Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

PEPTIDE CONDENSATION AND HYDROLYSIS MECHANISMS FROM PROTON-TRANSFER NETWORK PERSPECTIVE

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SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral *cis* Diglycine
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral *trans* Diglycine
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized pre-TS1A for formation of INT1
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT1
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT1 with dielectric constant of 32
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT1 with UltraFine Grid Integration
PCM| Atomic positions in Å of MN15/Def2TZVPP optimized INT1 with 4x H2O
Gas| Atomic positions in Å of MN15/Def2TZVPP optimized INT1 with 4x H2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT2
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized PEP1
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized PEP2
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS1A
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS2A
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS2B
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3B
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS2C
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3C
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS(Neut)1
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS(Neut2)

Scenario III (pp. 38-46)

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized *trans* Zwitterionic Diglycine
PCM| Atomic positions in Å of MN15/Def2TZVPP optimized INT3 with 4x H2O
Gas| Atomic positions in Å of MN15/Def2TZVPP optimized INT3 with 4x H2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT3
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT4
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT5
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT6
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS1D
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS2D
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3D
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3E
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3F
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3G
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3I
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS4D
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS4E
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS4F
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS4G
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS5D
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS5E
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS5F
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS5G
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6E
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6F

Scenario IV (pg. 47-74)

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral Glycine with 3xH_2O
Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral Glycine with 4xH_2O
Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral Glycine with 5xH_2O
Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral Glycine with 6xH_2O
Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral Glycine with 7xH_2O

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 3xH_2O
Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 4xH_2O
Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 5xH_2O
Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 6xH_2O
Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 7xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 1xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 2xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 3xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT6 solvated by 1xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT6 solvated by 2xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT6 solvated by 3xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT6 solvated by 4xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized *trans* zwitter diglycine solvated by 2xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized *trans* zwitter diglycine solvated by 3xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized *trans* zwitter diglycine solvated by 4xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized *trans* zwitter diglycine solvated by 5xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized *trans* zwitter diglycine solvated by 6xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D solvated by 1xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D catalyzed by 2xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D solvated by 3xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D solvated by 4xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D with 5x H_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D with 4xH_2O and 1 catalytic H_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D with 6x H_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D with 5xH_2O and 1 catalytic H_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS1D with 5xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS1D with 6xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS2D with 5xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS2D with 6xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3D with 5xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3D with 6xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS4D with 5xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS4D with 6xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS5D with 5xH_2O
SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS5D with 6xH_2O

Scenario I

Table S1: *In vacuo* changes in Gibbs free energy and enthalpy values for the condensation of two neutral glycine molecules at all levels of theory considered in this study relative to the infinitely dissociated neutral glycine pair. Pre/post-TS structures were obtained from Intrinsic Reaction Coordinate (IRC) calculation starting from each transition state.

Step	Level of Theory	ΔH°, kJ/mol	ΔG°, kJ/mol
trans pre-TS(C-N)$^{1\text{-step}}$	B3LYP/def2TZVPP	3	41
	M06-2X/def2TZVPP	-6	32
	MN15/def2TZVPP	-12	31
	ωB97xD/def2TZVPP	-10	30
	cam-B3LYP+D3BJ/def2TZVPP	-25	18
	B3LYP+D3BJ/def2TZVPP	-24	19
	cam-B3LYP/def2TZVPP	-16	27
	MN15/def2SVP	-33	18
	CBS-QB3	-9	32
trans TS(C-N)$^{1\text{-step}}$	B3LYP/def2TZVPP	151	208
	M06-2X/def2TZVPP	134	192
	MN15/def2TZVPP	132	192
	ωB97xD/def2TZVPP	140	198
	cam-B3LYP+D3BJ/def2TZVPP	132	190
	B3LYP+D3BJ/def2TZVPP	125	183
	cam-B3LYP/def2TZVPP	146	204
	MN15/def2SVP	116	175
	CBS-QB3	127	185
trans post-TS(C-N)$^{1\text{-step}}$	B3LYP/def2TZVPP	-25	15
	M06-2X/def2TZVPP	-45	-4
	MN15/def2TZVPP	-44	-3
	ωB97xD/def2TZVPP	-40	1
	cam-B3LYP+D3BJ/def2TZVPP	-43	0
	B3LYP+D3BJ/def2TZVPP	-44	-1
	cam-B3LYP/def2TZVPP	-31	10
	MN15/def2SVP	-46	-2
	CBS-QB3	-47	-4
cis pre-TS(C-N)$^{1\text{-step}}$	B3LYP/def2TZVPP	-11	25
	M06-2X/def2TZVPP	-21	17
	MN15/def2TZVPP	-12	28
	ωB97xD/def2TZVPP	-14	23
	cam-B3LYP+D3BJ/def2TZVPP	-15	23
	B3LYP+D3BJ/def2TZVPP	-16	22
	cam-B3LYP/def2TZVPP	-6	29
	MN15/def2SVP	-19	21
	CBS-QB3	-19	19

Table S1: continued

Step	Level of Theory	ΔH°, kJ/mol	ΔG°, kJ/mol
cis TS(C-N)$^{1\text{-step}}$	B3LYP/def2TZVPP	179	233
	M06-2X/def2TZVPP	166	221
	MN15/def2TZVPP	165	222
	ωB97xD/def2TZVPP	169	224
	cam-B3LYP+D3BJ/def2TZVPP	164	220
	B3LYP+D3BJ/def2TZVPP	155	210
	cam-B3LYP/def2TZVPP	177	232
	MN15/def2SVP	154	210
	CBS-QB3	161	216
cis post- TS(C-N)$^{1\text{-step}}$	B3LYP/def2TZVPP	-19	22
	M06-2X/def2TZVPP	-33	4
	MN15/def2TZVPP	-33	8
	ωB97xD/def2TZVPP	-20	18
	cam-B3LYP+D3BJ/def2TZVPP	-33	15
	B3LYP+D3BJ/def2TZVPP	-35	13
	cam-B3LYP/def2TZVPP	-19	28
	MN15/def2SVP	-35	10
	CBS-QB3	-34	10
cis pre-TS(C-N)$^{2\text{-step}}$	B3LYP/def2TZVPP	-4	32
	M06-2X/def2TZVPP	-19	20
	MN15/def2TZVPP	-16	26
	ωB97xD/def2TZVPP	-14	24
	cam-B3LYP+D3BJ/def2TZVPP	-9	24
	B3LYP+D3BJ/def2TZVPP	-9	24
	cam-B3LYP/def2TZVPP	-3	29
	MN15/def2SVP	-24	18
	CBS-QB3	-19	19
cis TS(C-N)$^{2\text{-step}}$	B3LYP/def2TZVPP	182	239
	M06-2X/def2TZVPP	146	203
	MN15/def2TZVPP	143	202
	ωB97xD/def2TZVPP	157	215
	cam-B3LYP+D3BJ/def2TZVPP	155	213
	B3LYP+D3BJ/def2TZVPP	160	218
	cam-B3LYP/def2TZVPP	167	224
	MN15/def2SVP	130	187
	CBS-QB3	143	199
cis post-TS(C-N)$^{2\text{-step}}$	B3LYP/def2TZVPP	53	107
	M06-2X/def2TZVPP	3	60
	MN15/def2TZVPP	1	60
	ωB97xD/def2TZVPP	21	78
	cam-B3LYP+D3BJ/def2TZVPP	17	74
	B3LYP+D3BJ/def2TZVPP	28	86
	cam-B3LYP/def2TZVPP	30	87
	MN15/def2SVP	-14	44
	CBS-QB3	3	60

Table S1: continued

Step	Level of Theory	ΔH°, kJ/mol	ΔG°, kJ/mol
cis INT2	B3LYP/def2TZVPP	55	110
	M06-2X/def2TZVPP	-2	56
	MN15/def2TZVPP	-5	55
	ωB97xD/def2TZVPP	16	74
	cam-B3LYP+D3BJ/def2TZVPP	11	69
	B3LYP+D3BJ/def2TZVPP	23	81
	cam-B3LYP/def2TZVPP	23	82
	MN15/def2SVP	-22	37
	CBS-QB3	-1	57
trans INT2	B3LYP/def2TZVPP	41	100
	M06-2X/def2TZVPP	-6	52
	MN15/def2TZVPP	-6	52
	ωB97xD/def2TZVPP	11	69
	cam-B3LYP+D3BJ/def2TZVPP	5	64
	B3LYP+D3BJ/def2TZVPP	18	76
	cam-B3LYP/def2TZVPP	17	76
	MN15/def2SVP	-29	31
	CBS-QB3	-7	52
cis TS3B	B3LYP/def2TZVPP	157	214
	M06-2X/def2TZVPP	136	193
	MN15/def2TZVPP	130	187
	ωB97xD/def2TZVPP	145	200
	cam-B3LYP+D3BJ/def2TZVPP	136	193
	B3LYP+D3BJ/def2TZVPP	134	191
	cam-B3LYP/def2TZVPP	148	205
	MN15/def2SVP	119	176
	CBS-QB3	139	196
trans TS3B	B3LYP/def2TZVPP	154	209
	M06-2X/def2TZVPP	134	189
	MN15/def2TZVPP	127	183
	ωB97xD/def2TZVPP	143	198
	cam-B3LYP+D3BJ/def2TZVPP	134	189
	B3LYP+D3BJ/def2TZVPP	132	187
	cam-B3LYP/def2TZVPP	145	201
	MN15/def2SVP	118	173
	CBS-QB3	139	194
cis post-TS3B	B3LYP/def2TZVPP	-19	22
	M06-2X/def2TZVPP	-33	4
	MN15/def2TZVPP	-33	8
	ωB97xD/def2TZVPP	-32	9
	cam-B3LYP+D3BJ/def2TZVPP	-35	7
	B3LYP+D3BJ/def2TZVPP	-36	7
	cam-B3LYP/def2TZVPP	-26	17
	MN15/def2SVP	-35	10
	CBS-QB3	-34	10

Table S1: continued

Step	Level of Theory	ΔHº, kJ/mol	ΔGº, kJ/mol
trans post-TS3B	B3LYP/def2TZVPP	-35	6
	M06-2X/def2TZVPP	-46	-7
	MN15/def2TZVPP	-46	-6
	ωB97xD/def2TZVPP	-46	-5
	cam-B3LYP+D3BJ/def2TZVPP	-50	-8
	B3LYP+D3BJ/def2TZVPP	-50	-8
	cam-B3LYP/def2TZVPP	-42	0
	MN15/def2SVP	-47	-4
	CBS-QB3	-50	-8
cis FP	B3LYP/def2TZVPP	4	9
	M06-2X/def2TZVPP	-2	2
	MN15/def2TZVPP	-4	1
	ωB97xD/def2TZVPP	-3	0
	cam-B3LYP+D3BJ/def2TZVPP	-2	3
	B3LYP+D3BJ/def2TZVPP	-4	1
	cam-B3LYP/def2TZVPP	3	1
	MN15/def2SVP	9	14
	CBS-QB3	-8	-4
trans FP	B3LYP/def2TZVPP	-16	-11
	M06-2X/def2TZVPP	-22	-16
	MN15/def2TZVPP	-21	-15
	ωB97xD/def2TZVPP	-22	-17
	cam-B3LYP+D3BJ/def2TZVPP	-23	-17
	B3LYP+D3BJ/def2TZVPP	-24	-19
	cam-B3LYP/def2TZVPP	-18	-12
	MN15/def2SVP	-8	0
	CBS-QB3	-28	-23

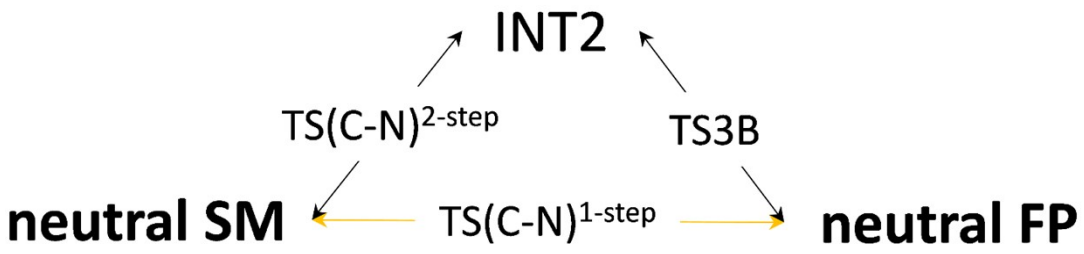

Figure S1: Graph representation of intermediates and transition states in *Scenario I* connecting two neutral glycine molecules (SM) and a neutral diglycine with one water molecule (FP) at the dissociation limit. Lowest free energy barrier pathway marked in orange.

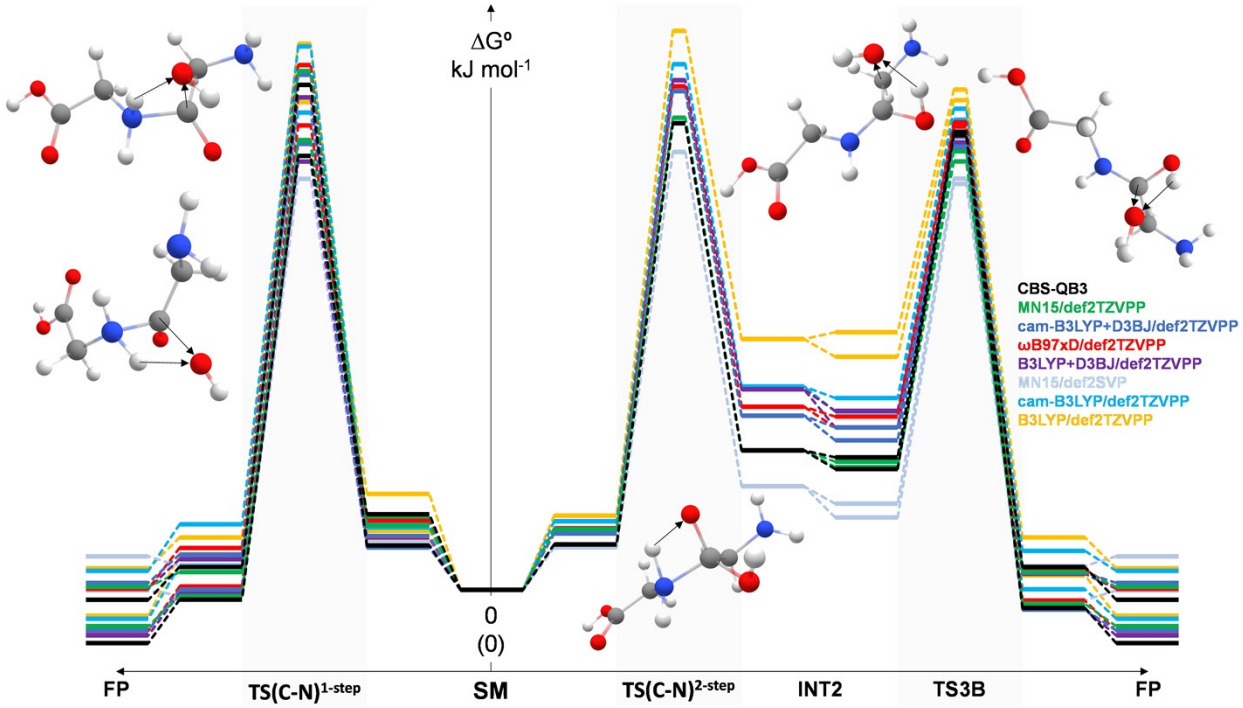

Figure S2: Gibbs free energy profiles of *in vacuo* pathways (*cis*/*trans* isomers for 1-step side and 2-step mechanisms on the left- and right-hand sides, respectively) for the condensation of two neutral glycine molecules as starting materials (SM) and ending in neutral diglycine and a dissociated water molecule as the final products (FP). The Gibbs free energy changes are relative to SM. Pre-/post-TS structures were obtained from Intrinsic Reaction Coordinate (IRC) calculation starting from each transition state. All levels of theory considered in this study are shown and color coded as shown in the legend.

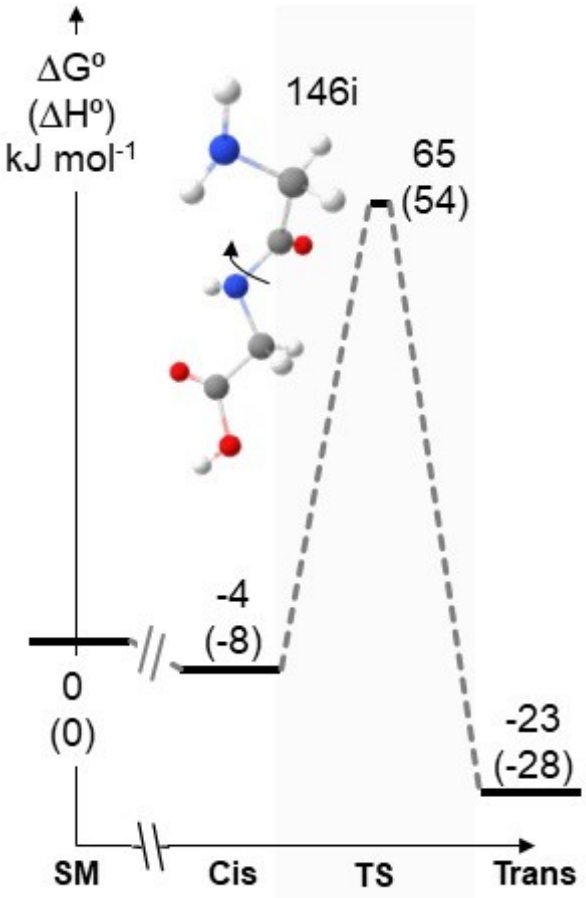

Figure S3: *In vacuo* free energy profile of peptide bond rotation in diglycine at CBS-QB3 level of theory. Pre-/post-TS structures were obtained from Intrinsic Reaction Coordinate (IRC) calculation. The reference energy is defined by two neutral glycine molecules at the dissociation limit.

Scenario II

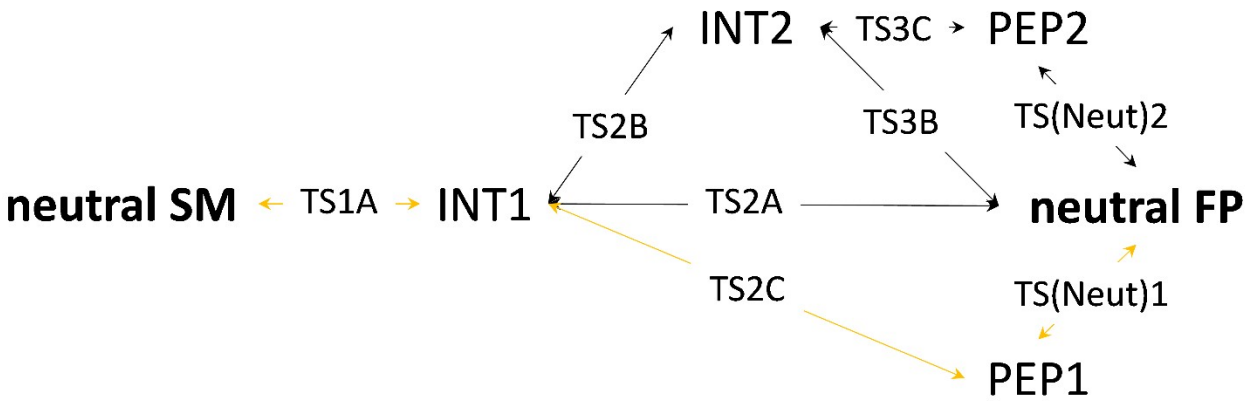

Figure S4: Graph representation of intermediates and transition states in *Scenario II* connecting two neutral glycine molecules (SM) and a neutral diglycine with one water molecule (FP) at the dissociation limit. Lowest free energy barrier pathway marked in orange.

Supplementary Analysis 1: To assess that INT1 is a true intermediate and not an artifact due to the specific parameters of a polarizable continuum model, we created an explicitly solvated derivatives of INT1 and INT3 with four water molecules and neutral and charged end-groups (see **Figure S3**). The INT1×4H_2O and INT3×4H_2O structural optimizations in gas phase resulted in equilibrium structures. The existence of these structures indicates that the PCM and COSMO models do not stabilize charged intermediates sufficiently enough. Evaluation of the size of the cavity used in PCM and COSMO models relative to the SMD revealed that by employing the United Atom Topological Model with atomic radii optimized for PBE1PBE/6-31G(d) level of theory (UAKS option in Gaussian16) makes the INT1 and INT3 structures also stationary with the PCM and COSMO models. However, a 10% decrease to the van der Waals radii of solute atoms in order to reduce the cavity size and thus increase the solute/solvent electrostatic interactions was insufficient to stabilize the intermediates in these PCM models.

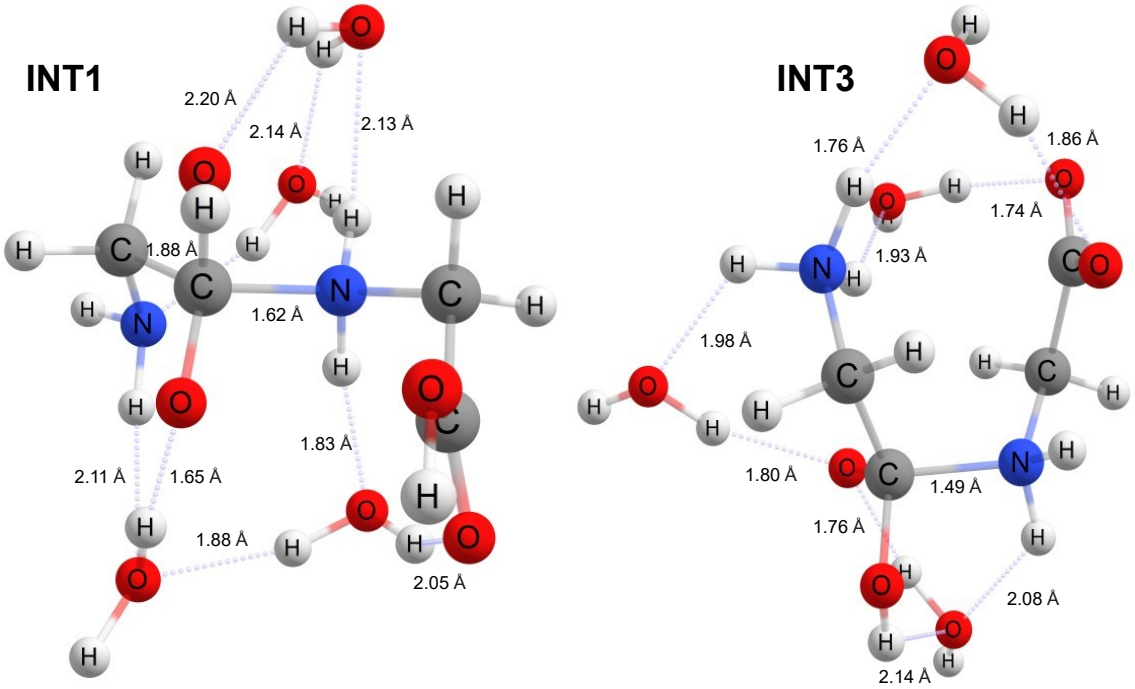

Figure S5: *In vacuo* structures of explicitly solvated INT1×4H_2O and INT3×4H_2O molecules at MN15/def2TZVPP level of theory.

An important caveat in finding the TS(C-N) leading to INT1 (and later INT3) is the flatness of the energy surface, which puts the post-TS intermediate energy level marginally higher than the TS. This anomaly could not be eliminated by applying finer integration grid or considering anharmonic corrections to the zero-point energy, which stabilizes INT1 and INT3 by 9 kJ mol^{-1}; however, the same correction stabilizes even more the TS by 12 kJ mol^{-1}. The post-TS IRC calculations clearly defines INT1 and INT3 being the intermediate that connects to the C–N TS; however, the instability of INT1 and INT3 has already been highlighted by the polarizable continuum dependence of its existence as equilibrium structure.

Scenario III

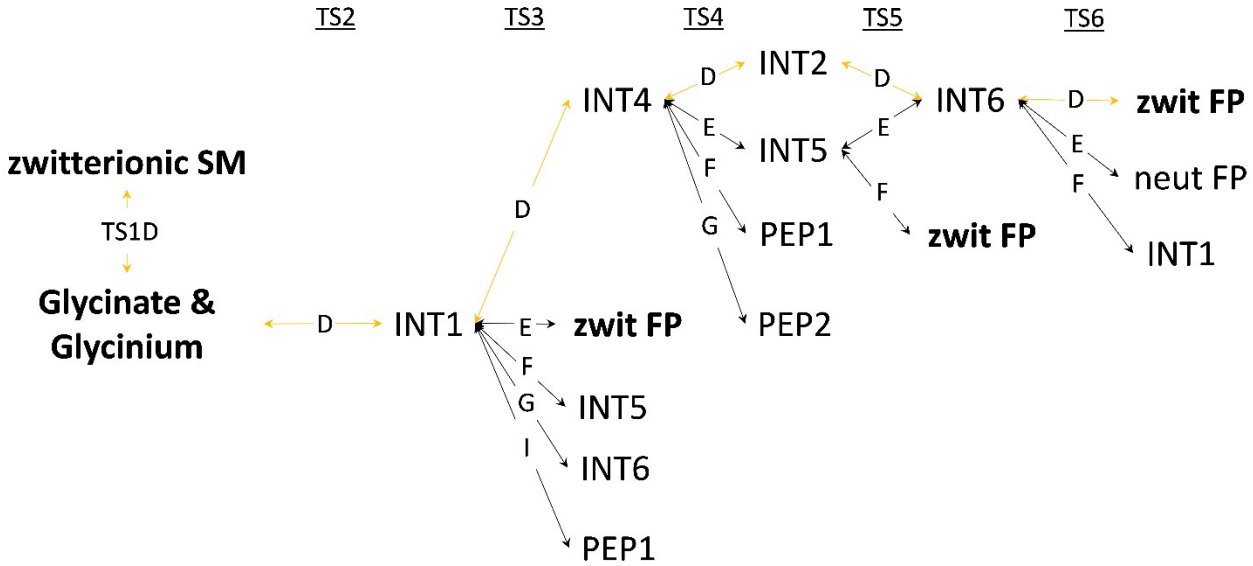

Figure S6: Graph representation of intermediates and transition states in *Scenario III* connecting two zwitterionic glycine molecules (SM) and a zwitterionic diglycine with one water molecule (FP) at the dissociation limit. Lowest free energy barrier pathway marked in orange.

Supplementary Analysis 2: *Scenario III* is aimed at zwitterionic forms of glycine as energetically more plausible model *in aquo* (**Figure S4**). Even so, it is possible, as in the case of **Figure S5** to switch back to the potential energy surface of the neutral system although we started from charged intermediates. The unexpected breaking of the C–N bond during search for TS10 is potentially indicative of the overall stabilization by the charged end-group and the conformational flexibility of the INT3 intermediate.

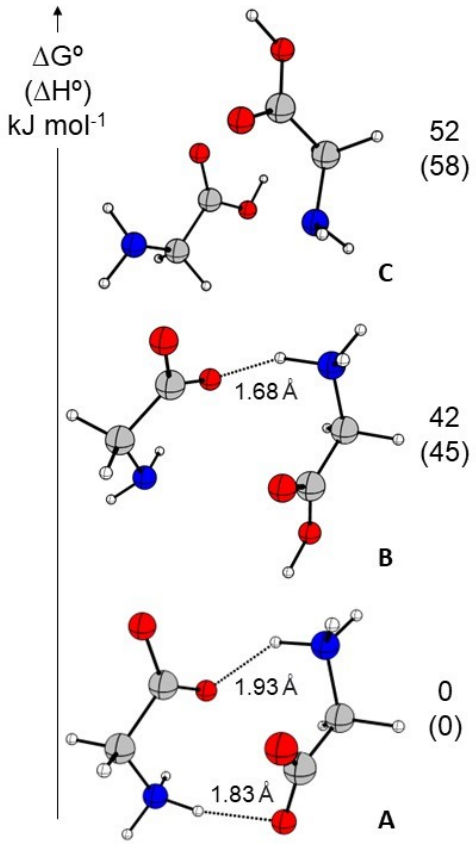

Figure S7: *In aquo* structure of pairs of zwitterionic glycine ions (A), glycinium/glycinate ions (B), and neutral glycine molecules (C) with relative free energy (enthalpy in parentheses, kJ mol^{-1}) calculated at MN15/def2TZVPP|SMD level of theory. The shorter H-bond (1.83 Å) in Panel A is set up for a proton transfer through TS(PT) in **Figure 4**.

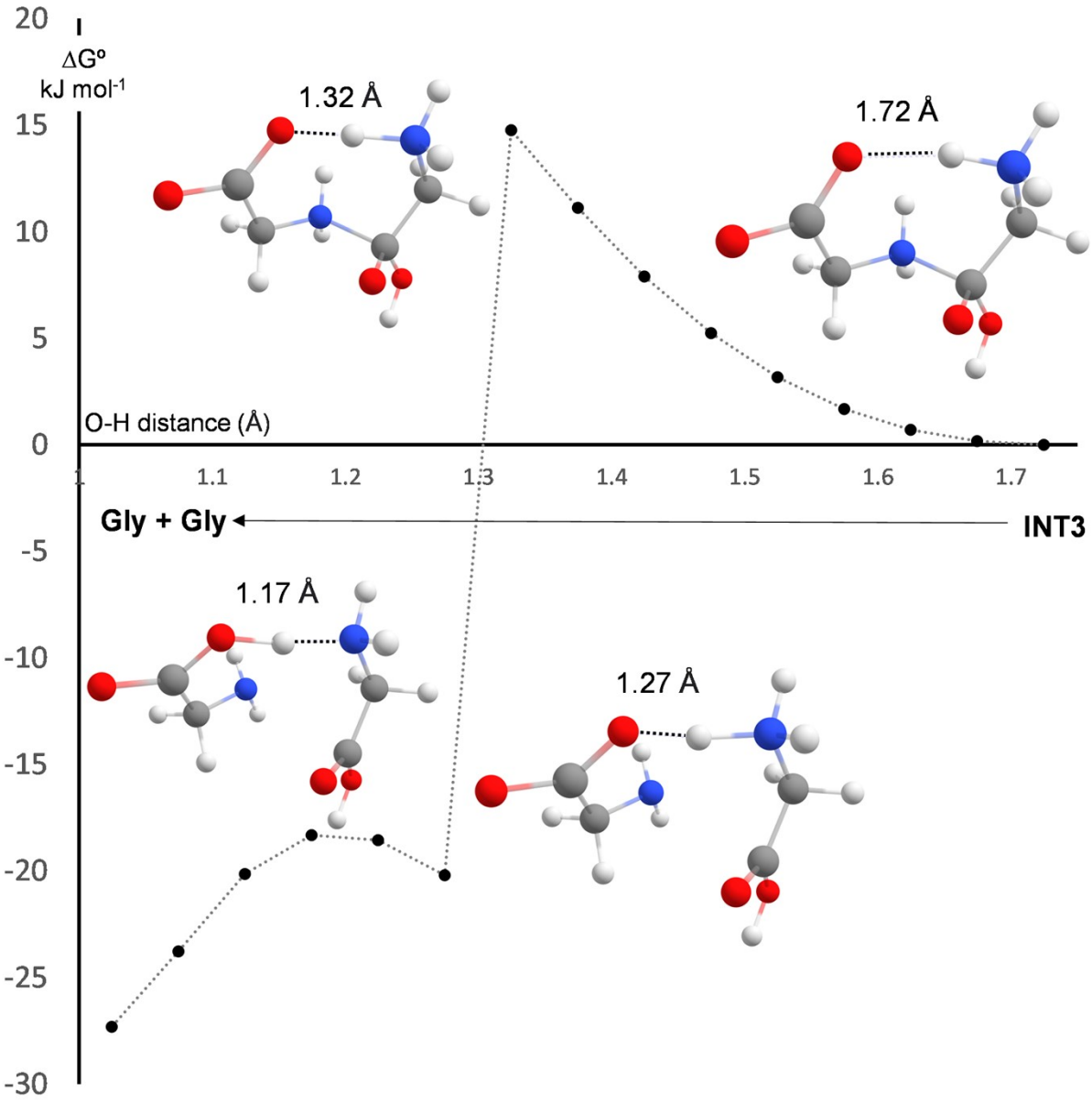

Figure S8: *In aquo* relaxed scan for searching TS10 as proton transfer transition state starting from INT4 (right side) using 0.05 Å steps from 1.72 Å to 1.02 Å H(ammonia)…O(carboxylate) distance at MN15/def2TZVP|SMD level. The scan results in the cleavage of the C–N bond and formation of the glycinium and glycinate pair, followed by a second TS to form neutral interacting glycine molecules as starting materials in *Scenario II* (**Figure 2**).

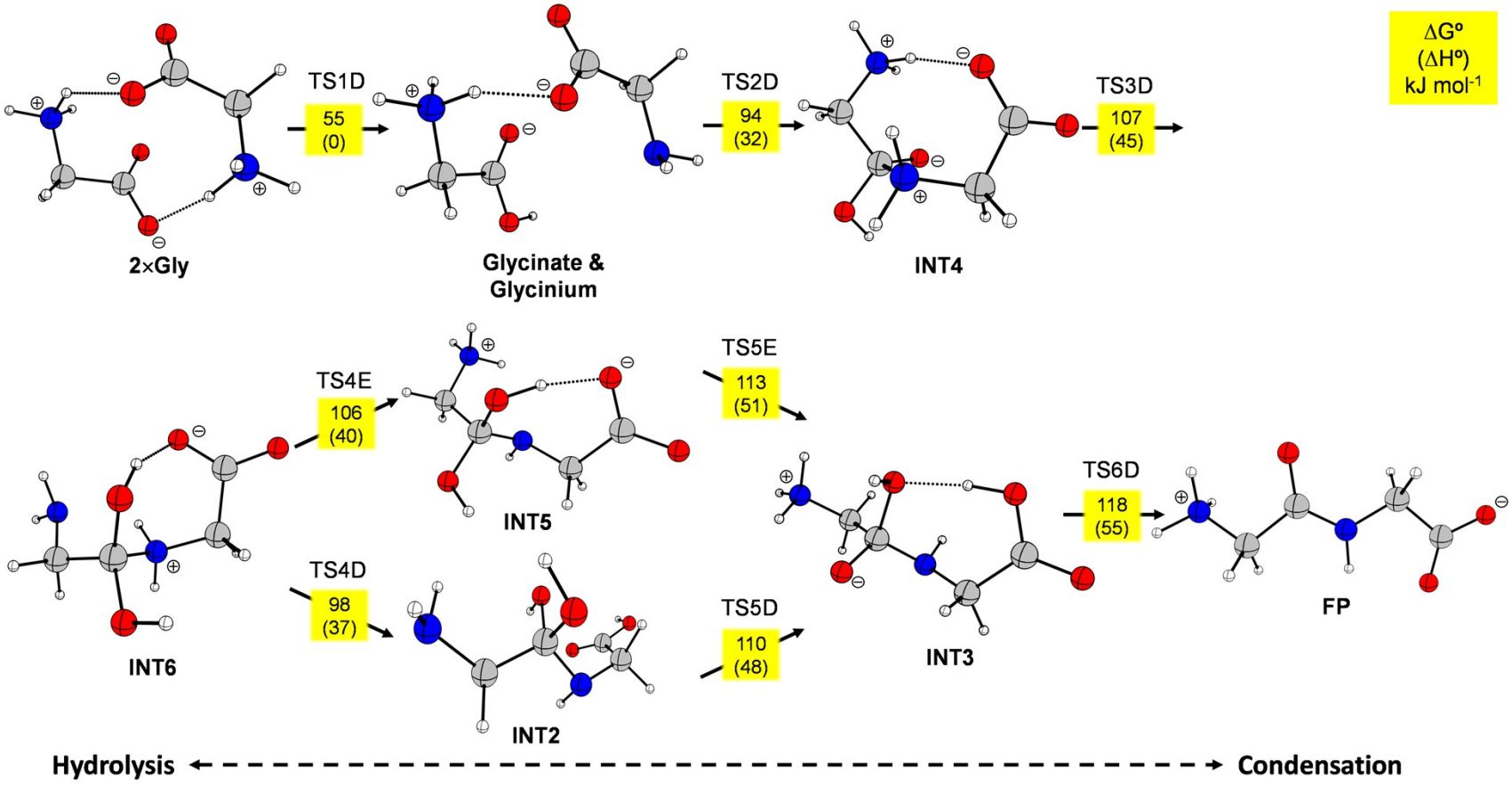

Figure S9: *In aquo* proton-transfer network for energetically most stable intermediates (free energy, enthalpy in parenthesis in kJ mol^{-1}) glycine condensation (forward) and hydrolysis (reverse) reactions calculated at MN15/def2TZVP|SMD level of theory. Transition states connecting the intermediates are shown in **Figure 4**.

Table S2: Gibbs free energy correction due to the lowering of translational entropy in aqueous water condensed phase using Whitesides' free volume method (S_{trans} = 11.1 + 12.5 ln (T) 12.5 ln (M_W) - 8.1 ln([analyte]/33.4); where analyte concentration is given in mM (200 mM in the given case) and 33.4 mL is the free volume available for analyte in 1 L of pure water using 3.10 Å water-water intersolvent distance parameter.

Species	G^o, a.u.	S^o, J mol^{-1} K^{-1}	S^o_{trans}, J mol^{-1} K^{-1}	M_w, g mol^{-1}	$S^{o,corr}_{trans}$, J mol^{-1} K^{-1}	$S^{o,corr}$, J mol^{-1} K^{-1}	$G^{o,corr}$, a.u.
SM: zwitterionic Gly	-284.21656	314	162	75	122	273	-284.21198
neutral Gly	-284.21347	312	167	75	127	271	-284.20889
TS21: rate-limiting step	-568.38796	415	176	150	136	375	-568.38338
FP: zwitterionic diGly	-492.04476	414	169	132	129	374	-492.04018
neutral diGly	-492.04518	431	174	132	134	391	-492.04060
water	-76.39384	189	144	18	86	130	-76.38721

Scenario IV

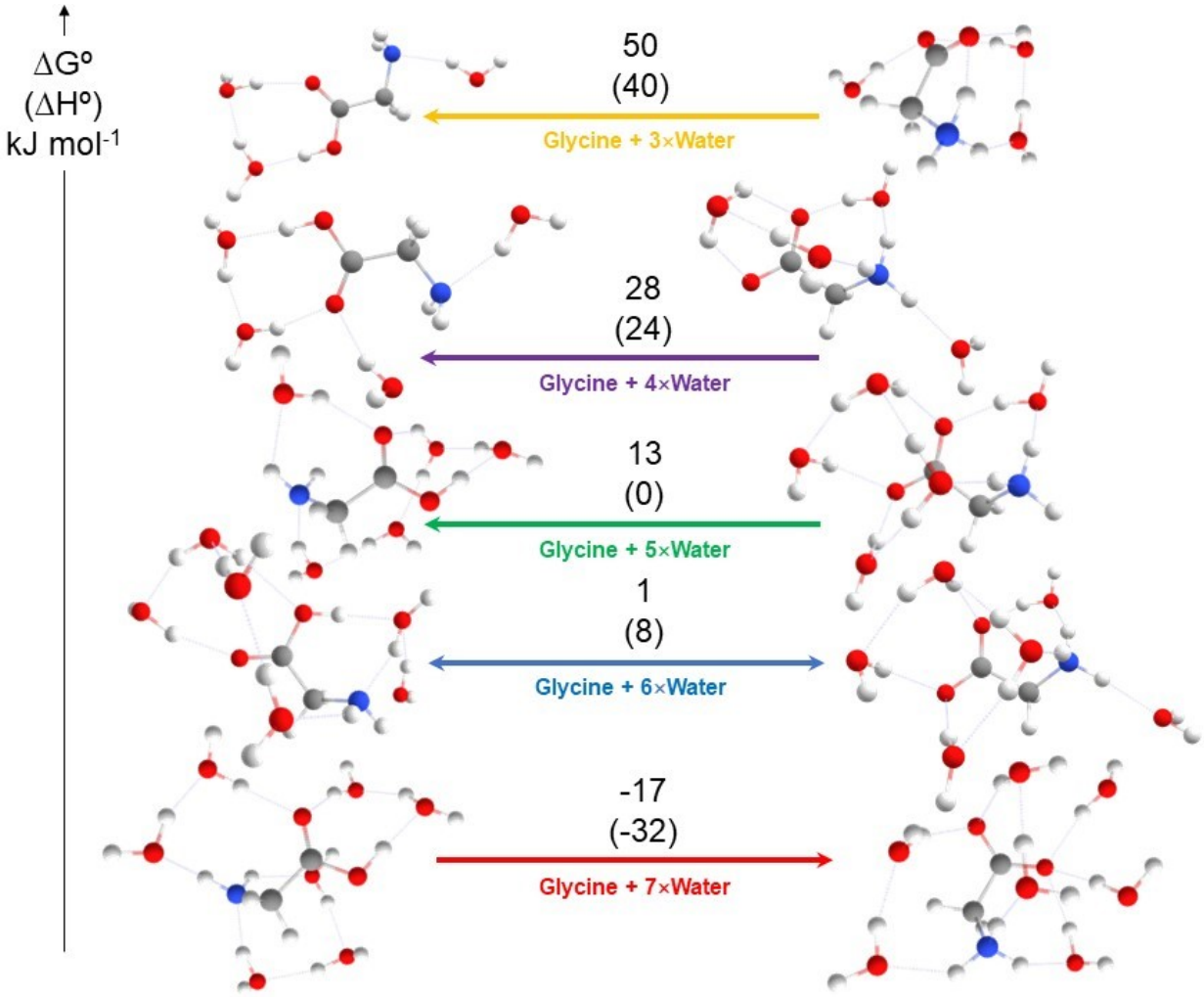

Figure S10: *In vacuo* relative Gibbs free energies and enthalpies (in parenthesis, kJ mol^{-1}) of micro-solvated zwitterionic and neutral glycine equilibrium structures calculated at MN15/def2TZVPP level of theory as function of the number of explicit solvent molecules.

Supplementary Analysis 3: The placement and the number of water molecules were determined by considering the strongest functional group/solvent interactions such as i) cationic ammonium end-group that is critical for reactivity, ii) carboxylic group which triggers the final water elimination step, iii) the leaving hydroxide group of *gem*-diol intermediate forming the eliminating water molecules, iv) and v) additional water molecules to attenuate the effects of varying protonation state of the end-groups. **Table S2** summarizes the numerical results for implicit and explicit solvation models with 5 and 6 water molecules (**Figure S8** and **S9**) in comparison to the implicit solvation-only model from **Figure 4**. The reference points (SM) were defined by combination of zwitterionic glycine molecules with two or three water molecules in their strongest first shell H-bonded interactions.

Table S3: Comparison of Gibbs free energies and enthalpies (in parenthesis, kJ mol^{-1}) using MN15/def2TZVPP|SMD level of theory between the solvation models considered in *Scenarios III* and *IV* for Steps 1-6 of the lowest energy pathway depicted in **Figure 4** in reference to combination of Gly´2H_2O and Gly´3H_2O models.

Steps		Implicit only	Implicit & Explicit w/5 H_2O	Implicit & Explicit w/6 H_2O
Step 1/TS1D[a]	Gly↔Gly TS1D	55(0)	50(-34)	59(-23)
Step 2/TS2D[a]	C–N bond formation	94(32)	109(20)	100(0)
Step 3/TS3D	$–NH_3^+$ end group neutralization	107(45)	122(37)	124(42)
Step 4/TS4D	$–COO^–$ end group neutralization	98(37)	117(31)	107(14)
Step 5/TS5D	*gem*-diol deprotonation	110(48)	118(28)	125(30)
Step 6/TS6D	non-catalytic condensation	118(55)	127(48)	124(44)
	catalytic condensation [a]	154(82)	143(49)	142(56)
FP	solvated diGly + H_2O	-14(-22)	-4(-49)	-10(-46)

[a] The low imaginary normal modes of implicit and explicit structures obtained from relaxed potential energy scans for Step 1, Step 2, and catalytic Step 6 did not allow for the refinement of the TS calculations. The TS candidates are localized on peaks that were noticeably broader relative to the other proton transfer pathways. Values reported here are our best estimates for the TS structures and upper limit for the barrier heights.

Looking at the transition states leading up to the rate-limiting step, TS6D, it is clear from the range of O…N distances spanning the various proton transfer pathways that they remain within 0.02 Å of each other. Similarly in the case of the rate limiting step TS6D, the O…O distance of the transition state remains within 0.06 Å uncatalyzed. Changes (±15 kJ mol^{-1}) seen in the free energies and enthalpies from the results of implicit-only solvation models in **Table S2** can be attributed to the specific placement of the water molecules.

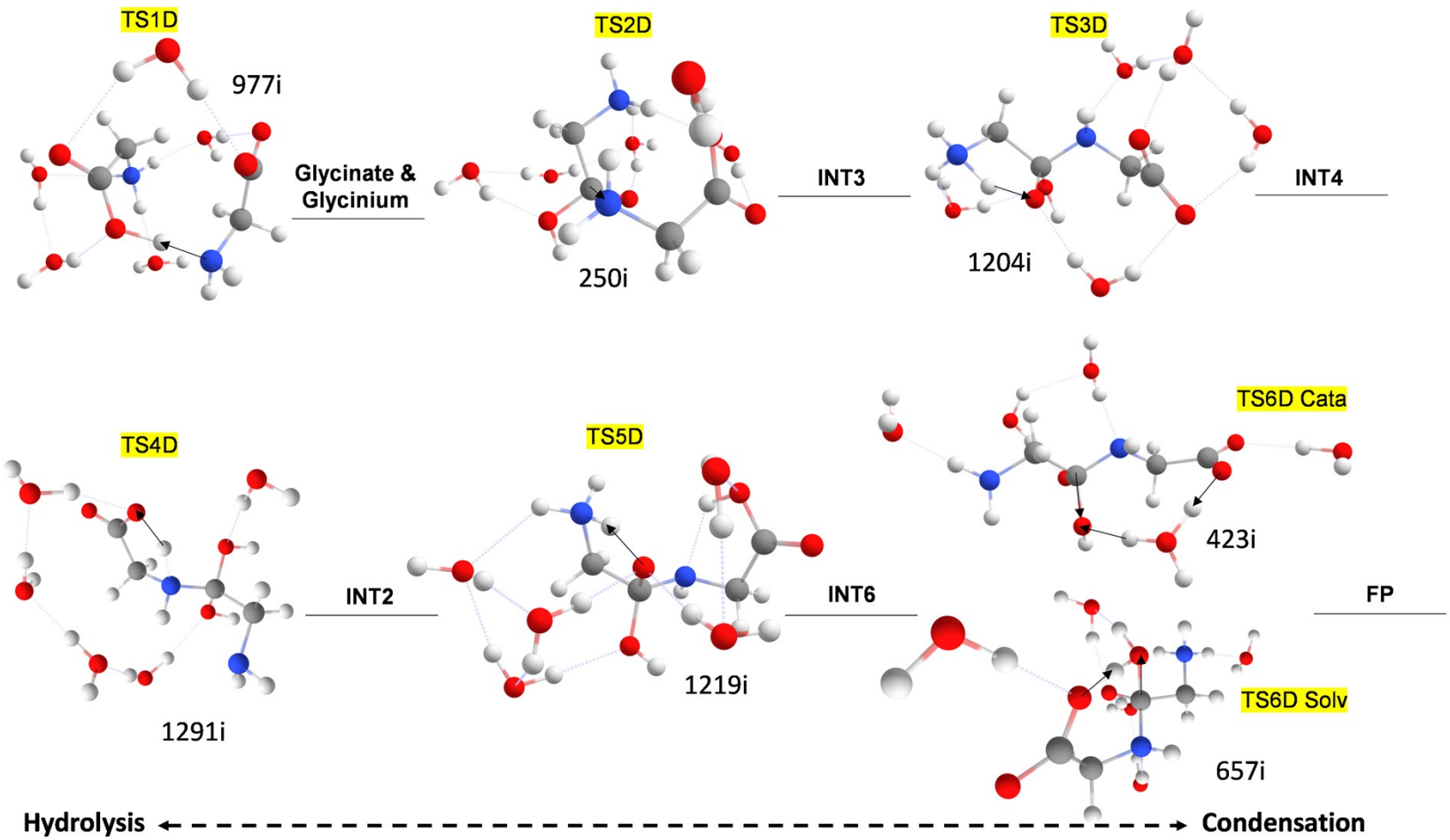

Figure S11: *In aquo* structures of transition states connecting Steps 1-6 solvated explicitly by five water molecules at MN15/def2TZVPP|SMD level of theory. Activation barrier heights are summarized in **Table S3**.

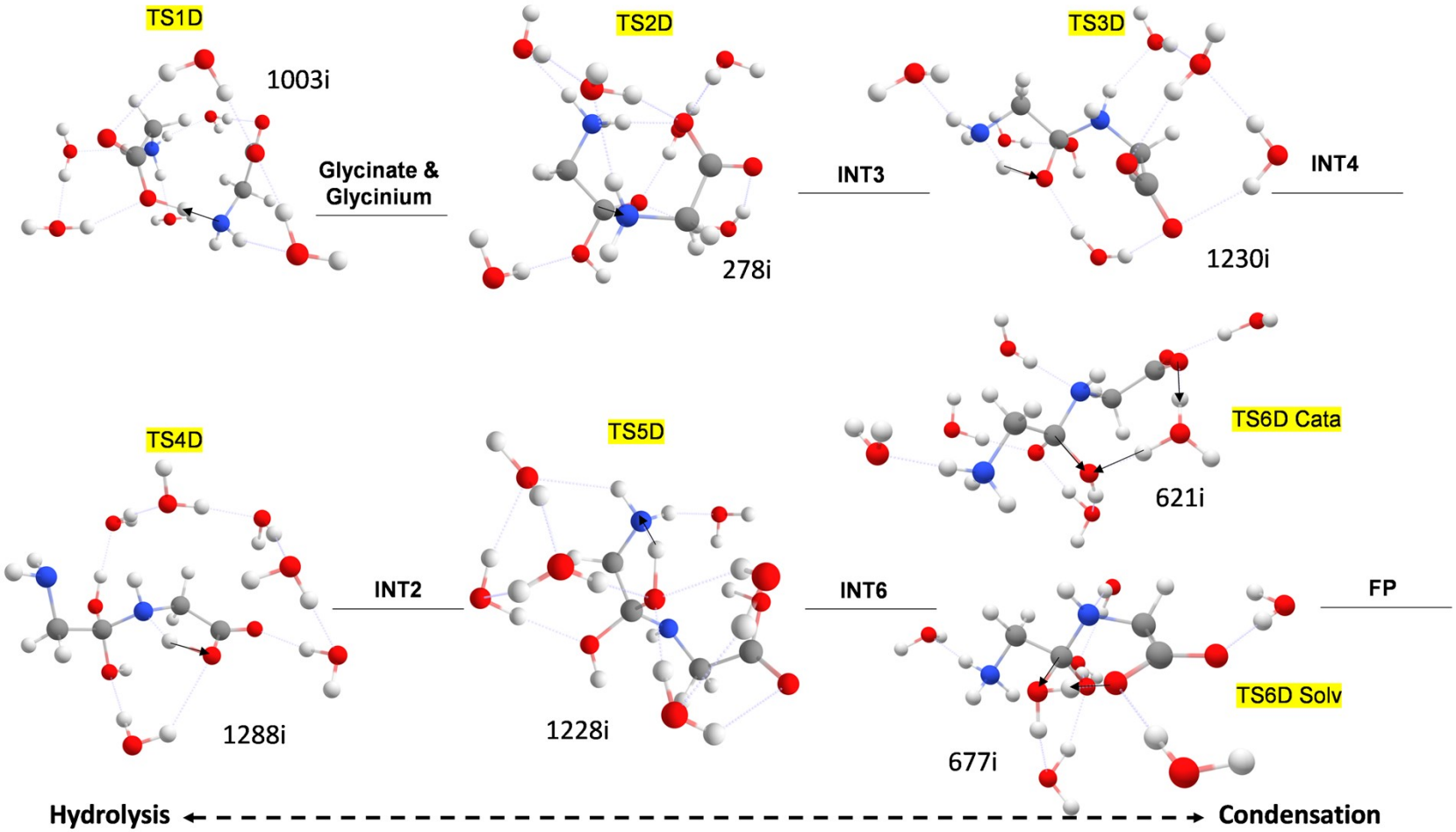

Figure S12: *In aquo* structures of transition states connecting Steps 1-6 solvated explicitly by six water molecules at MN15/def2TZVPP|SMD level of theory. Activation barrier heights are summarized in **Table S3**.

Cartesian Coordinates

Scenario I

Gas| Atomic positions in Å of CBS-QB3 optimized Water (Escf: -76.3586)

8	0.000000000	0.000000000	0.118695000
1	0.000000000	0.757069000	-0.474782000
1	0.000000000	-0.757069000	-0.474782000

Gas| Atomic positions in Å of CBS-QB3 optimized Neutral Glycine (Escf: -284.1103)

7	1.971165000	0.011954000	-0.000011000
6	0.726631000	-0.732469000	-0.000010000
6	-0.542042000	0.112130000	0.000036000
8	-1.653534000	-0.661296000	-0.000009000
8	-0.579380000	1.315585000	0.000006000
1	-2.413580000	-0.060123000	-0.000021000
1	2.001377000	0.625918000	-0.808342000
1	2.001415000	0.625857000	0.808364000
1	0.684189000	-1.393779000	-0.871450000
1	0.684217000	-1.393825000	0.871396000

Gas| Atomic positions in Å of CBS-QB3 optimized Neutral *cis* Diglycine (Escf: -491.8639)

1	4.093170000	-0.659082000	-0.000019000
8	3.204700000	-1.046088000	0.000068000
6	2.325716000	-0.026106000	-0.000033000
8	2.642771000	1.133845000	-0.000144000
6	0.900737000	-0.543039000	0.000062000
1	0.787083000	-1.189331000	-0.879053000
1	0.787170000	-1.189312000	0.879201000
7	-0.014946000	0.572239000	0.000070000
6	-1.381923000	0.519119000	0.000009000
8	-2.063294000	1.528601000	0.000070000
6	-2.017764000	-0.882181000	-0.000060000
1	-1.656871000	-1.437318000	-0.874076000
1	-1.656823000	-1.437389000	0.873901000
7	-3.470292000	-0.887726000	-0.000039000
1	-3.796481000	-0.356083000	-0.802605000
1	-3.796462000	-0.356010000	0.802484000
1	0.401863000	1.495310000	0.000136000

Gas| Atomic positions in Å of CBS-QB3 optimized Neutral *trans* Diglycine (Escf: -491.8719)

7	-2.443092000	1.470000000	0.179886000
6	-2.613393000	0.048663000	-0.135108000
6	-1.297270000	-0.735354000	-0.075424000
8	-1.187515000	-1.835595000	-0.589215000
1	-2.169030000	1.994570000	-0.644097000
1	-3.302922000	1.876210000	0.527874000
1	-3.276267000	-0.402540000	0.609093000
1	-3.051632000	-0.161142000	-1.117559000
7	-0.311818000	-0.106221000	0.620883000
6	1.031272000	-0.614569000	0.658588000
6	2.011422000	0.294487000	-0.062391000
8	3.263084000	-0.212448000	-0.003050000
8	1.742255000	1.333626000	-0.604665000
1	3.839978000	0.407405000	-0.473648000
1	-0.513875000	0.848165000	0.894752000
1	1.391240000	-0.757841000	1.683298000
1	1.032116000	-1.595309000	0.176355000

Gas| Atomic positions in Å of CBS-QB3 optimized pre-TS(C-N)$^{1\text{-step}}$ *cis* Pathway (Escf: -568.2303)

1	-4.753058000	-0.655342000	-0.711252000
8	-4.096832000	0.049260000	-0.820269000
6	-3.079146000	-0.228393000	0.027731000
8	-3.065865000	-1.195148000	0.744917000
6	-1.997856000	0.842057000	-0.029132000
1	-1.738596000	1.013753000	-1.076978000
1	-2.453986000	1.774429000	0.323016000
7	-0.801438000	0.543186000	0.736485000
1	-1.062271000	0.216664000	1.662170000
6	2.652643000	-0.561788000	-0.172747000
8	1.588145000	-0.964006000	-0.579111000
6	2.987733000	0.876756000	0.209544000
1	3.191211000	0.872582000	1.286641000
1	3.943341000	1.124663000	-0.263406000
7	1.991649000	1.878055000	-0.099723000
1	1.097800000	1.649111000	0.336228000
1	1.826128000	1.907137000	-1.100591000
8	3.711876000	-1.382250000	0.006165000
1	3.420582000	-2.275050000	-0.233606000
1	-0.281472000	-0.211273000	0.294446000

Gas| Atomic positions in Å of CBS-QB3 optimized pre-TS(C-N)$^{1\text{-step}}$ *trans* Pathway (Escf: -568.2264)

7	-0.886998000	-0.912106000	0.562371000
6	-1.667190000	-0.492647000	-0.600305000
6	-3.010530000	0.099418000	-0.232038000
8	-3.585275000	0.959000000	-0.847566000
8	-3.548269000	-0.494960000	0.863349000
1	-4.409940000	-0.076312000	1.006665000
1	-1.400107000	-1.592460000	1.111767000
1	-0.015207000	-1.330693000	0.248567000
1	-1.112862000	0.274982000	-1.141206000
1	-1.887771000	-1.301088000	-1.318873000
7	1.040566000	1.444159000	0.207595000
6	2.448812000	1.162401000	0.410430000
6	2.821152000	-0.214763000	-0.096217000
8	4.162139000	-0.346513000	-0.204580000
8	2.063148000	-1.120154000	-0.344349000
1	4.330993000	-1.257683000	-0.487173000
1	0.446077000	0.790669000	0.718296000
1	0.823054000	2.382040000	0.523013000
1	3.060982000	1.886557000	-0.134298000
1	2.802394000	1.194183000	1.457432000

Gas| Atomic positions in Å of CBS-QB3 optimized pre-TS(C-N)$^{2\text{-step}}$ Trans/*cis* Pathway (Escf: -568.2303)

1	4.508307000	-1.205255000	-0.325016000
8	3.751919000	-0.880594000	-0.836347000
6	2.990410000	-0.150271000	0.011888000
8	3.267214000	0.009061000	1.172359000
6	1.785548000	0.451746000	-0.698378000
1	2.175714000	1.153533000	-1.444659000
1	1.288930000	-0.340531000	-1.264088000
7	0.831483000	1.115422000	0.170844000
1	1.325436000	1.713087000	0.826858000
6	-2.477649000	-0.656091000	0.142017000
8	-1.511169000	-0.802935000	0.852037000
6	-2.947476000	0.651240000	-0.488926000
1	-2.846879000	0.525372000	-1.573245000
1	-4.023932000	0.731119000	-0.307121000
7	-2.269838000	1.856598000	-0.067779000
1	-1.264236000	1.783562000	-0.223649000
1	-2.398252000	2.000122000	0.928613000
8	-3.283630000	-1.687110000	-0.198190000
1	-2.918088000	-2.480956000	0.220726000
1	0.321812000	0.428710000	0.721655000

Gas| Atomic positions in Å of CBS-QB3 optimized INT2 for 2-step *cis* Pathway (Escf: -568.2238)

7	-3.134884000	-0.795236000	0.763598000
6	-1.997306000	-0.968949000	-0.133288000
6	-1.031041000	0.227351000	-0.225417000
7	0.043040000	-0.033001000	-1.167091000
6	1.183357000	-0.791786000	-0.711645000
6	2.215604000	-0.006927000	0.092883000
8	2.098240000	1.132949000	0.477930000
8	3.322322000	-0.740016000	0.317845000
8	-0.604050000	0.491965000	1.098634000
8	-1.675208000	1.368268000	-0.766122000
1	-2.811571000	-0.487906000	1.675441000
1	-3.771968000	-0.091380000	0.405128000
1	0.120097000	1.134598000	1.043708000
1	-2.270469000	1.685864000	-0.079203000
1	-1.433371000	-1.848746000	0.192051000
1	-2.358731000	-1.165973000	-1.143649000
1	0.312728000	0.841231000	-1.603465000
1	0.862145000	-1.634167000	-0.094492000
1	1.709058000	-1.230088000	-1.566078000
1	3.930883000	-0.189243000	0.833523000

Gas| Atomic positions in Å of CBS-QB3 optimized INT2 for 2-step *trans* Pathway (Escf: -568.2259)

7	-3.496949000	0.202012000	0.153099000
6	-2.398294000	-0.553744000	-0.436535000
6	-0.984637000	-0.084474000	-0.045929000
7	0.002824000	-0.914856000	-0.713937000
6	1.313073000	-1.097256000	-0.133466000
6	2.213076000	0.129206000	-0.048207000
8	1.892040000	1.276305000	-0.267950000
8	3.462587000	-0.203802000	0.322965000
8	-0.755338000	-0.254251000	1.347161000
8	-0.912586000	1.284748000	-0.380968000
1	-3.511695000	0.073016000	1.159981000
1	-3.362341000	1.192330000	-0.026648000
1	-2.483614000	-1.603026000	-0.149091000
1	-2.482371000	-0.500730000	-1.526994000
1	-1.155131000	0.515086000	1.764716000
1	0.027837000	1.534400000	-0.352920000
1	0.035853000	-0.684259000	-1.698241000
1	1.853806000	-1.862502000	-0.697624000
1	1.210687000	-1.479020000	0.884250000
1	3.972908000	0.618219000	0.383592000

Gas| Atomic positions in Å of CBS-QB3 optimized post-TS(C-N)$^{1\text{-step}}$ *cis* Pathway (Escf: -568.2350)

1	-4.707157000	0.177215000	0.360536000
8	-3.882350000	0.686180000	0.361135000
6	-2.882609000	-0.170304000	0.084737000
8	-3.037736000	-1.345626000	-0.116928000
6	-1.548361000	0.549877000	0.059240000
1	-1.618063000	1.344176000	-0.693873000
1	-1.420243000	1.045795000	1.028106000
7	-0.499304000	-0.401968000	-0.223727000
1	3.417739000	-1.155254000	0.062395000
6	0.841500000	-0.166251000	-0.269393000
8	1.623194000	-1.074963000	-0.526462000
6	1.301349000	1.272161000	0.028175000
1	0.676403000	1.965933000	-0.545978000
1	1.070800000	1.475556000	1.082476000
7	2.695115000	1.570906000	-0.218103000
1	2.910003000	1.433548000	-1.200731000
1	3.299630000	0.925889000	0.289082000
8	4.226064000	-0.958977000	0.567627000
1	4.092458000	-1.406128000	1.408585000
1	-0.796897000	-1.355118000	-0.397318000

Gas| Atomic positions in Å of CBS-QB3 optimized post-TS(C-N)$^{1\text{-step}}$ *trans* Pathway (Escf: -568.2401)

7	2.221226000	-1.151408000	-1.028589000
6	1.895588000	-1.229329000	0.393698000
6	0.768663000	-0.277280000	0.798540000
8	0.511428000	-0.034377000	1.962215000
8	2.849031000	1.780478000	-0.580692000
1	3.073384000	2.037640000	0.319385000
1	2.846721000	-0.367155000	-1.195044000
1	2.667346000	-2.001058000	-1.350310000
1	1.524140000	-2.232511000	0.624700000
1	2.730101000	-1.034203000	1.078424000
7	0.099051000	0.284508000	-0.265281000
6	-1.182358000	0.914539000	-0.061420000
6	-2.345286000	-0.046827000	-0.260600000
8	-3.522438000	0.588084000	-0.069875000
8	-2.253760000	-1.207837000	-0.555880000
1	-4.222653000	-0.067821000	-0.204877000
1	0.296720000	-0.177391000	-1.149309000
1	1.887745000	1.677103000	-0.563115000
1	-1.219210000	1.290335000	0.963273000
1	-1.319947000	1.765963000	-0.733499000

Gas| Atomic positions in Å of CBS-QB3 optimized post-TS(C-N)$^{2\text{-step}}$ Trans/*cis* Pathway (Escf: -568.2223)

1	3.795936000	-0.987958000	0.401222000
8	3.209991000	-0.306112000	0.763296000
6	2.194745000	-0.151767000	-0.112158000
8	2.099650000	-0.782382000	-1.134184000
6	1.235078000	0.937805000	0.335047000
1	0.928087000	0.755295000	1.366096000
1	1.809354000	1.872271000	0.348932000
7	0.063653000	1.069731000	-0.517755000
1	0.289060000	0.747662000	-1.455247000
6	-1.166803000	0.409118000	-0.076501000
8	-1.486064000	0.875329000	1.218333000
6	-1.140052000	-1.127594000	0.013788000
1	-0.823331000	-1.511268000	-0.958534000
1	-0.376602000	-1.415885000	0.741638000
7	-2.403195000	-1.751726000	0.390785000
1	-3.112800000	-1.482108000	-0.284497000
1	-2.704745000	-1.364917000	1.280635000
8	-2.153071000	0.745311000	-1.022980000
1	-1.987683000	1.660699000	-1.281736000
1	-1.542348000	1.837646000	1.173506000

Gas| Atomic positions in Å of CBS-QB3 optimized post-TS3B for 2-step *cis* Pathway (Escf: -568.2350)

7	2.695077000	1.570874000	-0.218425000
6	1.301376000	1.272188000	0.028189000
6	0.841488000	-0.166260000	-0.269201000
7	-0.499308000	-0.402022000	-0.223391000
6	-1.548362000	0.549810000	0.059609000
6	-2.882656000	-0.170298000	0.084651000
8	-3.037797000	-1.345587000	-0.117209000
8	-3.882418000	0.686200000	0.360940000
8	4.226192000	-0.958851000	0.567443000
8	1.623200000	-1.074969000	-0.526213000
1	3.299675000	0.926057000	0.288907000
1	2.909833000	1.433086000	-1.201023000
1	4.092762000	-1.406212000	1.408315000
1	3.417939000	-1.155349000	0.062183000
1	1.071073000	1.475647000	1.082528000
1	0.676277000	1.965931000	-0.545851000
1	-0.796892000	-1.355186000	-0.396932000
1	-1.420432000	1.045483000	1.028635000
1	-1.617857000	1.344316000	-0.693306000
1	-4.707247000	0.177272000	0.360078000

Gas| Atomic positions in Å of CBS-QB3 optimized post-TS3B for 2-step *trans* Pathway (Escf: -568.2412)

7	3.020266000	1.366478000	0.373125000
6	1.706104000	1.398816000	-0.237786000
6	0.801340000	0.184360000	0.027014000
7	-0.530415000	0.423750000	-0.036238000
6	-1.505888000	-0.631859000	0.114763000
6	-2.894133000	-0.051362000	-0.028062000
8	-3.137735000	1.111246000	-0.232007000
8	-3.836419000	-1.001137000	0.102475000
8	1.234267000	-0.942168000	0.261909000
8	3.926929000	-1.476770000	-0.408815000
1	2.935780000	1.265752000	1.379732000
1	3.545720000	0.559725000	0.038185000
1	1.179001000	2.310092000	0.067040000
1	1.827497000	1.466706000	-1.325477000
1	2.977527000	-1.464173000	-0.190298000
1	4.345015000	-1.841310000	0.377084000
1	-0.893088000	1.351654000	-0.206937000
1	-1.422214000	-1.121732000	1.090565000
1	-1.367678000	-1.419574000	-0.633353000
1	-4.697395000	-0.567836000	0.001178000

Gas| Atomic positions in Å of CBS-QB3 optimized TS(C-N)$^{1\text{-step}}$ *cis* Pathway (Escf: -568.1568)

1	-4.350898000	0.678517000	0.087026000
8	-3.462610000	1.058099000	0.170730000
6	-2.578520000	0.069127000	-0.041398000
8	-2.878392000	-1.071464000	-0.276460000
6	-1.153708000	0.590386000	0.020257000
1	-0.994663000	1.216986000	-0.863718000
1	-1.033361000	1.226057000	0.898085000
7	-0.208733000	-0.528180000	0.060461000
1	0.231491000	-0.813014000	1.063644000
6	1.344751000	-0.365589000	-0.372319000
8	1.753560000	-1.235589000	-1.096618000
6	1.868551000	1.064707000	-0.302402000
1	1.650372000	1.544507000	-1.265028000
1	1.352380000	1.620779000	0.480959000
7	3.299892000	1.122345000	-0.054039000
1	3.777127000	0.570132000	-0.761788000
1	3.458587000	0.648058000	0.832502000
8	1.579546000	-0.757764000	1.523515000
1	2.020336000	-1.615279000	1.537485000
1	-0.572762000	-1.333939000	-0.448293000

Gas| Atomic positions in Å of CBS-QB3 optimized TS(C-N)$^{1\text{-step}}$ *trans* Pathway (Escf: -568.1697)

7	-2.128594000	1.525557000	-0.542558000
6	-1.801544000	0.939610000	0.753278000
6	-1.026829000	-0.352179000	0.585860000
8	-0.679926000	-1.097164000	1.467032000
8	-2.277984000	-1.205584000	-0.721739000
1	-2.488395000	-2.053993000	-0.317596000
1	-2.811312000	0.923609000	-0.995749000
1	-2.514531000	2.455740000	-0.435374000
1	-1.141464000	1.622975000	1.300548000
1	-2.655710000	0.704958000	1.399441000
7	-0.135720000	-0.319284000	-0.724307000
6	1.212738000	-0.842595000	-0.557204000
6	2.168044000	0.242693000	-0.106585000
8	3.405215000	-0.251565000	0.082089000
8	1.872003000	1.397683000	0.055759000
1	3.967011000	0.482954000	0.372165000
1	-0.195901000	0.626843000	-1.112516000
1	-0.935673000	-0.969307000	-1.179211000
1	1.178197000	-1.624993000	0.205580000
1	1.579053000	-1.284832000	-1.486456000

Gas| Atomic positions in Å of CBS-QB3 optimized TS(C-N)$^{2\text{-step}}$ Trans/*cis* Pathway (Escf: -568.1637)

1	4.354072000	-0.685581000	0.040549000
8	3.465177000	-1.056128000	0.152257000
6	2.585526000	-0.063760000	-0.074442000
8	2.897660000	1.065433000	-0.346934000
6	1.157387000	-0.567774000	0.017839000
1	0.970102000	-1.175696000	-0.874819000
1	1.052622000	-1.220659000	0.885827000
7	0.229556000	0.556969000	0.116436000
1	0.518615000	1.319608000	-0.494882000
6	-1.373182000	0.356697000	0.091776000
8	-1.545143000	0.627133000	1.392261000
6	-1.824783000	-1.019183000	-0.404544000
1	-1.602385000	-1.128827000	-1.470718000
1	-1.275435000	-1.791154000	0.140539000
7	-3.252875000	-1.232907000	-0.188504000
1	-3.765181000	-0.528320000	-0.712389000
1	-3.447506000	-1.045362000	0.792769000
8	-1.882409000	1.344864000	-0.775513000
1	-2.157595000	2.054492000	-0.180033000
1	-0.236056000	0.846765000	1.217288000

Gas| Atomic positions in Å of CBS-QB3 optimized TS3B for 2-step *trans* Pathway (Escf: -568.1649)

7	-3.518592000	0.584344000	0.065568000
6	-2.174762000	1.105849000	-0.091514000
6	-1.091807000	0.061779000	-0.329879000
7	0.177431000	0.470311000	-0.319839000
6	1.267998000	-0.486745000	-0.390994000
6	2.542002000	0.193679000	0.049339000
8	2.606001000	1.311395000	0.497300000
8	3.606343000	-0.611167000	-0.106841000
8	-1.378234000	-1.050210000	-0.987550000
8	-1.370859000	-1.198749000	1.256781000
1	-3.791397000	0.105573000	-0.787860000
1	-3.488164000	-0.131483000	0.786222000
1	-2.156384000	1.782676000	-0.955367000
1	-1.903078000	1.701156000	0.784601000
1	-1.645390000	-1.577208000	-0.100832000
1	-1.837712000	-1.112273000	2.094234000
1	0.407572000	1.331184000	0.162850000
1	1.391993000	-0.885858000	-1.399423000
1	1.062188000	-1.326602000	0.281174000
1	4.381900000	-0.127277000	0.215062000

Gas| Atomic positions in Å of CBS-QB3 optimized TS3B for 2-step *cis* Pathway (Escf: -568.1645)

7	3.164514000	1.153498000	-0.001418000
6	1.759377000	1.127999000	-0.349818000
6	1.110578000	-0.251791000	-0.366469000
7	-0.223091000	-0.345938000	-0.479610000
6	-1.167530000	0.633742000	0.011764000
6	-2.557091000	0.028419000	0.005505000
8	-2.806465000	-1.117091000	-0.264527000
8	-3.479432000	0.940931000	0.354260000
8	1.804925000	-0.828976000	1.446734000
8	1.804732000	-1.296898000	-0.791619000
1	3.251229000	0.712524000	0.911634000
1	3.677085000	0.562951000	-0.650066000
1	1.122887000	-1.262933000	1.972005000
1	2.114974000	-1.493277000	0.233936000
1	1.210179000	1.783737000	0.329285000
1	1.626815000	1.533935000	-1.363185000
1	-0.593437000	-1.278886000	-0.626650000
1	-0.936619000	0.933850000	1.041751000
1	-1.183325000	1.542787000	-0.596291000
1	-4.341839000	0.498450000	0.350095000

Gas| Atomic positions in Å of CBS-QB3 optimized TS for Rotation Between *cis* and *trans* Diglycine (Escf: -491.8384)

7	2.756718000	-1.426410000	0.146081000
6	2.595843000	-0.126128000	-0.502284000
6	1.439012000	0.639603000	0.109996000
8	1.488228000	1.806426000	0.397545000
1	1.878316000	-1.932127000	0.084821000
1	3.468614000	-1.970325000	-0.329341000
1	3.496067000	0.477266000	-0.375558000
1	2.381816000	-0.173465000	-1.588627000
7	0.238797000	-0.163744000	0.288181000
6	-0.869432000	0.290565000	-0.556265000
6	-2.185210000	-0.147728000	0.048702000
8	-3.182225000	-0.106649000	-0.858239000
8	-2.344155000	-0.458926000	1.200115000
1	-3.998127000	-0.344706000	-0.392526000
1	-0.065282000	-0.061057000	1.256493000
1	-0.918442000	1.387336000	-0.644483000
1	-0.787628000	-0.116526000	-1.566878000

Scenario II

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Water (Escf: -76.3975)

8	0.000000000	0.000000000	0.117599000
1	0.000000000	0.764267000	-0.470396000
1	0.000000000	-0.764267000	-0.470396000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral Glycine (Escf: -284.2643)

6	0.000000000	0.542833000	0.000000000
8	1.187253000	0.792838000	0.000000000
8	-0.937898000	1.494713000	0.000000000
1	-0.514655000	2.370085000	0.000000000
6	-0.592114000	-0.841176000	0.000000000
1	-1.245447000	-0.908034000	0.870922000
7	0.372914000	-1.915527000	0.000000000
1	0.976496000	-1.827842000	0.812526000
1	0.976496000	-1.827842000	-0.812526000
1	-1.245447000	-0.908034000	-0.870922000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral *cis* Diglycine (Escf: -492.1401)

7	-3.396862000	-0.925566000	-0.000074000
6	-1.951652000	-0.877164000	-0.000210000
6	-1.366493000	0.520060000	-0.000098000
7	-0.025288000	0.606985000	0.000187000
6	0.872191000	-0.520397000	0.000516000
6	2.292143000	-0.036617000	0.000122000
8	2.622311000	1.128936000	-0.000278000
8	3.153271000	-1.048886000	0.000038000
8	-2.083235000	1.526351000	-0.000224000
1	-3.744760000	-0.419102000	0.809424000
1	-3.744907000	-0.419101000	-0.809507000
1	-1.558093000	-1.405477000	0.870876000
1	-1.558296000	-1.405218000	-0.871547000
1	0.394914000	1.531096000	0.000330000
1	0.743392000	-1.155564000	0.879884000
1	0.743098000	-1.156275000	-0.878283000
1	4.063792000	-0.706799000	-0.000230000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral *trans* Diglycine (Escf: -492.1425)

6	2.347584000	-0.160537000	-0.000061000
8	2.397339000	-1.371581000	-0.000264000
8	3.423912000	0.619902000	-0.000373000
1	4.227117000	0.071141000	-0.000629000
6	1.079370000	0.638230000	0.000656000
1	1.088036000	1.288895000	0.877816000
7	-0.055782000	-0.244684000	0.000605000
1	0.118758000	-1.243056000	0.000932000
1	1.087391000	1.289688000	-0.875904000
1	-3.874162000	0.301685000	-0.810501000
7	-3.751441000	-0.299190000	-0.000248000
6	-2.404926000	-0.827059000	-0.000072000
1	-2.251406000	-1.463144000	0.872686000
1	-2.251156000	-1.463187000	-0.872761000
6	-1.311835000	0.225020000	0.000041000
8	-1.556332000	1.435415000	-0.000333000
1	-3.874529000	0.301281000	0.810247000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized pre-TS1A for formation of INT1 (Escf: -568.5314)

6	-1.503800000	-0.459440000	-0.551979000
8	-0.722857000	0.045993000	-1.332045000
8	-1.628651000	-1.782501000	-0.416251000
1	-1.014230000	-2.227089000	-1.025336000
6	-2.468511000	0.297585000	0.306462000
1	-3.458235000	0.100924000	-0.124729000
7	-2.108331000	1.699809000	0.380782000
1	-2.838631000	2.207544000	0.868963000
1	-2.055109000	2.083041000	-0.558729000
1	-2.467779000	-0.155413000	1.296854000
6	1.953023000	0.337731000	-0.084209000
8	1.754958000	1.463255000	0.323350000
8	2.562440000	0.088032000	-1.246395000
1	2.808509000	0.928182000	-1.669254000
6	1.604047000	-0.918988000	0.652665000
1	1.124812000	-1.599168000	-0.053065000
7	0.728809000	-0.639392000	1.773039000
1	1.165820000	0.044915000	2.383497000
1	0.593020000	-1.486283000	2.314790000
1	2.562799000	-1.379133000	0.923357000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT1 (Escf: -568.5172)

6	-1.098275000	-0.502490000	-0.253530000
8	-0.357197000	-0.271644000	-1.285093000
8	-1.522710000	-1.839872000	-0.106740000
1	-0.923634000	-2.371991000	-0.651510000
6	-2.302888000	0.405169000	-0.043350000
1	-2.985267000	0.197332000	-0.873815000
7	-1.839262000	1.782450000	0.024981000
1	-2.619090000	2.416336000	0.160157000
1	-1.393855000	2.023544000	-0.856620000
1	-2.809750000	0.139760000	0.885566000
6	1.920219000	0.263109000	0.093575000
8	1.731714000	1.459509000	0.155991000
8	2.883608000	-0.298097000	-0.627142000
1	3.398341000	0.391502000	-1.081400000
6	1.144999000	-0.740425000	0.899134000
1	1.121838000	-1.706582000	0.401291000
7	-0.217327000	-0.248732000	1.087026000
1	-0.226108000	0.771621000	1.220397000
1	-0.677253000	-0.700176000	1.878283000
1	1.643249000	-0.848710000	1.862498000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT1 in Electrostatic Pressure environment of 32 (Escf: -568.5153)

6	-1.098441000	-0.502126000	-0.254682000
8	-0.353357000	-0.275491000	-1.281907000
8	-1.523031000	-1.838993000	-0.103050000
1	-0.935905000	-2.368362000	-0.663146000
6	-2.300717000	0.409420000	-0.048579000
1	-2.978625000	0.205361000	-0.883639000
7	-1.830545000	1.784148000	0.024343000
1	-2.608564000	2.425169000	0.132648000
1	-1.356530000	2.014751000	-0.845272000
1	-2.814246000	0.144147000	0.876774000
6	1.915975000	0.261319000	0.092989000
8	1.731734000	1.457866000	0.159060000
8	2.875111000	-0.301566000	-0.632814000
1	3.385694000	0.388138000	-1.091338000
6	1.142304000	-0.740642000	0.902534000
1	1.115806000	-1.707083000	0.405411000
7	-0.218462000	-0.246272000	1.092139000
1	-0.226427000	0.774612000	1.221642000
1	-0.679847000	-0.696097000	1.883107000
1	1.643316000	-0.848125000	1.864555000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT1 with UltraFine Grid Integration
(Escf: -568.5172)

6	-1.098275000	-0.502490000	-0.253530000
8	-0.357197000	-0.271644000	-1.285093000
8	-1.522710000	-1.839872000	-0.106740000
1	-0.923634000	-2.371991000	-0.651510000
6	-2.302888000	0.405169000	-0.043350000
1	-2.985267000	0.197332000	-0.873815000
7	-1.839262000	1.782450000	0.024981000
1	-2.619090000	2.416336000	0.160157000
1	-1.393855000	2.023544000	-0.856620000
1	-2.809750000	0.139760000	0.885566000
6	1.920219000	0.263109000	0.093575000
8	1.731714000	1.459509000	0.155991000
8	2.883608000	-0.298097000	-0.627142000
1	3.398341000	0.391502000	-1.081400000
6	1.144999000	-0.740425000	0.899134000
1	1.121838000	-1.706582000	0.401291000
7	-0.217327000	-0.248732000	1.087026000
1	-0.226108000	0.771621000	1.220397000
1	-0.677253000	-0.700176000	1.878283000
1	1.643249000	-0.848710000	1.862498000

PCM| Atomic positions in Å of MN15/Def2TZVPP optimized INT1 with 4x H2O(Escf: -874.1087)

6	-0.458276000	0.123472000	-0.958764000
8	0.701438000	0.054889000	-1.514714000
8	-1.338630000	-0.917578000	-1.343016000
1	-0.792427000	-1.547311000	-1.835674000
6	-1.235953000	1.435167000	-1.049199000
1	-1.386448000	1.613111000	-2.120239000
7	-0.513072000	2.480854000	-0.348478000
1	-1.043517000	3.343487000	-0.323459000
1	0.377326000	2.669903000	-0.802878000
1	-2.219773000	1.301956000	-0.591999000
6	1.648306000	-1.643675000	0.285443000
8	2.635055000	-1.006916000	0.584658000
8	1.682628000	-2.700013000	-0.515483000
1	2.590576000	-2.828471000	-0.836398000
6	0.279196000	-1.439974000	0.904291000
1	-0.418485000	-2.184612000	0.534695000
7	-0.266845000	-0.108216000	0.623101000
1	0.363587000	0.641724000	0.946495000
1	-1.166177000	0.018195000	1.114875000
1	0.395028000	-1.559363000	1.980930000
8	-4.108411000	-0.788529000	-0.426633000
1	-3.255358000	-0.936778000	-0.863047000
1	-3.867451000	-0.456069000	0.450776000
8	-2.842286000	0.255247000	2.032506000
1	-3.046684000	1.167503000	2.270085000
1	-2.946778000	-0.261478000	2.840158000
8	2.071547000	1.383444000	1.842049000
1	2.272533000	1.600855000	2.757937000
1	2.484171000	0.523134000	1.644564000
8	2.595078000	1.986267000	-1.022031000
1	2.590066000	2.039507000	-0.055919000
1	1.958228000	1.261821000	-1.222587000

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized INT1 with 4x H2O(Escf: -874.0937)

6	-0.283489000	-0.093990000	-1.027550000
8	0.859437000	0.437960000	-1.283097000
8	-0.482505000	-1.357670000	-1.626973000
1	0.386754000	-1.603151000	-1.976330000
6	-1.546493000	0.717408000	-1.323437000
1	-1.476467000	0.951739000	-2.389448000
7	-1.646026000	1.889450000	-0.459909000
1	-2.376896000	2.510388000	-0.791606000
1	-0.777780000	2.425502000	-0.477825000
1	-2.425805000	0.084832000	-1.172993000
6	2.047608000	-1.130593000	0.458679000
8	2.755613000	-0.323266000	1.007659000
8	2.481011000	-1.934282000	-0.517532000
1	3.380500000	-1.655619000	-0.749893000
6	0.633874000	-1.471233000	0.899098000
1	0.293590000	-2.395924000	0.443149000
7	-0.319282000	-0.408661000	0.556661000
1	-0.049155000	0.476950000	1.037034000
1	-1.256469000	-0.700710000	0.861569000
1	0.656869000	-1.584214000	1.982141000
8	-2.491969000	-2.370840000	0.361678000
1	-2.173849000	-2.274763000	-0.546327000
1	-3.104530000	-1.639913000	0.526347000
8	-3.122346000	0.342150000	1.349525000
1	-2.611835000	1.074742000	0.933813000
1	-3.360810000	0.622215000	2.237074000
8	0.941291000	1.761623000	1.883504000
1	1.089700000	2.402623000	1.162532000
1	1.750699000	1.227757000	1.886442000
8	1.254143000	2.958023000	-0.624542000
1	1.923043000	3.447318000	-1.108262000
1	1.223190000	2.025563000	-0.977194000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT2 (Escf: -568.5312)

7	-3.253761000	-0.749743000	-0.194604000
6	-2.119371000	-0.534361000	0.681734000
6	-0.982814000	0.265681000	0.048839000
7	0.022720000	0.523646000	1.039640000
6	1.300710000	0.928762000	0.501141000
6	2.171876000	-0.219947000	0.065644000
8	1.946823000	-1.389846000	0.300040000
8	3.264354000	0.191488000	-0.577822000
8	-1.421547000	1.507888000	-0.432895000
8	-0.496087000	-0.412057000	-1.098732000
1	-3.695652000	0.138406000	-0.415595000
1	-2.937260000	-1.153628000	-1.072311000
1	-2.445859000	-0.007140000	1.577224000
1	-1.705650000	-1.496375000	0.994385000
1	-1.986765000	1.350579000	-1.203128000
1	-0.166956000	-1.282618000	-0.829228000
1	0.127842000	-0.296574000	1.632106000
1	1.877943000	1.483933000	1.243504000
1	1.159941000	1.599993000	-0.345071000
1	3.818954000	-0.574490000	-0.806013000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized PEP1 (Escf: -492.1078)

7	2.921813000	-0.978790000	-0.054304000
6	2.535498000	0.387796000	0.232879000
6	1.085012000	0.636564000	-0.059238000
8	0.566599000	1.680148000	-0.322104000
1	3.294551000	-1.059708000	-0.993837000
1	2.644544000	0.590337000	1.301694000
1	3.099581000	1.156328000	-0.296600000
7	0.243465000	-0.573322000	0.054288000
6	-0.974864000	-0.575145000	-0.790420000
6	-2.148567000	-0.158224000	0.098557000
8	-3.245316000	0.017101000	-0.464348000
8	-1.883977000	-0.055378000	1.325860000
1	3.629839000	-1.297925000	0.595334000
1	-0.182712000	-0.544681000	1.021708000
1	0.868976000	-1.387628000	-0.046199000
1	-0.855598000	0.109809000	-1.624465000
1	-1.137041000	-1.582661000	-1.163442000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized PEP2 (Escf: -492.1298)

7	-3.150232000	0.623125000	0.089676000
6	-2.321048000	-0.385747000	-0.541441000
6	-0.961457000	-0.323036000	0.101332000
8	-0.810746000	0.575131000	1.013460000
1	-1.722185000	1.014899000	1.046217000
1	-3.488998000	1.307191000	-0.575332000
1	-2.709635000	-1.395395000	-0.417200000
1	-2.192721000	-0.212724000	-1.609149000
7	0.013715000	-1.118702000	-0.206412000
6	1.346766000	-0.977805000	0.351467000
6	2.107030000	0.253446000	-0.164449000
8	3.256113000	0.385431000	0.321870000
8	1.546165000	1.001913000	-0.994468000
1	-3.938750000	0.216398000	0.577797000
1	-0.148261000	-1.784878000	-0.954594000
1	1.280621000	-0.907642000	1.436031000
1	1.915548000	-1.869752000	0.105029000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS1A for formation of INT1 (Escf: -568.5155)

6	-1.185411000	-0.511494000	-0.338801000
8	-0.423219000	-0.283061000	-1.308718000
8	-1.586936000	-1.820309000	-0.124562000
1	-0.989348000	-2.386503000	-0.637409000
6	-2.306653000	0.441912000	0.007326000
1	-3.079468000	0.269728000	-0.751416000
7	-1.801403000	1.804518000	0.036729000
1	-2.570673000	2.458628000	0.132880000
1	-1.344803000	2.001887000	-0.850342000
1	-2.728213000	0.171792000	0.975233000
6	1.933202000	0.254511000	0.077341000
8	1.721799000	1.447906000	0.126493000
8	2.899874000	-0.289409000	-0.657279000
1	3.392152000	0.410704000	-1.119715000
6	1.188160000	-0.764273000	0.889421000
1	1.114009000	-1.697325000	0.330358000
7	-0.134020000	-0.264659000	1.203563000
1	-0.131371000	0.741564000	1.375670000
1	-0.566093000	-0.760311000	1.978247000
1	1.783832000	-0.954122000	1.785254000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS2A (Escf: -568.5155)

7	-2.218793000	1.354304000	-0.747234000
6	-1.707926000	1.051863000	0.573343000
6	-0.827777000	-0.161366000	0.572783000
8	-0.357243000	-0.692572000	1.551292000
8	-2.333370000	-1.476966000	-0.264104000
1	-2.254114000	-2.177452000	0.393661000
1	-2.951606000	0.691003000	-0.980628000
1	-2.608727000	2.289434000	-0.767563000
1	-1.063829000	1.870229000	0.907250000
1	-2.462129000	0.890291000	1.346341000
7	-0.180600000	-0.438253000	-0.762351000
6	1.206762000	-0.889154000	-0.685259000
6	2.064754000	0.214499000	-0.134013000
8	3.320375000	-0.172230000	0.035763000
8	1.650055000	1.326039000	0.109832000
1	3.853533000	0.566310000	0.378573000
1	-0.319436000	0.391364000	-1.353909000
1	-0.883510000	-1.179206000	-1.053402000
1	1.275180000	-1.766298000	-0.046628000
1	1.556979000	-1.157251000	-1.679980000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS2B (Escf: -568.4761)

1	4.284457000	-0.765701000	0.000083000
8	3.370278000	-1.087595000	0.084948000
6	2.522445000	-0.072550000	-0.050111000
8	2.867709000	1.073654000	-0.233396000
6	1.094764000	-0.531775000	0.022081000
1	0.923167000	-1.189668000	-0.832738000
1	0.955820000	-1.117990000	0.930003000
7	0.194999000	0.613483000	0.020578000
1	0.456766000	1.294053000	-0.692594000
6	-1.308835000	0.361101000	0.053803000
8	-1.478144000	0.699365000	1.376642000
6	-1.736021000	-1.045327000	-0.325670000
1	-1.477874000	-1.227461000	-1.369759000
1	-1.178842000	-1.753176000	0.285954000
7	-3.159245000	-1.257821000	-0.122632000
1	-3.676757000	-0.575026000	-0.669790000
1	-3.380141000	-1.067409000	0.851963000
8	-1.928197000	1.259796000	-0.823887000
1	-2.016555000	2.104341000	-0.357826000
1	-0.227599000	0.977954000	1.134018000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3B (Escf: -568.5155)

1	-3.994293000	-0.243400000	-0.841405000
8	-3.401794000	0.394077000	-0.406955000
6	-2.286486000	-0.219196000	-0.021270000
8	-2.066912000	-1.394909000	-0.200924000
6	-1.354332000	0.745389000	0.667251000
1	-1.175031000	1.588333000	-0.000872000
1	-1.853081000	1.127204000	1.555327000
7	-0.105007000	0.132402000	1.047941000
1	0.073416000	-0.060701000	2.027275000
6	0.857070000	-0.092709000	0.187967000
8	0.544057000	-0.025781000	-1.101332000
6	2.088236000	-0.829429000	0.639297000
1	2.413690000	-0.391724000	1.581547000
1	1.755033000	-1.847748000	0.857018000
7	3.166212000	-0.866097000	-0.317655000
1	3.371794000	0.090217000	-0.596570000
1	2.867637000	-1.363211000	-1.151761000
8	2.017304000	1.730127000	-0.266802000
1	1.298500000	2.366434000	-0.166263000
1	1.245736000	0.618020000	-1.407661000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS2C (Escf: -568.5096)

6	2.254840000	0.128502000	0.034795000
8	1.763687000	1.253194000	-0.306103000
8	3.391455000	-0.043457000	0.492438000
1	-0.297877000	-1.812968000	-1.031291000
6	1.416186000	-1.126728000	-0.142429000
1	1.968730000	-1.823688000	-0.767933000
7	0.095989000	-0.901317000	-0.774060000
1	0.189661000	-0.365667000	-1.643716000
1	1.249265000	-1.585825000	0.828398000
1	-3.293985000	1.205538000	0.107955000
7	-3.404985000	0.205117000	0.251395000
6	-2.343893000	-0.508549000	-0.424892000
1	-2.490979000	-1.585822000	-0.313621000
1	-2.349717000	-0.281410000	-1.489786000
6	-0.967592000	-0.221703000	0.152948000
8	-0.729211000	-0.301648000	1.361933000
1	-3.335136000	0.039898000	1.252213000
8	-0.675177000	1.354699000	-0.411506000
1	0.395248000	1.404861000	-0.368564000
1	-1.035526000	1.947043000	0.268380000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3C (Escf: -568.4969)

6	2.324625000	0.143026000	-0.044208000
8	1.807349000	1.295835000	-0.207774000
8	3.535003000	-0.067296000	0.142510000
1	0.105679000	-0.672407000	-1.655060000
6	1.407450000	-1.077343000	-0.056157000
1	1.930218000	-1.877321000	-0.575564000
7	0.105023000	-0.888524000	-0.664873000
1	-1.838305000	-0.456748000	1.698996000
1	1.280090000	-1.401106000	0.976057000
1	-3.061912000	1.311795000	0.166936000
7	-3.334178000	0.374232000	-0.110784000
6	-2.251027000	-0.320062000	-0.762437000
1	-2.536064000	-1.357843000	-0.934628000
1	-2.032935000	0.128556000	-1.731027000
6	-0.948440000	-0.365314000	0.009431000
8	-1.001790000	-0.743075000	1.296856000
1	-3.675452000	-0.127435000	0.702592000
8	-0.633777000	1.353787000	0.129638000
1	0.421399000	1.382789000	-0.010326000
1	-0.838555000	1.673914000	1.022013000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS(Neut)1 (Escf: -492.1072)

7	2.846361000	-1.066308000	-0.185689000
6	2.528328000	0.255458000	0.316715000
6	1.110100000	0.657383000	0.025297000
8	0.689690000	1.781125000	-0.008195000
1	3.269348000	-1.011746000	-1.105561000
1	2.606183000	0.269528000	1.406606000
1	3.163439000	1.060236000	-0.055975000
7	0.202912000	-0.459929000	-0.158093000
6	-1.017756000	-0.205669000	-0.950483000
6	-2.153243000	-0.192971000	0.076623000
8	-3.306348000	0.059386000	-0.289588000
8	-1.753874000	-0.467945000	1.254054000
1	3.495431000	-1.538879000	0.431239000
1	-0.360651000	-0.613474000	0.814250000
1	0.757460000	-1.289153000	-0.408069000
1	-0.952380000	0.748135000	-1.466132000
1	-1.164062000	-1.006730000	-1.668965000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS(Neut)2 (Escf: -492.1080)

7	2.842288000	-0.943913000	-0.254407000
6	2.377393000	0.430202000	-0.246901000
6	0.963036000	0.472071000	0.224273000
8	0.644140000	-0.117662000	1.367400000
1	0.430821000	-1.060165000	1.243968000
1	2.605807000	-1.390222000	-1.134046000
1	2.945578000	1.001045000	0.490207000
1	2.452117000	0.951686000	-1.202726000
7	0.050227000	1.131142000	-0.398567000
6	-1.353187000	1.074239000	-0.027840000
6	-1.947425000	-0.340473000	-0.171822000
8	-3.179072000	-0.399247000	0.042740000
8	-1.179627000	-1.284459000	-0.463856000
1	3.849920000	-0.969499000	-0.153581000
1	0.316831000	1.604767000	-1.258635000
1	-1.469862000	1.381905000	1.009595000
1	-1.901245000	1.764593000	-0.660496000

Scenario III

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine (Escf: -284.2690)

6	0.000000000	0.710834000	0.000000000
8	1.252336000	0.666492000	0.000000000
8	-0.728903000	1.728497000	0.000000000
6	-0.740436000	-0.622522000	0.000000000
1	-1.365585000	-0.703330000	0.884543000
7	0.224144000	-1.749158000	0.000000000
1	0.832550000	-1.691346000	0.820648000
1	0.832550000	-1.691346000	-0.820648000
1	-1.365585000	-0.703330000	-0.884543000
1	-0.247794000	-2.656327000	0.000000000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized *trans* Zwitterionic Diglycine (Escf: -492.1460)

6	2.507862000	0.125427000	0.028870000
8	2.421759000	1.377624000	0.019190000
8	3.564380000	-0.550896000	0.066628000
1	-4.336833000	0.766398000	-0.136124000
6	1.209777000	-0.677578000	-0.008271000
1	1.222734000	-1.319052000	-0.890939000
7	0.067519000	0.206509000	-0.030367000
1	0.280299000	1.200001000	-0.014596000
1	1.180053000	-1.329375000	0.866231000
1	-3.629497000	0.125932000	1.221534000
7	-3.544689000	0.218182000	0.205781000
6	-2.253773000	0.831667000	-0.172913000
1	-2.326105000	1.173493000	-1.202597000
1	-2.049063000	1.679677000	0.472367000
6	-1.182072000	-0.233547000	-0.078957000
8	-1.499287000	-1.428787000	-0.081528000
1	-3.586973000	-0.729253000	-0.190464000

PCM| Atomic positions in Å of MN15/Def2TZVPP optimized INT3 with 4x H2O(Escf: -874.1188)

6	1.107769000	0.359955000	-0.439827000
8	1.187716000	0.931379000	0.714652000
8	2.267137000	0.459854000	-1.265447000
1	2.575419000	1.374030000	-1.201300000
6	-0.084252000	0.830464000	-1.315519000
1	0.272289000	1.679918000	-1.892203000
7	-1.233642000	1.298774000	-0.493530000
1	-1.210739000	2.324180000	-0.437665000
1	-1.154718000	0.999905000	0.493438000
1	-0.431382000	0.062194000	-2.000909000
6	-1.235242000	-1.642866000	0.424139000
8	-1.470403000	-1.882311000	-0.787958000
8	-2.058683000	-1.358322000	1.314720000
1	-2.140282000	0.949816000	-0.875144000
6	0.243711000	-1.700845000	0.817073000
1	0.465705000	-1.108804000	1.699128000
7	1.073585000	-1.210479000	-0.295361000
1	0.717877000	-1.635113000	-1.158727000
1	2.064741000	-1.485163000	-0.158861000
1	0.509794000	-2.738747000	1.012728000
8	0.363766000	3.507167000	0.158822000
1	0.309609000	4.146823000	0.875634000
1	0.789322000	2.700473000	0.523790000
8	3.902598000	-1.563315000	0.035029000
1	4.286624000	-1.480669000	0.914939000
1	3.933564000	-0.679964000	-0.359227000
8	-3.380265000	-0.141799000	-1.560869000
1	-4.202579000	-0.164438000	-1.060149000
1	-2.863450000	-0.938551000	-1.292728000
8	-1.000841000	0.959035000	2.517931000
1	-1.380730000	0.072344000	2.364138000
1	-0.100778000	0.929943000	2.145122000

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized INT3 with 4x H2O(Escf: -874.1000)

6	1.334299000	0.015842000	-0.563924000
8	1.689770000	0.475727000	0.592111000
8	2.331683000	-0.215361000	-1.512008000
1	3.119536000	-0.517226000	-1.030946000
6	0.270413000	0.849221000	-1.296414000
1	0.817381000	1.631866000	-1.814983000
7	-0.660418000	1.489196000	-0.331597000
1	-0.387524000	2.470973000	-0.200826000
1	-0.588407000	1.096992000	0.626622000
1	-0.302197000	0.260901000	-2.007953000
6	-1.649173000	-1.391179000	0.111611000
8	-1.723714000	-1.493320000	-1.135677000
8	-2.553834000	-1.091965000	0.914131000
1	-1.658099000	1.391650000	-0.641917000
6	-0.251732000	-1.633695000	0.706379000
1	-0.020072000	-0.921216000	1.496971000
7	0.751675000	-1.489975000	-0.358377000
1	0.299152000	-1.794704000	-1.231266000
1	1.599305000	-2.031387000	-0.161070000
1	-0.215381000	-2.640999000	1.119576000
8	1.408955000	3.172365000	0.245849000
1	1.966872000	3.825648000	0.672729000
1	1.717473000	2.277743000	0.515574000
8	3.366128000	-1.553262000	0.822796000
1	2.895200000	-0.718225000	1.062567000
1	4.041121000	-1.735624000	1.480760000
8	-3.214375000	0.820343000	-1.234994000
1	-3.727942000	0.669013000	-0.431032000
1	-2.902691000	-0.084377000	-1.453804000
8	-1.569796000	0.975828000	2.287869000
1	-2.048575000	0.155710000	2.023782000
1	-1.345315000	0.904754000	3.218516000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT3 (Escf: -568.5254)

6	1.231409000	-0.405945000	0.220911000
8	0.651646000	-0.327771000	1.354872000
8	2.192190000	-1.420842000	0.065319000
1	1.969901000	-2.108903000	0.710616000
6	1.872176000	0.886224000	-0.291338000
1	2.822807000	1.020807000	0.216481000
7	0.975183000	2.003414000	0.077822000
1	1.288298000	2.888668000	-0.323152000
1	0.947110000	2.086632000	1.097045000
1	2.031040000	0.892146000	-1.366307000
6	-1.985592000	0.051118000	-0.022046000
8	-1.593178000	1.162786000	-0.481387000
8	-2.996807000	-0.137533000	0.682346000
1	-0.008473000	1.793442000	-0.225678000
6	-1.188934000	-1.185813000	-0.413245000
1	-1.044213000	-1.825999000	0.452110000
7	0.115585000	-0.815520000	-0.968044000
1	-0.022738000	-0.029626000	-1.609078000
1	0.532611000	-1.586594000	-1.489618000
1	-1.756883000	-1.732467000	-1.165752000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT4 (Escf: -568.5310)

7	-1.883129000	1.713099000	-0.375110000
6	-2.322303000	0.341498000	-0.187945000
6	-1.121680000	-0.508133000	0.186901000
8	-0.519411000	-0.109664000	1.361231000
8	-1.497424000	-1.828263000	0.264875000
1	-0.850882000	-2.317945000	0.796836000
1	0.159676000	0.589212000	1.166592000
1	-2.579389000	2.246245000	-0.882816000
1	-3.058310000	0.198313000	0.606583000
1	-2.742497000	-0.042401000	-1.116974000
7	-0.112071000	-0.335816000	-0.944032000
6	1.266713000	-0.817493000	-0.682458000
6	2.122583000	0.252493000	-0.008122000
8	3.339641000	0.009923000	0.065775000
8	1.524779000	1.282196000	0.416967000
1	-1.739979000	2.163974000	0.523511000
1	-0.107706000	0.682752000	-1.129283000
1	-0.509446000	-0.807916000	-1.761902000
1	1.226299000	-1.707982000	-0.056037000
1	1.716062000	-1.088956000	-1.633555000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT5 (Escf: -568.5359)

7	-2.054935000	1.625704000	-0.399460000
6	-2.345324000	0.177349000	-0.289528000
6	-1.058630000	-0.514781000	0.141854000
8	-0.572313000	0.060942000	1.314092000
8	-1.434300000	-1.843620000	0.406111000
1	-0.688871000	-2.296872000	0.826579000
1	0.233665000	0.614095000	1.090455000
1	-2.835683000	2.143467000	-0.808480000
1	-3.118174000	0.032961000	0.458375000
1	-2.679670000	-0.186683000	-1.256887000
7	-0.088530000	-0.361832000	-0.913706000
6	1.266906000	-0.816927000	-0.618184000
6	2.178840000	0.252271000	-0.021253000
8	3.410230000	0.068680000	-0.136219000
8	1.639337000	1.232148000	0.574834000
1	-1.850695000	2.014117000	0.526204000
1	-1.218105000	1.759548000	-0.980084000
1	-0.446564000	-0.829637000	-1.741174000
1	1.288650000	-1.670458000	0.071937000
1	1.725317000	-1.160310000	-1.542642000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT6 (Escf: -568.5179)

6	2.394391000	0.088497000	-0.029408000
8	1.929718000	1.324475000	-0.116729000
8	3.595381000	-0.120508000	-0.013886000
1	-4.179817000	0.225548000	-0.482810000
6	1.380489000	-1.031208000	0.052366000
1	1.899685000	-1.934652000	-0.264769000
7	0.147130000	-0.834524000	-0.683164000
1	0.295408000	-0.309442000	-1.541691000
1	1.130644000	-1.160951000	1.109029000
1	-3.122239000	1.355683000	0.132761000
7	-3.262537000	0.360062000	-0.056433000
6	-2.152802000	-0.175296000	-0.876610000
1	-2.431248000	-1.169528000	-1.211760000
1	-1.978116000	0.480928000	-1.724574000
6	-0.954104000	-0.269035000	0.076584000
8	-1.248025000	-0.895239000	1.196264000
1	-3.208203000	-0.140891000	0.844389000
8	-0.631665000	1.158846000	0.385841000
1	0.933943000	1.339879000	0.016995000
1	-0.703328000	1.216325000	1.350098000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS1D (Escf: -568.5363)

6	-1.231628000	0.876792000	0.347894000
8	-0.731836000	0.531966000	1.397199000
8	-0.987603000	2.026605000	-0.256443000
1	-0.240323000	2.467981000	0.191696000
6	-2.233397000	0.029880000	-0.391747000
1	-3.235440000	0.265934000	-0.039549000
7	-1.924015000	-1.385569000	-0.109771000
1	-2.633555000	-2.009861000	-0.497697000
1	-1.851551000	-1.547915000	0.899411000
1	-2.171473000	0.200959000	-1.460980000
6	1.243549000	-0.944873000	-0.162994000
8	0.543977000	-0.679416000	-1.183158000
8	1.140415000	-2.001661000	0.507203000
1	-0.993795000	-1.588114000	-0.534176000
6	2.286734000	0.065688000	0.283588000
1	2.276033000	0.081290000	1.374231000
7	2.050139000	1.399242000	-0.257260000
1	1.677893000	1.295580000	-1.197937000
1	2.924067000	1.909078000	-0.329225000
1	3.254112000	-0.355507000	-0.015416000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS2D (Escf: -568.5249)

6	1.318192000	-0.389235000	0.277145000
8	0.715539000	-0.343448000	1.374888000
8	2.227338000	-1.409891000	0.048313000
1	2.011629000	-2.128518000	0.662673000
6	1.889058000	0.899724000	-0.292852000
1	2.844399000	1.094290000	0.188640000
7	0.952802000	1.991315000	0.046186000
1	1.217534000	2.867391000	-0.406216000
1	0.946473000	2.131752000	1.059369000
1	2.029278000	0.860396000	-1.368637000
6	-2.010149000	0.045125000	-0.005494000
8	-1.619080000	1.175187000	-0.420547000
8	-3.028204000	-0.164579000	0.685344000
1	-0.033364000	1.728728000	-0.223333000
6	-1.207546000	-1.178468000	-0.422966000
1	-1.023203000	-1.798496000	0.452720000
7	0.064404000	-0.807846000	-1.027806000
1	-0.079183000	-0.027138000	-1.668968000
1	0.480835000	-1.581805000	-1.540811000
1	-1.816907000	-1.751896000	-1.123083000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3D (Escf: -568.5173)

7	-2.299621000	-1.529286000	-0.212045000
6	-2.266992000	-0.268282000	0.537970000
6	-1.067478000	0.500867000	-0.091847000
8	-0.677366000	-0.127924000	-1.194892000
8	-1.423761000	1.840681000	-0.261175000
1	-0.884602000	2.214673000	-0.973623000
1	-1.443228000	-1.127186000	-1.003404000
1	-1.993661000	-2.329705000	0.334314000
1	-3.172204000	0.300373000	0.355502000
1	-2.149873000	-0.430149000	1.605294000
7	0.085512000	0.498440000	0.932253000
6	1.382967000	0.925012000	0.366125000
6	2.213347000	-0.310140000	0.014283000
8	3.249229000	-0.100409000	-0.653018000
8	1.798611000	-1.411882000	0.452830000
1	-3.204894000	-1.725963000	-0.627401000
1	0.245112000	-0.482997000	1.223692000
1	-0.192216000	1.059326000	1.740325000
1	1.229058000	1.541185000	-0.515790000
1	1.920492000	1.507896000	1.110490000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3E (Escf: -568.4785)

7	-1.023229000	2.218393000	-0.043890000
6	-1.785011000	0.955846000	-0.257559000
6	-0.942884000	-0.156923000	0.316667000
8	-0.653593000	-0.227219000	1.487113000
8	-2.373581000	-1.674089000	-0.228886000
1	-2.507036000	-2.102181000	0.624991000
1	-0.032658000	2.062468000	-0.324345000
1	-1.427654000	2.990859000	-0.577207000
1	-2.723678000	1.013643000	0.280771000
1	-1.965916000	0.829513000	-1.319541000
7	-0.158519000	-0.951396000	-0.667042000
6	1.203437000	-1.266103000	-0.222822000
6	2.030049000	0.011172000	-0.086438000
8	3.184766000	-0.125685000	0.363032000
8	1.489036000	1.090478000	-0.454276000
1	-1.026616000	2.473694000	0.947518000
1	-0.134129000	-0.467374000	-1.567923000
1	-0.942787000	-1.732492000	-0.689801000
1	1.161814000	-1.789952000	0.727590000
1	1.664317000	-1.918988000	-0.960473000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3F (Escf: -568.4815)

7	3.092859000	1.025361000	-0.137710000
6	1.621234000	1.006801000	-0.315310000
6	1.175235000	-0.397169000	0.048686000
7	-0.304530000	-0.528467000	0.264567000
6	-1.200031000	0.620031000	0.118910000
6	-2.649208000	0.163150000	-0.050999000
8	-2.850981000	-1.051548000	-0.291386000
8	-3.515986000	1.065956000	0.032043000
8	1.557200000	-0.771830000	1.316686000
8	1.641092000	-1.252049000	-0.953868000
1	3.318271000	0.690418000	0.806640000
1	3.544796000	0.398338000	-0.809991000
1	1.193011000	1.733912000	0.367436000
1	1.386543000	1.263883000	-1.343973000
1	0.274519000	-0.835871000	1.347654000
1	1.716976000	-2.139374000	-0.571635000
1	-0.692057000	-1.309235000	-0.271681000
1	-0.948640000	1.197640000	-0.773652000
1	-1.122983000	1.275855000	0.983340000
1	3.477275000	1.965069000	-0.257644000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3G (Escf: -568.5067)

7	-1.019197000	1.992150000	0.212969000
6	-1.119187000	0.723286000	0.986385000
6	-1.299642000	-0.502782000	0.074150000
8	-1.655782000	-1.556069000	0.761191000
8	-2.234536000	-0.134162000	-0.954527000
1	-3.089743000	-0.464772000	-0.646190000
1	-1.705700000	1.960658000	-0.549788000
1	-1.215097000	2.805996000	0.799835000
1	-0.239905000	0.633385000	1.620713000
1	-2.008403000	0.786986000	1.606146000
7	-0.038322000	-0.700681000	-0.736054000
6	1.109438000	-1.168294000	0.044726000
6	2.128816000	-0.035492000	-0.032058000
8	3.204099000	-0.049708000	0.551240000
8	1.691627000	0.918302000	-0.802557000
1	-0.087043000	2.116099000	-0.195226000
1	0.673657000	0.374836000	-1.070686000
1	-0.275416000	-1.339622000	-1.491665000
1	0.843586000	-1.370254000	1.081882000
1	1.546875000	-2.070808000	-0.375426000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3I (Escf: -568.4901)

7	-3.051725000	0.313001000	-0.621770000
6	-2.108486000	0.915418000	0.324704000
6	-0.884850000	-0.000066000	0.476140000
8	-0.262412000	-0.049904000	1.552785000
8	-1.544095000	-1.436224000	0.044259000
1	-1.746914000	-1.907490000	0.869389000
1	-2.455719000	-0.964177000	-0.376213000
1	-4.016459000	0.458233000	-0.343898000
1	-1.779662000	1.913652000	0.038257000
1	-2.566637000	0.964126000	1.308603000
7	0.021529000	0.145629000	-0.761393000
6	1.232950000	-0.698988000	-0.682882000
6	2.387411000	0.130911000	-0.121355000
8	3.423603000	-0.500973000	0.176987000
8	2.198693000	1.370489000	-0.039897000
1	-2.929124000	0.660008000	-1.569241000
1	0.384164000	1.117555000	-0.732528000
1	-0.497999000	-0.005180000	-1.629369000
1	1.038486000	-1.561586000	-0.052199000
1	1.492775000	-1.036314000	-1.683380000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS4D (Escf: -568.5190)

7	2.734496000	-1.087966000	-0.648945000
6	2.172741000	-0.528927000	0.568295000
6	1.010437000	0.387605000	0.229279000
8	0.381127000	0.871358000	1.377773000
8	1.412494000	1.429657000	-0.617337000
1	2.192683000	1.864349000	-0.243490000
1	3.299275000	-0.391008000	-1.124332000
1	3.339029000	-1.871243000	-0.427766000
1	1.790769000	-1.329608000	1.199637000
1	2.876707000	0.064809000	1.164021000
7	-0.006778000	-0.369295000	-0.486997000
6	-1.196939000	0.384122000	-0.910346000
6	-2.332627000	-0.212894000	-0.078167000
8	-3.486101000	0.203064000	-0.155955000
8	-1.906595000	-1.171197000	0.670667000
1	1.041550000	1.281295000	1.954912000
1	-0.717368000	-1.070173000	0.283470000
1	0.454224000	-0.882806000	-1.238793000
1	-1.100931000	1.447011000	-0.702686000
1	-1.399037000	0.245704000	-1.968934000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS4E (Escf: -568.5178)

7	-1.346454000	1.808467000	-0.446396000
6	-2.195488000	0.664379000	-0.091232000
6	-1.199124000	-0.475067000	0.162639000
8	-0.568515000	-0.356193000	1.390515000
8	-1.861466000	-1.685692000	0.089944000
1	-1.268336000	-2.383784000	0.409007000
1	0.204946000	0.270307000	1.296557000
1	-1.782133000	2.444894000	-1.105968000
1	-2.804170000	0.826032000	0.793199000
1	-2.826199000	0.412467000	-0.940521000
7	-0.193572000	-0.283051000	-0.916917000
6	1.152567000	-0.834843000	-0.712896000
6	2.089750000	0.114890000	0.028774000
8	3.311770000	-0.086474000	-0.109182000
8	1.559669000	1.016595000	0.742987000
1	-1.028518000	2.325007000	0.370497000
1	-0.414890000	0.988742000	-0.899917000
1	-0.601541000	-0.656092000	-1.775178000
1	1.102145000	-1.773898000	-0.155206000
1	1.580991000	-1.053637000	-1.687104000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS4F (Escf: -568.4607)

7	1.844122000	1.844167000	-0.030755000
6	2.284182000	0.470247000	0.128238000
6	1.078886000	-0.413471000	-0.104909000
8	0.541037000	-0.446217000	-1.317352000
8	1.392326000	-1.861208000	-0.003490000
1	2.348657000	-2.056283000	0.025323000
1	0.951775000	-1.730032000	-1.062425000
1	2.549661000	2.483010000	0.317958000
1	3.054592000	0.145972000	-0.577388000
1	2.655753000	0.316088000	1.141111000
7	0.068872000	-0.141471000	0.980482000
6	-1.262067000	-0.743197000	0.744795000
6	-2.138040000	0.259154000	-0.006984000
8	-3.195575000	-0.192966000	-0.495135000
8	-1.730003000	1.446627000	-0.030398000
1	1.697074000	2.048978000	-1.014628000
1	-0.078007000	0.888306000	0.938930000
1	0.466858000	-0.396101000	1.888235000
1	-1.161433000	-1.670235000	0.188666000
1	-1.715931000	-0.954863000	1.710294000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS4G (Escf: -568.4676)

7	-1.265453000	2.051951000	0.220242000
6	-1.658053000	0.904428000	-0.575887000
6	-1.072027000	-0.362581000	0.064315000
8	-0.715141000	-0.157682000	1.345469000
8	-2.065754000	-1.477027000	-0.015179000
1	-2.328166000	-1.786788000	0.871592000
1	-0.852929000	0.821670000	1.473343000
1	-0.384090000	2.435152000	-0.104809000
1	-2.740457000	0.806829000	-0.548111000
1	-1.347202000	0.954788000	-1.619782000
7	-0.068047000	-1.121241000	-0.718154000
6	1.269457000	-1.213760000	-0.138546000
6	1.983745000	0.134589000	-0.078481000
8	3.082249000	0.148153000	0.528847000
8	1.435257000	1.105547000	-0.655692000
1	-1.979114000	2.769614000	0.213398000
1	-0.006214000	-0.724977000	-1.655463000
1	-1.135291000	-1.985652000	-0.496108000
1	1.217449000	-1.647682000	0.856082000
1	1.858890000	-1.885919000	-0.760719000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS5D (Escf: -568.5149)

7	-1.946928000	-1.661147000	-0.135885000
6	-2.260604000	-0.319065000	0.380984000
6	-1.040192000	0.514522000	-0.082765000
8	-0.535421000	-0.071350000	-1.194824000
8	-1.524008000	1.826227000	-0.320417000
1	-0.838275000	2.319196000	-0.792415000
1	-1.164095000	-1.222452000	-0.921314000
1	-1.488700000	-2.253090000	0.553920000
1	-3.152294000	0.047737000	-0.118241000
1	-2.400533000	-0.305016000	1.457565000
7	-0.034485000	0.504613000	0.986106000
6	1.267427000	0.967561000	0.546712000
6	2.091791000	-0.172737000	0.000140000
8	3.074100000	-0.023116000	-0.698992000
8	1.704471000	-1.380448000	0.397167000
1	-2.746869000	-2.148971000	-0.527689000
1	0.859521000	-1.239356000	0.885720000
1	-0.370698000	1.033588000	1.784963000
1	1.246325000	1.755698000	-0.210550000
1	1.821842000	1.356205000	1.402596000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS5E (Escf: -568.5168)

7	-2.227783000	-1.558483000	0.175798000
6	-2.366652000	-0.089118000	0.304153000
6	-1.025301000	0.504047000	-0.158313000
8	-0.595361000	-0.064833000	-1.280314000
8	-1.288927000	1.909377000	-0.326063000
1	-0.824609000	2.162540000	-1.135594000
1	-1.682248000	-1.691404000	-0.694304000
1	-1.686533000	-1.953041000	0.948518000
1	-3.143284000	0.230849000	-0.383592000
1	-2.633363000	0.169012000	1.325392000
7	-0.059173000	0.308613000	0.934641000
6	1.260120000	0.817649000	0.614900000
6	2.197079000	-0.215904000	0.038598000
8	3.367190000	0.021152000	-0.195456000
8	1.693312000	-1.422840000	-0.184576000
1	-3.124224000	-2.043134000	0.116917000
1	0.721252000	-1.358081000	-0.058353000
1	-0.405954000	0.749522000	1.781438000
1	1.239842000	1.651870000	-0.095023000
1	1.746618000	1.188062000	1.516777000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS5F (Escf: -568.4764)

7	-0.921776000	2.047337000	0.075346000
6	-1.832116000	0.949604000	-0.336836000
6	-1.102655000	-0.337476000	-0.004234000
8	-0.767830000	-0.485267000	1.290290000
8	-2.292941000	-1.422062000	0.103819000
1	-2.036271000	-2.228633000	-0.373772000
1	-1.743088000	-1.337829000	1.127197000
1	-1.142121000	2.920967000	-0.404047000
1	-2.757675000	1.022239000	0.224166000
1	-2.031559000	1.033218000	-1.401723000
7	-0.159612000	-0.698412000	-0.962846000
6	1.155158000	-1.111627000	-0.523703000
6	2.050626000	0.009647000	0.000524000
8	3.159341000	-0.342630000	0.461535000
8	1.646674000	1.205413000	-0.088795000
1	-0.999662000	2.203865000	1.082512000
1	0.088212000	1.767849000	-0.109485000
1	-0.147213000	-0.085447000	-1.769391000
1	1.072593000	-1.871626000	0.249790000
1	1.678473000	-1.571595000	-1.362045000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS5G (Escf: -568.4968)

7	1.955022000	1.667241000	0.036249000
6	2.273483000	0.316247000	-0.426604000
6	1.074480000	-0.572104000	-0.104772000
8	1.349809000	-1.876591000	0.166766000
8	0.605961000	0.063645000	1.276262000
1	1.043531000	-0.373556000	2.028668000
1	1.052502000	1.015518000	1.098788000
1	2.787609000	2.177920000	0.308966000
1	2.492479000	0.246724000	-1.490161000
1	3.126032000	-0.058910000	0.136197000
7	0.028668000	-0.447816000	-1.006537000
6	-1.280473000	-0.893255000	-0.547263000
6	-2.160987000	0.247634000	-0.034774000
8	-3.244054000	-0.099041000	0.501562000
8	-1.765548000	1.426663000	-0.212643000
1	1.459103000	2.204245000	-0.670374000
1	-0.043394000	0.511040000	-1.342327000
1	-1.822621000	-1.377496000	-1.360269000
1	-1.166886000	-1.633622000	0.242421000
1	2.177448000	-1.956382000	0.665006000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D (Escf: -568.5130)

6	2.344668000	0.117976000	-0.026622000
8	1.815339000	1.305903000	-0.149499000
8	3.557787000	-0.040631000	0.052694000
1	-4.129249000	0.361818000	-0.424300000
6	1.412157000	-1.076363000	0.024446000
1	1.967971000	-1.924509000	-0.371640000
7	0.146806000	-0.918919000	-0.655223000
1	0.223607000	-0.487937000	-1.571117000
1	1.212727000	-1.285238000	1.077226000
1	-2.898770000	1.366131000	0.106192000
7	-3.199941000	0.392027000	-0.001922000
6	-2.186356000	-0.336392000	-0.791609000
1	-2.560758000	-1.337754000	-0.989311000
1	-2.007882000	0.192571000	-1.722299000
6	-0.943981000	-0.429109000	0.081915000
8	-1.113851000	-0.805140000	1.280372000
1	-3.231113000	-0.026583000	0.935866000
8	-0.628492000	1.331571000	0.162143000
1	0.747866000	1.321829000	-0.037074000
1	-0.757635000	1.517624000	1.102012000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6E (Escf: -568.4974)

7	-3.007555000	0.481579000	-0.516251000
6	-2.032581000	0.872374000	0.526157000
6	-0.751590000	0.066548000	0.378581000
8	-0.031858000	-0.071681000	1.397678000
8	-1.654176000	-1.590754000	0.086332000
1	-1.900531000	-1.835297000	0.987009000
1	-2.849017000	-0.566551000	-0.540484000
1	-3.967388000	0.715603000	-0.261473000
1	-1.819155000	1.936951000	0.466571000
1	-2.463236000	0.633948000	1.493470000
7	-0.112343000	0.199324000	-0.863256000
6	1.108220000	-0.567744000	-0.960029000
6	2.239146000	-0.003924000	-0.144383000
8	3.103231000	-0.694649000	0.359662000
8	2.270306000	1.327514000	-0.090434000
1	-2.803792000	0.898138000	-1.426412000
1	3.053387000	1.604764000	0.415107000
1	-0.718450000	0.051241000	-1.662068000
1	0.982000000	-1.606524000	-0.645898000
1	1.446281000	-0.565557000	-1.997139000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6F (Escf: -568.4993)

7	1.379939000	1.824902000	0.089426000
6	2.166197000	0.623299000	-0.228515000
6	1.114031000	-0.504710000	-0.228231000
8	0.318515000	-0.518423000	-1.271156000
8	1.796491000	-1.726885000	0.000503000
1	1.230638000	-2.415978000	-0.377484000
1	-2.393983000	1.722166000	-0.617673000
1	1.912528000	2.558433000	0.545645000
1	2.657368000	0.669266000	-1.196713000
1	2.901762000	0.472815000	0.559514000
7	0.309165000	-0.149046000	1.027744000
6	-1.032856000	-0.701698000	0.999241000
6	-1.939440000	0.004270000	0.033180000
8	-2.836253000	-0.547381000	-0.572337000
8	-1.747381000	1.323323000	-0.010653000
1	0.908315000	2.197898000	-0.731038000
1	0.561678000	1.116563000	0.795033000
1	0.811823000	-0.467093000	1.854874000
1	-1.027294000	-1.759805000	0.735612000
1	-1.485134000	-0.597307000	1.987146000

Scenario IV

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral Glycine with 3x H2O(Escf: -513.4517)

6	0.012160000	-0.171194000	0.026031000
8	0.644366000	0.870440000	-0.015294000
8	0.542305000	-1.370666000	0.065202000
1	1.543142000	-1.346749000	0.052484000
6	-1.499649000	-0.199535000	0.034911000
1	-1.834747000	-0.798639000	-0.813763000
1	-1.827477000	-0.751406000	0.917416000
7	-2.125049000	1.106695000	0.001069000
1	-1.816703000	1.622398000	-0.816943000
1	-1.838527000	1.655635000	0.805031000
8	3.385577000	1.373906000	-0.090727000
1	3.664132000	1.960985000	0.616767000
1	2.408186000	1.355882000	-0.079640000
8	3.207320000	-1.330736000	0.041742000
1	3.672420000	-1.781869000	-0.667828000
8	-4.562137000	-0.451845000	-0.040111000
1	-5.447115000	-0.080799000	-0.064989000
1	-3.943944000	0.300698000	-0.027437000
1	3.481453000	-0.387414000	0.019266000

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral Glycine with 4x H2O(Escf: -589.8482)

6	-0.073250000	-0.492911000	-0.058850000
8	-0.700225000	0.508034000	0.269564000
8	-0.632153000	-1.606344000	-0.456026000
1	-1.633250000	-1.550058000	-0.479180000
6	1.436985000	-0.569279000	-0.042694000
1	1.713075000	-1.474792000	0.501887000
1	1.767357000	-0.751028000	-1.067655000
7	2.123667000	0.578445000	0.502182000
1	1.815904000	0.775070000	1.448324000
1	1.955452000	1.415341000	-0.050967000
8	-3.430118000	0.805435000	0.910847000
1	-3.790845000	1.667099000	0.686854000
1	-2.464565000	0.852703000	0.781579000
8	-3.284738000	-1.494964000	-0.518864000
1	-3.777467000	-2.233771000	-0.151466000
8	0.544581000	2.907276000	-0.762115000
1	0.184112000	3.110002000	-1.629146000
1	-0.021630000	2.217700000	-0.380639000
8	4.445323000	-1.104574000	0.164990000
1	5.351671000	-0.800342000	0.251223000
1	3.874793000	-0.337232000	0.354758000
1	-3.564054000	-0.685574000	-0.038753000

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral Glycine with 5x H2O(Escf: -666.2557)

6	0.117650000	0.662465000	0.573235000
8	0.446131000	1.180994000	-0.481119000
8	0.961304000	0.322291000	1.521118000
1	1.910906000	0.456285000	1.228539000
6	-1.319402000	0.332488000	0.908874000
1	-1.317370000	-0.579806000	1.509463000
1	-1.698622000	1.134705000	1.544926000
7	-2.156682000	0.188897000	-0.272405000
1	-1.561068000	0.016014000	-1.079627000
1	-2.646822000	1.056642000	-0.465833000
8	2.267007000	-0.798397000	-1.644699000
1	1.617824000	-1.436134000	-1.295958000
1	1.751024000	0.011045000	-1.761064000
8	3.418885000	0.351144000	0.542026000
1	4.178500000	-0.083002000	0.938386000
8	0.267414000	-2.230358000	-0.195593000
1	-0.668022000	-2.516262000	-0.190770000
1	0.535236000	-2.187778000	0.728148000
8	-1.719758000	3.102679000	-0.592220000
1	-1.508908000	4.037347000	-0.658835000
1	-0.898140000	2.617179000	-0.769440000
8	-2.482062000	-2.552367000	0.097374000
1	-3.159876000	-3.088675000	-0.320849000
1	-2.691484000	-1.607652000	-0.079754000
1	3.192736000	-0.129788000	-0.288242000

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral Glycine with 6x H2O(Escf: -742.6579)

6	0.603239000	-1.330644000	-0.709911000
8	0.720836000	-0.213706000	-1.409353000
8	-0.417021000	-1.984811000	-0.747562000
6	1.779576000	-1.718005000	0.165907000
1	1.657367000	-2.774675000	0.412508000
1	2.706153000	-1.581589000	-0.394632000
7	1.791719000	-0.831662000	1.328186000
1	0.916948000	-0.916594000	1.850197000
1	1.778172000	1.122653000	1.204341000
1	2.569279000	-1.054967000	1.938943000
8	-0.884198000	1.809567000	0.027839000
1	-1.836658000	1.947346000	-0.146457000
1	-0.566036000	1.230472000	-0.679011000
8	-3.600667000	1.539370000	-0.468381000
1	-4.067220000	1.743453000	-1.282586000
1	-3.538153000	0.567130000	-0.409799000
8	-2.995777000	-1.190238000	-0.183743000
1	-2.131063000	-1.469082000	-0.547836000
1	-3.564312000	-1.964954000	-0.194853000
8	-1.047016000	-0.299841000	2.026860000
1	-1.794797000	-0.776104000	1.643839000
1	-0.997519000	0.520130000	1.505334000
8	1.844265000	2.063333000	0.935390000
1	0.931749000	2.335874000	0.750428000
1	1.629150000	0.206338000	-1.347459000
8	3.043984000	1.004944000	-1.182308000
1	3.402785000	1.554246000	-1.884289000
1	2.749988000	1.594914000	-0.441874000

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Neutral Glycine with 7x H2O(Escf: -819.0544)

6	-0.177338000	-0.370135000	0.751665000
8	-0.259750000	-1.391265000	0.077593000
8	-1.153452000	0.057874000	1.517619000
1	-1.960617000	-0.528355000	1.455685000
6	1.050737000	0.505020000	0.800019000
1	0.749031000	1.468573000	1.215990000
1	1.742966000	0.050605000	1.514237000
7	1.716628000	0.658151000	-0.477350000
1	1.060249000	0.536301000	-1.245563000
1	2.509481000	0.030259000	-0.554718000
8	-2.581804000	-1.520770000	-1.436045000
1	-2.643369000	-2.133340000	-2.174120000
1	-1.688710000	-1.612905000	-1.047781000
8	3.771711000	-1.309908000	0.683022000
1	3.296708000	-2.010355000	0.197210000
1	4.705133000	-1.415095000	0.483939000
8	-3.393464000	-1.374591000	1.188543000
1	-4.226034000	-0.939221000	1.392164000
8	-1.004370000	1.075307000	-1.681124000
1	-1.248577000	1.826255000	-1.106027000
1	-1.786779000	0.519714000	-1.776335000
8	1.977972000	-2.889495000	-0.749468000
1	1.748361000	-3.783468000	-0.481686000
1	1.199627000	-2.337342000	-0.541581000
8	1.494317000	3.453764000	-0.228860000
1	1.790347000	4.015399000	-0.949628000
1	1.775429000	2.534149000	-0.446095000
1	-3.375892000	-1.536371000	0.224899000
8	-1.258378000	3.131474000	0.215855000
1	-1.331494000	2.662954000	1.053910000
1	-0.314913000	3.376751000	0.119765000

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 3x H2O(Escf: -513.4368)

6	0.317710000	-0.232389000	0.776939000
8	-0.637365000	-0.096046000	1.585579000
8	0.898739000	-1.266930000	0.425569000
6	0.757421000	1.097707000	0.117632000
1	1.658716000	1.479126000	0.590647000
1	0.937765000	0.967269000	-0.944224000
7	-0.389694000	2.013222000	0.353760000
1	-0.815912000	1.541667000	1.205086000
1	-1.079343000	1.856190000	-0.406981000
1	-0.156393000	2.993055000	0.479021000
8	3.134254000	-0.295453000	-0.897028000
1	2.431603000	-0.826610000	-0.469461000
1	3.908153000	-0.860782000	-0.950912000
8	-1.932487000	0.631808000	-1.415794000
1	-2.244643000	0.586024000	-2.322639000
1	-1.970277000	-0.285574000	-1.049085000
8	-1.904388000	-1.854638000	-0.234504000
1	-1.862053000	-1.502973000	0.670810000
1	-1.000557000	-2.181782000	-0.356581000

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 4x H2O(Escf: -589.8398)

6	0.850825000	0.379232000	0.956802000
8	1.135117000	1.170426000	0.010541000
8	1.611474000	-0.163079000	1.759789000
6	-0.644521000	0.021467000	1.067948000
1	-0.759083000	-0.911018000	1.612632000
1	-1.189392000	0.817738000	1.573247000
7	-1.208200000	-0.139914000	-0.300585000
1	-0.583729000	-0.791314000	-0.824667000
1	-1.202109000	0.784116000	-0.776739000
1	-2.169184000	-0.499315000	-0.266985000
8	3.170779000	-0.652191000	-0.548968000
1	2.817068000	0.247144000	-0.664936000
1	3.065308000	-0.749525000	0.413403000
8	0.792054000	-1.770508000	-1.321733000
1	0.902529000	-2.719726000	-1.414930000
1	1.681762000	-1.403656000	-1.084291000
8	-0.913683000	2.551671000	-0.901972000
1	-0.768306000	3.127254000	-1.656588000
1	-0.024634000	2.243829000	-0.580864000
8	-3.987354000	-1.043732000	0.121742000
1	-4.296451000	-1.884203000	0.472235000
1	-4.721300000	-0.426830000	0.198890000

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 5x H2O(Escf: -666.2564)

6	0.377194000	-0.144534000	-1.022437000
8	0.949682000	0.947006000	-0.810702000
8	-0.729752000	-0.340193000	-1.560127000
6	1.133751000	-1.402321000	-0.551744000
1	0.440915000	-2.230900000	-0.427120000
1	1.899871000	-1.662364000	-1.280659000
7	1.775338000	-1.117594000	0.758516000
1	0.980467000	-0.810536000	1.406666000
1	2.478422000	-0.356475000	0.648628000
1	2.240039000	-1.937966000	1.141609000
8	-0.878771000	2.094609000	1.085583000
1	-1.728607000	2.010343000	0.612480000
1	-0.214175000	2.022559000	0.379489000
8	-2.952688000	1.200171000	-0.616998000
1	-2.236084000	0.887516000	-1.197565000
1	-3.256194000	0.396134000	-0.178104000
8	-2.259329000	-1.725290000	0.175090000
1	-1.777077000	-1.377512000	-0.609842000
1	-2.767115000	-2.494022000	-0.096080000
8	-0.468306000	-0.430588000	1.998898000
1	-1.188199000	-0.944325000	1.592782000
1	-0.661593000	0.519664000	1.791208000
8	3.538364000	0.803878000	-0.174537000
1	4.020385000	1.577236000	0.129244000
1	2.682304000	1.108197000	-0.554925000

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 6x H2O(Escf: -742.6552)

6	-0.264441000	0.564254000	-1.036699000
8	-0.230443000	1.688598000	-0.489022000
8	-1.242006000	0.005389000	-1.573664000
6	1.057624000	-0.224169000	-1.044085000
1	0.861494000	-1.283929000	-1.187909000
1	1.695953000	0.144035000	-1.846207000
7	1.752359000	-0.044289000	0.254367000
1	1.065726000	-0.361264000	0.993985000
1	1.993772000	0.955258000	0.387045000
1	2.609425000	-0.608772000	0.304506000
8	-1.984172000	1.187331000	1.732828000
1	-2.771492000	0.831815000	1.278956000
1	-1.497688000	1.645521000	1.026157000
8	-3.701825000	-0.101676000	-0.121114000
1	-3.039406000	0.167316000	-0.782778000
1	-3.500637000	-1.033732000	0.029291000
8	-1.640645000	-2.385147000	-0.407890000
1	-1.502978000	-1.624774000	-1.020250000
1	-1.773342000	-3.176503000	-0.935335000
8	-0.309836000	-0.977085000	1.725642000
1	-0.777319000	-1.628205000	1.175345000
1	-0.944380000	-0.229795000	1.856947000
8	2.213930000	2.699138000	-0.101423000
1	2.324111000	3.509753000	0.401707000
1	1.253195000	2.595706000	-0.295886000
8	4.118324000	-1.797537000	0.295262000
1	4.182221000	-2.587070000	0.841011000
1	5.009112000	-1.597934000	-0.007398000

Gas| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 7x H2O(Escf: -819.0684)

6	0.020731000	0.064497000	-1.335548000
8	1.126407000	-0.500526000	-1.104768000
8	-0.162863000	1.260047000	-1.619758000
6	-1.220055000	-0.827302000	-1.202406000
1	-2.124048000	-0.271329000	-1.427438000
1	-1.138685000	-1.685007000	-1.868513000
7	-1.309109000	-1.327318000	0.197981000
1	-0.926322000	-0.609953000	0.873637000
1	-0.720178000	-2.176156000	0.291200000
1	-2.294448000	-1.484731000	0.446522000
8	2.289726000	-1.167396000	1.409982000
1	1.928604000	-0.879258000	0.551448000
1	3.140164000	-0.715511000	1.463826000
8	1.017745000	2.528571000	0.562867000
1	0.704323000	2.309196000	-0.335071000
1	1.965708000	2.324272000	0.519479000
8	-2.266258000	1.870978000	0.156801000
1	-1.633544000	1.835617000	-0.587723000
1	-1.783272000	2.258766000	0.894915000
8	-0.048614000	0.386760000	1.942676000
1	0.312233000	1.198834000	1.517240000
1	0.740347000	-0.137574000	2.161518000
8	0.769843000	-3.167250000	-0.191667000
1	1.396600000	-3.186511000	0.543540000
1	1.076858000	-2.419994000	-0.739745000
8	-3.872446000	-0.364306000	0.484470000
1	-3.456576000	0.521025000	0.432931000
1	-4.800109000	-0.243565000	0.698230000
8	3.320281000	1.062127000	-0.357832000
1	2.612340000	0.600725000	-0.854036000
1	3.969139000	1.357160000	-1.002259000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 1x Solvating H2O(Escf: -360.6755)

7	1.802358000	-1.221907000	0.003535000
6	0.383158000	-0.787145000	0.027926000
6	0.332897000	0.740683000	-0.000502000
8	1.430158000	1.341241000	-0.025949000
8	-0.811670000	1.253469000	0.005857000
1	2.030838000	-1.765887000	-0.829414000
1	2.349943000	-0.340721000	-0.006010000
1	-0.138584000	-1.189368000	-0.835581000
1	-0.096594000	-1.152875000	0.930788000
1	2.059481000	-1.769440000	0.825674000
8	-2.909123000	-0.563654000	0.047799000
1	-2.619424000	-1.285180000	-0.522032000
1	-2.173420000	0.087140000	0.025628000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 2x Solvating H2O(Escf: -437.0795)

7	1.396014000	-0.442252000	0.923896000
6	0.052187000	0.079376000	0.583679000
6	-0.734500000	-0.985986000	-0.178135000
8	-0.180731000	-2.095429000	-0.342133000
8	-1.879219000	-0.648054000	-0.567310000
1	1.596039000	-0.390708000	1.922556000
1	1.393093000	-1.432055000	0.626205000
1	-0.485369000	0.340916000	1.491234000
1	0.153342000	0.970649000	-0.030902000
1	2.134800000	0.072224000	0.402107000
8	3.195623000	1.133880000	-0.598449000
1	3.065618000	0.946420000	-1.536422000
1	2.923497000	2.052833000	-0.482640000
8	-2.631039000	1.954498000	0.018686000
1	-2.128134000	2.186109000	0.807861000
1	-2.368182000	1.029868000	-0.186882000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized Zwitterionic Glycine with 3x Solvating H2O(Escf: -513.4834)

7	-1.909525000	-0.792467000	-0.293978000
6	-0.855987000	-0.031537000	0.410370000
6	0.461289000	-0.790901000	0.406746000
8	0.501001000	-1.900250000	-0.156823000
8	1.417584000	-0.203468000	0.987793000
1	-1.628828000	-0.969824000	-1.260941000
1	-2.038692000	-1.705495000	0.147326000
1	-2.814350000	-0.272228000	-0.286952000
1	-1.177203000	0.147500000	1.433004000
1	-0.725423000	0.927640000	-0.086713000
8	-4.305562000	0.704874000	-0.164034000
1	-4.088109000	1.634016000	-0.018572000
1	-4.816964000	0.686661000	-0.982436000
8	1.709072000	2.432469000	0.007645000
1	1.136459000	2.445437000	-0.768018000
1	1.590747000	1.540891000	0.391655000
8	3.646600000	-0.309031000	-0.714240000
1	2.904695000	-0.355731000	-0.077656000
1	3.642961000	0.606286000	-1.018268000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT6 solvated by 1x Water Molecule (Escf: -644.9266)

6	-2.608584000	0.119662000	0.090879000
8	-2.088923000	0.506882000	1.243551000
8	-3.801110000	0.253554000	-0.126098000
1	3.803459000	-1.375214000	0.575901000
6	-1.669039000	-0.476815000	-0.934372000
1	-2.288991000	-1.073858000	-1.601805000
7	-0.549418000	-1.242081000	-0.425217000
1	-0.795818000	-1.781902000	0.400633000
1	-1.273753000	0.354103000	-1.524552000
1	2.891437000	-0.164621000	1.264598000
7	2.990697000	-0.770763000	0.444627000
6	1.741319000	-1.532935000	0.211969000
1	1.919656000	-2.230555000	-0.600211000
1	1.476301000	-2.063356000	1.122710000
6	0.681171000	-0.507533000	-0.207249000
8	1.074383000	0.224108000	-1.239451000
1	3.140847000	-0.163544000	-0.371921000
8	0.497682000	0.346538000	0.994308000
1	-1.085135000	0.443637000	1.224997000
1	0.900129000	1.213656000	0.803369000
8	2.080468000	2.469811000	-0.262199000
1	1.521536000	3.218181000	-0.500805000
1	1.732189000	1.691959000	-0.777032000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT6 solvated by 2x Water Molecule (Escf: -721.3288)

6	2.045803000	-0.721711000	0.332662000
8	1.854077000	0.213448000	-0.583329000
8	3.171953000	-0.987044000	0.715904000
1	-4.299668000	-0.131786000	-1.379221000
6	0.823186000	-1.426850000	0.877178000
1	1.171633000	-2.388773000	1.250718000
7	-0.298160000	-1.584927000	-0.024932000
1	-0.002071000	-1.793414000	-0.975344000
1	0.487088000	-0.851825000	1.743664000
1	-3.044263000	0.961457000	-1.387180000
7	-3.421840000	0.127858000	-0.926490000
6	-2.423525000	-0.967007000	-0.940306000
1	-2.895949000	-1.856658000	-0.535785000
1	-2.097321000	-1.135967000	-1.962912000
6	-1.282549000	-0.520868000	-0.018753000
8	-1.715821000	-0.178182000	1.184556000
1	-3.597735000	0.371667000	0.057423000
8	-0.688575000	0.655426000	-0.709531000
1	0.871938000	0.418856000	-0.704997000
1	-0.940413000	1.449919000	-0.203338000
8	-2.046352000	2.451762000	1.159333000
1	-1.432961000	2.884094000	1.764481000
1	-1.966107000	1.475644000	1.335183000
8	4.450813000	1.637605000	-0.853638000
1	3.577944000	1.217511000	-0.812624000
1	5.021653000	1.053249000	-0.341155000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT6 solvated by 3x H2O(Escf: -797.7381)

6	-2.459644000	-0.744203000	-0.330023000
8	-2.340935000	0.157071000	0.633057000
8	-3.554263000	-1.004327000	-0.797123000
1	3.519169000	-0.097980000	2.210278000
6	-1.195626000	-1.416174000	-0.818704000
1	-1.505977000	-2.371590000	-1.239496000
7	-0.129872000	-1.585621000	0.146117000
1	-0.479645000	-1.828060000	1.069580000
1	-0.817625000	-0.811857000	-1.646963000
1	2.386310000	0.980720000	1.648582000
7	2.884994000	0.110119000	1.436723000
6	1.915050000	-0.990389000	1.217620000
1	2.454540000	-1.835913000	0.800120000
1	1.477154000	-1.259241000	2.175685000
6	0.842923000	-0.514484000	0.230567000
8	1.326217000	-0.130882000	-0.946601000
1	3.446182000	0.248811000	0.576683000
8	0.202072000	0.637747000	0.908146000
1	-1.375397000	0.370833000	0.819571000
1	0.448918000	1.439244000	0.417313000
8	2.076715000	2.465947000	-0.697751000
1	1.653534000	3.014456000	-1.368233000
1	1.848923000	1.532255000	-0.927067000
8	3.993315000	-0.204650000	-1.242758000
1	3.003224000	-0.262122000	-1.264761000
1	4.200024000	0.671352000	-1.591337000
8	-4.813767000	1.821199000	0.301609000
1	-3.993788000	1.341813000	0.493448000
1	-5.282435000	1.250460000	-0.318676000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized INT6 solvated by 4x H2O(Escf: -874.1445)

6	2.360366000	-0.953492000	0.030294000
8	2.505081000	0.236187000	-0.531456000
8	3.335199000	-1.576371000	0.410761000
1	-3.457943000	1.639602000	-1.784605000
6	0.955882000	-1.494915000	0.186931000
1	1.045404000	-2.580862000	0.171948000
7	-0.037978000	-1.047629000	-0.767151000
1	0.310322000	-1.032988000	-1.722538000
1	0.617446000	-1.215839000	1.187901000
1	-2.010923000	2.346776000	-1.371080000
7	-2.626752000	1.545898000	-1.197074000
6	-1.907921000	0.273228000	-1.449547000
1	-2.602502000	-0.545849000	-1.280551000
1	-1.560360000	0.270735000	-2.479147000
6	-0.748700000	0.182792000	-0.449474000
8	-1.154917000	0.254831000	0.813538000
1	-2.912762000	1.583681000	-0.211156000
8	0.139962000	1.309449000	-0.773251000
1	1.622759000	0.694933000	-0.682846000
1	0.008415000	1.998292000	-0.094444000
8	-1.002300000	2.858111000	1.430707000
1	-0.392695000	3.021524000	2.159606000
1	-1.124816000	1.876806000	1.390005000
8	-3.654252000	-0.662572000	1.253469000
1	-2.731699000	-0.310259000	1.157513000
1	-3.820438000	-0.720110000	2.201428000
8	5.254832000	1.104604000	0.284808000
1	4.362036000	0.896348000	-0.029126000
1	5.576529000	0.275155000	0.657149000
8	-2.171331000	-2.912159000	0.141589000
1	-1.468322000	-2.346211000	-0.231971000
1	-2.783299000	-2.281930000	0.560946000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized *trans* Zwitterionic Diglycine solvated by 2x H2O(Escf: -644.9631)

6	-2.260541000	0.248729000	0.194348000
8	-1.475745000	0.826233000	0.988344000
8	-3.333023000	0.718649000	-0.252733000
1	3.693554000	-0.838549000	0.410763000
6	-1.932629000	-1.171056000	-0.283869000
1	-2.696216000	-1.840565000	0.105580000
7	-0.636442000	-1.655974000	0.126371000
1	-0.559820000	-2.251441000	0.940648000
1	-2.006458000	-1.181399000	-1.370609000
1	2.428193000	0.243644000	0.723136000
7	2.764389000	-0.533543000	0.115041000
6	1.777928000	-1.629611000	0.195769000
1	2.130309000	-2.472172000	-0.394905000
1	1.674362000	-1.933608000	1.233173000
6	0.473077000	-1.125928000	-0.378835000
8	0.477011000	-0.290488000	-1.292177000
1	2.817420000	-0.177208000	-0.844559000
8	1.202100000	1.343165000	1.561624000
1	0.284980000	1.016636000	1.440951000
1	1.309894000	1.969737000	0.822372000
8	1.379835000	2.435737000	-1.080115000
1	0.660483000	3.046722000	-1.279329000
1	1.019236000	1.545645000	-1.241126000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized *trans* Zwitterionic Diglycine solvated by 3x H2O(Escf: -721.3745)

6	-1.375833000	1.277417000	-0.234607000
8	-1.143232000	0.372207000	-1.086553000
8	-2.466374000	1.472465000	0.340855000
1	3.738893000	-1.721253000	-0.409963000
6	-0.247476000	2.255617000	0.105138000
1	-0.458652000	3.196938000	-0.398271000
7	1.056699000	1.789922000	-0.302899000
1	1.447527000	2.104282000	-1.181469000
1	-0.265626000	2.438748000	1.177937000
1	2.044890000	-1.748088000	-0.398604000
7	2.901598000	-1.286804000	-0.017265000
6	2.839310000	0.152737000	-0.342707000
1	3.705632000	0.655996000	0.079917000
1	2.846356000	0.271561000	-1.422207000
6	1.571884000	0.703489000	0.269028000
8	1.073774000	0.153485000	1.257783000
1	2.900164000	-1.420346000	0.997480000
8	0.348613000	-2.016164000	-1.005400000
1	-0.104641000	-1.147776000	-1.043639000
1	-0.057996000	-2.460228000	-0.248003000
8	-1.249903000	-1.577546000	1.723219000
1	-1.869522000	-1.589144000	0.970877000
1	-0.559889000	-0.938208000	1.482050000
8	-3.011024000	-1.590604000	-0.606555000
1	-2.419778000	-0.851952000	-0.881411000
1	-3.797576000	-1.158655000	-0.251451000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized *trans* Zwitterionic Diglycine solvated by 4x H2O(Escf: -797.7804)

6	-1.940116000	-1.018763000	-0.213504000
8	-1.755998000	-0.464464000	0.908254000
8	-2.824485000	-0.711969000	-1.038966000
1	3.548911000	0.212352000	1.595943000
6	-1.043562000	-2.203915000	-0.584673000
1	-1.572170000	-3.118184000	-0.321943000
7	0.231211000	-2.193697000	0.094997000
1	0.398451000	-2.809551000	0.879651000
1	-0.894063000	-2.196720000	-1.662794000
1	1.918018000	0.640791000	1.464406000
7	2.728172000	0.184138000	0.988759000
6	2.370215000	-1.212004000	0.656199000
1	3.167319000	-1.650735000	0.059914000
1	2.260150000	-1.777421000	1.576559000
6	1.092990000	-1.212684000	-0.150435000
8	0.884108000	-0.345023000	-1.011179000
1	2.926914000	0.734173000	0.132139000
8	0.252378000	1.228822000	1.856164000
1	-0.395703000	0.547554000	1.577500000
1	0.180439000	1.903380000	1.163178000
8	-0.500276000	2.236679000	-0.947112000
1	-1.344446000	2.215505000	-0.456070000
1	-0.202074000	1.313597000	-0.988008000
8	2.818767000	1.658366000	-1.551844000
1	2.085397000	1.024296000	-1.645499000
1	2.393934000	2.507538000	-1.376169000
8	-2.859456000	2.057057000	0.691850000
1	-2.573882000	1.123605000	0.823996000
1	-3.610338000	2.005182000	0.088049000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized *trans* Zwitterionic Diglycine solvated by 5x H2O(Escf: -874.1840)

6	1.708298000	-1.447651000	-0.321281000
8	2.055476000	-0.406573000	-0.949828000
8	2.393152000	-2.044235000	0.534432000
1	-2.184369000	2.911613000	-1.436058000
6	0.349917000	-2.069474000	-0.659210000
1	0.524249000	-2.920983000	-1.313764000
7	-0.548791000	-1.151491000	-1.317057000
1	-0.692553000	-1.203614000	-2.317036000
1	-0.099203000	-2.438971000	0.262675000
1	-0.658985000	2.422692000	-0.884518000
7	-1.684452000	2.214376000	-0.880721000
6	-1.898200000	0.853390000	-1.419864000
1	-2.941632000	0.573686000	-1.282319000
1	-1.661999000	0.853081000	-2.479534000
6	-1.021110000	-0.105724000	-0.649908000
8	-0.784623000	0.091779000	0.551977000
1	-2.014946000	2.273679000	0.086894000
8	1.144835000	2.251826000	-0.836563000
1	1.396994000	1.309575000	-0.937418000
1	1.331041000	2.443774000	0.093685000
8	1.508111000	1.080580000	2.092017000
1	2.357498000	0.986122000	1.622418000
1	0.845178000	0.664692000	1.517416000
8	-3.384705000	0.644534000	1.661346000
1	-2.421385000	0.561808000	1.556883000
1	-3.544298000	0.678822000	2.612283000
8	3.980060000	0.816076000	0.581467000
1	3.389233000	0.328777000	-0.038863000
1	4.449512000	0.128268000	1.068977000
8	-3.339119000	-2.053180000	0.592985000
1	-2.416481000	-2.281988000	0.761601000
1	-3.444084000	-1.160929000	0.970029000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized *trans* Zwitterionic Diglycine solvated by 6x H2O(Escf: -950.5854)

6	2.860519000	0.864342000	-0.768485000
8	2.464193000	1.995776000	-0.401053000
8	4.048473000	0.453259000	-0.731498000
1	-3.697504000	0.315983000	0.097513000
6	1.850921000	-0.120717000	-1.350314000
1	2.149450000	-0.319512000	-2.381317000
7	0.491671000	0.367744000	-1.296918000
1	0.343885000	1.348750000	-1.508770000
1	1.919748000	-1.061048000	-0.806881000
1	-2.354370000	-0.075643000	1.053872000
7	-2.787540000	-0.190043000	0.122587000
6	-1.874538000	0.370716000	-0.889337000
1	-2.306295000	0.219972000	-1.877376000
1	-1.761210000	1.438109000	-0.714341000
6	-0.536990000	-0.332772000	-0.832012000
8	-0.453815000	-1.497367000	-0.408480000
1	-2.952962000	-1.194522000	-0.057975000
8	-5.224441000	1.260571000	-0.096581000
1	-5.023755000	2.191889000	-0.251483000
1	-5.754676000	1.244254000	0.709745000
8	-2.842271000	-2.998242000	-0.787952000
1	-3.026353000	-3.633303000	-0.085568000
1	-1.898662000	-2.776697000	-0.701406000
8	-0.919483000	0.604493000	2.142214000
1	-1.101570000	0.844161000	3.059094000
1	-0.140762000	0.012589000	2.163071000
8	0.079951000	2.936150000	0.734280000
1	-0.289875000	2.171123000	1.209889000
1	0.896249000	2.596408000	0.316528000
8	3.918085000	-1.871336000	0.894060000
1	4.062733000	-1.119249000	0.288136000
1	3.035363000	-1.703334000	1.266768000
8	1.225638000	-1.253024000	1.880096000
1	0.725248000	-1.569681000	1.104910000
1	1.076286000	-1.905810000	2.576112000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized *trans* Zwitterionic Diglycine solvated by 7x H2O(Escf: -1026.9912)

6	-2.524592000	-0.279755000	-0.844786000
8	-2.308295000	-1.464434000	-0.507296000
8	-3.644911000	0.300852000	-0.805678000
1	4.015978000	-0.755023000	0.099085000
6	-1.379692000	0.564303000	-1.391356000
1	-1.637852000	0.834542000	-2.416938000
7	-0.107524000	-0.118437000	-1.346653000
1	-0.094394000	-1.095428000	-1.619027000
1	-1.315731000	1.488620000	-0.820287000
1	2.725861000	-0.217365000	1.059474000
7	3.189806000	-0.121836000	0.140121000
6	2.224864000	-0.486323000	-0.912418000
1	2.691972000	-0.342725000	-1.885421000
1	1.957311000	-1.534677000	-0.802729000
6	1.001496000	0.398738000	-0.827158000
8	1.077803000	1.536303000	-0.335789000
1	3.505191000	0.855008000	0.015921000
8	5.397774000	-1.896419000	-0.107030000
1	5.085196000	-2.804034000	-0.207578000
1	5.948473000	-1.902131000	0.685592000
8	3.683967000	2.683035000	-0.618846000
1	3.939611000	3.260429000	0.110536000
1	2.715876000	2.606460000	-0.564813000
8	1.221850000	-0.695384000	2.127596000
1	1.356476000	-0.989071000	3.036907000
1	0.525789000	-0.008946000	2.160260000
8	-0.088971000	-2.788150000	0.604897000
1	0.382683000	-2.108634000	1.118728000
1	-0.840399000	-2.313941000	0.198346000
8	-3.186349000	2.574487000	0.857584000
1	-3.448386000	1.873307000	0.232419000
1	-2.374445000	2.226678000	1.264587000
8	-0.698021000	1.406858000	1.902659000
1	-0.144853000	1.699229000	1.154793000
1	-0.491725000	2.006088000	2.631703000
8	-5.480786000	-1.537464000	0.213596000
1	-4.969493000	-2.344935000	0.339177000
1	-4.834060000	-0.890789000	-0.144234000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D solvated by 1x Water Molecule (Escf: -644.9202)

6	-2.541017000	-0.171299000	-0.113642000
8	-1.942390000	-0.607658000	-1.184232000
8	-3.727484000	-0.399821000	0.106277000
1	3.754785000	1.226182000	-0.730025000
6	-1.731963000	0.635694000	0.884613000
1	-2.419797000	1.339602000	1.349644000
7	-0.574160000	1.321100000	0.359104000
1	-0.755057000	1.856812000	-0.483640000
1	-1.402532000	-0.052935000	1.664119000
1	2.712746000	0.011544000	-1.216123000
7	2.930865000	0.681018000	-0.469625000
6	1.749559000	1.534120000	-0.223636000
1	2.013490000	2.273352000	0.528598000
1	1.466833000	2.022999000	-1.150419000
6	0.646621000	0.641872000	0.322241000
8	0.953573000	-0.139933000	1.277580000
1	3.138362000	0.139789000	0.377801000
8	0.484987000	-0.386902000	-1.148266000
1	-0.849686000	-0.493768000	-1.179250000
1	0.836098000	-1.252547000	-0.886700000
8	2.109241000	-2.469524000	0.421091000
1	1.532902000	-3.210715000	0.640118000
1	1.712310000	-1.686761000	0.862469000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D catalyzed by 2x Water Molecule (Escf: -721.3235)

6	1.997763000	-0.740964000	0.278525000
8	1.738713000	0.231377000	-0.538801000
8	3.134874000	-0.978017000	0.687446000
1	-4.259393000	0.103597000	-1.291841000
6	0.839318000	-1.604014000	0.746055000
1	1.235028000	-2.605593000	0.905575000
7	-0.318866000	-1.645369000	-0.119624000
1	-0.088310000	-1.818768000	-1.093489000
1	0.529315000	-1.224649000	1.721201000
1	-2.928754000	1.103153000	-1.255377000
7	-3.363031000	0.276337000	-0.833055000
6	-2.453947000	-0.887734000	-0.921988000
1	-2.996370000	-1.765013000	-0.580298000
1	-2.136732000	-1.015495000	-1.952145000
6	-1.287922000	-0.629583000	0.025551000
8	-1.606189000	-0.261289000	1.214338000
1	-3.525224000	0.486301000	0.160155000
8	-0.604033000	0.707799000	-0.761154000
1	0.590467000	0.482619000	-0.667650000
1	-0.822676000	1.488490000	-0.217098000
8	-1.818186000	2.439146000	1.230258000
1	-1.174004000	2.856804000	1.813731000
1	-1.781515000	1.475291000	1.429674000
8	4.202346000	1.708168000	-0.832632000
1	3.357972000	1.228663000	-0.756274000
1	4.821999000	1.184130000	-0.311913000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D solvated by 3x H2O(Escf: -797.7314)

6	-2.370299000	0.727173000	0.380658000
8	-2.190443000	-0.234481000	-0.467235000
8	-3.449952000	0.928410000	0.939711000
1	3.506867000	-0.089373000	-2.155992000
6	-1.191045000	1.631801000	0.695422000
1	-1.593364000	2.630867000	0.854370000
7	-0.126263000	1.667439000	-0.282699000
1	-0.451408000	1.841233000	-1.228836000
1	-0.778139000	1.300203000	1.648985000
1	2.295682000	-1.077354000	-1.598290000
7	2.830009000	-0.225198000	-1.402133000
6	1.921554000	0.938682000	-1.288370000
1	2.512924000	1.796360000	-0.976892000
1	1.473575000	1.128417000	-2.259358000
6	0.860716000	0.662552000	-0.230137000
8	1.270359000	0.291555000	0.933492000
1	3.352860000	-0.353692000	-0.514729000
8	0.116850000	-0.682311000	-0.949041000
1	-1.045753000	-0.472947000	-0.732728000
1	0.390319000	-1.463367000	-0.433480000
8	1.739531000	-2.423532000	0.796599000
1	1.280470000	-2.925416000	1.480406000
1	1.648303000	-1.480018000	1.048731000
8	3.976882000	0.021997000	1.274652000
1	3.012932000	0.208985000	1.330064000
1	4.082464000	-0.862545000	1.646539000
8	-4.590364000	-1.823930000	-0.449296000
1	-3.772283000	-1.295397000	-0.478682000
1	-5.150131000	-1.364570000	0.187236000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D solvated by 4x H2O(Escf: -874.1366)

6	-2.274293000	1.005319000	0.108337000
8	-2.406264000	-0.170721000	-0.401214000
8	-3.209488000	1.634778000	0.614016000
1	3.297496000	-1.893056000	-1.685051000
6	-0.894116000	1.644975000	0.086237000
1	-1.034622000	2.700886000	-0.141472000
7	0.073093000	1.072362000	-0.828178000
1	-0.253646000	1.026178000	-1.789119000
1	-0.492847000	1.590255000	1.099343000
1	1.806326000	-2.487941000	-1.261318000
7	2.465995000	-1.716778000	-1.116495000
6	1.843395000	-0.415287000	-1.451379000
1	2.609217000	0.353806000	-1.370770000
1	1.458826000	-0.459350000	-2.465665000
6	0.751144000	-0.110767000	-0.430280000
8	1.099967000	-0.197555000	0.812047000
1	2.739144000	-1.722487000	-0.125725000
8	-0.317154000	-1.322719000	-0.741936000
1	-1.323512000	-0.811237000	-0.604251000
1	-0.209160000	-1.997361000	-0.033427000
8	0.613401000	-2.808849000	1.451114000
1	-0.016289000	-2.922488000	2.173177000
1	0.901174000	-1.870811000	1.487404000
8	3.717332000	0.501702000	1.239468000
1	2.776297000	0.215985000	1.192434000
1	3.917053000	0.607674000	2.176912000
8	-5.109131000	-0.972070000	0.071844000
1	-4.184546000	-0.711179000	-0.099469000
1	-5.500517000	-0.201702000	0.499539000
8	2.430353000	2.819934000	0.022334000
1	1.661157000	2.334607000	-0.323446000
1	2.965922000	2.137700000	0.464742000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D with 5x Solvating H2O(Escf: -950.5411)

6	-2.811311000	0.723900000	-0.323978000
8	-2.682151000	-0.540604000	-0.532285000
8	-3.903137000	1.274559000	-0.144749000
1	3.360370000	-1.446439000	-0.699845000
6	-1.551538000	1.576021000	-0.287807000
1	-1.794758000	2.529396000	-0.755041000
7	-0.368757000	1.013956000	-0.908138000
1	-0.514227000	0.721751000	-1.870179000
1	-1.330258000	1.783421000	0.760552000
1	1.900700000	-2.204741000	-0.328852000
7	2.416664000	-1.322212000	-0.267950000
6	1.677453000	-0.232390000	-0.938953000
1	2.302082000	0.659157000	-0.922986000
1	1.473740000	-0.525110000	-1.965038000
6	0.396721000	0.072396000	-0.167905000
8	0.537602000	0.299288000	1.098499000
1	2.530200000	-1.098610000	0.727344000
8	-0.416920000	-1.343557000	-0.340963000
1	-1.493851000	-1.003178000	-0.442300000
1	-0.316129000	-1.841803000	0.501087000
8	0.383696000	-2.181714000	2.219122000
1	-0.348563000	-2.273937000	2.840486000
1	0.499182000	-1.216104000	2.077880000
8	4.900695000	-1.478369000	-1.577584000
1	5.531866000	-0.879435000	-1.159557000
1	5.310044000	-2.351650000	-1.537649000
8	2.944603000	1.470946000	1.686235000
1	2.066076000	1.037334000	1.582235000
1	2.976121000	1.793436000	2.594511000
8	-5.249619000	-1.721577000	-0.117879000
1	-4.368696000	-1.330037000	-0.270148000
1	-5.833154000	-0.963194000	-0.000099000
8	1.539653000	3.285378000	-0.119941000
1	0.916832000	2.621260000	-0.462064000
1	2.093753000	2.791902000	0.510500000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D with 4x solvating and 1x catalyzing H2O(Escf: -950.5332)

6	-2.763436000	0.377258000	0.008892000
8	-2.914024000	-0.762931000	-0.565878000
8	-3.660854000	1.229212000	0.066199000
1	3.957217000	-1.100373000	-0.382441000
6	-1.425903000	0.660680000	0.667243000
1	-1.385615000	1.718925000	0.919174000
7	-0.299578000	0.283093000	-0.181900000
1	-0.575080000	-0.400051000	-0.884322000
1	-1.423581000	0.093836000	1.608803000
1	2.953629000	-1.791112000	0.785429000
7	3.154896000	-0.934562000	0.263122000
6	1.949747000	-0.494289000	-0.468404000
1	2.196925000	0.408911000	-1.021849000
1	1.645110000	-1.282354000	-1.152766000
6	0.862948000	-0.178552000	0.562039000
8	1.251157000	0.669428000	1.505158000
1	3.409568000	-0.210177000	0.942936000
8	0.564561000	-1.489371000	1.180224000
1	-2.185301000	-1.724037000	-0.168004000
1	0.455757000	-1.321523000	2.132182000
8	-1.536532000	-2.600335000	0.185251000
1	-2.015262000	-3.137850000	0.833193000
1	-0.696605000	-2.225807000	0.624774000
8	5.296739000	-1.355503000	-1.531351000
1	5.586512000	-0.522797000	-1.924233000
1	5.048931000	-1.918720000	-2.274956000
8	-6.009018000	-0.077163000	-0.853856000
1	-5.246952000	0.444048000	-0.530699000
1	-5.626020000	-0.933631000	-1.076218000
8	0.724410000	2.920190000	-0.963681000
1	0.398740000	2.022024000	-0.740075000
1	0.796931000	2.927430000	-1.925170000
8	3.236058000	2.320771000	0.734515000
1	2.486625000	1.755418000	1.054103000
1	2.871142000	2.733156000	-0.059691000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D with 6x Solvating H2O(Escf: -1026.9463)

6	-2.551602000	-0.103909000	-0.384516000
8	-2.181705000	-1.324941000	-0.529176000
8	-3.730033000	0.222078000	-0.179147000
1	3.937946000	-0.969890000	-0.537789000
6	-1.498476000	0.989953000	-0.466524000
1	-1.931972000	1.803847000	-1.048307000
7	-0.216266000	0.623813000	-1.030038000
1	-0.282009000	0.236601000	-1.967092000
1	-1.346575000	1.371633000	0.544956000
1	2.663187000	-1.995460000	-0.144136000
7	2.970746000	-1.018835000	-0.143253000
6	2.043066000	-0.169623000	-0.919714000
1	2.456336000	0.837000000	-0.953533000
1	1.954632000	-0.569843000	-1.925696000
6	0.694078000	-0.103819000	-0.208377000
8	0.735668000	0.229167000	1.044729000
1	2.988834000	-0.702304000	0.832853000
8	0.194911000	-1.641027000	-0.309286000
1	-0.933675000	-1.535947000	-0.434049000
1	0.377966000	-2.065008000	0.559999000
8	1.089647000	-2.172148000	2.300162000
1	0.393767000	-2.403134000	2.927106000
1	0.991126000	-1.210472000	2.126509000
8	5.492301000	-0.791974000	-1.360564000
1	6.075142000	-0.190589000	-0.880612000
1	5.962156000	-1.634565000	-1.391668000
8	2.778679000	1.961990000	1.608745000
1	2.031314000	1.327239000	1.505973000
1	2.682668000	2.344318000	2.488878000
8	-4.539617000	-2.931911000	-0.144493000
1	-3.731603000	-2.403195000	-0.277030000
1	-5.219505000	-2.281690000	0.066700000
8	1.114308000	3.277539000	-0.390339000
1	0.683179000	2.464530000	-0.707815000
1	1.727390000	2.969238000	0.300571000
8	-4.151591000	2.959911000	0.302898000
1	-3.299599000	3.378395000	0.134147000
1	-4.004996000	2.009372000	0.119625000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS6D with 5x solvating and 1x catalyzing H2O(Escf: -1026.9407)

6	-2.784013000	0.434266000	-0.218720000
8	-2.900259000	-0.590655000	-0.976362000
8	-3.718502000	1.215473000	0.028438000
1	3.920382000	-1.060337000	-0.744061000
6	-1.438856000	0.680386000	0.442083000
1	-1.407186000	1.714960000	0.780448000
7	-0.312046000	0.380397000	-0.435440000
1	-0.595420000	-0.216844000	-1.209347000
1	-1.427500000	0.042273000	1.336950000
1	2.884797000	-1.863698000	0.319211000
7	3.110342000	-0.955757000	-0.095188000
6	1.925877000	-0.407852000	-0.786818000
1	2.201476000	0.543227000	-1.236646000
1	1.610935000	-1.109584000	-1.555293000
6	0.833813000	-0.180716000	0.259728000
8	1.232265000	0.565172000	1.286661000
1	3.367256000	-0.323076000	0.669794000
8	0.508967000	-1.544065000	0.734288000
1	-2.163720000	-1.685031000	-0.663230000
1	0.367305000	-1.488302000	1.699676000
8	-1.554650000	-2.552827000	-0.400670000
1	-2.045140000	-3.144148000	0.190543000
1	-0.714425000	-2.213873000	0.082597000
8	5.272473000	-1.202721000	-1.899100000
1	5.586630000	-0.330547000	-2.167905000
1	5.013834000	-1.645973000	-2.716540000
8	0.131283000	-0.594923000	3.430583000
1	0.572329000	-0.005755000	2.766778000
1	0.807383000	-0.815468000	4.081725000
8	-6.057030000	0.002161000	-0.960447000
1	-5.258642000	0.447767000	-0.607519000
1	-5.715882000	-0.788602000	-1.393580000
8	0.802203000	3.047733000	-0.965867000
1	0.442759000	2.147136000	-0.815009000
1	0.829098000	3.148101000	-1.924581000
8	3.230513000	2.288932000	0.689471000
1	2.498709000	1.681848000	0.963935000
1	2.837918000	2.762697000	-0.057139000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS1D with 5x Solvating H2O(Escf: -950.5725)

7	1.172426000	-0.909221000	-1.828838000
6	1.924178000	0.317067000	-1.534527000
6	2.245596000	0.450094000	-0.054460000
8	2.179724000	-0.584492000	0.663165000
8	2.553190000	1.595766000	0.353291000
1	-1.034453000	1.083382000	-1.448531000
1	-0.979985000	2.564296000	-0.715026000
1	0.952795000	-0.957757000	-2.821747000
1	2.865984000	0.347093000	-2.085053000
1	1.337524000	1.182109000	-1.843219000
7	-1.399593000	1.621488000	-0.657502000
6	-1.011209000	0.999982000	0.627680000
6	-1.199130000	-0.506431000	0.613537000
8	-1.629169000	-1.059095000	1.622236000
8	-0.905425000	-1.136617000	-0.477254000
1	1.733293000	-1.729867000	-1.591231000
1	0.079732000	-0.958249000	-1.126108000
1	-2.431456000	1.623932000	-0.726697000
1	0.035057000	1.231806000	0.823149000
1	-1.615482000	1.432808000	1.418611000
8	-3.698112000	-1.985600000	-0.901512000
1	-3.951877000	-2.502471000	-0.126788000
1	-2.727885000	-1.953907000	-0.877502000
8	-4.072402000	0.741737000	-0.174674000
1	-4.025273000	0.763774000	0.789566000
1	-3.984789000	-0.204180000	-0.413824000
8	0.964609000	-0.035556000	3.160585000
1	0.068188000	-0.368308000	3.019936000
1	1.429469000	-0.211097000	2.317465000
8	3.037989000	-3.037114000	-0.347340000
1	3.952235000	-2.927875000	-0.632951000
1	2.799899000	-2.194172000	0.089737000
8	0.693338000	3.559029000	-0.515171000
1	0.966669000	3.851512000	-1.392698000
1	1.373986000	2.912560000	-0.232692000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS1D with 6x Solvating H2O(Escf: -1026.9769)

7	1.119445000	-0.364338000	-1.890345000
6	1.830389000	0.771369000	-1.293377000
6	2.326580000	0.462080000	0.110665000
8	2.380414000	-0.744364000	0.472316000
8	2.641053000	1.445452000	0.823585000
1	-1.193048000	1.315537000	-0.768009000
1	-1.030555000	2.468300000	0.417574000
1	0.799954000	-0.126910000	-2.827365000
1	2.691558000	1.065343000	-1.895745000
1	1.158614000	1.629357000	-1.241197000
7	-1.429126000	1.537343000	0.217098000
6	-0.865666000	0.567457000	1.180200000
6	-1.029610000	-0.868992000	0.718333000
8	-1.353685000	-1.724924000	1.537460000
8	-0.825065000	-1.120932000	-0.533837000
1	1.738325000	-1.174530000	-1.958132000
1	0.092060000	-0.688818000	-1.162741000
1	-2.457625000	1.521340000	0.297778000
1	0.193785000	0.784485000	1.309490000
1	-1.362246000	0.697661000	2.136783000
8	-3.616234000	-1.824480000	-1.053686000
1	-3.800010000	-2.605574000	-0.517305000
1	-2.647436000	-1.750973000	-1.070197000
8	-4.011286000	0.361804000	0.725448000
1	-3.806684000	0.010521000	1.601328000
1	-3.918535000	-0.400269000	0.117225000
8	1.353917000	-1.045356000	3.103051000
1	0.467282000	-1.390603000	2.933347000
1	1.750896000	-0.931439000	2.216442000
8	3.135041000	-2.759902000	-1.298681000
1	4.019831000	-2.552964000	-1.620356000
1	2.944071000	-2.088534000	-0.612618000
8	0.641062000	3.440291000	0.826537000
1	0.830581000	4.087874000	0.137502000
1	1.376184000	2.792229000	0.788028000
8	-1.196052000	1.428699000	-2.712416000
1	-1.987195000	1.889814000	-3.017905000
1	-0.455501000	1.995337000	-2.964353000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS2D with 5x Solvating H2O(Escf: -950.5546)

6	-0.750793000	-0.556068000	-0.437168000
8	-0.417388000	0.549383000	-0.915974000
8	-1.580534000	-1.378889000	-1.157149000
1	-1.576837000	-1.075462000	-2.079324000
6	-1.077502000	-0.681732000	1.039000000
1	-2.102763000	-0.344956000	1.189741000
7	-0.176035000	0.203079000	1.806890000
1	-0.199064000	-0.024830000	2.802237000
1	-0.478762000	1.181619000	1.686984000
1	-0.981349000	-1.704176000	1.390388000
6	2.398507000	0.243275000	-0.595272000
8	2.362287000	0.252545000	0.672250000
8	2.889854000	1.147362000	-1.304170000
1	0.810753000	0.138566000	1.455339000
6	1.846366000	-0.984117000	-1.301316000
1	1.405798000	-0.686012000	-2.250357000
7	0.837623000	-1.651144000	-0.489910000
1	1.210600000	-1.869687000	0.434528000
1	0.523592000	-2.517338000	-0.922031000
1	2.688432000	-1.650295000	-1.509192000
8	-4.121335000	-1.852201000	0.242715000
1	-3.348824000	-1.883232000	-0.344412000
1	-4.843723000	-2.251099000	-0.256982000
8	-1.679820000	2.437035000	0.662190000
1	-1.531067000	3.384914000	0.557053000
1	-1.212256000	1.999383000	-0.077789000
8	-4.103293000	1.029015000	-0.291989000
1	-3.317866000	1.436343000	0.107668000
1	-4.093662000	0.092127000	-0.030145000
8	3.625309000	-2.210489000	1.407172000
1	3.251487000	-1.322382000	1.256590000
1	3.797013000	-2.552365000	0.521249000
8	1.514375000	3.305175000	0.001962000
1	0.890426000	2.791560000	0.530748000
1	2.061831000	2.634148000	-0.448666000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS2D with 6x Solvating H2O(Escf: -1026.9669)

6	0.813892000	-1.280918000	0.794136000
8	-0.397703000	-1.416024000	1.076106000
8	1.636838000	-2.379393000	0.821916000
1	1.090323000	-3.176129000	0.729820000
6	1.577831000	-0.076228000	1.311765000
1	1.921191000	-0.293411000	2.320623000
7	0.667208000	1.084785000	1.354955000
1	1.211367000	1.967359000	1.418433000
1	0.015890000	1.010928000	2.140514000
1	2.435863000	0.159550000	0.685825000
6	-1.412079000	-0.040374000	-1.339223000
8	-0.936686000	1.088779000	-1.000395000
8	-2.627479000	-0.294326000	-1.457574000
1	0.088681000	1.125790000	0.486995000
6	-0.423974000	-1.141710000	-1.680568000
1	-0.814138000	-2.096160000	-1.330852000
7	0.881595000	-0.903665000	-1.083732000
1	1.201427000	0.046966000	-1.279953000
1	1.582350000	-1.550621000	-1.441295000
1	-0.356139000	-1.186380000	-2.770006000
8	4.142250000	-1.737379000	-0.665963000
1	3.424578000	-2.016753000	-0.077013000
1	4.294411000	-0.809971000	-0.448548000
8	-2.461039000	0.331025000	2.030653000
1	-2.668601000	1.040424000	1.396911000
1	-1.815166000	-0.248388000	1.588370000
8	2.398575000	3.306730000	0.880906000
1	2.026409000	4.174445000	1.078312000
1	2.171877000	3.124809000	-0.053073000
8	1.575169000	2.278564000	-1.595993000
1	0.635405000	2.018892000	-1.572262000
1	1.742355000	2.621204000	-2.482038000
8	-3.074474000	2.470194000	0.113492000
1	-2.319319000	2.066935000	-0.368331000
1	-3.858159000	2.072985000	-0.285771000
8	-2.900916000	-2.616353000	0.250281000
1	-2.025705000	-2.432444000	0.630743000
1	-2.996826000	-1.907026000	-0.410064000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3D with 5x Solvating H2O(Escf: -950.5476)

7	3.061065000	-0.566357000	1.651046000
6	2.262619000	-1.325686000	0.685416000
6	1.420443000	-0.227137000	-0.029173000
8	1.478642000	0.893371000	0.699674000
8	1.879865000	-0.072961000	-1.344545000
1	1.726573000	0.845436000	-1.617956000
1	2.368577000	0.470741000	1.452679000
1	3.041671000	-0.955320000	2.588068000
1	2.873454000	-1.863138000	-0.033420000
1	1.617412000	-2.024534000	1.210148000
7	-0.015892000	-0.706454000	-0.115735000
6	-0.955382000	0.293527000	-0.666573000
6	-1.615987000	1.075980000	0.465484000
8	-2.112663000	2.184148000	0.155784000
8	-1.663536000	0.514226000	1.587589000
1	4.021327000	-0.436233000	1.340082000
1	-0.343133000	-0.881735000	0.849669000
1	-0.094434000	-1.597292000	-0.636160000
1	-0.446730000	0.953523000	-1.363065000
1	-1.743323000	-0.236064000	-1.204515000
8	4.852413000	-0.054553000	-0.916659000
1	3.926796000	-0.003779000	-1.203721000
1	5.029775000	-0.999125000	-0.829758000
8	0.571855000	3.305885000	-0.579873000
1	-0.382953000	3.156847000	-0.486846000
1	0.967951000	2.531858000	-0.138223000
8	-4.521491000	0.469657000	-0.722397000
1	-4.144484000	-0.312293000	-0.282461000
1	-3.918004000	1.194111000	-0.500780000
8	-1.400021000	-2.957269000	-1.222586000
1	-1.136593000	-3.836370000	-0.926467000
1	-2.069189000	-2.651609000	-0.578803000
8	-3.191270000	-1.769698000	0.647061000
1	-3.718624000	-2.315739000	1.242996000
1	-2.712790000	-1.132168000	1.208043000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS3D with 6x Solvating H2O(Escf: -1026.9490)

7	-3.140251000	-0.444791000	-0.702007000
6	-2.244088000	-0.823854000	0.391039000
6	-1.174207000	0.303383000	0.383855000
8	-1.208726000	0.901187000	-0.815522000
8	-1.405658000	1.179307000	1.453688000
1	-1.143480000	2.072460000	1.179367000
1	-2.277731000	0.398224000	-1.135125000
1	-3.353607000	-1.236208000	-1.314211000
1	-2.738553000	-0.880465000	1.356292000
1	-1.782837000	-1.781830000	0.161154000
7	0.188416000	-0.316932000	0.608568000
6	1.315201000	0.632253000	0.474663000
6	1.870708000	0.594530000	-0.947203000
8	2.530337000	1.595617000	-1.311282000
8	1.676737000	-0.460598000	-1.600565000
1	-3.990557000	0.004164000	-0.371026000
1	0.337903000	-1.022539000	-0.132525000
1	0.241307000	-0.809755000	1.516735000
1	1.006187000	1.635010000	0.755642000
1	2.112044000	0.314039000	1.148616000
8	-4.353611000	1.429711000	1.779760000
1	-3.383238000	1.419003000	1.742546000
1	-4.603156000	0.507937000	1.918336000
8	0.175496000	3.413923000	-1.072479000
1	1.073972000	3.054729000	-1.155724000
1	-0.381950000	2.617010000	-1.002416000
8	4.828615000	0.249043000	0.281631000
1	4.312762000	-0.575793000	0.311381000
1	4.285275000	0.861948000	-0.234928000
8	1.462900000	-1.905757000	2.625259000
1	1.039669000	-2.749159000	2.824580000
1	2.062950000	-2.083357000	1.874681000
8	3.097798000	-2.130372000	0.290531000
1	3.485336000	-2.970752000	0.016861000
1	2.608793000	-1.789029000	-0.481196000
8	-3.184888000	-3.011729000	-2.215842000
1	-3.572740000	-2.910204000	-3.093461000
1	-2.233193000	-3.063895000	-2.367059000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS4D with 5x Solvating H2O(Escf: -950.5478)

7	-2.648902000	0.818588000	1.575457000
6	-2.651649000	-0.471967000	0.910635000
6	-1.846775000	-0.390977000	-0.374793000
8	-1.748690000	-1.636287000	-1.004543000
8	-2.382719000	0.568687000	-1.245679000
1	-3.341192000	0.446641000	-1.318163000
1	-3.217682000	1.482557000	1.057818000
1	-3.041295000	0.736302000	2.506654000
1	-2.181231000	-1.217039000	1.551810000
1	-3.645678000	-0.844225000	0.633487000
7	-0.484307000	0.009643000	-0.074367000
6	0.390077000	0.281326000	-1.225124000
6	1.548567000	-0.698972000	-1.059548000
8	2.512601000	-0.720678000	-1.816775000
8	1.363720000	-1.463017000	-0.031614000
1	-2.639121000	-1.960674000	-1.206684000
1	0.292812000	-0.936599000	0.296513000
1	-0.500524000	0.791789000	0.589475000
1	-0.116904000	0.090674000	-2.168706000
1	0.758955000	1.305344000	-1.219954000
8	-0.831311000	-3.583171000	1.066802000
1	-1.071677000	-2.975284000	0.348742000
1	-1.549578000	-3.503647000	1.705483000
8	3.934195000	-0.891666000	1.213419000
1	3.117087000	-1.300618000	0.880646000
1	4.620341000	-1.154902000	0.587765000
8	3.210789000	1.719750000	0.360918000
1	3.156501000	1.664322000	-0.601682000
1	3.480213000	0.825286000	0.656029000
8	0.673041000	2.458622000	1.248876000
1	1.578517000	2.202460000	0.969685000
1	0.742825000	2.770775000	2.158173000
8	-1.327270000	3.291401000	-0.620724000
1	-1.755676000	2.446784000	-0.830102000
1	-0.630390000	3.066861000	0.022923000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS4D with 6x Solvating H2O(Escf: -1026.9581)

7	-2.964090000	0.587767000	1.626031000
6	-2.919084000	-0.708398000	0.971134000
6	-2.149536000	-0.588708000	-0.333657000
8	-2.096254000	-1.851806000	-0.916296000
8	-2.772767000	0.273824000	-1.235378000
1	-2.543919000	1.213617000	-1.026520000
1	-3.618531000	1.199597000	1.146434000
1	-3.283260000	0.490406000	2.583038000
1	-2.399851000	-1.424758000	1.608095000
1	-3.897962000	-1.123113000	0.715239000
7	-0.792762000	-0.113401000	-0.020290000
6	0.077486000	0.223276000	-1.151368000
6	1.340985000	-0.596326000	-0.909043000
8	2.346088000	-0.490712000	-1.611751000
8	1.194493000	-1.387902000	0.097420000
1	-1.880470000	-1.770523000	-1.857624000
1	0.073756000	-1.001094000	0.373752000
1	-0.870434000	0.663316000	0.643956000
1	-0.360705000	-0.079368000	-2.102444000
1	0.307856000	1.284941000	-1.205630000
8	-0.735368000	-3.678354000	0.925740000
1	-1.187478000	-3.119946000	0.271333000
1	0.176522000	-3.362716000	0.920226000
8	3.191782000	0.603187000	1.649063000
1	2.285017000	0.289950000	1.764217000
1	3.646898000	-0.113314000	1.159955000
8	2.618623000	2.559887000	-0.270058000
1	2.507487000	2.105435000	-1.115190000
1	2.909016000	1.863681000	0.357960000
8	0.128148000	2.604744000	1.072450000
1	0.977255000	2.669106000	0.587169000
1	0.175357000	3.249359000	1.788461000
8	-2.044634000	2.862400000	-0.688932000
1	-1.717935000	3.254881000	-1.507858000
1	-1.276336000	2.842337000	-0.079086000
8	4.446498000	-1.373150000	0.039553000
1	3.762503000	-1.179154000	-0.633476000
1	4.201198000	-2.229204000	0.410916000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS5D with 5x Solvating H2O(Escf: -950.5495)

7	-1.112944000	-0.725803000	-1.996251000
6	-1.336658000	-1.558004000	-0.807196000
6	-0.290463000	-1.036548000	0.211090000
8	0.065604000	0.221462000	-0.186769000
8	-0.916708000	-1.025130000	1.481826000
1	-0.369764000	-0.517033000	2.099534000
1	-0.412792000	0.082076000	-1.327580000
1	-0.599377000	-1.201233000	-2.732803000
1	-2.336372000	-1.372053000	-0.425194000
1	-1.213403000	-2.617996000	-1.007928000
7	0.883214000	-1.897288000	0.182364000
6	2.027719000	-1.358874000	0.890697000
6	2.880061000	-0.492740000	-0.006178000
8	3.713127000	0.285853000	0.413332000
8	2.698645000	-0.671275000	-1.309183000
1	-1.975339000	-0.329691000	-2.362231000
1	1.935772000	-1.287477000	-1.399776000
1	0.642936000	-2.830830000	0.500961000
1	1.788292000	-0.771261000	1.781960000
1	2.670057000	-2.178942000	1.214548000
8	-3.863156000	0.600143000	-1.256106000
1	-3.221310000	1.194399000	-0.816985000
1	-4.583721000	1.168480000	-1.552827000
8	-2.019116000	2.018197000	0.370467000
1	-2.489926000	1.684246000	1.146614000
1	-1.272979000	1.395326000	0.239606000
8	1.287273000	1.988585000	1.634799000
1	0.821502000	1.319774000	1.092911000
1	2.160994000	1.607250000	1.795897000
8	1.970999000	2.629765000	-1.245928000
1	1.792645000	2.525907000	-0.296625000
1	2.028490000	1.725739000	-1.581065000
8	-3.767281000	-0.291393000	1.631112000
1	-3.969616000	-0.066667000	0.708200000
1	-2.827038000	-0.541026000	1.621117000

SMD| Atomic positions in Å of MN15/Def2TZVPP optimized TS5D with 6x Solvating H2O(Escf: -1026.9532)

7	-0.822499000	1.853852000	0.741207000
6	-1.076026000	1.637211000	-0.686715000
6	-0.239209000	0.379192000	-1.023067000
8	-0.057194000	-0.299894000	0.152750000
8	-0.976814000	-0.381593000	-1.959082000
1	-0.525492000	-1.226082000	-2.110530000
1	-0.359412000	0.656839000	0.844814000
1	-0.111355000	2.569221000	0.910984000
1	-2.129868000	1.417740000	-0.837003000
1	-0.788237000	2.485662000	-1.302400000
7	1.060370000	0.782464000	-1.540698000
6	2.037785000	-0.287149000	-1.572294000
6	2.751748000	-0.420940000	-0.247731000
8	3.352000000	-1.421891000	0.089796000
8	2.738945000	0.664563000	0.517654000
1	-1.672570000	2.038607000	1.265845000
1	2.134931000	1.310192000	0.084774000
1	0.955178000	1.232801000	-2.444420000
1	1.642103000	-1.272405000	-1.835151000
1	2.808462000	-0.046416000	-2.306069000
8	-3.738094000	0.873645000	1.233414000
1	-3.255463000	0.043691000	1.413937000
1	-4.528340000	0.841949000	1.785760000
8	-2.324281000	-1.628310000	1.170565000
1	-2.895281000	-1.809899000	0.409633000
1	-1.532154000	-1.200947000	0.783873000
8	0.581106000	-3.080593000	-0.035548000
1	0.322758000	-2.138341000	-0.042853000
1	1.525989000	-3.069836000	-0.240125000
8	1.058189000	-1.693047000	2.609457000
1	0.935405000	-2.382943000	1.938400000
1	0.992113000	-0.873589000	2.100478000
8	-3.843797000	-0.668994000	-1.335721000
1	-3.949827000	-0.074298000	-0.574480000
1	-2.900265000	-0.608332000	-1.566090000
8	1.548313000	3.740410000	0.924592000
1	1.968335000	3.725503000	0.055478000
1	2.145124000	3.242424000	1.497407000