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Regioselective Nucleophilic Aromatic Substitution reaction of 5,7-Dinitroquinazoline-4-one and 5,7-Dinitroquinazoline-4-thione with Methylamine: A Mechanistic Consideration

Amritpal Singh,[a] Neetu Goel*[a]

[a]Department of Chemistry & Centre of Advanced Studies in Chemistry, Panjab University, Chandigarh-160014, India
Fax: 0172-2545074 Phone No +91-9815970112
* corresponding author E-mail: neetugoel@pu.ac.in

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Optimized Structure	B3LYP		B3PW91	
	Gas Phase			
	Gibbs free energies (a.u.)	Relative Free Energies (kcal/mol)	Gibbs free energies (a.u.)	Relative Free Energies (kcal/mol)
R	-1076.5198	0.00	-1076.1147	0.00
RP1	-1076.5108	5.65	-1076.1053	5.89
RP2	-1076.5134	4.02	-1076.1066	5.08
TS1	-1076.4492	44.31	-1076.0470	42.48
TS2	-1076.4771	26.75	-1076.0754	24.66
P1	-1076.5301	-6.46	-1076.1232	-5.33
P2	-1076.5487	-18.14	-1076.1414	-16.75
	Solvent Phase			
R’	-1076.5461	0.00	-1076.1409	0.00
RP1’	-1076.5343	7.40	-1076.1283	8.88
RP2’	-1076.5338	7.72	-1076.1268	7.91
TS1’	-1076.4912	34.75	-1076.0893	32.37
TS2’	-1076.5026	27.30	-1076.1000	25.66
P1’	-1076.5586	-7.82	-1076.1523	-7.15
P2’	-1076.5679	-13.66	-1076.1609	-12.55

Table 1 Comparison of the energies using B3LYP and B3PW91 functionals in gas phase and solvent phase (ethanol) without dispersion effects for the reaction of methylamine with 5,7-dinitroquinazoline-4-one.

Optimized Structure	B3LYP-D			
	Gas Phase		Solvent Phase	
	Gibbs free energies (a.u.)	Relative Free Energies (kcal/mol)	Gibbs free energies (a.u.)	Relative Free Energies (kcal/mol)
R/R’	-1076.5557	0.00	-1076.5823	0.00
RP1/RP1’	-1076.5517	2.50	-1076.5747	4.77
RP2/RP2’	-1076.5546	0.69	1076.57770	3.33
TS1/TS1’	-1076.4971	36.77	-1076.5402	26.42
TS2/TS2’	-1076.5268	18.14	-1076.5534	18.14
P1/P1’	-1076.5727	-10.67	-1076.6014	-11.98
P2/P2’	-1076.5922	-22.90	-1076.6115	-18.32

Table 2 Energies using B3LYP-D functional in gas phase and solvent phase (ethanol) with dispersion effects for the reaction of methylamine with 5,7-dinitroquinazoline-4-one.

Optimized Structure	B3LYP-D			
	Gas Phase		Solvent Phase	
	Gibbs free energies (a.u.)	Relative Free Energies (kcal/mol)	Gibbs free energies (a.u.)	Relative Free Energies (kcal/mol)
R1/R1’	-1399.5062	0.00	-1399.5341	0.00
RP3/RP3’	-1399.5042	1.26	-1399.5287	3.39
RP4/RP4’	-1399.5070	-0.50	-1399.5298	2.70
TS3/TS3’	-1399.4489	35.95	-1399.4949	24.60
TS4/TS4’	-1399.4817	15.37	-1399.5080	16.38
P3/P3’	-1399.5250	-11.80	-1399.5556	-13.49
P4/P4’	-1399.5441	-23.16	-1076.5632	-18.26

Table 3 Energies using B3LYP-D functional in gas phase and solvent phase (ethanol) with dispersion effects for the reaction of methylamine with 5,7-dinitroquinazoline-4-thione.