

**Supporting Information for  
Grignard reagents in solution:  
Theoretical study of the equilibria  
and the reaction with a carbonyl compound  
in diethyl ether solvent**

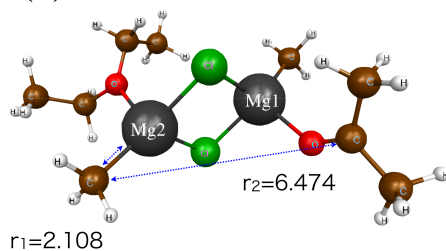
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Table SI 1: Potential parameters for solvent and solute molecules.

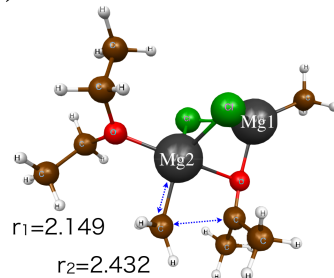
Site (s)	Solvent		
	$\sigma_{ss}$ (Å)	$\epsilon_{ss}$ kcal/mol	$Q_s$ ( $e$ )
O	3.000	0.170	-0.50
CH <sub>2</sub>	3.800	0.118	0.25
CH <sub>3</sub>	3.905	0.175	0.00
	Solute		
	$\sigma_{ss}$ (Å)	$\epsilon_{ss}$ kcal/mol	$Q_s$ ( $e$ )
Mg	3.0000	0.8947	
Cl	3.4709	0.2650	
Br	3.9556	0.3200	
C	3.4000	0.1094	
C (in acetone, attatched to O)	3.4000	0.0860	
H	2.6500	0.0157	
O (in acetone)	2.9600	0.2100	
O (in Et <sub>2</sub> O)	3.0000	0.1700	
CH <sub>2</sub> (in Et <sub>2</sub> O)	3.8000	0.1180	
CH <sub>3</sub> (in Et <sub>2</sub> O)	3.9050	0.1750	

Figure SI 1: Geometries of (a) reactant, (b) transition state, (c) intermediate, and (d) product for the reaction of cyclic dimer with acetone. Distances are in Å.

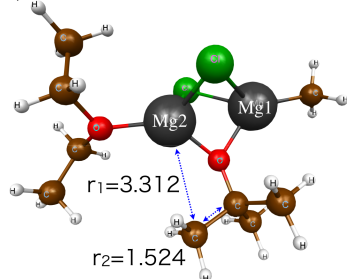
(a) Reactant



(b) Transition State



(c) Intermediate



(d) Product

