

SUPPLEMENTARY MATERIAL

# Glycine conformers: a never-ending story?

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## 1 Methodology and Computational details

### 1.1 Molecular structure determination: best-estimated ab initio geometry

To account simultaneously for basis-set and electron-correlation effects, equilibrium structures have been determined by making use of a composite scheme, in which the various contributions are evaluated separately at the highest possible level and then combined in order to obtain best theoretical estimates. The approach used is based on additivity at the energy-gradient level.<sup>1,2</sup> Coupled-cluster (CC) theory within the singles and doubles (CCSD) approximation augmented by a perturbative treatment of triple excitations (CCSD(T))<sup>3</sup> has been employed in conjunction with correlation-consistent sets, (aug)-cc-p(C)VnZ ( $n=T, Q, 5$ ).<sup>4-6</sup> The contributions considered are: the Hartree-Fock self-consistent-field (HF-SCF) energy extrapolated to the basis-set limit, the valence correlation energy at the CCSD(T) level extrapolated to the basis-set limit as well, and the core-correlation correction. The energy gradient used in the geometry optimization is given by

$$\frac{dE_{\text{CBS+CV}}}{dx} = \frac{dE^{\infty}(\text{HF} - \text{SCF})}{dx} + \frac{d\Delta E^{\infty}(\text{CCSD(T)})}{dx} + \frac{d\Delta E(\text{CV})}{dx}, \quad (1)$$

where  $dE^{\infty}(\text{HF-SCF})/dx$  and  $d\Delta E^{\infty}(\text{CCSD(T)})/dx$  are the energy gradients corresponding to the  $\exp(-Cn)$  extrapolation scheme for HF-SCF<sup>7</sup> and to the  $n^{-3}$  extrapolation formula for the CCSD(T) correlation contribution,<sup>8</sup> respectively. In the expression given above,  $n=T, Q$  and 5 have been chosen for the HF-SCF extrapolation, while  $n=T$  and  $Q$  have been used for CCSD(T). Core-correlation effects have been included by adding the corresponding correction,  $d\Delta E(\text{CV})/dx$ , where the core-correlation energy correction,  $\Delta E(\text{CV})$ , is obtained as difference of all-electron and frozen-core CCSD(T) energies using the core-valence cc-pCVTZ basis set.

### 1.2 Molecular structure determination: semi-experimental equilibrium geometry

The so-called semi-experimental structure of the conformer Ip has been obtained by a least-squares fit of the molecular structural parameters to the equilibrium moments of inertia,  $I_e^i$ . The latter are straightforwardly obtained from the corresponding equilibrium rotational constants,  $B_e^i$ , which in turn are derived from the experimental ground-state constants,  $B_0^i$ , by correcting them for vibrational effects:

$$B_e^i = B_0^i + \frac{1}{2} \sum_r \alpha_r^i. \quad (2)$$

In the fitting procedure, the weighting scheme has been chosen in order to have the moments of inertia equally weighted. Experimental ground-state rotational constants for five isotopic species are known,<sup>9</sup> which means that, in addition to the main isotopologue, data for the isotopic substitution at both carbons, nitrogen and hydrogens bonded to carbon are available. In Eq. (2),  $\alpha_r^i$  are the computed vibration-rotation interaction constants, with  $r$  and  $i$  denoting the normal mode and the inertial axis, respectively. These constants have been obtained by means of vibrational second-order perturbation theory (VPT2).<sup>10,11</sup> The required cubic force field has been computed at the density functional theory (DFT) level. Within the DFT approach, the standard B3LYP functional has been used in conjunction with the double- $\zeta$  SNSD<sup>12</sup> basis set.

The fitting procedure deserves a few comments. First of all, it should be noted that the non-determinable geometrical parameters have been kept fixed at the corresponding best-estimated values. The fit has been carried out in three steps. First, only the determinable angles have been fitted with all the other parameters kept fixed at the best-estimated values. Then, the obtained

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angle values have been introduced in the input and kept fixed during the fitting of all determinable distances. Once the obtained values have been included in the input, all the determinable distances and angles have been relaxed. For all three steps, no convergence problem has been encountered. This positive outcome also depends on the chosen Z-matrix. In fact, the used Z-matrix does not contain variable dihedral angles. A previous definition of the Z-matrix involving variable dihedral angles led to serious convergence issues.

### 1.3 Rotational spectra: best-estimated spectroscopic parameters

Moving to the field of rotational spectroscopy, best-estimated ground-state rotational constants have been obtained by adding to the equilibrium rotational constants corresponding to the best-estimated equilibrium structure the vibrational corrections,  $\Delta B_0^i$ , computed at the B3LYP/SNSD level. From Eq. (2), the corresponding expression is:

$$\Delta B_0^i = -\frac{1}{2} \sum_r \alpha_r^i . \quad (3)$$

By making use of the harmonic force fields obtained at different levels of theory in the frame of the best-estimated harmonic frequency and intensity determination, best estimates for quartic centrifugal-distortion constants,  $D(\text{best})$ , have been derived by means of the following composite scheme:

$$\begin{aligned} D(\text{best}) &= D(\text{CCSD(T)}/\text{VTZ}) + [D(\text{MP2}/\text{CVTZ}, \text{all}) - D(\text{MP2}/\text{CVTZ}, \text{fc})] \\ &+ [D(\text{MP2}/\text{augVTZ}, \text{fc}) - D(\text{MP2}/\text{VTZ}, \text{fc})] + [D(\text{MP2}/\text{VQZ}, \text{fc}) - D(\text{MP2}/\text{VTZ}, \text{fc})] , \end{aligned} \quad (4)$$

where  $D$  denotes a generic quartic centrifugal-distortion constant. The first difference (in square brackets) provides the CV correction ( $\Delta D(\text{CV})$ ), the second one the contribution of diffuse functions ( $\Delta D(\text{aug})$ ), and the last one the effect of enlarging the basis set from a triple-zeta to a quadruple-zeta set. Watson's  $S$ -reduced Hamiltonian in the  $I^r$  representation<sup>13</sup> has been employed.

An analogous composite scheme:

$$\begin{aligned} \chi_{ij}(\text{best}) &= \chi_{ij}(\text{CCSD(T)}/\text{VTZ}) + [\chi_{ij}(\text{MP2}/\text{CVTZ}, \text{all}) - \chi_{ij}(\text{MP2}/\text{CVTZ}, \text{fc})] \\ &+ [\chi_{ij}(\text{MP2}/\text{augVTZ}, \text{fc}) - \chi_{ij}(\text{MP2}/\text{VTZ}, \text{fc})] + [\chi_{ij}(\text{MP2}/\text{VQZ}, \text{fc}) - \chi_{ij}(\text{MP2}/\text{VTZ}, \text{fc})] , \end{aligned} \quad (5)$$

has been considered for the nitrogen quadrupole-coupling constants  $\chi_{ij}$ , where  $ij$  refers to the principal inertial axes. The additivity scheme has actually been applied to the electric field-gradient components  $q_{ij}$ , which are the quantities computed by electronic-structure calculations. The latter are transformed to nuclear quadrupole-coupling constants by means of

$$\chi_{ij} = eQq_{ij}, \quad (6)$$

where  $eQ$  in the present case is the nitrogen quadrupole moment,  $Q(^{14}\text{N}) = 0.02044(3)$  barn, taken from Ref.<sup>14</sup>. The electric field-gradient tensors have been initially obtained for the main isotopic species and then transformed in order to obtain those for the tri-deuterated [OD,NH<sub>2</sub>] species considered.

In Ref.<sup>15</sup>, Halkier *et al.* showed that the molecular electric dipole moment can be extrapolated to the complete basis set (CBS) limit (provided that a hierarchical sequence of basis sets is employed) using the following  $n^{-3}$  extrapolation form for the correlation contribution:

$$\Delta\mu^{\text{corr}}(n) = \Delta\mu_{\infty}^{\text{corr}} + A n^{-3} . \quad (7)$$

In our investigation, this formula has been applied with  $n=3$  (triple-zeta, i.e., MP2/cc-pVTZ) and 4 (quadruple-zeta, i.e., MP2/cc-pVQZ). To obtain the extrapolated dipole moment, the CBS limit of the correlation contribution should then be added to the HF-SCF CBS limit, which is assumed in the present case to be reached at the HF-SCF/cc-pV5Z level:

$$\mu(\text{CBS}) = \mu_{\infty}^{\text{SCF}} + \Delta\mu_{\infty}^{\text{corr}} . \quad (8)$$

The best estimate of the dipole moment has then been derived by applying a composite scheme aiming at accounting for core-correlation, diffuse function and high-order electron correlation effects. The best estimates for electric dipole-moment components have been obtained by the following expression:

$$\mu(\text{best}) = \mu(\text{CBS}) + \Delta\mu(\text{CV}) + \Delta\mu(\text{aug}) + \Delta\mu(\text{T}) . \quad (9)$$

To directly predict experiment, zero-point vibrational (ZPV) corrections have been computed and added to the best-estimated values. ZPV corrections have been obtained at the B3LYP/SNSD level using the perturbational approach described in Ref.<sup>11</sup>. The latter have been found to be non-negligible, as they are of the order of 5-10 %.

#### 1.4 Energy: best-estimated energy differences

In view of accurately establishing the energy difference between the VI<sub>p</sub> and Ip conformers, single-point energy calculations at the best-estimated equilibrium structures have been carried out employing the same composite scheme used for the molecular structure determination. CBS total energies have been determined by extrapolating the CCSD(T) correlation contribution to the CBS limit by means of the  $n^{-3}$  formula<sup>8</sup>:

$$\Delta E^{\text{corr}}(n) = \Delta E_{\infty}^{\text{corr}} + A' n^{-3} \quad (10)$$

and adding the HF-SCF CBS limit, evaluated by the expression<sup>7</sup>

$$E^{\text{SCF}}(n) = E_{\infty}^{\text{SCF}} + B' \exp(-C' n) . \quad (11)$$

The cc-pVTZ and cc-pVQZ basis sets have been employed in the former equation, whereas the cc-pV $n$ Z sets, with  $n=T, Q, 5$ , have been used in the latter. Making use of the additivity approximation, corrections to take into account CV effects have then been added to CBS energies. This involves carrying out energy computations using the core-valence correlation-consistent cc-pCVTZ basis set in conjunction with the CCSD(T) method. The CV corrections to the total energies are thus given as

$$\Delta E_{CV} = E_{\text{core+val}} - E_{\text{val}} , \quad (12)$$

where  $E_{\text{core+val}}$  is the CCSD(T) total energy obtained by correlating all electrons and  $E_{\text{val}}$  is the CCSD(T) total energy obtained in the frozen-core approximation.

#### 1.5 Harmonic force field: best-estimated harmonic frequencies and intensities

Best-estimated harmonic force fields for the VI<sub>p</sub> conformer of glycine (both main and tri-deuterated isotopologues) have been evaluated by means of a composite scheme. This scheme mainly involves the second-order Møller-Plesset perturbation theory (MP2)<sup>16</sup> level, used in conjunction with the standard cc-pV $n$ Z<sup>4</sup> basis sets ( $n=T, Q$ ) as well as a triple-zeta basis set augmented by diffuse functions, aug-cc-pVTZ.<sup>4,5</sup> In both cases, the frozen-core (fc) approximation has been adopted. To account for core-correlation effects, the core-valence correlation consistent cc-pCVTZ basis set<sup>4,6</sup> has been employed, whereas the CCSD(T) method has been used together with the cc-pVTZ basis set in order to improve the electron-correlation treatment. At the various optimized geometries, harmonic force fields have been obtained using analytic second derivatives.<sup>17</sup> Following the procedure introduced in Ref.<sup>18</sup>, the harmonic frequencies,  $\omega$ , have been extrapolated to the complete basis set (CBS) limit starting from the results obtained at the MP2/cc-pVTZ and MP2/cc-pVQZ levels. The extrapolated correlation contribution has been added to the HF-SCF CBS limit, which is assumed to be reached at the HF/cc-pV5Z level. Corrections due to core correlation and effects of diffuse functions in the basis set have then been evaluated at the MP2/cc-pCVTZ ( $\Delta\omega(\text{CV})=\omega(\text{MP2/cc-pCVTZ,all})-\omega(\text{MP2/cc-pCVTZ,fc})$ ) and MP2/aug-cc-pVTZ levels ( $\Delta\omega(\text{aug})=\omega(\text{MP2/aug-cc-pVTZ,fc})-\omega(\text{MP2/cc-pVTZ,fc})$ ), respectively. The latter correction has been introduced since diffuse functions are required to properly describe electronegative atoms and also to recover the corresponding limitations affecting the extrapolation procedure when small- to medium-sized basis sets are employed. Higher-order electron-correlation energy contributions,  $\Delta\omega((\text{T}))$ , have been derived by comparing the harmonic frequencies at the MP2 and CCSD(T) levels, both in conjunction with the cc-pVTZ basis set. The best-estimated harmonic frequencies,  $\omega(\text{best})$ , are then provided by

$$\omega(\text{best}) = \omega(\text{CBS}(T, Q)) + \Delta\omega(\text{CV}) + \Delta\omega(\text{aug}) + \Delta\omega((\text{T})) . \quad (13)$$

An analogous composite scheme has also been used to determine the best estimates for IR intensities,  $I(\text{best})$ , within the harmonic approximation. As extrapolation schemes have not been formulated for such a property yet, Eq. (13) has been rearranged as follows:

$$I(\text{best}) = I(\text{CCSD}(T)/\text{VTZ}) + \Delta I(\text{CV}) + \Delta I(\text{QZ} - \text{TZ}) + \Delta I(\text{aug}) , \quad (14)$$

where  $\Delta I(\text{QZ} - \text{TZ})$  is the correction due to the enlargement of the basis set from triple- to quadruple-zeta.

## 1.6 Anharmonic force field calculations

Computations of IR spectra beyond harmonic approximations, the vibrational corrections to rotational constants and vibrational contributions to thermodynamic properties, have been performed by means of a Hindered-Rotor Anharmonic Oscillator (HRAO) model, within the vibrational second-order perturbation theory (VPT2)<sup>10</sup>. In order to compute accurately the vibrational spectra and vibrational corrections for the VIp conformer of glycine, a hybrid CCSD(T)/DFT approach has been employed.<sup>19–25</sup> It is based on the assumption that the differences between CCSD(T) and B3LYP results are mainly due to the harmonic terms, and it has already been validated for vibrational frequencies of several closed- and open-shell systems (see for instance Ref.<sup>21–24</sup>), as well as for thermodynamic properties.<sup>26</sup> Anharmonic DFT semi-diagonal quartic force fields (i.e., the cubic ( $K_{ijk}$ ) and semi-diagonal quartic ( $K_{iijk}$ ) force constants) have been obtained by numerical differentiation of the analytical second derivatives of the energy (with the standard 0.01 Å step), starting from equilibrium structures optimized using tight convergence criteria. Within the DFT approach, the standard B3LYP functional<sup>27</sup> has been used in conjunction with the double- $\zeta$  SNSD<sup>12</sup> basis set, developed for spectroscopic studies of medium-to-large molecular systems. This basis set has been constructed from the polarized double- $\zeta$  N07D basis set<sup>12,28–30</sup> by consistently including diffuse  $s$  functions on all atoms, and one set of diffuse polarized functions ( $d$  on heavy atoms and  $p$  on hydrogens). This basis set allows cost-effective prediction of a broad range of spectroscopic properties, including electron-spin resonance (ESR)<sup>28–31</sup>, vibrational (IR, Raman, VCD)<sup>25,31–34</sup> and electronic (absorption, emission, ECD)<sup>25,31,34,35</sup> spectra.

With respect to VPT2 computations, the generalized second-order vibrational perturbation model (GVPT2) as well as the corresponding deperturbed approach (DVPT2)<sup>10,11,36</sup>, as implemented in the GAUSSIAN package<sup>11,37,38</sup>, have been applied to compute anharmonic frequencies and IR intensities, respectively. In the present work, the criteria chosen to define Fermi resonances involving frequencies are those proposed by Martin *et al.*<sup>39</sup>, while for the 1-1 resonances present in the perturbative treatment of intensities<sup>38,40</sup>, the criteria proposed by Bloino and Barone<sup>40</sup> have been adopted. Vibrational contributions to thermodynamic properties have been evaluated by resonance-free perturbative approach within the hybrid degeneracy corrected second-order perturbation theory (HDCPT2).<sup>26</sup> The latter provides an automatic treatment of internal rotations through the hindered-rotor model in conjunction with simple perturbation theory (SPT)<sup>41</sup> reformulated to treat consistently both energy minima and transition states. In all cases the best-estimated harmonic frequencies have been introduced directly into the VPT2 computations along with the cubic and quartic force constants obtained at the DFT level.

MP2 and CCSD(T) calculations have been carried out with the quantum-chemical CFOUR program package.<sup>42</sup> All DFT and VPT2 computations have been performed employing a locally modified version of the GAUSSIAN suite of programs for quantum chemistry.<sup>43</sup>

## 2 Supplementary results

### References

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**Table 1** Best-estimated and DFT harmonic frequencies ( $\text{cm}^{-1}$ ) of the Ip and VIp conformers of glycine.

	Composite scheme							DFT	
	MP2/TZ	MP2/QZ	MP2/CBS	$\Delta\omega(\text{CV})$	$\Delta\omega(\text{diff})$	$\Delta\omega((\text{T}))$	best	B3LYP/SNSD	
<i>glycine-<math>I_p</math></i>									
A''	65.11	65.82	66.83	0.63	1.64	-1.75	67.35	A''	65.58
A''	217.93	212.79	209.37	0.01	-7.58	-1.40	200.38	A''	212.24
A'	259.77	257.93	256.83	1.19	-2.62	-1.16	254.24	A'	256.69
A'	468.05	468.75	469.14	1.93	-0.96	-3.49	466.62	A'	463.06
A''	514.63	514.69	514.97	1.38	-3.45	-4.95	507.95	A''	508.16
A'	639.24	639.74	641.16	2.23	-3.48	-1.67	638.23	A'	634.61
A''	657.03	654.72	652.80	1.61	-9.76	-5.41	639.24	A''	654.65
A'	842.94	839.21	838.02	1.79	-9.24	-4.00	826.57	A'	820.93
A''	925.49	923.28	921.95	2.29	-5.51	-3.00	915.72	A''	915.73
A'	955.75	941.91	935.35	-0.73	-22.49	6.58	918.72	A'	920.30
A'	1141.63	1140.71	1140.13	3.42	-6.42	0.34	1137.48	A'	1124.50
A'	1181.34	1181.13	1181.61	3.10	-5.78	-1.93	1177.00	A'	1162.27
A''	1194.76	1193.61	1192.86	2.52	-0.18	-3.52	1191.68	A''	1183.55
A'	1317.23	1314.15	1312.37	2.30	-8.00	6.52	1313.19	A'	1303.24
A''	1398.95	1397.13	1395.93	1.60	-4.10	-2.02	1391.40	A''	1382.83
A'	1420.72	1417.77	1416.45	3.61	-8.22	1.07	1412.92	A'	1395.61
A'	1472.60	1471.02	1469.96	1.47	1.52	-3.50	1469.44	A'	11452.96
A'	1677.28	1676.37	1675.79	1.91	-5.93	3.23	1675.00	A'	1673.10
A'	1826.92	1820.16	1817.63	5.18	-19.24	4.44	1808.01	A'	1817.29
A'	3099.97	3100.08	3099.81	5.51	-5.73	-37.90	3061.70	A'	3045.14
A''	3148.32	3150.85	3152.14	5.66	-4.67	-46.00	3107.13	A''	3080.75
A'	3537.42	3545.56	3549.78	7.62	-5.75	-35.92	3515.73	A'	3503.32
A''	3622.39	3631.26	3636.41	8.01	-4.74	-47.21	3592.48	A''	3576.75
A'	3770.06	3772.46	3773.55	5.49	-20.23	3.86	3762.67	A'	3740.04
<i>glycine-<math>V_{I_p}</math></i>									
A''	77.97	81.17	83.35	0.61	2.75	-2.50	84.21	A''	77.98
A''	207.37	204.33	200.63	-0.20	-5.50	-1.64	193.28	A''	203.02
A'	262.73	261.36	260.45	1.20	-2.81	-1.37	257.47	A'	260.21
A''	462.96	470.61	472.92	1.31	1.77	-5.88	470.11	A''	462.77
A'	471.50	471.20	470.79	1.85	-3.42	-3.87	465.36	A'	467.77
A''	571.13	572.42	572.32	1.51	-1.50	-5.28	567.05	A''	573.56
A'	651.97	652.00	651.25	2.41	-5.49	-1.73	646.43	A'	647.35
A'	849.93	847.20	845.94	2.18	-8.46	-3.18	836.48	A'	830.19
A''	928.91	927.99	926.76	2.33	-4.58	-3.44	921.07	A''	919.88
A'	956.00	943.09	934.89	-0.67	-21.55	6.78	919.45	A'	921.37
A'	1151.70	1148.50	1146.17	3.38	-11.10	-2.66	1135.79	A'	1120.57
A'	1185.17	1184.32	1184.02	3.06	-7.73	-3.96	1175.39	A'	1157.44
A''	1192.79	1193.24	1193.62	2.53	1.41	-3.78	1193.77	A''	1183.79
A'	1296.05	1293.80	1292.13	1.79	-7.81	11.65	1297.79	A'	1283.94
A'	1394.60	1393.37	1393.58	3.17	-4.05	1.35	1394.05	A'	1377.90
A''	1406.68	1406.59	1405.89	1.69	-2.38	-2.68	1402.52	A''	1392.16
A'	1477.96	1477.26	1477.12	1.68	1.78	-4.51	1476.06	A'	1458.81
A'	1677.65	1676.98	1676.68	1.91	-5.56	3.23	1676.27	A'	1673.78
A'	1853.74	1847.99	1845.00	5.48	-19.78	8.72	1839.41	A'	1851.01
A'	3072.73	3073.64	3074.77	5.46	-4.33	-38.47	3037.42	A'	3017.69
A''	3121.98	3125.49	3128.28	5.67	-3.32	-47.27	3083.35	A''	3053.87
A'	3535.92	3543.65	3548.78	7.57	-6.21	-34.53	3515.61	A'	3502.95
A''	3619.60	3628.02	3635.17	7.95	-5.22	-45.55	3592.36	A''	3575.53
A'	3822.99	3823.80	3824.80	5.85	-24.93	-7.08	3798.64	A'	3781.17

<sup>a</sup> See text.

**Table 2** Best-estimated and DFT harmonic IR intensities (km/mol) of the Ip and VIp conformers of glycine.

	Composite scheme					DFT	
	CCSD(T)/TZ	$\Delta I(\text{CV})$	$\Delta I(\text{QZ-TZ})$	$\Delta I(\text{diff})$	best	B3LYP/SNSD	
<i>glycine-<math>I_p</math></i>							
A''	5.62	0.10	0.01	-0.61	5.11	A''	5.01
A''	43.71	0.07	-0.07	0.59	44.31	A''	43.35
A'	8.95	0.10	0.73	0.46	10.25	A'	10.04
A'	30.03	0.19	0.64	-0.03	30.84	A''	30.04
A''	30.10	0.56	-0.74	-1.07	28.84	A'	29.45
A'	9.10	-0.22	-1.30	-1.70	5.88	A''	5.92
A''	89.19	0.01	0.20	-1.09	88.32	A'	89.91
A'	63.32	4.84	11.73	8.59	88.48	A'	75.32
A''	1.60	0.16	0.12	-0.21	1.67	A''	2.92
A'	135.93	-2.57	-15.40	-29.10	88.85	A'	120.39
A'	138.81	3.64	25.90	29.19	197.53	A'	189.89
A'	139.92	-4.49	-16.77	-12.41	106.26	A''	112.71
A''	1.19	0.02	0.03	-0.06	1.18	A'	1.34
A'	9.78	0.43	0.81	2.92	13.94	A'	13.40
A''	0.20	-0.01	-0.06	-0.07	0.06	A'	0.07
A'	26.54	1.13	-1.39	-3.59	22.69	A''	14.44
A'	10.88	0.53	1.10	1.27	13.78	A'	15.16
A'	15.83	0.40	0.81	0.27	17.31	A'	18.59
A'	244.96	1.37	11.04	19.63	277.00	A'	299.88
A'	15.10	-0.13	-0.23	-0.03	14.71	A'	16.97
A''	6.93	-0.24	-1.19	-1.39	4.10	A''	5.89
A'	1.42	0.25	1.47	0.87	4.00	A'	2.17
A''	2.72	0.53	3.52	4.11	10.88	A'	5.76
A'	61.09	1.10	5.40	2.76	70.35	A''	58.41
<i>glycine-<math>V_{I_p}</math></i>							
A''	7.97	0.13	-0.39	-1.40	6.31	A''	6.34
A''	56.01	-0.02	0.44	0.98	57.41	A''	58.22
A'	26.77	0.21	0.50	-0.45	27.03	A'	26.84
A''	83.03	-0.00	0.14	0.26	1.73	A''	1.49
A'	1.33	0.74	0.22	0.41	84.40	A'	77.99
A''	8.08	-0.04	1.28	0.27	9.60	A''	14.39
A'	12.99	0.04	0.37	0.27	13.66	A'	12.94
A'	15.97	2.43	7.28	7.60	33.28	A'	22.56
A''	0.66	0.09	0.08	-0.08	0.75	A''	1.13
A'	174.49	-0.28	-9.72	-25.11	139.38	A'	166.27
A'	21.08	-1.36	5.47	11.26	36.44	A'	44.09
A'	14.41	-0.58	-1.18	-1.61	11.05	A''	3.90
A''	0.64	0.01	0.10	0.07	0.83	A'	0.77
A'	320.77	1.62	3.11	7.17	332.67	A'	357.25
A'	53.66	1.16	-5.90	-11.63	37.29	A'	23.42
A''	0.32	-0.01	-0.12	-0.14	0.05	A''	0.11
A'	5.76	0.22	1.01	1.54	8.53	A'	8.19
A'	18.38	0.40	0.92	0.28	19.98	A'	20.61
A'	198.27	1.48	11.38	19.39	230.52	A'	251.92
A'	23.98	-0.11	0.04	0.40	24.31	A'	27.99
A''	10.98	-0.31	-1.84	-2.25	6.58	A''	9.80
A'	2.39	0.31	1.75	1.10	5.55	A'	3.45
A''	3.94	0.59	3.74	4.29	12.55	A'	7.34
A'	47.36	0.95	3.88	1.61	53.80	A''	44.19

<sup>a</sup> See text.

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