Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
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Supplementary Informations

Table S1 Main geometrical parameters of the GLY1 isomer of isolated glycine. Semi-Experimental parameters have been reported with the same number of decimals as in the original work [32]. Asterisks indicate data constrained to CCSD(T) values during the fitting procedure.

Equilibrium parameters

Atom labels	Double Zeta		Triple Zeta			Semi-Exp.
	B3LYP/ aug-N07D	MP2/ DZP[a]	B3LYP/ TZ2P[b]	MP2/ 6-311++G** [c]	CCSD(T)/ cc-pVTZ[d]	(Fit 2)[d]
bond lengths (Å)						
N-H2	1.017	1.016	1.012	1.014	1.012	1.0065
N-C2	1.450	1.455	1.451	1.447	1.446	1.441
C2-H4	1.097	1.093	1.091	1.094	1.088	1.0907
C1-C2	1.524	1.524	1.522	1.519	1.511	1.511
C1-O1	1.356	1.362	1.356	1.356	1.349	1.353
O1-H1	0.971	0.973	0.968	0.968	0.966	0.966*
O2-N	2.880	-	2.867	-	-	-
C1-O2	1.209	1.221	1.204	1.209	1.204	1.207
angles (°)						
H2-N-H3	105.7	-	105.7	106.2	104.98	104.98*
H2-N-C2	110.2	-	109.9	110.2	-	-
N-C2-C1	115.9	115	115.5	115.6	115.2	115.4
H4-C2-H5	105.5	-	105.6	106.1	105.9	105.95
H4-C2-C1	107.5	-	107.7	107.4	-	-
O1-C1-O2	122.8	123	-	-	123.1	123.2
C2-C1-O1	111.5	-	111.5	110.9	111.4	111.9
C1-O1-H1	107.1	-	107.1	106.6	106.04	106.04*
C2-C1-O2	125.6	126	125.7	125.7	-	-

[a] geometry at MP2/DZP level [31];

[b] Ref [16];

[c] geometries at MP2(full)/6-311++G** level [30];

[d] Ref. [32].

Table S2 Main geometrical parameters of adsorbed glycine for (a) Si_9H_{12}, (b) $Si_{15}H_{16}$ and (c) $Si_{60}H_{44}$ cluster, compared to isolated molecule.

	GLY1	Adsorbed glycine			
		Cluster	Ads(COOH)	TS	Ads(COO+H)
O1-H1 (Å)	0.971	a	1.069	1.136	-
		b	1.045	1.176	-
		c	1.041	-	-
Si1-H1 (Å)	-	a	2.069	1.936	1.494
		b	2.131	1.873	1.493
		c	2.147	-	1.493
C1-O1 (Å)	1.356	a	1.284	1.274	1.216
		b	1.289	1.269	1.216
		c	1.291	-	1.216
C1-O2 (Å)	1.209	a	1.266	1.276	1.343
		b	1.262	1.280	1.343
		c	1.261	-	1.342
C1-C2 (Å)	1.524	a	1.523	1.525	1.530
		b	1.521	1.525	1.530
		c	1.522	-	1.531
C2-N (Å)	1.450	a	1.444	1.445	1.452
		b	1.443	1.445	1.453
		c	1.442	-	1.451
N-H2 (Å)	0.017	a	1.015	1.015	1.016
		b	1.016	1.016	1.016
		c	1.017	-	1.017
Si2-O2 (Å)	-	a	1.894	1.871	1.769
		b	1.898	1.857	1.768
		c	1.900	-	1.771
Si1-Si2 (Å)	-	a	2.383	2.384	2.399
		b	2.389	2.387	2.394
		c	2.420	-	2.422
Si5-H2	-	a	-	-	-
		b	-	-	-
		c	3.248	-	3.481
θ[O1-C1-O2] (°)	122.8	a	125.7	125.9	122.6
		b	125.5	125.8	122.9
		c	125.2	-	122.8
φ[Si1-Si2-O2-C1] (°)	-	a	0.0	0.0	58.6
		b	7.4	6.2	50.4
		c	3.8	-	52.6
φ[O2-C1-C2-N] (°)	0.0	a	0.0	0.0	8.2
		b	5.8	4.3	13.7
		c	19.4	-	6.1