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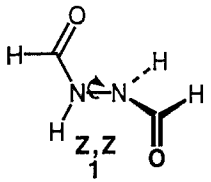
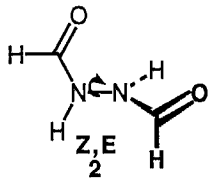
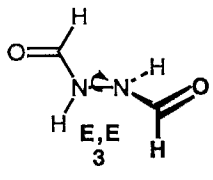
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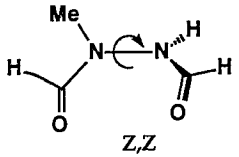
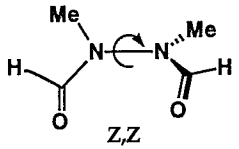
Total energies for rotamers of **1-5** in Hartrees

Structure		θ	HF/6-31G*	rel. E[a]	HF/6-31+G**	rel. E[a]	MP2/6-31+G**	rel. E[a]
	1 a	min	-336.663943	0.0	-336.687125	0.0	-337.646677	0.0
		45	-336.647317		-336.670736			
	**1 b**	0	-336.632557	19.7	-336.654264	20.6	-337.619551	17.0
		-45	-336.647317		-336.670737			
		-90	-336.663298		-336.686475			
		-135	-336.661076		-336.684558			
	1 c	180	-336.658839	3.2	-336.683408	2.3	-337.645326	0.8
		135	-336.661076		-336.684558			
	2 a	min	-336.663497	0.0	-336.686376	0.0	-337.645022	0.0
		45	-336.652985		-336.675977			
	**2 b**	0	-336.643228	12.7	-336.665960	12.8	-337.627795	10.8
		-45	-336.652985		-336.675977			
		-90	-336.663494		-336.686370			
		-135	-336.657321		-336.680192			
	2 c	180	-336.648025	9.7	-336.671334	9.4	-337.633432	7.3
		135	-336.657321		-336.680192			
	3 a	min	-336.663910	0.0	-336.687007	0.0	-337.644668	0.0
		45	-336.651451		-336.674464			
	**3 b**	0	-336.636241	17.4	-336.658770	17.7	-337.621089	14.8
		-45	-336.651451		-336.674464			
		-90	-336.663907		-336.687005			
		-135	-336.651937		-336.675011			
	3 c	180	-336.642172	13.6	-336.664771	13.9	-337.625520	12.0
		135	-336.651937		-336.675012			

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Supplemental Material

Total energies (continued)

Structure		θ	HF/6-31G*	rel. E[a]	HF/6-31+G**	rel. E[a]	MP2/6-31+G**	rel. E[a]
 Z,Z	**4 a**	min			-375.718539	0.0		
	4 c	180			-375.707368	7.0		
 Z,Z	**5 a**	min			-414.749161	0.0		
	5 c	180			-414.718767	19.1		

(a) Energies relative to the minimum energy for **1-5** in kcal/mol.

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