Supporting Information

A DFT assisted mechanism evolution of the Carbonylation of Ethylene glycol to ethylene carbonate by urea over $Zn(NCO)_2.(NH_3)_2$ catalyst.

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Table-S1. Optimized geometrical parameter of $Zn(NCO)_2$ $2NH_3$.

S.No.	Atom	Calculated Bond Length	Atoms	Calculated Bond Angle
1	$r_{Zn\text{-}NH3}$	2.106	$\beta_{N2\text{-}Zn1\text{-}N3}$	127.2
2	$r_{Zn\text{-}NH3}$	2.108	$\beta_{N2\text{-}Zn1\text{-}N'8}$	102.8
3	$r_{Zn\text{-}NCO}$	1.895	$\beta_{N2\text{-}Zn1\text{-}N'12}$	102.7
4	$r_{Zn\text{-}NCO}$	1.894	$\beta_{Zn1\text{-}N2\text{-}C5}$	174.7
5	r_{NH}	1.018	$\beta_{N3\text{-}Zn1\text{-}N'8}$	102.7
6	r_{NH}	1.019	$\beta_{NC3\text{-}Zn1\text{-}N'12}$	102.8
7	r_{NH}	1.018	$\beta_{Zn1\text{-}NC3\text{-}C4}$	174.7
8	r_{NH}	1.019	$\beta_{N'8\text{-}Zn1\text{-}N'12}$	120.5
9	r_{NH}	1.019	$\beta_{Zn1\text{-}N'8\text{-}H9}$	103.4
10	r_{NH}	1.017	$\beta_{Zn1\text{-}N'8\text{-}H10}$	103.5
11	$r_{N=C}$	1.225	$\beta_{Zn1\text{-}N'8\text{-}H11}$	122.1
12	$r_{N=C}$	1.225	$\beta_{Zn1\text{-}N'12\text{-}H13}$	122.1
13	$r_{C=O}$	1.223	$\beta_{Zn1\text{-}N'12\text{-}H14}$	103.4
14	$r_{C=O}$	1.223	$\beta_{Zn1\text{-}N'12\text{-}H15}$	103.5
15			$\beta_{N2\text{-}C5\text{-}O7}$	179.2
16			$\beta_{N3\text{-}C4\text{-}O6}$	179.2
17			$\beta_{H9\text{-}N8\text{-}H10}$	109.4
18			$\beta_{H9\text{-}N8\text{-}H11}$	109
19			$\beta_{H10\text{-}N8\text{-}H11}$	109
20			$\beta_{H13\text{-}N12\text{-}H14}$	109
21			$\beta_{H13\text{-}N12\text{-}H15}$	109
22			$\beta_{H14\text{-}N12\text{-}H15}$	109.4

r =Bond length in Angstrom, Beta=Bond angle in degree, N="N" atom of NCO group, N'="N"atom of NH_3 group

Table-S2. Mullikan atomic charges in cis-cis and cis-trans conformers of 2-HEC.

S.No.	Atom	2-HEC (S-Trans)	2-HEC (S-cis)
1	Amino “N”	-0.733	-0.819
2	Carbonyl “C”	0.686	0.621
3	Hydroxyl “O”	-0.605	-0.633
4	Hydroxyl “H”	0.379	0.417

Table-S3. Charge distribution in HNCO, EG and -NCO group in catalyst.

S.No.	Atom	HNCO	EG	NCO^- in catalyst
1	H	0.364	0.368	
2	N	-0.474		-.732
3	C	0.416	-0.093	.651
4	O	-0.306	-0.617	-512

Table-S4. Charge distribution in associative mechanism when 2-HEC adsorbed via both ammonia group of the catalyst.

S.No.	Atom	2-HEC	2-HEC on Catalyst Via NH_3
1	Amino "N"	-0.723	-0.704
2	Carbonyl "C"	0.683	0.726
3	Hydroxyl "O"	-0.618	-0.637
4	Hydroxyl "H"	0.365	0.410

Table-S5 The electronic energies of optimized structure of 2-HEC adsorbed through different functional groups.

S.No.	Adsorption via Functional Group Atom	Energy of optimized Geometry (a.u.)	Dipole Moment (Debye)
1	Amino "N"Atom	-2570.66940275	4.9496
2	Carbonyl "O"Atom	-2570.68679039	9.9923
3	Hydroxyl "O"Atom	-2570.67393107	11.1311
4	Bidentate	-2514.1040531	7.3975

Table-S6 The charge distributions on various atoms in different mode of adsorptions.

Atom	2-HEC (Gaseous Phase)		2-HEC (Adsorbed Via Ammino N site)		2-HEC (Adsorbed Via Carbonyl O site)		2-HEC (Adsorbed Via Hydroxy O site)		2-HEC (Adsorbed as bidentate ligand)
	Trans	Cis	Trans	Cis	Trans	Cis	Trans	Cis	
N(Amino)	-0.733	-0.671	-0.892	-0.948	-0.452	-0.635	-0.727	-0.766	-0.815
C(Carbonyl)	0.686	0.707	0.683	0.702	0.613	0.768	0.681	0.556	0.672
O(Carbonyl)	-0.425	-0.465	-0.404	-0.44	-0.565	-0.565	-0.411	-0.366	-0.362
O(Alkoxy)	-0.524	-0.503	-0.451	-0.48	-0.332	-0.482	-0.536	-0.473	-0.484
C(Alkyl)	-0.057	-0.107	-0.208	-0.018	-0.116	-0.052	-0.054	-0.072	0.083
C(Alkyl)	-0.021	-0.081	-0.083	-0.216	-0.014	-0.087	-0.023	-0.051	0.008
O(Hydroxy)	-0.605	-0.568	-0.578	-0.561	-0.398	-0.633	-0.678	-0.688	-0.684

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