Journal Name

ARTICLE TYPE

Cite this: DOI: 00.0000/xxxxxxxxxx

Supplementary Material: A high level theory investigation on the lowest-lying ionization potentials of glycine ($C_2H_5NO_2$)

Gabriel L. C. de Souza*[a,b] and Kirk A. Peterson*[b]

[a] *Departamento de Química, Universidade Federal de Mato Grosso, Cuiabá, Mato Grosso, 78060-900 Brazil; E-mail: gabriellcs@pq.cnpq.br*
[b] *Department of Chemistry, Washington State University, Pullman, Washington, 99164 USA. E-mail: kipeters@wsu.edu*

Table S1 Vertical ionization potentials (IPs) for NH_2CH_2COOH as determined using the frozen-core EOMIP-CCSD/AVXZ (X = D, T, and Q) approach.[a] All values are given in eV.

			AVDZ			
IP	Ip	IIn	IIp	IIIn	IIIp	IVn
1	9.92	9.99	9.93	9.63	9.63	9.78
2	10.90	11.32	11.37	11.42	11.44	10.80
3	12.09	11.41	11.40	12.02	11.95	12.04
4	13.57	13.44	13.42	13.70	13.71	13.92
5	14.41	13.90	13.84	14.39	14.34	14.35
6	15.05	15.07	15.06	14.71	14.79	14.96
7	15.69	15.66	15.64	15.82	15.68	15.58
8	16.94	16.72	16.73	16.94	16.99	16.81
9	17.19	17.71	17.87	16.99	17.02	17.04
10	17.69	18.44	18.37	17.75	17.74	17.95
11	20.36	19.86	19.83	20.73	20.76	20.27
12	22.05	22.33	22.32	21.44	21.66	21.90
			AVTZ			
IP	Ip	IIn	IIp	IIIn	IIIp	IVn
1	10.13	10.22	10.16	9.85	9.85	9.99
2	11.12	11.52	11.58	11.64	11.66	11.02
3	12.29	11.62	11.61	12.23	12.15	12.25
4	13.72	13.62	13.61	13.86	13.88	14.08
5	14.57	14.07	14.00	14.55	14.51	14.51
6	15.20	15.22	15.21	14.86	14.94	15.11
7	15.85	15.80	15.79	15.97	15.83	15.72
8	17.09	16.86	16.87	17.09	17.14	16.95
9	17.34	17.86	18.02	17.14	17.17	17.19
10	17.81	18.57	18.49	17.87	17.86	18.07
11	20.47	19.98	19.95	20.84	20.87	20.38
12	22.60	22.88	22.87	21.99	22.21	22.41
			AVQZ			
IP	Ip	IIn	IIp	IIIn	IIIp	IVn
1	10.20	—	—	—	—	—
2	11.21	—	—	—	—	—
3	12.38	—	—	—	—	—
4	13.78	—	—	—	—	—
5	14.65	—	—	—	—	—
6	15.27	—	—	—	—	—
7	15.91	—	—	—	—	—
8	17.17	—	—	—	—	—
9	17.41	—	—	—	—	—
10	17.86	—	—	—	—	—
11	20.54	—	—	—	—	—
12	22.75	—	—	—	—	—

[a] The CCSD(T)/AVTZ value for the first vertical IP of the Ip conformer (MP2 geometry of neutral) is 10.11 eV with the first adiabatic IP [CCSD(T)/AVTZ optimized geometry and harmonic zero-point corrections) at 9.34 eV

Table S2 CBS extrapolation using Eq.1 at the [DT], [TQ], and [DTQ] levels for the vertical IPs. Again, all values given in eV.

			CBS[DT]			
IP	Ip	IIn	IIp	IIIn	IIIp	IVn
1	10.20	10.30	10.24	9.93	9.93	10.06
2	11.20	11.59	11.65	11.72	11.73	11.10
3	12.37	11.69	11.68	12.30	12.22	12.32
4	13.77	13.69	13.67	13.91	13.93	14.13
5	14.63	14.13	14.06	14.61	14.57	14.57
6	15.25	15.28	15.26	14.92	14.99	15.17
7	15.90	15.85	15.84	16.02	15.88	15.77
8	17.15	16.91	16.92	17.14	17.19	17.00
9	17.39	17.91	18.08	17.20	17.22	17.24
10	17.85	18.62	18.53	17.92	17.90	18.12
11	20.51	20.02	19.99	20.88	20.90	20.42
12	22.79	23.07	23.06	22.19	22.41	22.60
			CBS[TQ]			
IP	Ip	IIn	IIp	IIIn	IIIp	IVn
1	10.23	—	—	—	—	—
2	11.26	—	—	—	—	—
3	12.43	—	—	—	—	—
4	13.81	—	—	—	—	—
5	14.69	—	—	—	—	—
6	15.30	—	—	—	—	—
7	15.95	—	—	—	—	—
8	17.21	—	—	—	—	—
9	17.45	—	—	—	—	—
10	17.89	—	—	—	—	—
11	20.57	—	—	—	—	—
12	22.83	—	—	—	—	—
			CBS[DTQ]			
IP	Ip	IIn	IIp	IIIn	IIIp	IVn
1	10.24	—	—	—	—	—
2	11.26	—	—	—	—	—
3	12.44	—	—	—	—	—
4	13.81	—	—	—	—	—
5	14.71	—	—	—	—	—
6	15.31	—	—	—	—	—
7	15.97	—	—	—	—	—
8	17.25	—	—	—	—	—
9	17.47	—	—	—	—	—
10	17.90	—	—	—	—	—
11	20.63	—	—	—	—	—
12	22.80	—	—	—	—	—

Table S3 Vertical ionization potentials (IPs) and Δ_{CV} for NH_2CH_2COOH as determined using the frozen-core EOMIP-CCSD/ACVXZ (X = D and T) approach. All values are given in eV.

			ACVDZ			
IP	Ip	IIn	IIp	IIIn	IIIp	IVn
1	9.93	10.01	9.95	9.64	9.64	9.79
2	10.91	11.33	11.38	11.43	11.45	10.81
3	12.10	11.42	11.42	12.03	11.95	12.05
4	13.57	13.45	13.44	13.71	13.70	13.92
5	14.42	13.90	13.85	14.40	14.35	14.35
6	15.06	15.08	15.10	14.72	14.80	14.96
7	15.70	15.66	15.65	15.82	15.68	15.59
8	16.95	16.73	16.75	16.95	17.00	16.82
9	17.21	17.72	17.88	17.00	17.03	17.06
10	17.69	18.45	18.38	17.76	17.74	17.95
11	20.37	19.87	19.85	20.74	20.77	20.28
12	22.07	22.35	22.41	21.46	21.68	21.92
			ACVTZ			
IP	Ip	IIn	IIp	IIIn	IIIp	IVn
1	10.14	10.23	10.20	9.86	9.86	9.99
2	11.13	11.53	11.61	11.65	11.67	11.03
3	12.30	11.63	11.64	12.24	12.16	12.26
4	13.72	13.63	13.64	13.86	13.88	14.08
5	14.58	14.07	14.03	14.56	14.52	14.52
6	15.21	15.23	15.25	14.87	14.94	15.12
7	15.85	15.81	15.82	15.98	15.84	15.73
8	17.10	16.87	16.90	17.10	17.15	16.96
9	17.35	17.87	18.05	17.15	17.17	17.20
10	17.81	18.57	18.51	17.88	17.86	18.08
11	20.48	19.99	19.98	20.85	20.87	20.39
12	22.62	22.90	23.01	22.02	22.23	22.43
			Δ_{CV}**(DZ)**			
IP	Ip	IIn	IIp	IIIn	IIIp	IVn
1	0.006	0.007	0.007	0.007	0.007	0.006
2	0.008	0.007	0.007	0.007	0.007	0.007
3	0.007	0.007	0.007	0.007	0.007	0.007
4	0.005	0.007	0.007	0.005	0.005	0.006
5	0.007	0.006	0.006	0.006	0.007	0.006
6	0.006	0.007	0.007	0.006	0.006	0.007
7	0.007	0.007	0.007	0.007	0.008	0.006
8	0.007	0.006	0.006	0.005	0.008	0.007
9	0.006	0.005	0.005	0.008	0.03	0.005
10	0.005	0.005	0.005	0.005	0.005	0.005
11	0.004	0.005	0.005	0.004	0.004	0.004
12	0.06	0.06	0.06	0.06	0.24	0.005
			Δ_{CV}**(TZ)**			
IP	Ip	IIn	IIp	IIIn	IIIp	IVn
1	0.02	0.03	0.03	0.03	0.03	0.02
2	0.03	0.02	0.03	0.03	0.03	0.03
3	0.03	0.03	0.03	0.03	0.03	0.03
4	0.02	0.03	0.03	0.02	0.02	0.03
5	0.03	0.02	0.02	0.02	0.03	0.02
6	0.02	0.03	0.03	0.02	0.02	0.02
7	0.02	0.02	0.02	0.02	0.02	0.02
8	0.02	0.02	0.02	0.02	0.03	0.02
9	0.02	0.02	0.02	0.03	0.05	0.02
10	0.02	0.02	0.02	0.01	0.02	0.02
11	0.01	0.02	0.02	0.02	0.02	0.01
12	0.12	0.12	0.12	0.12	0.12	0.11

Table S4 Raw values used for computing the vertical ionization potentials (IPs) for the Ip conformation of the $C_2H_5NO_2$ molecule determined using the frozen-core EOMIP-CCSD/AVXZ (X = D, T, and Q) approach. The values are given in hartrees.

	AVDZ
Ground state	-283.76458648730500
1IP	-283.40013538407982
2IP	-283.36417474944994
3IP	-283.32039406358166
4IP	-283.26603449284943
5IP	-283.23520933298903
6IP	-283.21135355705047
7IP	-283.18799921118506
8IP	-283.14200148967439
9IP	-283.13291171149785
10IP	-283.11466159615844
11IP	-283.01645562176350
12IP	-282.95441025588900
	AVTZ
Ground state	-283.99780932359988
1IP	-283.62560706077602
2IP	-283.58914629123126
3IP	-283.54605345003671
4IP	-283.49360357220354
5IP	-283.46237688616293
6IP	-283.43915680738627
7IP	-283.41551625164846
8IP	-283.36969703769631
9IP	-283.36056401092964
10IP	-283.34345460106050
11IP	-283.24553625919037
12IP	-283.16742970371342
	AVQZ
Ground state	-284.06844263002432
1IP	-283.69374951379910
2IP	-283.65662864020305
3IP	-283.61360058139093
4IP	-283.56221983560857
5IP	-283.53018871891794
6IP	-283.50747595854847
7IP	-283.48365289391973
8IP	-283.43748116355255
9IP	-283.42858431329444
10IP	-283.41216707627234
11IP	-283.31376359182212
12IP	-283.23255310659516

Table S5 Raw values used for computing the vertical ionization potentials (IPs) for the Ip conformation of the $C_2H_5NO_2$ molecule determined using the EOMIP-CCSD/ACVXZ (X = D, T, and Q) approach. The values are given in hartrees.

	ACVDZ
Ground state	-283.96557220655882
1IP	-283.60046211949475
2IP	-283.56449224880998
3IP	-283.52078946655649
4IP	-283.46663346785959
5IP	-283.43552478769124
6IP	-283.41180386669822
7IP	-283.38847343068130
8IP	-283.34228853704997
9IP	-283.33308700599918
10IP	-283.31523838302417
11IP	-283.21687543289863
12IP	-283.15217791314114
	ACVTZ
Ground state	-284.26525818019900
1IP	-283.89184118147045
2IP	-283.85506597350451
3IP	-283.81203466575687
4IP	-283.76024725874186
5IP	-283.72842177772691
6IP	-283.70559920258302
7IP	-283.68181300399260
8IP	-283.63586559422816
9IP	-283.62685862792199
10IP	-283.61019076434042
11IP	-283.51218499044762
12IP	-283.42960516768773

Table S6 Raw values used for computing the vertical ionization potentials (IPs) for the Ip conformation of the $C_2H_5NO_2$ molecule determined using the frozen-core EOMIP-CCSD/ACVXZ (X = D, T, and Q) approach. The values are given in hartrees.

	ACVDZ
Ground state	-283.77590849919676
1IP	-283.41103039269268
2IP	-283.37511035299008
3IP	-283.33139550800649
4IP	-283.27714959765126
5IP	-283.24611376857860
6IP	-283.22235111485469
7IP	-283.19908395282590
8IP	-283.15288792592253
9IP	-283.14362775479350
10IP	-283.12576594073295
11IP	-283.02734639164163
12IP	-282.96473193315290
	ACVTZ
Ground state	-284.00731226359278
1IP	-283.63475962654491
2IP	-283.59822382399341
3IP	-283.55514278055284
4IP	-283.50294100255013
5IP	-283.47148519368682
6IP	-283.44843352348016
7IP	-283.42476654486410
8IP	-283.37882512967917
9IP	-283.36965962464637
10IP	-283.35283407342467
11IP	-283.25478726653921
12IP	-283.17611862236021

Table S7 Raw values used for computing the vertical ionization potentials (IPs) for the IIn conformation of the $C_2H_5NO_2$ molecule determined using the frozen core EOMIP-CCSD/AVXZ (X = D and T) approach. The values are given in hartrees.

	AVDZ
Ground state	-283.76277250132756
1IP	-283.39546846035512
2IP	-283.34687968503954
3IP	-283.34342730187353
4IP	-283.26879293585097
5IP	-283.25200396717332
6IP	-283.20897841365343
7IP	-283.18736946546494
8IP	-283.14828373814368
9IP	-283.11189828671007
10IP	-283.08496001694840
11IP	-283.03283933943089
12IP	-282.94211823236287
	AVTZ
Ground state	-283.99605985804442
1IP	-283.62043463794225
2IP	-283.57263118876625
3IP	-283.56905518212943
4IP	-283.49540846908957
5IP	-283.47912378317568
6IP	-283.43666918983087
7IP	-283.41531678355045
8IP	-283.37635921543603
9IP	-283.33968914094527
10IP	-283.31359934392867
11IP	-283.26185965497672
12IP	-283.15528732804040

Table S8 Raw values used for computing the vertical ionization potentials (IPs) for the IIn conformation of the $C_2H_5NO_2$ molecule determined using the EOMIP-CCSD/ACVXZ (X = D and T) approach. The values are given in hartrees.

	ACVDZ
Ground state	-283.96379938033778
1IP	-283.59581066249257
2IP	-283.54727284975115
3IP	-283.54383913067477
4IP	-283.46915463511203
5IP	-283.45256024355729
6IP	-283.40918882357352
7IP	-283.38789695183323
8IP	-283.34868261343712
9IP	-283.31235175894960
10IP	-283.28556513923184
11IP	-283.23321107669130
12IP	-283.13993791925952
	ACVTZ
Ground state	-284.26346998074905
1IP	-283.88639509902691
2IP	-283.83876072662406
3IP	-283.83503993357419
4IP	-283.76145980039672
5IP	-283.74551429431739
6IP	-283.70261135716191
7IP	-283.68168748163203
8IP	-283.64269045907884
9IP	-283.60623343891660
10IP	-283.58025713614177
11IP	-283.52828988503745
12IP	-283.41739578624441

Table S9 Raw values used for computing the vertical ionization potentials (IPs) for the IIn conformation of the $C_2H_5NO_2$ molecule determined using the frozen-core EOMIP-CCSD/ACVXZ (X = D and T) approach. The values are given in hartrees.

	ACVDZ
Ground state	-283.77410245735530
1IP	-283.40637077881036
2IP	-283.35783620487769
3IP	-283.35440254377818
4IP	-283.27970741088342
5IP	-283.26309276158094
6IP	-283.21974757842196
7IP	-283.19845478153746
8IP	-283.15922001530402
9IP	-283.12284472833653
10IP	-283.09606095476067
11IP	-283.04369728068929
12IP	-282.95245971663462
	ACVTZ
Ground state	-284.00551581738580
1IP	-283.62947111842146
2IP	-283.58174567022382
3IP	-283.57808991375737
4IP	-283.50446413083398
5IP	-283.48834995837217
6IP	-283.44566607198601
7IP	-283.42455466357387
8IP	-283.38555035243513
9IP	-283.34889707667810
10IP	-283.32291336085052
11IP	-283.27098641418399
12IP	-283.16394085848998

Table S10 Raw values used for computing the vertical ionization potentials (IPs) for the IIp conformation of the $C_2H_5NO_2$ molecule determined using the frozen core EOMIP-CCSD/AVXZ (X = D and T) approach. The values are given in hartrees.

	AVDZ
Ground state	-283.76259179411295
1IP	-283.39767271885535
2IP	-283.34485972259358
3IP	-283.34360637637485
4IP	-283.26930521693737
5IP	-283.25414535376871
6IP	-283.20923341286914
7IP	-283.18777303955318
8IP	-283.14769571176390
9IP	-283.10595154391797
10IP	-283.08762231456154
11IP	-283.03369309197791
12IP	-282.94235098837783
	AVTZ
Ground state	-283.99598980901681
1IP	-283.62274502024411
2IP	-283.57061328137445
3IP	-283.56943101935047
4IP	-283.49602386963841
5IP	-283.48135892677868
6IP	-283.43702072051053
7IP	-283.41582293659252
8IP	-283.37588704398178
9IP	-283.33373336540257
10IP	-283.31647622212739
11IP	-283.26279256768879
12IP	-283.15563788111643

Table S11 Raw values used for computing the vertical ionization potentials (IPs) for the IIp conformation of the $C_2H_5NO_2$ molecule determined using the EOMIP-CCSD/ACVXZ (X = D and T) approach. The values are given in hartrees.

	ACVDZ
Ground state	-283.96365442304239
1IP	-283.59804954240190
2IP	-283.54530853848081
3IP	-283.54402754948114
4IP	-283.46970230749173
5IP	-283.45474526533206
6IP	-283.40946923966595
7IP	-283.38834296786638
8IP	-283.34813564722316
9IP	-283.30639976582034
10IP	-283.28830238930567
11IP	-283.23410103831435
12IP	-283.14018418302589
	ACVTZ
Ground state	-284.26344691263733
1IP	-283.88874984278442
2IP	-283.83664035360022
3IP	-283.83559439587549
4IP	-283.76211985319111
5IP	-283.74781286721174
6IP	-283.70299971837233
7IP	-283.68224191790529
8IP	-283.64226704456598
9IP	-283.60028146646624
10IP	-283.58322326350054
11IP	-283.52926485365788
12IP	-283.41774557441659

Table S12 Raw values used for computing the vertical ionization potentials (IPs) for the IIp conformation of the $C_2H_5NO_2$ molecule determined using the frozen-core EOMIP-CCSD/ACVXZ (X = D and T) approach. The values are given in hartrees.

	ACVDZ
Ground state	-283.77393055198615
1IP	-283.40858360543228
2IP	-283.35584427120938
3IP	-283.35456961166875
4IP	-283.28022809590368
5IP	-283.26524680625357
6IP	-283.22000001481609
7IP	-283.19887658743932
8IP	-283.15864671541607
9IP	-283.11687003835465
10IP	-283.09876742499830
11IP	-283.04456117192711
12IP	-282.95269886167102
	ACVTZ
Ground state	-284.00545755411912
1IP	-283.63179299950156
2IP	-283.57965674751159
3IP	-283.57855631581191
4IP	-283.50508920356992
5IP	-283.49060111681905
6IP	-283.44602021015606
7IP	-283.42507724716279
8IP	-283.38509280171502
9IP	-283.34292138672845
10IP	-283.32583287595412
11IP	-283.27192960098370
12IP	-283.16429889307886

Table S13 Raw values used for computing the vertical ionization potentials (IPs) for the IIIn conformation of the $C_2H_5NO_2$ molecule determined using the frozen core EOMIP-CCSD/AVXZ (X = D and T) approach. The values are given in hartrees.

	AVDZ
Ground state	-283.76186972103420
1IP	-283.40791410788711
2IP	-283.34211471056739
3IP	-283.31998733863173
4IP	-283.25839882017567
5IP	-283.23314452613249
6IP	-283.22136513101100
7IP	-283.18057207830100
8IP	-283.13943701894175
9IP	-283.13734881030041
10IP	-283.10960044602382
11IP	-283.00005945981059
12IP	-282.97406120789583
	AVTZ
Ground state	-283.99494753436761
1IP	-283.63284952327541
2IP	-283.56721750094272
3IP	-283.54558113145202
4IP	-283.48569737635404
5IP	-283.46013732676136
6IP	-283.44877111108485
7IP	-283.40804270896831
8IP	-283.36707023178417
9IP	-283.36495017677117
10IP	-283.33814257501263
11IP	-283.22910723830472
12IP	-283.18668271445227

Table S14 Raw values used for computing the vertical ionization potentials (IPs) for the IIIn conformation of the $C_2H_5NO_2$ molecule determined using the EOMIP-CCSD/ACVXZ (X = D and T) approach. The values are given in hartrees.

	ACVDZ
Ground state	-283.96282425158660
1IP	-283.60821064140396
2IP	-283.54240212212460
3IP	-283.52035394412974
4IP	-283.45896016879749
5IP	-283.43346499711163
6IP	-283.42176355390211
7IP	-283.38100222188592
8IP	-283.33956340176638
9IP	-283.33766962230288
10IP	-283.31011538422723
11IP	-283.20046677791777
12IP	-283.17179313153576
	ACVTZ
Ground state	-284.26234642450873
1IP	-283.89888760112962
2IP	-283.83323464616331
3IP	-283.81152990907196
4IP	-283.75226020899083
5IP	-283.72626422270190
6IP	-283.71503911139172
7IP	-283.67428864425676
8IP	-283.63330204171410
9IP	-283.63108607869538
10IP	-283.60481705457261
11IP	-283.49569088652817
12IP	-283.44874943731458

Table S15 Raw values used for computing the vertical ionization potentials (IPs) for the IIIn conformation of the $C_2H_5NO_2$ molecule determined using the frozen-core EOMIP-CCSD/ACVXZ (X = D and T) approach. The values are given in hartrees.

	ACVDZ
Ground state	-283.77317114660298
1IP	-283.41881332563992
2IP	-283.35300424674875
3IP	-283.33096964850336
4IP	-283.26948776087767
5IP	-283.24405012766277
6IP	-283.23234348742591
7IP	-283.19162431909666
8IP	-283.15008970069334
9IP	-283.14830806772346
10IP	-283.12064197256910
11IP	-283.01096951549425
12IP	-282.98437186682605
	ACVTZ
Ground state	-284.00442241519880
1IP	-283.64194390310809
2IP	-283.57628586975829
3IP	-283.55465335398196
4IP	-283.49498962244957
5IP	-283.46925811539182
6IP	-283.45798688129884
7IP	-283.41726589650301
8IP	-283.37609047144775
9IP	-283.37412521807778
10IP	-283.34745966242588
11IP	-283.23834552242300
12IP	-283.19534008469464

Table S16 Raw values used for computing the vertical ionization potentials (IPs) for the IIIp conformation of the $C_2H_5NO_2$ molecule determined using the frozen core EOMIP-CCSD/AVXZ (X = D and T) approach. The values are given in hartrees.

	AVDZ
Ground state	-283.76183756483130
1IP	-283.40810074607566
2IP	-283.34139975440513
3IP	-283.32286597602007
4IP	-283.25783848001089
5IP	-283.23478050019048
6IP	-283.21830581507743
7IP	-283.18579918634379
8IP	-283.13764701226017
9IP	-283.13635082496012
10IP	-283.11010292991148
11IP	-282.99902076967516
12IP	-282.96604476153243
	AVTZ
Ground state	-283.99497882595477
1IP	-283.63309844842541
2IP	-283.56661022860635
3IP	-283.54858665099056
4IP	-283.48503372819334
5IP	-283.46177994958015
6IP	-283.44597697498722
7IP	-283.41323739308029
8IP	-283.36522486713704
9IP	-283.36410278899655
10IP	-283.33878263388823
11IP	-283.22818780491258
12IP	-283.17874541816172

Table S17 Raw values used for computing the vertical ionization potentials (IPs) for the IIIp conformation of the $C_2H_5NO_2$ molecule determined using the EOMIP-CCSD/ACVXZ (X = D and T) approach. The values are given in hartrees.

	ACVDZ
Ground state	-283.96280050958535
1IP	-283.60840525439988
2IP	-283.54169620484919
3IP	-283.52324166228772
4IP	-283.45841322971575
5IP	-283.43509016407626
6IP	-283.41872533820759
7IP	-283.38624603402991
8IP	-283.33774636029983
9IP	-283.33667765650847
10IP	-283.31066929749852
11IP	-283.19944070720550
12IP	-283.15719465934654
	ACVTZ
Ground state	-284.26239179315564
1IP	-283.89914946533634
2IP	-283.83265542251530
3IP	-283.81456558752706
4IP	-283.75160213422799
5IP	-283.72786217106386
6IP	-283.71231071564262
7IP	-283.67948669824489
8IP	-283.63143199713494
9IP	-283.63026955017659
10IP	-283.60549237877899
11IP	-283.49477817087831
12IP	-283.44082484594082

Table S18 Raw values used for computing the vertical ionization potentials (IPs) for the IIIp conformation of the $C_2H_5NO_2$ molecule determined using the frozen-core EOMIP-CCSD/ACVXZ (X = D and T) approach. The values are given in hartrees.

	ACVDZ
Ground state	-283.77313584942908
1IP	-283.41899700229203
2IP	-283.35228356197797
3IP	-283.33384451795303
4IP	-283.26893076997101
5IP	-283.24567003235745
6IP	-283.22928547897459
7IP	-283.19686094799818
8IP	-283.14825382309732
9IP	-283.14730362819756
10IP	-283.12119227440093
11IP	-283.00993396013274
12IP	-282.97634859171325
	ACVTZ
Ground state	-284.00446249974539
1IP	-283.64220248949135
2IP	-283.57568973637103
3IP	-283.55767549187453
4IP	-283.49432827014294
5IP	-283.47088496819953
6IP	-283.45522376138877
7IP	-283.42246818201988
8IP	-283.37419157882357
9IP	-283.37331324467738
10IP	-283.34814157640398
11IP	-283.23743363618826
12IP	-283.18741371972186

Table S19 Raw values used for computing the vertical ionization potentials (IPs) for the IVn conformation of the $C_2H_5NO_2$ molecule determined using the frozen core EOMIP-CCSD/AVXZ (X = D and T) approach. The values are given in hartrees.

	AVDZ
Ground state	-283.76247447740150
1IP	-283.40304582159621
2IP	-283.36567295599644
3IP	-283.31987441792228
4IP	-283.25109782246454
5IP	-283.23526077469182
6IP	-283.21281001059759
7IP	-283.19009798098637
8IP	-283.14473338853065
9IP	-283.13632361574469
10IP	-283.10298676064980
11IP	-283.01762915921734
12IP	-282.95784880168048
	AVTZ
Ground state	-283.99572117282821
1IP	-283.62874144666915
2IP	-283.59081312495425
3IP	-283.54563345464510
4IP	-283.47844164816479
5IP	-283.46244624243928
6IP	-283.44030343778240
7IP	-283.41793967323491
8IP	-283.37280400799017
9IP	-283.36419347909936
10IP	-283.33151589906333
11IP	-283.24673303178844
12IP	-283.17204037219562

Table S20 Raw values used for computing the vertical ionization potentials (IPs) for the IVn conformation of the $C_2H_5NO_2$ molecule determined using the EOMIP-CCSD/ACVXZ (X = D and T) approach. The values are given in hartrees.

	ACVDZ
Ground state	-283.96347065300949
1IP	-283.60343856519683
2IP	-283.56601662814143
3IP	-283.52027833574653
4IP	-283.45149907311742
5IP	-283.43575139807695
6IP	-283.41326852532973
7IP	-283.39049603064149
8IP	-283.34523181157181
9IP	-283.33648880419702
10IP	-283.30346666747090
11IP	-283.21805891499440
12IP	-283.15594012678071
	ACVTZ
Ground state	-284.26316993288350
1IP	-283.89508401735822
2IP	-283.85676854962338
3IP	-283.81163289769262
4IP	-283.74461429258298
5IP	-283.72887517216236
6IP	-283.70664420812318
7IP	-283.68423925016992
8IP	-283.63930633031936
9IP	-283.63044793731626
10IP	-283.59810056677605
11IP	-283.51338032222361
12IP	-283.43469853830055

Table S21 Raw values used for computing the vertical ionization potentials (IPs) for the IVn conformation of the $C_2H_5NO_2$ molecule determined using the frozen-core EOMIP-CCSD/ACVXZ (X = D and T) approach. The values are given in hartrees.

	ACVDZ
Ground state	-283.77379758151915
1IP	-283.41398007091777
2IP	-283.37661220230183
3IP	-283.33086948225241
4IP	-283.26206599345670
5IP	-283.24630635997238
6IP	-283.22383931612075
7IP	-283.20104742722827
8IP	-283.15580914713991
9IP	-283.14699235306477
10IP	-283.11400257982280
11IP	-283.02851697059145
12IP	-282.96826438447971
	ACVTZ
Ground state	-284.00521791877918
1IP	-283.63791509036128
2IP	-283.59989140988415
3IP	-283.55471421579779
4IP	-283.48760981773347
5IP	-283.47171016516404
6IP	-283.44955304977680
7IP	-283.42712692400613
8IP	-283.38211605373635
9IP	-283.37319528733298
10IP	-283.34082083573975
11IP	-283.25597479260068
12IP	-283.18078495669778

Table S22 Cartesian coordinates of the neutral Ip conformation of glycine as optimized at the CCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	0.4977693494	-0.0854849807	0.0000000000
C	-0.7706473044	0.7516340973	0.0000000000
N	-2.0106622419	-0.0038659951	0.0000000000
O	1.6031519118	0.6990120572	0.0000000000
O	0.5454055687	-1.2931850324	0.0000000000
H	2.3639032771	0.0988622189	0.0000000000
H	-0.7318780623	1.4072283373	-0.8741914261
H	-0.7318780623	1.4072283373	0.8741914261
H	-2.0300182181	-0.6197150199	0.8067621318
H	-2.0300182181	-0.6197150199	-0.8067621318

Table S23 Cartesian coordinates of the cation Ip conformation of glycine as optimized at the CCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	0.6102776369	-0.1580837630	0.0000000000
C	-0.7535109536	0.7137481407	0.0000000000
N	-1.8798272638	-0.1170840362	0.0000000000
O	1.5890606574	0.7327336687	0.0000000000
O	0.6387404218	-1.3471136754	0.0000000000
H	2.4444231910	0.2662503015	0.0000000000
H	-0.7089800959	1.3154530509	-0.9093098452
H	-0.7089800959	1.3154530509	0.9093098452
H	-2.2630377490	-0.4896788691	0.8673937820
H	-2.2630377490	-0.4896788691	-0.8673937820

Table S24 Cartesian coordinates of the neutral IIn conformation of glycine as optimized at the MP2/6-311++G* level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	0.0059004863	-0.0448955524	-0.6074176658
C	0.1002871437	-0.8244187993	0.7103018081
N	-0.0723681513	0.0682451461	1.8618139662
O	0.0403479605	1.2875760988	-0.4514712568
O	-0.0637149456	-0.5909995281	-1.6818081694
H	0.0762059911	1.4126000962	0.5206135683
H	-0.6233440060	-1.6427094097	0.6622517480
H	1.0980620138	-1.2713982783	0.7298791393
H	-1.0114058093	0.0114453042	2.2406782803
H	0.5716760294	-0.1562279627	2.6104518385