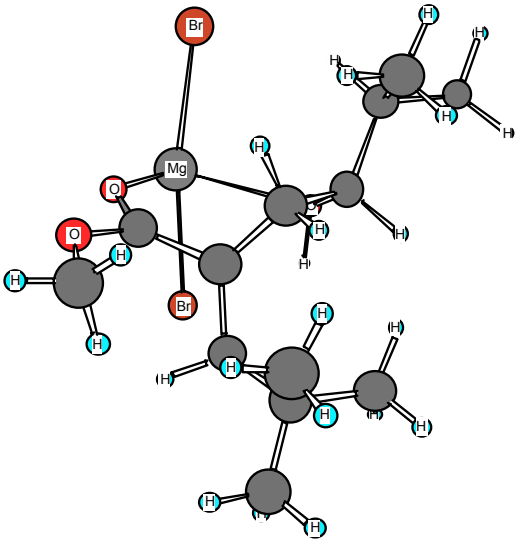
46D-1 (-224.5)

Supplementary data

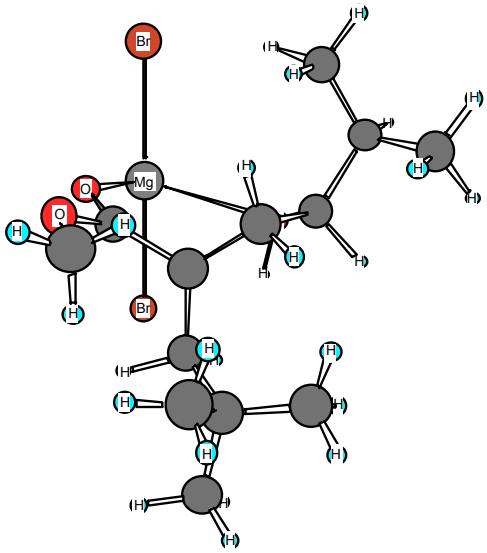
Fig. S3 Low energy conformers of **47A** and their heats of formation (kcal mol^{-1})



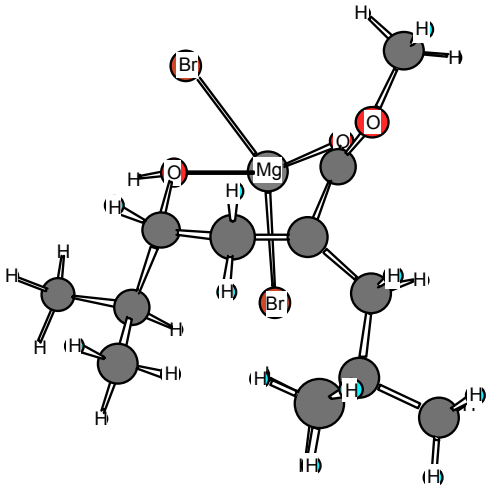
47A



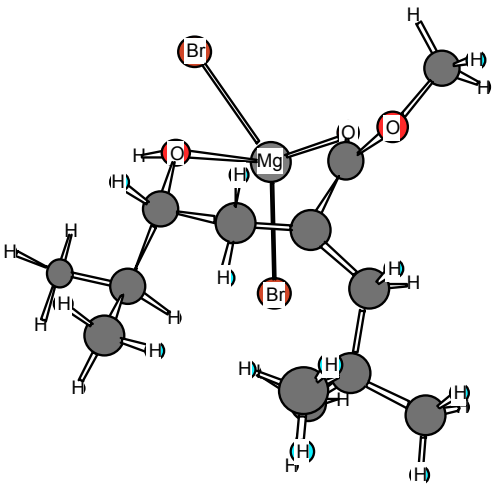
47A-3 (-233.6)



47A-4 (-231.1)



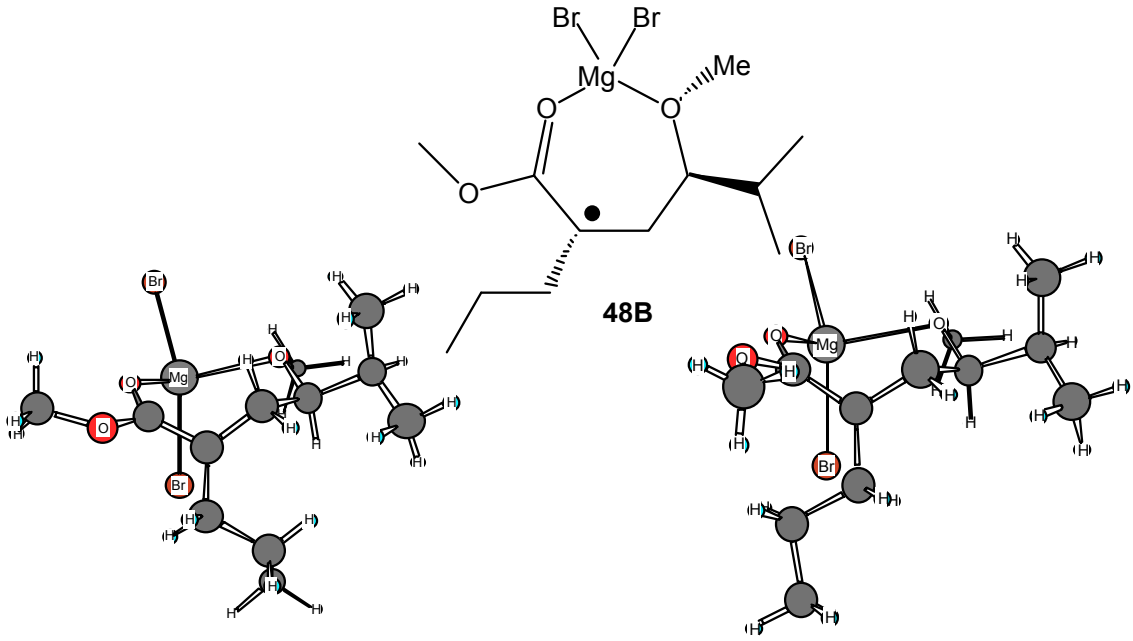
47A-1 (-235.8)



47A-2 (-234.2)

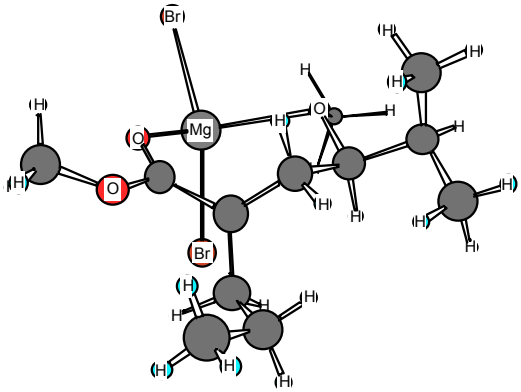
Supplementary data

Fig. S4 Low energy conformers of **48B** and their heats of formation (kcal mol^{-1})

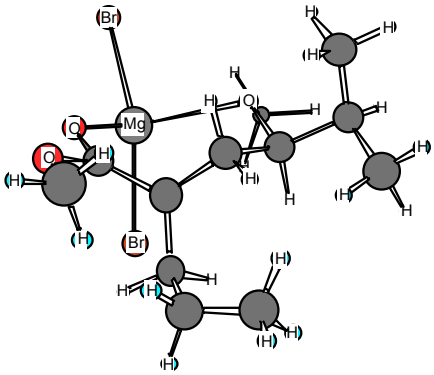


48B-5 (-223.2)

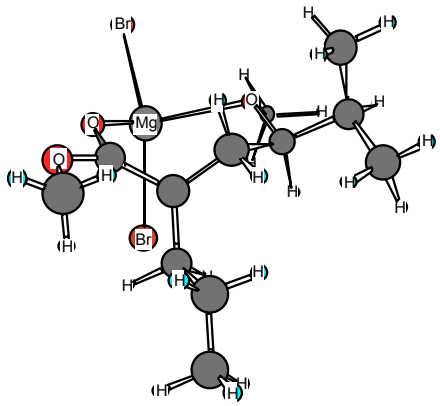
48B-6 (-223.0)



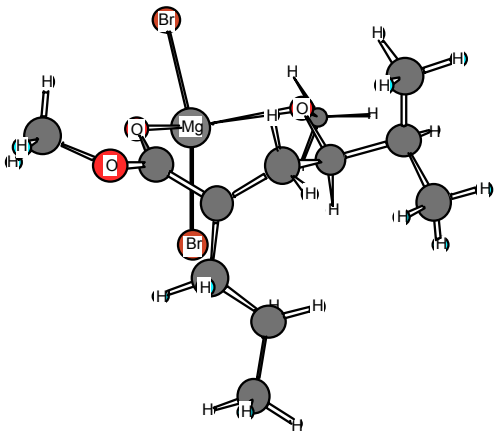
48B-3 (-223.4)



48B-4 (-223.2)



48B-1 (-224.4)



48B-2 (-224.0)

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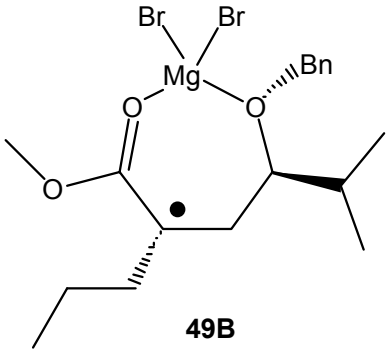
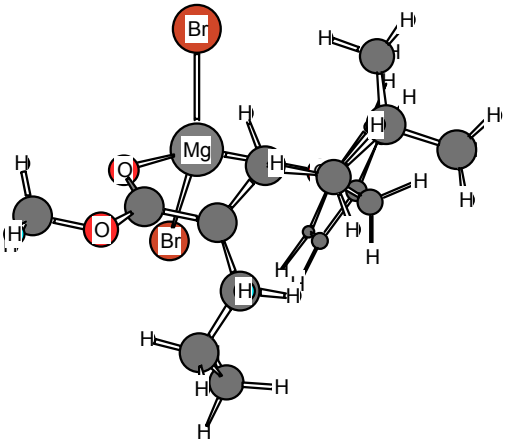
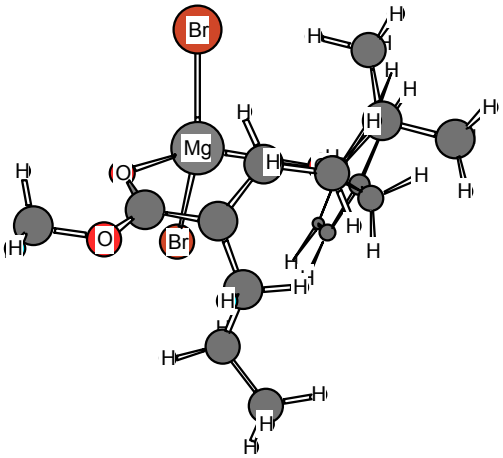
Fig. S5 Low energy conformers of **49B** and their heats of formation (kcal mol^{-1})



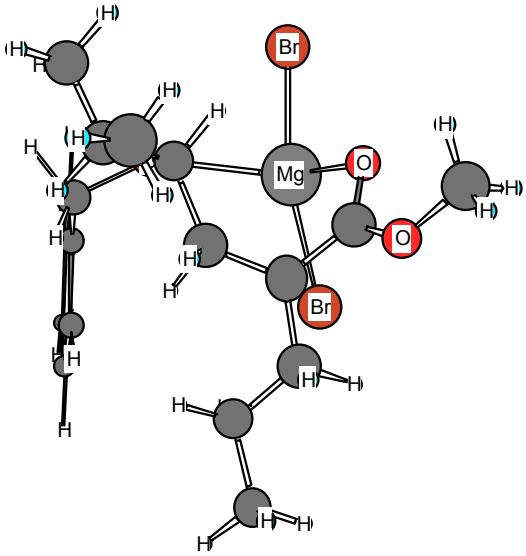
49B



49B-3 (-182.3)



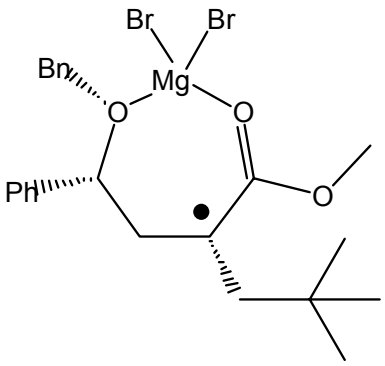
49B-1 (-183.6)



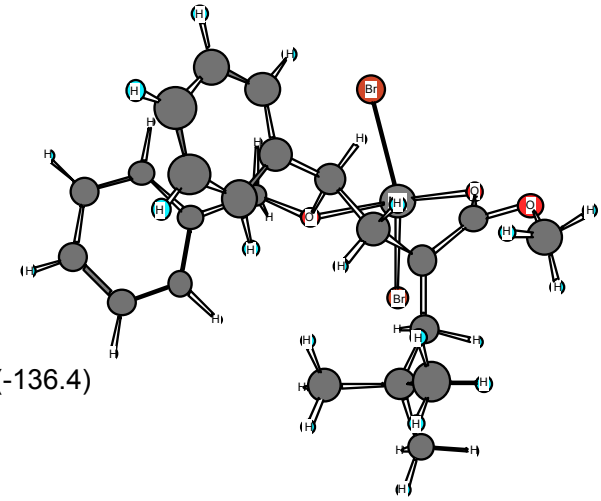
49B-2 (-182.6)

Supplementary data

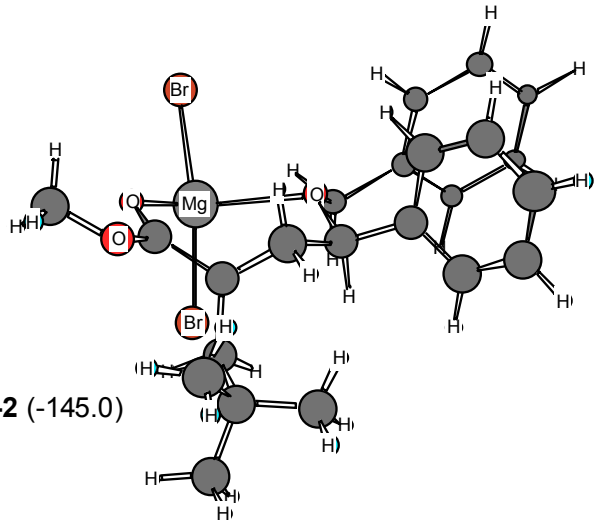
Fig. S6 Low energy conformers of **50A** and **50B** and their heats of formation (kcal mol^{-1})



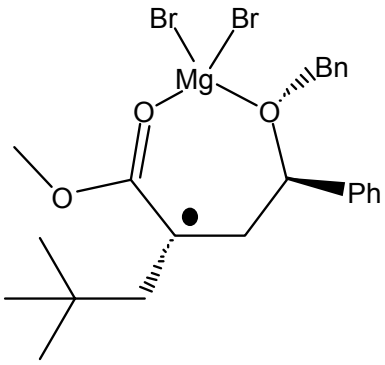
50A



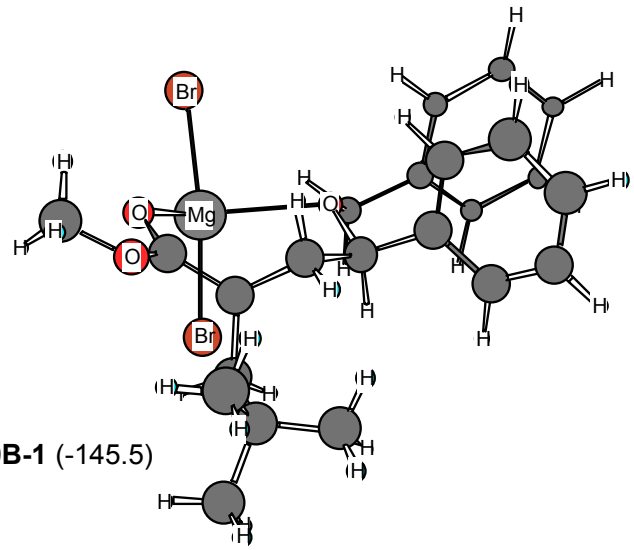
50A-1 (-136.4)



50B-2 (-145.0)



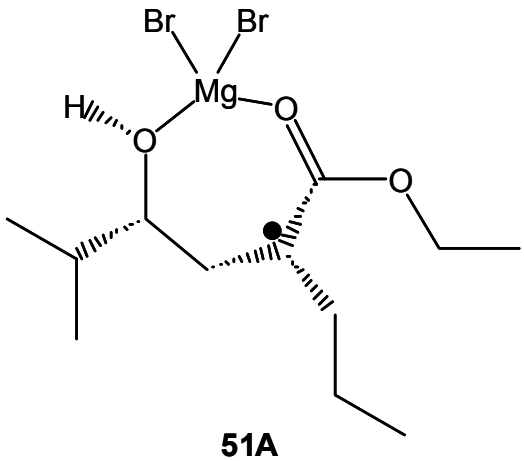
50B



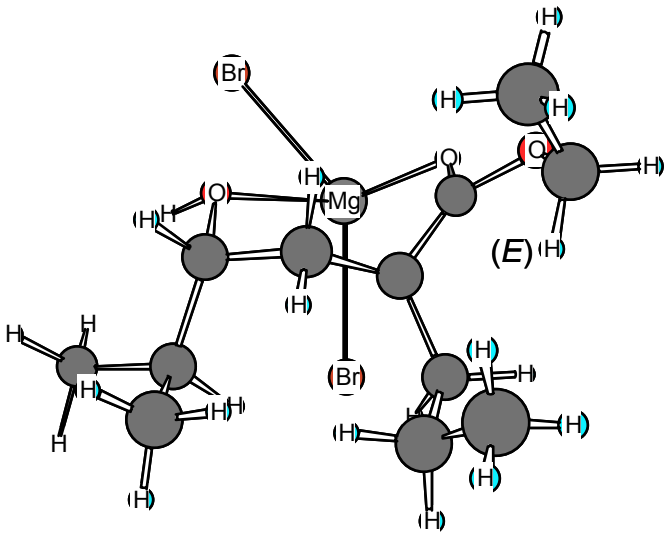
50B-1 (-145.5)

Supplementary data

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



51A



51A-3 (-234.5)

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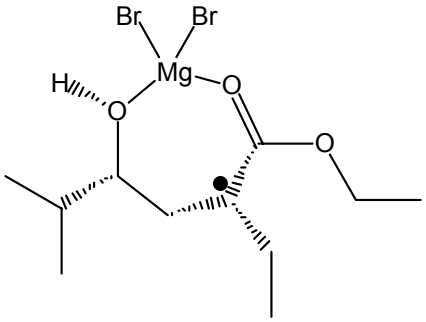
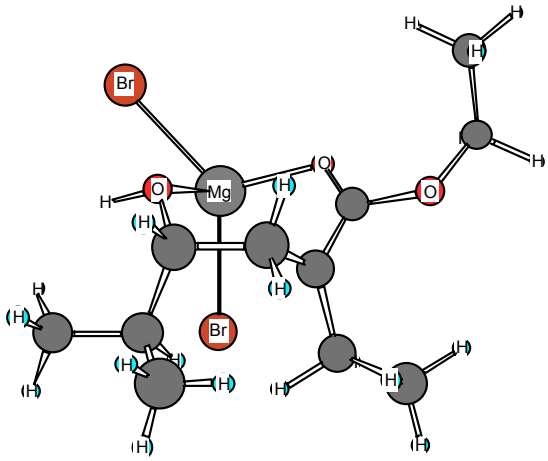
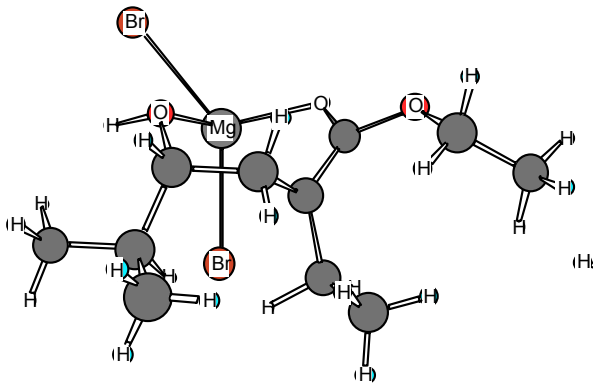
Fig. S8 Low energy conformers of **52A** and their heats of formation (kcal mol^{-1})



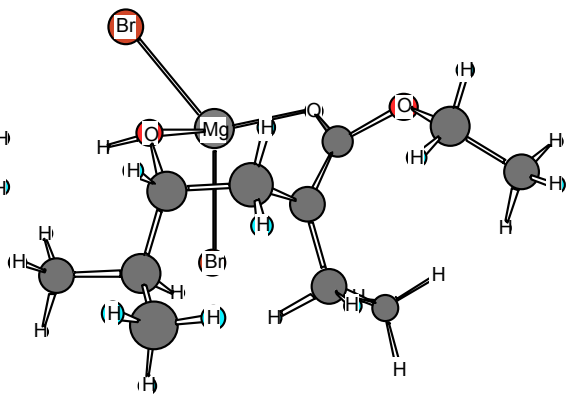
52A



52A-3 (-226.6)



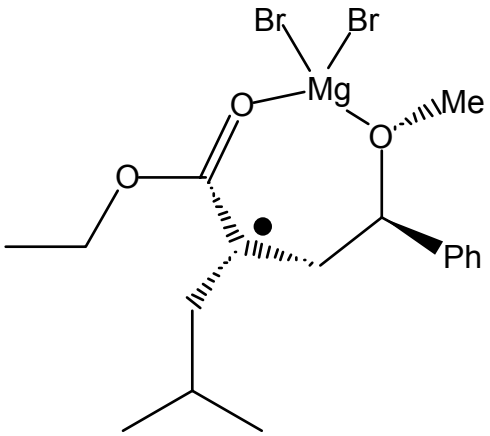
52A-1 (-227.5)



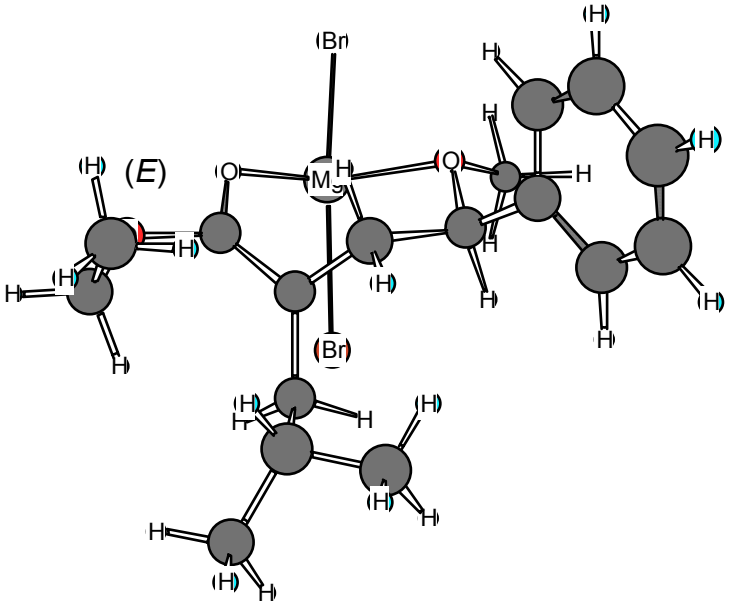
52A-2 (-226.9)

Supplementary data

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



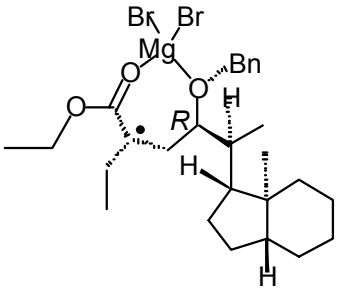
55B



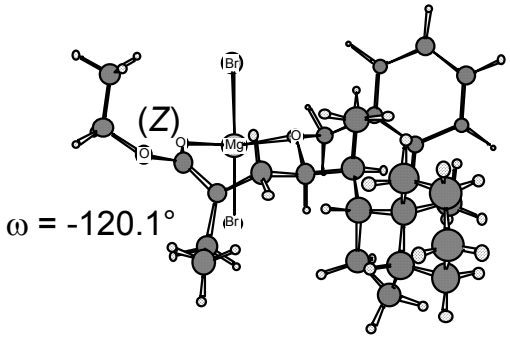
55B-1 (-192.0)

Supplementary data

Fig. S10 Low energy conformers of 68**B** and their heats of formation (kcal mol^{-1})

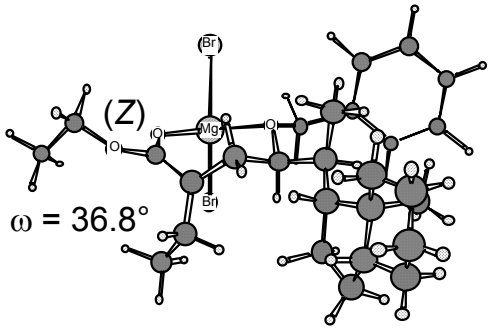


68B



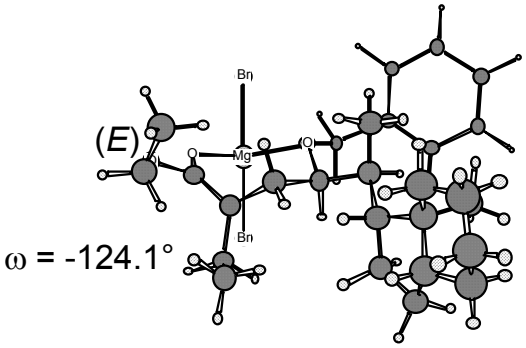
θ = 107.0°

68B-3 (-210.6)



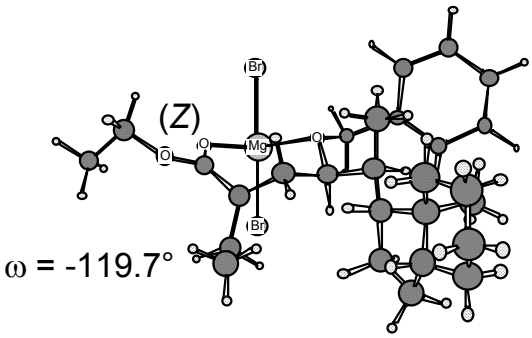
θ = 110.1°

68B-4 (-210.4)



θ = 107.6°

68B-1 (-211.4)



θ = 108.2°

68B-2 (-210.9)

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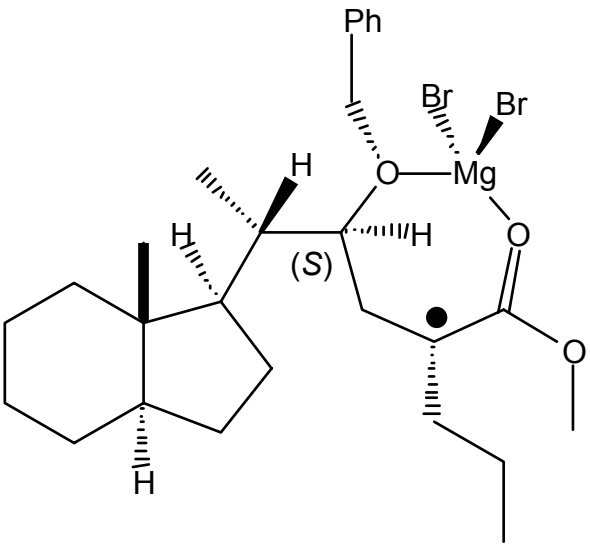
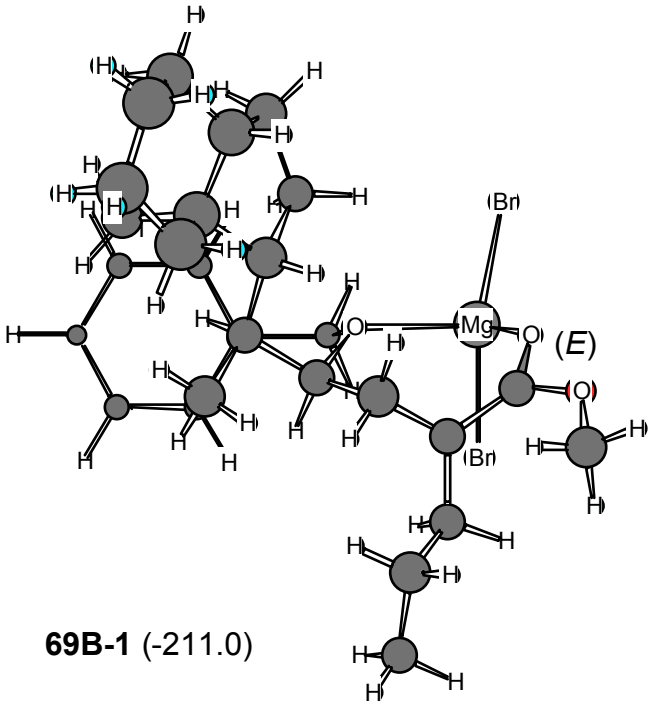
Fig. S11 Global minimum conformer **69B-1** and its heat of formation (kca mol^{-1})





69B-1 (-211.0)

Supplementary data

Fig. S12. Global minimum energy conformers for the model in the ethyl radical addition to compound **4**