What Rules the Relative Stability of α-, β- and γ-Glycine Polymorphs?

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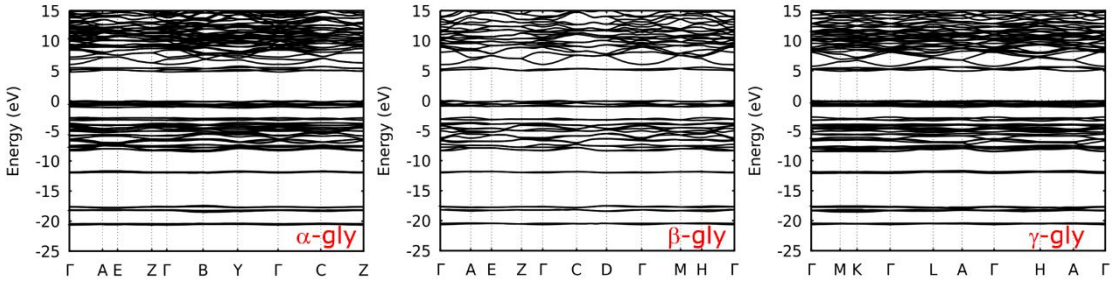

Figure 1. Full electronic band structure in the -25 to 15 eV energy range for α-, β- and γ-glycine polymorphs.

Calculation of lattice energy from experimental enthalpy of sublimation

The lattice energy is frequently related to experimental sublimation enthalpies assuming the zero-point vibrational energy difference and thermal corrections between the 0 K and the reference temperature:

$$\Delta H_{sub}(T) = -E_{latt} + \int_0^T \Delta C_p dT \quad (1)$$

where $\Delta C_p = C_p^g - C_p^s$, the difference of the heat capacities of gas and the crystal. Assuming that vibrational motions does not change from the molecule in the crystal phase to the gas phase, the vibrational contributions of both phases are canceled ($C_{p,vib}^g = C_{p,vib}^s$), only translational and rotational contributions are considered. The heat capacity of the crystal can be approximated by C_p^s= 6R and for the gas-phase, $C_{p,trans}^g$ = 5/2 R and $C_{p,rot}^g$ = 3/2 R. The simplified expression is:

$$\Delta H_{sub}(T) = -E_{latt} - 2RT \quad (2)$$

In this work, the experimental lattice energy value (-144 kJ mol^{-1}) and the sublimation enthalpy adjusted to 298.15 K, 139 kJ mol^{-1} were obtained from Equation (2), using the experimental value, Δ_{sub}H = (137 ± 2) kJ/mol, at Tsub = 419 K.

Lattice energy calculation models

Different models for obtaining the ΔE_{pt} and ΔE_{conf} terms, as described below, were investigated.

$$E_{latt} = \left(\frac{E^*_{crystal,QE}}{N} - E^*_{ZW,QE}\right) + \left(E^*_{ZW,ccsd(t)} - E_{102,ccsd(t)}\right) + \left(E_{102,ccsd(t)} - E_{011,ccsd(t)}\right) \quad (1)$$

$$E_{latt} = \left(\frac{E^*_{crystal,QE}}{N} - E^*_{ZW,QE}\right) + \left(E^*_{ZW,ccsd(t)} - E^*_{102,ccsd(t)}\right) + \left(E^*_{102,QE} - E_{011,QE}\right) \quad (2)$$

$$E_{latt} = \left(\frac{E^*_{crystal,QE}}{N} - E^*_{ZW,QE}\right) + \left(E^*_{ZW,QE} - E^*_{102,QE}\right) + \left(E^*_{102,ccsd(t)} - E_{011,ccsd(t)}\right) \quad (3)$$

$$E_{latt} = \left(\frac{E^*_{crystal,QE}}{N} - E^*_{ZW,QE}\right) + \left(E^*_{ZW,QE} - E^*_{102,QE}\right) + \left(E^*_{102,QE} - E_{011,QE}\right) \quad (4)$$

Electronic energy with *(ccsd(t))* labels were obtained at the CCSD(T)/6-311G++(2d,2p) level, in Gaussian09 [2] package, whereas electronic energies with (QE) labels were obtained at the PBE-D3 level in Quantum ESPRESSO. All energy terms marked with a star (*) were performed in the optimized geometries resulting from the Quantum ESPRESSO calculations, otherwise geometries obtained from optimizations at the B3LYP/6-311++G(2d,2p) level in Gaussian09 were assumed. Lattice energies calculated for the model (i) are reported in **Table 1**.

Table 1*: Calculated lattice energy values.*

	Elatt (kJ/mol)			
	(1)	(2)	(3)	(4)
α-glycine	-129.81	-141.19	-144.93	-156.30
β-glycine	-127.20	-138.58	-143.13	-154.51
γ-glycine	-129.19	-140.57	-144.12	-155.50

Taking into account the reference value for the lattice energy, -144 kJ/mol, the best calculated lattice energy values were obtained from model (3) deviation only -0.93, 0.87

and -0.12 kJ/mol for the α-, β- and γ-glycine, respectively, with respect to the global minimum.

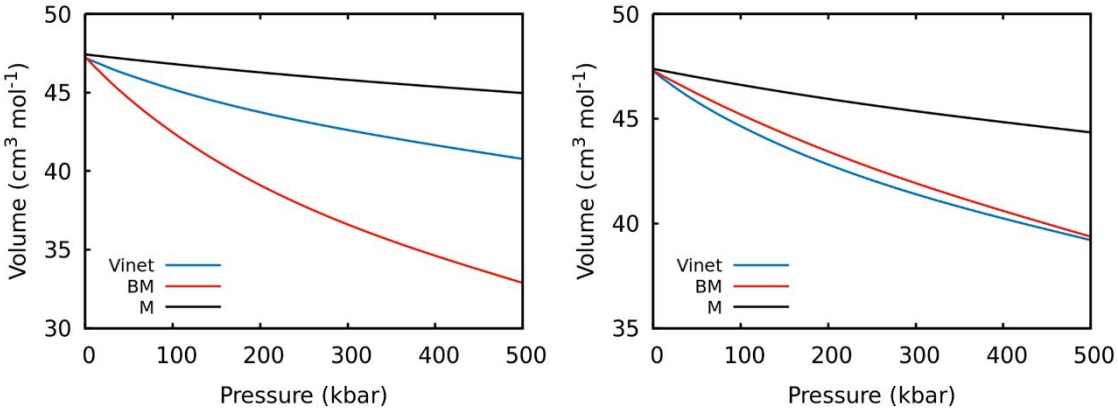

Figure 2. Volume x pressure diagrams for the β-glycine (left) and γ-glycine (right), obtained from a fit in the Murnaghan (M), third-order Birch-Murnaghan (BM) and Vinet equations of state.

Table 2. Bulk modulus (**B_0**) and its first derivative (B'), equilibrium volume (V_0) and minimized electronic energy (E_{min}) parameters obtained for the β-glycine and γ-glycine, obtained from a fit in the Murnaghan (M), third-order Birch-Murnaghan (BM) and Vinet (V) equations of state.

	β-glycine			**γ-glycine**		
	M	**BM**	**V**	**M**	**BM**	**V**
V_0 (a.u.^{3})	1063.07	1058.75	1057.87	1593.10	1589.40	1589.04
B_0 (kbar)	7314.84	530.61	1896.46	5755.62	1380.99	1393.90
B'	9.04	20.45	9.57	7.89	8.33	8.31
E_{min} (Ry)	-232.34367	-231.54273	-232.37129	-348.51362	-348.51419	-348.51682

Table 3. Equilibrium volume (V_0), dV/dT, thermal expansion (α) bulk modulus **(**B_0) and its first derivative (B') parameters obtained for the α-glycine from a fit in the Vinet equations of state.

	V_0 (au^3/cell)	**dV/dT**	**α (K^{-1})**	**B_0 (kbar)**	**B_1**
25	2189.186339	7.95E-02	3.63E-05	71.3561	15.81722
50	2190.386201	1.01E-01	4.60E-05	70.65169	15.85229
75	2192.757645	1.22E-01	5.56E-05	69.36881	15.91086
100	2195.993469	1.43E-01	6.51E-05	67.7637	15.9754
125	2199.849898	1.64E-01	7.46E-05	65.95835	16.0425
150	2204.346151	1.85E-01	8.40E-05	63.95355	16.11715
175	2209.445265	2.06E-01	9.34E-05	61.72618	16.20436
200	2215.136547	2.27E-01	1.03E-04	59.31527	16.30364
225	2221.359374	2.48E-01	1.12E-04	56.78386	16.41182
250	2228.030781	2.69E-01	1.21E-04	54.2284	16.51956
275	2235.408335	2.90E-01	1.30E-04	51.467	16.65125
300	2242.808358	3.11E-01	1.39E-04	48.92956	16.76504
325	2250.555449	3.32E-01	1.48E-04	46.46772	16.87238
350	2258.023385	3.53E-01	1.56E-04	44.27329	16.96546
375	2267.911816	3.74E-01	1.65E-04	41.31913	17.12716
400	2276.951133	3.95E-01	1.73E-04	38.9412	17.2431
425	2286.082004	4.16E-01	1.82E-04	36.75154	17.34311
450	2296.81164	4.36E-01	1.90E-04	34.22519	17.48701
475	2309.889463	4.57E-01	1.98E-04	31.32293	17.67258
500	2321.936792	4.78E-01	2.06E-04	28.96774	17.81827

Table 4. Equilibrium volume (V_0), dV/dT, thermal expansion (α) bulk modulus **(**B_0) and its first derivative (B') parameters obtained for the β-glycine from a fit in the Vinet equation of state.

	V_0 (au^3/cell)	**dV/dT**	**α (K^{-1})**	**B_0 (kbar)**	**B_1**
25	1083.809312	2.10E-02	1.94E-05	65.85584	5.134622
50	1084.157556	2.68E-02	2.47E-05	65.73851	5.137609
75	1084.795407	3.22E-02	2.97E-05	65.55642	5.141592
100	1085.664515	3.71E-02	3.42E-05	65.32557	5.146254
125	1086.70094	4.17E-02	3.84E-05	65.06249	5.151288
150	1087.859699	4.58E-02	4.21E-05	64.77843	5.156499
175	1089.110615	4.95E-02	4.55E-05	64.48079	5.16176
200	1090.433088	5.28E-02	4.85E-05	64.17467	5.166985
225	1091.812693	5.57E-02	5.10E-05	63.86369	5.172107
250	1093.23892	5.82E-02	5.32E-05	63.55051	5.17708
275	1094.704361	6.03E-02	5.50E-05	63.23702	5.181829
300	1096.201623	6.19E-02	5.65E-05	62.92499	5.186442
325	1097.727115	6.31E-02	5.75E-05	62.61524	5.190788
350	1099.276387	6.39E-02	5.82E-05	62.30867	5.194894
375	1100.846085	6.43E-02	5.84E-05	62.00592	5.198753
400	1102.433342	6.43E-02	5.83E-05	61.70743	5.202359
425	1104.034804	6.39E-02	5.79E-05	61.41356	5.205701
450	1105.650707	6.30E-02	5.70E-05	61.1246	5.208754
475	1107.278331	6.18E-02	5.58E-05	60.84074	5.211464
500	1108.916111	6.01E-02	5.42E-05	60.56192	5.213798

Table 5. Equilibrium volume (V_0), dV/dT, thermal expansion (α) bulk modulus **(**B_0) and its first derivative (B') parameters obtained for the γ-glycine from a fit in the Vinet equations of state.

	V_0 (au^3/cell)	**dV/dT**	**α (K^{-1})**	**B_0 (kbar)**	**B_1**
25	1639.599468	1.65E-02	1.00E-05	153.8662	2.346788
50	1639.814556	2.13E-02	1.30E-05	153.6996	2.34715
75	1640.355025	2.59E-02	1.58E-05	153.3046	2.348914
100	1640.992427	3.01E-02	1.84E-05	152.8685	2.356198
125	1641.876261	3.41E-02	2.07E-05	152.3523	2.358675
150	1642.865931	3.77E-02	2.30E-05	151.7632	2.362358
175	1643.867623	4.10E-02	2.50E-05	151.1813	2.370686
200	1644.989572	4.41E-02	2.68E-05	150.5692	2.375531
225	1646.135387	4.68E-02	2.84E-05	149.9376	2.382499
250	1647.340358	4.93E-02	2.99E-05	149.2939	2.38888
275	1648.567918	5.14E-02	3.12E-05	148.6361	2.397285
300	1649.867069	5.32E-02	3.23E-05	147.9875	2.402333
325	1651.175944	5.47E-02	3.31E-05	147.3091	2.409987
350	1652.514579	5.60E-02	3.39E-05	146.6151	2.418319
375	1653.903582	5.69E-02	3.44E-05	145.9229	2.424812
400	1655.316059	5.75E-02	3.47E-05	145.2189	2.432873
425	1656.752163	5.78E-02	3.49E-05	144.5182	2.440139
450	1658.22838	5.78E-02	3.49E-05	143.7925	2.448292
475	1659.733907	5.75E-02	3.47E-05	143.0741	2.455489
500	1661.259796	5.69E-02	3.43E-05	142.326	2.465185

Table 6. Equilibrium volume (V_0), dV/dT, thermal expansion (α) bulk modulus **(**B_0) and its first derivative (B') parameters obtained for the α-glycine from a fit in the Birch-Murnaghan equation of state.

	V_0 (au^3/cell)	dV/dT	α (K^{-1})	B_0 (kbar)	B_1
25	2199.252792	4.32E-01	1.96E-04	161.2173	48.21195
50	2202.511094	4.03E-01	1.83E-04	148.2172	51.94724
75	2209.498319	3.76E-01	1.70E-04	121.9326	61.86254
100	2221.496179	3.51E-01	1.58E-04	80.37815	90.4748
125	2233.486205	3.30E-01	1.48E-04	47.8851	145.6268
150	2242.869769	3.10E-01	1.38E-04	29.88104	224.8633
175	2250.37313	2.93E-01	1.30E-04	20.73344	313.6066
200	2255.873683	2.78E-01	1.23E-04	18.94084	334.09
225	2262.151003	2.66E-01	1.18E-04	16.01747	383.3426
250	2268.109983	2.56E-01	1.13E-04	14.50298	411.2832
275	2274.014685	2.49E-01	1.09E-04	13.64096	424.8718
300	2280.041604	2.44E-01	1.07E-04	13.17704	427.0664
325	2285.887127	2.41E-01	1.05E-04	13.26476	412.3565
350	2292.179497	2.41E-01	1.05E-04	12.65389	419.6069
375	2298.668508	2.43E-01	1.06E-04	12.11576	425.0998
400	2305.003011	2.48E-01	1.07E-04	11.97291	417.718
425	2311.514931	2.55E-01	1.10E-04	11.79053	411.7043
450	2318.073602	2.64E-01	1.14E-04	11.61551	405.7329
475	2324.734771	2.76E-01	1.19E-04	11.43769	400.0196
500	2331.406794	2.90E-01	1.25E-04	11.28411	393.8169

Table 7. Equilibrium volume (V_0), dV/dT, thermal expansion (α) bulk modulus **(**B_0) and its first derivative (B') parameters obtained for the β-glycine from a fit in the Birch-Murnaghan equation of state.

	V_0 (au^3/cell)	**dV/dT**	**α (K^{-1})**	**B_0 (kbar)**	**B_1**
25	1084.090399	2.17E-02	2.00E-05	292.203	5.101892
50	1084.442742	2.88E-02	2.66E-05	291.6827	5.104209
75	1085.088422	3.64E-02	3.35E-05	290.875	5.106928
100	1085.968374	4.44E-02	4.08E-05	289.8512	5.10985
125	1087.017858	5.28E-02	4.85E-05	288.6849	5.112796
150	1088.191347	6.16E-02	5.66E-05	287.4263	5.115656
175	1089.458246	7.08E-02	6.50E-05	286.1084	5.118364
200	1090.79773	8.05E-02	7.38E-05	284.7542	5.120852
225	1092.194192	9.06E-02	8.30E-05	283.3788	5.123155
250	1093.637343	1.01E-01	9.25E-05	281.9883	5.125485
275	1095.122489	1.12E-01	1.02E-04	280.6039	5.127187
300	1096.639874	1.23E-01	1.13E-04	279.2275	5.128599
325	1098.185316	1.35E-01	1.23E-04	277.8621	5.129744
350	1099.754904	1.47E-01	1.34E-04	276.5119	5.130592
375	1101.345194	1.60E-01	1.45E-04	275.1798	5.131143
400	1102.953293	1.73E-01	1.57E-04	273.8677	5.131397
425	1104.576674	1.87E-01	1.69E-04	272.5773	5.131355
450	1106.212481	2.00E-01	1.81E-04	271.3092	5.131082
475	1107.858386	2.15E-01	1.94E-04	270.0636	5.130636
500	1109.513335	2.29E-01	2.07E-04	268.8414	5.129966

Table 8. Equilibrium volume (V_0), dV/dT, thermal expansion (α) bulk modulus **(**B_0) and its first derivative (B') parameters obtained for the γ-glycine from a fit in the Birch-Murnaghan equation of state.

	V_0 (au^3/cell)	dV/dT	α (K^{-1})	B_0 (kbar)	B_1
25	1641.579642	1.54E-02	9.38E-06	711.9975	2.178073
50	1641.801841	2.02E-02	1.23E-05	710.9632	2.180917
75	1642.273086	2.47E-02	1.51E-05	709.2374	2.185709
100	1642.948536	2.90E-02	1.76E-05	707.0741	2.191799
125	1643.76751	3.29E-02	2.00E-05	704.6481	2.1986
150	1644.690477	3.65E-02	2.22E-05	702.0382	2.20596
175	1645.698357	3.98E-02	2.42E-05	699.3018	2.213689
200	1646.768754	4.28E-02	2.60E-05	696.4673	2.221694
225	1647.892376	4.55E-02	2.76E-05	693.5571	2.229961
250	1649.06188	4.79E-02	2.91E-05	690.5844	2.23839
275	1650.272158	5.00E-02	3.03E-05	687.5572	2.246978
300	1651.517549	5.18E-02	3.14E-05	684.4826	2.255712
325	1652.799392	5.33E-02	3.23E-05	681.3648	2.264568
350	1654.113921	5.45E-02	3.30E-05	678.2073	2.273541
375	1655.459696	5.54E-02	3.35E-05	675.013	2.282621
400	1656.835731	5.60E-02	3.38E-05	671.7839	2.291804
425	1658.241206	5.63E-02	3.40E-05	668.5216	2.301083
450	1659.675496	5.63E-02	3.39E-05	665.2274	2.310454
475	1661.138142	5.60E-02	3.37E-05	661.9019	2.319915
500	1662.628826	5.54E-02	3.33E-05	658.5455	2.329466

Table 9. Equilibrium volume (V_0), dV/dT, thermal expansion (α) bulk modulus **(**B_0) and its first derivative (B') parameters obtained for the α-glycine from a fit in the Murnaghan equation of state.

	V_0 (au^3/cell)	**dV/dT**	**α (K^{-1})**	**B_0 (kbar)**	**B_1**
25	2196.473831	1.04E-01	4.76E-05	349.3522	11.80823
50	2197.810594	1.22E-01	5.57E-05	346.0158	11.82244
75	2200.493248	1.41E-01	6.40E-05	339.8435	11.8433
100	2204.222943	1.60E-01	7.27E-05	331.791	11.86604
125	2208.723269	1.80E-01	8.16E-05	322.5769	11.88872
150	2213.835304	2.01E-01	9.08E-05	312.6025	11.91092
175	2219.51393	2.22E-01	1.00E-04	301.9853	11.93353
200	2225.623208	2.45E-01	1.10E-04	291.1357	11.95437
225	2232.249091	2.68E-01	1.20E-04	279.857	11.97608
250	2239.271818	2.91E-01	1.30E-04	268.56	11.99505
275	2246.767876	3.16E-01	1.40E-04	257.1036	12.01323
300	2254.80185	3.41E-01	1.51E-04	245.4301	12.03152
325	2263.400598	3.67E-01	1.62E-04	233.602	12.04953
350	2272.630817	3.93E-01	1.73E-04	221.6106	12.06751
375	2282.383429	4.20E-01	1.84E-04	209.7913	12.08225
400	2293.055558	4.48E-01	1.96E-04	197.5212	12.101
425	2304.750022	4.77E-01	2.07E-04	184.9482	12.12077
450	2317.240094	5.06E-01	2.19E-04	172.5915	12.13721
475	2330.759117	5.37E-01	2.30E-04	160.28	12.15201
500	2345.248277	5.68E-01	2.42E-04	148.2639	12.16262

Table 10. Equilibrium volume (V_0), dV/dT, thermal expansion (α) bulk modulus **(**B_0) and its first derivative (B') parameters obtained for the β-glycine from a fit in the Murnaghan equation of state.

	V_0 (au^3/cell)	dV/dT	α (K^{-1})	B_0 (kbar)	B_1
25	1085.715126	2.20E-02	2.03E-05	282.4517	4.904083
50	1086.079781	2.81E-02	2.58E-05	281.9562	4.904395
75	1086.747675	3.37E-02	3.10E-05	281.1973	4.90349
100	1087.657563	3.89E-02	3.57E-05	280.2422	4.901509
125	1088.742326	4.36E-02	4.01E-05	279.16	4.898648
150	1089.954744	4.79E-02	4.40E-05	277.9974	4.895062
175	1091.263067	5.18E-02	4.75E-05	276.7855	4.890868
200	1092.645681	5.52E-02	5.06E-05	275.5455	4.886138
225	1094.086501	5.82E-02	5.32E-05	274.2926	4.880915
250	1095.576699	6.08E-02	5.55E-05	273.0382	4.875223
275	1097.107115	6.29E-02	5.73E-05	271.7909	4.869055
300	1098.671541	6.46E-02	5.88E-05	270.5565	4.862393
325	1100.263466	6.58E-02	5.98E-05	269.3366	4.8554
350	1101.877738	6.66E-02	6.05E-05	268.132	4.848475
375	1103.509585	6.70E-02	6.07E-05	266.9528	4.841335
400	1105.160909	6.69E-02	6.05E-05	265.8023	4.833559
425	1106.829962	6.64E-02	6.00E-05	264.6695	4.825431
450	1108.507635	6.54E-02	5.90E-05	263.5774	4.817039
475	1110.196303	6.40E-02	5.77E-05	262.503	4.808514
500	1111.892707	6.22E-02	5.59E-05	261.4549	4.799844

Table 11. Equilibrium volume (V_0), dV/dT, thermal expansion (α) bulk modulus **(**B_0) and its first derivative (B') parameters obtained for the γ-glycine from a fit in the Murnaghan equation of state.

	V_0 (au^3/cell)	dV/dT	α (K^{-1})	B_0 (kbar)	B_1
25	1633.201913	1.63E-02	9.95E-06	685.1933	3.348023
50	1633.437561	2.13E-02	1.30E-05	684.1101	3.349069
75	1633.938975	2.61E-02	1.59E-05	682.2448	3.350683
100	1634.650132	3.05E-02	1.86E-05	679.8693	3.352598
125	1635.513287	3.46E-02	2.12E-05	677.1641	3.354682
150	1636.485798	3.84E-02	2.35E-05	674.2297	3.357211
175	1637.540102	4.19E-02	2.56E-05	671.1359	3.36018
200	1638.664713	4.51E-02	2.75E-05	667.9477	3.362611
225	1639.847929	4.79E-02	2.92E-05	664.6548	3.364904
250	1641.078451	5.05E-02	3.08E-05	661.2904	3.367478
275	1642.351404	5.27E-02	3.21E-05	657.8577	3.370343
300	1643.664684	5.46E-02	3.32E-05	654.3747	3.373229
325	1645.020688	5.62E-02	3.42E-05	650.8881	3.374558
350	1646.406419	5.75E-02	3.49E-05	647.3115	3.377336
375	1647.826371	5.85E-02	3.55E-05	643.6975	3.380095
400	1649.280255	5.92E-02	3.59E-05	640.0515	3.382861
425	1650.763989	5.95E-02	3.61E-05	636.3589	3.385741
450	1652.277813	5.96E-02	3.60E-05	632.6328	3.388755
475	1653.821014	5.93E-02	3.58E-05	628.8494	3.392436
500	1655.400284	5.87E-02	3.55E-05	625.0602	3.395355

Figure 3. Calculated volume in the temperature range of 25 and 500 K, at ambient pressure, obtained from a fit in the Vinet EOS for a-, b- and g-glycine polymorphs. The experimental data were retrieved from the ref. [45] of the manuscript.